wwPDB NMR Structure Validation Summary Report (i)

Jun 5, 2023 – 04:07 PM JST

PDB ID	:	6JXV
BMRB ID	:	36031
Title	:	SUMO1 bound to phosphorylated SLS4-SIM peptide from ICP0
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Deposited on	:	2019-04-25

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:

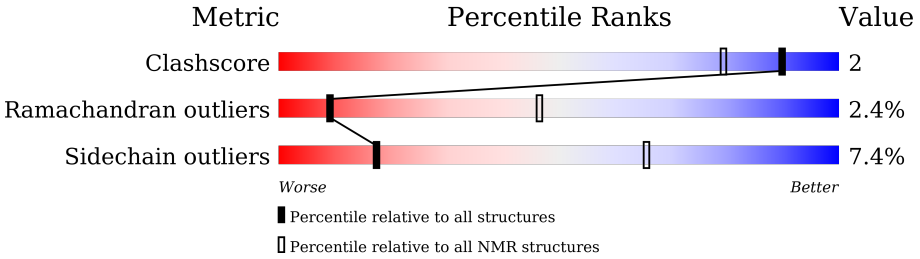
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (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 75%.

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	101	69% 7% 24%
2	B	20	45% 5% 10% 40%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:21-A:97, B:357-B:364, B:366-B:366, B:368-B:368 (87)	0.36	11

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

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

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

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1440 atoms, of which 713 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Small ubiquitin-related modifier.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	77	1254	395	627	108	120	4	0

- Molecule 2 is a protein called Phosphorylated SLS4-SIM from ubiquitin E3 ligase ICP0.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	12	186	55	86	17	26	2	0

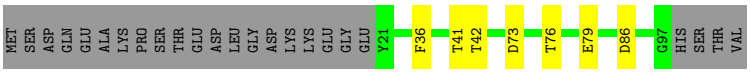
4 Residue-property plots (i)

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.

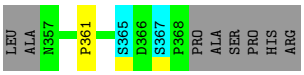
• Molecule 1: Small ubiquitin-related modifier

Chain A: 69% 7% 24%



• Molecule 2: Phosphorylated SLS4-SIM from ubiquitin E3 ligase ICP0

Chain B: 45% 5% 10% 40%

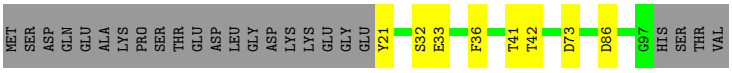


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 11. Colouring as in section 4.1 above.

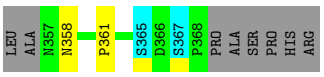
• Molecule 1: Small ubiquitin-related modifier

Chain A: 68% 8% 24%



• Molecule 2: Phosphorylated SLS4-SIM from ubiquitin E3 ligase ICP0

Chain B: 40% 10% 10% 40%



5 Refinement protocol and experimental data overview (i)

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

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 calculation	

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	1101
Number of shifts mapped to atoms	916
Number of unparsed shifts	0
Number of shifts with mapping errors	185
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality (i)

6.1 Standard geometry (i)

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

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	627	627	626	2±1
2	B	80	78	77	1±1
All	All	14140	14100	14060	49

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 2.

5 of 19 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLU:HB2	2:B:358:ASN:O	0.53	2.03	4	5
1:A:23:LYS:HE2	1:A:35:HIS:ND1	0.53	2.18	10	1
1:A:26:VAL:HA	1:A:88:ILE:O	0.49	2.06	17	2
1:A:76:THR:O	1:A:79:GLU:HG2	0.49	2.08	1	9
1:A:42:THR:OG1	2:B:366:ASP:HB2	0.48	2.06	18	3

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	75/101 (74%)	70±1 (94±2%)	4±1 (5±2%)	1±0 (1±1%)	16 63
2	B	8/20 (40%)	7±0 (88±0%)	0±0 (0±0%)	1±0 (12±0%)	1 6
All	All	1660/2420 (69%)	1547 (93%)	73 (4%)	40 (2%)	9 46

All 3 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	361	PRO	20
1	A	41	THR	18
1	A	81	GLY	2

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	70/91 (77%)	64±1 (92±2%)	6±1 (8±2%)	16 63
2	B	10/16 (62%)	10±1 (96±6%)	0±1 (4±6%)	39 86
All	All	1600/2140 (75%)	1482 (93%)	118 (7%)	17 65

5 of 22 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	36	PHE	20
1	A	42	THR	20
1	A	86	ASP	14
1	A	73	ASP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	32	SER	9

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	SEP	B	367	2	8,9,10	1.01±0.02	0±0 (0±0%)
2	SEP	B	365	2	8,9,10	1.03±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	SEP	B	367	2	8,12,14	1.89±0.13	3±0 (36±2%)
2	SEP	B	365	2	8,12,14	1.89±0.08	3±0 (36±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	B	365	2	-	0±0,5,8,10	-
2	SEP	B	367	2	-	0±0,5,8,10	-

There are no bond-length outliers.

5 of 6 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
2	B	367	SEP	OG-CB-CA	3.64	111.68	108.14	11	19
2	B	365	SEP	OG-CB-CA	3.35	111.41	108.14	2	19
2	B	365	SEP	O2P-P-OG	3.13	115.05	106.73	5	20
2	B	367	SEP	OG-P-O1P	3.03	114.98	106.47	13	20
2	B	367	SEP	O2P-P-OG	3.02	114.76	106.73	11	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 (i)

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *final_SUMO1_ppSLS4_nmrstar21.str*

7.1.1 Bookkeeping (i)

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	1101
Number of shifts mapped to atoms	916
Number of unparsed shifts	0
Number of shifts with mapping errors	185
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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 185) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	ASP	CA	54.7	0.200	1
1	A	3	ASP	CB	40.9	0.200	1
1	A	3	ASP	HA	4.566	0.020	1
1	A	3	ASP	HB2	2.672	0.020	2
1	A	3	ASP	HB3	2.672	0.020	2
1	A	4	GLN	N	119.687	0.20	1
1	A	4	GLN	H	8.122	0.02	1
1	A	4	GLN	C	176.013	0.20	1
1	A	4	GLN	CA	56.0	0.200	1
1	A	4	GLN	CB	29.5	0.200	1
1	A	4	GLN	CG	33.659	0.200	1
1	A	4	GLN	HA	4.262	0.020	1
1	A	4	GLN	HB2	2.16	0.020	2
1	A	4	GLN	HB3	1.984	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	GLN	HG2	2.336	0.020	2
1	A	4	GLN	HG3	2.336	0.020	2
1	A	5	GLU	N	121.361	0.20	1
1	A	5	GLU	H	8.262	0.02	1
1	A	5	GLU	C	176.037	0.20	1
1	A	5	GLU	CA	56.5	0.200	1
1	A	5	GLU	CB	30.3	0.200	1
1	A	5	GLU	CG	36.649	0.200	1
1	A	5	GLU	HA	4.213	0.020	1
1	A	5	GLU	HB2	1.979	0.020	2
1	A	5	GLU	HB3	1.979	0.020	2
1	A	5	GLU	HG2	2.186	0.020	2
1	A	5	GLU	HG3	2.186	0.020	2
1	A	6	ALA	N	125.183	0.20	1
1	A	6	ALA	H	8.221	0.02	1
1	A	6	ALA	C	177.249	0.20	1
1	A	6	ALA	CA	52.2	0.200	1
1	A	6	ALA	CB	19.1	0.200	1
1	A	6	ALA	HA	4.261	0.020	1
1	A	6	ALA	HB1	1.319	0.020	1
1	A	6	ALA	HB2	1.319	0.020	1
1	A	6	ALA	HB3	1.319	0.020	1
1	A	7	LYS	N	122.168	0.20	1
1	A	7	LYS	H	8.266	0.02	1
1	A	7	LYS	HB2	1.798	0.020	2
1	A	7	LYS	HB3	1.665	0.020	2
1	A	7	LYS	HG2	1.439	0.020	2
1	A	7	LYS	HG3	1.449	0.020	2
1	A	7	LYS	HD2	1.676	0.020	2
1	A	7	LYS	HD3	1.676	0.020	2
1	A	7	LYS	HE2	2.98	0.020	2
1	A	7	LYS	HE3	2.98	0.020	2
1	A	7	LYS	CA	56.3	0.200	1
1	A	7	LYS	CB	32.4	0.200	1
1	A	7	LYS	CE	42.1	0.200	1
1	A	8	PRO	C	176.954	0.20	1
1	A	8	PRO	CA	63.0	0.200	1
1	A	8	PRO	CB	32.1	0.200	1
1	A	8	PRO	CG	27.357	0.200	1
1	A	8	PRO	CD	50.704	0.200	1
1	A	8	PRO	HA	4.425	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	PRO	HB2	2.268	0.020	1
1	A	8	PRO	HB3	1.892	0.020	1
1	A	8	PRO	HG2	1.929	0.020	2
1	A	8	PRO	HG3	1.929	0.020	2
1	A	8	PRO	HD2	3.793	0.020	1
1	A	8	PRO	HD3	3.617	0.020	1
1	A	9	SER	N	116.699	0.20	1
1	A	9	SER	H	8.563	0.02	1
1	A	9	SER	C	174.969	0.20	1
1	A	9	SER	CA	58.2	0.200	1
1	A	9	SER	CB	63.9	0.200	1
1	A	10	THR	N	115.54	0.20	1
1	A	10	THR	H	8.217	0.02	1
1	A	10	THR	HA	4.334	0.020	1
1	A	10	THR	HB	4.249	0.020	1
1	A	10	THR	HG21	1.181	0.020	1
1	A	10	THR	HG22	1.181	0.020	1
1	A	10	THR	HG23	1.181	0.020	1
1	A	10	THR	C	174.577	0.20	1
1	A	10	THR	CA	61.9	0.200	1
1	A	10	THR	CB	69.6	0.200	1
1	A	10	THR	CG2	21.499	0.200	1
1	A	11	GLU	N	122.694	0.20	1
1	A	11	GLU	H	8.368	0.02	1
1	A	11	GLU	C	175.822	0.20	1
1	A	11	GLU	CA	56.6	0.200	1
1	A	11	GLU	CB	30.2	0.200	1
1	A	11	GLU	CG	36.24	0.200	1
1	A	11	GLU	HB2	1.898	0.020	2
1	A	11	GLU	HB3	1.898	0.020	2
1	A	11	GLU	HG2	2.219	0.020	2
1	A	11	GLU	HG3	2.219	0.020	2
1	A	12	ASP	N	121.754	0.20	1
1	A	12	ASP	H	8.363	0.02	1
1	A	12	ASP	C	176.307	0.20	1
1	A	12	ASP	CA	54.1	0.200	1
1	A	12	ASP	CB	41.1	0.200	1
1	A	12	ASP	HA	4.562	0.020	1
1	A	12	ASP	HB2	2.594	0.020	2
1	A	12	ASP	HB3	2.594	0.020	2
1	A	13	LEU	N	123.466	0.20	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	LEU	H	8.305	0.02	1
1	A	13	LEU	C	178.151	0.20	1
1	A	13	LEU	CA	55.2	0.200	1
1	A	13	LEU	CB	42.1	0.200	1
1	A	13	LEU	CG	26.93	0.200	1
1	A	13	LEU	CD1	24.935	0.200	1
1	A	13	LEU	CD2	23.064	0.200	1
1	A	13	LEU	HA	4.306	0.020	1
1	A	13	LEU	HB2	1.591	0.020	1
1	A	13	LEU	HB3	1.653	0.020	1
1	A	13	LEU	HG	1.602	0.020	1
1	A	13	LEU	HD11	0.889	0.020	2
1	A	13	LEU	HD12	0.889	0.020	2
1	A	13	LEU	HD13	0.889	0.020	2
1	A	13	LEU	HD21	0.81	0.020	2
1	A	13	LEU	HD22	0.81	0.020	2
1	A	13	LEU	HD23	0.81	0.020	2
1	A	14	GLY	N	108.955	0.20	1
1	A	14	GLY	H	8.421	0.02	1
1	A	14	GLY	C	173.974	0.20	1
1	A	14	GLY	CA	45.4	0.200	1
1	A	14	GLY	HA2	3.892	0.020	2
1	A	14	GLY	HA3	3.892	0.020	2
1	A	15	ASP	N	120.558	0.20	1
1	A	15	ASP	H	8.248	0.02	1
1	A	15	ASP	C	176.357	0.20	1
1	A	15	ASP	CB	41.1	0.200	1
1	A	15	ASP	HA	4.544	0.020	1
1	A	15	ASP	HB2	2.62	0.020	2
1	A	15	ASP	HB3	2.62	0.020	2
1	A	16	LYS	N	121.153	0.20	1
1	A	16	LYS	H	8.273	0.02	1
1	A	16	LYS	C	176.755	0.20	1
1	A	16	LYS	CA	57.1	0.200	1
1	A	16	LYS	CB	32.7	0.200	1
1	A	16	LYS	CG	27.435	0.200	1
1	A	16	LYS	CD	28.764	0.200	1
1	A	16	LYS	CE	43.023	0.200	1
1	A	16	LYS	HA	4.269	0.020	1
1	A	16	LYS	HB2	1.82	0.020	2
1	A	16	LYS	HB3	1.82	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	16	LYS	HG2	1.57	0.020	2
1	A	16	LYS	HG3	1.57	0.020	2
1	A	16	LYS	HD2	1.646	0.020	2
1	A	16	LYS	HD3	1.646	0.020	2
1	A	17	LYS	N	122.255	0.20	1
1	A	17	LYS	H	8.351	0.02	1
1	A	17	LYS	C	177.447	0.20	1
1	A	17	LYS	CA	58.6	0.200	1
1	A	17	LYS	CB	29.9	0.200	1
1	A	17	LYS	CG	24.651	0.200	1
1	A	17	LYS	CD	29.0	0.200	1
1	A	17	LYS	CE	42.104	0.200	1
1	A	17	LYS	HA	4.267	0.020	1
1	A	17	LYS	HB2	1.784	0.020	2
1	A	17	LYS	HB3	1.784	0.020	2
1	A	17	LYS	HG2	1.38	0.020	2
1	A	17	LYS	HG3	1.38	0.020	2
1	A	17	LYS	HD2	1.635	0.020	2
1	A	17	LYS	HD3	1.635	0.020	2
1	A	17	LYS	HE2	2.945	0.020	2
1	A	17	LYS	HE3	2.945	0.020	2
1	A	18	GLU	N	121.862	0.20	1
1	A	18	GLU	H	8.489	0.02	1
1	A	18	GLU	C	176.298	0.20	1
1	A	18	GLU	CB	30.5	0.200	1
1	A	18	GLU	CG	36.277	0.200	1
1	A	18	GLU	CA	57.094	0.200	1
1	A	18	GLU	HA	4.252	0.020	1
1	A	18	GLU	HB2	1.945	0.020	2
1	A	18	GLU	HB3	1.945	0.020	2
1	A	18	GLU	HG2	2.237	0.020	2
1	A	18	GLU	HG3	2.237	0.020	2
1	A	19	GLY	N	109.421	0.20	1
1	A	19	GLY	H	8.442	0.02	1
1	A	19	GLY	HA2	3.957	0.020	2
1	A	19	GLY	HA3	3.957	0.020	2
1	A	20	GLU	N	121.726	0.20	1
1	A	20	GLU	H	8.272	0.02	1
1	A	98	HIS	N	122.166	0.20	1
1	A	98	HIS	H	8.341	0.02	1
1	A	98	HIS	C	176.43	0.20	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	98	HIS	CA	55.7	0.200	1
1	A	98	HIS	CB	32.6	0.200	1
1	A	99	SER	N	116.387	0.20	1
1	A	99	SER	H	8.293	0.02	1
1	A	99	SER	C	174.969	0.20	1
1	A	99	SER	CA	58.2	0.200	1
1	A	99	SER	CB	63.9	0.200	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
$^{13}C_{\alpha}$	90	-0.47 ± 0.20	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	87	0.11 ± 0.24	None needed (< 0.5 ppm)
$^{13}C'$	88	-0.17 ± 0.18	None needed (< 0.5 ppm)
^{15}N	89	0.40 ± 0.60	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 916 atoms were assigned a chemical shift out of a possible 1223. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	368/433 (85%)	152/176 (86%)	145/174 (83%)	71/83 (86%)
Sidechain	520/712 (73%)	353/457 (77%)	167/225 (74%)	0/30 (0%)
Aromatic	28/78 (36%)	14/39 (36%)	14/36 (39%)	0/3 (0%)
Overall	916/1223 (75%)	519/672 (77%)	326/435 (75%)	71/116 (61%)

7.1.4 Statistically unusual chemical shifts (i)

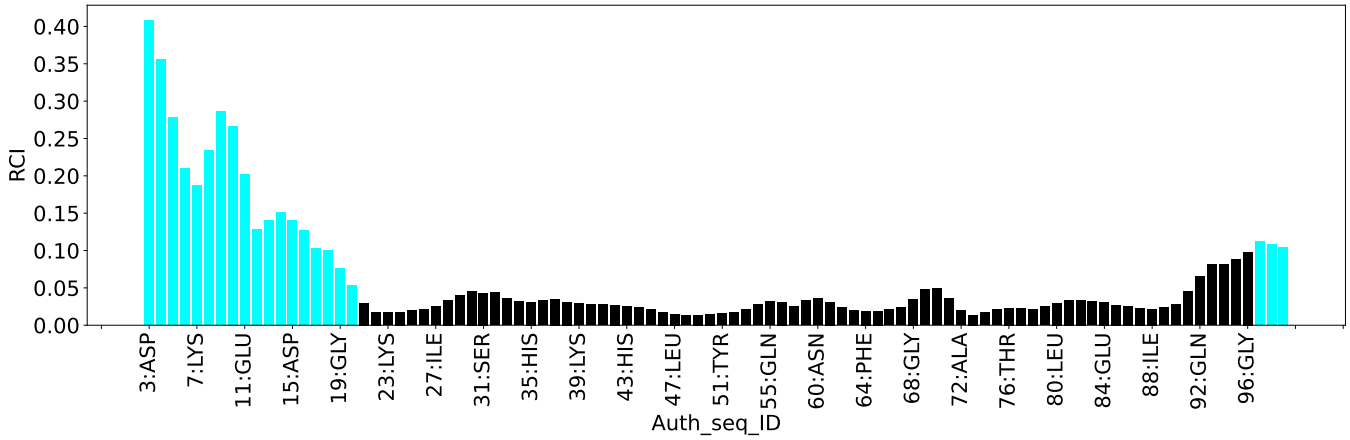
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	72	ALA	N	104.50	106.13 – 140.55	-5.5
1	A	67	GLU	HG2	1.14	1.24 – 3.30	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	61
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	61
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.5
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 (i)

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 (i)

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)	1.1	0.18
0.2-0.5 (Medium)	1.8	0.5
>0.5 (Large)	8.7	4.83

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)

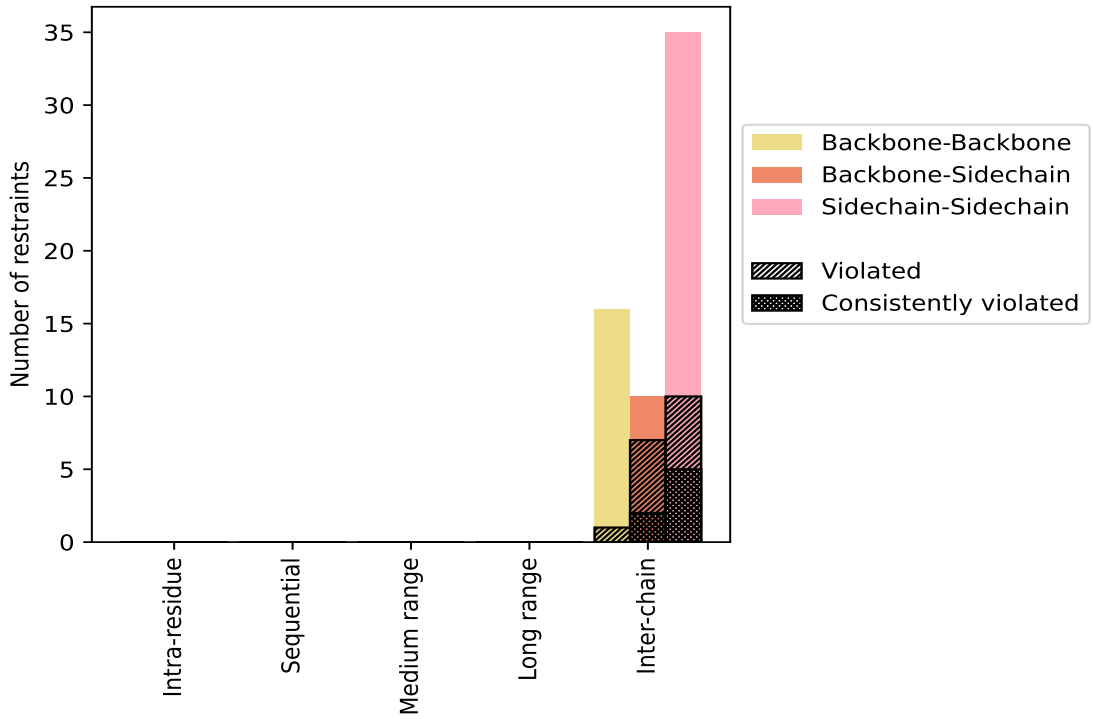
9.1 Summary of distance violations (i)

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	61	100.0	18	29.5	29.5	7	11.5	11.5
Backbone-Backbone	16	26.2	1	6.2	1.6	0	0.0	0.0
Backbone-Sidechain	10	16.4	7	70.0	11.5	2	20.0	3.3
Sidechain-Sidechain	35	57.4	10	28.6	16.4	5	14.3	8.2
Hydrogen bond	0	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	61	100.0	18	29.5	29.5	7	11.5	11.5
Backbone-Backbone	16	26.2	1	6.2	1.6	0	0.0	0.0
Backbone-Sidechain	10	16.4	7	70.0	11.5	2	20.0	3.3
Sidechain-Sidechain	35	57.4	10	28.6	16.4	5	14.3	8.2

[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 (i)



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 (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[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	10	10	0.85	1.71	0.56	0.89
2	0	0	0	0	10	10	1.16	2.15	0.62	1.34
3	0	0	0	0	12	12	1.42	4.04	1.15	1.18
4	0	0	0	0	11	11	1.33	2.92	0.69	1.23
5	0	0	0	0	10	10	0.92	1.98	0.56	0.89
6	0	0	0	0	11	11	1.38	3.79	1.14	0.75
7	0	0	0	0	11	11	1.48	3.69	1.06	1.2
8	0	0	0	0	11	11	1.54	4.13	1.27	1.07
9	0	0	0	0	13	13	1.34	4.53	1.34	0.97
10	0	0	0	0	13	13	1.37	4.83	1.29	0.92
11	0	0	0	0	11	11	1.53	4.22	1.27	1.2

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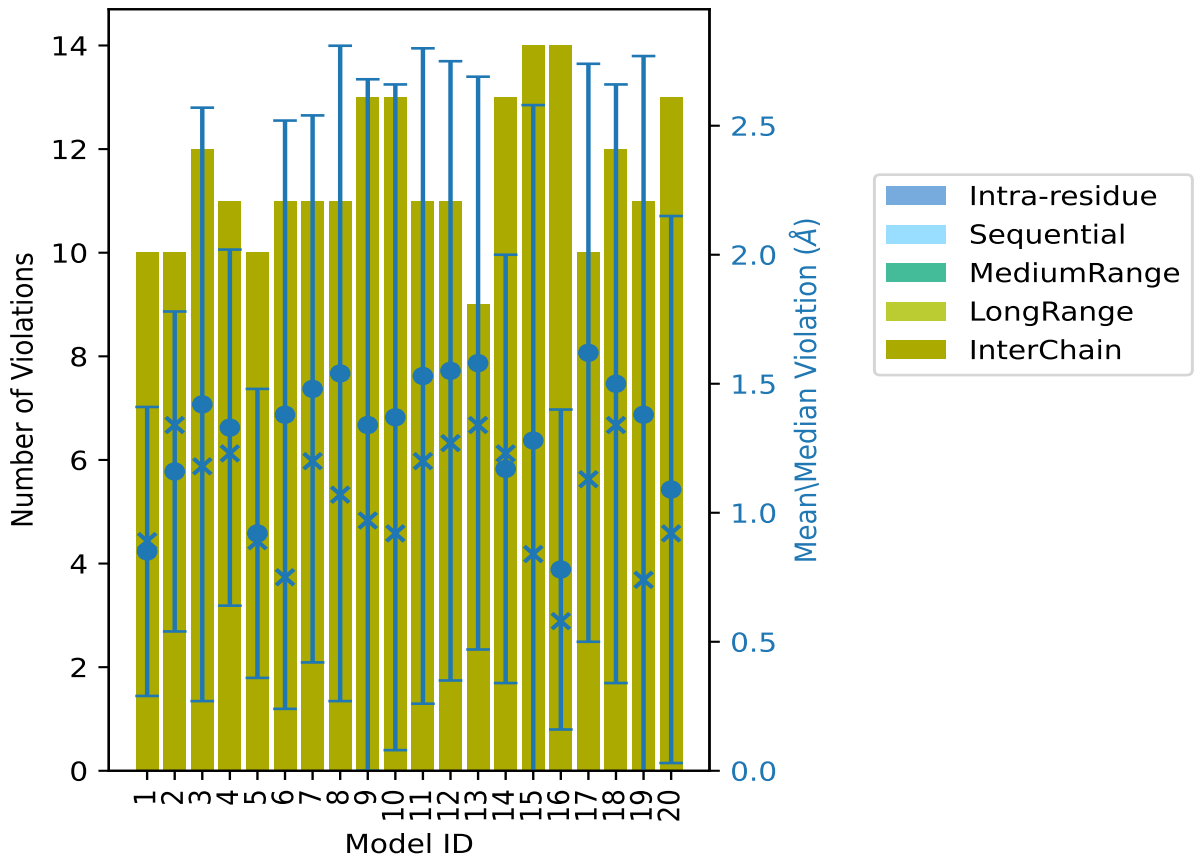
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	0	0	0	11	11	1.55	4.12	1.2	1.27
13	0	0	0	0	9	9	1.58	3.59	1.11	1.34
14	0	0	0	0	13	13	1.17	2.67	0.83	1.23
15	0	0	0	0	14	14	1.28	4.43	1.3	0.84
16	0	0	0	0	14	14	0.78	1.86	0.62	0.58
17	0	0	0	0	10	10	1.62	3.73	1.12	1.13
18	0	0	0	0	12	12	1.5	3.89	1.16	1.34
19	0	0	0	0	11	11	1.38	4.64	1.39	0.74
20	0	0	0	0	13	13	1.09	3.53	1.06	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 (i)



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

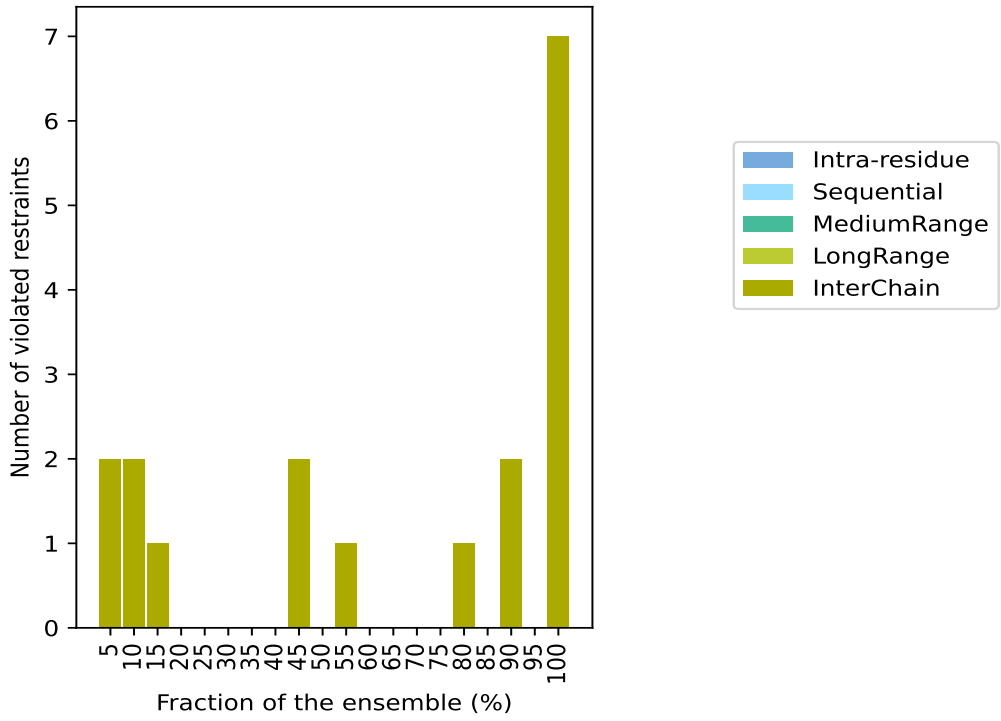
9.3 Distance violation statistics for the ensemble (i)

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, 43(IR:0, SQ:0, MR:0, LR:0, IC:43) 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	2	2	1	5.0
0	0	0	0	2	2	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	2	2	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	1	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	2	2	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	7	7	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

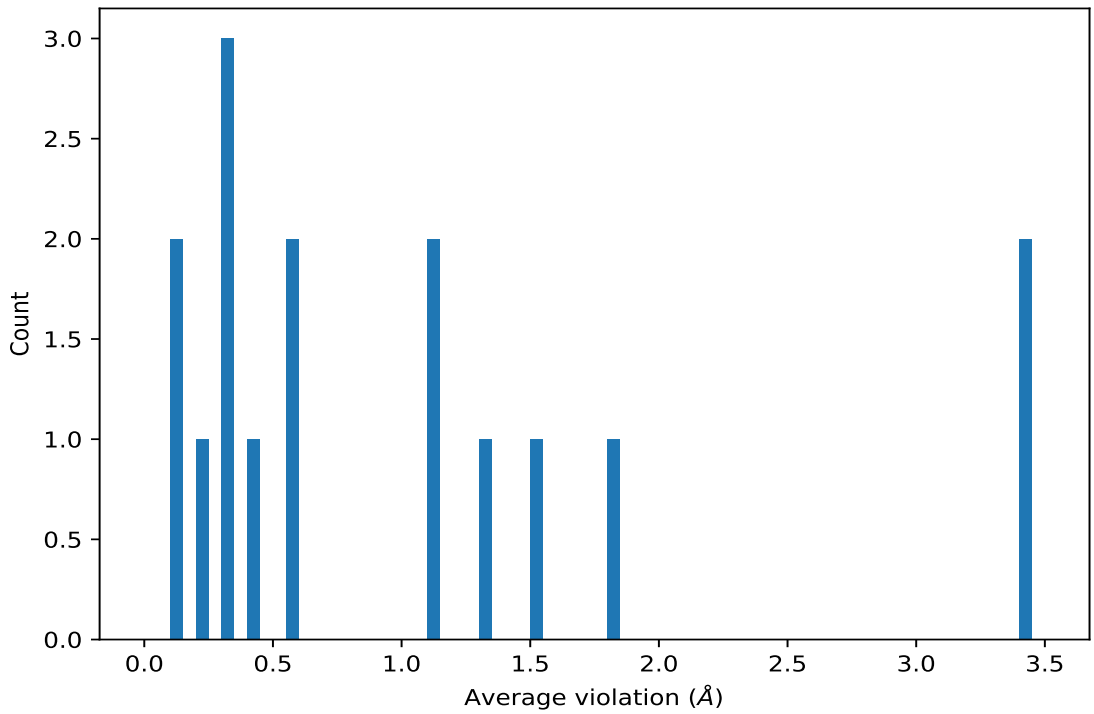
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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.

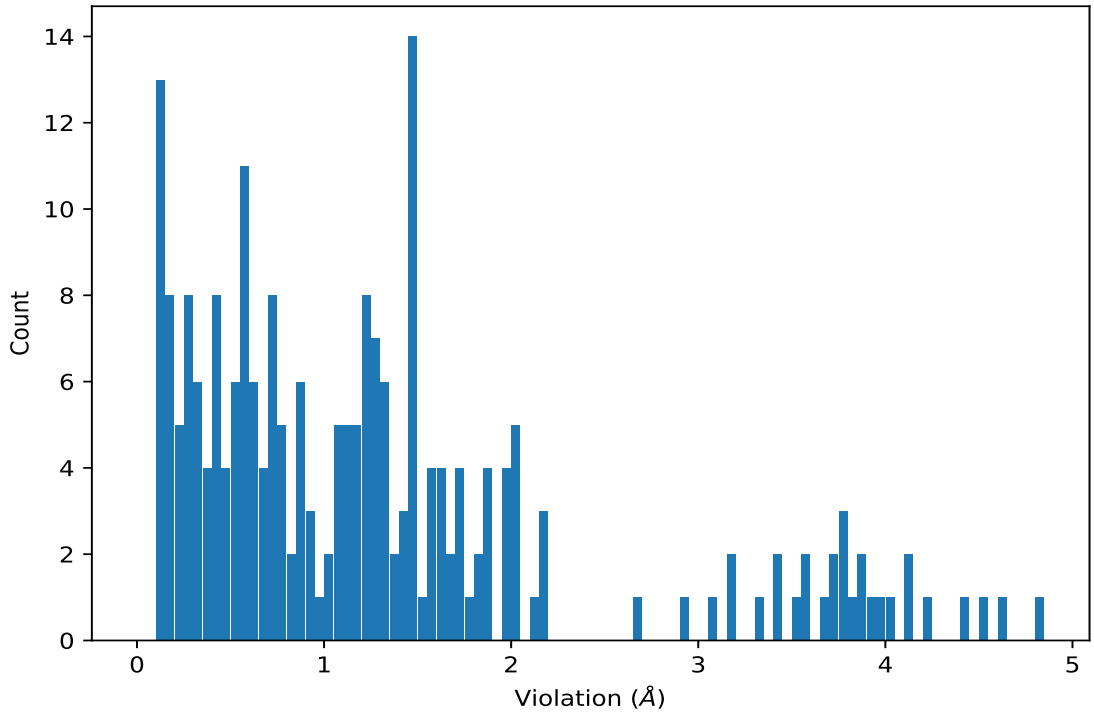
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	20	3.41	1.12	3.74
(1,52)	1:A:46:LYS:HD3	2:B:365:SEP:HA	20	1.8	0.18	1.82
(1,53)	1:A:46:LYS:HD3	2:B:365:SEP:HB2	20	1.51	0.39	1.51
(1,19)	1:A:36:PHE:HD1	2:B:362:ILE:HB	20	1.33	0.15	1.32
(1,47)	1:A:46:LYS:HD3	2:B:364:ILE:HB	20	1.13	0.28	1.18
(1,51)	1:A:46:LYS:HD3	2:B:364:ILE:HB	20	1.13	0.28	1.18
(1,24)	1:A:37:LYS:HB3	2:B:363:VAL:HA	20	0.43	0.18	0.42
(1,46)	1:A:46:LYS:HD3	2:B:364:ILE:HA	18	0.59	0.16	0.58
(1,50)	1:A:46:LYS:HD3	2:B:364:ILE:HA	18	0.59	0.16	0.58
(1,42)	1:A:43:HIS:HD2	2:B:367:SEP:HB2	16	3.41	0.54	3.58

[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)
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	10	4.83
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	19	4.64
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	9	4.53
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	15	4.43
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	11	4.22
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	8	4.13
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	12	4.12
(1,43)	1:A:43:HIS:HD2	2:B:366:ASP:HB3	3	4.04
(1,42)	1:A:43:HIS:HD2	2:B:367:SEP:HB2	9	3.96
(1,42)	1:A:43:HIS:HD2	2:B:367:SEP:HB2	15	3.93

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found