wwPDB NMR Structure Validation Summary Report

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BMRB ID	:	17668
Title	:	NMR solution structure of ZiaAN sub mutant
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Deposited on	:	2011-05-26

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:

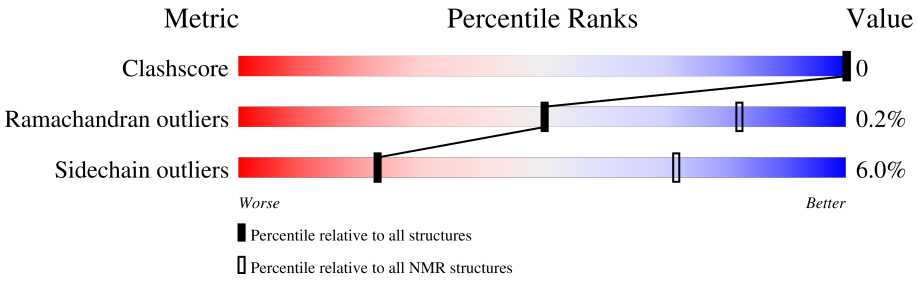
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 83%.

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	106	58% · 5% 33%

2 Ensemble composition and analysis

This entry contains 30 models. Model 26 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:7-A:17, A:22-A:76 (66)	0.78	26

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 7 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 15, 19, 25, 26, 28, 30
2	7, 10, 18, 22, 23, 27
3	13, 16
4	2, 29
5	3, 24
6	9, 21
7	14, 20
Single-model clusters	6; 8; 11; 12; 17

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 996 atoms, of which 469 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc-transporting ATPase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	71	996	326	469	94	103	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ARG	ASP	conflict	UNP Q59998
A	20	ALA	THR	conflict	UNP Q59998
A	21	ALA	SER	conflict	UNP Q59998
A	23	ALA	LYS	conflict	UNP Q59998
A	24	SER	LEU	conflict	UNP Q59998
A	25	SER	LYS	conflict	UNP Q59998
A	28	ARG	GLY	conflict	UNP Q59998
A	29	ALA	SER	conflict	UNP Q59998

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: Zinc-transporting ATPase

Chain A:

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

The representative model is number 26. Colouring as in section 4.1 above.

- Molecule 1: Zinc-transporting ATPase

Chain A:

5 Refinement protocol and experimental data overview

The models were refined using the following method: *restrained energy minimization.*

Of the 300 calculated structures, 30 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
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	1014
Number of shifts mapped to atoms	689
Number of unparsed shifts	0
Number of shifts with mapping errors	325
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality

6.1 Standard geometry

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	0.62±0.01	0±0/496 (0.0± 0.0%)	1.03±0.03	3±1/670 (0.4± 0.1%)
All	All	0.62	0/14880 (0.0%)	1.03	78/20100 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.5
All	All	0	7

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
1	A	47	ARG	NE-CZ-NH1	8.31	124.46	120.30	16	18
1	A	65	ARG	NE-CZ-NH1	7.85	124.23	120.30	27	23
1	A	65	ARG	NE-CZ-NH2	-7.74	116.43	120.30	27	4
1	A	28	ARG	NE-CZ-NH1	7.56	124.08	120.30	4	21
1	A	32	ARG	NE-CZ-NH1	7.29	123.95	120.30	15	11

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	71	TYR	Sidechain	2
1	A	65	ARG	Sidechain	2
1	A	47	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	75	GLU	Peptide	1
1	A	35	GLY	Peptide	1

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
All	All	14790	13200	15420	-

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 -.

There are no clashes.

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	65/106 (61%)	59±2 (90±3%)	6±2 (10±3%)	0±0 (0±1%)	50	82
All	All	1950/3180 (61%)	1759 (90%)	187 (10%)	4 (0%)	50	82

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	57	VAL	3
1	A	16	GLY	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	53/86 (62%)	50±1 (94±3%)	3±1 (6±3%)	23	72
All	All	1590/2580 (62%)	1495 (94%)	95 (6%)	23	72

5 of 25 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	48	LEU	19
1	A	59	GLU	10
1	A	75	GLU	10
1	A	12	MET	9
1	A	65	ARG	7

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no 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 83% for the well-defined parts and 81% 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	1014
Number of shifts mapped to atoms	689
Number of unparsed shifts	0
Number of shifts with mapping errors	325
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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 325) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	PRO	HB2	1.804	0.020	1
1	A	6	PRO	HG2	1.859	0.020	1
1	A	6	PRO	HD2	3.629	0.020	1
1	A	7	LEU	HB2	1.396	0.020	2
1	A	8	LYS	HB2	1.014	0.020	2
1	A	8	LYS	HG2	1.096	0.020	2
1	A	8	LYS	HD2	1.45	0.020	1
1	A	8	LYS	HE2	2.813	0.020	1
1	A	10	GLN	HB2	1.886	0.020	1
1	A	10	GLN	HG2	2.267	0.020	1
1	A	11	GLN	HB2	1.858	0.020	2
1	A	11	GLN	HG2	2.241	0.020	1
1	A	12	MET	HB2	1.996	0.020	2
1	A	12	MET	HG2	2.486	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	13	GLN	HB2	1.913	0.020	2
1	A	17	MET	HB2	2.16	0.020	2
1	A	17	MET	HG2	2.049	0.020	2
1	A	18	ARG	HB2	1.831	0.020	2
1	A	18	ARG	HG2	1.696	0.020	2
1	A	18	ARG	HD2	3.193	0.020	2
1	A	19	CYS	HB2	3.003	0.020	2
1	A	22	CYS	HB2	3.112	0.020	2
1	A	24	SER	HB2	3.847	0.020	1
1	A	26	ILE	HG12	1.586	0.020	2
1	A	28	ARG	HB2	1.831	0.020	2
1	A	28	ARG	HG2	1.723	0.020	2
1	A	28	ARG	HD2	3.112	0.020	1
1	A	30	LEU	HB2	1.668	0.020	2
1	A	31	GLU	HB2	1.94	0.020	1
1	A	31	GLU	HG2	2.484	0.020	1
1	A	32	ARG	HB2	1.913	0.020	1
1	A	32	ARG	HG2	1.75	0.020	1
1	A	32	ARG	HD2	3.085	0.020	1
1	A	33	LEU	HB2	1.722	0.020	1
1	A	34	LYS	HB2	1.694	0.020	1
1	A	34	LYS	HG2	1.369	0.020	2
1	A	34	LYS	HD2	1.614	0.020	1
1	A	34	LYS	HE2	2.921	0.020	1
1	A	38	GLU	HB2	1.817	0.020	1
1	A	38	GLU	HG2	2.021	0.020	2
1	A	40	SER	HB2	3.522	0.020	1
1	A	47	ARG	HB2	1.641	0.020	2
1	A	47	ARG	HG2	1.368	0.020	1
1	A	47	ARG	HD2	3.003	0.020	1
1	A	48	LEU	HB2	1.504	0.020	2
1	A	52	TYR	HB2	2.621	0.020	2
1	A	53	ASP	HB2	2.921	0.020	2
1	A	54	PRO	HB2	2.212	0.020	1
1	A	54	PRO	HD2	4.065	0.020	2
1	A	55	LYS	HB2	1.886	0.020	1
1	A	55	LYS	HG2	1.423	0.020	2
1	A	55	LYS	HD2	1.614	0.020	1
1	A	55	LYS	HE2	2.895	0.020	1
1	A	56	GLN	HB2	2.022	0.020	2
1	A	56	GLN	HG2	2.186	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	SER	HB2	4.147	0.020	2
1	A	59	GLU	HB2	2.131	0.020	2
1	A	59	GLU	HG2	2.458	0.020	2
1	A	60	ILE	HG12	1.408	0.020	2
1	A	62	ILE	HG12	1.259	0.020	2
1	A	63	GLN	HB2	2.159	0.020	2
1	A	63	GLN	HG2	2.485	0.020	1
1	A	64	GLU	HB2	2.077	0.020	2
1	A	64	GLU	HG2	2.458	0.020	2
1	A	65	ARG	HB2	1.805	0.020	1
1	A	65	ARG	HG2	1.614	0.020	2
1	A	65	ARG	HD2	3.194	0.020	2
1	A	66	ILE	HG12	0.905	0.020	2
1	A	69	LEU	HB2	1.466	0.020	1
1	A	71	TYR	HB2	3.385	0.020	2
1	A	73	LEU	HB2	1.504	0.020	1
1	A	75	GLU	HB2	1.914	0.020	2
1	A	75	GLU	HG2	2.187	0.020	2
1	A	76	PRO	HB2	2.104	0.020	1
1	A	76	PRO	HG2	1.94	0.020	2
1	A	76	PRO	HD2	3.766	0.020	2
1	A	77	LYS	C	176.93	0.3	1
1	A	77	LYS	CA	56.246	0.3	1
1	A	77	LYS	CB	30.616	0.3	1
1	A	77	LYS	CG	24.837	0.3	1
1	A	77	LYS	CD	29.331	0.3	1
1	A	77	LYS	CE	42.144	0.3	1
1	A	77	LYS	HA	4.158	0.020	1
1	A	77	LYS	HB2	1.695	0.020	2
1	A	77	LYS	HB3	1.614	0.020	2
1	A	77	LYS	HG2	1.314	0.020	1
1	A	77	LYS	HD2	1.532	0.020	1
1	A	77	LYS	HE2	2.867	0.020	1
1	A	77	LYS	N	121.367	0.3	1
1	A	78	SER	C	174.857	0.3	1
1	A	78	SER	CA	58.258	0.3	1
1	A	78	SER	CB	63.76	0.3	1
1	A	78	SER	H	8.285	0.020	1
1	A	78	SER	HB2	3.656	0.020	1
1	A	78	SER	N	116.445	0.3	1
1	A	79	SER	C	174.515	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	SER	CA	58.257	0.3	1
1	A	79	SER	CB	63.76	0.3	1
1	A	79	SER	H	8.313	0.020	1
1	A	79	SER	HB2	3.712	0.020	1
1	A	79	SER	N	118.086	0.3	1
1	A	80	VAL	C	176.241	0.3	1
1	A	80	VAL	CA	62.251	0.3	1
1	A	80	VAL	CB	32.753	0.3	1
1	A	80	VAL	CG1	21.031	0.3	1
1	A	80	VAL	CG2	20.438	0.3	1
1	A	80	VAL	H	8.032	0.020	1
1	A	80	VAL	HA	4.093	0.020	1
1	A	80	VAL	HB	1.941	0.020	1
1	A	80	VAL	HG21	0.796	0.020	1
1	A	80	VAL	HG22	0.796	0.020	1
1	A	80	VAL	HG23	0.796	0.020	1
1	A	80	VAL	N	121.367	0.3	1
1	A	81	THR	C	176.589	0.3	1
1	A	81	THR	CA	61.725	0.3	1
1	A	81	THR	CB	69.776	0.3	1
1	A	81	THR	CG2	21.903	0.3	1
1	A	81	THR	H	8.172	0.020	1
1	A	81	THR	HA	4.229	0.020	1
1	A	81	THR	HB	4.038	0.020	1
1	A	81	THR	HG21	1.042	0.020	1
1	A	81	THR	HG22	1.042	0.020	1
1	A	81	THR	HG23	1.042	0.020	1
1	A	81	THR	N	118.633	0.3	1
1	A	82	LEU	C	176.241	0.3	1
1	A	82	LEU	CA	55.247	0.3	1
1	A	82	LEU	CB	42.701	0.3	1
1	A	82	LEU	CG	26.948	0.3	1
1	A	82	LEU	CD1	24.823	0.3	1
1	A	82	LEU	CD2	23.592	0.3	1
1	A	82	LEU	H	8.257	0.020	1
1	A	82	LEU	HA	4.256	0.020	1
1	A	82	LEU	HB2	1.463	0.020	1
1	A	82	LEU	HG	1.475	0.020	1
1	A	82	LEU	HD11	0.795	0.020	1
1	A	82	LEU	HD12	0.795	0.020	1
1	A	82	LEU	HD13	0.795	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	82	LEU	HD21	0.742	0.020	1
1	A	82	LEU	HD22	0.742	0.020	1
1	A	82	LEU	HD23	0.742	0.020	1
1	A	82	LEU	N	125.195	0.3	1
1	A	83	ASN	C	176.583	0.3	1
1	A	83	ASN	CA	54.753	0.3	1
1	A	83	ASN	CB	41.23	0.3	1
1	A	83	ASN	H	7.92	0.020	1
1	A	83	ASN	HB2	2.649	0.020	2
1	A	83	ASN	HB3	2.54	0.020	2
1	A	83	ASN	N	124.102	0.3	1
1	A	84	GLY	C	174.343	0.3	1
1	A	84	GLY	CA	45.625	0.3	1
1	A	84	GLY	H	8.257	0.020	1
1	A	84	GLY	HA2	3.739	0.020	1
1	A	84	GLY	N	113.711	0.3	1
1	A	85	HIS	CA	56.246	0.3	1
1	A	85	HIS	CB	30.241	0.3	1
1	A	85	HIS	H	8.229	0.020	1
1	A	85	HIS	N	118.633	0.3	1
1	A	86	LYS	C	176.07	0.3	1
1	A	86	LYS	CA	56.242	0.3	1
1	A	86	LYS	CB	32.71	0.3	1
1	A	86	LYS	CG	24.72	0.3	1
1	A	86	LYS	CE	42.145	0.3	1
1	A	86	LYS	HG2	1.232	0.020	1
1	A	86	LYS	N	121.914	0.3	1
1	A	87	HIS	H	8.201	0.020	1
1	A	87	HIS	N	116.992	0.3	1
1	A	88	PRO	C	177.79	0.3	1
1	A	88	PRO	CA	66.239	0.3	1
1	A	88	PRO	CB	31.719	0.3	1
1	A	88	PRO	CG	27.169	0.3	1
1	A	88	PRO	CD	50.653	0.3	1
1	A	88	PRO	HB2	1.668	0.020	1
1	A	88	PRO	HG2	1.832	0.020	1
1	A	88	PRO	HD2	3.33	0.020	1
1	A	89	HIS	C	175.554	0.3	1
1	A	89	HIS	CA	56.236	0.3	1
1	A	89	HIS	CB	30.257	0.3	1
1	A	89	HIS	H	8.538	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	89	HIS	N	119.18	0.3	1
1	A	90	SER	CA	58.565	0.3	1
1	A	90	SER	CB	63.886	0.3	1
1	A	90	SER	H	8.144	0.020	1
1	A	90	SER	HB2	3.957	0.020	1
1	A	90	SER	N	116.445	0.3	1
1	A	91	HIS	C	175.204	0.3	1
1	A	91	HIS	CA	56.242	0.3	1
1	A	91	HIS	CB	30.235	0.3	1
1	A	92	ARG	C	177.447	0.3	1
1	A	92	ARG	CA	56.257	0.3	1
1	A	92	ARG	CB	30.241	0.3	1
1	A	92	ARG	CG	27.772	0.3	1
1	A	92	ARG	H	8.144	0.020	1
1	A	92	ARG	HB2	1.913	0.020	1
1	A	92	ARG	N	122.461	0.3	1
1	A	93	GLU	CA	56.224	0.3	1
1	A	93	GLU	CB	30.723	0.3	1
1	A	93	GLU	H	8.088	0.020	1
1	A	93	GLU	HA	4.202	0.020	1
1	A	93	GLU	N	121.367	0.3	1
1	A	94	GLU	C	177.274	0.3	1
1	A	94	GLU	CA	56.702	0.3	1
1	A	94	GLU	CB	30.252	0.3	1
1	A	94	GLU	CG	36.274	0.3	1
1	A	94	GLU	HA	4.147	0.020	1
1	A	94	GLU	HB2	1.912	0.020	2
1	A	94	GLU	HB3	1.777	0.020	2
1	A	94	GLU	HG2	1.967	0.020	2
1	A	94	GLU	HG3	1.914	0.020	2
1	A	94	GLU	N	122.461	0.3	1
1	A	95	GLY	C	174.213	0.3	1
1	A	95	GLY	CA	45.276	0.3	1
1	A	95	GLY	H	8.341	0.020	1
1	A	95	GLY	N	109.336	0.3	1
1	A	96	HIS	C	178.658	0.3	1
1	A	96	HIS	H	8.06	0.020	1
1	A	96	HIS	N	118.633	0.3	1
1	A	97	SER	CA	58.258	0.3	1
1	A	97	SER	CB	63.754	0.3	1
1	A	97	SER	H	8.116	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	97	SER	N	115.812	0.3	1
1	A	98	HIS	N	118.633	0.3	1
1	A	99	SER	C	179.517	0.3	1
1	A	99	SER	CA	58.256	0.3	1
1	A	99	SER	CB	63.755	0.3	1
1	A	100	HIS	C	175.896	0.3	1
1	A	100	HIS	CA	56.254	0.3	1
1	A	100	HIS	CB	30.254	0.3	1
1	A	100	HIS	H	8.312	0.020	1
1	A	100	HIS	N	120.82	0.3	1
1	A	101	GLY	CA	45.266	0.3	1
1	A	101	GLY	H	8.313	0.020	1
1	A	101	GLY	N	109.883	0.3	1
1	A	102	ALA	C	178.484	0.3	1
1	A	102	ALA	CA	52.736	0.3	1
1	A	102	ALA	CB	19.237	0.3	1
1	A	102	ALA	HA	4.214	0.020	1
1	A	102	ALA	HB1	1.259	0.020	1
1	A	102	ALA	HB2	1.259	0.020	1
1	A	102	ALA	HB3	1.259	0.020	1
1	A	102	ALA	N	123.555	0.3	1
1	A	103	GLY	C	174.342	0.3	1
1	A	103	GLY	CA	45.241	0.3	1
1	A	103	GLY	H	8.285	0.020	1
1	A	103	GLY	N	107.696	0.3	1
1	A	104	GLU	C	176.413	0.3	1
1	A	104	GLU	CA	56.759	0.3	1
1	A	104	GLU	CB	30.236	0.3	1
1	A	104	GLU	H	8.06	0.020	1
1	A	104	GLU	N	119.727	0.3	1
1	A	105	PHE	C	175.547	0.3	1
1	A	105	PHE	CA	57.743	0.3	1
1	A	105	PHE	CB	39.499	0.3	1
1	A	105	PHE	H	8.117	0.020	1
1	A	105	PHE	HA	4.474	0.020	1
1	A	105	PHE	HB2	3.003	0.020	2
1	A	105	PHE	HB3	2.84	0.020	2
1	A	105	PHE	N	120.273	0.3	1
1	A	106	ASN	C	175.547	0.3	1
1	A	106	ASN	CA	53.225	0.3	1
1	A	106	ASN	CB	38.753	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	106	ASN	H	8.172	0.020	1
1	A	106	ASN	HA	4.528	0.020	1
1	A	106	ASN	N	119.727	0.3	1
1	A	107	LEU	C	177.446	0.3	1
1	A	107	LEU	CA	55.249	0.3	1
1	A	107	LEU	CB	42.261	0.3	1
1	A	107	LEU	CG	26.901	0.3	1
1	A	107	LEU	CD1	24.834	0.3	1
1	A	107	LEU	CD2	23.512	0.3	1
1	A	107	LEU	H	8.06	0.020	1
1	A	107	LEU	HD11	0.747	0.020	1
1	A	107	LEU	HD12	0.747	0.020	1
1	A	107	LEU	HD13	0.747	0.020	1
1	A	107	LEU	HD21	0.688	0.020	1
1	A	107	LEU	HD22	0.688	0.020	1
1	A	107	LEU	HD23	0.688	0.020	1
1	A	107	LEU	N	121.914	0.3	1
1	A	108	LYS	C	176.413	0.3	1
1	A	108	LYS	CA	56.24	0.3	1
1	A	108	LYS	CB	32.733	0.3	1
1	A	108	LYS	CG	24.836	0.3	1
1	A	108	LYS	CD	28.888	0.3	1
1	A	108	LYS	CE	42.144	0.3	1
1	A	108	LYS	H	8.145	0.020	1
1	A	108	LYS	HA	4.229	0.020	1
1	A	108	LYS	HB2	1.559	0.020	2
1	A	108	LYS	HB3	1.505	0.020	2
1	A	108	LYS	HG2	1.181	0.020	2
1	A	108	LYS	HG3	1.123	0.020	2
1	A	108	LYS	HD2	1.482	0.020	1
1	A	108	LYS	N	121.914	0.3	1
1	A	109	GLN	C	175.716	0.3	1
1	A	109	GLN	CA	55.756	0.3	1
1	A	109	GLN	CB	29.732	0.3	1
1	A	109	GLN	CG	36.499	0.3	1
1	A	109	GLN	H	8.256	0.020	1
1	A	109	GLN	HA	4.201	0.020	1
1	A	109	GLN	HB2	1.995	0.020	1
1	A	109	GLN	HG2	2.077	0.020	1
1	A	109	GLN	N	121.914	0.3	1
1	A	110	GLU	C	175.545	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	110	GLU	CA	56.246	0.3	1
1	A	110	GLU	CB	30.241	0.3	1
1	A	110	GLU	CG	36.279	0.3	1
1	A	110	GLU	HA	4.147	0.020	1
1	A	110	GLU	HB2	1.913	0.020	2
1	A	110	GLU	HB3	1.695	0.020	2
1	A	110	GLU	HG2	2.13	0.020	1
1	A	110	GLU	N	123.008	0.3	1
1	A	111	LEU	CA	56.821	0.3	1
1	A	111	LEU	CB	43.447	0.3	1
1	A	111	LEU	CG	27.188	0.3	1
1	A	111	LEU	CD1	25.136	0.3	1
1	A	111	LEU	CD2	23.668	0.3	1
1	A	111	LEU	H	7.835	0.020	1
1	A	111	LEU	HA	4.065	0.020	1
1	A	111	LEU	HB2	1.45	0.020	1
1	A	111	LEU	HG	1.45	0.020	1
1	A	111	LEU	HD11	0.769	0.020	1
1	A	111	LEU	HD12	0.769	0.020	1
1	A	111	LEU	HD13	0.769	0.020	1
1	A	111	LEU	HD21	0.715	0.020	1
1	A	111	LEU	HD22	0.715	0.020	1
1	A	111	LEU	HD23	0.715	0.020	1
1	A	111	LEU	N	129.023	0.3	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	103	-0.05 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	94	-0.02 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	93	-0.18 ± 0.21	None needed (< 0.5 ppm)
^{15}N	99	0.30 ± 0.56	None needed (< 0.5 ppm)

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 83%, i.e. 727 atoms were assigned a chemical shift out of a possible 879. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	315/331 (95%)	122/135 (90%)	129/132 (98%)	64/64 (100%)
Sidechain	412/530 (78%)	268/348 (77%)	144/162 (89%)	0/20 (0%)
Aromatic	0/18 (0%)	0/8 (0%)	0/10 (0%)	0/0 (—%)
Overall	727/879 (83%)	390/491 (79%)	273/304 (90%)	64/84 (76%)

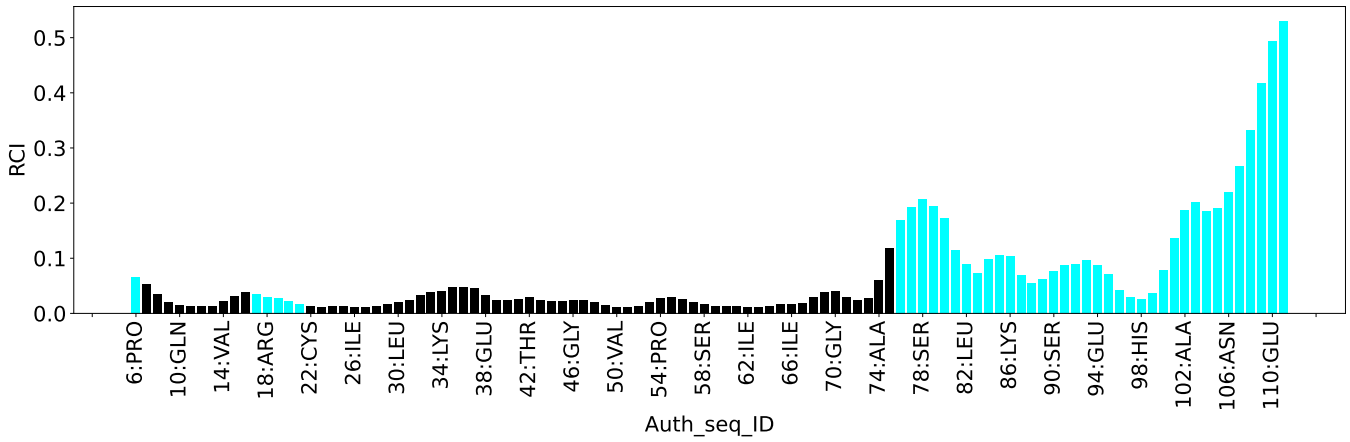
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	759
Intra-residue (|i-j|=0)	172
Sequential (|i-j|=1)	193
Medium range (|i-j|>1 and |i-j|<5)	135
Long range (|i-j|≥5)	245
Inter-chain	0
Hydrogen bond restraints	14
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	191
Number of restraints per residue	7.2
Number of long range restraints per residue[1]	2.4

[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)	16.3	0.2
0.2-0.5 (Medium)	24.0	0.5
>0.5 (Large)	57.2	4.59

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)

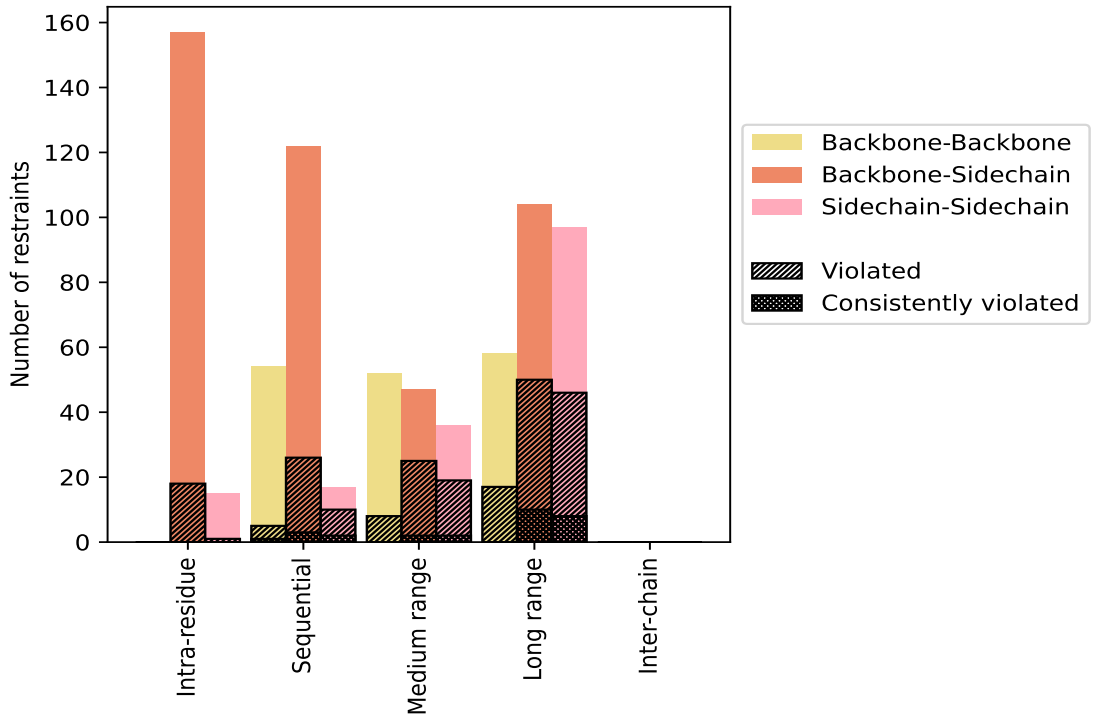
9.1 Summary of distance violations (i)

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)	172	22.7	19	11.0	2.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	157	20.7	18	11.5	2.4	0	0.0	0.0
Sidechain-Sidechain	15	2.0	1	6.7	0.1	0	0.0	0.0
Sequential (|i-j|=1)	193	25.4	41	21.2	5.4	6	3.1	0.8
Backbone-Backbone	54	7.1	5	9.3	0.7	1	1.9	0.1
Backbone-Sidechain	122	16.1	26	21.3	3.4	3	2.5	0.4
Sidechain-Sidechain	17	2.2	10	58.8	1.3	2	11.8	0.3
Medium range (|i-j|>1 & |i-j|<5)	135	17.8	52	38.5	6.9	4	3.0	0.5
Backbone-Backbone	52	6.9	8	15.4	1.1	0	0.0	0.0
Backbone-Sidechain	47	6.2	25	53.2	3.3	2	4.3	0.3
Sidechain-Sidechain	36	4.7	19	52.8	2.5	2	5.6	0.3
Long range (|i-j|≥5)	245	32.3	101	41.2	13.3	18	7.3	2.4
Backbone-Backbone	44	5.8	5	11.4	0.7	0	0.0	0.0
Backbone-Sidechain	104	13.7	50	48.1	6.6	10	9.6	1.3
Sidechain-Sidechain	97	12.8	46	47.4	6.1	8	8.2	1.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	14	1.8	12	85.7	1.6	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	759	100.0	225	29.6	29.6	28	3.7	3.7
Backbone-Backbone	164	21.6	30	18.3	4.0	1	0.6	0.1
Backbone-Sidechain	430	56.7	119	27.7	15.7	15	3.5	2.0
Sidechain-Sidechain	165	21.7	76	46.1	10.0	12	7.3	1.6

[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	6	21	18	51	0	96	0.99	4.05	0.84	0.82
2	8	20	19	54	0	101	0.86	3.46	0.69	0.73
3	9	23	24	59	0	115	0.8	4.16	0.79	0.58
4	7	15	22	56	0	100	0.85	3.31	0.74	0.74
5	6	13	21	55	0	95	0.81	3.5	0.63	0.64
6	7	14	18	45	0	84	0.87	4.59	0.79	0.66
7	6	17	19	50	0	92	0.9	3.14	0.7	0.72
8	8	20	18	50	0	96	0.83	3.34	0.61	0.7
9	6	17	23	48	0	94	0.85	4.07	0.7	0.68
10	5	20	21	54	0	100	0.81	2.67	0.59	0.68
11	7	16	20	48	0	91	0.77	2.6	0.6	0.65

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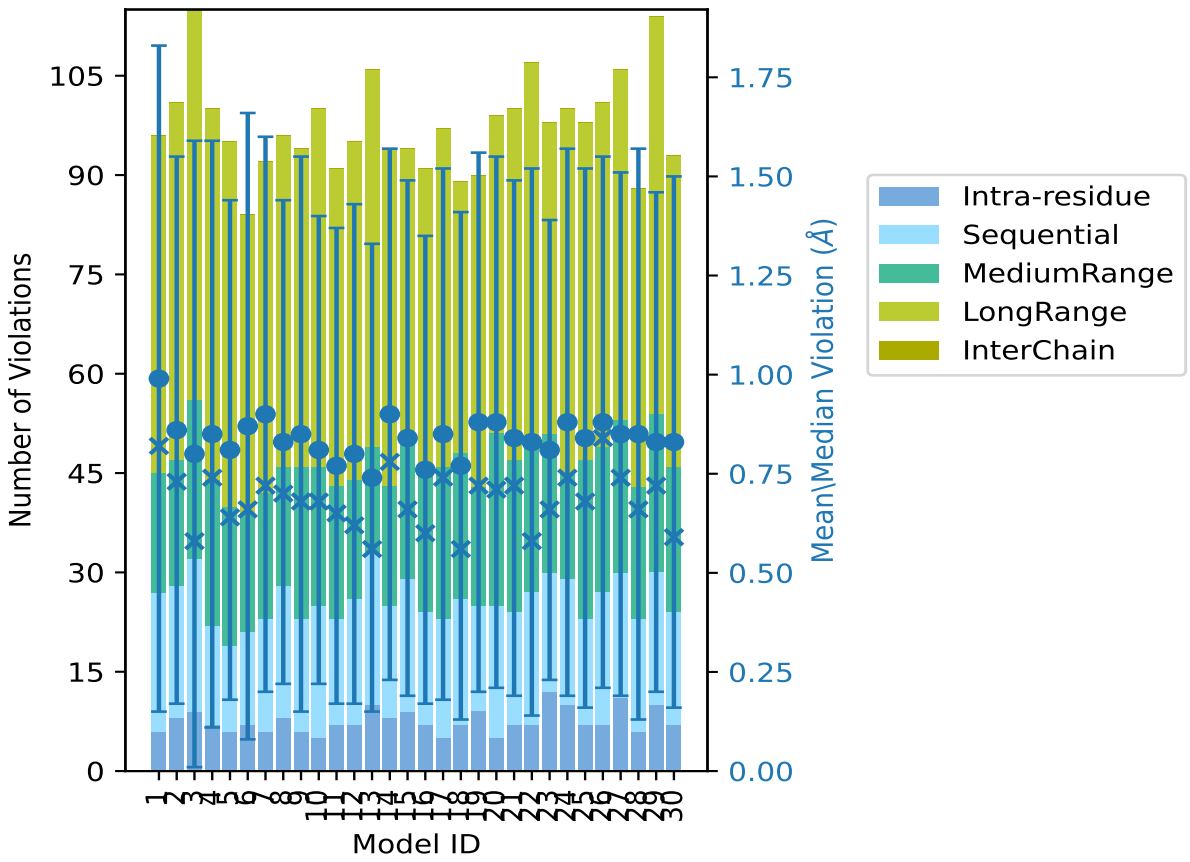
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	7	19	18	51	0	95	0.8	2.55	0.63	0.62
13	10	23	16	57	0	106	0.74	2.55	0.59	0.56
14	8	17	18	51	0	94	0.9	2.82	0.67	0.78
15	9	20	22	43	0	94	0.84	3.1	0.65	0.66
16	7	17	22	45	0	91	0.76	2.6	0.59	0.6
17	5	18	23	51	0	97	0.85	2.87	0.67	0.74
18	7	19	22	41	0	89	0.77	2.89	0.64	0.56
19	9	16	18	47	0	90	0.88	3.01	0.68	0.72
20	5	20	26	48	0	99	0.88	3.11	0.67	0.71
21	7	17	23	53	0	100	0.84	3.38	0.65	0.72
22	7	20	22	58	0	107	0.83	3.04	0.69	0.58
23	12	18	21	47	0	98	0.81	2.56	0.58	0.66
24	10	19	16	55	0	100	0.88	3.52	0.69	0.74
25	7	16	24	51	0	98	0.84	2.94	0.68	0.68
26	7	20	22	52	0	101	0.88	2.88	0.67	0.84
27	11	19	23	53	0	106	0.85	2.72	0.66	0.74
28	6	17	20	45	0	88	0.85	4.2	0.72	0.66
29	10	20	24	60	0	114	0.83	2.63	0.63	0.72
30	7	17	22	47	0	93	0.83	3.08	0.67	0.59

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

9.2.1 Bar graph : Distance Violation statistics for each model



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

9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 532(IR:153, SQ:152, MR:83, LR:144, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
2	7	10	6	0	25	1	3.3
1	3	5	10	0	19	2	6.7
0	3	2	6	0	11	3	10.0
2	0	1	4	0	7	4	13.3
0	2	0	4	0	6	5	16.7
1	2	1	6	0	10	6	20.0

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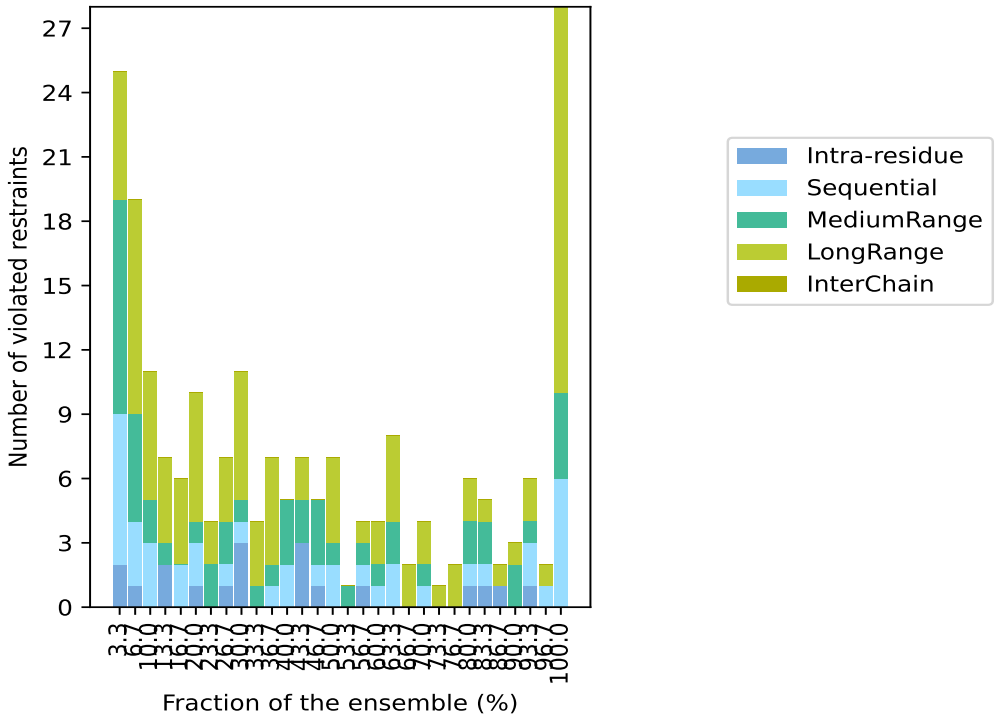
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	2	2	0	4	7	23.3
1	1	2	3	0	7	8	26.7
3	1	1	6	0	11	9	30.0
0	0	1	3	0	4	10	33.3
0	1	1	5	0	7	11	36.7
0	2	3	0	0	5	12	40.0
3	0	2	2	0	7	13	43.3
1	1	3	0	0	5	14	46.7
0	2	1	4	0	7	15	50.0
0	0	1	0	0	1	16	53.3
1	1	1	1	0	4	17	56.7
0	1	1	2	0	4	18	60.0
0	2	2	4	0	8	19	63.3
0	0	0	2	0	2	20	66.7
0	1	1	2	0	4	21	70.0
0	0	0	1	0	1	22	73.3
0	0	0	2	0	2	23	76.7
1	1	2	2	0	6	24	80.0
1	1	2	1	0	5	25	83.3
1	0	0	1	0	2	26	86.7
0	0	2	1	0	3	27	90.0
1	2	1	2	0	6	28	93.3
0	1	0	1	0	2	29	96.7
0	6	4	18	0	28	30	100.0

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

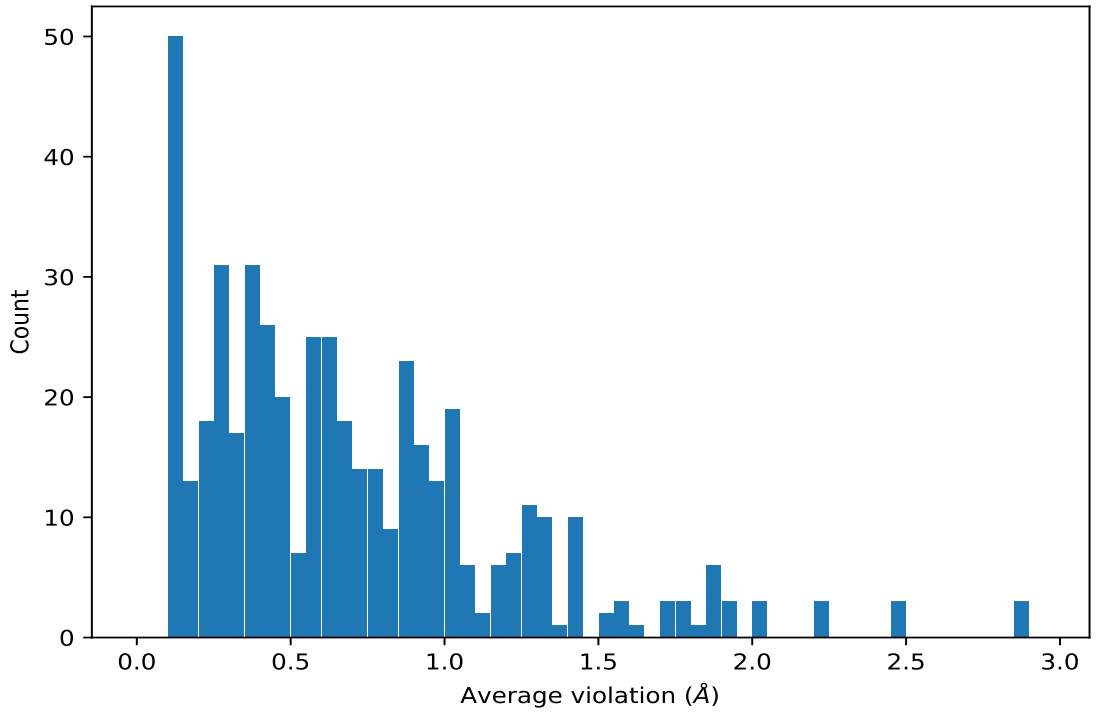
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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



9.4.2 Table: Most violated distance restraints

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG21	30	2.24	0.92	2.37
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG22	30	2.24	0.92	2.37
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG23	30	2.24	0.92	2.37
(1,371)	1:A:11:GLN:H	1:A:50:VAL:HG21	30	2.01	0.14	2.03
(1,371)	1:A:11:GLN:H	1:A:50:VAL:HG22	30	2.01	0.14	2.03
(1,371)	1:A:11:GLN:H	1:A:50:VAL:HG23	30	2.01	0.14	2.03
(1,65)	1:A:50:VAL:HG21	1:A:75:GLU:HG3	30	1.91	0.55	1.94
(1,65)	1:A:50:VAL:HG22	1:A:75:GLU:HG3	30	1.91	0.55	1.94
(1,65)	1:A:50:VAL:HG23	1:A:75:GLU:HG3	30	1.91	0.55	1.94
(1,191)	1:A:14:VAL:HG21	1:A:48:LEU:HA	30	1.86	0.84	2.05
(1,191)	1:A:14:VAL:HG22	1:A:48:LEU:HA	30	1.86	0.84	2.05
(1,191)	1:A:14:VAL:HG23	1:A:48:LEU:HA	30	1.86	0.84	2.05
(1,129)	1:A:10:GLN:HG3	1:A:50:VAL:HG21	30	1.86	0.68	1.91
(1,129)	1:A:10:GLN:HG3	1:A:50:VAL:HG22	30	1.86	0.68	1.91
(1,129)	1:A:10:GLN:HG3	1:A:50:VAL:HG23	30	1.86	0.68	1.91
(1,46)	1:A:36:VAL:HG21	1:A:50:VAL:HB	30	1.77	0.92	1.6

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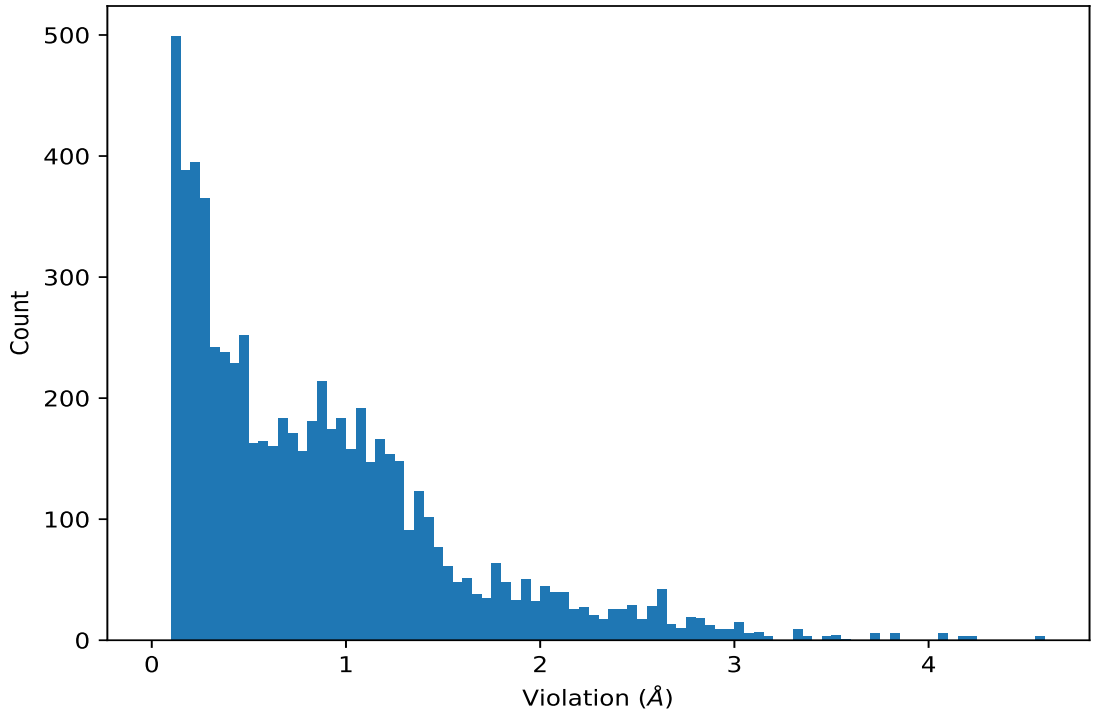
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,46)	1:A:36:VAL:HG22	1:A:50:VAL:HB	30	1.77	0.92	1.6
(1,46)	1:A:36:VAL:HG23	1:A:50:VAL:HB	30	1.77	0.92	1.6
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD21	30	1.71	1.15	1.42
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD22	30	1.71	1.15	1.42
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD23	30	1.71	1.15	1.42
(1,370)	1:A:11:GLN:H	1:A:75:GLU:HG3	30	1.65	0.57	1.74
(1,214)	1:A:62:ILE:HG21	1:A:64:GLU:HG3	30	1.59	0.47	1.28
(1,214)	1:A:62:ILE:HG22	1:A:64:GLU:HG3	30	1.59	0.47	1.28
(1,214)	1:A:62:ILE:HG23	1:A:64:GLU:HG3	30	1.59	0.47	1.28
(1,47)	1:A:36:VAL:HG21	1:A:50:VAL:HG11	30	1.41	0.82	1.02

[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)
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG21	6	4.59
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG22	6	4.59
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG23	6	4.59
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD21	28	4.2
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD22	28	4.2
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD23	28	4.2
(1,186)	1:A:30:LEU:HD11	1:A:62:ILE:HG13	3	4.16
(1,186)	1:A:30:LEU:HD12	1:A:62:ILE:HG13	3	4.16
(1,186)	1:A:30:LEU:HD13	1:A:62:ILE:HG13	3	4.16
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD21	9	4.07
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD22	9	4.07
(1,294)	1:A:6:PRO:HG3	1:A:7:LEU:HD23	9	4.07
(1,186)	1:A:30:LEU:HD11	1:A:62:ILE:HG13	1	4.05
(1,186)	1:A:30:LEU:HD12	1:A:62:ILE:HG13	1	4.05
(1,186)	1:A:30:LEU:HD13	1:A:62:ILE:HG13	1	4.05
(1,184)	1:A:30:LEU:HD11	1:A:62:ILE:HA	3	3.83
(1,184)	1:A:30:LEU:HD12	1:A:62:ILE:HA	3	3.83
(1,184)	1:A:30:LEU:HD13	1:A:62:ILE:HA	3	3.83
(1,184)	1:A:30:LEU:HD11	1:A:62:ILE:HA	1	3.81
(1,184)	1:A:30:LEU:HD12	1:A:62:ILE:HA	1	3.81
(1,184)	1:A:30:LEU:HD13	1:A:62:ILE:HA	1	3.81
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG21	9	3.74
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG22	9	3.74
(1,268)	1:A:18:ARG:HB3	1:A:43:VAL:HG23	9	3.74
(1,46)	1:A:36:VAL:HG21	1:A:50:VAL:HB	3	3.73
(1,46)	1:A:36:VAL:HG22	1:A:50:VAL:HB	3	3.73
(1,46)	1:A:36:VAL:HG23	1:A:50:VAL:HB	3	3.73
(1,247)	1:A:11:GLN:HG3	1:A:47:ARG:HD3	6	3.58

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found