wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2LRC
BMRB ID	:	18130
Title	:	Structure of thioredoxin 2 from Pseudomonas aeruginosa PAO1 in its reduced form
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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 (1)) were used in the production of this report:

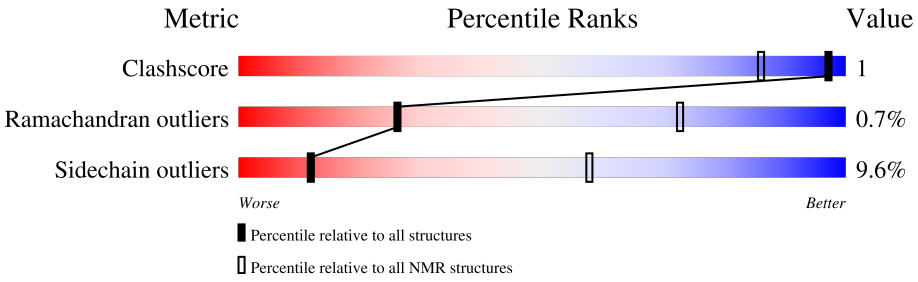
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 92%.

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	114	77% 6% • 10% 5%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:57, A:65-A:108 (97)	0.41	13

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1531 atoms, of which 690 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Probable thioredoxin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	108	1531	531	690	150	157	3	0

There are 6 discrepancies between the modelled and reference sequences:

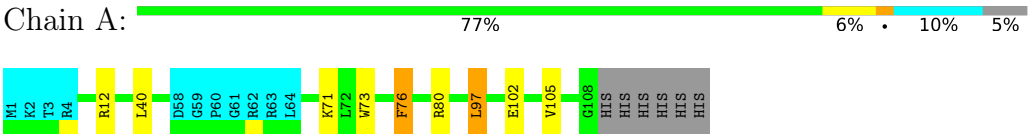
Chain	Residue	Modelled	Actual	Comment	Reference
A	109	HIS	-	expression tag	UNP Q9I0E8
A	110	HIS	-	expression tag	UNP Q9I0E8
A	111	HIS	-	expression tag	UNP Q9I0E8
A	112	HIS	-	expression tag	UNP Q9I0E8
A	113	HIS	-	expression tag	UNP Q9I0E8
A	114	HIS	-	expression tag	UNP Q9I0E8

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.

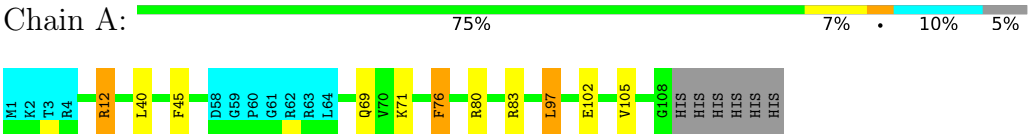
- Molecule 1: Probable thioredoxin



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

The representative model is number 13. Colouring as in section 4.1 above.

- Molecule 1: Probable thioredoxin



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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	
CYANA	structure solution	

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	1296
Number of shifts mapped to atoms	1163
Number of unparsed shifts	0
Number of shifts with mapping errors	133
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality (i)

6.1 Standard geometry (i)

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	0.69±0.01	0±0/772 (0.0± 0.0%)	1.02±0.02	2±1/1049 (0.2± 0.1%)
All	All	0.69	0/15440 (0.0%)	1.02	47/20980 (0.2%)

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	0.1±0.2
All	All	0	1

There are no bond-length outliers.

5 of 7 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	12	ARG	NE-CZ-NH1	6.72	123.66	120.30	12	10
1	A	83	ARG	NE-CZ-NH1	6.63	123.62	120.30	3	4
1	A	17	ARG	NE-CZ-NH1	6.11	123.36	120.30	9	4
1	A	80	ARG	NE-CZ-NH1	6.10	123.35	120.30	16	15
1	A	66	ARG	NE-CZ-NH1	6.03	123.32	120.30	8	5

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	17	ARG	Sidechain	1

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	753	614	722	1±0
All	All	15060	12280	14440	19

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 1.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:VAL:HG21	1:A:97:LEU:HB3	0.49	1.84	7	3
1:A:76:PHE:CE2	1:A:97:LEU:HD21	0.47	2.44	12	16

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/114 (84%)	90±1 (94±1%)	5±1 (6±1%)	1±0 (1±0%)	26	73
All	All	1920/2280 (84%)	1797 (94%)	109 (6%)	14 (1%)	26	73

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	73	TRP	11
1	A	71	LYS	3

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	78/93 (84%)	71±1 (90±1%)	7±1 (10±1%)	12	58
All	All	1560/1860 (84%)	1411 (90%)	149 (10%)	12	58

5 of 14 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	40	LEU	20
1	A	76	PHE	20
1	A	97	LEU	20
1	A	102	GLU	19
1	A	105	VAL	17

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 92% for the well-defined parts and 88% 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	1296
Number of shifts mapped to atoms	1163
Number of unparsed shifts	0
Number of shifts with mapping errors	133
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

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 133) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	ARG	HB2	1.893	0.020	2
1	A	4	ARG	HG2	1.687	0.020	2
1	A	4	ARG	HD2	3.212	0.020	1
1	A	5	TYR	HB2	2.814	0.020	2
1	A	6	SER	HB2	3.942	0.020	1
1	A	8	GLU	HB2	1.96	0.020	1
1	A	8	GLU	HG2	2.312	0.020	2
1	A	10	PRO	HB2	1.835	0.020	2
1	A	10	PRO	HG2	1.964	0.020	2
1	A	10	PRO	HD2	3.759	0.020	2
1	A	12	ARG	HB2	2.003	0.020	2
1	A	12	ARG	HG2	2.249	0.020	2
1	A	12	ARG	HD2	2.382	0.020	1
1	A	13	ASP	HB2	2.655	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	GLU	HB2	2.321	0.020	2
1	A	14	GLU	HG2	2.266	0.020	2
1	A	15	LEU	HB2	1.879	0.020	2
1	A	16	ASP	HB2	2.74	0.020	1
1	A	17	ARG	HB2	2.024	0.020	2
1	A	17	ARG	HG2	1.694	0.020	2
1	A	17	ARG	HD2	3.237	0.020	1
1	A	18	LEU	HB2	1.662	0.020	1
1	A	21	PRO	HB2	2.089	0.020	1
1	A	21	PRO	HG2	2.031	0.020	1
1	A	21	PRO	HD2	3.453	0.020	2
1	A	23	LEU	HB2	1.985	0.020	2
1	A	25	GLU	HB2	2.007	0.020	2
1	A	25	GLU	HG2	1.788	0.020	2
1	A	26	PHE	HB2	2.771	0.020	1
1	A	29	ASP	HB2	2.745	0.020	2
1	A	30	TRP	HB2	3.551	0.020	2
1	A	34	CYS	HB2	3.583	0.020	2
1	A	35	GLN	HB2	2.176	0.020	1
1	A	35	GLN	HG2	2.708	0.020	2
1	A	38	GLN	HB2	2.406	0.020	2
1	A	38	GLN	HG2	3.284	0.020	2
1	A	39	PRO	HB2	1.907	0.020	2
1	A	39	PRO	HG2	2.109	0.020	1
1	A	39	PRO	HD2	4.069	0.020	1
1	A	40	LEU	HB2	1.964	0.020	2
1	A	41	LEU	HB2	2.122	0.020	2
1	A	43	GLU	HB2	2.253	0.020	2
1	A	43	GLU	HG2	2.357	0.020	2
1	A	45	PHE	HB2	3.166	0.020	1
1	A	46	SER	HB2	3.936	0.020	1
1	A	47	ASP	HB2	2.406	0.020	2
1	A	48	TYR	HB2	3.186	0.020	2
1	A	49	PRO	HB2	2.058	0.020	2
1	A	49	PRO	HG2	2.025	0.020	1
1	A	49	PRO	HD2	3.65	0.020	2
1	A	50	GLU	HB2	2.193	0.020	1
1	A	50	GLU	HG2	2.431	0.020	2
1	A	54	LEU	HB2	1.461	0.020	2
1	A	55	LYS	HB2	1.512	0.020	2
1	A	55	LYS	HG2	0.669	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	55	LYS	HD2	0.259	0.020	2
1	A	55	LYS	HE2	1.962	0.020	2
1	A	57	GLU	HB2	1.773	0.020	2
1	A	57	GLU	HG2	2.094	0.020	2
1	A	58	ASP	HB2	2.409	0.020	2
1	A	60	PRO	HB2	2.06	0.020	2
1	A	60	PRO	HG2	2.029	0.020	1
1	A	60	PRO	HD2	3.802	0.020	2
1	A	64	LEU	HB2	2.089	0.020	2
1	A	66	ARG	HB2	2.03	0.020	2
1	A	66	ARG	HG2	1.916	0.020	2
1	A	66	ARG	HD2	3.377	0.020	1
1	A	67	SER	HB2	4.079	0.020	1
1	A	68	PHE	HB2	3.388	0.020	2
1	A	69	GLN	HB2	2.336	0.020	2
1	A	69	GLN	HG2	2.329	0.020	1
1	A	71	LYS	HB2	1.801	0.020	2
1	A	71	LYS	HG2	1.38	0.020	2
1	A	71	LYS	HD2	1.6	0.020	1
1	A	71	LYS	HE2	2.914	0.020	1
1	A	72	LEU	HB2	1.357	0.020	2
1	A	73	TRP	HB2	3.46	0.020	2
1	A	74	PRO	HB2	1.467	0.020	2
1	A	74	PRO	HG2	2.257	0.020	1
1	A	74	PRO	HD2	4.058	0.020	2
1	A	76	PHE	HB2	3.337	0.020	2
1	A	78	PHE	HB2	3.091	0.020	2
1	A	79	LEU	HB2	1.961	0.020	2
1	A	80	ARG	HB2	1.897	0.020	2
1	A	80	ARG	HG2	1.668	0.020	2
1	A	80	ARG	HD2	3.275	0.020	1
1	A	81	ASP	HB2	2.975	0.020	2
1	A	83	ARG	HB2	1.888	0.020	2
1	A	83	ARG	HG2	1.691	0.020	2
1	A	83	ARG	HD2	3.271	0.020	1
1	A	84	GLU	HB2	2.09	0.020	2
1	A	84	GLU	HG2	2.395	0.020	1
1	A	87	ARG	HB2	2.357	0.020	2
1	A	87	ARG	HG2	1.584	0.020	2
1	A	87	ARG	HD2	3.18	0.020	1
1	A	90	ARG	HB2	2.122	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	90	ARG	HG2	1.882	0.020	2
1	A	90	ARG	HD2	2.88	0.020	1
1	A	91	PRO	HB2	1.948	0.020	1
1	A	91	PRO	HG2	2.065	0.020	2
1	A	91	PRO	HD2	3.79	0.020	2
1	A	93	SER	HB2	4.035	0.020	1
1	A	95	SER	HB2	3.986	0.020	1
1	A	97	LEU	HB2	2.2	0.020	2
1	A	98	GLU	HB2	2.197	0.020	1
1	A	98	GLU	HG2	2.433	0.020	2
1	A	99	GLU	HB2	2.014	0.020	2
1	A	99	GLU	HG2	2.421	0.020	2
1	A	101	PHE	HB2	2.4	0.020	2
1	A	102	GLU	HB2	2.017	0.020	2
1	A	102	GLU	HG2	2.227	0.020	2
1	A	103	SER	HB2	3.76	0.020	2
1	A	104	LEU	HB2	2.122	0.020	2
1	A	107	GLU	HB2	2.105	0.020	2
1	A	107	GLU	HG2	2.316	0.020	1
1	A	109	HIS	C	173.585	0.3	1
1	A	109	HIS	CA	55.483	0.3	1
1	A	109	HIS	CB	29.783	0.3	1
1	A	109	HIS	H	8.184	0.020	1
1	A	109	HIS	HA	4.578	0.020	1
1	A	109	HIS	HB2	3.088	0.020	2
1	A	109	HIS	HB3	3.018	0.020	2
1	A	109	HIS	HD2	7.083	0.020	1
1	A	109	HIS	N	118.701	0.3	1
1	A	110	HIS	C	178.966	0.3	1
1	A	110	HIS	CA	56.626	0.3	1
1	A	110	HIS	CB	29.714	0.3	1
1	A	110	HIS	H	8.141	0.020	1
1	A	110	HIS	HA	4.46	0.020	1
1	A	110	HIS	HB2	3.238	0.020	2
1	A	110	HIS	HB3	3.088	0.020	2
1	A	110	HIS	HD2	6.984	0.020	1
1	A	110	HIS	N	125.473	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
$^{13}C_{\alpha}$	108	0.29 ± 0.16	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	97	0.84 ± 0.13	Should be checked
$^{13}C'$	108	0.50 ± 0.18	None needed (< 0.5 ppm)
^{15}N	100	0.04 ± 0.48	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 92%, i.e. 1192 atoms were assigned a chemical shift out of a possible 1289. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	482/482 (100%)	197/197 (100%)	194/194 (100%)	91/91 (100%)
Sidechain	625/691 (90%)	414/450 (92%)	208/215 (97%)	3/26 (12%)
Aromatic	85/116 (73%)	49/58 (84%)	34/54 (63%)	2/4 (50%)
Overall	1192/1289 (92%)	660/705 (94%)	436/463 (94%)	96/121 (79%)

7.1.4 Statistically unusual chemical shifts

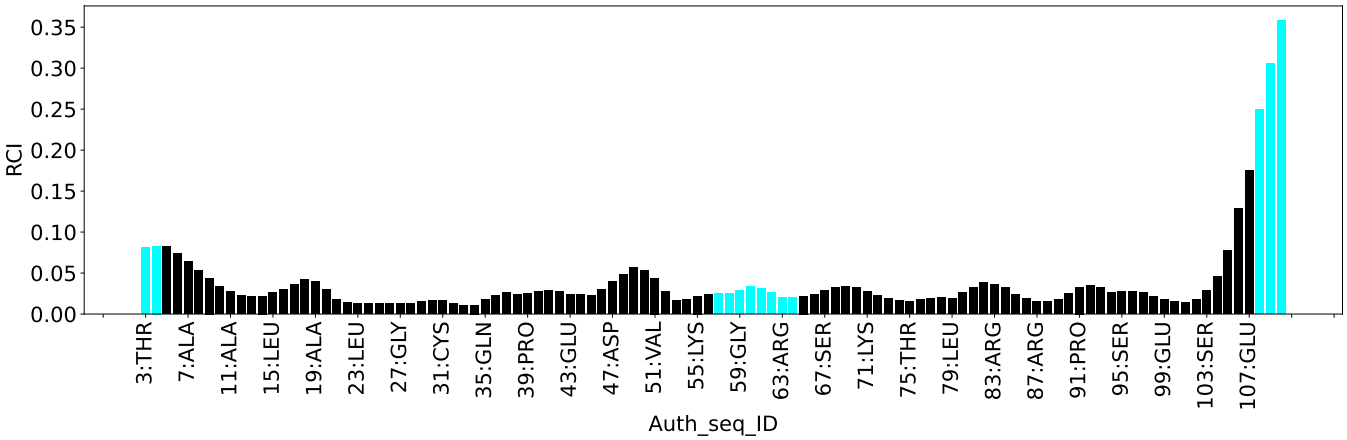
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	12	ARG	CD	35.58	38.57 – 47.75	-8.3
1	A	55	LYS	HD3	0.01	0.54 – 2.65	-7.5
1	A	55	LYS	HD2	0.26	0.58 – 2.64	-6.5
1	A	55	LYS	HE3	1.67	1.92 – 3.89	-6.3
1	A	55	LYS	HB3	0.31	0.46 – 3.04	-5.6
1	A	28	THR	HG21	0.06	0.08 – 2.19	-5.1
1	A	28	THR	HG22	0.06	0.08 – 2.19	-5.1
1	A	28	THR	HG23	0.06	0.08 – 2.19	-5.1

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:



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	2304
Intra-residue (|i-j|=0)	497
Sequential (|i-j|=1)	590
Medium range (|i-j|>1 and |i-j|<5)	409
Long range (|i-j|≥5)	808
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	701
Number of restraints per residue	20.2
Number of long range restraints per residue[1]	7.1

[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)	43.6	0.2
0.2-0.5 (Medium)	74.0	0.5
>0.5 (Large)	91.5	2.99

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)

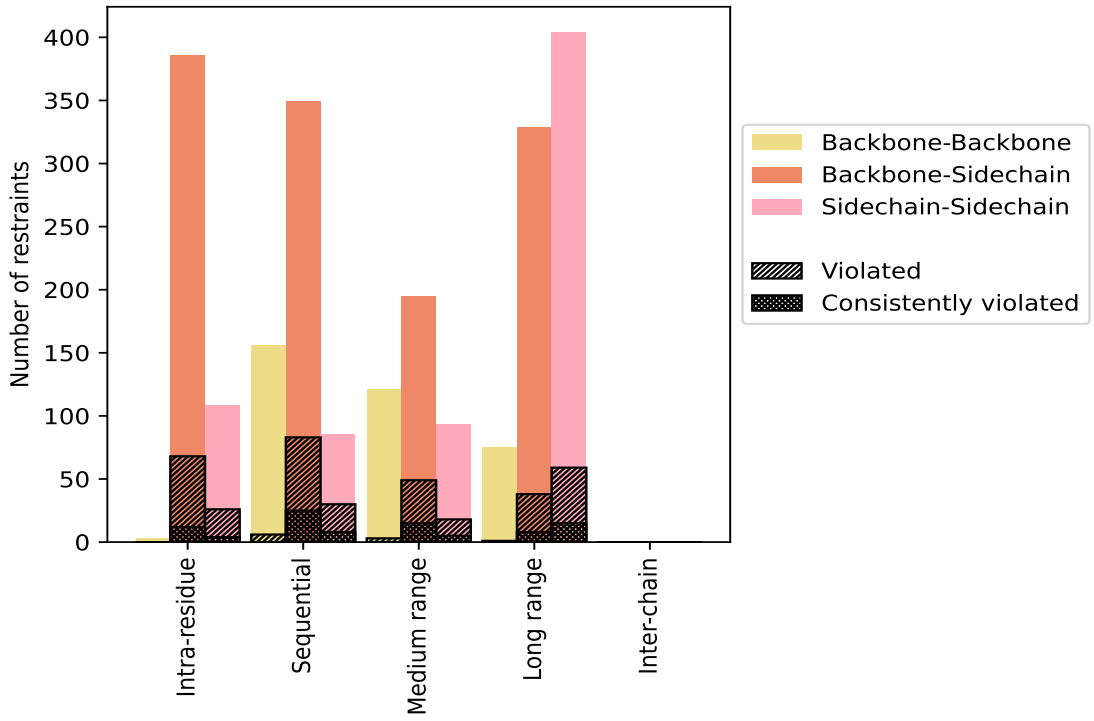
9.1 Summary of distance violations (i)

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)	497	21.6	94	18.9	4.1	16	3.2	0.7
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	386	16.8	68	17.6	3.0	12	3.1	0.5
Sidechain-Sidechain	108	4.7	26	24.1	1.1	4	3.7	0.2
Sequential (|i-j|=1)	590	25.6	119	20.2	5.2	33	5.6	1.4
Backbone-Backbone	156	6.8	6	3.8	0.3	0	0.0	0.0
Backbone-Sidechain	349	15.1	83	23.8	3.6	25	7.2	1.1
Sidechain-Sidechain	85	3.7	30	35.3	1.3	8	9.4	0.3
Medium range (|i-j|>1 & |i-j|<5)	409	17.8	70	17.1	3.0	20	4.9	0.9
Backbone-Backbone	121	5.3	3	2.5	0.1	0	0.0	0.0
Backbone-Sidechain	195	8.5	49	25.1	2.1	15	7.7	0.7
Sidechain-Sidechain	93	4.0	18	19.4	0.8	5	5.4	0.2
Long range (|i-j|≥5)	808	35.1	98	12.1	4.3	23	2.8	1.0
Backbone-Backbone	75	3.3	1	1.3	0.0	0	0.0	0.0
Backbone-Sidechain	329	14.3	38	11.6	1.6	8	2.4	0.3
Sidechain-Sidechain	404	17.5	59	14.6	2.6	15	3.7	0.7
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	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	2304	100.0	381	16.5	16.5	92	4.0	4.0
Backbone-Backbone	355	15.4	10	2.8	0.4	0	0.0	0.0
Backbone-Sidechain	1259	54.6	238	18.9	10.3	60	4.8	2.6
Sidechain-Sidechain	690	29.9	133	19.3	5.8	32	4.6	1.4

[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	46	67	36	50	0	199	0.61	2.98	0.47	0.49
2	54	65	38	55	0	212	0.6	2.98	0.49	0.47
3	53	71	39	56	0	219	0.59	2.97	0.49	0.45
4	60	66	38	48	0	212	0.59	2.93	0.47	0.44
5	46	62	35	48	0	191	0.6	2.99	0.49	0.45
6	53	73	40	46	0	212	0.6	2.99	0.49	0.48
7	52	63	42	53	0	210	0.59	2.98	0.5	0.43
8	47	65	36	54	0	202	0.6	2.98	0.49	0.44
9	53	67	41	55	0	216	0.54	2.97	0.47	0.4
10	58	61	43	51	0	213	0.57	2.89	0.48	0.41
11	50	66	36	50	0	202	0.6	2.92	0.49	0.44

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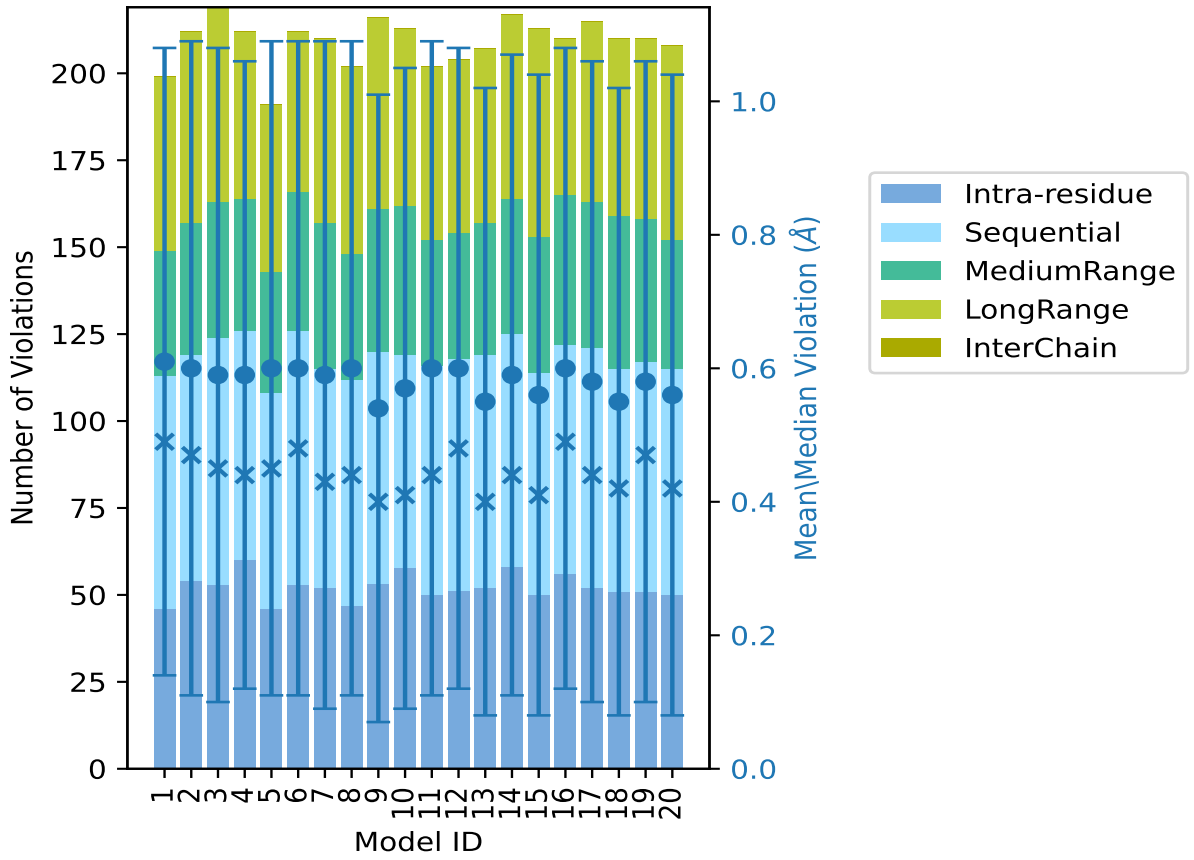
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	51	67	36	50	0	204	0.6	2.93	0.48	0.48
13	52	67	38	50	0	207	0.55	2.98	0.47	0.4
14	58	67	39	53	0	217	0.59	2.97	0.48	0.44
15	50	64	39	60	0	213	0.56	2.98	0.48	0.41
16	56	66	43	45	0	210	0.6	2.91	0.48	0.49
17	52	69	42	52	0	215	0.58	2.93	0.48	0.44
18	51	64	44	51	0	210	0.55	2.87	0.47	0.42
19	51	66	41	52	0	210	0.58	2.91	0.48	0.47
20	50	65	37	56	0	208	0.56	2.99	0.48	0.42

[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

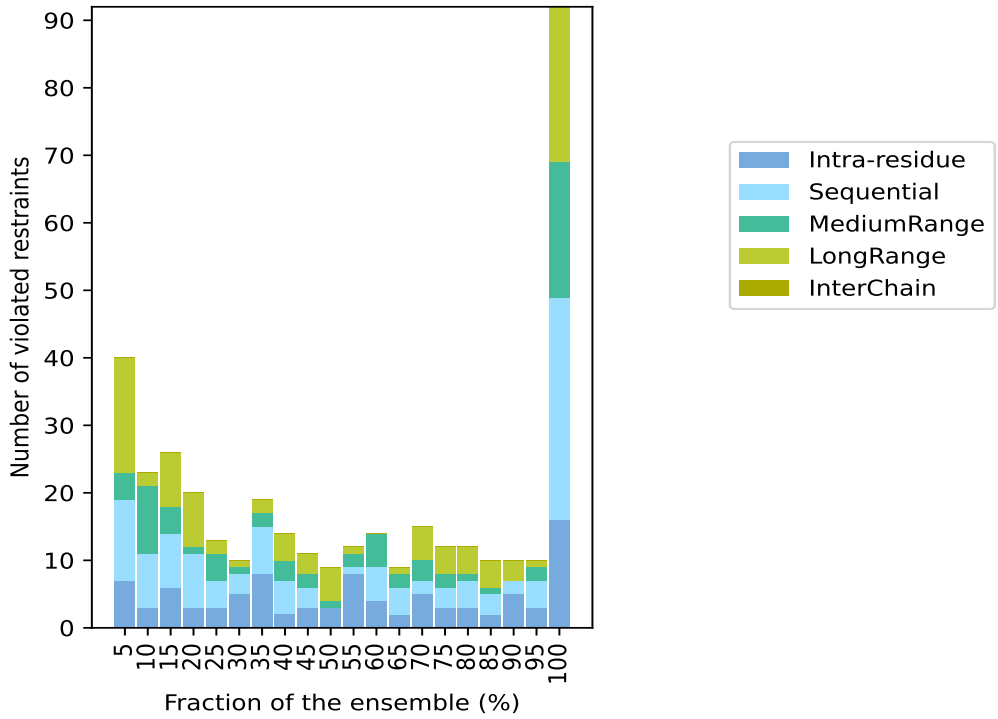
9.3 Distance violation statistics for the ensemble (i)

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, 1923(IR:403, SQ:471, MR:339, LR:710, 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]	%
7	12	4	17	0	40	1	5.0
3	8	10	2	0	23	2	10.0
6	8	4	8	0	26	3	15.0
3	8	1	8	0	20	4	20.0
3	4	4	2	0	13	5	25.0
5	3	1	1	0	10	6	30.0
8	7	2	2	0	19	7	35.0
2	5	3	4	0	14	8	40.0
3	3	2	3	0	11	9	45.0
3	0	1	5	0	9	10	50.0
8	1	2	1	0	12	11	55.0
4	5	5	0	0	14	12	60.0
2	4	2	1	0	9	13	65.0
5	2	3	5	0	15	14	70.0
3	3	2	4	0	12	15	75.0
3	4	1	4	0	12	16	80.0
2	3	1	4	0	10	17	85.0
5	2	0	3	0	10	18	90.0
3	4	2	1	0	10	19	95.0
16	33	20	23	0	92	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

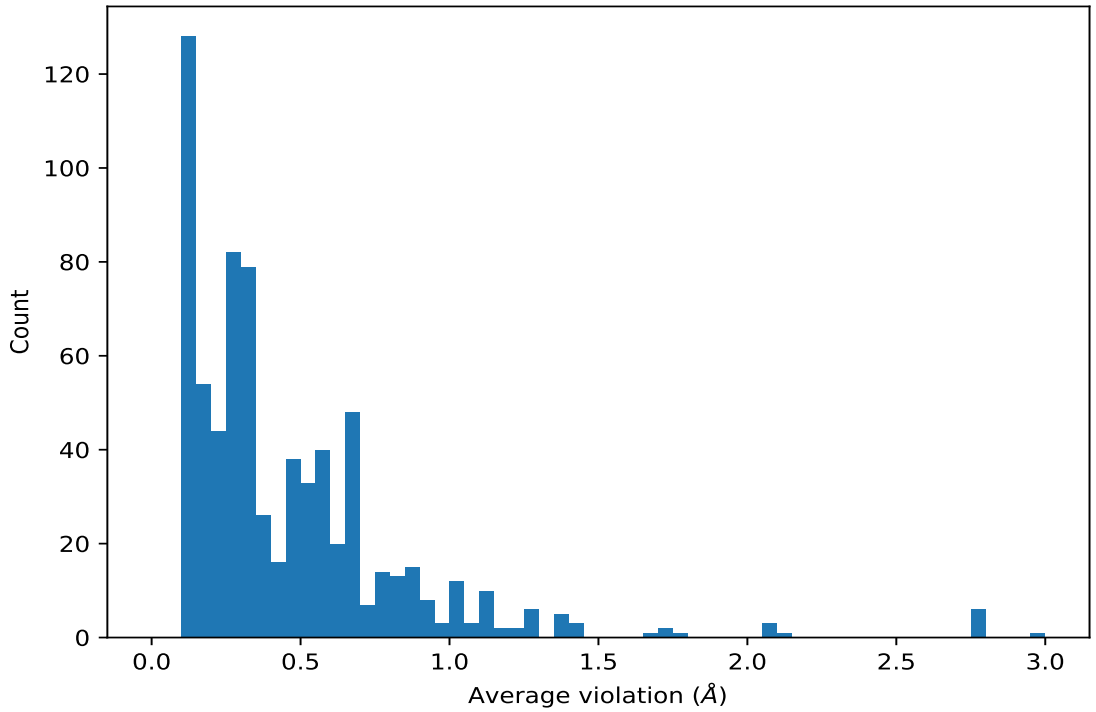
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	20	2.95	0.04	2.97
(1,2063)	1:A:51:VAL:HG11	1:A:78:PHE:HD1	20	2.76	0.03	2.76
(1,2063)	1:A:51:VAL:HG12	1:A:78:PHE:HD1	20	2.76	0.03	2.76
(1,2063)	1:A:51:VAL:HG13	1:A:78:PHE:HD1	20	2.76	0.03	2.76
(1,2063)	1:A:51:VAL:HG21	1:A:78:PHE:HD1	20	2.76	0.03	2.76
(1,2063)	1:A:51:VAL:HG22	1:A:78:PHE:HD1	20	2.76	0.03	2.76
(1,2063)	1:A:51:VAL:HG23	1:A:78:PHE:HD1	20	2.76	0.03	2.76
(1,231)	1:A:78:PHE:HD1	1:A:101:PHE:HZ	20	2.1	0.04	2.09
(1,229)	1:A:78:PHE:HD2	1:A:88:VAL:HG21	20	2.09	0.03	2.09
(1,229)	1:A:78:PHE:HD2	1:A:88:VAL:HG22	20	2.09	0.03	2.09
(1,229)	1:A:78:PHE:HD2	1:A:88:VAL:HG23	20	2.09	0.03	2.09
(1,233)	1:A:78:PHE:HD1	1:A:104:LEU:HB3	20	1.77	0.11	1.73
(1,570)	1:A:32:GLY:HA3	1:A:35:GLN:HB3	20	1.72	0.02	1.72
(1,500)	1:A:39:PRO:HG3	1:A:40:LEU:HA	20	1.71	0.05	1.72
(1,1951)	1:A:37:ALA:H	1:A:38:GLN:HB3	20	1.68	0.03	1.68
(1,1253)	1:A:37:ALA:H	1:A:39:PRO:HD3	20	1.43	0.07	1.44

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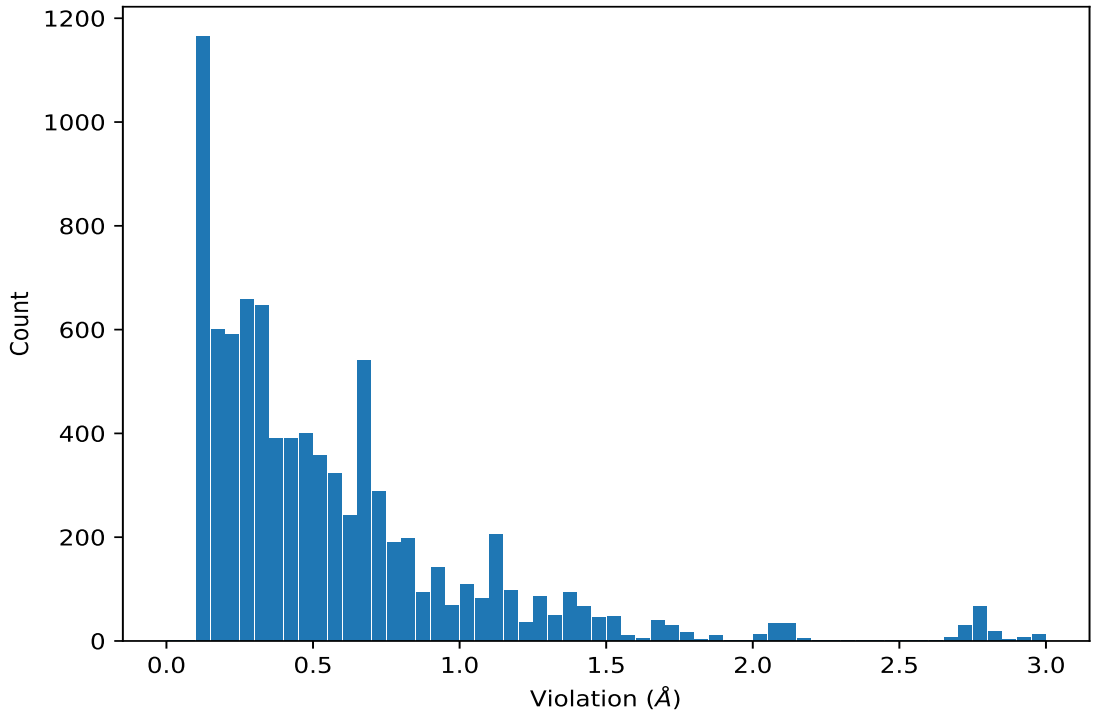
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,293)	1:A:95:SER:HA	1:A:98:GLU:HB3	20	1.42	0.16	1.44

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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



9.5.2 Table : All distance violations

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)
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	5	2.99
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	6	2.99
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	20	2.99
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	1	2.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	2	2.98
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	7	2.98
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	8	2.98
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	13	2.98
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	15	2.98
(1,227)	1:A:78:PHE:HD2	1:A:88:VAL:HB	3	2.97

10 Dihedral-angle violation analysis (i)

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