



Full wwPDB NMR Structure Validation Report ⓘ

Sep 9, 2026 – 09:09 PM JST

PDB ID : 23SS / pdb_000023ss
BMRB ID : 36832
Title : The lasso structure of jiangxilassin A
Authors : Kumeta, H.; Kawakami, A.; Tsunoda, T.; Dairi, T.; Ogasawara, Y.
Deposited on : 2026-02-16

This is a Full wwPDB NMR Structure Validation 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

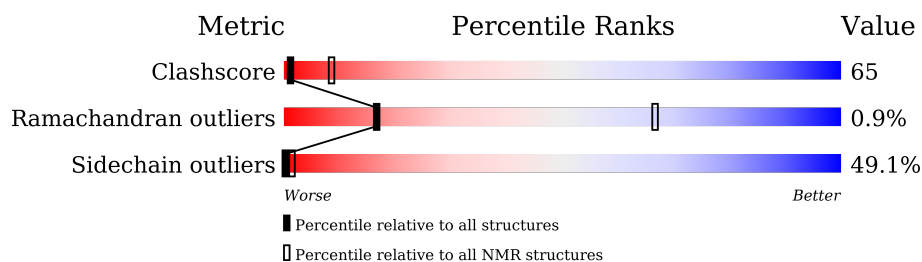
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 66%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	17	

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:1-A:9, A:14-A:17 (13)	0.13	19

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 256 atoms, of which 117 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP.

Mol	Chain	Residues	Atoms						Trace
1	A	17	Total	C	H	N	O	S	0
			256	94	117	20	22	3	

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: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

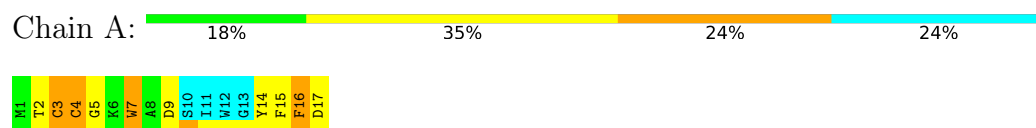
4.2.1 Score per residue for model 1

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.2 Score per residue for model 2

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.3 Score per residue for model 3

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



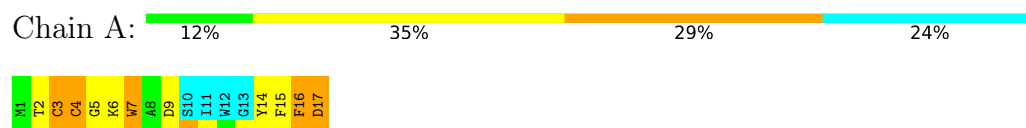
4.2.4 Score per residue for model 4

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.5 Score per residue for model 5

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.6 Score per residue for model 6

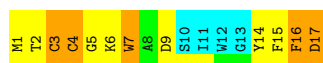
- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.7 Score per residue for model 7

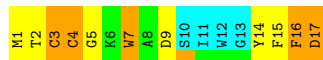
- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP





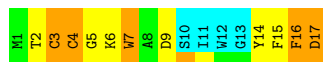
4.2.8 Score per residue for model 8

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



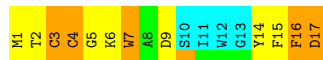
4.2.9 Score per residue for model 9

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.10 Score per residue for model 10

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.11 Score per residue for model 11

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



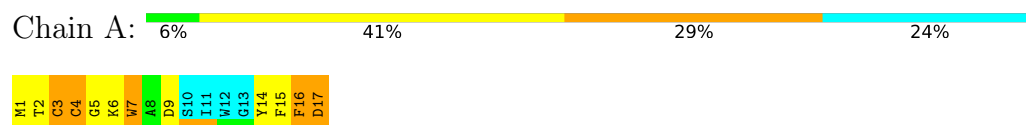
4.2.12 Score per residue for model 12

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.13 Score per residue for model 13

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



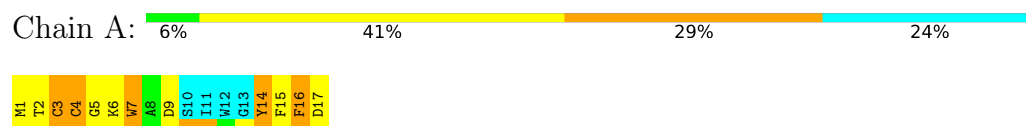
4.2.14 Score per residue for model 14

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.15 Score per residue for model 15

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP



4.2.16 Score per residue for model 16

- Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP

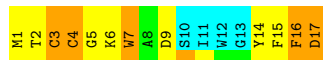




4.2.17 Score per residue for model 17

• Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP

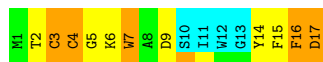
Chain A: 6% 41% 29% 24%



4.2.18 Score per residue for model 18

• Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP

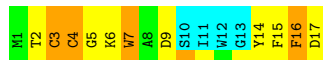
Chain A: 12% 35% 29% 24%



4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP

Chain A: 12% 41% 24% 24%



4.2.20 Score per residue for model 20

• Molecule 1: MET-THR-CYS-CYS-GLY-LYS-TRP-ALA-ASP-DHA-ILE-TRP-GLY-TYR-PHE-PHE-ASP

Chain A: 6% 47% 24% 24%



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 authors did not provide any information on software used for structure solution, optimization or 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	192
Number of shifts mapped to atoms	190
Number of unparsed shifts	0
Number of shifts with mapping errors	2
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

6 Model quality

6.1 Standard geometry

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

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

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	108	90	90	13±2
All	All	2160	1800	1800	257

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 65.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:TYR:C	1:A:15:PHE:CD2	0.65	2.75	18	8
1:A:14:TYR:C	1:A:15:PHE:CD1	0.65	2.75	11	10
1:A:5:GLY:C	1:A:15:PHE:CD2	0.62	2.77	9	4
1:A:16:PHE:O	1:A:16:PHE:CD1	0.60	2.55	6	12
1:A:16:PHE:O	1:A:16:PHE:CD2	0.60	2.55	3	8
1:A:5:GLY:O	1:A:15:PHE:CD2	0.60	2.55	2	11
1:A:7:TRP:CE3	1:A:16:PHE:O	0.60	2.54	8	20
1:A:2:THR:O	1:A:14:TYR:CD2	0.59	2.55	2	6
1:A:2:THR:HG23	1:A:15:PHE:O	0.59	1.97	2	20
1:A:5:GLY:O	1:A:15:PHE:CD1	0.59	2.55	7	9
1:A:2:THR:O	1:A:14:TYR:CG	0.54	2.60	7	2
1:A:5:GLY:N	1:A:15:PHE:CG	0.54	2.76	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:THR:O	1:A:14:TYR:CD1	0.53	2.61	11	4
1:A:3:CYS:SG	1:A:4:CYS:N	0.52	2.83	16	20
1:A:16:PHE:CD1	1:A:16:PHE:C	0.50	2.89	17	12
1:A:5:GLY:C	1:A:15:PHE:CD1	0.50	2.90	15	2
1:A:16:PHE:CD2	1:A:16:PHE:C	0.50	2.89	8	8
1:A:7:TRP:CH2	1:A:17:ASP:HB3	0.49	2.43	1	14
1:A:4:CYS:HA	1:A:15:PHE:CD1	0.48	2.43	9	1
1:A:2:THR:HG1	1:A:15:PHE:C	0.47	2.17	9	1
1:A:2:THR:N	1:A:15:PHE:O	0.47	2.48	13	16
1:A:5:GLY:O	1:A:15:PHE:CE2	0.47	2.68	9	2
1:A:7:TRP:CH2	1:A:17:ASP:HB2	0.46	2.45	16	6
1:A:15:PHE:CD1	1:A:15:PHE:N	0.46	2.82	11	10
1:A:2:THR:O	1:A:3:CYS:C	0.46	2.59	1	8
1:A:7:TRP:CZ3	1:A:17:ASP:HB3	0.46	2.46	15	3
1:A:2:THR:O	1:A:14:TYR:CB	0.45	2.64	7	3
1:A:9:ASP:OD1	1:A:9:ASP:C	0.45	2.60	7	13
1:A:1:MET:N	1:A:15:PHE:O	0.44	2.50	1	7
1:A:15:PHE:CD2	1:A:15:PHE:N	0.44	2.85	10	7
1:A:7:TRP:CE3	1:A:16:PHE:C	0.42	2.98	3	3
1:A:5:GLY:HA3	1:A:15:PHE:CB	0.41	2.45	13	1
1:A:1:MET:CG	1:A:9:ASP:CG	0.41	2.94	11	1
1:A:2:THR:OG1	1:A:15:PHE:O	0.40	2.40	2	1

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	11/17 (65%)	9±0 (85±4%)	2±0 (14±5%)	0±0 (1±3%)	16	66
All	All	220/340 (65%)	188 (85%)	30 (14%)	2 (1%)	16	66

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	14	TYR	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	11/13 (85%)	6±1 (51±8%)	5±1 (49±8%)	0	1
All	All	220/260 (85%)	112 (51%)	108 (49%)	0	1

All 7 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	3	CYS	20
1	A	4	CYS	20
1	A	7	TRP	20
1	A	16	PHE	20
1	A	6	LYS	16
1	A	17	ASP	9
1	A	1	MET	3

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	DHA	A	10	1	4,4,5	2.47±0.01	2±0 (50±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
1	DHA	A	10	1	2,4,6	2.23±0.01	1±0 (50±0%)

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
1	DHA	A	10	1	-	0±0,0,2,4	-

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	10	DHA	C-CA	4.05	1.51	1.45	19	20
1	A	10	DHA	CA-N	2.62	1.41	1.35	14	20

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	10	DHA	O-C-CA	2.98	119.99	125.54	11	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 68% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *D_1300070379_cs_P1.str.V1*

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	192
Number of shifts mapped to atoms	190
Number of unparsed shifts	0
Number of shifts with mapping errors	2
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

- Can not parse the chemical shift value. All 36 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HB2	1.774	.	.
1	A	1	MET	HB3	2.220	.	.
1	A	1	MET	HG2	2.270	.	.
1	A	1	MET	HG3	2.364	.	.
1	A	3	CYS	HB2	3.440	.	.
1	A	3	CYS	HB3	3.742	.	.
1	A	4	CYS	HB2	3.029	.	.
1	A	4	CYS	HB3	3.111	.	.
1	A	5	GLY	HA2	3.415	.	.
1	A	6	LYS	HB2	1.045	.	.
1	A	6	LYS	HB3	1.087	.	.
1	A	6	LYS	HE2	2.553	.	.
1	A	6	LYS	HE3	2.606	.	.
1	A	7	TRP	HB2	2.981	.	.
1	A	7	TRP	HB3	3.388	.	.
1	A	9	ASP	HB2	2.446	.	.
1	A	9	ASP	HB3	2.988	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ILE	HG12	1.099	.	.
1	A	11	ILE	HG13	1.422	.	.
1	A	12	TRP	HB2	3.195	.	.
1	A	12	TRP	HB3	3.317	.	.
1	A	13	GLY	HA2	3.061	.	.
1	A	14	TYR	HB2	2.986	.	.
1	A	14	TYR	HB3	3.106	.	.
1	A	14	TYR	CD1	130.491	.	.
1	A	14	TYR	CE1	114.322	.	.
1	A	15	PHE	HB2	2.314	.	.
1	A	15	PHE	HB3	2.720	.	.
1	A	15	PHE	CD1	129.836	.	.
1	A	15	PHE	CE1	127.866	.	.
1	A	16	PHE	HB2	3.484	.	.
1	A	16	PHE	HB3	3.874	.	.
1	A	16	PHE	CD1	129.421	.	.
1	A	16	PHE	CE1	128.706	.	.
1	A	17	ASP	HB2	2.589	.	.
1	A	17	ASP	HB3	3.007	.	.

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 2 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	H	7.729	.	1
1	A	17	ASP	CE2	51.345	.	.

7.1.2 Chemical shift referencing ⓘ

No chemical shift referencing corrections were calculated (not enough data).

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 66%, i.e. 110 atoms were assigned a chemical shift out of a possible 166. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	49/66 (74%)	23/27 (85%)	26/26 (100%)	0/13 (0%)
Sidechain	34/59 (58%)	14/38 (37%)	20/20 (100%)	0/1 (0%)
Aromatic	27/41 (66%)	19/20 (95%)	8/20 (40%)	0/1 (0%)
Overall	110/166 (66%)	56/85 (66%)	54/66 (82%)	0/15 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 142 atoms were assigned a chemical shift out of a possible 210. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	59/82 (72%)	27/34 (79%)	32/32 (100%)	0/16 (0%)
Sidechain	46/75 (61%)	21/49 (43%)	25/25 (100%)	0/1 (0%)
Aromatic	37/53 (70%)	24/26 (92%)	13/25 (52%)	0/2 (0%)
Overall	142/210 (68%)	72/109 (66%)	70/82 (85%)	0/19 (0%)

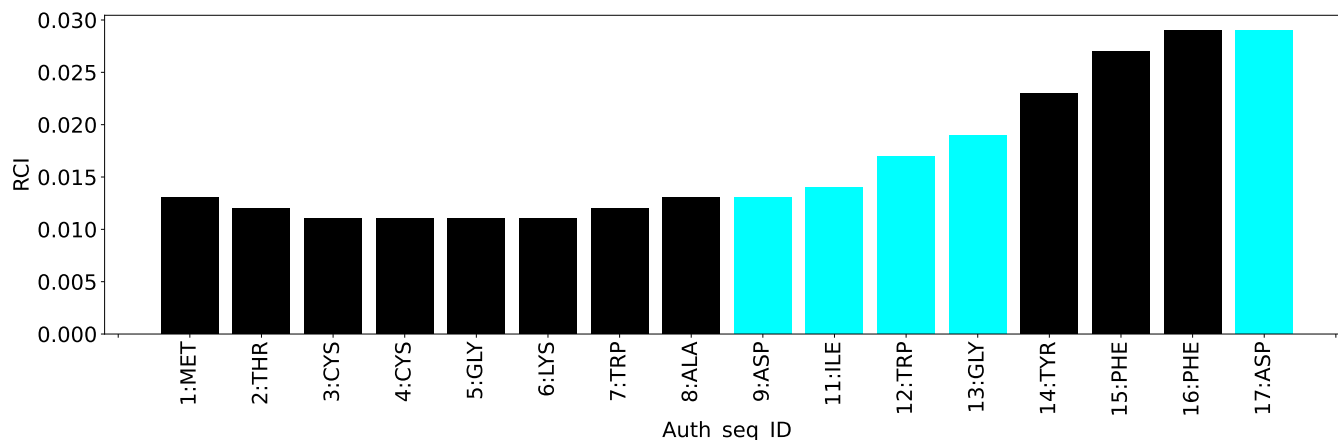
7.1.4 Statistically unusual chemical shifts [i](#)

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	333
Intra-residue ($ i-j =0$)	60
Sequential ($ i-j =1$)	53
Medium range ($ i-j >1$ and $ i-j <5$)	36
Long range ($ i-j \geq 5$)	184
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	19.6
Number of long range restraints per residue ¹	10.8

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.3	0.2
0.2-0.5 (Medium)	0.3	0.26
>0.5 (Large)	2.0	1.37

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](#)

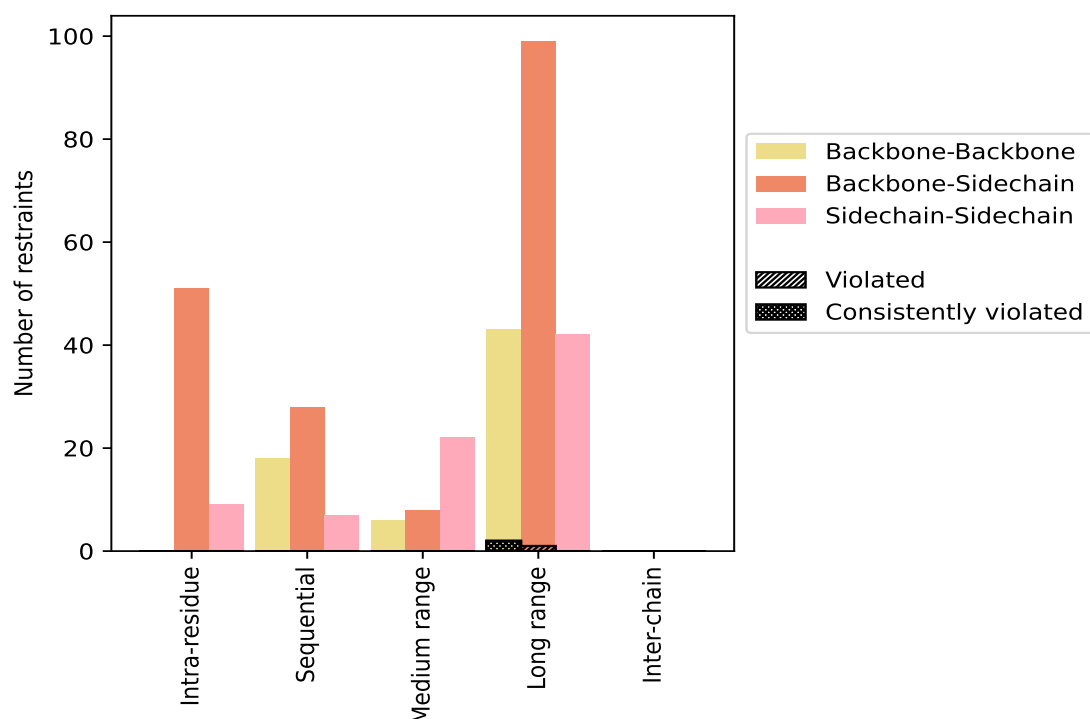
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	60	18.0	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	51	15.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	9	2.7	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	53	15.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	18	5.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	28	8.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	2.1	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	36	10.8	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	6	1.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	2.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	22	6.6	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	184	55.3	3	1.6	0.9	2	1.1	0.6
Backbone-Backbone	43	12.9	2	4.7	0.6	2	4.7	0.6
Backbone-Sidechain	99	29.7	1	1.0	0.3	0	0.0	0.0
Sidechain-Sidechain	42	12.6	0	0.0	0.0	0	0.0	0.0
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	333	100.0	3	0.9	0.9	2	0.6	0.6
Backbone-Backbone	67	20.1	2	3.0	0.6	2	3.0	0.6
Backbone-Sidechain	186	55.9	1	0.5	0.3	0	0.0	0.0
Sidechain-Sidechain	80	24.0	0	0.0	0.0	0	0.0	0.0

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	2	0	2	1.02	1.05	0.03	1.02
2	0	0	0	3	0	3	0.8	1.13	0.41	1.05
3	0	0	0	3	0	3	0.73	1.06	0.37	0.92
4	0	0	0	2	0	2	1.14	1.2	0.06	1.14
5	0	0	0	2	0	2	1.13	1.18	0.05	1.13
6	0	0	0	3	0	3	0.75	1.08	0.38	0.95
7	0	0	0	3	0	3	0.83	1.19	0.46	1.13
8	0	0	0	3	0	3	0.94	1.31	0.51	1.29
9	0	0	0	2	0	2	1.37	1.37	0.01	1.37
10	0	0	0	3	0	3	0.75	1.07	0.37	0.95

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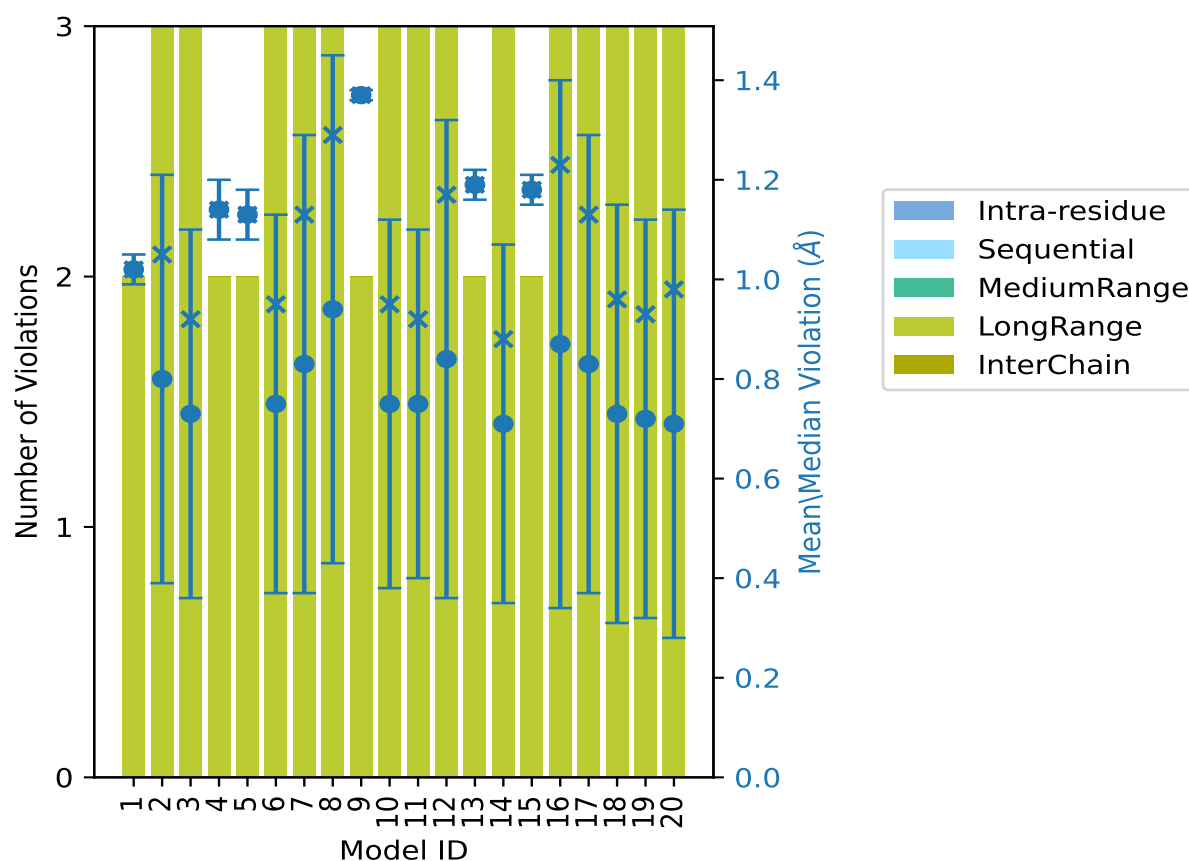
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	0	3	0	3	0.75	1.06	0.35	0.92
12	0	0	0	3	0	3	0.84	1.19	0.48	1.17
13	0	0	0	2	0	2	1.19	1.22	0.03	1.19
14	0	0	0	3	0	3	0.71	1.04	0.36	0.88
15	0	0	0	2	0	2	1.18	1.21	0.03	1.18
16	0	0	0	3	0	3	0.87	1.25	0.53	1.23
17	0	0	0	3	0	3	0.83	1.18	0.46	1.13
18	0	0	0	3	0	3	0.73	1.1	0.42	0.96
19	0	0	0	3	0	3	0.72	1.08	0.4	0.93
20	0	0	0	3	0	3	0.71	1.04	0.43	0.98

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard 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

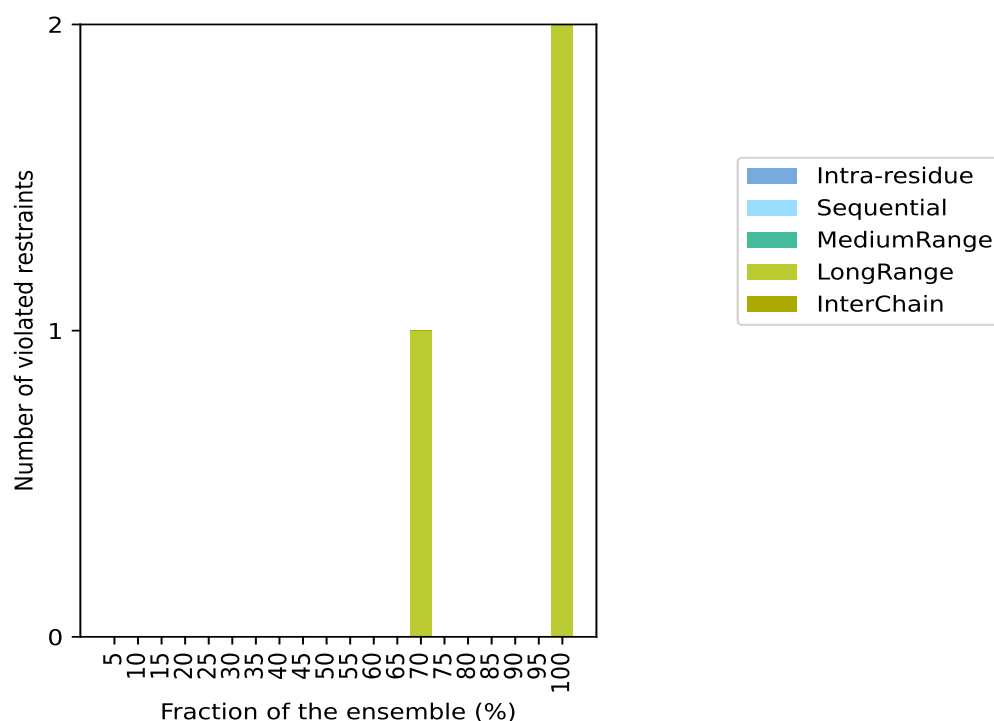
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 330(IR:60, SQ:53, MR:36, LR:181, IC:0) restraints are not 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	%
0	0	0	0	0	0	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	1	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	2	0	2	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

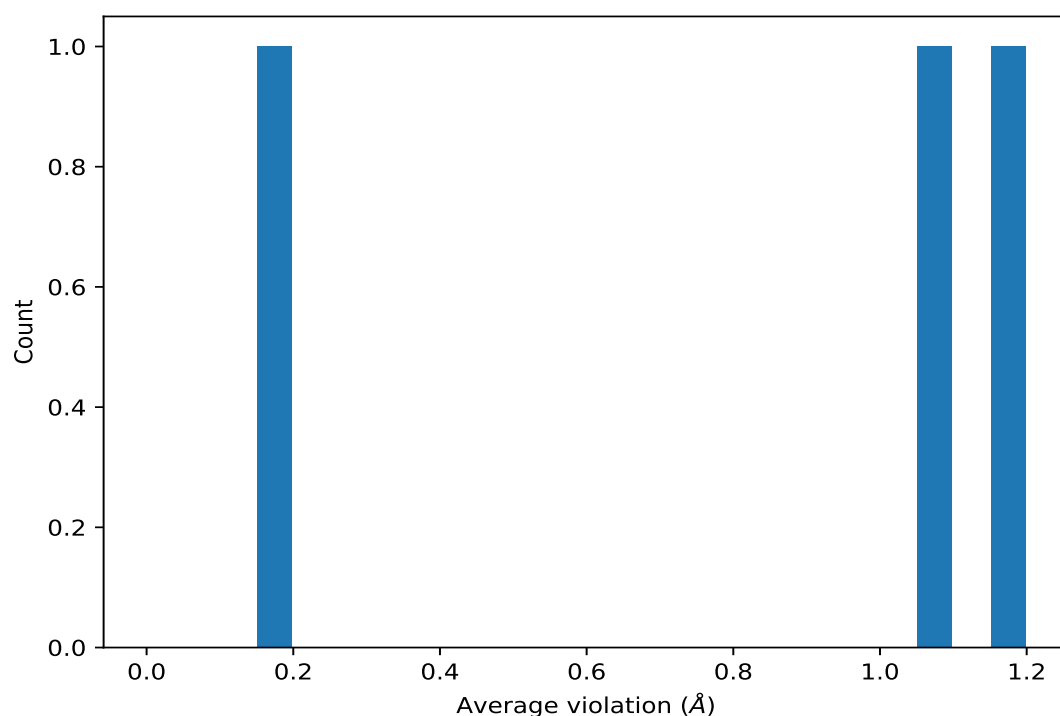
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violation for each restraint sorted by number of violated models and the mean 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.

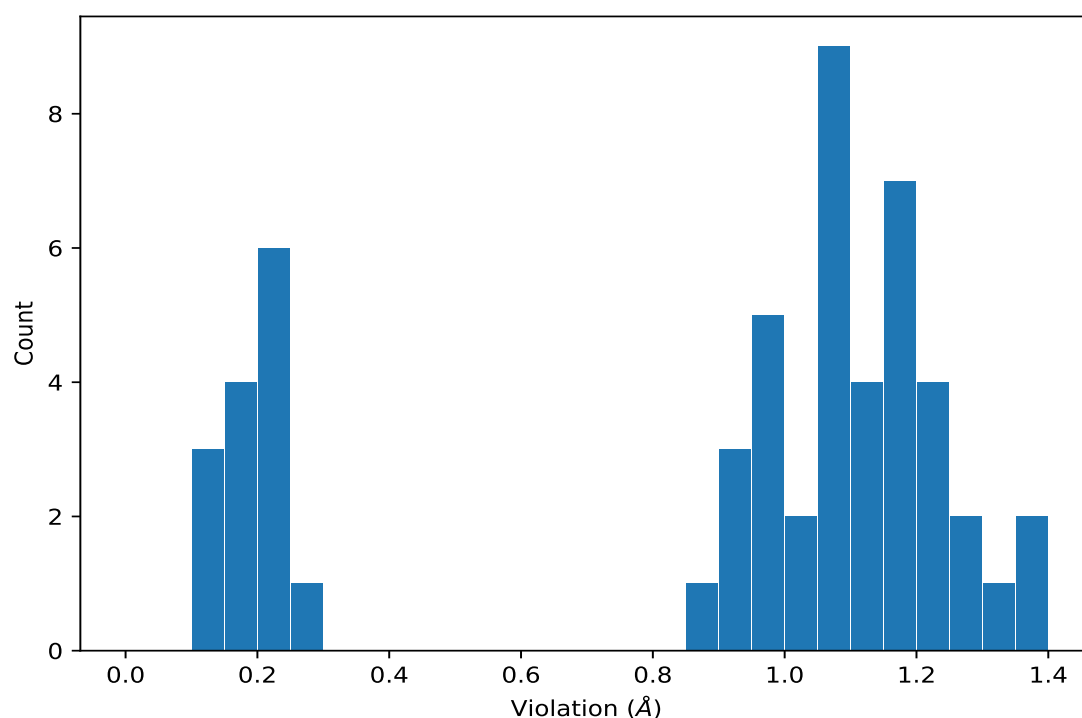
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	20	1.15	0.09	1.15
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	20	1.07	0.13	1.06
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	14	0.19	0.04	0.19

¹Number of violated models, ²Standard 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 lists the absolute value of the violation for each restraint in the ensemble sorted by its 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)
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	9	1.37
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	9	1.36
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	8	1.31
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	8	1.29
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	16	1.25
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	16	1.23
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	13	1.22
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	15	1.21
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	4	1.2
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	7	1.19
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	12	1.19
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	5	1.18
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	17	1.18
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	12	1.17
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	13	1.16
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	15	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	7	1.13
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	17	1.13
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	2	1.13
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	18	1.1
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	4	1.08
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	5	1.08
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	6	1.08
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	19	1.08
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	10	1.07
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	3	1.06
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	11	1.06
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	2	1.05
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	1	1.05
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	14	1.04
(1,23)	1:5:A:GLY:HA2	1:16:A:PHE:H	20	1.04
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	1	0.99
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	20	0.98
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	18	0.96
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	6	0.95
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	10	0.95
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	19	0.93
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	3	0.92
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	11	0.92
(1,163)	1:5:A:GLY:HA2	1:16:A:PHE:HA	14	0.88
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	11	0.26
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	10	0.24
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	2	0.22
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	3	0.21
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	6	0.21
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	8	0.21
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	14	0.2
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	7	0.18
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	17	0.18
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	12	0.17
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	19	0.16
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	18	0.14
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	16	0.12
(1,182)	1:5:A:GLY:HA2	1:15:A:PHE:HB3	20	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found