



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 9X71 / pdb_00009x71
BMRB ID : 36797
Title : the closed-form Hsp90a NTD
Authors : Wan, C.J.
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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 ⓘ 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
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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

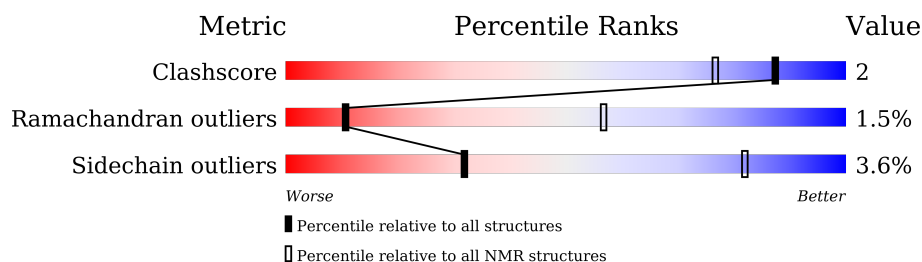
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 8%.

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	237	85% .. 13%

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:16-A:132, A:136-A:222 (204)	2.37	8

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 and 1 single-model cluster was found.

Cluster number	Models
1	1, 3, 4, 5, 9
2	6, 7, 8, 10
Single-model clusters	2

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3259 atoms, of which 1633 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms						Trace
1	A	207	Total	C	H	N	O	S	0
			3259	1033	1633	268	320	5	

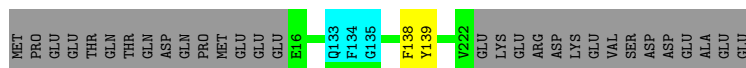
4 Residue-property plots [i](#)

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: Heat shock protein HSP 90-alpha

Chain A:  85% .. 13%

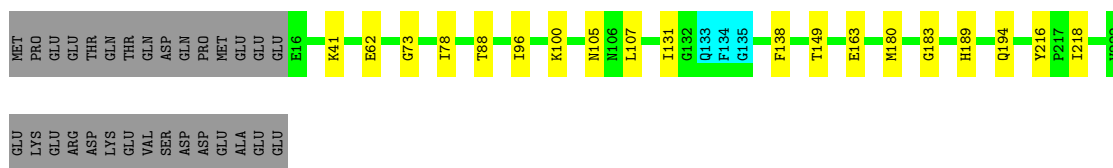


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Heat shock protein HSP 90-alpha

Chain A:  78% 8% • 13%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *back calculated data agree with experimental NOESY spectrum*.

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

Software name	Classification	Version
CYANA	refinement	
X-PLOR NIH	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	448
Number of shifts mapped to atoms	448
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

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	1.25±0.02	0±0/1627 (0.0± 0.0%)	0.96±0.02	0±0/2195 (0.0± 0.0%)
All	All	1.25	3/16270 (0.0%)	0.96	1/21950 (0.0%)

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	81	ILE	CA-CB	5.87	1.59	1.53	3	1
1	A	33	ILE	CA-CB	5.53	1.61	1.54	7	1
1	A	17	VAL	CA-CB	5.29	1.59	1.53	5	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	138	PHE	CA-CB-CG	5.21	119.01	113.80	6	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1602	1613	1608	6±2
All	All	16020	16130	16080	65

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

5 of 61 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:MET:SD	1:A:183:GLY:HA3	0.61	2.36	6	2
1:A:62:GLU:HG3	1:A:69:LYS:HG3	0.59	1.74	1	1
1:A:16:GLU:N	1:A:174:THR:HG1	0.59	1.95	10	1
1:A:205:GLU:HA	1:A:208:LYS:HE2	0.57	1.77	7	1
1:A:78:ILE:HB	1:A:218:ILE:HG22	0.57	1.76	8	1

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	202/237 (85%)	182±3 (90±2%)	17±3 (8±2%)	3±1 (1±1%)	11	57
All	All	2020/2370 (85%)	1820 (90%)	170 (8%)	30 (1%)	11	57

5 of 16 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	114	GLY	4
1	A	73	GLY	4
1	A	217	PRO	3
1	A	97	GLY	3
1	A	110	ILE	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	176/207 (85%)	170±3 (96±1%)	6±3 (4±1%)	32	82
All	All	1760/2070 (85%)	1696 (96%)	64 (4%)	32	82

5 of 43 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	45	LEU	3
1	A	69	LYS	3
1	A	150	VAL	3
1	A	182	ARG	3
1	A	198	LEU	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](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	448
Number of shifts mapped to atoms	448
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

- Can not parse the chemical shift value. First 5 (of 224) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	17	VAL	HG11	0.78	.	.
1	A	17	VAL	HG12	0.78	.	.
1	A	17	VAL	HG13	0.78	.	.
1	A	17	VAL	HG21	0.76	.	.
1	A	17	VAL	HG22	0.76	.	.
1	A	17	VAL	HG23	0.76	.	.
1	A	17	VAL	CG1	18.06	.	.
1	A	17	VAL	CG2	18.15	.	.
1	A	29	LEU	HD11	0.76	.	.
1	A	29	LEU	HD12	0.76	.	.
1	A	29	LEU	HD13	0.76	.	.
1	A	29	LEU	HD21	0.88	.	.
1	A	29	LEU	HD22	0.88	.	.
1	A	29	LEU	HD23	0.88	.	.
1	A	29	LEU	CD1	23.55	.	.
1	A	29	LEU	CD2	21.04	.	.
1	A	32	LEU	HD11	0.68	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	32	LEU	HD12	0.68	.	.
1	A	32	LEU	HD13	0.68	.	.
1	A	32	LEU	HD21	0.71	.	.
1	A	32	LEU	HD22	0.71	.	.
1	A	32	LEU	HD23	0.71	.	.
1	A	32	LEU	CD1	21.75	.	.
1	A	32	LEU	CD2	22.66	.	.
1	A	45	LEU	HD11	0.64	.	.
1	A	45	LEU	HD12	0.64	.	.
1	A	45	LEU	HD13	0.64	.	.
1	A	45	LEU	HD21	0.6	.	.
1	A	45	LEU	HD22	0.6	.	.
1	A	45	LEU	HD23	0.6	.	.
1	A	45	LEU	CD1	20.77	.	.
1	A	45	LEU	CD2	22.86	.	.
1	A	48	LEU	HD11	0.8	.	.
1	A	48	LEU	HD12	0.8	.	.
1	A	48	LEU	HD13	0.8	.	.
1	A	48	LEU	HD21	0.81	.	.
1	A	48	LEU	HD22	0.81	.	.
1	A	48	LEU	HD23	0.81	.	.
1	A	48	LEU	CD1	19.82	.	.
1	A	48	LEU	CD2	24.99	.	.
1	A	56	LEU	HD11	0.3	.	.
1	A	56	LEU	HD12	0.3	.	.
1	A	56	LEU	HD13	0.3	.	.
1	A	56	LEU	HD21	-0.02	.	.
1	A	56	LEU	HD22	-0.02	.	.
1	A	56	LEU	HD23	-0.02	.	.
1	A	56	LEU	CD1	23.37	.	.
1	A	56	LEU	CD2	22.67	.	.
1	A	64	LEU	HD11	0.75	.	.
1	A	64	LEU	HD12	0.75	.	.
1	A	64	LEU	HD13	0.75	.	.
1	A	64	LEU	HD21	0.85	.	.
1	A	64	LEU	HD22	0.85	.	.
1	A	64	LEU	HD23	0.85	.	.
1	A	64	LEU	CD1	22.45	.	.
1	A	64	LEU	CD2	19.33	.	.
1	A	70	LEU	HD11	0.9	.	.
1	A	70	LEU	HD12	0.9	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	70	LEU	HD13	0.9	.	.
1	A	70	LEU	HD21	0.68	.	.
1	A	70	LEU	HD22	0.68	.	.
1	A	70	LEU	HD23	0.68	.	.
1	A	70	LEU	CD1	22.76	.	.
1	A	70	LEU	CD2	19.52	.	.
1	A	76	LEU	HD11	0.48	.	.
1	A	76	LEU	HD12	0.48	.	.
1	A	76	LEU	HD13	0.48	.	.
1	A	76	LEU	HD21	0.85	.	.
1	A	76	LEU	HD22	0.85	.	.
1	A	76	LEU	HD23	0.85	.	.
1	A	76	LEU	CD1	20.84	.	.
1	A	76	LEU	CD2	23.05	.	.
1	A	80	LEU	HD11	0.73	.	.
1	A	80	LEU	HD12	0.73	.	.
1	A	80	LEU	HD13	0.73	.	.
1	A	80	LEU	HD21	0.63	.	.
1	A	80	LEU	HD22	0.63	.	.
1	A	80	LEU	HD23	0.63	.	.
1	A	80	LEU	CD1	22.78	.	.
1	A	80	LEU	CD2	23.89	.	.
1	A	89	LEU	HD11	1.04	.	.
1	A	89	LEU	HD12	1.04	.	.
1	A	89	LEU	HD13	1.04	.	.
1	A	89	LEU	HD21	0.79	.	.
1	A	89	LEU	HD22	0.79	.	.
1	A	89	LEU	HD23	0.79	.	.
1	A	89	LEU	CD1	22.88	.	.
1	A	89	LEU	CD2	19.34	.	.
1	A	92	VAL	HG11	0.82	.	.
1	A	92	VAL	HG12	0.82	.	.
1	A	92	VAL	HG13	0.82	.	.
1	A	92	VAL	HG21	0.83	.	.
1	A	92	VAL	HG22	0.83	.	.
1	A	92	VAL	HG23	0.83	.	.
1	A	92	VAL	CG1	19.41	.	.
1	A	92	VAL	CG2	18.33	.	.
1	A	103	LEU	HD11	0.67	.	.
1	A	103	LEU	HD12	0.67	.	.
1	A	103	LEU	HD13	0.67	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	LEU	HD21	0.59	.	.
1	A	103	LEU	HD22	0.59	.	.
1	A	103	LEU	HD23	0.59	.	.
1	A	103	LEU	CD1	22.21	.	.
1	A	103	LEU	CD2	22.2	.	.
1	A	107	LEU	HD11	-0.94	.	.
1	A	107	LEU	HD12	-0.94	.	.
1	A	107	LEU	HD13	-0.94	.	.
1	A	107	LEU	HD21	-0.73	.	.
1	A	107	LEU	HD22	-0.73	.	.
1	A	107	LEU	HD23	-0.73	.	.
1	A	107	LEU	CD1	18.81	.	.
1	A	107	LEU	CD2	20.91	.	.
1	A	122	LEU	HD11	0.29	.	.
1	A	122	LEU	HD12	0.29	.	.
1	A	122	LEU	HD13	0.29	.	.
1	A	122	LEU	HD21	0.21	.	.
1	A	122	LEU	HD22	0.21	.	.
1	A	122	LEU	HD23	0.21	.	.
1	A	122	LEU	CD1	19.64	.	.
1	A	122	LEU	CD2	22.41	.	.
1	A	136	VAL	HG11	0.46	.	.
1	A	136	VAL	HG12	0.46	.	.
1	A	136	VAL	HG13	0.46	.	.
1	A	136	VAL	HG21	0.86	.	.
1	A	136	VAL	HG22	0.86	.	.
1	A	136	VAL	HG23	0.86	.	.
1	A	136	VAL	CG1	14.91	.	.
1	A	136	VAL	CG2	19.73	.	.
1	A	143	LEU	HD11	0.91	.	.
1	A	143	LEU	HD12	0.91	.	.
1	A	143	LEU	HD13	0.91	.	.
1	A	143	LEU	HD21	0.94	.	.
1	A	143	LEU	HD22	0.94	.	.
1	A	143	LEU	HD23	0.94	.	.
1	A	143	LEU	CD1	23.95	.	.
1	A	143	LEU	CD2	21.46	.	.
1	A	144	VAL	HG11	-0.71	.	.
1	A	144	VAL	HG12	-0.71	.	.
1	A	144	VAL	HG13	-0.71	.	.
1	A	144	VAL	HG21	0.33	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	144	VAL	HG22	0.33	.	.
1	A	144	VAL	HG23	0.33	.	.
1	A	144	VAL	CG1	12.72	.	.
1	A	144	VAL	CG2	19.58	.	.
1	A	148	VAL	HG11	0.05	.	.
1	A	148	VAL	HG12	0.05	.	.
1	A	148	VAL	HG13	0.05	.	.
1	A	148	VAL	HG21	0.85	.	.
1	A	148	VAL	HG22	0.85	.	.
1	A	148	VAL	HG23	0.85	.	.
1	A	148	VAL	CG1	19.93	.	.
1	A	148	VAL	CG2	19.45	.	.
1	A	150	VAL	HG11	0.75	.	.
1	A	150	VAL	HG12	0.75	.	.
1	A	150	VAL	HG13	0.75	.	.
1	A	150	VAL	HG21	0.5	.	.
1	A	150	VAL	HG22	0.5	.	.
1	A	150	VAL	HG23	0.5	.	.
1	A	150	VAL	CG1	19.39	.	.
1	A	150	VAL	CG2	18.25	.	.
1	A	172	VAL	HG11	1.14	.	.
1	A	172	VAL	HG12	1.14	.	.
1	A	172	VAL	HG13	1.14	.	.
1	A	172	VAL	HG21	0.9	.	.
1	A	172	VAL	HG22	0.9	.	.
1	A	172	VAL	HG23	0.9	.	.
1	A	172	VAL	CG1	20.35	.	.
1	A	172	VAL	CG2	19.4	.	.
1	A	186	VAL	HG11	0.97	.	.
1	A	186	VAL	HG12	0.97	.	.
1	A	186	VAL	HG13	0.97	.	.
1	A	186	VAL	HG21	0.77	.	.
1	A	186	VAL	HG22	0.77	.	.
1	A	186	VAL	HG23	0.77	.	.
1	A	186	VAL	CG1	18.27	.	.
1	A	186	VAL	CG2	19.39	.	.
1	A	188	LEU	HD11	0.67	.	.
1	A	188	LEU	HD12	0.67	.	.
1	A	188	LEU	HD13	0.67	.	.
1	A	188	LEU	HD21	0.45	.	.
1	A	188	LEU	HD22	0.45	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	188	LEU	HD23	0.45	.	.
1	A	188	LEU	CD1	24.01	.	.
1	A	188	LEU	CD2	23.92	.	.
1	A	190	LEU	HD11	0.49	.	.
1	A	190	LEU	HD12	0.49	.	.
1	A	190	LEU	HD13	0.49	.	.
1	A	190	LEU	HD21	0.7	.	.
1	A	190	LEU	HD22	0.7	.	.
1	A	190	LEU	HD23	0.7	.	.
1	A	190	LEU	CD1	20.06	.	.
1	A	190	LEU	CD2	23.85	.	.
1	A	198	LEU	HD11	0.87	.	.
1	A	198	LEU	HD12	0.87	.	.
1	A	198	LEU	HD13	0.87	.	.
1	A	198	LEU	HD21	0.59	.	.
1	A	198	LEU	HD22	0.59	.	.
1	A	198	LEU	HD23	0.59	.	.
1	A	198	LEU	CD1	24.24	.	.
1	A	198	LEU	CD2	22.1	.	.
1	A	207	VAL	HG11	0.77	.	.
1	A	207	VAL	HG12	0.77	.	.
1	A	207	VAL	HG13	0.77	.	.
1	A	207	VAL	HG21	0.75	.	.
1	A	207	VAL	HG22	0.75	.	.
1	A	207	VAL	HG23	0.75	.	.
1	A	207	VAL	CG1	20.53	.	.
1	A	207	VAL	CG2	18.93	.	.
1	A	220	LEU	HD11	0.8	.	.
1	A	220	LEU	HD12	0.8	.	.
1	A	220	LEU	HD13	0.8	.	.
1	A	220	LEU	HD21	0.79	.	.
1	A	220	LEU	HD22	0.79	.	.
1	A	220	LEU	HD23	0.79	.	.
1	A	220	LEU	CD1	21.95	.	.
1	A	220	LEU	CD2	24.04	.	.
1	A	222	VAL	HG11	0.78	.	.
1	A	222	VAL	HG12	0.78	.	.
1	A	222	VAL	HG13	0.78	.	.
1	A	222	VAL	HG21	0.81	.	.
1	A	222	VAL	HG22	0.81	.	.
1	A	222	VAL	HG23	0.81	.	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	222	VAL	CG1	17.39	.	.
1	A	222	VAL	CG2	18.57	.	.

7.1.2 Chemical shift referencing [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 224 atoms were assigned a chemical shift out of a possible 2783. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1026 (0%)	0/418 (0%)	0/408 (0%)	0/200 (0%)
Sidechain	224/1560 (14%)	168/1016 (17%)	56/493 (11%)	0/51 (0%)
Aromatic	0/197 (0%)	0/95 (0%)	0/93 (0%)	0/9 (0%)
Overall	224/2783 (8%)	168/1529 (11%)	56/994 (6%)	0/260 (0%)

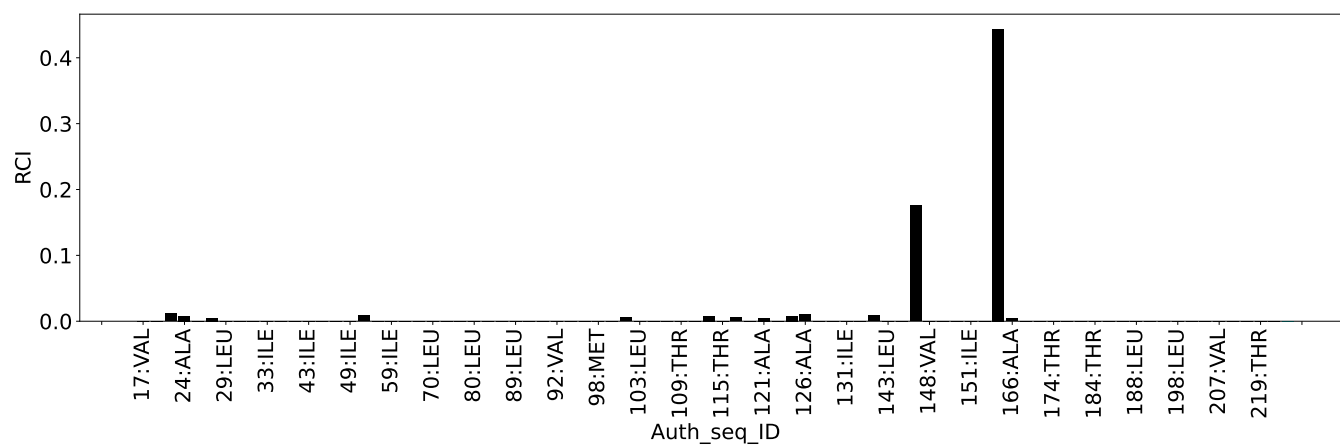
7.1.4 Statistically unusual chemical shifts [i](#)

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	1792
Intra-residue ($ i-j =0$)	273
Sequential ($ i-j =1$)	452
Medium range ($ i-j >1$ and $ i-j <5$)	533
Long range ($ i-j \geq 5$)	534
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	7.6
Number of long range restraints per residue ¹	2.3

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)	35.5	0.2
0.2-0.5 (Medium)	7.8	0.5
>0.5 (Large)	1.0	1.57

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 ⓘ

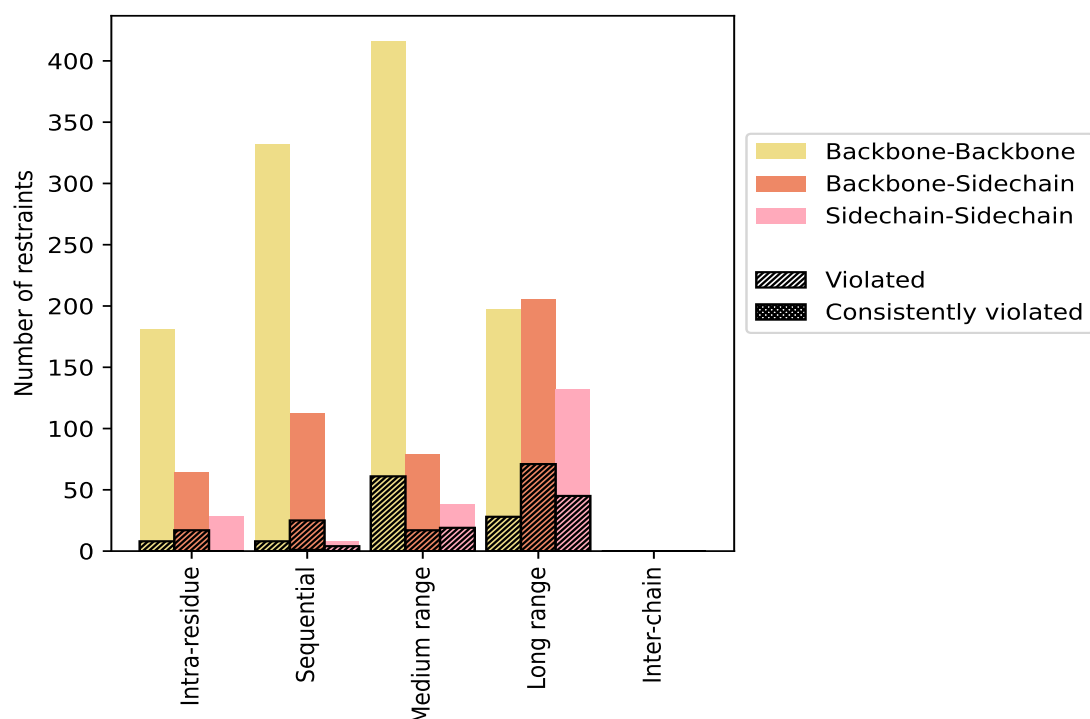
9.1 Summary of distance violations ⓘ

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)	273	15.2	25	9.2	1.4	0	0.0	0.0
Backbone-Backbone	181	10.1	8	4.4	0.4	0	0.0	0.0
Backbone-Sidechain	64	3.6	17	26.6	0.9	0	0.0	0.0
Sidechain-Sidechain	28	1.6	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	452	25.2	37	8.2	2.1	1	0.2	0.1
Backbone-Backbone	332	18.5	8	2.4	0.4	0	0.0	0.0
Backbone-Sidechain	112	6.2	25	22.3	1.4	1	0.9	0.1
Sidechain-Sidechain	8	0.4	4	50.0	0.2	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	533	29.7	97	18.2	5.4	0	0.0	0.0
Backbone-Backbone	416	23.2	61	14.7	3.4	0	0.0	0.0
Backbone-Sidechain	79	4.4	17	21.5	0.9	0	0.0	0.0
Sidechain-Sidechain	38	2.1	19	50.0	1.1	0	0.0	0.0
Long range (i-j ≥5)	534	29.8	144	27.0	8.0	0	0.0	0.0
Backbone-Backbone	197	11.0	28	14.2	1.6	0	0.0	0.0
Backbone-Sidechain	205	11.4	71	34.6	4.0	0	0.0	0.0
Sidechain-Sidechain	132	7.4	45	34.1	2.5	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	1792	100.0	303	16.9	16.9	1	0.1	0.1
Backbone-Backbone	1126	62.8	105	9.3	5.9	0	0.0	0.0
Backbone-Sidechain	460	25.7	130	28.3	7.3	1	0.2	0.1
Sidechain-Sidechain	206	11.5	68	33.0	3.8	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

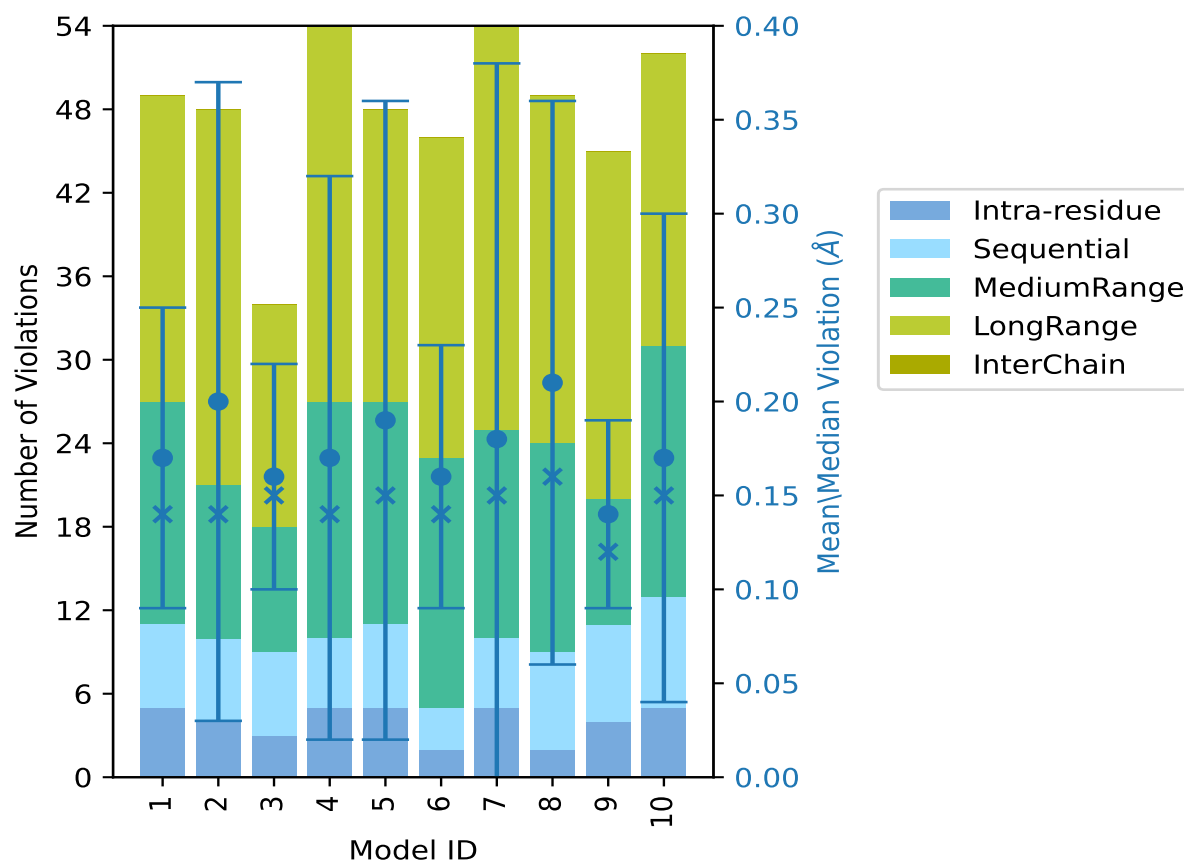
9.2 Distance violation statistics for each model [i](#)

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	5	6	16	22	0	49	0.17	0.52	0.08	0.14
2	4	6	11	27	0	48	0.2	1.09	0.17	0.14
3	3	6	9	16	0	34	0.16	0.34	0.06	0.15
4	5	5	17	27	0	54	0.17	1.18	0.15	0.14
5	5	6	16	21	0	48	0.19	1.26	0.17	0.15
6	2	3	18	23	0	46	0.16	0.39	0.07	0.14
7	5	5	15	29	0	54	0.18	1.57	0.2	0.15
8	2	7	15	25	0	49	0.21	0.81	0.15	0.16
9	4	7	9	25	0	45	0.14	0.32	0.05	0.12
10	5	8	18	21	0	52	0.17	1.0	0.13	0.15

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 [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1489(IR:248, SQ:415, MR:436, LR:390, 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	%
17	26	63	94	0	200	1	10.0
4	7	26	32	0	69	2	20.0
2	3	5	7	0	17	3	30.0

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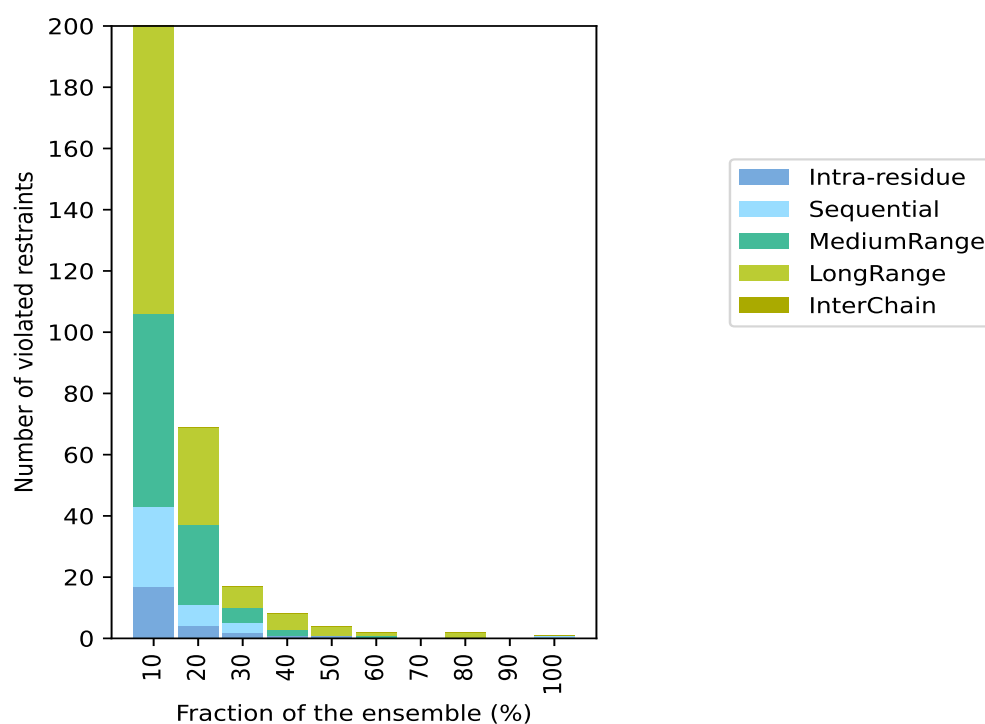
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	0	2	5	0	8	4	40.0
1	0	0	3	0	4	5	50.0
0	0	1	1	0	2	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	2	0	2	8	80.0
0	0	0	0	0	0	9	90.0
0	1	0	0	0	1	10	100.0

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 ⓘ

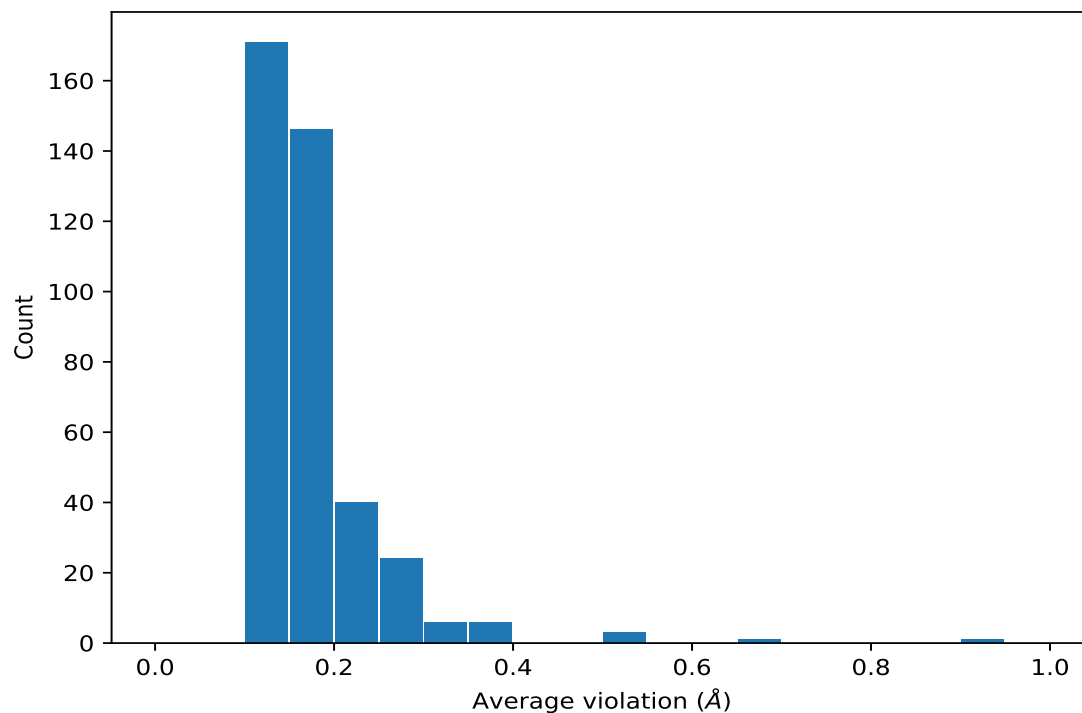


9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

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

in the ensemble



9.4.2 Table: Most violated distance restraints [i](#)

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,732)	1:71:A:ASP:H	1:70:A:LEU:HD11	10	0.28	0.06	0.29
(1,732)	1:71:A:ASP:H	1:70:A:LEU:HD12	10	0.28	0.06	0.29
(1,732)	1:71:A:ASP:H	1:70:A:LEU:HD13	10	0.28	0.06	0.29
(1,732)	1:71:A:ASP:H	1:70:A:LEU:HD21	10	0.28	0.06	0.29
(1,732)	1:71:A:ASP:H	1:70:A:LEU:HD22	10	0.28	0.06	0.29
(1,732)	1:71:A:ASP:H	1:70:A:LEU:HD23	10	0.28	0.06	0.29
(1,1689)	1:98:A:MET:H	1:153:A:LYS:HA	8	0.91	0.4	0.88
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD11	8	0.38	0.12	0.39
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD12	8	0.38	0.12	0.39
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD13	8	0.38	0.12	0.39
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD21	8	0.38	0.12	0.39
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD22	8	0.38	0.12	0.39
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD23	8	0.38	0.12	0.39
(1,578)	1:207:A:VAL:HG11	1:218:A:ILE:HD11	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG11	1:218:A:ILE:HD12	6	0.18	0.05	0.18

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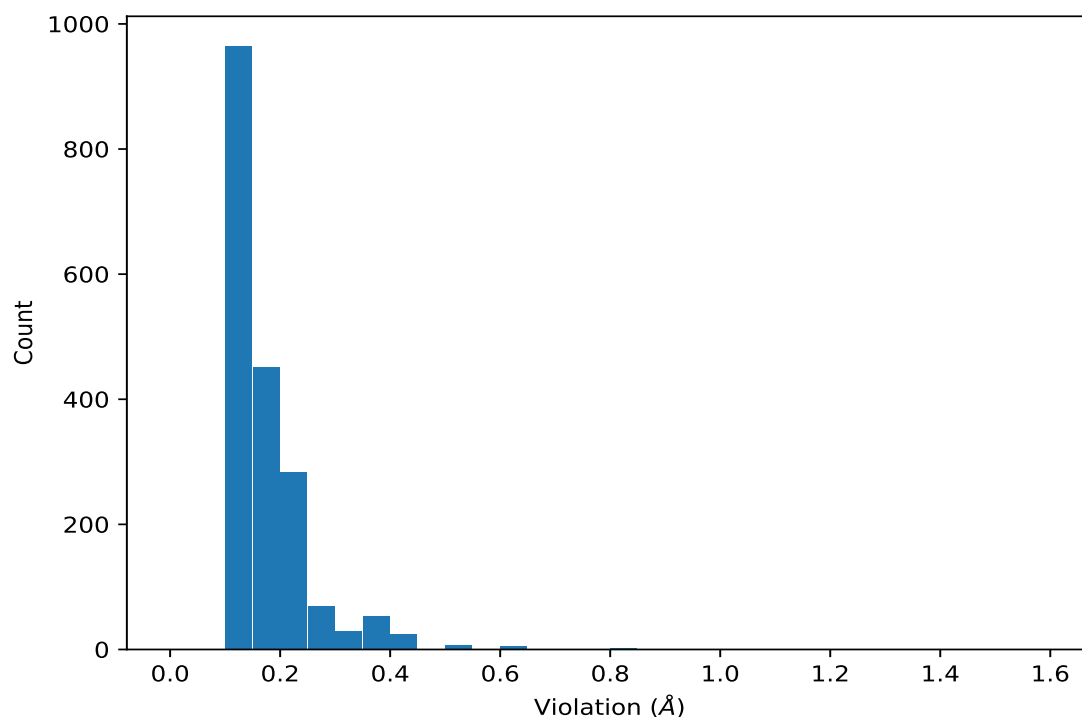
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,578)	1:207:A:VAL:HG11	1:218:A:ILE:HD13	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG12	1:218:A:ILE:HD11	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG12	1:218:A:ILE:HD12	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG12	1:218:A:ILE:HD13	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG13	1:218:A:ILE:HD11	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG13	1:218:A:ILE:HD12	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG13	1:218:A:ILE:HD13	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG21	1:218:A:ILE:HD11	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG21	1:218:A:ILE:HD12	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG21	1:218:A:ILE:HD13	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG22	1:218:A:ILE:HD11	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG22	1:218:A:ILE:HD12	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG22	1:218:A:ILE:HD13	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG23	1:218:A:ILE:HD11	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG23	1:218:A:ILE:HD12	6	0.18	0.05	0.18
(1,578)	1:207:A:VAL:HG23	1:218:A:ILE:HD13	6	0.18	0.05	0.18
(1,318)	1:62:A:GLU:H	1:65:A:THR:H	6	0.18	0.04	0.16
(1,1688)	1:97:A:GLY:H	1:183:A:GLY:HA2	5	0.2	0.04	0.2
(1,1688)	1:97:A:GLY:H	1:183:A:GLY:HA3	5	0.2	0.04	0.2
(1,505)	1:70:A:LEU:HD11	1:76:A:LEU:HD11	5	0.18	0.04	0.19
(1,505)	1:70:A:LEU:HD11	1:76:A:LEU:HD12	5	0.18	0.04	0.19
(1,505)	1:70:A:LEU:HD11	1:76:A:LEU:HD13	5	0.18	0.04	0.19
(1,505)	1:70:A:LEU:HD12	1:76:A:LEU:HD11	5	0.18	0.04	0.19
(1,505)	1:70:A:LEU:HD12	1:76:A:LEU:HD12	5	0.18	0.04	0.19
(1,505)	1:70:A:LEU:HD12	1:76:A:LEU:HD13	5	0.18	0.04	0.19
(1,505)	1:70:A:LEU:HD13	1:76:A:LEU:HD11	5	0.18	0.04	0.19
(1,505)	1:70:A:LEU:HD13	1:76:A:LEU:HD12	5	0.18	0.04	0.19
(1,505)	1:70:A:LEU:HD13	1:76:A:LEU:HD13	5	0.18	0.04	0.19
(1,735)	1:75:A:GLU:H	1:70:A:LEU:HD11	5	0.16	0.04	0.14
(1,735)	1:75:A:GLU:H	1:70:A:LEU:HD12	5	0.16	0.04	0.14
(1,735)	1:75:A:GLU:H	1:70:A:LEU:HD13	5	0.16	0.04	0.14
(1,1693)	1:114:A:GLY:H	1:114:A:GLY:HA2	5	0.11	0.0	0.11
(1,1693)	1:114:A:GLY:H	1:114:A:GLY:HA3	5	0.11	0.0	0.11
(1,770)	1:86:A:ASP:H	1:198:A:LEU:HD11	4	0.34	0.14	0.37

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 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)
(1,1689)	1:98:A:MET:H	1:153:A:LYS:HA	7	1.57
(1,1689)	1:98:A:MET:H	1:153:A:LYS:HA	5	1.26
(1,1689)	1:98:A:MET:H	1:153:A:LYS:HA	4	1.18
(1,1479)	1:141:A:ALA:H	1:138:A:PHE:HA	2	1.09
(1,1689)	1:98:A:MET:H	1:153:A:LYS:HA	10	1.0
(1,1046)	1:123:A:GLN:HE21	1:122:A:LEU:HD21	8	0.81
(1,1046)	1:123:A:GLN:HE21	1:122:A:LEU:HD22	8	0.81
(1,1046)	1:123:A:GLN:HE21	1:122:A:LEU:HD23	8	0.81
(1,1689)	1:98:A:MET:H	1:153:A:LYS:HA	2	0.76
(1,1689)	1:98:A:MET:H	1:153:A:LYS:HA	8	0.71
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD11	8	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD12	8	0.61
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD13	8	0.61
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD21	8	0.61
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD22	8	0.61
(1,768)	1:85:A:GLN:H	1:198:A:LEU:HD23	8	0.61
(1,1689)	1:98:A:MET:H	1:153:A:LYS:HA	1	0.52

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found