wwPDB NMR Structure Validation Summary Report

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PDB ID	:	1NR3
BMRB ID	:	5657
Title	:	SOLUTION STRUCTURE OF THE PROTEIN MTH0916: THE NORTH-EAST STRUCTURAL GENOMICS CONSORTIUM TARGET TT212
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Deposited on	:	2003-01-23

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

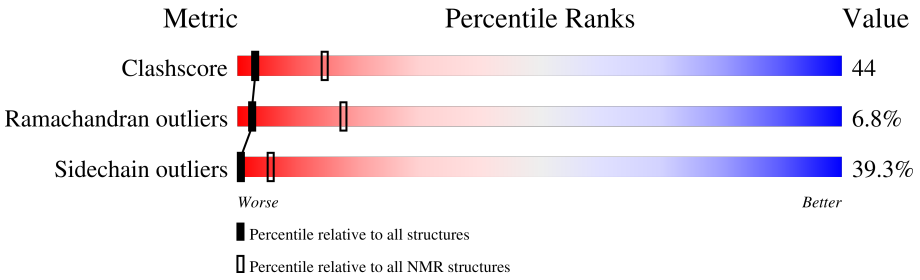
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 77%.

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	122	16% 52% 18% • 12%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:6-A:29, A:40-A:122 (107)	0.74	1

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 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1854 atoms, of which 861 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding protein tfx.

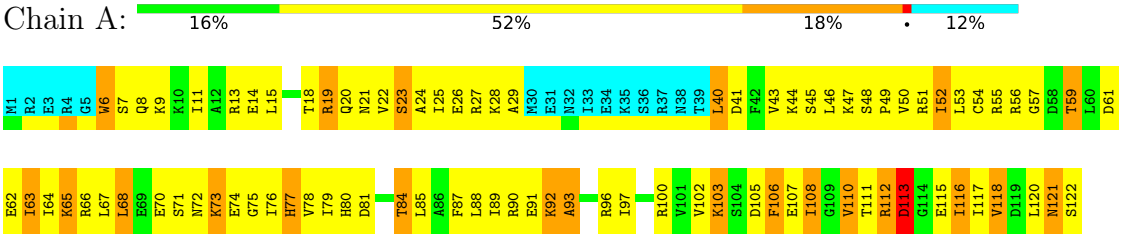
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	122	1854	616	861	191	183	3	0

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.

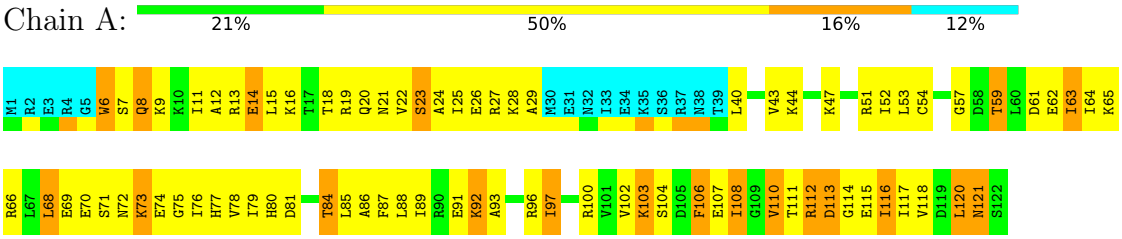
• Molecule 1: DNA-binding protein tfx



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

The representative model is number 1. Colouring as in section 4.1 above.

• Molecule 1: DNA-binding protein tfx



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS, 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
DYANA	refinement	1.5
CYANA	refinement	1.0.3

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	1345
Number of shifts mapped to atoms	1190
Number of unparsed shifts	0
Number of shifts with mapping errors	155
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality

6.1 Standard geometry

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	867	763	917	79±9
All	All	17340	15260	18340	1579

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 44.

5 of 482 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:VAL:HG23	1:A:116:ILE:HG22	0.95	1.38	7	18
1:A:22:VAL:HG21	1:A:78:VAL:CG2	0.93	1.93	18	3
1:A:116:ILE:HD12	1:A:117:ILE:N	0.90	1.82	1	5
1:A:76:ILE:O	1:A:78:VAL:HG23	0.88	1.68	5	3
1:A:15:LEU:HD11	1:A:81:ASP:OD2	0.88	1.68	12	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	106/122 (87%)	78±2 (73±2%)	21±2 (20±2%)	7±1 (7±1%)	2 17
All	All	2120/2440 (87%)	1557 (73%)	419 (20%)	144 (7%)	2 17

5 of 18 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	103	LYS	20
1	A	113	ASP	20
1	A	77	HIS	19
1	A	19	ARG	17
1	A	121	ASN	17

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	98/112 (88%)	59±4 (61±4%)	39±4 (39±4%)	0 5
All	All	1960/2240 (88%)	1189 (61%)	771 (39%)	0 5

5 of 81 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	6	TRP	20
1	A	59	THR	20
1	A	63	ILE	20
1	A	73	LYS	20
1	A	84	THR	20

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 77% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *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	1345
Number of shifts mapped to atoms	1190
Number of unparsed shifts	0
Number of shifts with mapping errors	155
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. First 5 (of 155) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ARG	HB2	2.08	0.01	2
1	A	3	GLU	HB2	2.01	0.01	2
1	A	3	GLU	HG2	2.43	0.01	2
1	A	4	ARG	HB2	1.92	0.01	2
1	A	4	ARG	HG2	1.73	0.01	2
1	A	6	TRP	HB2	3.36	0.01	2
1	A	7	SER	HB2	3.72	0.01	2
1	A	8	GLN	HB2	2.15	0.01	2
1	A	8	GLN	HG2	2.42	0.01	1
1	A	9	LYS	HB2	1.79	0.01	1
1	A	9	LYS	HG2	1.51	0.01	1
1	A	10	LYS	HB2	1.88	0.01	2
1	A	10	LYS	HG2	1.48	0.01	1
1	A	10	LYS	HD2	1.7	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	ILE	HG12	1.26	0.01	2
1	A	13	ARG	HB2	1.88	0.01	1
1	A	13	ARG	HG2	1.7	0.01	1
1	A	13	ARG	HD2	3.12	0.01	1
1	A	14	GLU	HB2	1.91	0.01	1
1	A	14	GLU	HG2	2.35	0.01	1
1	A	15	LEU	HB2	1.66	0.01	2
1	A	16	LYS	HB2	1.95	0.01	2
1	A	16	LYS	HG2	1.48	0.01	2
1	A	16	LYS	HD2	1.75	0.01	1
1	A	19	ARG	HB2	1.96	0.01	2
1	A	19	ARG	HG2	1.73	0.01	2
1	A	19	ARG	HD2	3.26	0.01	1
1	A	20	GLN	HB2	2.16	0.01	2
1	A	20	GLN	HG2	2.43	0.01	1
1	A	21	ASN	HB2	2.96	0.01	2
1	A	23	SER	HB2	3.98	0.01	2
1	A	25	ILE	HG12	1.27	0.01	1
1	A	26	GLU	HB2	2.12	0.01	2
1	A	26	GLU	HG2	2.36	0.01	2
1	A	27	ARG	HB2	1.89	0.01	2
1	A	27	ARG	HG2	1.73	0.01	2
1	A	27	ARG	HD2	3.28	0.01	1
1	A	28	LYS	HB2	1.94	0.01	1
1	A	28	LYS	HG2	1.48	0.01	2
1	A	28	LYS	HD2	1.76	0.01	1
1	A	30	MET	HB2	2.18	0.01	2
1	A	30	MET	HG2	2.64	0.01	2
1	A	31	GLU	HB2	2.05	0.01	1
1	A	31	GLU	HG2	2.32	0.01	2
1	A	32	ASN	HB2	2.87	0.01	1
1	A	33	ILE	HG12	1.28	0.01	2
1	A	34	GLU	HB2	2.12	0.01	2
1	A	34	GLU	HG2	2.43	0.01	1
1	A	35	LYS	HB2	1.87	0.01	2
1	A	35	LYS	HG2	1.47	0.01	2
1	A	35	LYS	HD2	1.74	0.01	1
1	A	36	SER	HB2	3.95	0.01	1
1	A	37	ARG	HB2	1.86	0.01	1
1	A	37	ARG	HG2	1.75	0.01	2
1	A	37	ARG	HD2	3.28	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	38	ASN	HB2	2.94	0.01	2
1	A	40	LEU	HB2	1.72	0.01	2
1	A	41	ASP	HB2	2.6	0.01	1
1	A	42	PHE	HB2	3.2	0.01	1
1	A	44	LYS	HB2	1.86	0.01	2
1	A	44	LYS	HG2	1.49	0.01	2
1	A	44	LYS	HD2	1.73	0.01	1
1	A	45	SER	HB2	3.92	0.01	1
1	A	46	LEU	HB2	1.67	0.01	2
1	A	47	LYS	HB2	1.91	0.01	1
1	A	49	PRO	HB2	2.35	0.01	2
1	A	49	PRO	HG2	2.01	0.01	2
1	A	49	PRO	HD2	3.69	0.01	2
1	A	51	ARG	HB2	1.68	0.01	2
1	A	51	ARG	HG2	1.54	0.01	2
1	A	51	ARG	HD2	3.18	0.01	1
1	A	52	ILE	HG12	1.29	0.01	2
1	A	53	LEU	HB2	1.58	0.01	2
1	A	54	CYS	HB2	1.8	0.01	1
1	A	55	ARG	HB2	1.75	0.01	2
1	A	55	ARG	HG2	1.65	0.01	2
1	A	55	ARG	HD2	3.2	0.01	1
1	A	56	ARG	HB2	1.68	0.01	2
1	A	56	ARG	HG2	1.52	0.01	2
1	A	56	ARG	HD2	3.33	0.01	1
1	A	58	ASP	HB2	2.86	0.01	2
1	A	60	LEU	HB2	1.39	0.01	1
1	A	61	ASP	HB2	2.63	0.01	2
1	A	62	GLU	HB2	2.1	0.01	2
1	A	62	GLU	HG2	2.43	0.01	1
1	A	63	ILE	HG12	1.33	0.01	1
1	A	64	ILE	HG12	1.83	0.01	1
1	A	65	LYS	HB2	1.99	0.01	1
1	A	65	LYS	HG2	1.46	0.01	2
1	A	65	LYS	HD2	1.77	0.01	1
1	A	66	ARG	HB2	2.04	0.01	2
1	A	66	ARG	HG2	1.96	0.01	1
1	A	66	ARG	HD2	3.2	0.01	2
1	A	67	LEU	HB2	1.79	0.01	2
1	A	68	LEU	HB2	2.04	0.01	2
1	A	69	GLU	HB2	2.33	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	GLU	HG2	2.35	0.01	2
1	A	70	GLU	HB2	2.0	0.01	1
1	A	70	GLU	HG2	2.44	0.01	2
1	A	71	SER	HB2	3.82	0.01	1
1	A	72	ASN	HB2	3.08	0.01	1
1	A	73	LYS	HB2	2.09	0.01	1
1	A	73	LYS	HG2	1.75	0.01	2
1	A	73	LYS	HD2	1.82	0.01	1
1	A	74	GLU	HB2	1.78	0.01	1
1	A	74	GLU	HG2	2.37	0.01	1
1	A	76	ILE	HG12	1.08	0.01	1
1	A	77	HIS	HB2	3.13	0.01	2
1	A	79	ILE	HG12	0.93	0.01	1
1	A	80	HIS	HB2	2.66	0.01	1
1	A	81	ASP	HB2	3.26	0.01	2
1	A	82	SER	HB2	4.01	0.01	2
1	A	83	ILE	HG12	1.33	0.01	1
1	A	85	LEU	HB2	2.03	0.01	1
1	A	87	PHE	HB2	3.33	0.01	1
1	A	88	LEU	HB2	1.43	0.01	1
1	A	89	ILE	HG12	1.04	0.01	2
1	A	90	ARG	HB2	1.9	0.01	1
1	A	90	ARG	HG2	1.9	0.01	2
1	A	90	ARG	HD2	3.22	0.01	2
1	A	91	GLU	HB2	2.04	0.01	1
1	A	91	GLU	HG2	2.05	0.01	2
1	A	92	LYS	HB2	1.77	0.01	2
1	A	92	LYS	HG2	1.63	0.01	2
1	A	92	LYS	HD2	1.77	0.01	1
1	A	94	SER	HB2	3.91	0.01	1
1	A	95	HIS	HB2	3.29	0.01	2
1	A	96	ARG	HB2	2.42	0.01	2
1	A	96	ARG	HG2	1.28	0.01	2
1	A	96	ARG	HD2	3.01	0.01	2
1	A	97	ILE	HG12	1.5	0.01	2
1	A	100	ARG	HB2	2.33	0.01	1
1	A	100	ARG	HG2	1.66	0.01	2
1	A	100	ARG	HD2	3.42	0.01	2
1	A	103	LYS	HB2	1.94	0.01	2
1	A	103	LYS	HG2	1.56	0.01	1
1	A	103	LYS	HD2	1.75	0.01	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	104	SER	HB2	3.85	0.01	2
1	A	105	ASP	HB2	2.73	0.01	2
1	A	106	PHE	HB2	3.38	0.01	2
1	A	107	GLU	HB2	2.01	0.01	1
1	A	107	GLU	HG2	2.3	0.01	2
1	A	108	ILE	HG12	1.09	0.01	1
1	A	112	ARG	HB2	2.0	0.01	1
1	A	112	ARG	HG2	1.91	0.01	1
1	A	112	ARG	HD2	3.29	0.01	1
1	A	113	ASP	HB2	2.92	0.01	2
1	A	115	GLU	HB2	1.92	0.01	2
1	A	115	GLU	HG2	2.37	0.01	1
1	A	116	ILE	HG12	1.5	0.01	2
1	A	117	ILE	HG12	1.4	0.01	2
1	A	119	ASP	HB2	2.42	0.01	2
1	A	120	LEU	HB2	1.66	0.01	2
1	A	121	ASN	HB2	2.97	0.01	1
1	A	122	SER	HB2	3.9	0.01	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	119	-0.35 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	113	0.19 ± 0.09	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	118	-0.00 ± 0.27	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 77%, i.e. 1214 atoms were assigned a chemical shift out of a possible 1569. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	422/537 (79%)	213/217 (98%)	105/214 (49%)	104/106 (98%)
Sidechain	761/962 (79%)	523/622 (84%)	238/292 (82%)	0/48 (0%)
Aromatic	31/70 (44%)	22/37 (59%)	8/28 (29%)	1/5 (20%)
Overall	1214/1569 (77%)	758/876 (87%)	351/534 (66%)	105/159 (66%)

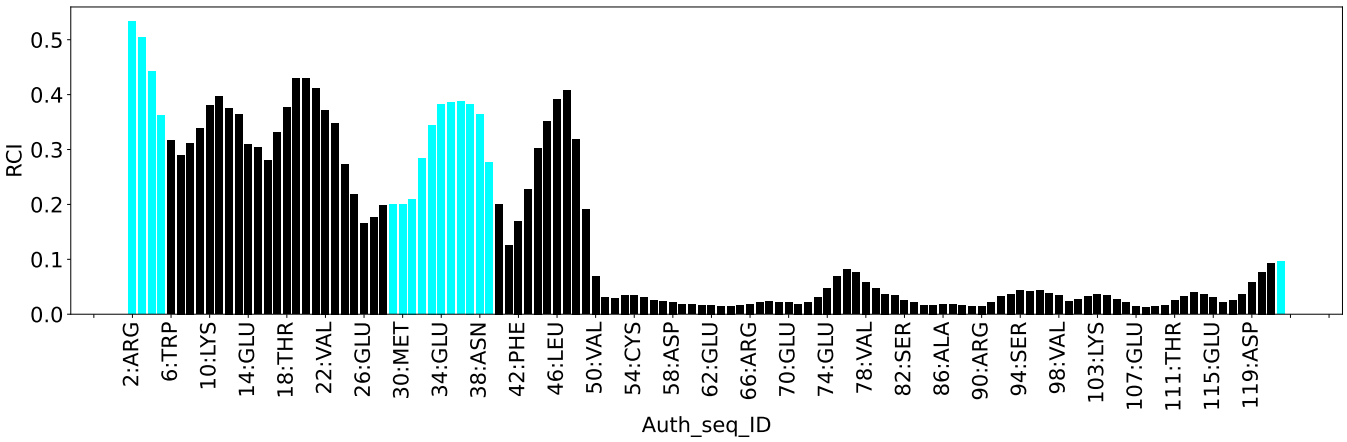
7.1.4 Statistically unusual chemical shifts (i)

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	1164
Intra-residue (|i-j|=0)	248
Sequential (|i-j|=1)	399
Medium range (|i-j|>1 and |i-j|<5)	294
Long range (|i-j|≥5)	223
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	415
Number of restraints per residue	9.5
Number of long range restraints per residue[1]	1.8

[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)	8.4	0.2
0.2-0.5 (Medium)	12.1	0.5
>0.5 (Large)	4.5	1.21

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)

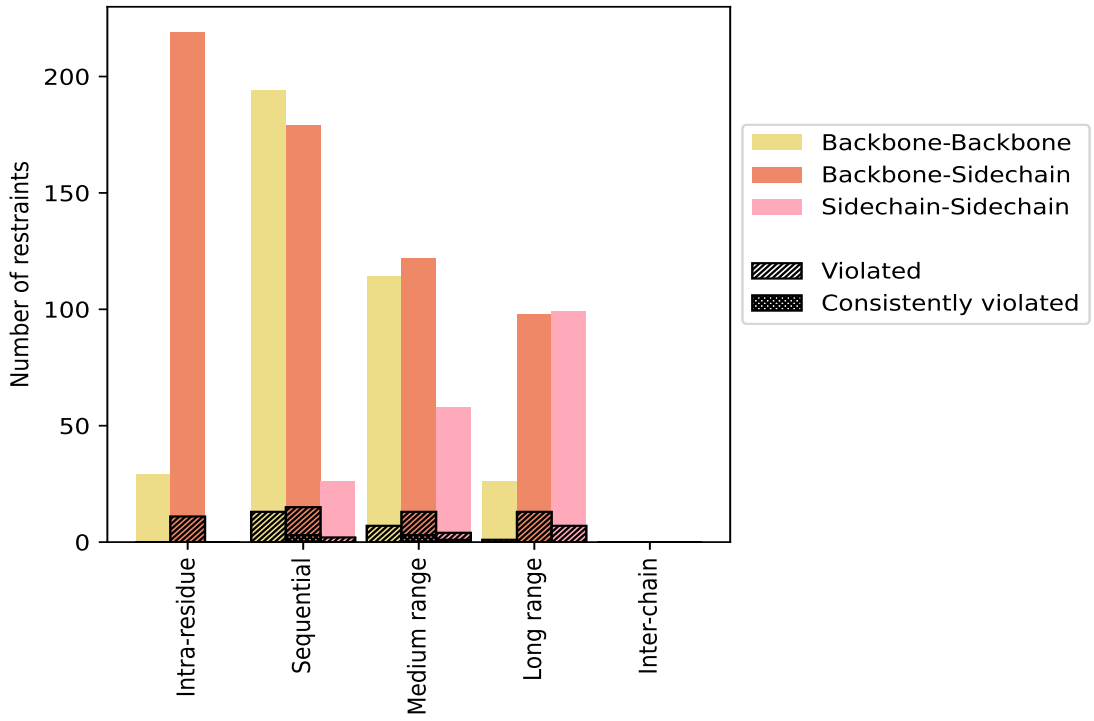
9.1 Summary of distance violations (i)

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)	248	21.3	11	4.4	0.9	0	0.0	0.0
Backbone-Backbone	29	2.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	219	18.8	11	5.0	0.9	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	399	34.3	30	7.5	2.6	3	0.8	0.3
Backbone-Backbone	194	16.7	13	6.7	1.1	0	0.0	0.0
Backbone-Sidechain	179	15.4	15	8.4	1.3	3	1.7	0.3
Sidechain-Sidechain	26	2.2	2	7.7	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	294	25.3	24	8.2	2.1	4	1.4	0.3
Backbone-Backbone	114	9.8	7	6.1	0.6	0	0.0	0.0
Backbone-Sidechain	122	10.5	13	10.7	1.1	3	2.5	0.3
Sidechain-Sidechain	58	5.0	4	6.9	0.3	1	1.7	0.1
Long range (|i-j|≥5)	223	19.2	21	9.4	1.8	0	0.0	0.0
Backbone-Backbone	26	2.2	1	3.8	0.1	0	0.0	0.0
Backbone-Sidechain	98	8.4	13	13.3	1.1	0	0.0	0.0
Sidechain-Sidechain	99	8.5	7	7.1	0.6	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	1164	100.0	86	7.4	7.4	7	0.6	0.6
Backbone-Backbone	363	31.2	21	5.8	1.8	0	0.0	0.0
Backbone-Sidechain	618	53.1	52	8.4	4.5	6	1.0	0.5
Sidechain-Sidechain	183	15.7	13	7.1	1.1	1	0.5	0.1

[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	1	10	8	6	0	25	0.33	0.74	0.18	0.27
2	4	5	8	7	0	24	0.3	0.79	0.17	0.24
3	2	8	7	5	0	22	0.34	0.57	0.14	0.37
4	2	8	8	5	0	23	0.31	0.65	0.16	0.28
5	4	8	8	7	0	27	0.29	0.79	0.19	0.22
6	2	7	9	5	0	23	0.33	0.8	0.19	0.3
7	1	5	10	8	0	24	0.37	0.83	0.19	0.32
8	3	3	9	9	0	24	0.43	0.98	0.23	0.41
9	0	6	8	7	0	21	0.34	0.78	0.17	0.3
10	0	8	9	5	0	22	0.32	0.79	0.16	0.26
11	1	10	10	6	0	27	0.34	1.21	0.26	0.25

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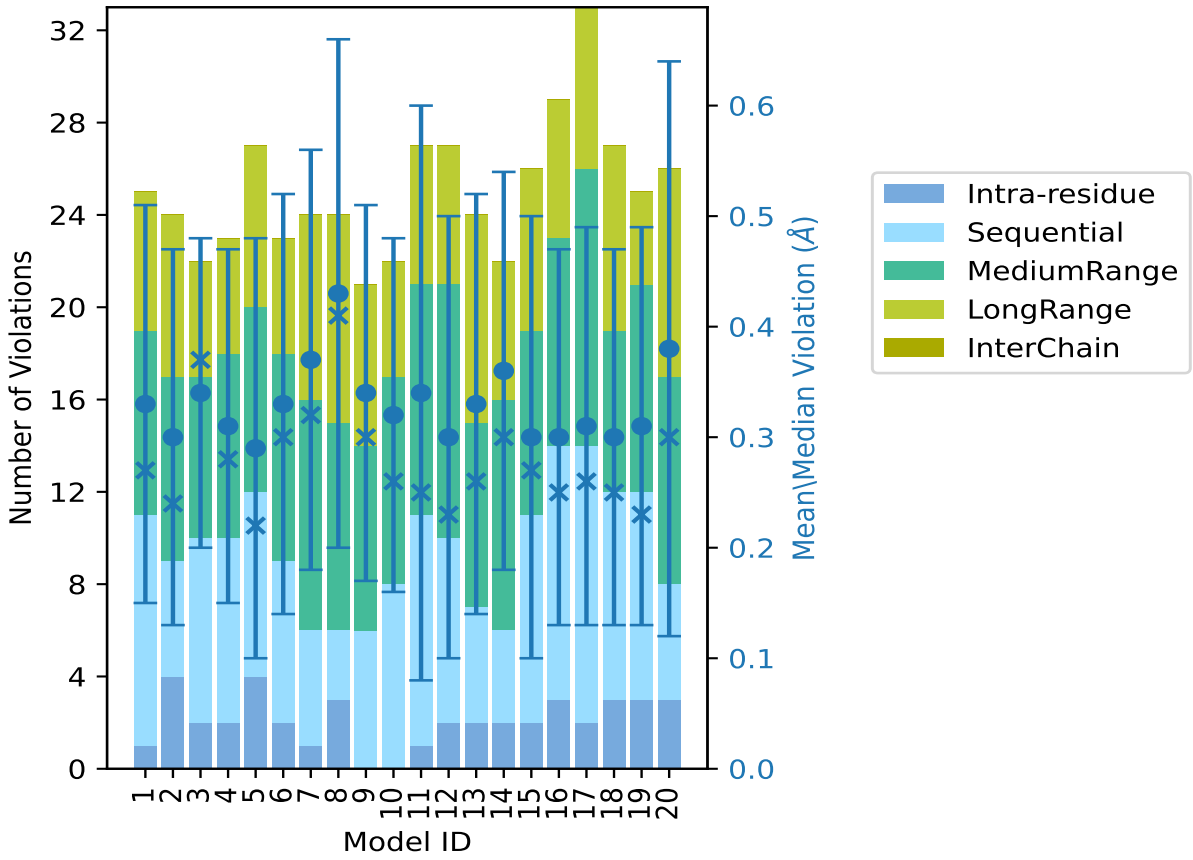
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	8	11	6	0	27	0.3	0.85	0.2	0.23
13	2	5	8	9	0	24	0.33	0.74	0.19	0.26
14	2	4	10	6	0	22	0.36	0.83	0.18	0.3
15	2	9	8	7	0	26	0.3	0.88	0.2	0.27
16	3	11	9	6	0	29	0.3	0.77	0.17	0.25
17	2	12	12	7	0	33	0.31	0.72	0.18	0.26
18	3	9	7	8	0	27	0.3	0.76	0.17	0.25
19	3	9	9	4	0	25	0.31	0.83	0.18	0.23
20	3	5	9	9	0	26	0.38	1.07	0.26	0.3

[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

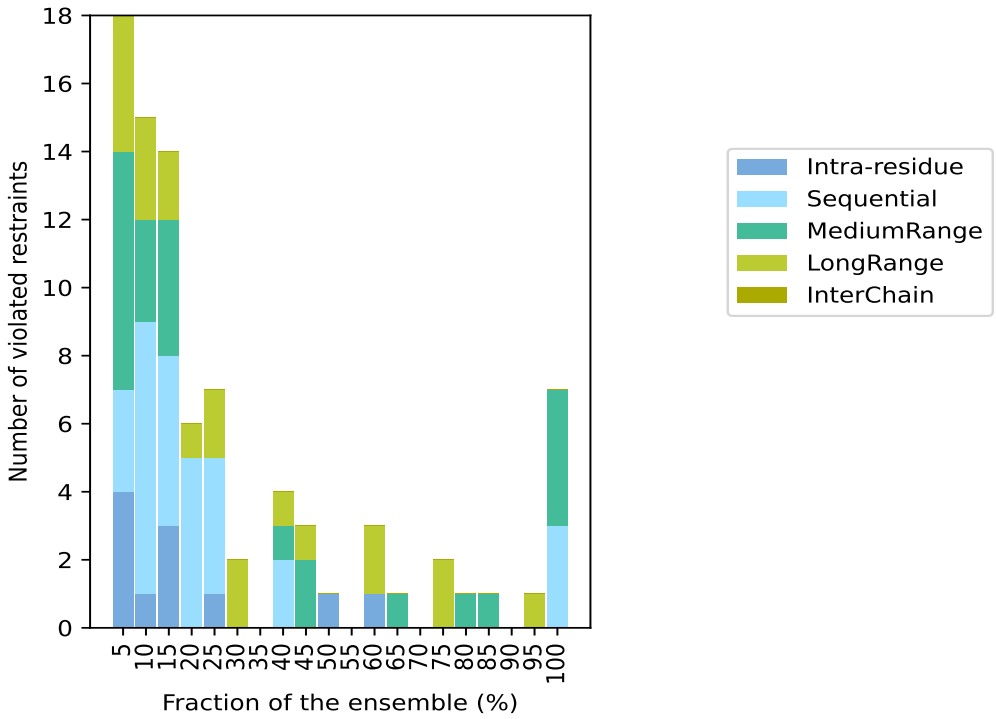
9.3 Distance violation statistics for the ensemble (i)

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, 1078(IR:237, SQ:369, MR:270, LR:202, 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]	%
4	3	7	4	0	18	1	5.0
1	8	3	3	0	15	2	10.0
3	5	4	2	0	14	3	15.0
0	5	0	1	0	6	4	20.0
1	4	0	2	0	7	5	25.0
0	0	0	2	0	2	6	30.0
0	0	0	0	0	0	7	35.0
0	2	1	1	0	4	8	40.0
0	0	2	1	0	3	9	45.0
1	0	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
1	0	0	2	0	3	12	60.0
0	0	1	0	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	2	0	2	15	75.0
0	0	1	0	0	1	16	80.0
0	0	1	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	1	0	1	19	95.0
0	3	4	0	0	7	20	100.0

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

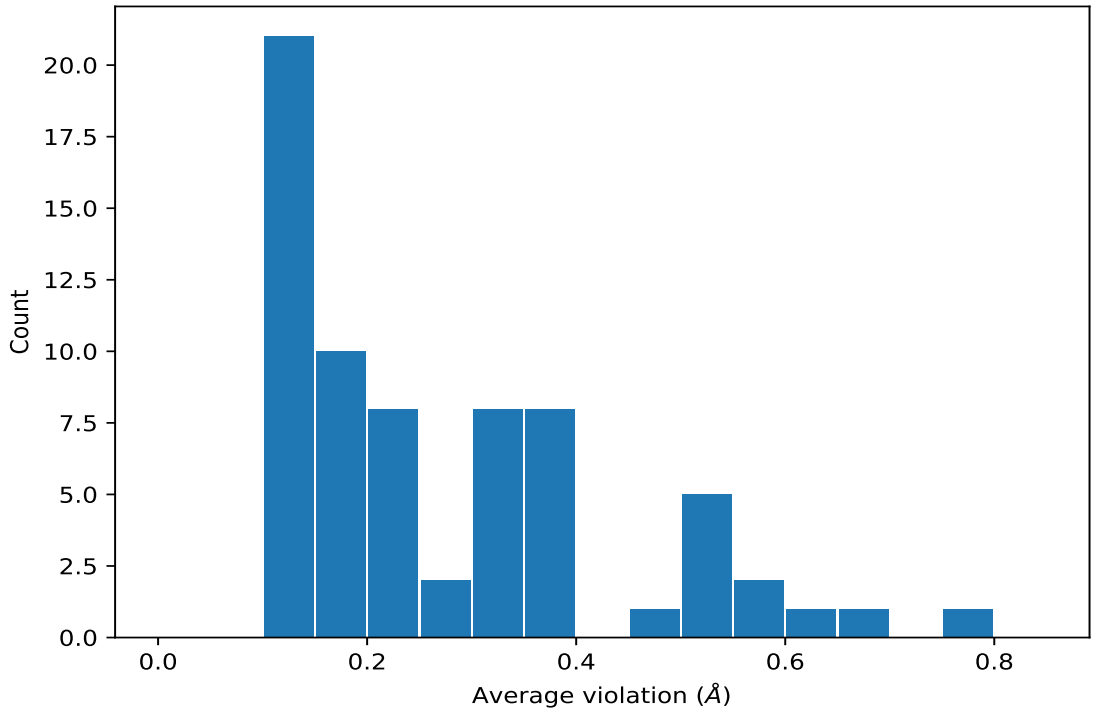
9.3.1 Bar graph : Distance violation statistics for the ensemble



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.

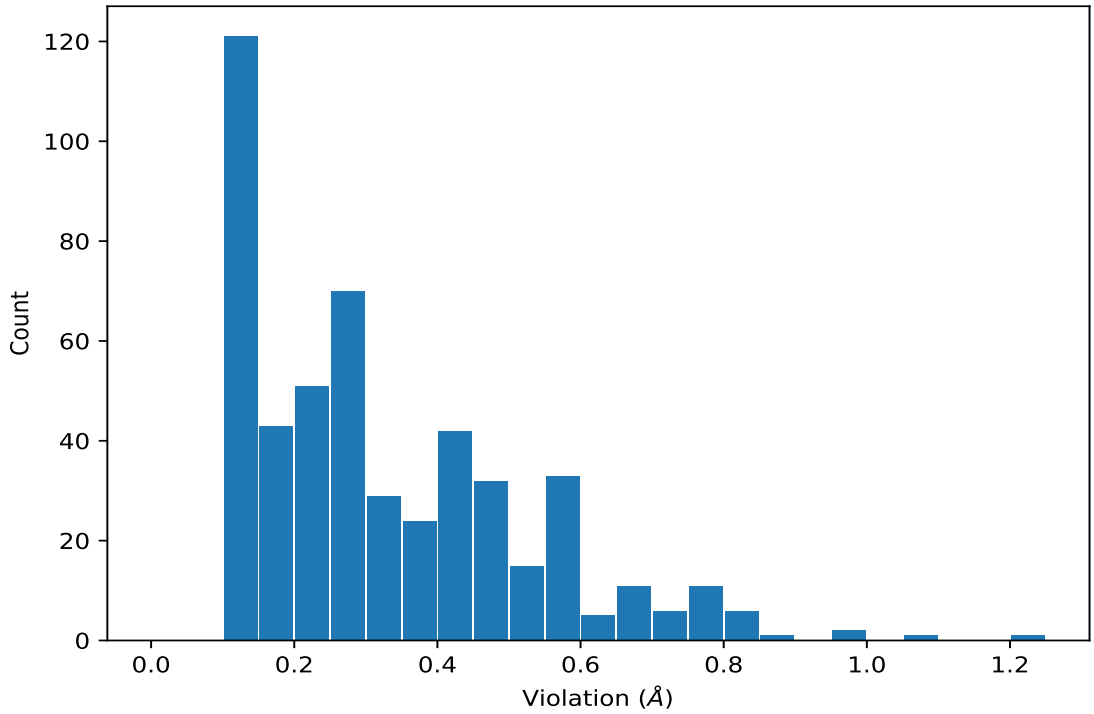
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,501)	1:A:69:GLU:HA	1:A:73:LYS:HB3	20	0.76	0.06	0.78
(1,504)	1:A:69:GLU:HB3	1:A:73:LYS:HB3	20	0.52	0.07	0.55
(1,477)	1:A:68:LEU:H	1:A:72:ASN:HB3	20	0.49	0.08	0.51
(1,676)	1:A:89:ILE:H	1:A:90:ARG:HB3	20	0.37	0.09	0.4
(1,497)	1:A:69:GLU:H	1:A:70:GLU:HG3	20	0.37	0.08	0.4
(1,656)	1:A:87:PHE:H	1:A:88:LEU:HB3	20	0.34	0.04	0.33
(1,511)	1:A:70:GLU:HA	1:A:73:LYS:HB3	20	0.31	0.11	0.27
(2,231)	1:A:107:GLU:HB3	1:A:118:VAL:H	19	0.51	0.16	0.49
(2,151)	1:A:69:GLU:HB3	1:A:73:LYS:HB3	17	0.21	0.04	0.22
(1,489)	1:A:68:LEU:HB3	1:A:71:SER:H	16	0.28	0.04	0.28

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:A:90:ARG:HD3	1:A:97:ILE:HG13	11	1.21
(2,231)	1:A:107:GLU:HB3	1:A:118:VAL:H	20	1.07
(1,321)	1:A:54:CYS:HB3	1:A:108:ILE:H	8	0.98
(2,229)	1:A:107:GLU:HB3	1:A:117:ILE:HB	20	0.97
(1,321)	1:A:54:CYS:HB3	1:A:108:ILE:H	15	0.88
(1,321)	1:A:54:CYS:HB3	1:A:108:ILE:H	12	0.85
(1,501)	1:A:69:GLU:HA	1:A:73:LYS:HB3	7	0.83
(1,501)	1:A:69:GLU:HA	1:A:73:LYS:HB3	14	0.83
(1,501)	1:A:69:GLU:HA	1:A:73:LYS:HB3	19	0.83
(1,501)	1:A:69:GLU:HA	1:A:73:LYS:HB3	8	0.81

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found