wwPDB NMR Structure Validation Summary Report

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PDB ID	:	8K2T
BMRB ID	:	36582
Title	:	Solution structure of full-length HtpG in complex with D131D
Authors	:	Qu, X.; Huang, C.
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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:

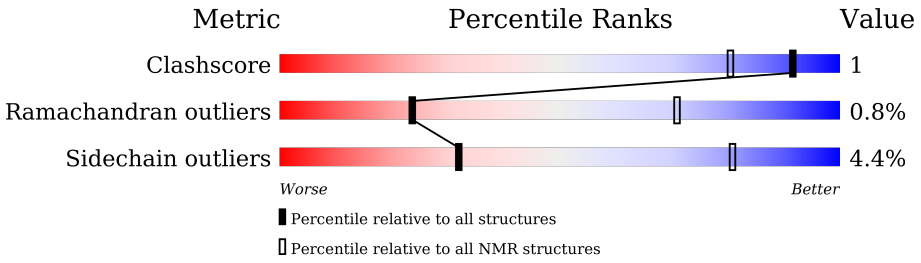
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 11%.

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	624	57% · 41%
1	B	624	65% · 33%
2	C	132	100%

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:15-A:381, B:14-B:415, B:435-B:439, B:459-B:469 (785)	3.43	5

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22181 atoms, of which 11056 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chaperone protein HtpG.

Mol	Chain	Residues	Atoms						Trace
1	A	624	Total	C	H	N	O	S	0
			10015	3174	4980	862	986	13	
1	B	624	Total	C	H	N	O	S	0
			10015	3174	4980	862	986	13	

- Molecule 2 is a protein called Nuclease A.

Mol	Chain	Residues	Atoms						Trace
2	C	132	Total	C	H	N	O	S	0
			2151	672	1096	184	194	5	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP P00644
C	2	ALA	-	expression tag	UNP P00644
C	3	THR	-	expression tag	UNP P00644
C	4	SER	-	expression tag	UNP P00644

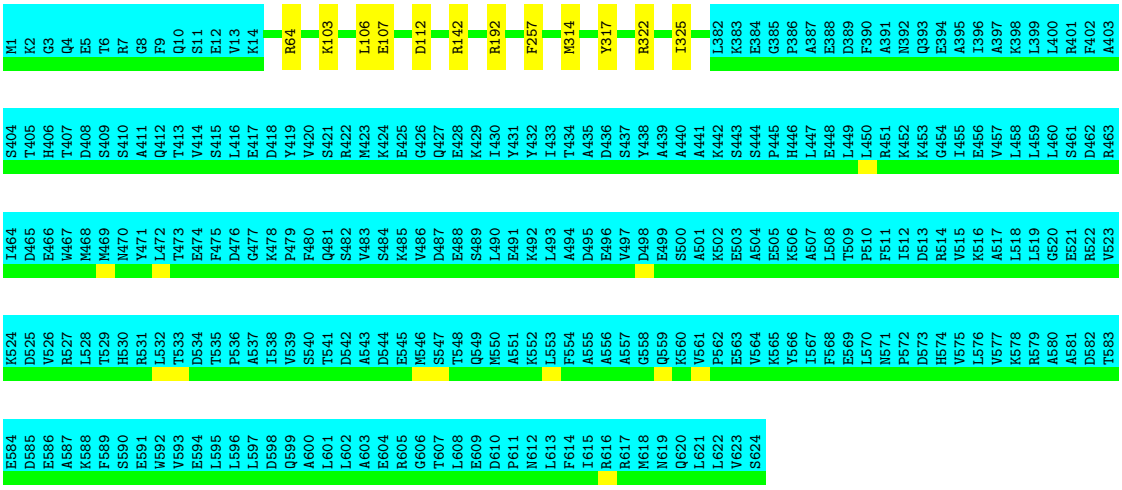
4 Residue-property plots

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.

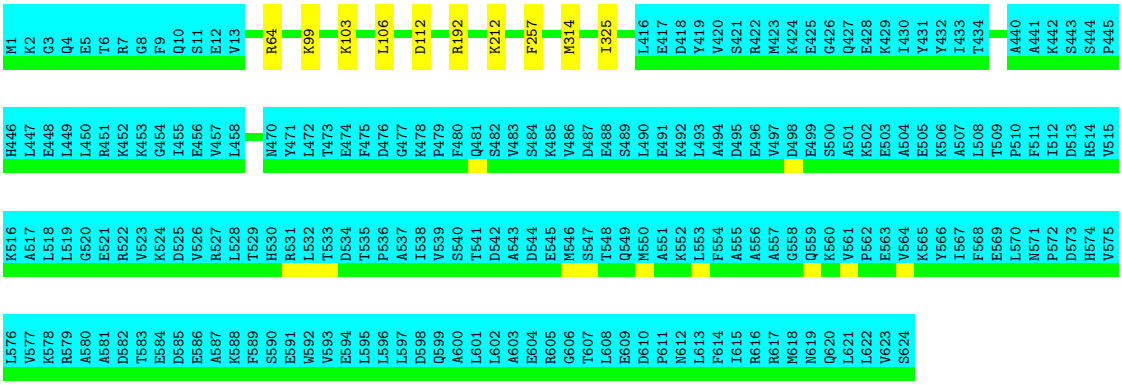
• Molecule 1: Chaperone protein HtpG

Chain A:



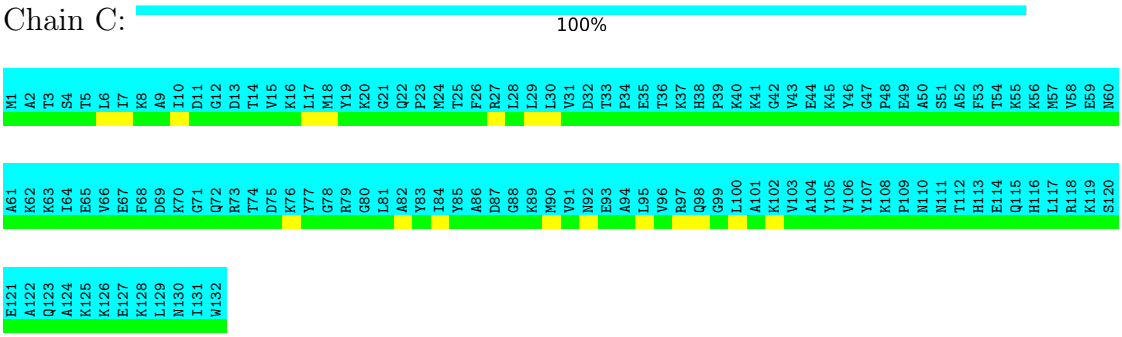
• Molecule 1: Chaperone protein HtpG

Chain B:



• Molecule 2: Nuclease A

Chain C:

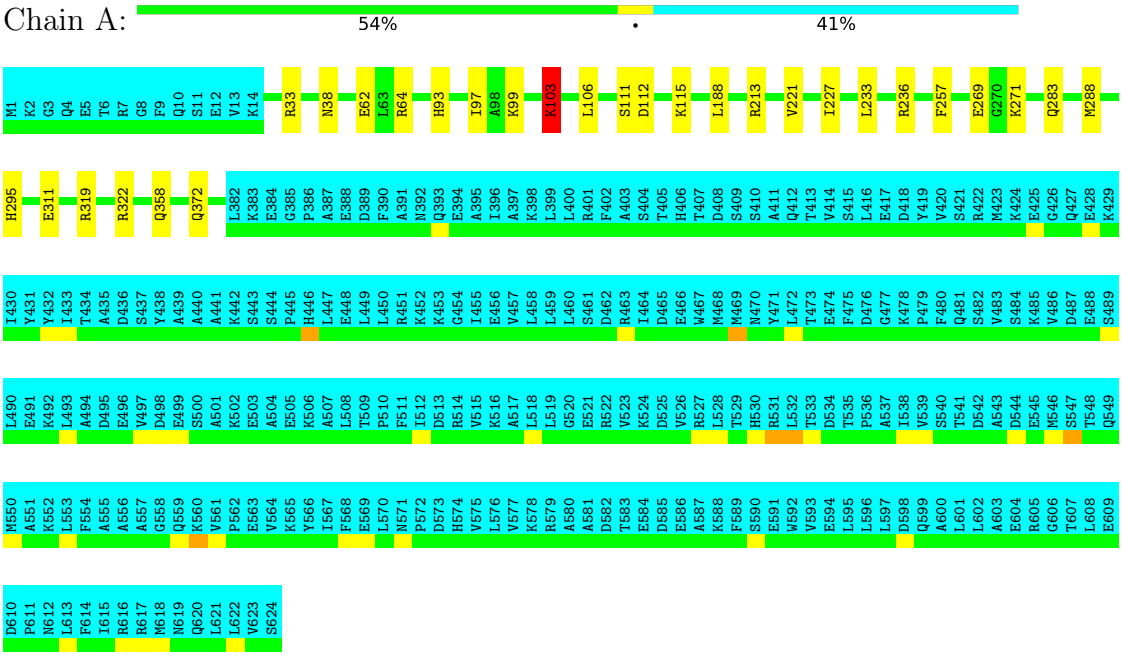


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

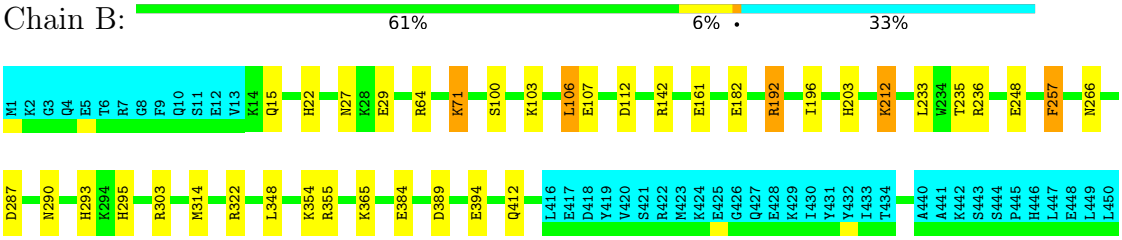
- Molecule 1: Chaperone protein HtpG

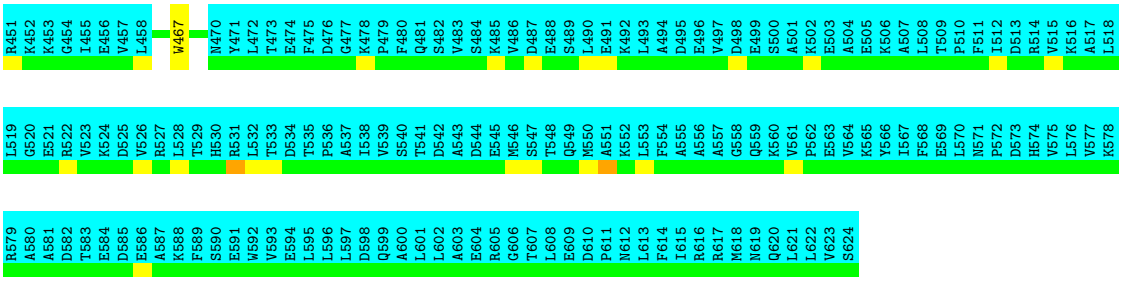
Chain A:



- Molecule 1: Chaperone protein HtpG

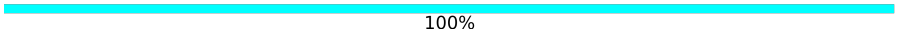
Chain B:

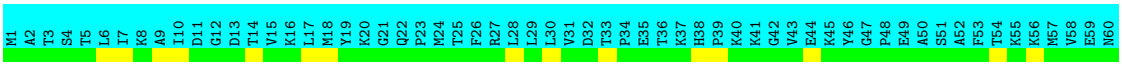


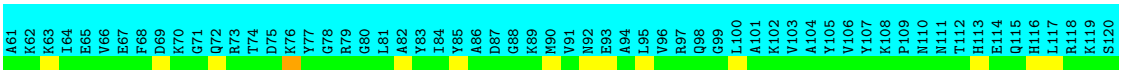


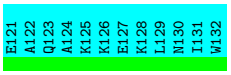
• Molecule 2: Nuclease A

Chain C:









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: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure calculation	
CNS	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	1687
Number of shifts mapped to atoms	1687
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	11%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.85±0.01	0±0/3057 (0.0± 0.0%)	0.63±0.01	0±0/4128 (0.0± 0.0%)
1	B	0.85±0.01	0±0/3460 (0.0± 0.0%)	0.63±0.01	0±0/4673 (0.0± 0.0%)
All	All	0.85	0/130340 (0.0%)	0.63	1/176020 (0.0%)

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.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	322	ARG	NE-CZ-NH2	-5.04	117.78	120.30	18	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	293	HIS	Peptide	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	2995	2936	2926	8±3
1	B	3391	3317	3306	11±4
2	C	0	0	0	0±0
All	All	127720	125060	124640	375

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.

5 of 264 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:318:LEU:HD11	1:A:353:THR:HG23	0.63	1.69	11	6
1:B:106:LEU:HD22	1:B:112:ASP:HB3	0.63	1.70	1	12
1:B:314:MET:SD	1:B:321:VAL:HB	0.63	2.33	12	2
1:B:460:LEU:HD23	1:B:465:ASP:HB3	0.62	1.72	16	4
1:B:460:LEU:HD21	1:B:469:MET:SD	0.61	2.35	16	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	367/624 (59%)	336±3 (91±1%)	28±3 (8±1%)	3±1 (1±0%)	21	69
1	B	418/624 (67%)	385±4 (92±1%)	29±4 (7±1%)	3±1 (1±0%)	24	71
2	C	0	-	-	-	-	
All	All	15700/27600 (57%)	14420 (92%)	1150 (7%)	130 (1%)	24	71

5 of 25 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	B	103	LYS	20
1	A	106	LEU	16

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Mol	Chain	Res	Type	Models (Total)
1	B	106	LEU	10
1	A	207	PRO	8

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	325/547 (59%)	310±3 (95±1%)	15±3 (5±1%)	31 79
1	B	367/547 (67%)	352±3 (96±1%)	15±3 (4±1%)	34 82
2	C	0	-	-	-
All	All	13840/24100 (57%)	13237 (96%)	603 (4%)	32 81

5 of 199 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	325	ILE	16
1	B	64	ARG	16
1	A	64	ARG	15
1	A	257	PHE	14
1	B	257	PHE	14

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

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 11% for the well-defined parts and 9% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_0*

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	1687
Number of shifts mapped to atoms	1687
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	442	0.09 ± 0.06	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	417	0.90 ± 0.10	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	414	-0.32 ± 0.15	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 11%, i.e. 1227 atoms were assigned a chemical shift out of a possible 10952. 0 out of 120 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	925/3934 (24%)	302/1596 (19%)	321/1570 (20%)	302/768 (39%)
Sidechain	302/6081 (5%)	0/3916 (0%)	302/1903 (16%)	0/262 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/937 (0%)	0/456 (0%)	0/422 (0%)	0/59 (0%)
Overall	1227/10952 (11%)	302/5968 (5%)	623/3895 (16%)	302/1089 (28%)

7.1.4 Statistically unusual chemical shifts (i)

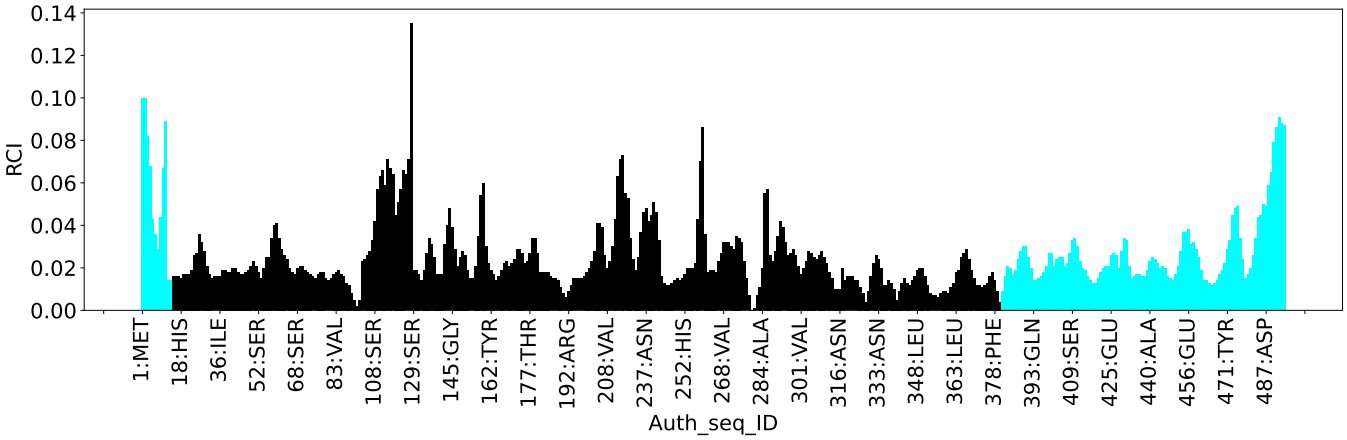
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	279	TYR	H	117.59	4.70 – 11.88	152.2
1	A	328	SER	H	31.14	5.45 – 11.10	40.5
1	A	340	GLN	H	29.41	5.39 – 11.05	37.5
1	A	279	TYR	N	9.63	100.12 – 140.79	-27.2
1	A	91	ILE	CA	30.54	48.30 – 75.08	-11.6
1	A	380	LEU	CB	57.53	33.11 – 51.34	8.4
1	A	335	SER	CB	51.64	56.28 – 71.32	-8.1
1	A	462	ASP	CB	53.22	32.98 – 48.76	7.8
1	A	181	ARG	CB	43.22	21.74 – 39.52	7.1
1	A	380	LEU	CA	40.90	45.17 – 66.21	-7.0
1	A	360	LEU	CB	30.11	33.11 – 51.34	-6.7
1	A	353	THR	CB	58.99	61.12 – 78.27	-6.2
1	A	91	ILE	CB	50.21	28.63 – 48.45	5.9
1	A	191	TRP	CA	43.57	45.21 – 70.26	-5.7

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:


RCI
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
1:MET
18:HIS
36:ILE
52:SER
68:SER
83:VAL
108:SER
129:SER
145:GLY
162:TYR
177:THR
192:ARG
208:VAL
237:ASN
252:HIS
268:VAL
284:ALA
301:VAL
316:ASN
333:ASN
348:LEU
363:LEU
378:PHE
393:GLN
409:SER
425:GLU
440:ALA
456:GLU
471:TYR
487:ASP
Auth_seq_ID

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	24243
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	6802
Medium range (|i-j|>1 and |i-j|<5)	6814
Long range (|i-j|≥5)	10540
Inter-chain	87
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	17.6
Number of long range restraints per residue[1]	7.6

[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)	99.5	0.2
0.2-0.5 (Medium)	46.7	0.5
>0.5 (Large)	25.1	92.03

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)

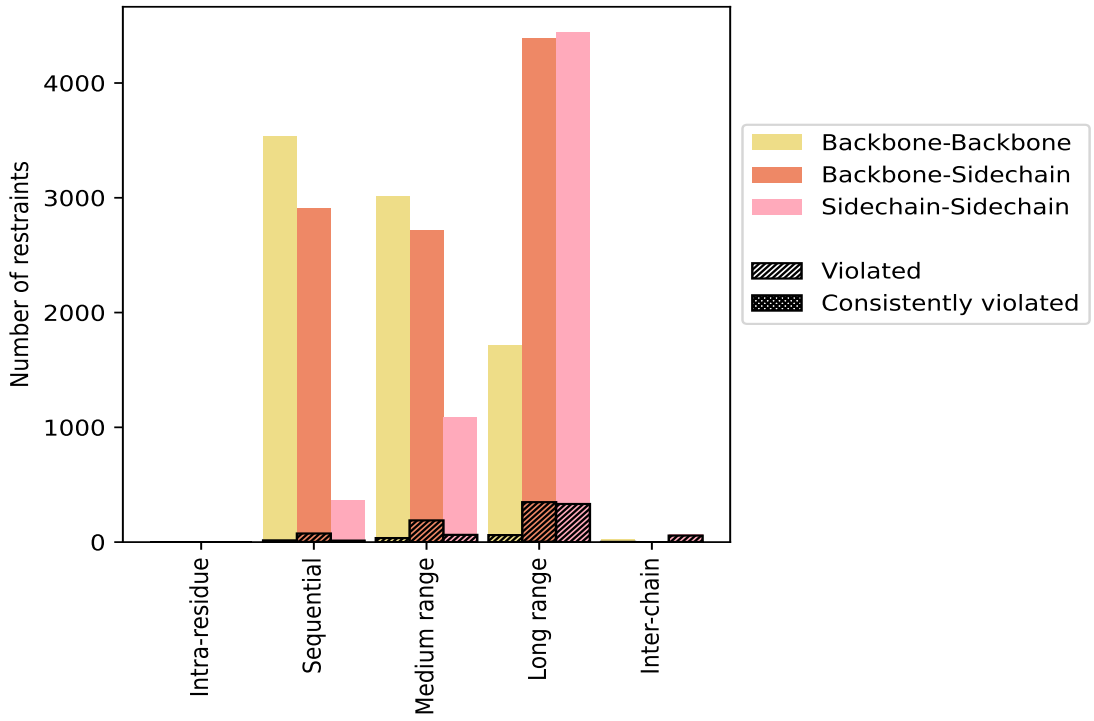
9.1 Summary of distance violations (i)

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)	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
Sequential (|i-j|=1)	6802	28.1	103	1.5	0.4	2	0.0	0.0
Backbone-Backbone	3532	14.6	15	0.4	0.1	0	0.0	0.0
Backbone-Sidechain	2910	12.0	75	2.6	0.3	2	0.1	0.0
Sidechain-Sidechain	360	1.5	13	3.6	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	6814	28.1	287	4.2	1.2	0	0.0	0.0
Backbone-Backbone	3014	12.4	35	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	2714	11.2	189	7.0	0.8	0	0.0	0.0
Sidechain-Sidechain	1086	4.5	63	5.8	0.3	0	0.0	0.0
Long range (|i-j|≥5)	10540	43.5	741	7.0	3.1	4	0.0	0.0
Backbone-Backbone	1712	7.1	61	3.6	0.3	0	0.0	0.0
Backbone-Sidechain	4386	18.1	348	7.9	1.4	4	0.1	0.0
Sidechain-Sidechain	4442	18.3	332	7.5	1.4	0	0.0	0.0
Inter-chain	87	0.4	58	66.7	0.2	2	2.3	0.0
Backbone-Backbone	21	0.1	1	4.8	0.0	1	4.8	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	66	0.3	57	86.4	0.2	1	1.5	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	24243	100.0	1189	4.9	4.9	8	0.0	0.0
Backbone-Backbone	8279	34.2	112	1.4	0.5	1	0.0	0.0
Backbone-Sidechain	10010	41.3	612	6.1	2.5	6	0.1	0.0
Sidechain-Sidechain	5954	24.6	465	7.8	1.9	1	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



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	0	16	32	122	26	196	0.75	90.94	6.47	0.17
2	0	21	27	97	16	161	0.85	90.19	7.07	0.19
3	0	12	19	121	17	169	0.84	90.41	6.92	0.17
4	0	16	28	102	15	161	0.84	89.95	7.05	0.18
5	0	17	30	109	18	174	0.8	90.34	6.81	0.16
6	0	16	37	107	19	179	0.79	90.24	6.71	0.18
7	0	12	32	109	17	170	0.81	89.38	6.82	0.16
8	0	14	34	104	21	173	0.79	90.3	6.83	0.17
9	0	12	30	102	10	154	0.9	91.49	7.33	0.18
10	0	16	36	111	18	181	0.82	91.84	6.79	0.17

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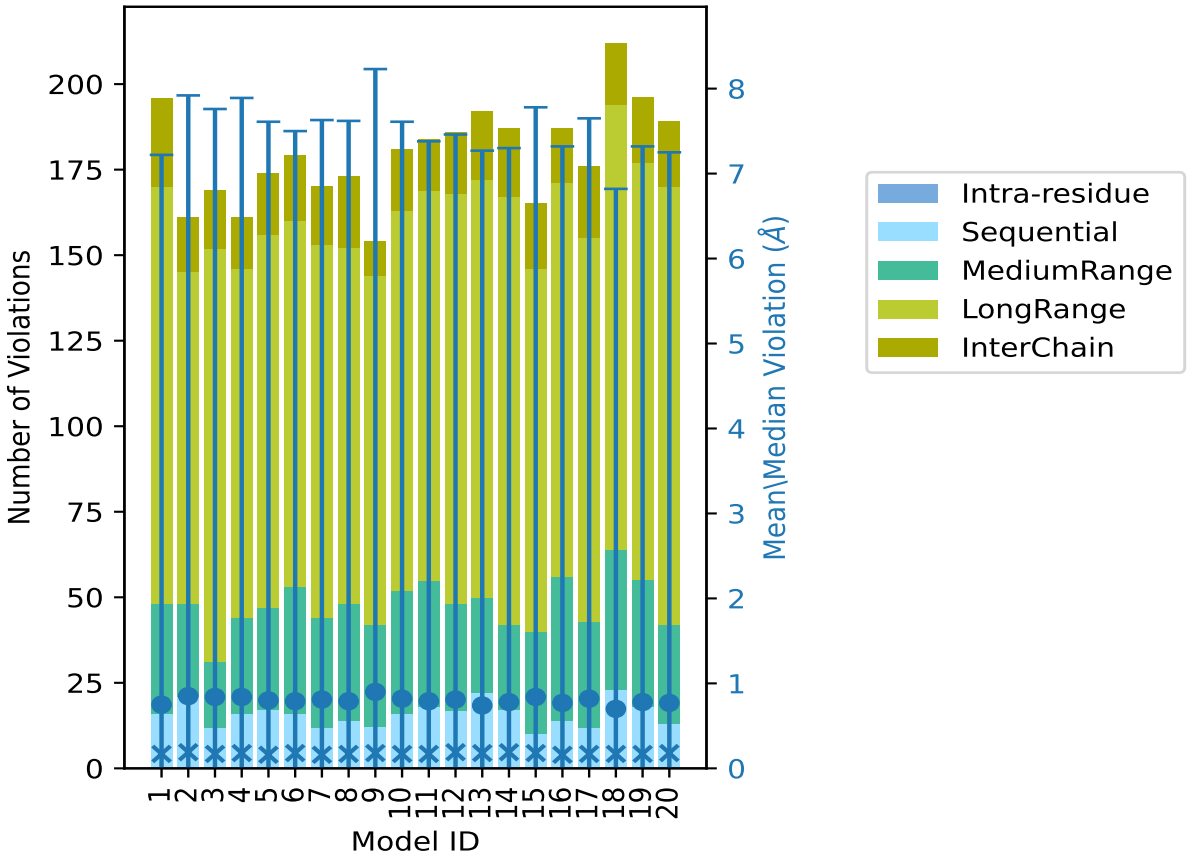
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	18	37	114	15	184	0.79	89.79	6.59	0.17
12	0	17	31	120	18	186	0.81	91.15	6.65	0.19
13	0	22	28	122	20	192	0.74	90.86	6.53	0.18
14	0	17	25	125	20	187	0.78	89.6	6.52	0.19
15	0	10	30	106	19	165	0.84	89.58	6.94	0.18
16	0	14	42	115	16	187	0.77	89.97	6.55	0.16
17	0	12	31	112	21	176	0.82	91.03	6.83	0.17
18	0	23	41	130	18	212	0.7	89.56	6.12	0.17
19	0	18	37	122	19	196	0.78	92.03	6.54	0.17
20	0	13	29	128	19	189	0.77	89.58	6.48	0.18

[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

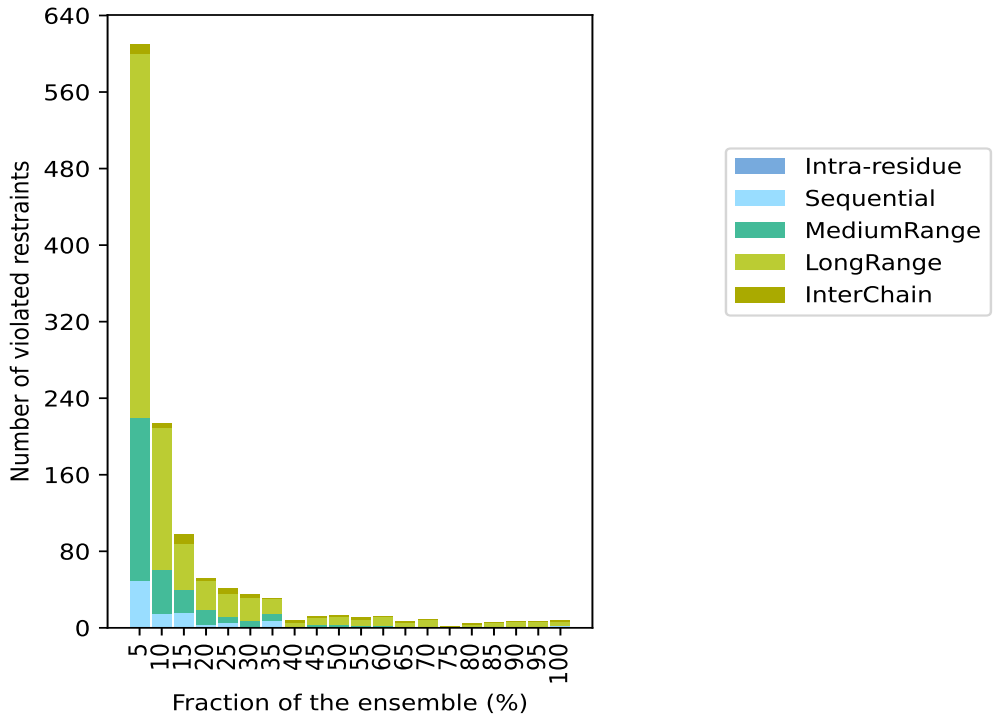
9.3 Distance violation statistics for the ensemble (i)

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, 23054(IR:0, SQ:6699, MR:6527, LR:9799, IC:29) 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	49	171	380	10	610	1	5.0
0	15	46	148	5	214	2	10.0
0	16	24	48	10	98	3	15.0
0	3	16	30	3	52	4	20.0
0	5	6	25	6	42	5	25.0
0	1	6	24	4	35	6	30.0
0	7	8	15	1	31	7	35.0
0	1	0	4	3	8	8	40.0
0	1	2	7	2	12	9	45.0
0	1	2	8	2	13	10	50.0
0	1	1	6	3	11	11	55.0
0	0	2	10	0	12	12	60.0
0	0	1	4	2	7	13	65.0
0	0	1	7	1	9	14	70.0
0	0	1	0	1	2	15	75.0
0	0	0	3	2	5	16	80.0
0	0	0	5	1	6	17	85.0
0	0	0	7	0	7	18	90.0
0	1	0	6	0	7	19	95.0
0	2	0	4	2	8	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

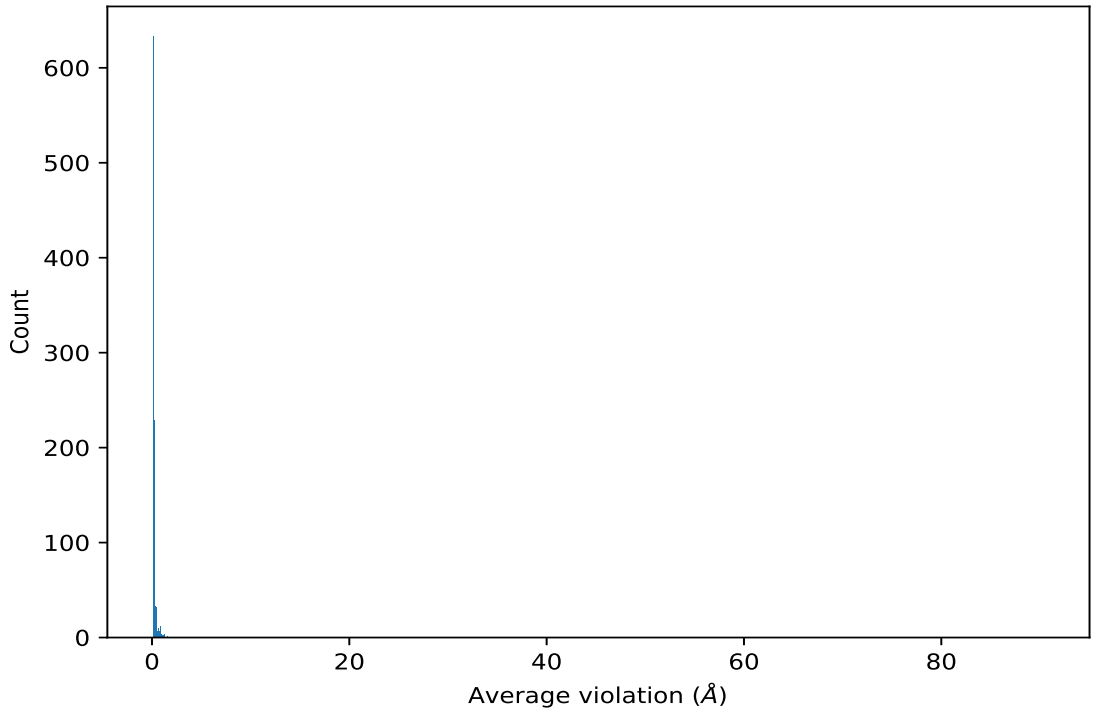
9.3.1 Bar graph : Distance violation statistics for the ensemble



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

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)
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	20	90.41	0.77	90.27
(1,16652)	1:202:B:ASP:HA	1:245:B:GLU:HG3	20	1.24	0.24	1.25
(1,1482)	1:66:A:ARG:HB2	1:211:A:GLU:H	20	0.57	0.21	0.55
(1,13560)	1:66:B:ARG:HB2	1:211:B:GLU:H	20	0.54	0.12	0.55
(1,16148)	1:177:B:THR:HA	1:178:B:LEU:HB3	20	0.35	0.04	0.36
(1,16915)	1:209:B:GLU:HA	1:224:B:TRP:HB2	20	0.35	0.15	0.32
(1,4070)	1:177:A:THR:HA	1:178:A:LEU:HB3	20	0.34	0.04	0.35
(1,24214)	1:458:B:LEU:HD11	2:95:C:LEU:HD21	20	0.32	0.12	0.29
(1,24214)	1:458:B:LEU:HD11	2:95:C:LEU:HD22	20	0.32	0.12	0.29
(1,24214)	1:458:B:LEU:HD11	2:95:C:LEU:HD23	20	0.32	0.12	0.29
(1,24214)	1:458:B:LEU:HD12	2:95:C:LEU:HD21	20	0.32	0.12	0.29
(1,24214)	1:458:B:LEU:HD12	2:95:C:LEU:HD22	20	0.32	0.12	0.29
(1,24214)	1:458:B:LEU:HD12	2:95:C:LEU:HD23	20	0.32	0.12	0.29
(1,24214)	1:458:B:LEU:HD13	2:95:C:LEU:HD21	20	0.32	0.12	0.29
(1,24214)	1:458:B:LEU:HD13	2:95:C:LEU:HD22	20	0.32	0.12	0.29
(1,24214)	1:458:B:LEU:HD13	2:95:C:LEU:HD23	20	0.32	0.12	0.29

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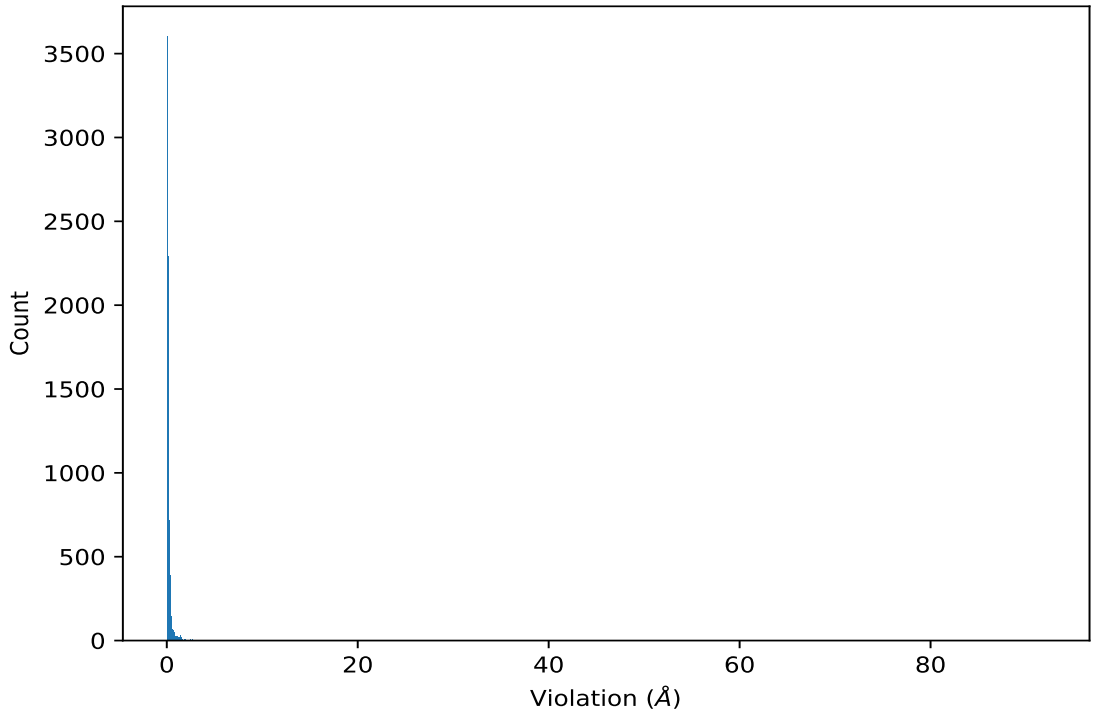
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,17572)	1:249:B:PHE:HE2	1:298:B:LYS:HD2	19	1.22	0.27	1.26
(1,17573)	1:249:B:PHE:HZ	1:298:B:LYS:HD2	19	1.16	0.3	1.3

[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)
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	19	92.03
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	10	91.84
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	9	91.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	12	91.15
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	17	91.03
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	1	90.94
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	13	90.86
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	3	90.41
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	5	90.34
(2,7)	1:218:A:GLY:H	1:218:B:GLY:H	8	90.3

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found