wwPDB NMR Structure Validation Summary Report (i)

Jun 3, 2023 – 06:40 PM EDT

PDB ID	:	2MQN
BMRB ID	:	25040
Title	:	Structural Investigation of hnRNP L
Authors	:	Blatter, M.; Allain, F.
Deposited on	:	2014-06-24

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

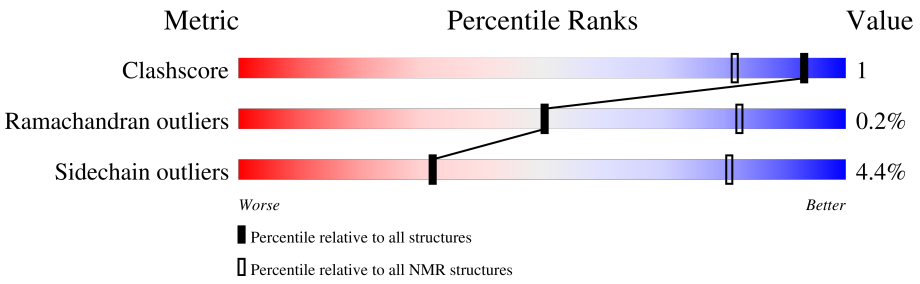
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 75%.

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	216	83% • 12%

2 Ensemble composition and analysis (i)

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:376-A:475, A:494-A:533, A:538-A:586 (189)	0.94	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 6 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3327 atoms, of which 1629 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heterogenous nuclear ribonucleoprotein L.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	216	3327	1069	1629	289	325	15	0

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: Heterogenous nuclear ribonucleoprotein L

Chain A: 83% • 12%

D371 Y372 G373 P374 H375 L386 L402 M412 F440 K445 E476 S477 R478 N479 N480 R481 F482 S483 T484 P485 E486 Q487 A488 A489 K490 N491 R492 I493 H501 G534 K535 S536 E537 Y562 G569 P570 S586

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: Heterogenous nuclear ribonucleoprotein L

Chain A: 81% 6% 12%

D371 Y372 G373 P374 H375 L386 K390 L402 M412 A418 R431 F440 K445 E476 S477 R478 N479 N480 R481 F482 S483 T484 P485 E486 Q487 A488 A489 K490 N491 R492 I493 H501 F502 F503 L507 G534 K535 S536 E537 G569 P570 Q583 S586

5 Refinement protocol and experimental data overview (i)

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

Of the 250 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
TopSpin	refinement	
CYANA	structure solution	
Amber	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	2075
Number of shifts mapped to atoms	2075
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	1481	1426	1426	4±2
All	All	29620	28520	28520	76

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:386:LEU:H	1:A:386:LEU:HD23	0.58	1.59	15	12
1:A:386:LEU:HD13	1:A:386:LEU:H	0.58	1.58	13	8
1:A:412:MET:HE3	1:A:418:ALA:HB1	0.53	1.80	14	5
1:A:501:HIS:CD2	1:A:503:PHE:CZ	0.53	2.97	1	2
1:A:445:LYS:H	1:A:445:LYS:CD	0.49	2.21	15	5

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	188/216 (87%)	178±2 (95±1%)	10±2 (5±1%)	0±1 (0±0%)	50 82
All	All	3760/4320 (87%)	3563 (95%)	190 (5%)	7 (0%)	50 82

All 4 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	461	SER	3
1	A	494	GLN	2
1	A	565	LYS	1
1	A	460	GLN	1

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	166/189 (88%)	159±2 (96±1%)	7±2 (4±1%)	32 81
All	All	3320/3780 (88%)	3173 (96%)	147 (4%)	32 81

5 of 29 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	440	PHE	20
1	A	445	LYS	17
1	A	402	LEU	13
1	A	562	TYR	13
1	A	501	HIS	11

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 (i)

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 73% 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 (i)

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	2075
Number of shifts mapped to atoms	2075
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 (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	186	2.46 ± 0.20	Should be applied
$^{13}C_{\beta}$	180	2.68 ± 0.13	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	203	-0.50 ± 0.30	None needed (< 0.5 ppm)

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 75%, i.e. 1866 atoms were assigned a chemical shift out of a possible 2495. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	700/937 (75%)	356/380 (94%)	165/378 (44%)	179/179 (100%)
Sidechain	1051/1309 (80%)	717/851 (84%)	324/413 (78%)	10/45 (22%)

Continued on next page...

Continued from previous page...

	Total	^{1}H	^{13}C	^{15}N
Aromatic	115/249 (46%)	74/123 (60%)	40/120 (33%)	1/6 (17%)
Overall	1866/2495 (75%)	1147/1354 (85%)	529/911 (58%)	190/230 (83%)

7.1.4 Statistically unusual chemical shifts (i)

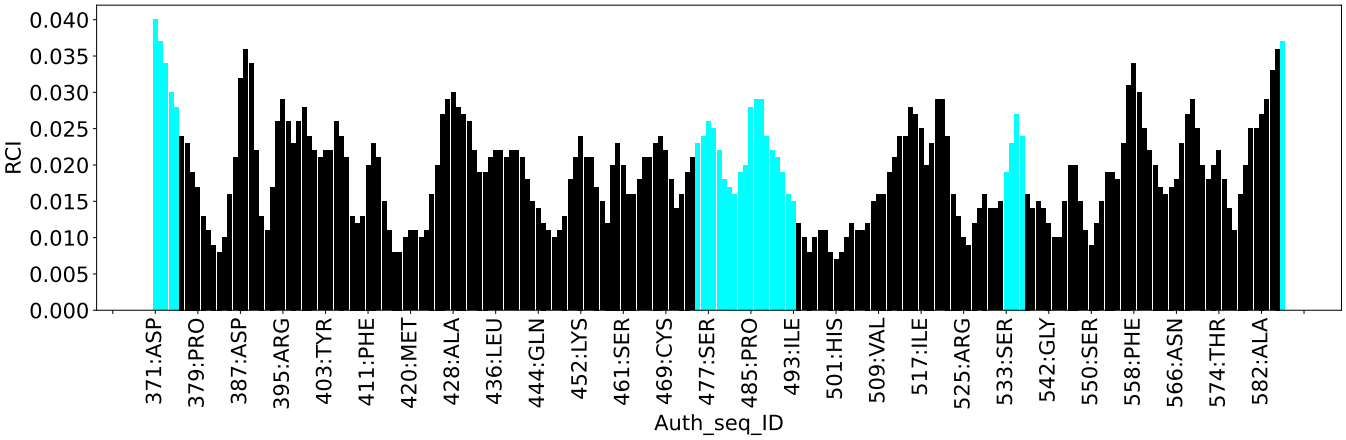
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	561	HIS	HE1	134.81	5.13 – 10.76	225.3
1	A	561	HIS	CE1	8.20	126.08 – 149.12	-56.2
1	A	478	ARG	CD	33.89	38.57 – 47.75	-10.1
1	A	554	GLU	HG2	0.31	1.24 – 3.30	-9.5
1	A	554	GLU	HG3	0.31	1.20 – 3.30	-9.2
1	A	496	PRO	HA	1.43	2.78 – 6.00	-9.2
1	A	472	LYS	HG2	-0.23	0.13 – 2.61	-6.4
1	A	470	SER	HB2	2.50	2.61 – 5.13	-5.5
1	A	526	PRO	HA	2.67	2.78 – 6.00	-5.3
1	A	576	LYS	HB2	0.51	0.58 – 2.97	-5.3
1	A	542	GLY	HA2	2.06	2.15 – 5.77	-5.2
1	A	419	ALA	HB1	0.12	0.14 – 2.58	-5.1
1	A	419	ALA	HB2	0.12	0.14 – 2.58	-5.1
1	A	419	ALA	HB3	0.12	0.14 – 2.58	-5.1

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
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
371:ASP
379:PRO
387:ASP
395:ARG
403:TYR
411:PHE
420:MET
428:ALA
436:LEU
444:GLN
452:LYS
461:SER
469:CYS
477:SER
485:PRO
493:ILE
501:HIS
509:VAL
517:ILE
525:ARG
533:SER
542:GLY
550:SER
558:PHE
566:ASN
574:THR
582:ALA
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	3758
Intra-residue (|i-j|=0)	481
Sequential (|i-j|=1)	1003
Medium range (|i-j|>1 and |i-j|<5)	574
Long range (|i-j|≥5)	1461
Inter-chain	0
Hydrogen bond restraints	239
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	3
Number of restraints per residue	17.4
Number of long range restraints per residue[1]	7.3

[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 (i)

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 (i)

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)	9.1	0.2
0.2-0.5 (Medium)	9.1	0.5
>0.5 (Large)	53.6	3.15

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)

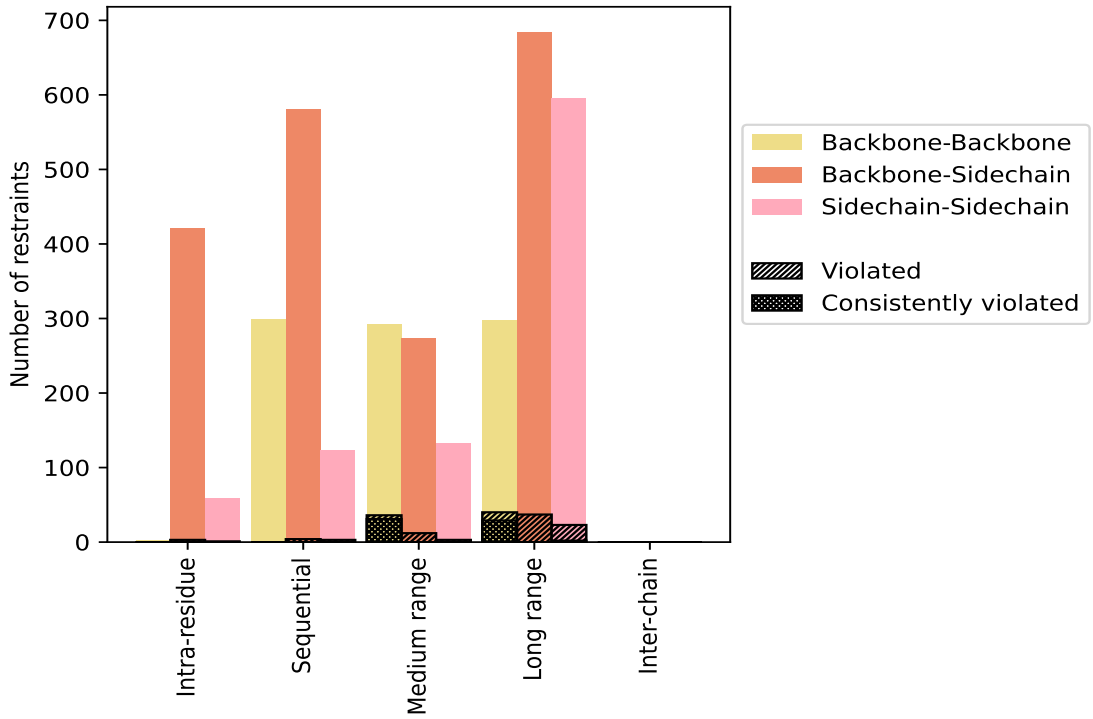
9.1 Summary of distance violations (i)

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)	481	12.8	4	0.8	0.1	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	421	11.2	3	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	58	1.5	1	1.7	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1003	26.7	7	0.7	0.2	0	0.0	0.0
Backbone-Backbone	299	8.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	581	15.5	4	0.7	0.1	0	0.0	0.0
Sidechain-Sidechain	123	3.3	3	2.4	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	574	15.3	16	2.8	0.4	0	0.0	0.0
Backbone-Backbone	168	4.5	1	0.6	0.0	0	0.0	0.0
Backbone-Sidechain	273	7.3	12	4.4	0.3	0	0.0	0.0
Sidechain-Sidechain	133	3.5	3	2.3	0.1	0	0.0	0.0
Long range (|i-j|≥5)	1461	38.9	71	4.9	1.9	2	0.1	0.1
Backbone-Backbone	182	4.8	11	6.0	0.3	0	0.0	0.0
Backbone-Sidechain	684	18.2	37	5.4	1.0	0	0.0	0.0
Sidechain-Sidechain	595	15.8	23	3.9	0.6	2	0.3	0.1
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	239	6.4	64	26.8	1.7	60	25.1	1.6
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3758	100.0	162	4.3	4.3	62	1.6	1.6
Backbone-Backbone	890	23.7	76	8.5	2.0	60	6.7	1.6
Backbone-Sidechain	1959	52.1	56	2.9	1.5	0	0.0	0.0
Sidechain-Sidechain	909	24.2	30	3.3	0.8	2	0.2	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 (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	1	2	34	33	0	70	0.67	1.47	0.26	0.68
2	0	1	33	38	0	72	0.65	1.24	0.27	0.69
3	2	0	32	40	0	74	0.64	1.31	0.28	0.71
4	0	1	33	33	0	67	0.7	1.38	0.24	0.71
5	1	2	32	35	0	70	0.68	2.28	0.33	0.7
6	0	2	33	39	0	74	0.62	1.67	0.3	0.6
7	0	0	34	36	0	70	0.69	2.5	0.35	0.68
8	0	0	32	36	0	68	0.69	1.68	0.27	0.74
9	0	0	34	41	0	75	0.62	1.18	0.27	0.66
10	0	2	33	37	0	72	0.65	1.06	0.26	0.7
11	0	0	34	39	0	73	0.63	1.14	0.27	0.7

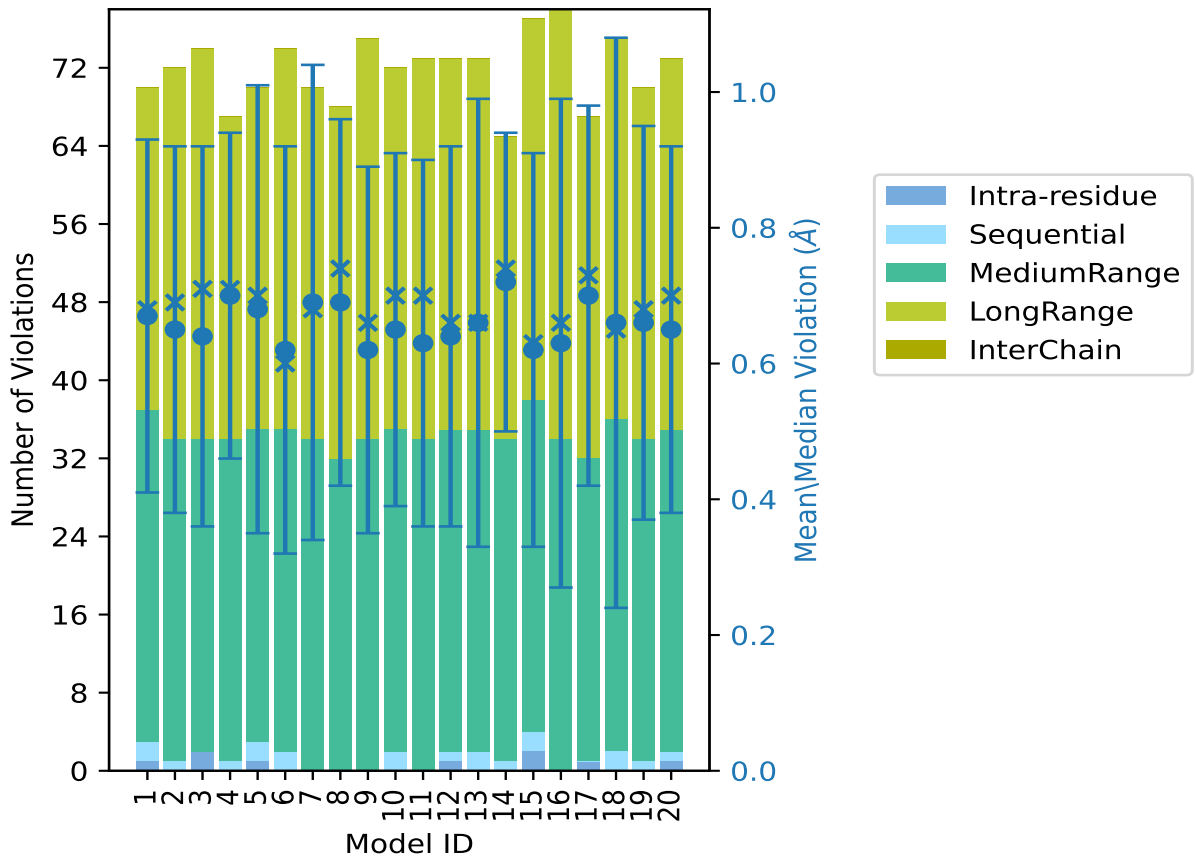
Continued on next page...

Continued from previous page...

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	1	1	33	38	0	73	0.64	1.55	0.28	0.66
13	0	2	33	38	0	73	0.66	1.99	0.33	0.66
14	0	1	33	31	0	65	0.72	1.18	0.22	0.74
15	2	2	34	39	0	77	0.62	1.38	0.29	0.63
16	0	0	34	44	0	78	0.63	2.1	0.36	0.66
17	1	0	31	35	0	67	0.7	1.81	0.28	0.73
18	0	2	34	39	0	75	0.66	3.15	0.42	0.65
19	0	1	33	36	0	70	0.66	1.79	0.29	0.68
20	1	1	33	38	0	73	0.65	1.23	0.27	0.7

[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 (i)



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

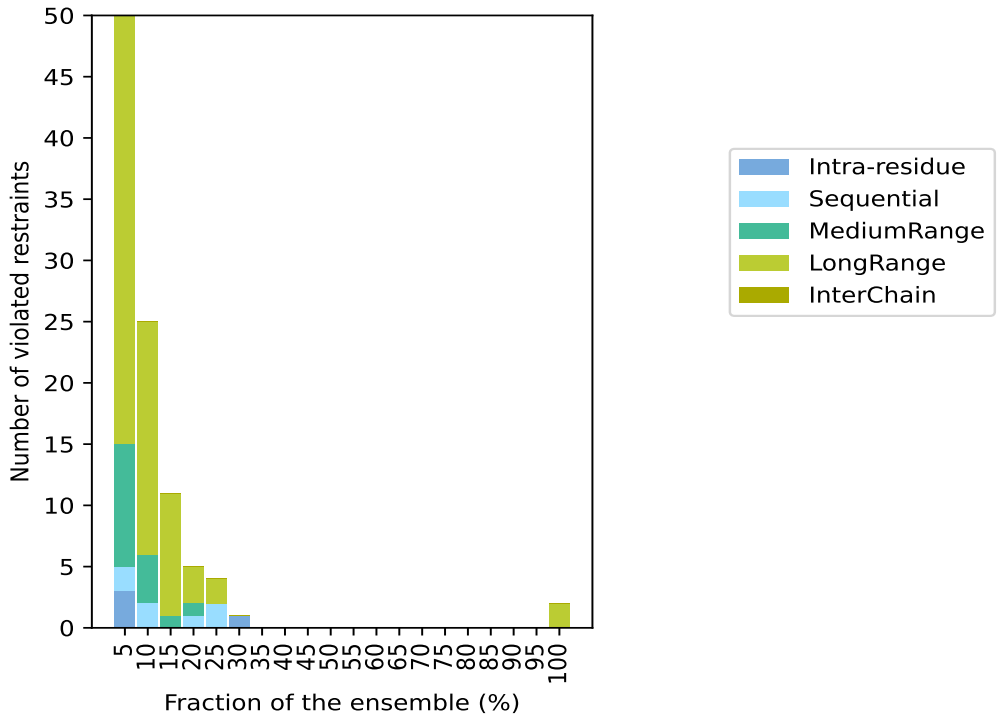
9.3 Distance violation statistics for the ensemble (i)

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, 3421(IR:477, SQ:996, MR:558, LR:1390, 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]	%
3	2	10	35	0	50	1	5.0
0	2	4	19	0	25	2	10.0
0	0	1	10	0	11	3	15.0
0	1	1	3	0	5	4	20.0
0	2	0	2	0	4	5	25.0
1	0	0	0	0	1	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	0	0	0	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

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

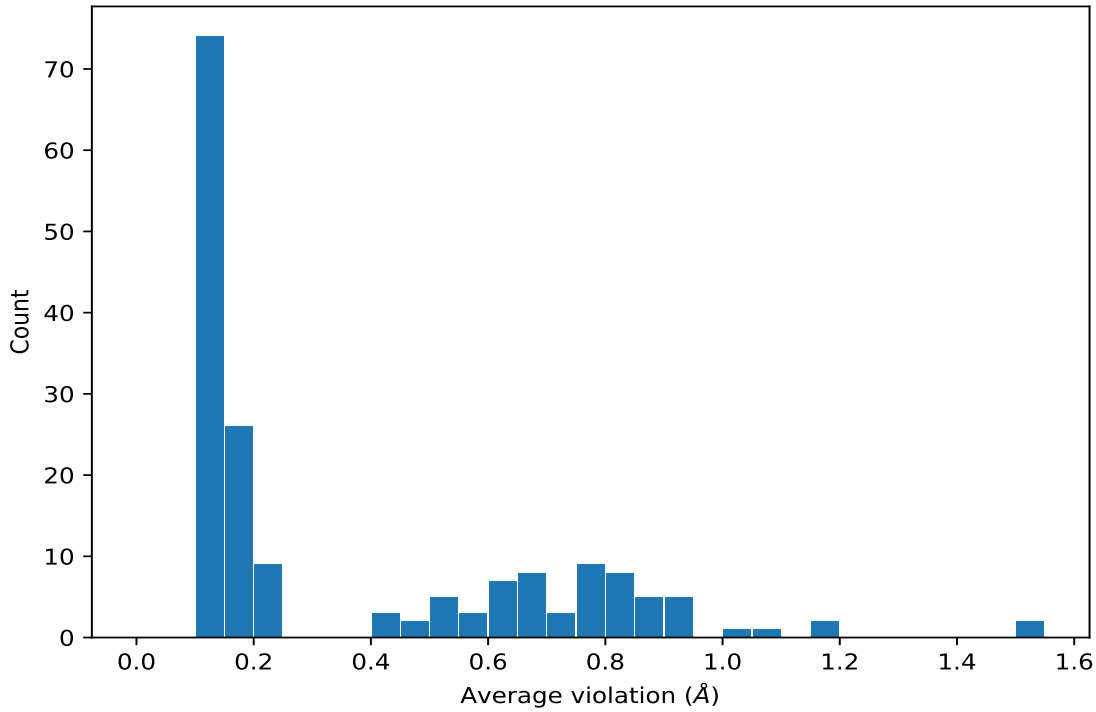
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

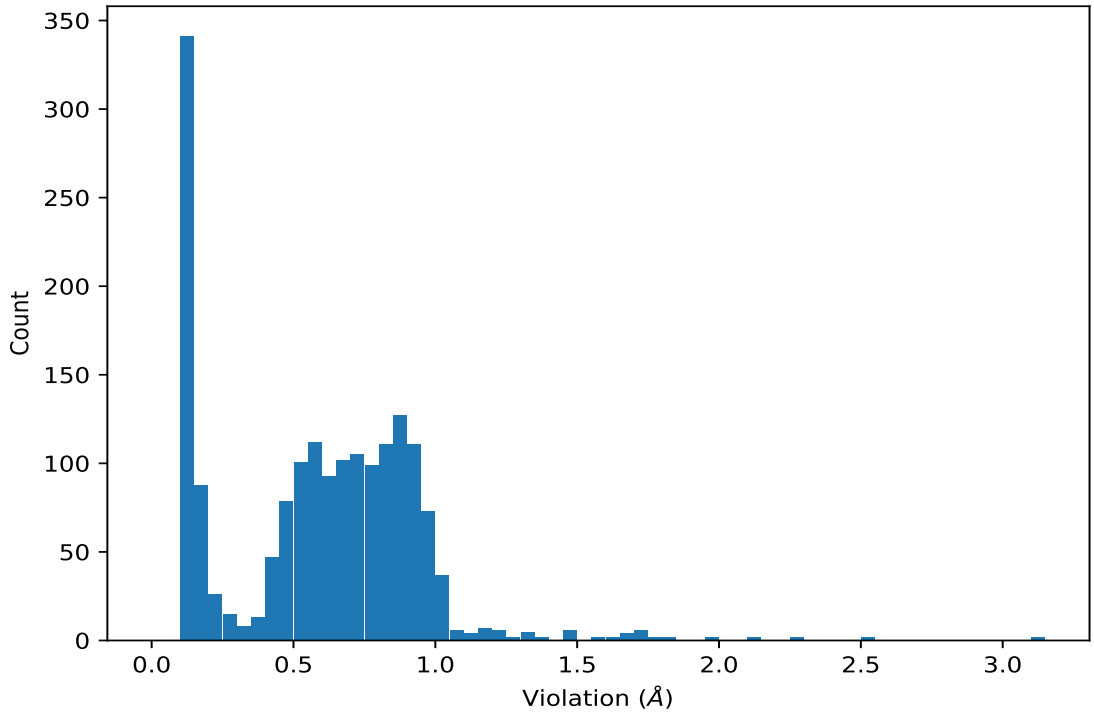
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD2	20	1.5	0.44	1.39
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD3	20	1.5	0.44	1.39
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE2	20	1.2	0.6	1.0
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE3	20	1.2	0.6	1.0
(3,144)	1:A:431:ARG:N	1:A:427:TYR:O	20	1.08	0.22	1.11
(3,173)	1:A:553:LEU:N	1:A:549:LYS:O	20	1.0	0.02	1.0
(3,164)	1:A:514:PHE:N	1:A:510:THR:O	20	0.94	0.03	0.95
(3,180)	1:A:560:ASN:N	1:A:556:LEU:O	20	0.94	0.1	0.98
(3,166)	1:A:516:GLU:N	1:A:512:GLU:O	20	0.94	0.02	0.94
(3,136)	1:A:397:PHE:N	1:A:393:CYS:O	20	0.93	0.04	0.94
(3,162)	1:A:578:CYS:N	1:A:501:HIS:O	20	0.93	0.05	0.94
(3,167)	1:A:517:ILE:N	1:A:513:ASN:O	20	0.89	0.03	0.9

[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)
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE2	18	3.15
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE3	18	3.15
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD2	7	2.5
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD3	7	2.5
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD2	5	2.28
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD3	5	2.28
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD2	16	2.1
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD3	16	2.1
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD2	13	1.99
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD3	13	1.99
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD2	17	1.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD3	17	1.81
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD2	19	1.79
(1,634)	1:A:397:PHE:HD1	1:A:472:LYS:HD3	19	1.79
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE2	13	1.73
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE3	13	1.73
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE2	5	1.72
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE3	5	1.72
(1,635)	1:A:397:PHE:HD1	1:A:472:LYS:HE2	16	1.7

10 Dihedral-angle violation analysis (i)

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