WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB NMR Structure Validation Summary Report (i)

Jun 4, 2023 – 06:33 AM EDT

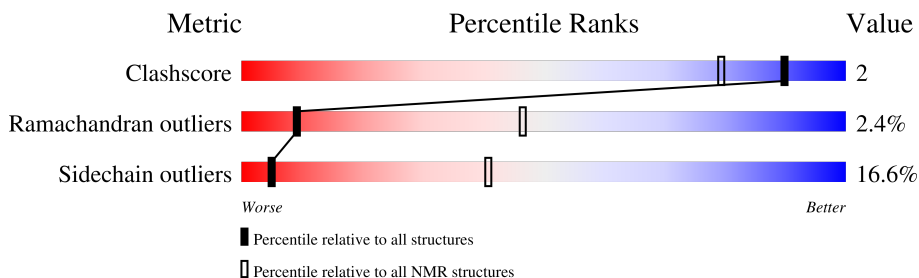|		
PDB ID	:	2L39
BMRB ID	:	17174
Title	:	Mouse prion protein fragment 121-231 AT 37 C
Authors	:	Christen, B.; Damberger, F.F.; Perez, D.R.; Hornemann, S.; Wuthrich, K.
Deposited on	:	2010-09-10

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 84%.

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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		2.4%
Sidechain outliers		16.6%

Worse — *Better*

▮ Percentile relative to all structures
⫾ Percentile relative to all NMR structures

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	114	74% 15% 11%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:125-A:225 (101)	0.51	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1809 atoms, of which 872 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	114	1809	580	872	165	183	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	SEE REMARK 999	UNP Q4FJQ7
A	120	SER	-	SEE REMARK 999	UNP Q4FJQ7

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.

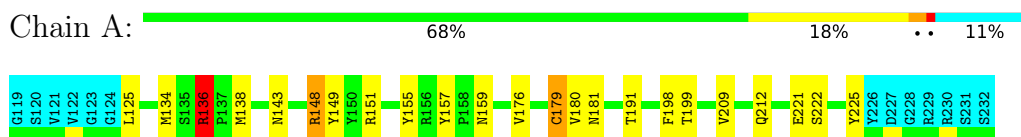• Molecule 1: Major prion protein

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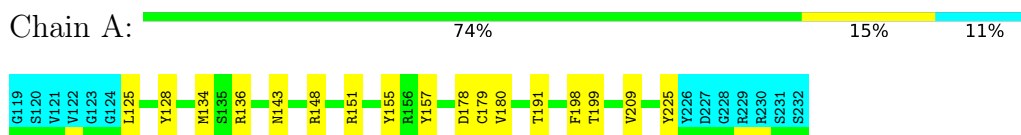
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

• Molecule 1: Major prion protein

Chain A:

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics*.

Of the 120 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	structure solution	1.0.3
OPALp	refinement	1.2

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	1294
Number of shifts mapped to atoms	1294
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	0.68±0.01	0±0/868 (0.0± 0.0%)	1.13±0.03	1±1/1175 (0.1± 0.1%)
All	All	0.68	0/17360 (0.0%)	1.13	29/23500 (0.1%)

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	3.9±1.7
All	All	0	77

There are no bond-length outliers.

5 of 15 unique angle 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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	209	VAL	CA-CB-CG2	12.57	129.76	110.90	2	2
1	A	136	ARG	NE-CZ-NH2	-7.96	116.32	120.30	10	5
1	A	215	VAL	CA-CB-CG1	7.02	121.44	110.90	17	3
1	A	225	TYR	CB-CG-CD2	-7.02	116.79	121.00	8	1
1	A	156	ARG	NE-CZ-NH2	-6.98	116.81	120.30	6	2

There are no chirality outliers.

5 of 17 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	157	TYR	Sidechain	12
1	A	128	TYR	Sidechain	12
1	A	149	TYR	Sidechain	9

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	136	ARG	Sidechain	7
1	A	155	TYR	Sidechain	5

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	847	788	788	3±2
All	All	16940	15760	15760	56

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:180:VAL:HG13	1:A:184:ILE:CD1	0.67	2.19	12	1
1:A:125:LEU:HD11	1:A:186:GLN:CD	0.60	2.17	10	1
1:A:180:VAL:HG13	1:A:184:ILE:HD12	0.56	1.77	12	1
1:A:130:LEU:HD13	1:A:162:TYR:CZ	0.56	2.35	18	1
1:A:176:VAL:HA	1:A:179:CYS:SG	0.55	2.42	3	4

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	101/114 (89%)	88±3 (87±3%)	11±3 (11±3%)	2±1 (2±1%)	9	46
All	All	2020/2280 (89%)	1758 (87%)	213 (11%)	49 (2%)	9	46

5 of 12 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	180	VAL	13
1	A	198	PHE	11
1	A	125	LEU	8
1	A	195	GLY	5
1	A	190	THR	3

6.3.2   Protein sidechains ⓘ

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	94/103 (91%)	78±3 (83±3%)	16±3 (17±3%)	5	41
All	All	1880/2060 (91%)	1567 (83%)	313 (17%)	5	41

5 of 47 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	155	TYR	20
1	A	209	VAL	20
1	A	225	TYR	20
1	A	199	THR	17
1	A	178	ASP	15

6.3.3   RNA ⓘ

There are no RNA molecules in this entry.

6.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5   Carbohydrates ⓘ

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 84% for the well-defined parts and 83% 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	1294
Number of shifts mapped to atoms	1294
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	114	-0.41 ± 0.15	None needed (< 0.5 ppm)
$^{13}C_\beta$	105	0.23 ± 0.15	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	110	0.13 ± 0.12	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 84%, i.e. 1176 atoms were assigned a chemical shift out of a possible 1405. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	397/504 (79%)	198/204 (97%)	101/202 (50%)	98/98 (100%)
Sidechain	673/748 (90%)	454/479 (95%)	197/231 (85%)	22/38 (58%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	106/153 (69%)	66/73 (90%)	39/76 (51%)	1/4 (25%)
Overall	1176/1405 (84%)	718/756 (95%)	337/509 (66%)	121/140 (86%)

### 7.1.4 Statistically unusual chemical shifts ⓘ

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	183	THR	HG1	6.48	0.08 – 2.19	25.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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:
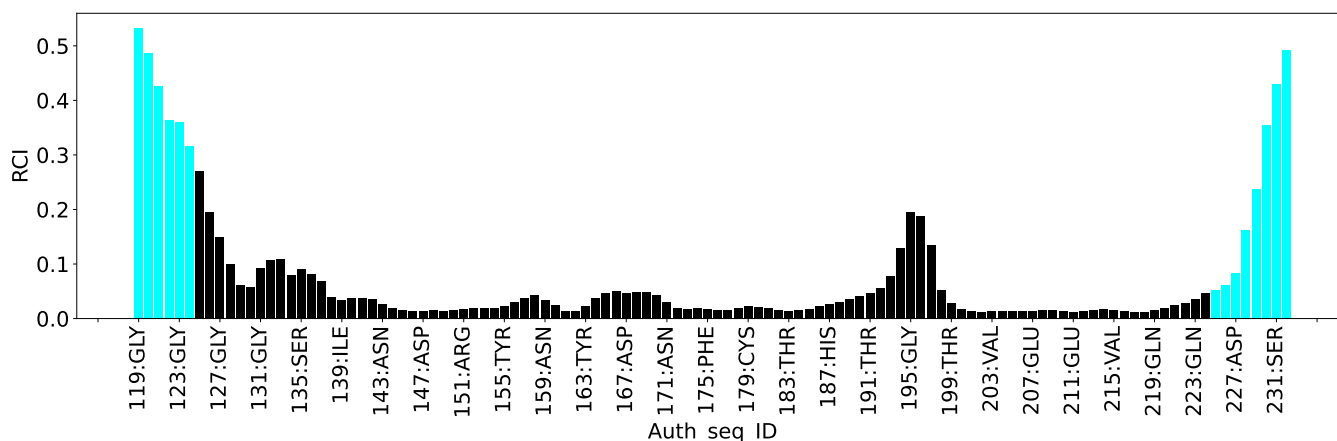
8 NMR restraints analysis ⓘ

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	6338
Intra-residue ($\lvert i-j \rvert$=0)	1134
Sequential ($\lvert i-j \rvert$=1)	1644
Medium range ($\lvert i-j \rvert$>1 and $\lvert i-j \rvert$<5)	1726
Long range ($\lvert i-j \rvert$≥5)	1834
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	55.6
Number of long range restraints per residue[1]	16.1

[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)	73.5	0.2
0.2-0.5 (Medium)	116.9	0.5
>0.5 (Large)	234.6	3.41

8.2.2 Average number of dihedral-angle violations per model ⓘ

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations
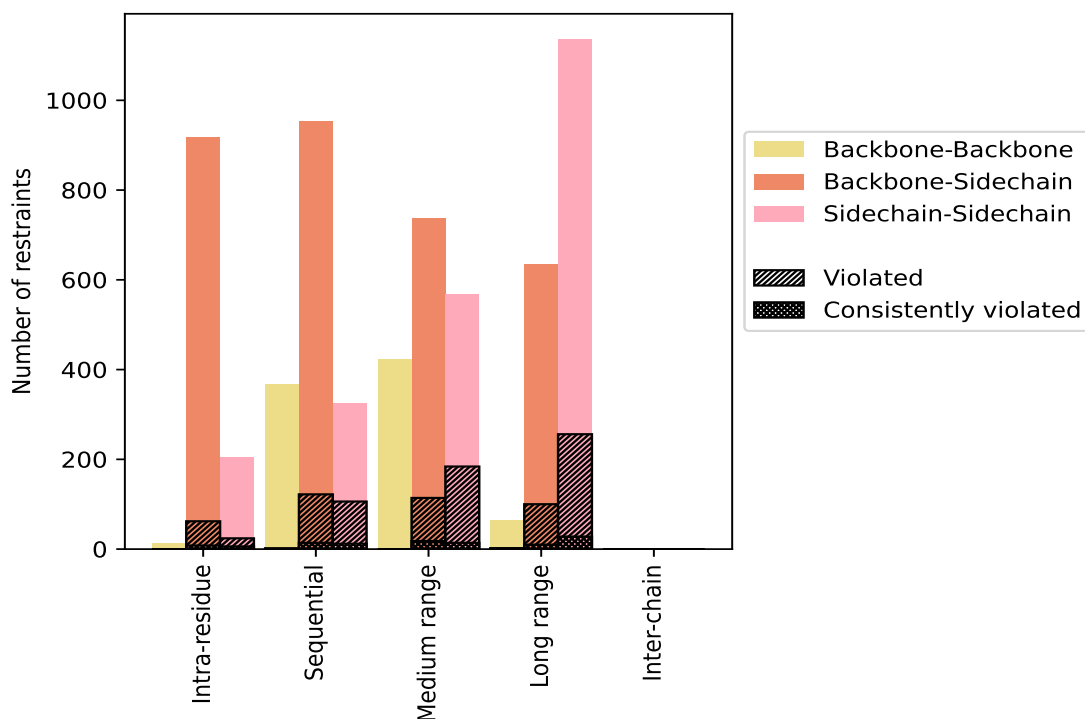
9 Distance violation analysis ⓘ

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)	1134	17.9	86	7.6	1.4	14	1.2	0.2
Backbone-Backbone	12	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	918	14.5	62	6.8	1.0	8	0.9	0.1
Sidechain-Sidechain	204	3.2	24	11.8	0.4	6	2.9	0.1
Sequential (|i-j|=1)	1644	25.9	230	14.0	3.6	26	1.6	0.4
Backbone-Backbone	366	5.8	2	0.5	0.0	0	0.0	0.0
Backbone-Sidechain	954	15.1	122	12.8	1.9	14	1.5	0.2
Sidechain-Sidechain	324	5.1	106	32.7	1.7	12	3.7	0.2
Medium range (|i-j|>1 & |i-j|<5)	1726	27.2	298	17.3	4.7	32	1.9	0.5
Backbone-Backbone	422	6.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	736	11.6	114	15.5	1.8	18	2.4	0.3
Sidechain-Sidechain	568	9.0	184	32.4	2.9	14	2.5	0.2
Long range (|i-j|≥5)	1834	28.9	358	19.5	5.6	40	2.2	0.6
Backbone-Backbone	64	1.0	2	3.1	0.0	2	3.1	0.0
Backbone-Sidechain	634	10.0	100	15.8	1.6	10	1.6	0.2
Sidechain-Sidechain	1136	17.9	256	22.5	4.0	28	2.5	0.4
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	6338	100.0	972	15.3	15.3	112	1.8	1.8
Backbone-Backbone	864	13.6	4	0.5	0.1	2	0.2	0.0
Backbone-Sidechain	3242	51.2	398	12.3	6.3	50	1.5	0.8
Sidechain-Sidechain	2232	35.2	570	25.5	9.0	60	2.7	0.9

[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	34	110	158	170	0	472	0.76	2.26	0.55	0.6
2	36	98	130	110	0	374	0.61	2.36	0.46	0.48
3	36	100	152	150	0	438	0.76	2.55	0.55	0.59
4	40	90	132	136	0	398	0.66	2.31	0.51	0.53
5	36	96	138	166	0	436	0.73	2.83	0.54	0.57
6	36	96	140	172	0	444	0.74	2.83	0.55	0.58
7	40	106	126	126	0	398	0.67	2.21	0.5	0.57
8	34	94	126	142	0	396	0.69	3.22	0.54	0.53
9	40	94	140	174	0	448	0.72	2.62	0.57	0.55
10	52	108	150	142	0	452	0.71	2.41	0.54	0.56
11	36	94	122	88	0	340	0.67	3.25	0.52	0.54

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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	34	92	158	138	0	422	0.73	2.45	0.54	0.57
13	40	104	160	134	0	438	0.68	2.6	0.52	0.53
14	36	116	150	180	0	482	0.74	2.55	0.56	0.58
15	28	112	142	150	0	432	0.69	3.41	0.58	0.52
16	40	98	150	150	0	438	0.73	2.45	0.53	0.58
17	28	96	128	136	0	388	0.67	3.04	0.53	0.52
18	34	118	132	170	0	454	0.74	2.44	0.56	0.62
19	40	100	142	110	0	392	0.72	2.64	0.53	0.54
20	36	102	176	144	0	458	0.71	2.58	0.49	0.61

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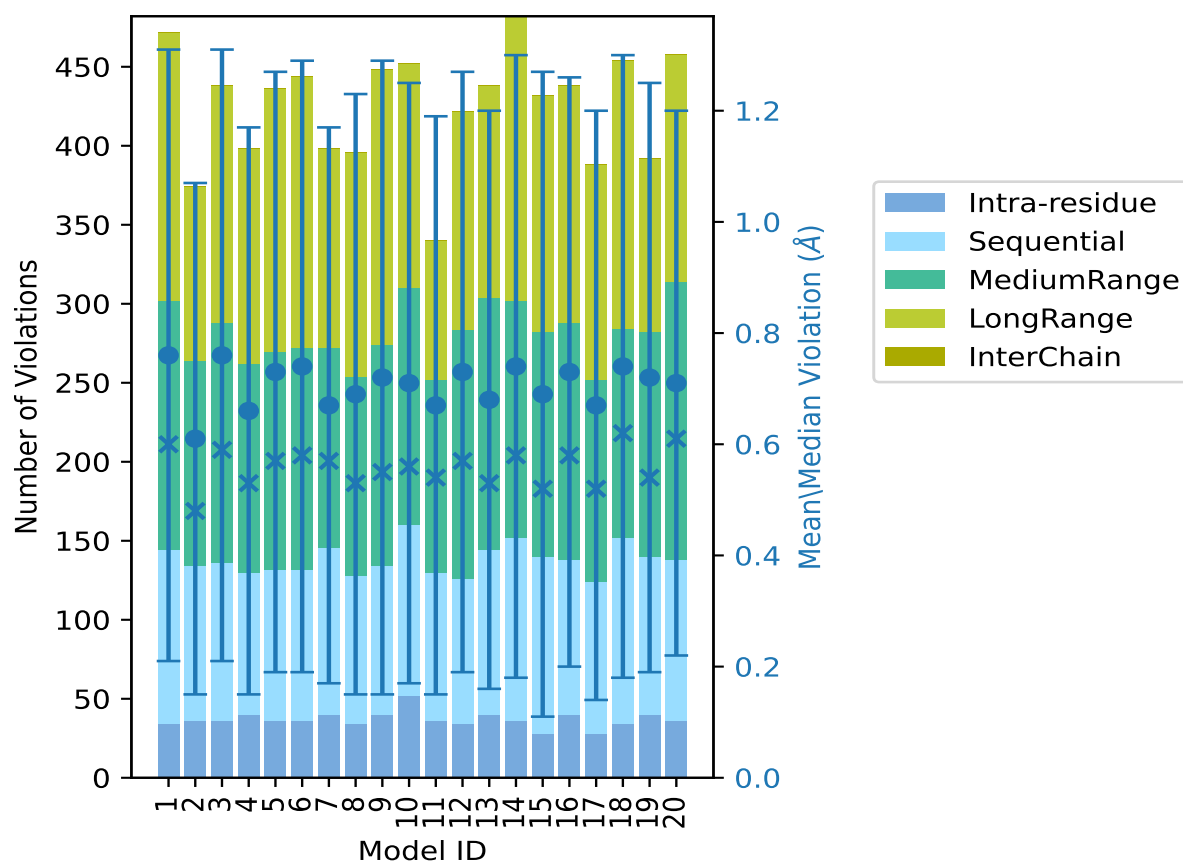
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3 Distance violation statistics for the ensemble ⓘ

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, 5366(IR:1048, SQ:1414, MR:1428, LR:1476, IC:0) restraints are not violated in the ensemble.

\multicolumn{6}{c}{Number of violated restraints}	\multicolumn{2}{c}{Fraction of the ensemble}
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
16	42	42	64	0	164	1	5.0
8	24	26	36	0	94	2	10.0
4	20	32	46	0	102	3	15.0
16	18	20	10	0	64	4	20.0
2	2	8	12	0	24	5	25.0
4	14	10	26	0	54	6	30.0
0	8	8	20	0	36	7	35.0
2	4	10	6	0	22	8	40.0
2	6	8	28	0	44	9	45.0
4	0	6	2	0	12	10	50.0
0	4	6	2	0	12	11	55.0
0	4	0	6	0	10	12	60.0
0	6	2	6	0	14	13	65.0
0	4	10	2	0	16	14	70.0
2	10	18	10	0	40	15	75.0
2	6	6	4	0	18	16	80.0
6	10	12	6	0	34	17	85.0
0	14	26	26	0	66	18	90.0
4	8	16	6	0	34	19	95.0
14	26	32	40	0	112	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 ⓘ
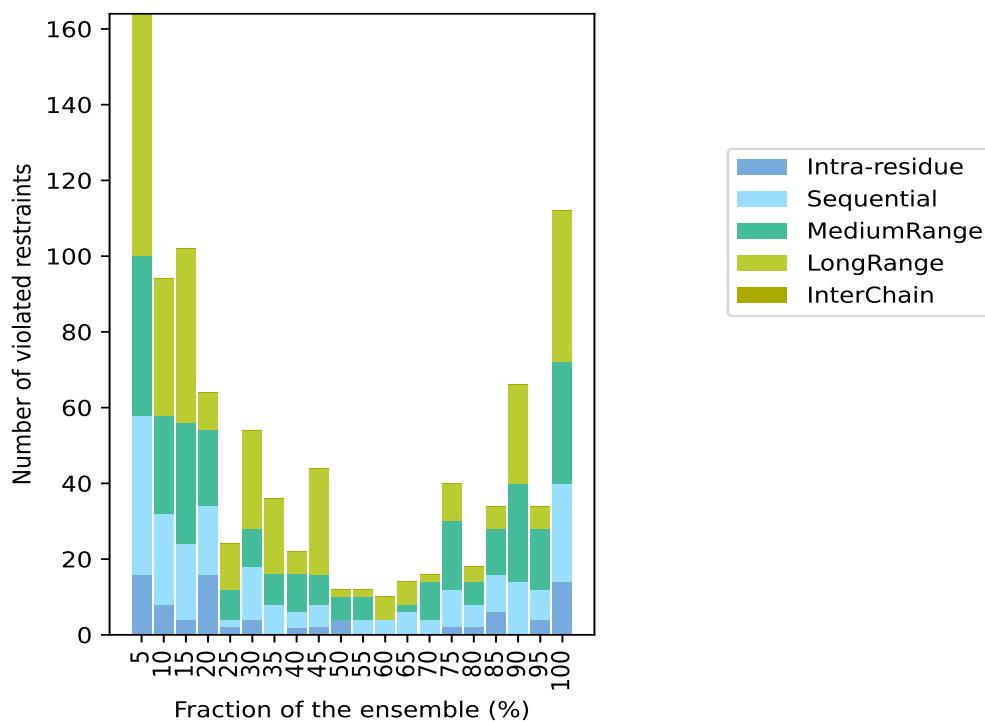
9.4   Most violated distance restraints in the ensemble ⓘ

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
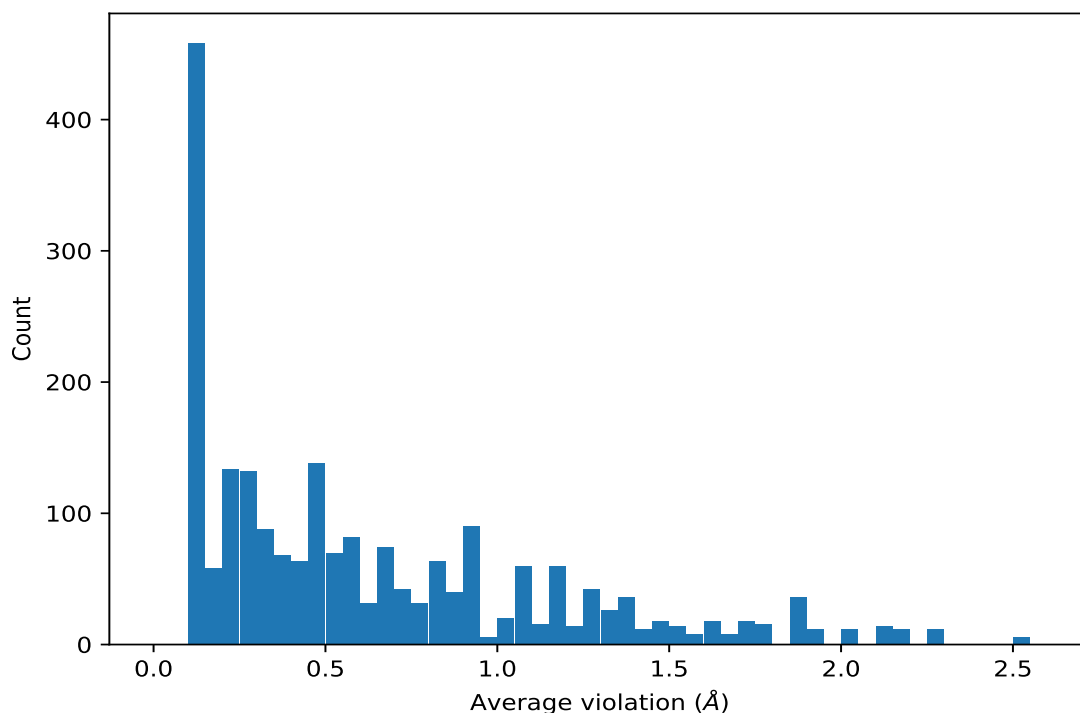
9.4.2   Table: Most violated distance restraints ⓘ

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)
(1,22)	1:A:203:VAL:HG21	1:A:204:LYS:HG2	20	2.11	0.08	2.11
(1,22)	1:A:203:VAL:HG22	1:A:204:LYS:HG2	20	2.11	0.08	2.11
(1,22)	1:A:203:VAL:HG23	1:A:204:LYS:HG2	20	2.11	0.08	2.11
(1,3191)	1:A:203:VAL:HG21	1:A:204:LYS:HG2	20	2.11	0.08	2.11
(1,3191)	1:A:203:VAL:HG22	1:A:204:LYS:HG2	20	2.11	0.08	2.11
(1,3191)	1:A:203:VAL:HG23	1:A:204:LYS:HG2	20	2.11	0.08	2.11
(1,1821)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	20	2.1	0.58	1.87
(1,4990)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	20	2.1	0.58	1.87
(1,2034)	1:A:198:PHE:H	1:A:203:VAL:HG11	20	1.95	0.52	2.2
(1,2034)	1:A:198:PHE:H	1:A:203:VAL:HG12	20	1.95	0.52	2.2
(1,2034)	1:A:198:PHE:H	1:A:203:VAL:HG13	20	1.95	0.52	2.2
(1,5203)	1:A:198:PHE:H	1:A:203:VAL:HG11	20	1.95	0.52	2.2
(1,5203)	1:A:198:PHE:H	1:A:203:VAL:HG12	20	1.95	0.52	2.2
(1,5203)	1:A:198:PHE:H	1:A:203:VAL:HG13	20	1.95	0.52	2.2
(1,381)	1:A:183:THR:HG21	1:A:209:VAL:HG21	20	1.9	0.59	2.1
(1,381)	1:A:183:THR:HG21	1:A:209:VAL:HG22	20	1.9	0.59	2.1

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,381)	1:A:183:THR:HG21	1:A:209:VAL:HG23	20	1.9	0.59	2.1
(1,381)	1:A:183:THR:HG22	1:A:209:VAL:HG21	20	1.9	0.59	2.1
(1,381)	1:A:183:THR:HG22	1:A:209:VAL:HG22	20	1.9	0.59	2.1
(1,381)	1:A:183:THR:HG22	1:A:209:VAL:HG23	20	1.9	0.59	2.1
(1,381)	1:A:183:THR:HG23	1:A:209:VAL:HG21	20	1.9	0.59	2.1
(1,381)	1:A:183:THR:HG23	1:A:209:VAL:HG22	20	1.9	0.59	2.1
(1,381)	1:A:183:THR:HG23	1:A:209:VAL:HG23	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG21	1:A:209:VAL:HG21	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG21	1:A:209:VAL:HG22	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG21	1:A:209:VAL:HG23	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG22	1:A:209:VAL:HG21	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG22	1:A:209:VAL:HG22	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG22	1:A:209:VAL:HG23	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG23	1:A:209:VAL:HG21	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG23	1:A:209:VAL:HG22	20	1.9	0.59	2.1
(1,3550)	1:A:183:THR:HG23	1:A:209:VAL:HG23	20	1.9	0.59	2.1
(1,2945)	1:A:198:PHE:HD1	1:A:203:VAL:HG11	20	1.88	0.11	1.9
(1,2945)	1:A:198:PHE:HD1	1:A:203:VAL:HG12	20	1.88	0.11	1.9
(1,2945)	1:A:198:PHE:HD1	1:A:203:VAL:HG13	20	1.88	0.11	1.9
(1,2945)	1:A:198:PHE:HD2	1:A:203:VAL:HG11	20	1.88	0.11	1.9
(1,2945)	1:A:198:PHE:HD2	1:A:203:VAL:HG12	20	1.88	0.11	1.9
(1,2945)	1:A:198:PHE:HD2	1:A:203:VAL:HG13	20	1.88	0.11	1.9
(1,6114)	1:A:198:PHE:HD1	1:A:203:VAL:HG11	20	1.88	0.11	1.9

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

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
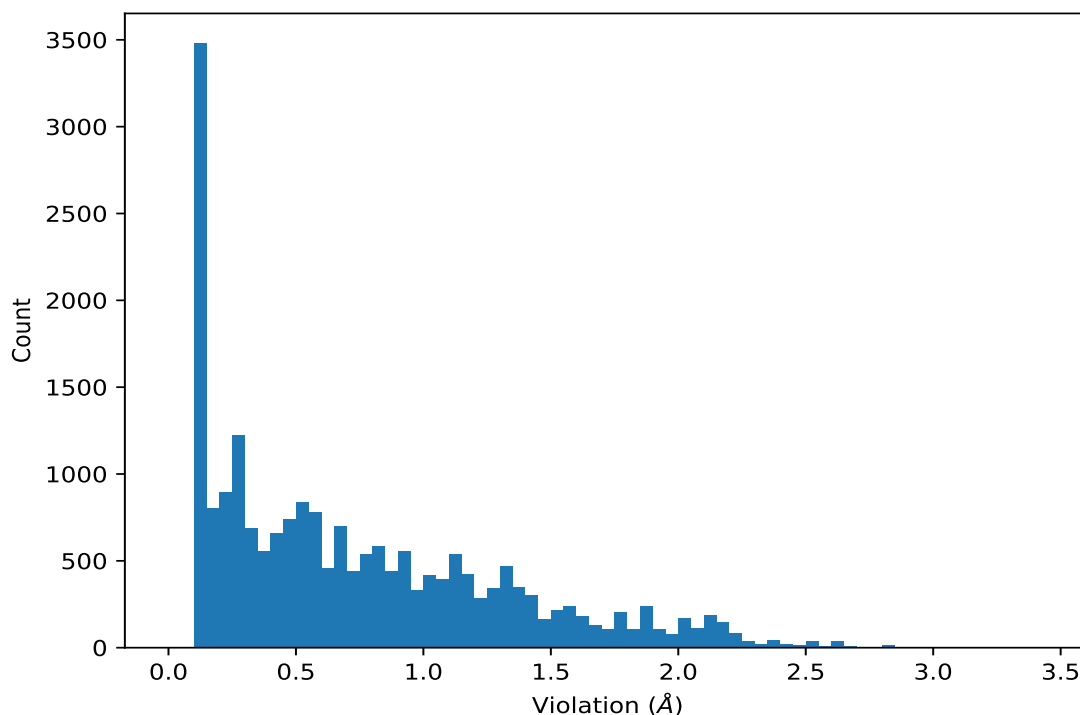
9.5.2 Table : All distance violations ⓘ

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)
(1,4990)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	15	3.41
(1,1821)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	15	3.41
(1,4990)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	11	3.25
(1,1821)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	11	3.25
(1,4990)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	8	3.22
(1,1821)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	8	3.22
(1,4990)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	17	3.04
(1,1821)	1:A:165:PRO:HG3	1:A:168:GLN:HB2	17	3.04
(1,468)	1:A:122:VAL:HG11	1:A:130:LEU:HB2	5	2.83
(1,468)	1:A:122:VAL:HG12	1:A:130:LEU:HB2	5	2.83
(1,468)	1:A:122:VAL:HG13	1:A:130:LEU:HB2	5	2.83
(1,468)	1:A:122:VAL:HG11	1:A:130:LEU:HB2	6	2.83

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found