



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:27 PM UTC

PDB ID : 2K1D / pdb_00002k1d
BMRB ID : 15676
Title : NMR Studies of a Pathogenic Mutant (D178N) of the Human Prion Protein
Authors : Mills, J.L.; Surewicz, K.; Surewicz, W.K.; Sonnichsen, F.D.
Deposited on : 2008-02-29

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

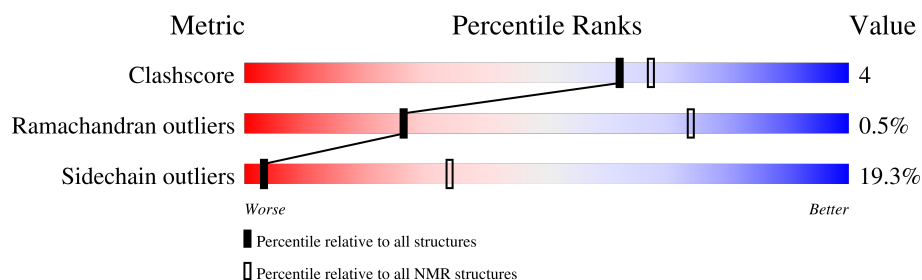
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	146	41% 10% 22% 27%

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: *closest to the average*.

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:133-A:162, A:174-A:218 (75)	0.98	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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1721 atoms, of which 829 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1721	552	829	157	175	8	

There are 6 discrepancies between the modelled and reference sequences:

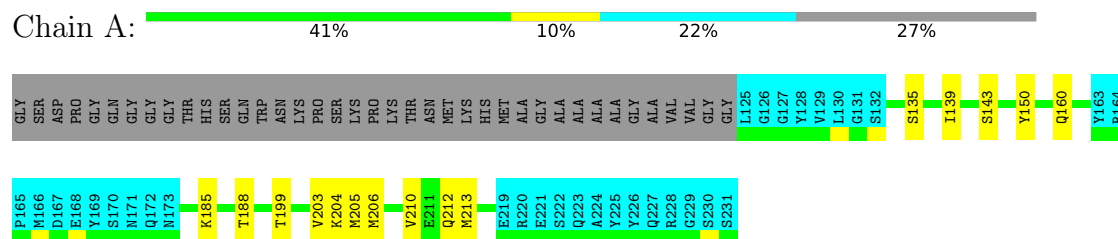
Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLY	-	expression tag	UNP P04156
A	87	SER	-	expression tag	UNP P04156
A	88	ASP	-	expression tag	UNP P04156
A	89	PRO	-	expression tag	UNP P04156
A	129	VAL	MET	variant	UNP P04156
A	178	ASN	ASP	engineered mutation	UNP P04156

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: Major prion protein

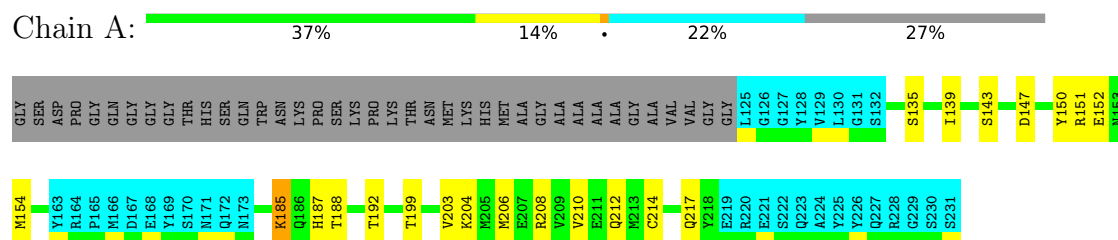


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

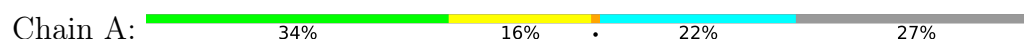
4.2.1 Score per residue for model 1

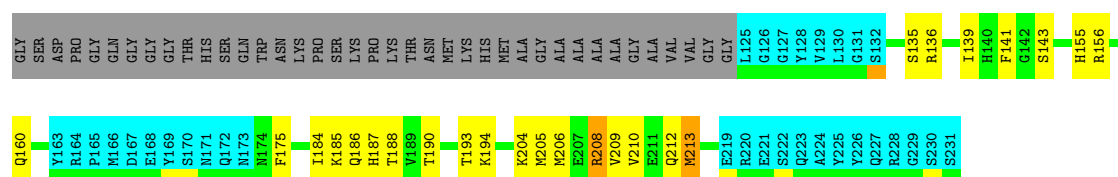
- Molecule 1: Major prion protein



4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein

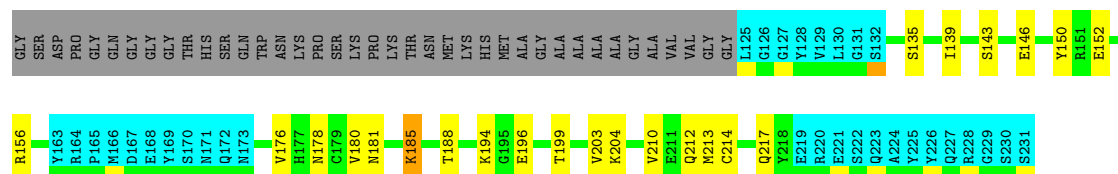




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Major prion protein

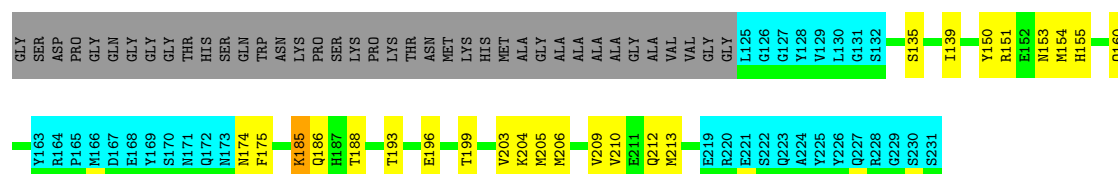
Chain A: 36% 15% • 22% 27%



4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein

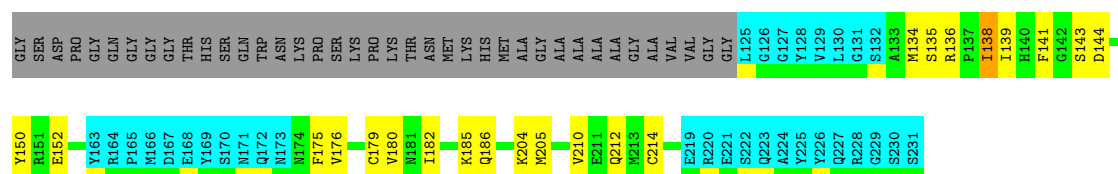
Chain A: 35% 16% • 22% 27%



4.2.5 Score per residue for model 5

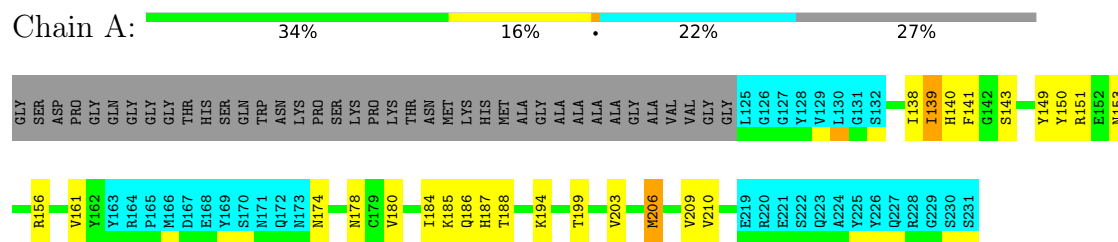
- Molecule 1: Major prion protein

Chain A: 36% 14% • 22% 27%



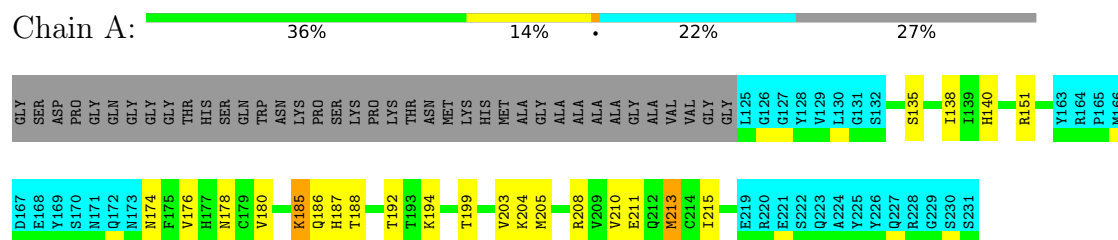
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



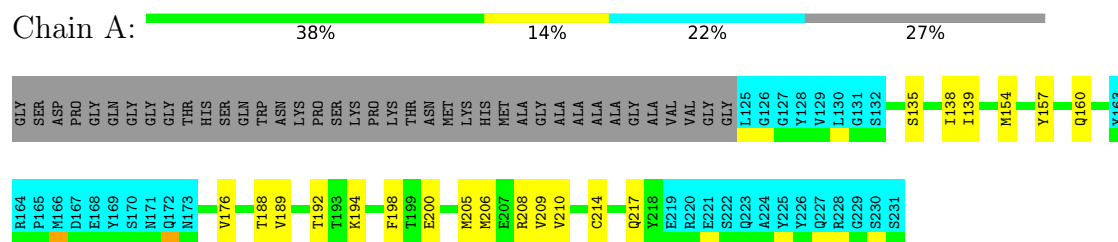
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



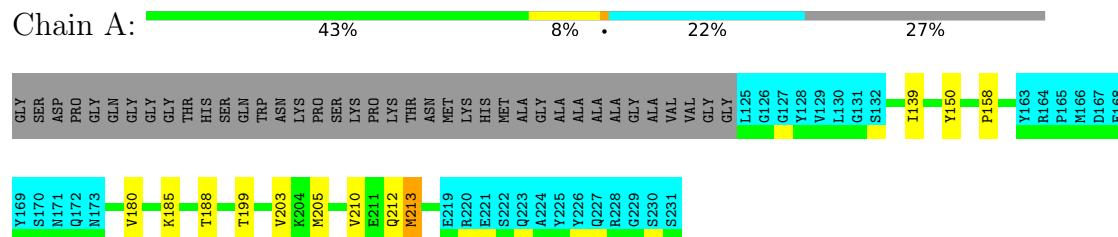
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



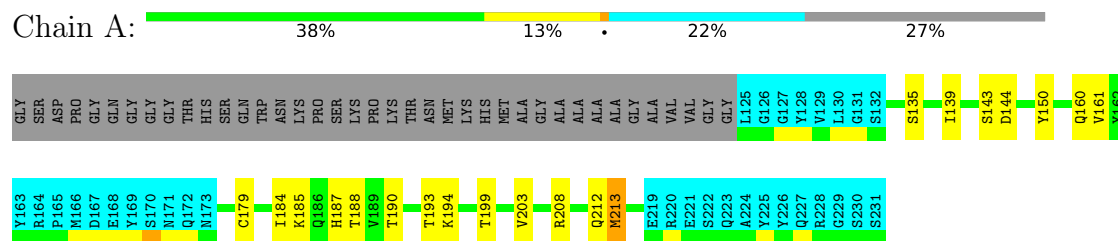
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



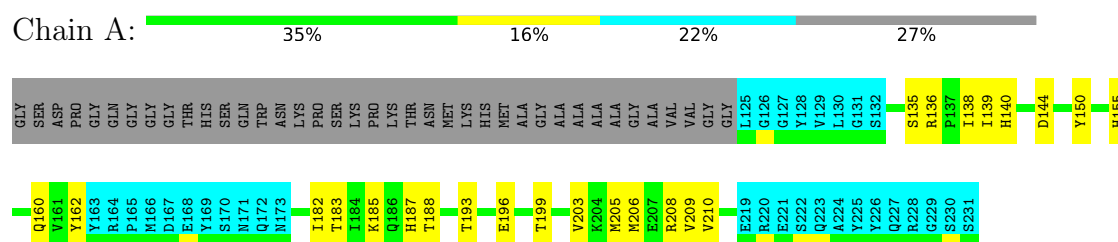
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



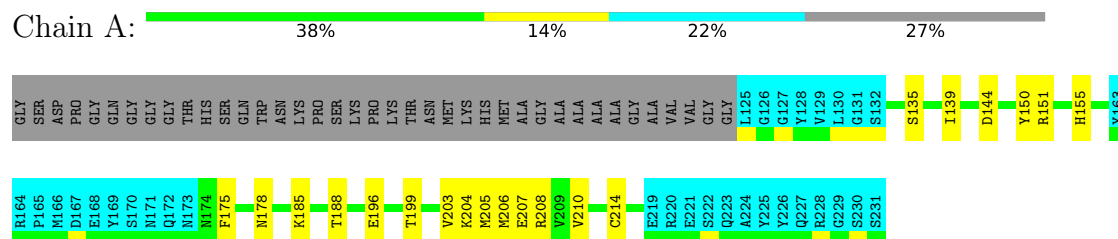
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



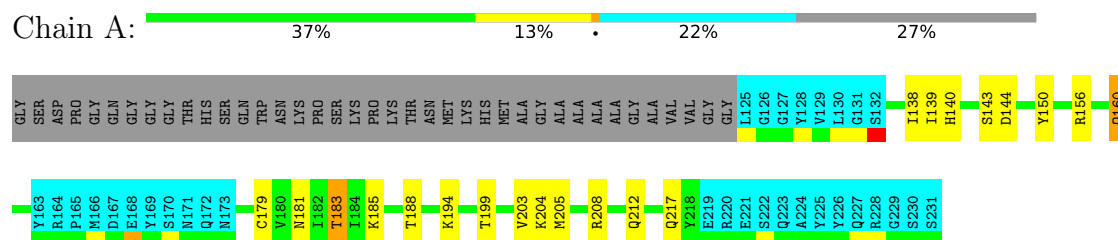
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



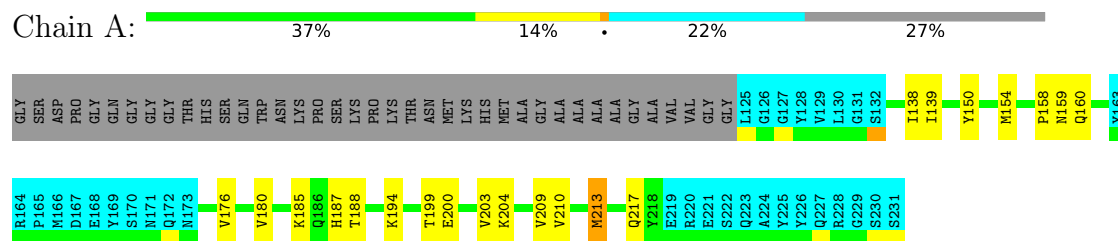
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



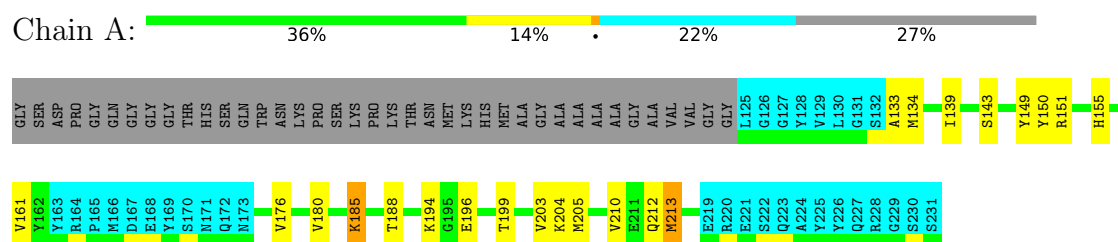
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



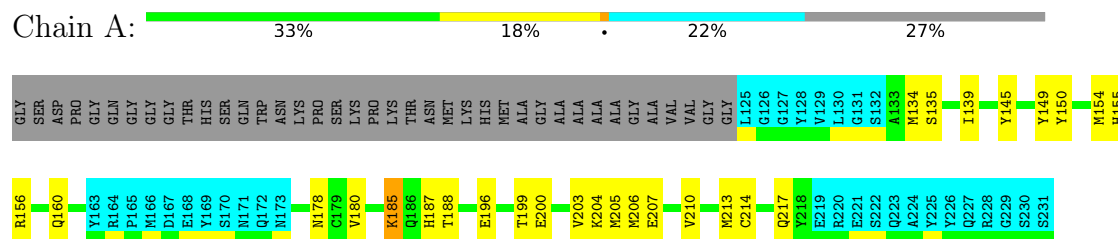
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



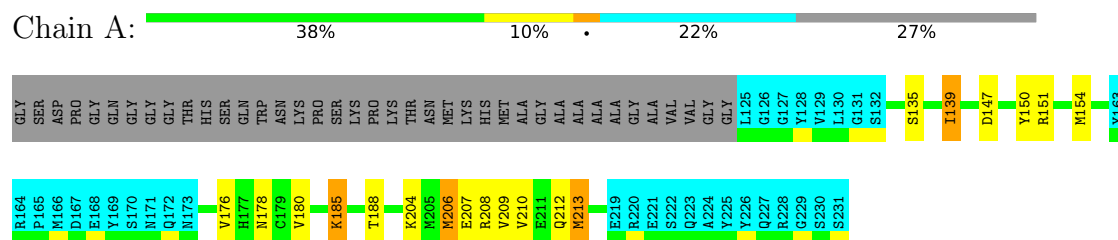
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



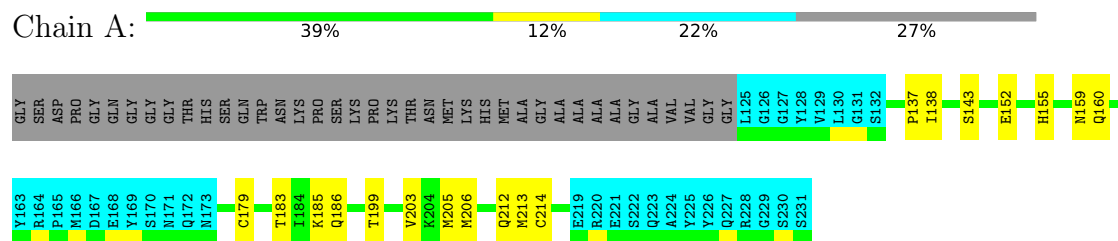
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



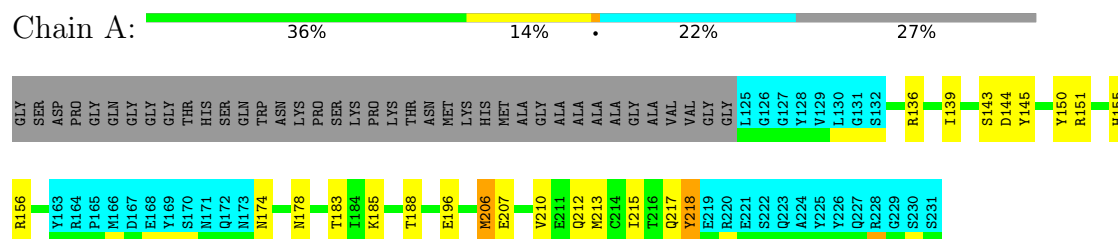
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



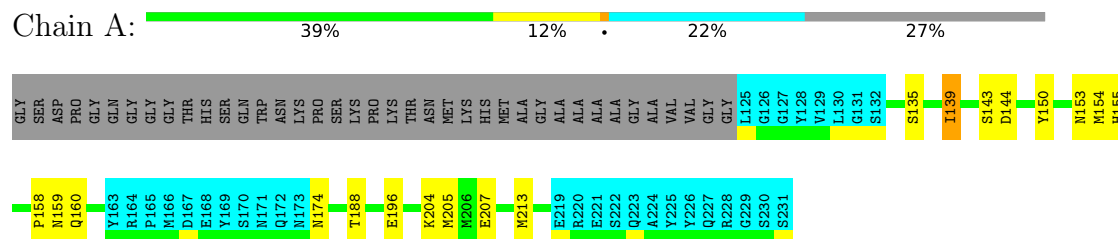
4.2.19 Score per residue for model 19

- Molecule 1: Major prion protein



4.2.20 Score per residue for model 20

- Molecule 1: Major prion protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, TORSION ANGLE DYNAMICS*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	1053
Number of shifts mapped to atoms	1053
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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	632	598	600	5±2
All	All	12640	11960	12000	107

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:ILE:HD12	1:A:209:VAL:HA	0.64	1.68	4	4
1:A:176:VAL:O	1:A:180:VAL:HG23	0.63	1.94	17	4
1:A:139:ILE:HG22	1:A:150:TYR:OH	0.62	1.95	1	15
1:A:206:MET:O	1:A:210:VAL:HG23	0.62	1.94	6	10
1:A:158:PRO:O	1:A:213:MET:HE1	0.61	1.93	14	2
1:A:139:ILE:HD12	1:A:209:VAL:CA	0.61	2.26	2	2
1:A:139:ILE:HG22	1:A:150:TYR:CZ	0.60	2.32	17	8
1:A:138:ILE:HD11	1:A:141:PHE:CZ	0.56	2.35	5	1
1:A:185:LYS:O	1:A:188:THR:HG22	0.56	2.01	19	12
1:A:180:VAL:HG13	1:A:210:VAL:HB	0.55	1.78	7	5
1:A:180:VAL:HG13	1:A:210:VAL:CG1	0.55	2.32	14	4
1:A:184:ILE:HD11	1:A:210:VAL:HG21	0.55	1.78	2	1
1:A:139:ILE:HD13	1:A:209:VAL:HA	0.55	1.78	6	3
1:A:176:VAL:HG13	1:A:214:CYS:SG	0.53	2.43	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:199:THR:O	1:A:203:VAL:HG12	0.50	2.07	12	14
1:A:210:VAL:HA	1:A:213:MET:HE2	0.50	1.83	17	4
1:A:161:VAL:HG13	1:A:213:MET:HG2	0.49	1.82	10	1
1:A:184:ILE:O	1:A:188:THR:HG23	0.48	2.09	10	2
1:A:211:GLU:O	1:A:215:ILE:HD12	0.48	2.08	7	1
1:A:137:PRO:HB2	1:A:138:ILE:HD12	0.47	1.86	18	1
1:A:179:CYS:HA	1:A:182:ILE:HD12	0.46	1.87	5	1
1:A:158:PRO:HB2	1:A:213:MET:HE1	0.46	1.88	20	1
1:A:190:THR:O	1:A:193:THR:HG22	0.46	2.11	2	2
1:A:139:ILE:HG22	1:A:150:TYR:CE1	0.45	2.46	6	1
1:A:162:TYR:CD2	1:A:182:ILE:HG22	0.43	2.48	11	1
1:A:189:VAL:O	1:A:192:THR:HG22	0.42	2.13	8	1
1:A:161:VAL:HG11	1:A:213:MET:HB3	0.42	1.91	15	1
1:A:180:VAL:HG13	1:A:210:VAL:CB	0.42	2.44	6	1
1:A:134:MET:HE2	1:A:213:MET:SD	0.42	2.54	16	1
1:A:139:ILE:HD11	1:A:208:ARG:HD2	0.42	1.90	2	1
1:A:198:PHE:CZ	1:A:206:MET:HE1	0.40	2.51	8	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	75/146 (51%)	69±3 (92±3%)	5±1 (6±2%)	0±0 (0±1%)	26	74
All	All	1486/2920 (51%)	1384 (93%)	95 (6%)	7 (0%)	26	74

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	138	ILE	4
1	A	133	ALA	1
1	A	143	SER	1
1	A	218	TYR	1

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	72/123 (59%)	56±9 (78±12%)	13±3 (19±4%)	3	35
All	All	1389/2460 (56%)	1121 (81%)	268 (19%)	3	34

All 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	135	SER	13
1	A	185	LYS	13
1	A	204	LYS	13
1	A	205	MET	13
1	A	212	GLN	12
1	A	213	MET	11
1	A	143	SER	10
1	A	160	GLN	10
1	A	208	ARG	9
1	A	155	HIS	9
1	A	194	LYS	9
1	A	151	ARG	8
1	A	187	HIS	8
1	A	196	GLU	8
1	A	154	MET	7
1	A	217	GLN	7
1	A	178	ASN	7
1	A	144	ASP	7
1	A	214	CYS	6
1	A	156	ARG	6
1	A	186	GLN	6
1	A	174	ASN	5
1	A	207	GLU	5
1	A	152	GLU	4
1	A	136	ARG	4
1	A	175	PHE	4
1	A	188	THR	4
1	A	140	HIS	4
1	A	206	MET	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	183	THR	4
1	A	153	ASN	3
1	A	138	ILE	3
1	A	139	ILE	3
1	A	149	TYR	3
1	A	200	GLU	3
1	A	179	CYS	3
1	A	159	ASN	3
1	A	147	ASP	2
1	A	192	THR	2
1	A	141	PHE	2
1	A	181	ASN	2
1	A	193	THR	2
1	A	134	MET	2
1	A	145	TYR	2
1	A	146	GLU	1
1	A	157	TYR	1
1	A	218	TYR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 71% 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	1053
Number of shifts mapped to atoms	1053
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	98	-0.22 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	87	0.15 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	94	0.24 ± 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 76%, i.e. 804 atoms were assigned a chemical shift out of a possible 1062. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	287/373 (77%)	140/150 (93%)	75/150 (50%)	72/73 (99%)
Sidechain	477/577 (83%)	317/371 (85%)	145/178 (81%)	15/28 (54%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	40/112 (36%)	26/55 (47%)	14/53 (26%)	0/4 (0%)
Overall	804/1062 (76%)	483/576 (84%)	234/381 (61%)	87/105 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1053 atoms were assigned a chemical shift out of a possible 1481. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	378/535 (71%)	186/217 (86%)	98/214 (46%)	94/104 (90%)
Sidechain	605/789 (77%)	403/505 (80%)	179/242 (74%)	23/42 (55%)
Aromatic	70/157 (45%)	46/75 (61%)	24/78 (31%)	0/4 (0%)
Overall	1053/1481 (71%)	635/797 (80%)	301/534 (56%)	117/150 (78%)

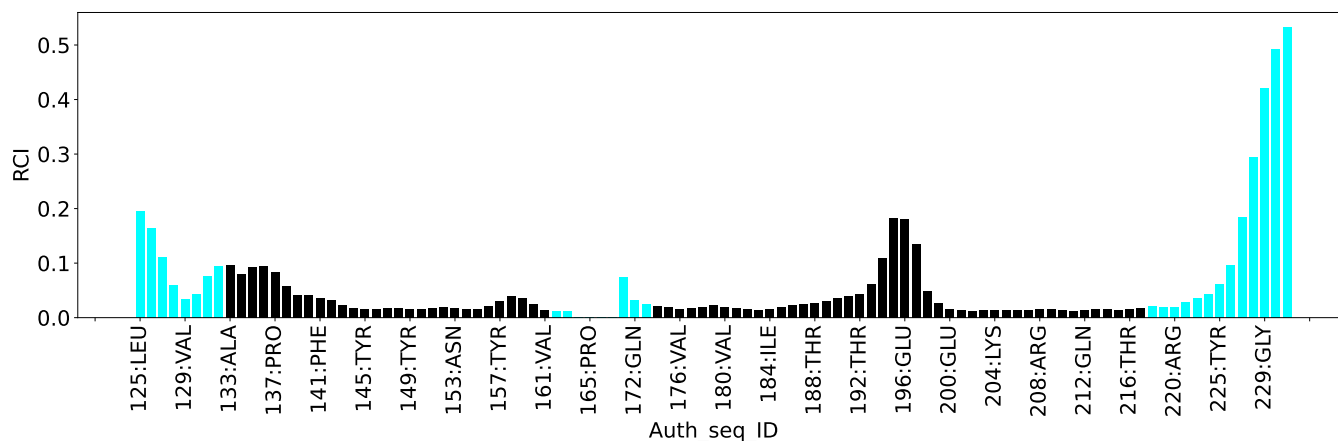
7.1.4 Statistically unusual chemical shifts [i](#)

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	806
Intra-residue ($ i-j =0$)	308
Sequential ($ i-j =1$)	256
Medium range ($ i-j >1$ and $ i-j <5$)	120
Long range ($ i-j \geq 5$)	122
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	5.5
Number of long range restraints per residue ¹	0.8

¹Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.3	0.17
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

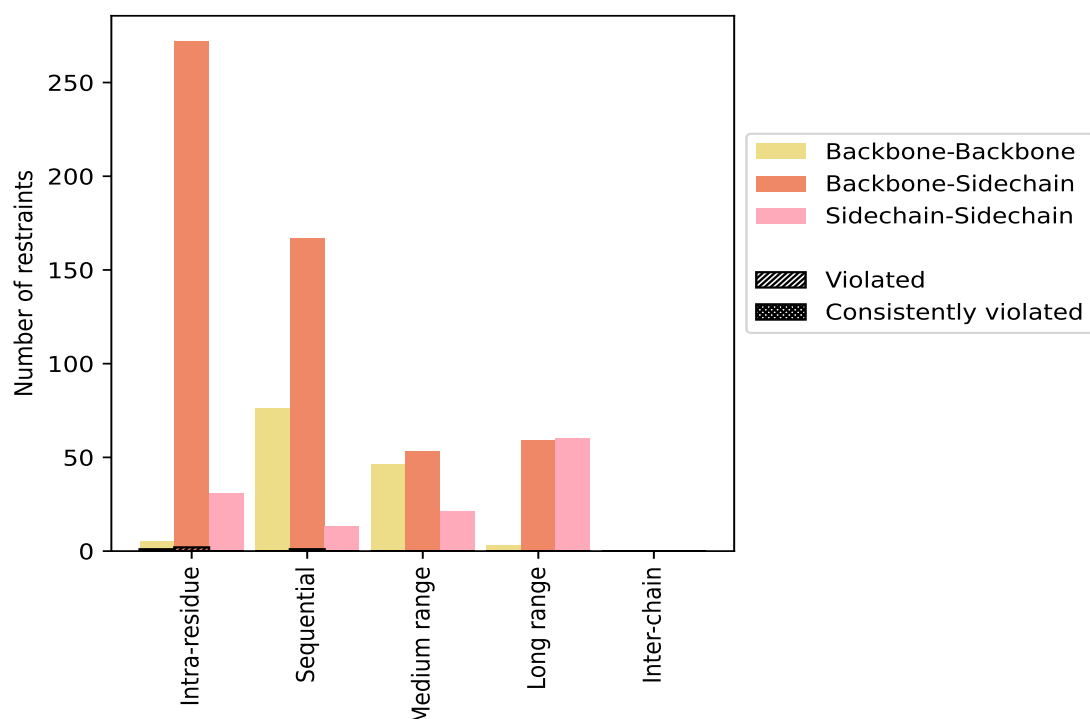
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	308	38.2	3	1.0	0.4	0	0.0	0.0
Backbone-Backbone	5	0.6	1	20.0	0.1	0	0.0	0.0
Backbone-Sidechain	272	33.7	2	0.7	0.2	0	0.0	0.0
Sidechain-Sidechain	31	3.8	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	256	31.8	1	0.4	0.1	0	0.0	0.0
Backbone-Backbone	76	9.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	167	20.7	1	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	13	1.6	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	120	14.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	46	5.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	53	6.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	21	2.6	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	122	15.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	3	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	59	7.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	60	7.4	0	0.0	0.0	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	806	100.0	4	0.5	0.5	0	0.0	0.0
Backbone-Backbone	130	16.1	1	0.8	0.1	0	0.0	0.0
Backbone-Sidechain	551	68.4	3	0.5	0.4	0	0.0	0.0
Sidechain-Sidechain	125	15.5	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	1	0	0	0	0	1	0.11	0.11	0.0	0.11
8	1	0	0	0	0	1	0.11	0.11	0.0	0.11
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

Continued on next page...

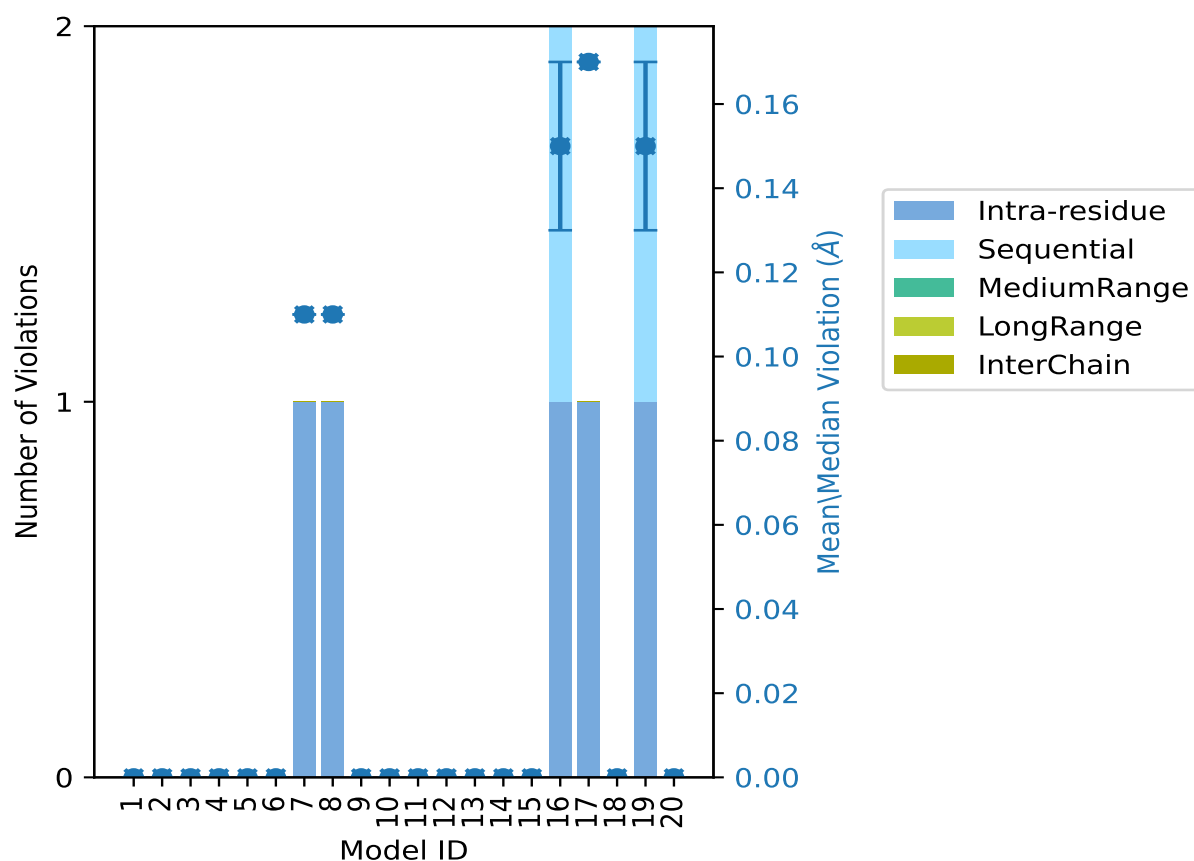
Continued from previous page...

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				
11	0	0	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	1	1	0	0	0	2	0.15	0.17	0.02	0.15
17	1	0	0	0	0	1	0.17	0.17	0.0	0.17
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	1	1	0	0	0	2	0.15	0.17	0.02	0.15
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

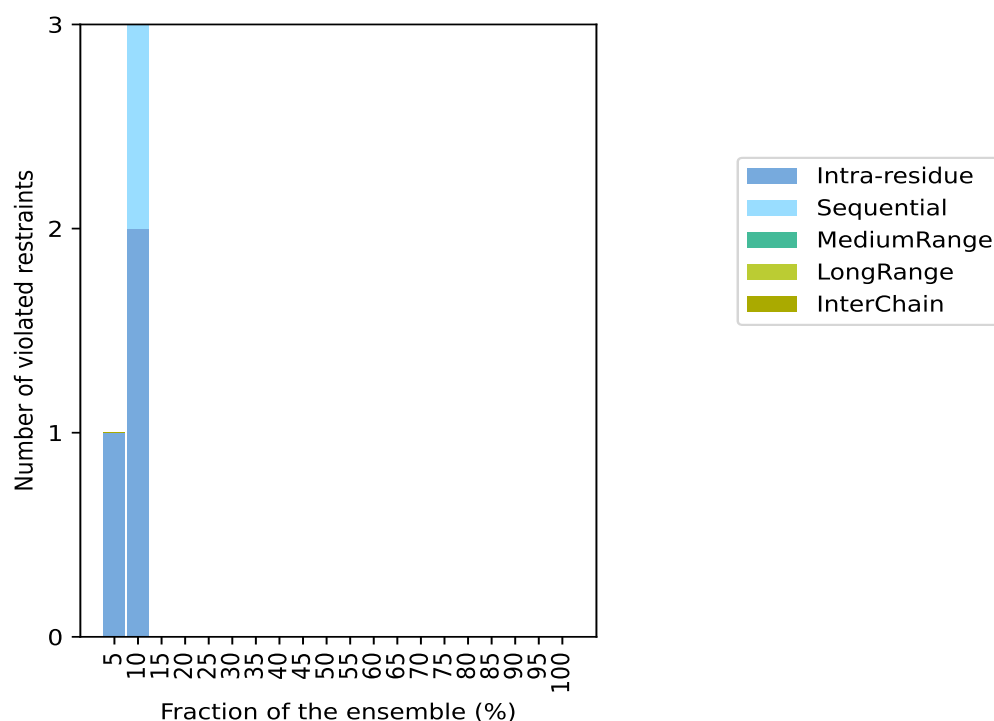
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 802(IR:305, SQ:255, MR:120, LR:122, IC:0) restraints are 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	%
1	0	0	0	0	1	1	5.0
2	1	0	0	0	3	2	10.0
0	0	0	0	0	0	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	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	0	0	0	20	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

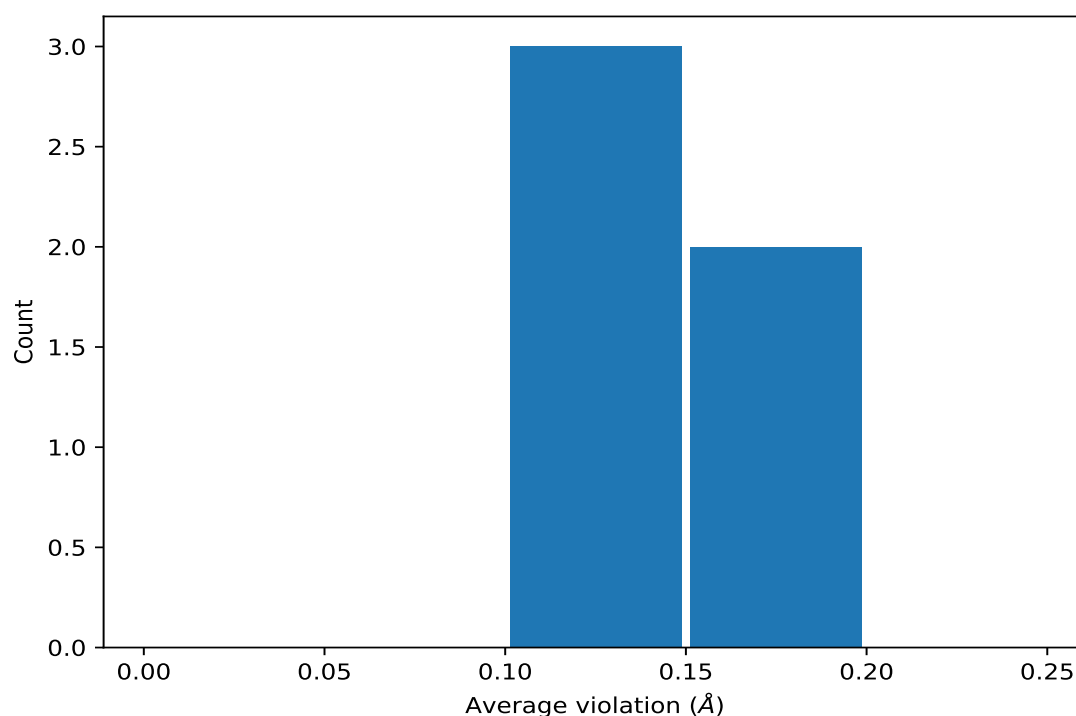
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violation for each restraint sorted by number of violated models and the mean 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.

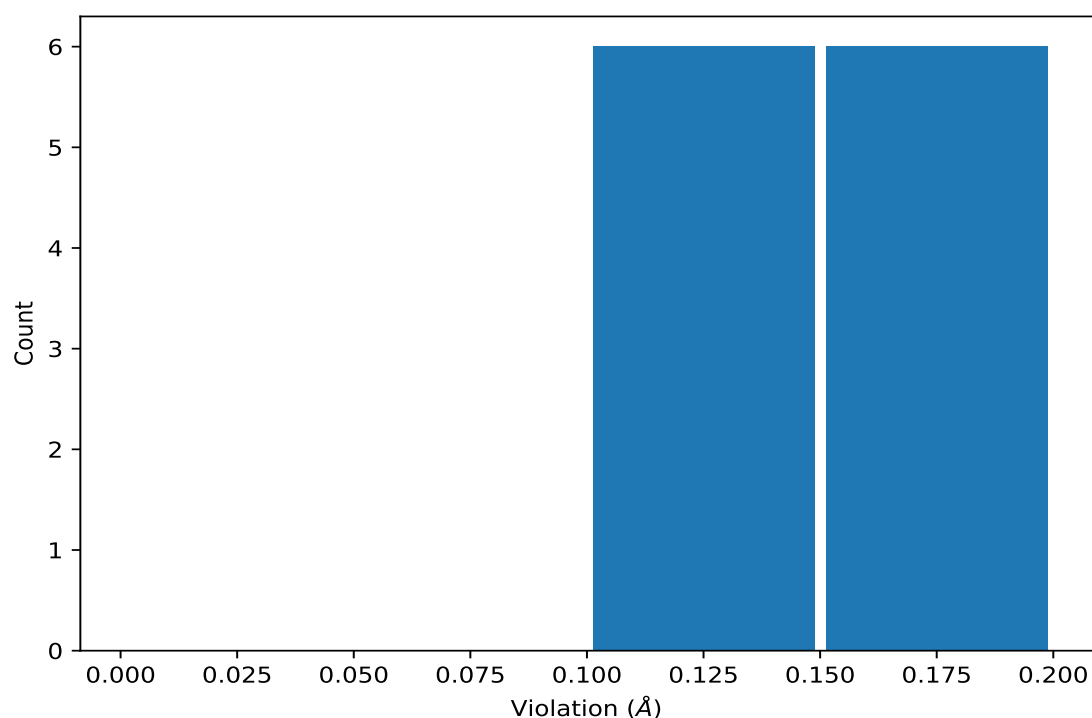
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,418)	1:145:A:TYR:HD1	1:146:A:GLU:H	2	0.17	0.0	0.17
(1,418)	1:145:A:TYR:HD2	1:146:A:GLU:H	2	0.17	0.0	0.17
(1,289)	1:145:A:TYR:H	1:145:A:TYR:HE1	2	0.13	0.0	0.13
(1,289)	1:145:A:TYR:H	1:145:A:TYR:HE2	2	0.13	0.0	0.13
(1,345)	1:132:A:SER:H	1:132:A:SER:HA	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

9.5.1 Histogram : Distribution of distance violations [i](#)

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



9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its 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)
(1,418)	1:145:A:TYR:HD1	1:146:A:GLU:H	16	0.17
(1,418)	1:145:A:TYR:HD2	1:146:A:GLU:H	16	0.17
(1,418)	1:145:A:TYR:HD1	1:146:A:GLU:H	19	0.17
(1,418)	1:145:A:TYR:HD2	1:146:A:GLU:H	19	0.17
(1,296)	1:128:A:TYR:H	1:128:A:TYR:HB2	17	0.17
(1,296)	1:128:A:TYR:H	1:128:A:TYR:HB3	17	0.17
(1,289)	1:145:A:TYR:H	1:145:A:TYR:HE1	16	0.13
(1,289)	1:145:A:TYR:H	1:145:A:TYR:HE2	16	0.13
(1,289)	1:145:A:TYR:H	1:145:A:TYR:HE1	19	0.13
(1,289)	1:145:A:TYR:H	1:145:A:TYR:HE2	19	0.13
(1,345)	1:132:A:SER:H	1:132:A:SER:HA	7	0.11
(1,345)	1:132:A:SER:H	1:132:A:SER:HA	8	0.11

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found