



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1E1U  
Title : Human prion protein variant R220K  
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Deposited on : 2000-05-11

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

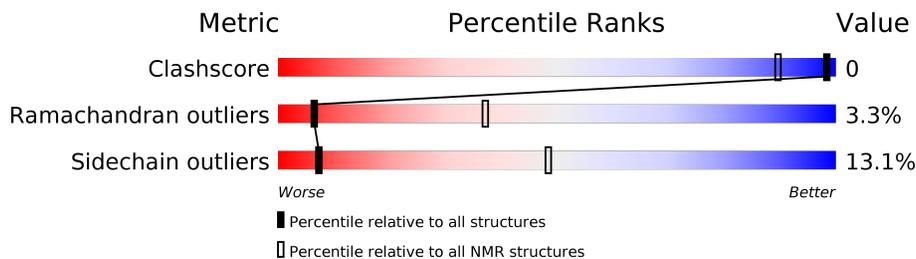
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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  $\geq 3$ , 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	104	

## 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 7 as representative.

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:128-A:219 (92)	0.54	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 5 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1689 atoms, of which 814 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRION PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	104	1689	544	814	151	171	9	0

There is a discrepancy between the modelled and reference sequences:

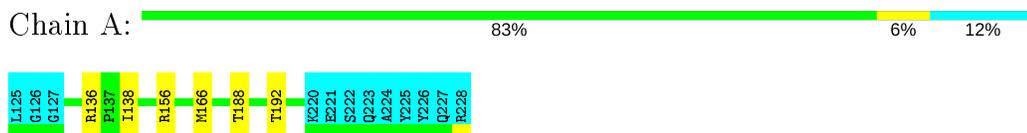
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	LYS	ARG	engineered mutation	UNP P78446

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: PRION PROTEIN

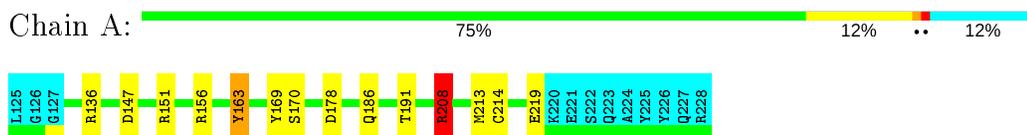


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: PRION PROTEIN



#### 4.2.2 Score per residue for model 2

- Molecule 1: PRION PROTEIN



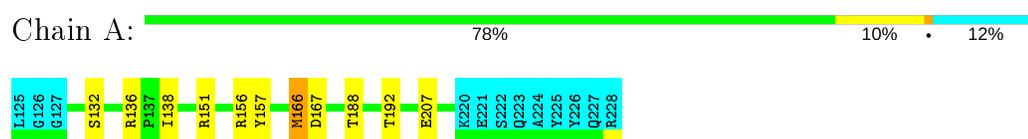
### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: PRION PROTEIN



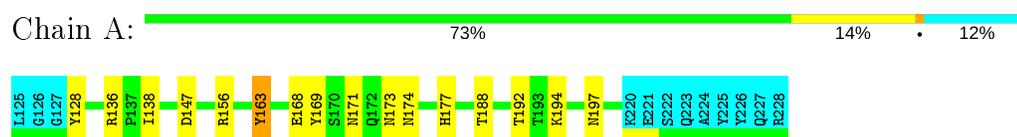
### 4.2.4 Score per residue for model 4

- Molecule 1: PRION PROTEIN



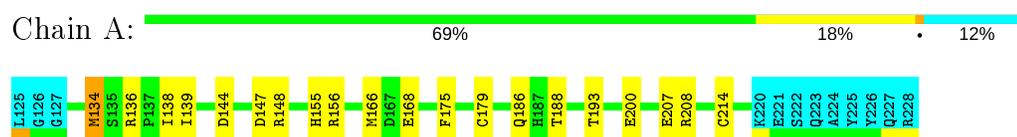
### 4.2.5 Score per residue for model 5

- Molecule 1: PRION PROTEIN



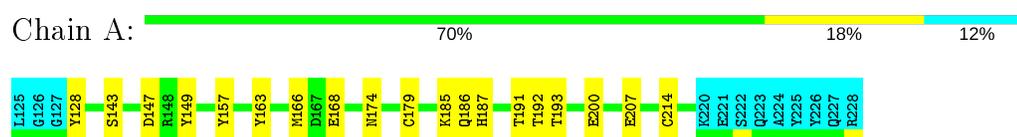
### 4.2.6 Score per residue for model 6

- Molecule 1: PRION PROTEIN



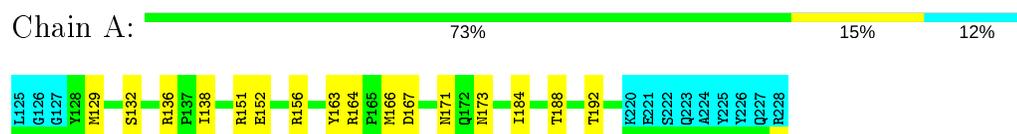
### 4.2.7 Score per residue for model 7

- Molecule 1: PRION PROTEIN



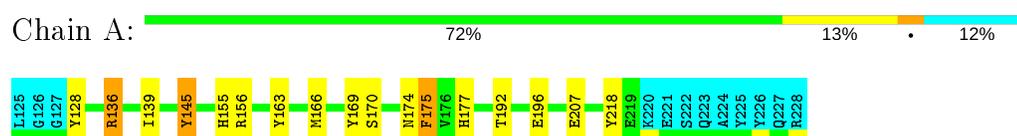
### 4.2.8 Score per residue for model 8

- Molecule 1: PRION PROTEIN



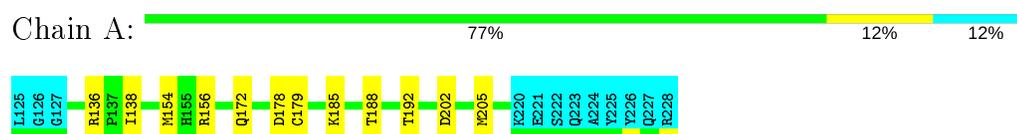
### 4.2.9 Score per residue for model 9

- Molecule 1: PRION PROTEIN



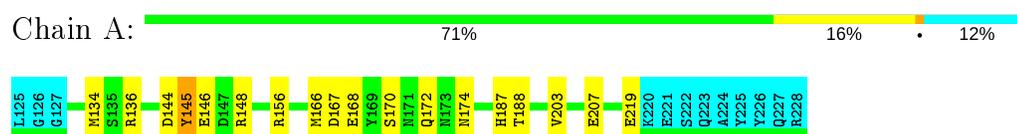
### 4.2.10 Score per residue for model 10

- Molecule 1: PRION PROTEIN



### 4.2.11 Score per residue for model 11

- Molecule 1: PRION PROTEIN



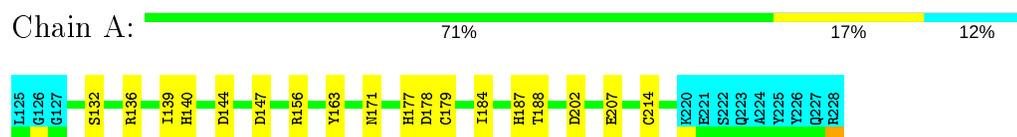
### 4.2.12 Score per residue for model 12

- Molecule 1: PRION PROTEIN



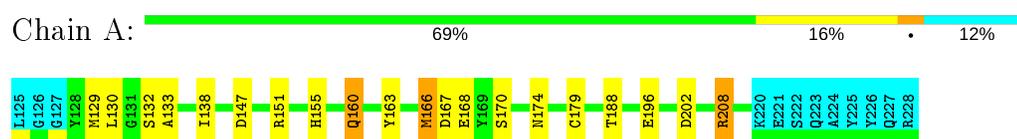
### 4.2.13 Score per residue for model 13

- Molecule 1: PRION PROTEIN



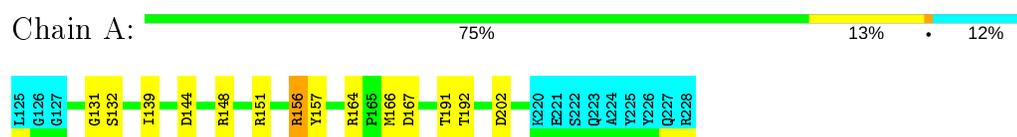
### 4.2.14 Score per residue for model 14

- Molecule 1: PRION PROTEIN



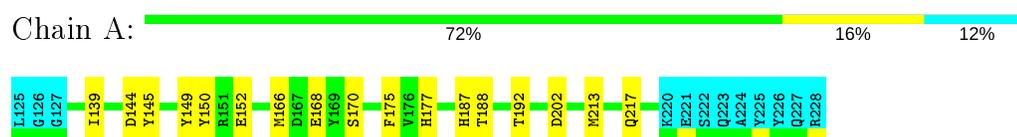
### 4.2.15 Score per residue for model 15

- Molecule 1: PRION PROTEIN



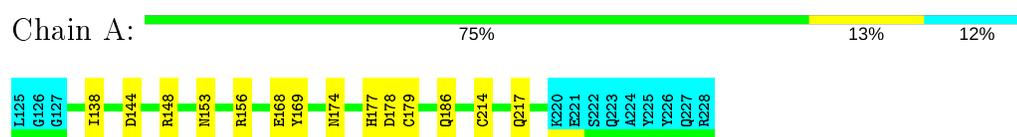
### 4.2.16 Score per residue for model 16

- Molecule 1: PRION PROTEIN



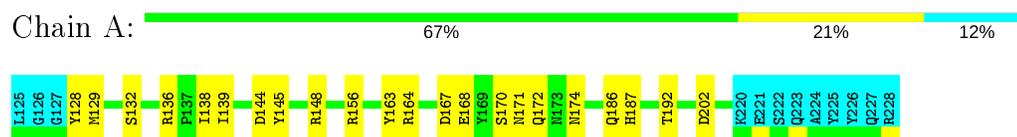
### 4.2.17 Score per residue for model 17

- Molecule 1: PRION PROTEIN



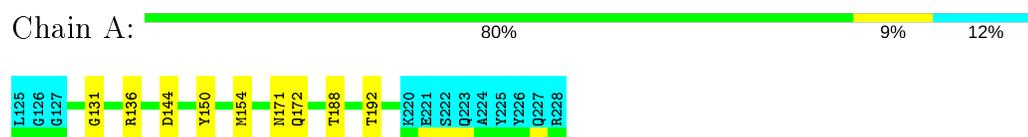
### 4.2.18 Score per residue for model 18

- Molecule 1: PRION PROTEIN



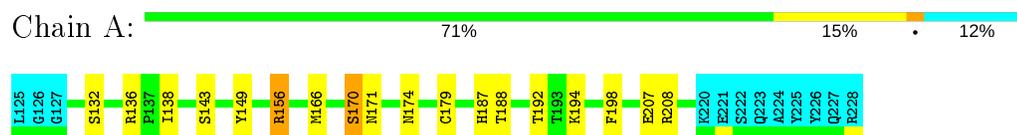
### 4.2.19 Score per residue for model 19

- Molecule 1: PRION PROTEIN



### 4.2.20 Score per residue for model 20

- Molecule 1: PRION PROTEIN



## 5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
OPALP	refinement	
DYANA	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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	777	721	721	0±1
All	All	15540	14420	14420	6

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:PHE:CD2	1:A:218:TYR:CE1	0.50	2.99	9	1
1:A:175:PHE:CD2	1:A:218:TYR:CD1	0.49	3.00	9	1
1:A:145:TYR:CE2	1:A:146:GLU:HG3	0.42	2.50	11	1
1:A:161:VAL:CG1	1:A:213:MET:SD	0.41	3.08	3	1
1:A:145:TYR:CE1	1:A:146:GLU:HG3	0.41	2.50	12	1
1:A:133:ALA:HA	1:A:160:GLN:CG	0.40	2.47	14	1

## 5.2 Torsion angles [i](#)

### 5.2.1 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	92/104 (88%)	81±2 (88±2%)	8±2 (9±2%)	3±1 (3±1%)	6	37
All	All	1840/2080 (88%)	1612 (88%)	168 (9%)	60 (3%)	6	37

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	138	ILE	11
1	A	139	ILE	6
1	A	170	SER	6
1	A	166	MET	5
1	A	167	ASP	5
1	A	168	GLU	4
1	A	169	TYR	3
1	A	198	PHE	3
1	A	172	GLN	3
1	A	136	ARG	2
1	A	132	SER	2
1	A	128	TYR	2
1	A	219	GLU	2
1	A	171	ASN	2
1	A	156	ARG	1
1	A	134	MET	1
1	A	140	HIS	1
1	A	131	GLY	1

### 5.2.2 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	88/97 (91%)	76±3 (87±3%)	12±3 (13±3%)	7	48
All	All	1760/1940 (91%)	1529 (87%)	231 (13%)	7	48

All 52 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	156	ARG	16
1	A	188	THR	14
1	A	192	THR	13
1	A	144	ASP	9
1	A	187	HIS	9
1	A	174	ASN	8
1	A	136	ARG	8
1	A	179	CYS	8
1	A	207	GLU	8
1	A	166	MET	8
1	A	202	ASP	8
1	A	177	HIS	7
1	A	214	CYS	7
1	A	163	TYR	6
1	A	186	GLN	6
1	A	147	ASP	6
1	A	132	SER	6
1	A	178	ASP	5
1	A	171	ASN	5
1	A	175	PHE	5
1	A	155	HIS	4
1	A	168	GLU	4
1	A	185	LYS	4
1	A	191	THR	4
1	A	217	GLN	3
1	A	151	ARG	3
1	A	208	ARG	3
1	A	194	LYS	3
1	A	173	ASN	3
1	A	129	MET	3
1	A	143	SER	3
1	A	152	GLU	2
1	A	170	SER	2
1	A	169	TYR	2
1	A	184	ILE	2
1	A	172	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	154	MET	2
1	A	213	MET	2
1	A	196	GLU	2
1	A	200	GLU	2
1	A	164	ARG	2
1	A	193	THR	2
1	A	160	GLN	1
1	A	204	LYS	1
1	A	140	HIS	1
1	A	134	MET	1
1	A	205	MET	1
1	A	145	TYR	1
1	A	130	LEU	1
1	A	149	TYR	1
1	A	197	ASN	1
1	A	148	ARG	1

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.6 Other polymers [i](#)

There are no such molecules in this entry.

## 5.7 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Chemical shift validation

No chemical shift data were provided