Full wwPDB NMR Structure Validation Report

Feb 23, 2022 – 12:35 PM EST

PDB ID	:	1XYU
Title	:	Solution structure of the sheep prion protein with polymorphism H168
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Deposited on	:	2004-11-11

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

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

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

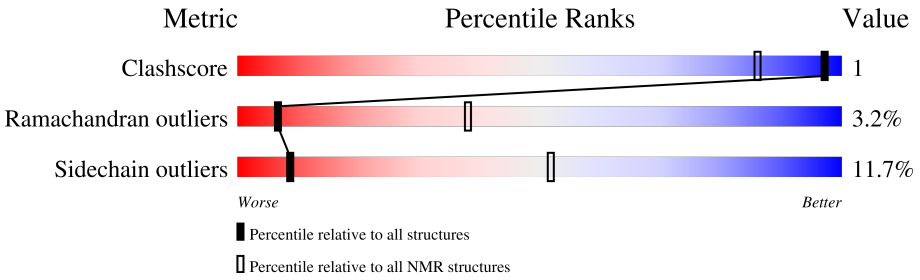
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 >=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	111	71% 11% 18%

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:128-A:189, A:198-A:226 (91)	0.35	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 3 clusters and 8 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1777 atoms, of which 859 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	111	1777	572	859	162	177	7	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	HIS	ARG	SEE REMARK 999	UNP P23907

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

Chain A: 

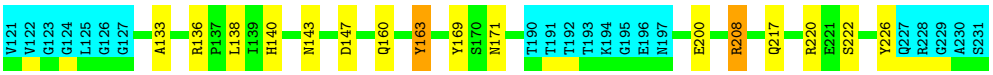
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Major prion protein

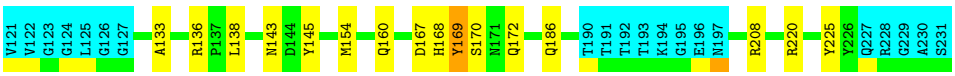
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Major prion protein

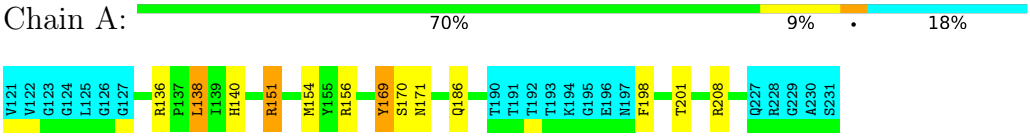
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: Major prion protein

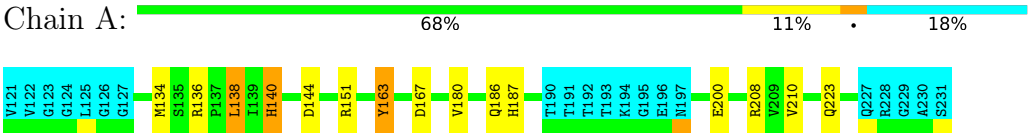
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Major prion protein

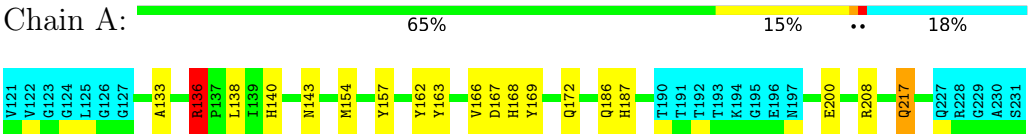
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Major prion protein

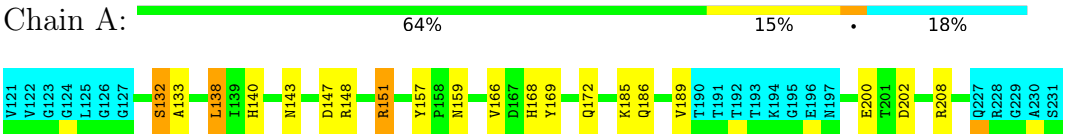
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Major prion protein

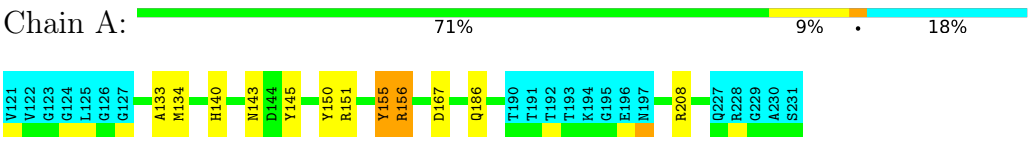
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Major prion protein

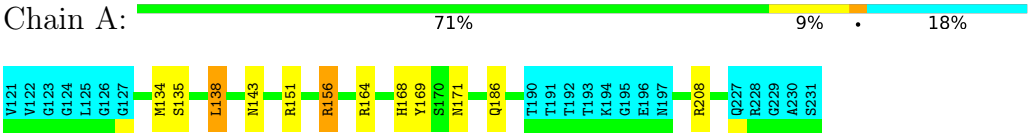
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Major prion protein

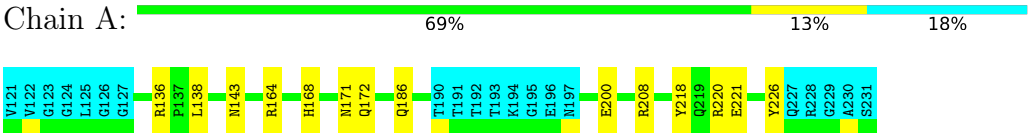
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Major prion protein

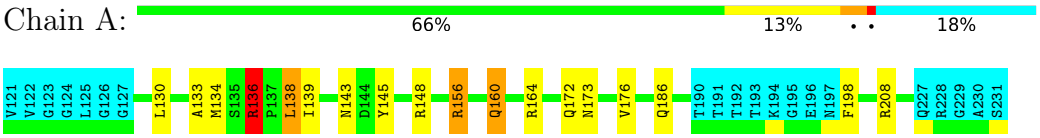
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Major prion protein

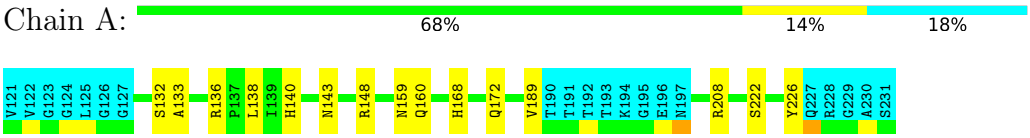
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Major prion protein

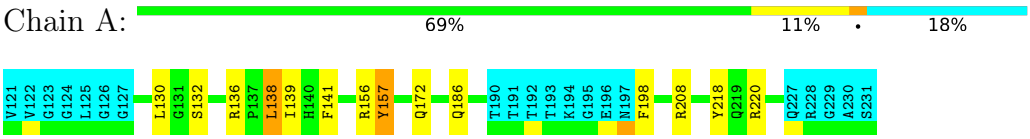
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Major prion protein

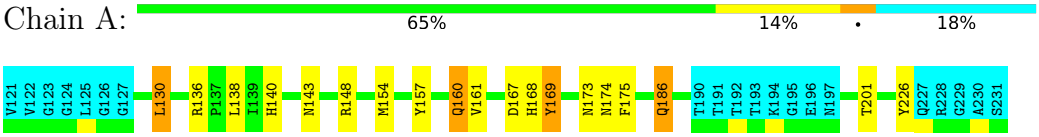
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Major prion protein

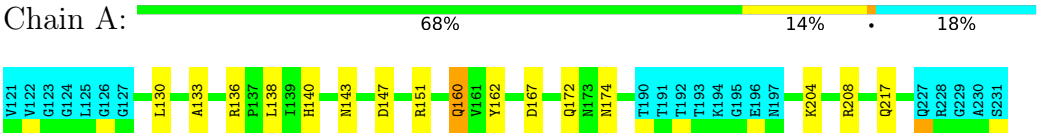
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Major prion protein

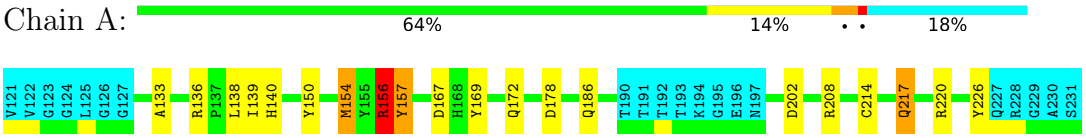
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Major prion protein

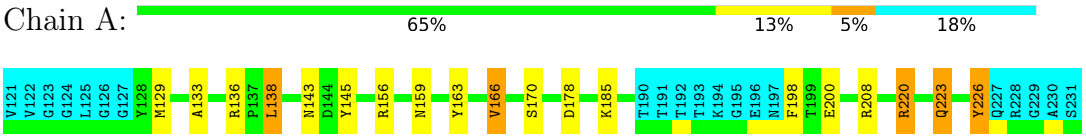
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Major prion protein

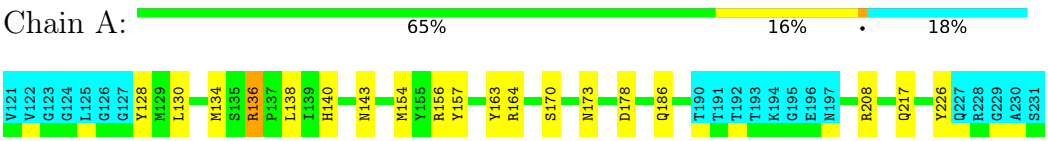
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Major prion protein

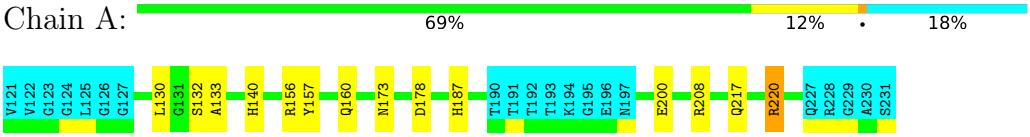
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Major prion protein

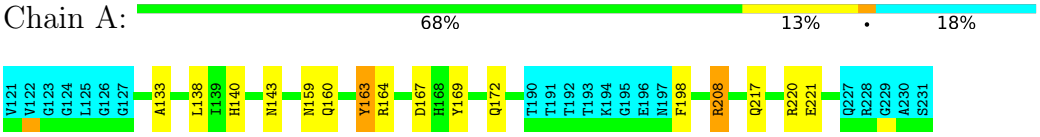
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Major prion protein

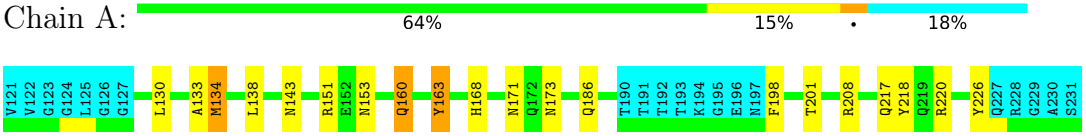
Chain A:



4.2.20 Score per residue for model 20

• 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 100 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	6.2
CANDID	refinement	1.0

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	0.70±0.01	0±0/809 (0.0± 0.0%)	1.08±0.03	2±2/1097 (0.2± 0.2%)
All	All	0.70	0/16180 (0.0%)	1.08	45/21940 (0.2%)

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	2.1±1.2
All	All	0	43

There are no bond-length outliers.

All 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	208	ARG	NE-CZ-NH2	-7.52	116.54	120.30	19	4
1	A	136	ARG	NE-CZ-NH1	7.41	124.00	120.30	17	5
1	A	157	TYR	CB-CG-CD2	-7.02	116.79	121.00	15	6
1	A	148	ARG	CD-NE-CZ	6.70	132.97	123.60	13	1
1	A	136	ARG	CD-NE-CZ	6.45	132.62	123.60	10	4
1	A	220	ARG	NE-CZ-NH2	-6.21	117.19	120.30	19	2
1	A	226	TYR	CB-CG-CD1	-6.20	117.28	121.00	15	2
1	A	148	ARG	NE-CZ-NH2	-6.18	117.21	120.30	13	2
1	A	148	ARG	NE-CZ-NH1	5.83	123.21	120.30	13	1
1	A	166	VAL	CG1-CB-CG2	-5.80	101.62	110.90	6	2
1	A	136	ARG	NE-CZ-NH2	-5.79	117.41	120.30	1	3
1	A	156	ARG	NE-CZ-NH2	-5.60	117.50	120.30	10	1
1	A	156	ARG	NE-CZ-NH1	5.60	123.10	120.30	15	1
1	A	163	TYR	CB-CG-CD2	-5.49	117.70	121.00	1	3
1	A	140	HIS	CA-CB-CG	5.44	122.85	113.60	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	166	VAL	CA-CB-CG1	5.43	119.04	110.90	16	1
1	A	226	TYR	CB-CG-CD2	-5.37	117.78	121.00	11	2
1	A	161	VAL	CA-CB-CG2	5.19	118.69	110.90	13	1
1	A	218	TYR	CB-CG-CD2	-5.17	117.90	121.00	20	1
1	A	132	SER	C-N-CA	5.15	134.57	121.70	11	1
1	A	155	TYR	CB-CG-CD2	-5.01	118.00	121.00	7	1

There are no chirality outliers.

All 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	151	ARG	Sidechain	6
1	A	156	ARG	Sidechain	6
1	A	220	ARG	Sidechain	5
1	A	164	ARG	Sidechain	4
1	A	145	TYR	Sidechain	3
1	A	157	TYR	Sidechain	3
1	A	136	ARG	Sidechain	2
1	A	162	TYR	Sidechain	2
1	A	148	ARG	Sidechain	2
1	A	218	TYR	Sidechain	2
1	A	163	TYR	Sidechain	2
1	A	225	TYR	Sidechain	1
1	A	150	TYR	Sidechain	1
1	A	140	HIS	Peptide	1
1	A	134	MET	Peptide	1
1	A	153	ASN	Peptide	1
1	A	226	TYR	Peptide	1

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	787	728	728	1±1
All	All	15740	14560	14560	19

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:VAL:HG22	1:A:210:VAL:HG23	0.58	1.74	4	1
1:A:130:LEU:HD11	1:A:160:GLN:NE2	0.55	2.15	14	4
1:A:172:GLN:HE21	1:A:176:VAL:HG21	0.52	1.64	10	1
1:A:133:ALA:HB1	1:A:159:ASN:HD22	0.49	1.68	16	1
1:A:139:ILE:HG21	1:A:141:PHE:CZ	0.48	2.43	12	1
1:A:169:TYR:CE1	1:A:175:PHE:CZ	0.42	3.08	13	1
1:A:130:LEU:HD11	1:A:160:GLN:HE22	0.42	1.74	18	1
1:A:223:GLN:HA	1:A:226:TYR:CD2	0.42	2.49	16	1
1:A:185:LYS:O	1:A:189:VAL:HG23	0.42	2.14	6	1
1:A:214:CYS:HA	1:A:217:GLN:CG	0.41	2.45	15	1
1:A:150:TYR:CE1	1:A:154:MET:HB3	0.41	2.50	15	1
1:A:169:TYR:CZ	1:A:175:PHE:CE1	0.41	3.08	13	1
1:A:172:GLN:HE21	1:A:176:VAL:CG2	0.41	2.29	10	1
1:A:136:ARG:HH11	1:A:136:ARG:CG	0.40	2.29	10	1
1:A:169:TYR:CE1	1:A:175:PHE:CE1	0.40	3.09	13	1
1:A:163:TYR:CD1	1:A:217:GLN:HG2	0.40	2.51	5	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	91/111 (82%)	80±3 (87±3%)	8±2 (9±2%)	3±1 (3±1%)	7	38
All	All	1820/2220 (82%)	1592 (87%)	170 (9%)	58 (3%)	7	38

All 10 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	143	ASN	15
1	A	133	ALA	12
1	A	138	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	198	PHE	6
1	A	170	SER	4
1	A	167	ASP	4
1	A	147	ASP	3
1	A	169	TYR	2
1	A	132	SER	2
1	A	171	ASN	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	87/100 (87%)	77±2 (88±2%)	10±2 (12±2%)	9 52
All	All	1740/2000 (87%)	1537 (88%)	203 (12%)	9 52

All 43 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	208	ARG	17
1	A	138	LEU	16
1	A	186	GLN	14
1	A	140	HIS	12
1	A	169	TYR	9
1	A	136	ARG	9
1	A	172	GLN	9
1	A	160	GLN	8
1	A	217	GLN	8
1	A	168	HIS	8
1	A	200	GLU	7
1	A	154	MET	6
1	A	134	MET	6
1	A	156	ARG	6
1	A	163	TYR	5
1	A	173	ASN	5
1	A	171	ASN	4
1	A	167	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	220	ARG	4
1	A	178	ASP	4
1	A	151	ARG	3
1	A	201	THR	3
1	A	187	HIS	3
1	A	159	ASN	3
1	A	130	LEU	3
1	A	226	TYR	3
1	A	222	SER	2
1	A	223	GLN	2
1	A	132	SER	2
1	A	202	ASP	2
1	A	221	GLU	2
1	A	139	ILE	2
1	A	174	ASN	2
1	A	144	ASP	1
1	A	155	TYR	1
1	A	135	SER	1
1	A	145	TYR	1
1	A	189	VAL	1
1	A	204	LYS	1
1	A	129	MET	1
1	A	166	VAL	1
1	A	185	LYS	1
1	A	164	ARG	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 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

No chemical shift data were provided