



Full wwPDB NMR Structure Validation Report ⓘ

Feb 28, 2026 – 07:31 PM UTC

PDB ID : 1XYU / pdb_00001xyu
Title : Solution structure of the sheep prion protein with polymorphism H168
Authors : Calzolari, L.; Lysek, D.A.; Guntert, P.; Wuthrich, K.
Deposited on : 2004-11-11

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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
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

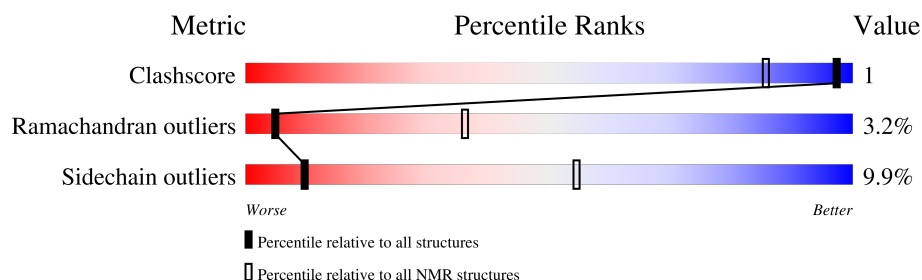
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	111	

2 Ensemble composition and analysis

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)	0.61	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
1	A	111	Total	C	H	N	O	S	0
			1777	572	859	162	177	7	

There is a discrepancy between the modelled and reference sequences:

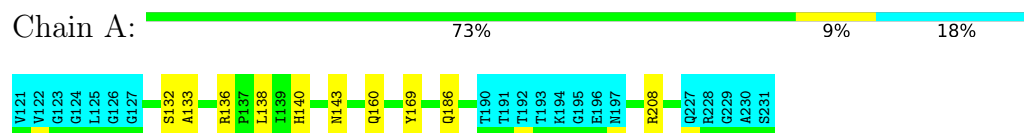
Chain	Residue	Modelled	Actual	Comment	Reference
A	168	HIS	ARG	SEE REMARK 999	UNP P23907

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

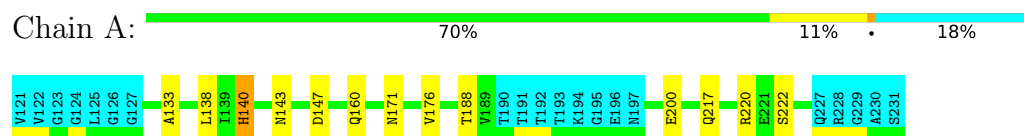


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

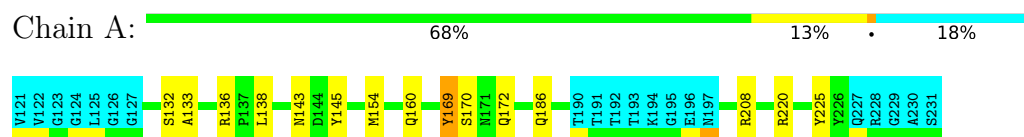
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Major prion protein



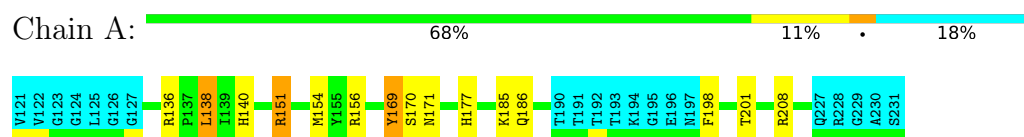
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



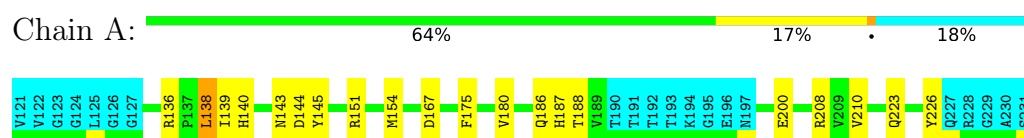
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



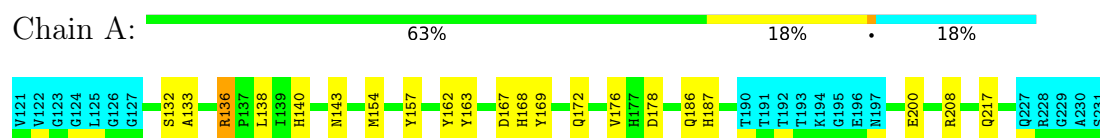
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



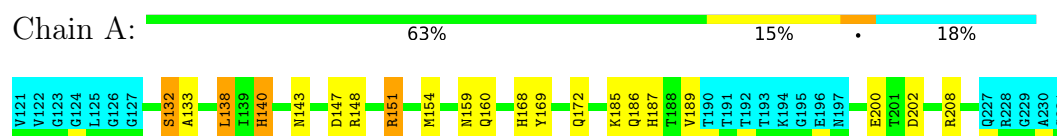
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



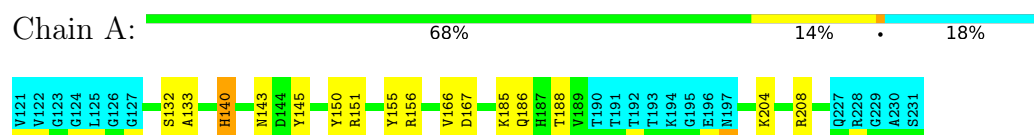
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



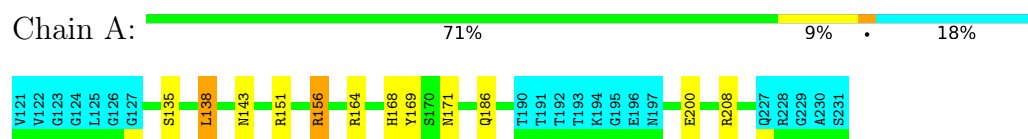
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



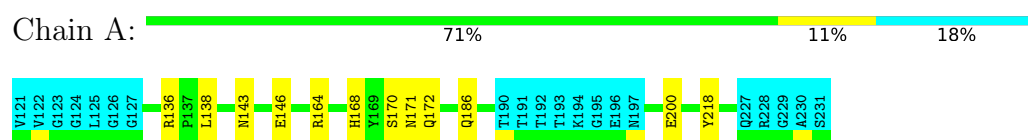
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



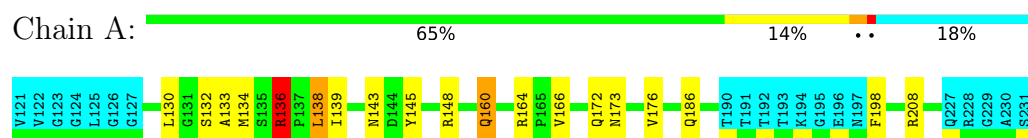
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



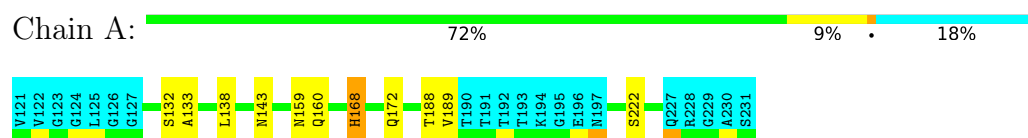
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



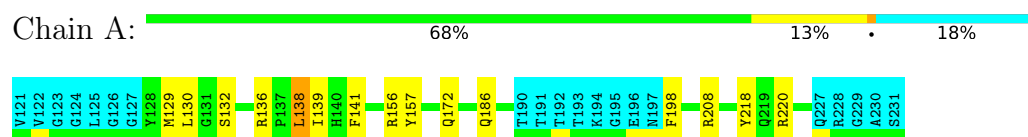
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



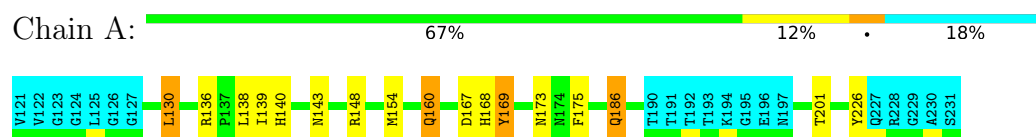
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



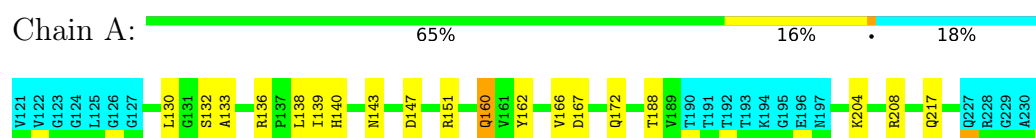
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



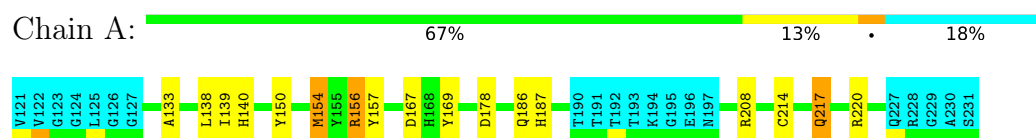
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



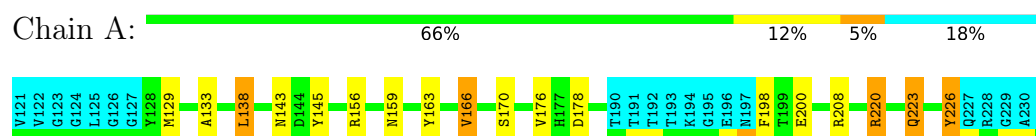
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



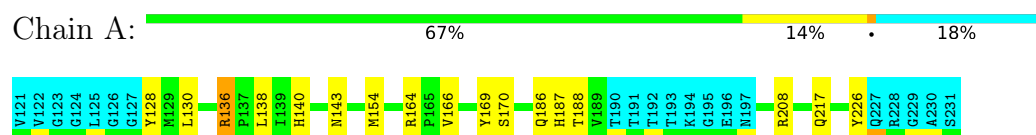
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



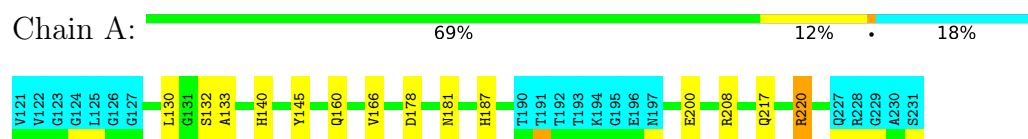
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



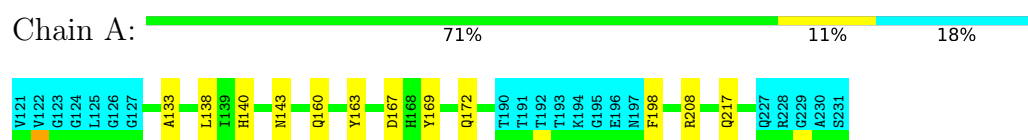
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



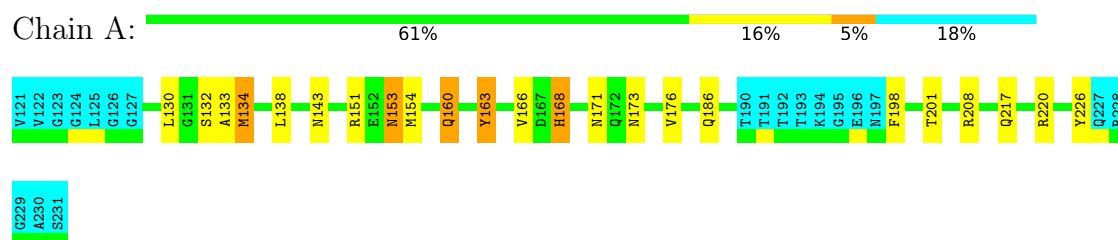
4.2.19 Score per residue for model 19

- 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: *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	0.71±0.01	0±0/809 (0.0± 0.0%)	1.48±0.03	4±3/1097 (0.4± 0.3%)
All	All	0.71	0/16180 (0.0%)	1.48	87/21940 (0.4%)

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	181	ASN	CA-C-N	9.77	132.87	120.56	18	1
1	A	181	ASN	C-N-CA	9.77	132.87	120.56	18	1
1	A	140	HIS	CA-CB-CG	9.05	122.85	113.80	4	11
1	A	202	ASP	CA-CB-CG	7.40	120.00	112.60	6	1
1	A	132	SER	CA-C-N	6.82	134.57	121.54	11	7
1	A	132	SER	C-N-CA	6.82	134.57	121.54	11	7
1	A	166	VAL	CA-C-N	6.65	130.09	120.38	17	4
1	A	166	VAL	C-N-CA	6.65	130.09	120.38	17	4
1	A	188	THR	CA-C-N	6.63	128.91	120.56	7	5
1	A	188	THR	C-N-CA	6.63	128.91	120.56	7	5
1	A	178	ASP	CA-CB-CG	6.16	118.75	112.60	5	1
1	A	148	ARG	CD-NE-CZ	6.12	132.97	124.40	13	1
1	A	168	HIS	CA-CB-CG	6.11	119.91	113.80	11	1
1	A	176	VAL	CB-CA-C	6.11	116.90	111.71	20	3
1	A	170	SER	CA-C-N	6.02	133.05	121.54	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	170	SER	C-N-CA	6.02	133.05	121.54	9	1
1	A	187	HIS	CB-CG-CD2	-5.92	123.50	131.20	17	4
1	A	136	ARG	CD-NE-CZ	5.87	132.62	124.40	10	4
1	A	168	HIS	CB-CG-CD2	-5.76	123.71	131.20	11	3
1	A	154	MET	CA-C-N	5.74	127.97	120.28	6	2
1	A	154	MET	C-N-CA	5.74	127.97	120.28	6	2
1	A	145	TYR	CA-C-N	5.72	128.22	120.38	18	2
1	A	145	TYR	C-N-CA	5.72	128.22	120.38	18	2
1	A	153	ASN	CA-CB-CG	5.69	118.29	112.60	20	1
1	A	169	TYR	CA-C-N	5.67	132.37	121.54	17	1
1	A	169	TYR	C-N-CA	5.67	132.37	121.54	17	1
1	A	143	ASN	CA-CB-CG	5.41	118.01	112.60	4	1
1	A	175	PHE	N-CA-C	-5.40	105.09	110.97	4	1
1	A	188	THR	CB-CA-C	5.38	119.22	110.24	1	1
1	A	177	HIS	CB-CG-CD2	-5.30	124.31	131.20	3	1
1	A	146	GLU	CA-C-N	5.22	127.53	120.38	9	1
1	A	146	GLU	C-N-CA	5.22	127.53	120.38	9	1
1	A	176	VAL	N-CA-C	-5.13	106.66	111.48	1	1
1	A	166	VAL	CA-CB-CG1	5.08	119.04	110.40	16	1
1	A	226	TYR	CA-C-N	5.03	131.15	121.54	4	1
1	A	226	TYR	C-N-CA	5.03	131.15	121.54	4	1
1	A	204	LYS	N-CA-CB	-5.03	102.72	110.16	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

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Mol	Chain	Res	Type	Group	Models (Total)
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

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%)	5	36
All	All	1820/2220 (82%)	1592 (87%)	170 (9%)	58 (3%)	5	36

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
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%)	78±2 (90±2%)	9±2 (10±2%)	10	54
All	All	1740/2000 (87%)	1568 (90%)	172 (10%)	10	54

All 39 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	138	LEU	16
1	A	208	ARG	16
1	A	186	GLN	14
1	A	160	GLN	9
1	A	200	GLU	8
1	A	169	TYR	8
1	A	172	GLN	8
1	A	217	GLN	7
1	A	136	ARG	7
1	A	154	MET	7
1	A	168	HIS	6
1	A	139	ILE	5
1	A	171	ASN	4
1	A	220	ARG	4
1	A	140	HIS	3
1	A	151	ARG	3
1	A	201	THR	3
1	A	167	ASP	3
1	A	166	VAL	3
1	A	173	ASN	3
1	A	130	LEU	3
1	A	226	TYR	3
1	A	178	ASP	3
1	A	222	SER	2
1	A	185	LYS	2
1	A	187	HIS	2
1	A	223	GLN	2
1	A	132	SER	2
1	A	159	ASN	2
1	A	156	ARG	2
1	A	134	MET	2
1	A	129	MET	2
1	A	163	TYR	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

6.3.3 RNA ⓘ

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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided