



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 02:45 AM UTC

PDB ID : 1U5L / pdb_00001u5l
Title : Solution Structure of the turtle prion protein fragment (121-226)
Authors : Lysek, D.A.; Calzolari, L.; Guntert, P.; Wuthrich, K.
Deposited on : 2004-07-28

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

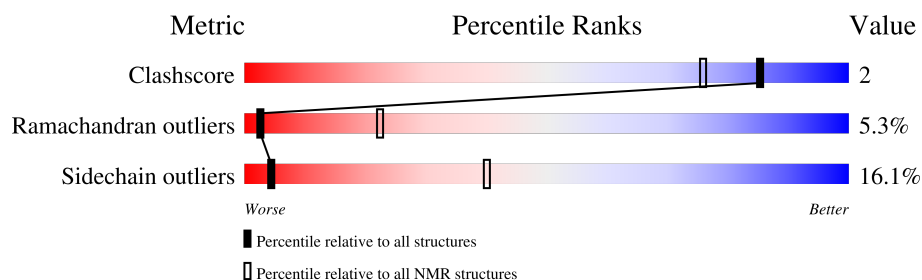
1 Overall quality at a glance

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	108	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:126-A:225 (100)	1.13	7

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1702 atoms, of which 825 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1702	541	825	157	171	8	

There are 4 discrepancies between the modelled and reference sequences:

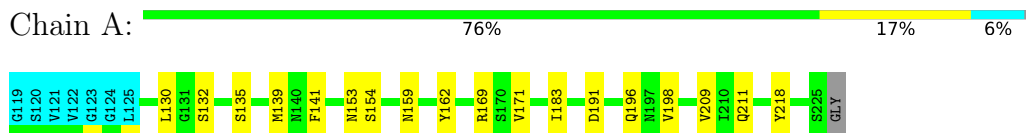
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	cloning artifact	UNP Q9I9C0
A	120	SER	-	cloning artifact	UNP Q9I9C0
A	181	VAL	LEU	SEE REMARK 999	UNP Q9I9C0
A	183	ILE	ASN	SEE REMARK 999	UNP Q9I9C0

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: prion protein

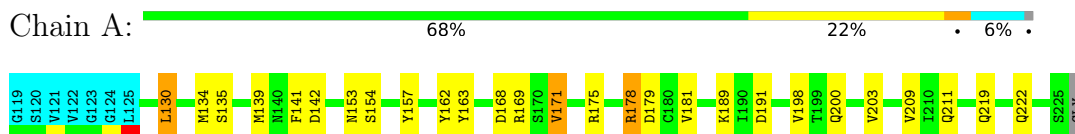


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

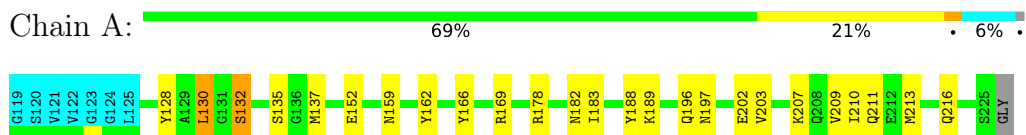
4.2.1 Score per residue for model 1

- Molecule 1: prion protein



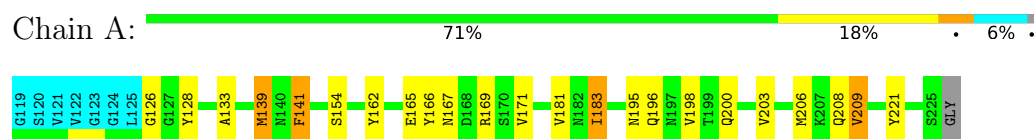
4.2.2 Score per residue for model 2

- Molecule 1: prion protein



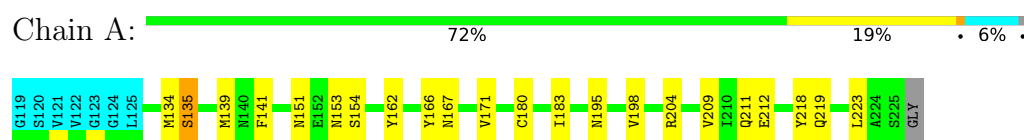
4.2.3 Score per residue for model 3

- Molecule 1: prion protein



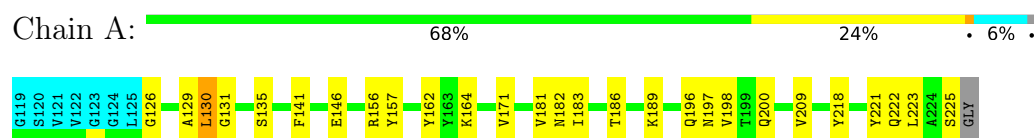
4.2.4 Score per residue for model 4

- Molecule 1: prion protein



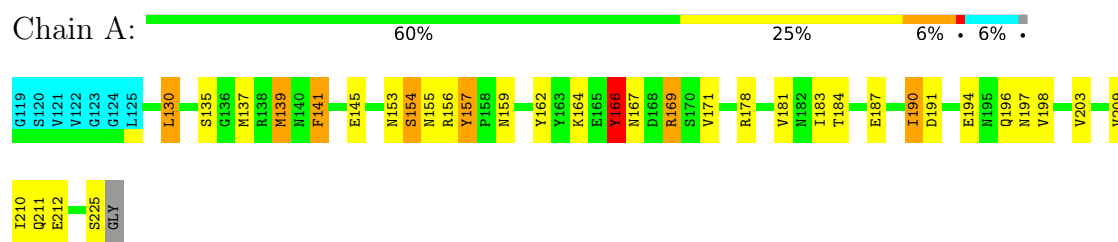
4.2.5 Score per residue for model 5

- 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 (medoid)

- 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



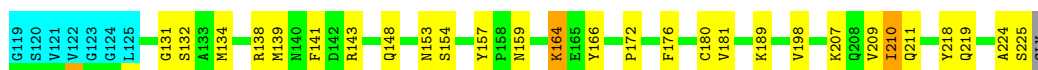
4.2.10 Score per residue for model 10

- Molecule 1: prion protein



4.2.11 Score per residue for model 11

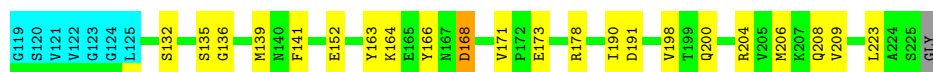
- Molecule 1: prion protein



4.2.12 Score per residue for model 12

- Molecule 1: prion protein

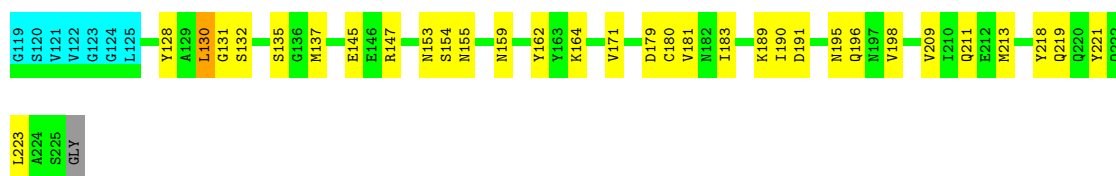
Chain A:  72% 19% • 6% •



4.2.13 Score per residue for model 13

- Molecule 1: prion protein

Chain A:  63% 29% • 6% •



4.2.14 Score per residue for model 14

- Molecule 1: prion protein

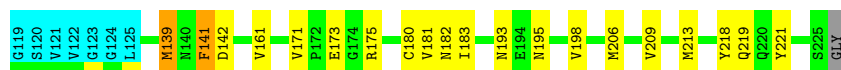
Chain A:  74% 17% • 6% •



4.2.15 Score per residue for model 15

- Molecule 1: prion protein

Chain A:  74% 17% • 6% •



4.2.16 Score per residue for model 16

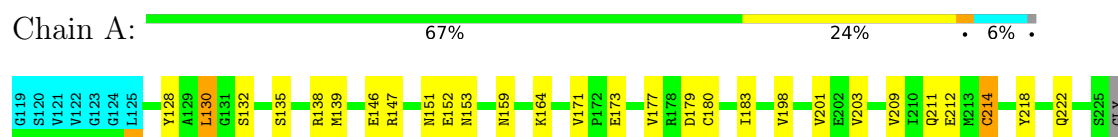
- Molecule 1: prion protein

Chain A:  66% 25% • 6% •



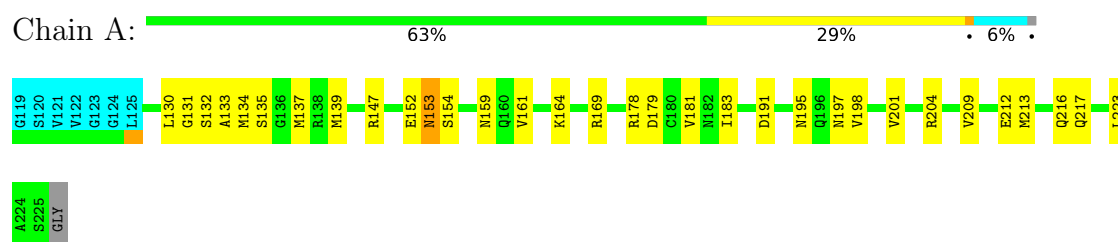
4.2.17 Score per residue for model 17

- Molecule 1: prion protein



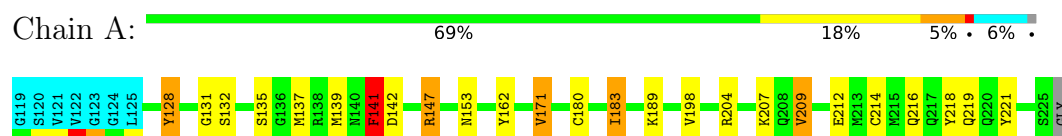
4.2.18 Score per residue for model 18

- Molecule 1: prion protein



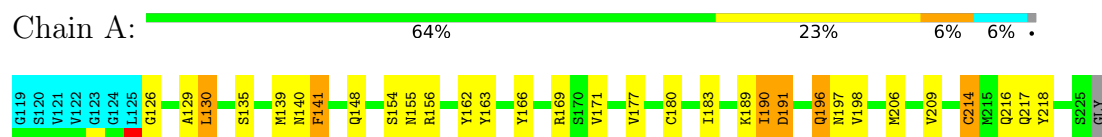
4.2.19 Score per residue for model 19

- Molecule 1: prion protein



4.2.20 Score per residue for model 20

- Molecule 1: prion protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *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
DYANA	structure solution	6.0
DYANA	refinement	6.0

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	0.65±0.01	0±0/854 (0.0± 0.0%)	1.46±0.04	4±2/1153 (0.4± 0.2%)
All	All	0.65	0/17080 (0.0%)	1.46	81/23060 (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	2.0±1.1
All	All	0	41

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	155	ASN	CA-CB-CG	7.92	120.52	112.60	8	1
1	A	153	ASN	CA-C-N	7.34	135.55	121.54	4	4
1	A	153	ASN	C-N-CA	7.34	135.55	121.54	4	4
1	A	171	VAL	CB-CA-C	6.38	117.29	110.53	14	2
1	A	181	VAL	CA-CB-CG2	6.13	120.83	110.40	3	3
1	A	203	VAL	CA-CB-CG2	6.03	120.65	110.40	7	5
1	A	134	MET	CA-C-N	6.01	133.03	121.54	9	2
1	A	134	MET	C-N-CA	6.01	133.03	121.54	9	2
1	A	131	GLY	CA-C-N	5.92	132.85	121.54	19	1
1	A	131	GLY	C-N-CA	5.92	132.85	121.54	19	1
1	A	145	GLU	CA-C-N	5.66	127.80	120.44	6	2
1	A	145	GLU	C-N-CA	5.66	127.80	120.44	6	2
1	A	181	VAL	CA-C-N	5.66	127.79	120.44	6	4
1	A	181	VAL	C-N-CA	5.66	127.79	120.44	6	4
1	A	168	ASP	CA-C-N	5.63	132.29	121.54	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	168	ASP	C-N-CA	5.63	132.29	121.54	1	1
1	A	168	ASP	CA-CB-CG	5.59	118.19	112.60	12	1
1	A	153	ASN	CA-CB-CG	5.54	118.14	112.60	18	2
1	A	151	ASN	CA-C-N	5.48	128.41	120.79	14	1
1	A	151	ASN	C-N-CA	5.48	128.41	120.79	14	1
1	A	141	PHE	CA-CB-CG	5.44	119.24	113.80	16	1
1	A	154	SER	CA-C-N	5.43	128.53	120.17	3	1
1	A	154	SER	C-N-CA	5.43	128.53	120.17	3	1
1	A	132	SER	CA-C-N	5.39	131.83	121.54	18	1
1	A	132	SER	C-N-CA	5.39	131.83	121.54	18	1
1	A	141	PHE	CA-C-N	5.31	131.69	121.54	19	1
1	A	141	PHE	C-N-CA	5.31	131.69	121.54	19	1
1	A	217	GLN	CA-C-N	5.28	128.09	120.38	8	1
1	A	217	GLN	C-N-CA	5.28	128.09	120.38	8	1
1	A	152	GLU	CA-C-N	5.27	131.61	121.54	16	2
1	A	152	GLU	C-N-CA	5.27	131.61	121.54	16	2
1	A	166	TYR	CA-C-N	5.26	131.58	121.54	6	1
1	A	166	TYR	C-N-CA	5.26	131.58	121.54	6	1
1	A	133	ALA	CA-C-N	5.22	128.05	120.79	14	1
1	A	133	ALA	C-N-CA	5.22	128.05	120.79	14	1
1	A	151	ASN	CA-CB-CG	-5.17	107.42	112.60	7	2
1	A	210	ILE	CA-C-O	-5.16	115.58	120.95	16	1
1	A	140	ASN	CA-C-N	5.16	131.39	121.54	20	1
1	A	140	ASN	C-N-CA	5.16	131.39	121.54	20	1
1	A	209	VAL	CA-C-O	-5.15	116.05	121.41	3	1
1	A	219	GLN	CA-C-N	5.15	127.70	120.28	11	1
1	A	219	GLN	C-N-CA	5.15	127.70	120.28	11	1
1	A	171	VAL	CA-C-N	5.13	126.25	119.84	1	2
1	A	171	VAL	C-N-CA	5.13	126.25	119.84	1	2
1	A	195	ASN	CA-C-N	5.12	131.31	121.54	13	1
1	A	195	ASN	C-N-CA	5.12	131.31	121.54	13	1
1	A	157	TYR	CA-C-N	5.08	125.09	120.21	6	1
1	A	157	TYR	C-N-CA	5.08	125.09	120.21	6	1
1	A	165	GLU	CA-C-N	5.05	131.19	121.54	3	1
1	A	165	GLU	C-N-CA	5.05	131.19	121.54	3	1
1	A	210	ILE	N-CA-C	-5.05	105.78	110.53	11	1
1	A	209	VAL	CB-CA-C	5.05	118.17	111.70	19	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	218	TYR	Sidechain	6
1	A	221	TYR	Sidechain	5
1	A	163	TYR	Sidechain	4
1	A	166	TYR	Sidechain	4
1	A	147	ARG	Sidechain	4
1	A	169	ARG	Sidechain	3
1	A	128	TYR	Sidechain	3
1	A	178	ARG	Sidechain	2
1	A	188	TYR	Sidechain	1
1	A	156	ARG	Sidechain	1
1	A	143	ARG	Sidechain	1
1	A	157	TYR	Sidechain	1
1	A	224	ALA	Peptide	1
1	A	136	GLY	Peptide	1
1	A	204	ARG	Sidechain	1
1	A	171	VAL	Peptide	1
1	A	164	LYS	Peptide	1
1	A	162	TYR	Sidechain	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	837	782	784	4±2
All	All	16740	15640	15680	72

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:HD12	1:A:162:TYR:CD1	0.62	2.29	5	5
1:A:139:MET:HE1	1:A:212:GLU:CB	0.60	2.27	18	1
1:A:177:VAL:HA	1:A:180:CYS:SG	0.56	2.40	17	2
1:A:181:VAL:HG11	1:A:211:GLN:HG3	0.55	1.78	1	2
1:A:139:MET:SD	1:A:141:PHE:CZ	0.55	3.00	6	4
1:A:171:VAL:HG12	1:A:175:ARG:HD3	0.54	1.80	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:HD12	1:A:162:TYR:CG	0.53	2.38	14	2
1:A:161:VAL:HG13	1:A:213:MET:SD	0.53	2.43	8	1
1:A:130:LEU:N	1:A:130:LEU:HD13	0.52	2.19	17	5
1:A:180:CYS:SG	1:A:214:CYS:SG	0.52	3.07	17	4
1:A:130:LEU:HD12	1:A:162:TYR:CB	0.52	2.35	14	2
1:A:171:VAL:HG21	1:A:176:PHE:HB2	0.51	1.81	9	1
1:A:128:TYR:CE1	1:A:183:ILE:HG12	0.51	2.40	7	3
1:A:157:TYR:CD2	1:A:206:MET:SD	0.51	3.03	10	1
1:A:130:LEU:HD12	1:A:162:TYR:HB3	0.49	1.83	14	1
1:A:139:MET:HG2	1:A:141:PHE:CE1	0.49	2.43	1	2
1:A:130:LEU:HD23	1:A:162:TYR:CD1	0.48	2.43	6	1
1:A:161:VAL:CG1	1:A:213:MET:HG3	0.48	2.39	14	3
1:A:161:VAL:HG21	1:A:214:CYS:HA	0.47	1.85	8	1
1:A:171:VAL:HG12	1:A:175:ARG:CD	0.47	2.39	10	1
1:A:180:CYS:HG	1:A:214:CYS:CB	0.47	2.23	19	2
1:A:129:ALA:C	1:A:130:LEU:HD13	0.47	2.34	20	2
1:A:188:TYR:HD2	1:A:190:ILE:HD11	0.46	1.71	16	1
1:A:164:LYS:HG3	1:A:166:TYR:CD1	0.46	2.44	6	1
1:A:181:VAL:HG12	1:A:210:ILE:HG22	0.46	1.86	11	1
1:A:139:MET:HB3	1:A:141:PHE:CE2	0.46	2.46	3	2
1:A:157:TYR:CD1	1:A:188:TYR:CD2	0.46	3.04	16	1
1:A:130:LEU:CD1	1:A:162:TYR:CD1	0.45	3.00	5	1
1:A:184:THR:HG22	1:A:210:ILE:HD13	0.45	1.89	6	1
1:A:130:LEU:HG	1:A:162:TYR:CD1	0.45	2.47	14	1
1:A:130:LEU:HD23	1:A:162:TYR:CD2	0.44	2.47	8	1
1:A:188:TYR:CD2	1:A:190:ILE:HD11	0.44	2.48	16	1
1:A:200:GLN:HA	1:A:203:VAL:HG22	0.44	1.88	1	2
1:A:137:MET:HE1	1:A:139:MET:HG3	0.43	1.90	6	1
1:A:139:MET:SD	1:A:141:PHE:CE1	0.42	3.12	4	2
1:A:164:LYS:HE2	1:A:166:TYR:CD1	0.42	2.49	12	1
1:A:210:ILE:HA	1:A:213:MET:HG2	0.42	1.92	2	1
1:A:190:ILE:HG22	1:A:191:ASP:H	0.41	1.74	20	1
1:A:128:TYR:CE1	1:A:183:ILE:HG23	0.41	2.50	2	1
1:A:139:MET:HE1	1:A:212:GLU:HB2	0.41	1.93	17	2
1:A:164:LYS:CG	1:A:166:TYR:CE1	0.40	3.04	6	1
1:A:139:MET:CB	1:A:141:PHE:CE1	0.40	3.04	20	1
1:A:164:LYS:HG3	1:A:166:TYR:CE1	0.40	2.51	11	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	99/108 (92%)	80±3 (81±3%)	14±3 (14±3%)	5±3 (5±3%)	2	22
All	All	1980/2160 (92%)	1600 (81%)	276 (14%)	104 (5%)	2	22

All 25 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	135	SER	14
1	A	196	GLN	10
1	A	132	SER	8
1	A	141	PHE	8
1	A	154	SER	7
1	A	191	ASP	7
1	A	169	ARG	6
1	A	197	ASN	6
1	A	155	ASN	6
1	A	126	GLY	4
1	A	133	ALA	4
1	A	131	GLY	4
1	A	157	TYR	2
1	A	166	TYR	2
1	A	189	LYS	2
1	A	190	ILE	2
1	A	198	VAL	2
1	A	172	PRO	2
1	A	173	GLU	2
1	A	134	MET	1
1	A	137	MET	1
1	A	167	ASN	1
1	A	127	GLY	1
1	A	176	PHE	1
1	A	153	ASN	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	92/96 (96%)	77±3 (84±4%)	15±3 (16±4%)	4 40
All	All	1840/1920 (96%)	1543 (84%)	297 (16%)	4 40

All 67 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	209	VAL	20
1	A	198	VAL	18
1	A	183	ILE	15
1	A	171	VAL	13
1	A	159	ASN	11
1	A	130	LEU	9
1	A	211	GLN	9
1	A	218	TYR	8
1	A	153	ASN	8
1	A	178	ARG	7
1	A	212	GLU	7
1	A	189	LYS	6
1	A	216	GLN	6
1	A	139	MET	6
1	A	223	LEU	6
1	A	190	ILE	6
1	A	179	ASP	5
1	A	219	GLN	5
1	A	207	LYS	5
1	A	162	TYR	5
1	A	195	ASN	5
1	A	206	MET	5
1	A	180	CYS	5
1	A	164	LYS	5
1	A	142	ASP	4
1	A	169	ARG	4
1	A	204	ARG	4
1	A	221	TYR	4
1	A	191	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	222	GLN	3
1	A	132	SER	3
1	A	152	GLU	3
1	A	182	ASN	3
1	A	208	GLN	3
1	A	146	GLU	3
1	A	156	ARG	3
1	A	225	SER	3
1	A	154	SER	3
1	A	217	GLN	3
1	A	148	GLN	3
1	A	196	GLN	3
1	A	137	MET	3
1	A	147	ARG	3
1	A	201	VAL	3
1	A	175	ARG	2
1	A	167	ASN	2
1	A	135	SER	2
1	A	200	GLN	2
1	A	187	GLU	2
1	A	155	ASN	2
1	A	140	ASN	2
1	A	197	ASN	2
1	A	213	MET	2
1	A	145	GLU	2
1	A	134	MET	2
1	A	138	ARG	2
1	A	168	ASP	2
1	A	173	GLU	2
1	A	214	CYS	2
1	A	202	GLU	1
1	A	151	ASN	1
1	A	186	THR	1
1	A	157	TYR	1
1	A	194	GLU	1
1	A	165	GLU	1
1	A	193	ASN	1
1	A	163	TYR	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