



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:35 AM UTC

PDB ID : 2L1K / pdb_00002l1k
Title : Mouse prion protein (121-231) containing the substitutions Y169A, Y225A, and Y226A
Authors : Christen, B.; Damberger, F.F.; Perez, D.R.; Hornemann, S.; Wuthrich, K.
Deposited on : 2010-07-28

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

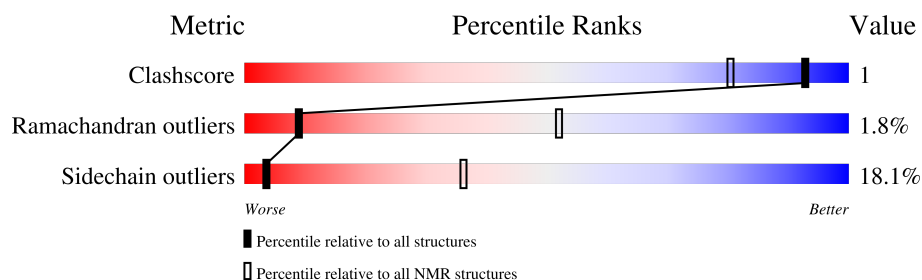
1 Overall quality at a glance

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	114	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 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:125-A:229 (105)	0.68	16

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 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1776 atoms, of which 860 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1776	562	860	165	180	9	

There are 5 discrepancies between the modelled and reference sequences:

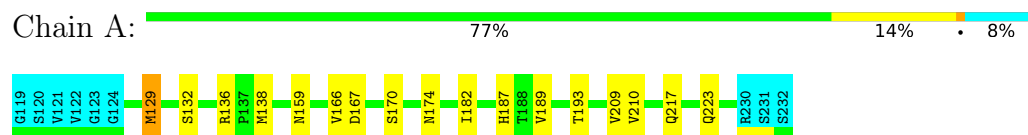
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP Q4FJQ7
A	120	SER	-	expression tag	UNP Q4FJQ7
A	169	ALA	TYR	engineered mutation	UNP Q4FJQ7
A	225	ALA	TYR	engineered mutation	UNP Q4FJQ7
A	226	ALA	TYR	engineered mutation	UNP Q4FJQ7

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

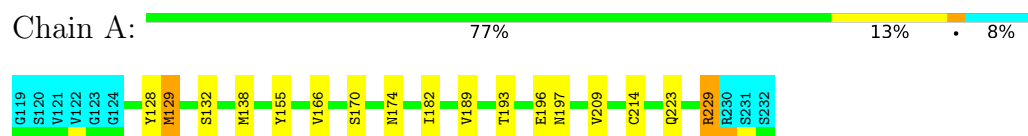


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

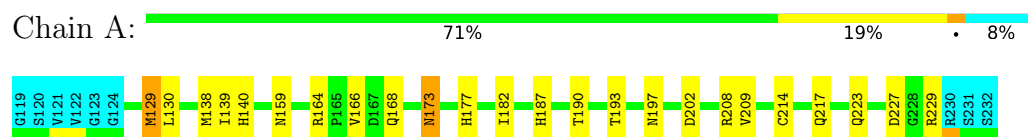
4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



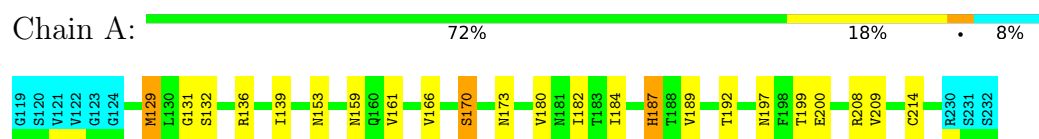
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



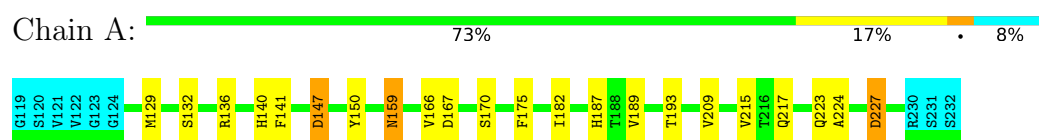
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



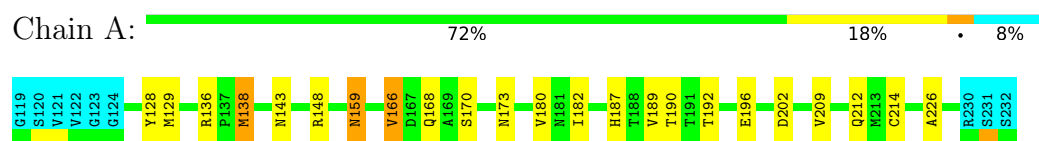
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



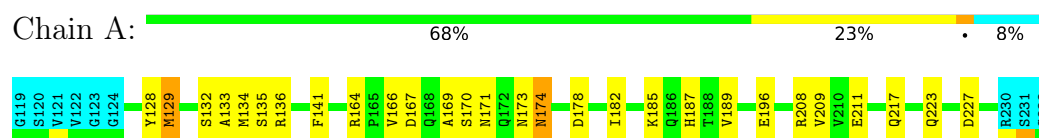
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



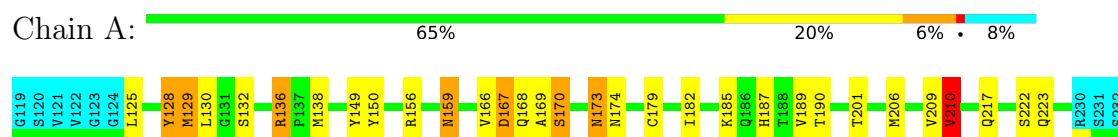
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



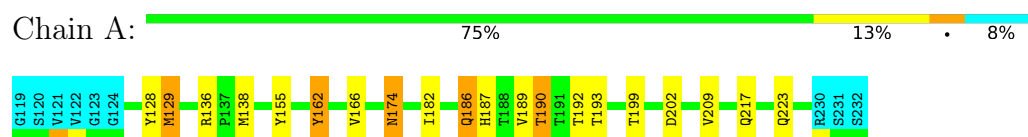
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



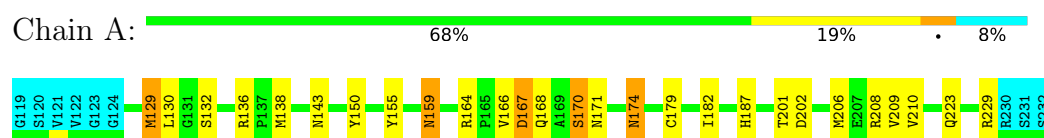
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



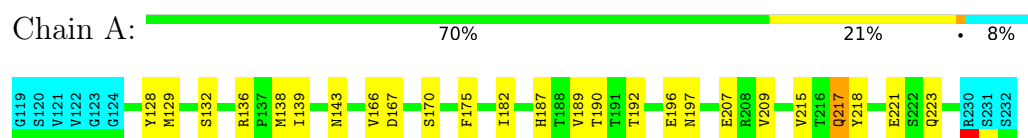
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



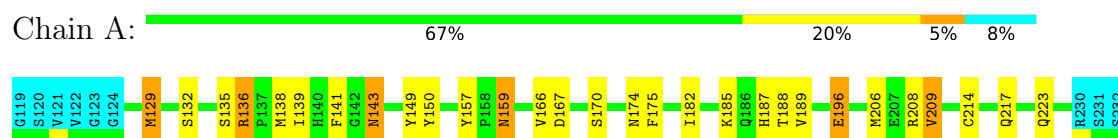
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



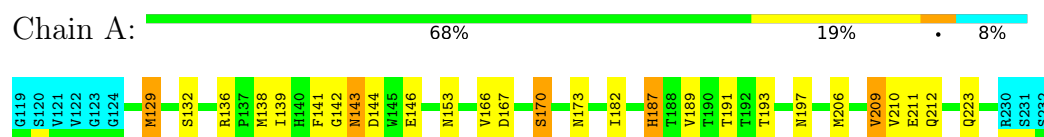
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



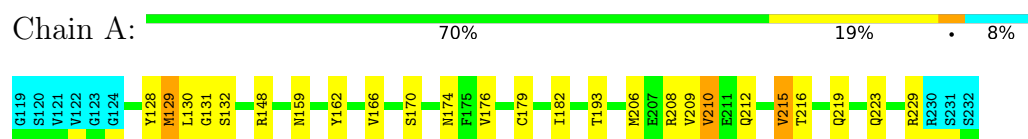
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



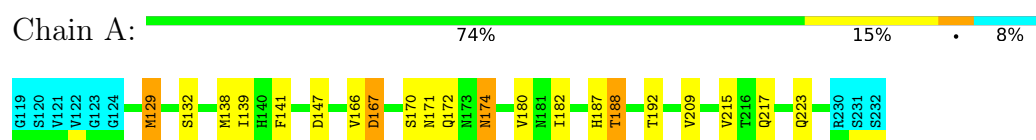
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



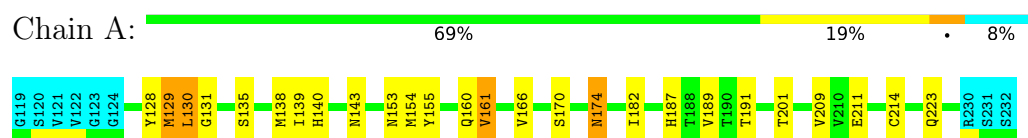
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



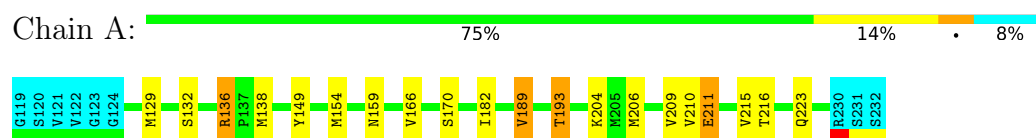
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



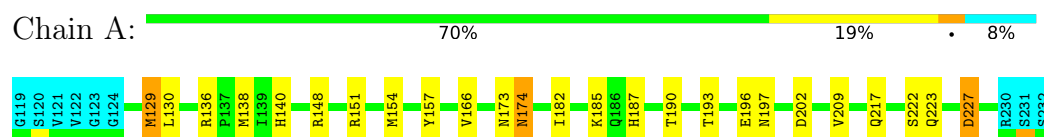
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Major prion protein



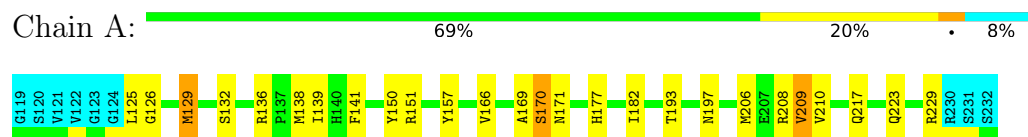
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



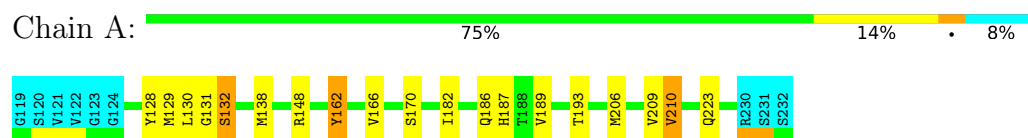
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



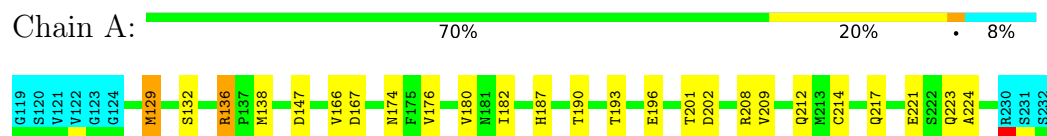
4.2.19 Score per residue for model 19

- 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 80 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	1.0.3
OPALp	refinement	

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	0.68±0.01	0±0/880 (0.0± 0.0%)	1.49±0.03	4±2/1190 (0.3± 0.2%)
All	All	0.68	0/17600 (0.0%)	1.49	82/23800 (0.3%)

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	2.4±1.5
All	All	0	47

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	159	ASN	CA-CB-CG	10.32	122.92	112.60	5	5
1	A	147	ASP	CA-CB-CG	9.97	122.57	112.60	4	1
1	A	209	VAL	CA-CB-CG2	8.85	125.45	110.40	11	1
1	A	187	HIS	CB-CG-CD2	-8.71	119.87	131.20	4	7
1	A	227	ASP	CA-CB-CG	8.08	120.68	112.60	17	3
1	A	174	ASN	CA-CB-CG	7.90	120.50	112.60	15	5
1	A	140	HIS	CA-CB-CG	6.89	120.69	113.80	2	3
1	A	167	ASP	CA-CB-CG	6.77	119.37	112.60	11	1
1	A	208	ARG	N-CA-C	-6.66	105.04	113.43	11	1
1	A	170	SER	CA-C-N	6.51	133.98	121.54	14	1
1	A	170	SER	C-N-CA	6.51	133.98	121.54	14	1
1	A	210	VAL	CA-CB-CG1	6.34	121.17	110.40	7	1
1	A	143	ASN	CA-CB-CG	6.28	118.88	112.60	12	3
1	A	177	HIS	CA-CB-CG	6.25	120.05	113.80	18	1
1	A	140	HIS	CB-CG-CD2	-6.17	123.18	131.20	4	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	202	ASP	CA-CB-CG	6.12	118.72	112.60	5	1
1	A	174	ASN	CA-C-N	6.07	128.73	120.54	6	1
1	A	174	ASN	C-N-CA	6.07	128.73	120.54	6	1
1	A	153	ASN	CA-C-N	6.04	130.80	121.19	15	1
1	A	153	ASN	C-N-CA	6.04	130.80	121.19	15	1
1	A	189	VAL	CA-CB-CG1	6.04	120.66	110.40	11	2
1	A	171	ASN	N-CA-CB	-5.94	102.31	111.46	9	1
1	A	217	GLN	CB-CG-CD	5.84	122.54	112.60	10	1
1	A	173	ASN	CA-CB-CG	-5.81	106.79	112.60	2	2
1	A	176	VAL	CA-CB-CG1	5.76	120.20	110.40	20	1
1	A	133	ALA	CA-C-N	5.76	129.76	122.16	6	1
1	A	133	ALA	C-N-CA	5.76	129.76	122.16	6	1
1	A	187	HIS	CB-CG-ND1	5.68	131.22	122.70	4	3
1	A	175	PHE	CA-CB-CG	5.55	119.35	113.80	4	3
1	A	229	ARG	CA-C-N	5.53	132.11	121.54	2	1
1	A	229	ARG	C-N-CA	5.53	132.11	121.54	2	1
1	A	192	THR	CA-CB-CG2	5.52	119.89	110.50	14	2
1	A	131	GLY	CA-C-N	5.44	131.93	121.54	19	1
1	A	131	GLY	C-N-CA	5.44	131.93	121.54	19	1
1	A	191	THR	CA-CB-CG2	5.43	119.74	110.50	12	2
1	A	153	ASN	CA-CB-CG	5.34	117.94	112.60	12	1
1	A	130	LEU	CA-C-N	5.29	127.74	122.30	7	1
1	A	130	LEU	C-N-CA	5.29	127.74	122.30	7	1
1	A	190	THR	CA-CB-CG2	5.28	119.48	110.50	5	1
1	A	210	VAL	CA-CB-CG2	5.23	119.28	110.40	7	1
1	A	215	VAL	CA-CB-CG1	5.20	119.24	110.40	13	1
1	A	188	THR	N-CA-C	-5.20	104.63	111.96	14	1
1	A	190	THR	CB-CA-C	5.19	119.11	111.17	8	1
1	A	170	SER	CB-CA-C	5.19	120.75	110.42	14	1
1	A	185	LYS	CA-C-N	5.19	127.50	120.65	11	1
1	A	185	LYS	C-N-CA	5.19	127.50	120.65	11	1
1	A	209	VAL	CA-CB-CG1	5.12	119.10	110.40	18	2
1	A	177	HIS	CB-CG-CD2	-5.10	124.57	131.20	2	1
1	A	169	ALA	CA-C-N	5.10	131.28	121.54	7	1
1	A	169	ALA	C-N-CA	5.10	131.28	121.54	7	1
1	A	193	THR	CB-CA-C	5.10	119.34	110.72	16	1
1	A	219	GLN	CA-C-N	5.10	127.38	120.65	13	1
1	A	219	GLN	C-N-CA	5.10	127.38	120.65	13	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	128	TYR	Sidechain	9
1	A	136	ARG	Sidechain	5
1	A	150	TYR	Sidechain	5
1	A	208	ARG	Sidechain	4
1	A	229	ARG	Sidechain	3
1	A	164	ARG	Sidechain	3
1	A	162	TYR	Sidechain	3
1	A	148	ARG	Sidechain	3
1	A	169	ALA	Peptide	2
1	A	196	GLU	Peptide	2
1	A	149	TYR	Sidechain	2
1	A	157	TYR	Sidechain	2
1	A	226	ALA	Peptide	1
1	A	156	ARG	Sidechain	1
1	A	218	TYR	Sidechain	1
1	A	151	ARG	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	861	805	805	2±1
All	All	17220	16100	16100	47

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:206:MET:HA	1:A:209:VAL:HG22	0.72	1.62	11	1
1:A:129:MET:HA	1:A:129:MET:HE2	0.68	1.65	10	15
1:A:206:MET:O	1:A:210:VAL:HG12	0.63	1.94	9	6
1:A:129:MET:HE3	1:A:129:MET:HA	0.61	1.72	12	2
1:A:130:LEU:HD21	1:A:160:GLN:HB3	0.58	1.76	15	1
1:A:206:MET:O	1:A:210:VAL:HG13	0.52	2.04	7	1
1:A:151:ARG:HA	1:A:154:MET:HE2	0.51	1.82	17	1
1:A:125:LEU:HB3	1:A:128:TYR:CD1	0.48	2.44	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ARG:HD3	1:A:154:MET:HE2	0.47	1.85	16	1
1:A:224:ALA:HA	1:A:227:ASP:OD1	0.47	2.10	4	1
1:A:211:GLU:O	1:A:215:VAL:HG23	0.45	2.12	16	1
1:A:129:MET:HE3	1:A:129:MET:CA	0.43	2.42	17	1
1:A:134:MET:CE	1:A:217:GLN:HG2	0.43	2.43	6	1
1:A:206:MET:HG3	1:A:210:VAL:HG12	0.43	1.89	7	1
1:A:130:LEU:HD13	1:A:130:LEU:C	0.43	2.39	15	1
1:A:172:GLN:HE21	1:A:215:VAL:HG13	0.42	1.74	14	1
1:A:134:MET:HE3	1:A:217:GLN:HG2	0.42	1.90	6	1
1:A:129:MET:HA	1:A:129:MET:CE	0.42	2.41	7	1
1:A:176:VAL:HA	1:A:179:CYS:SG	0.41	2.54	13	1
1:A:130:LEU:HD22	1:A:161:VAL:O	0.41	2.16	15	1
1:A:130:LEU:HD21	1:A:160:GLN:CB	0.41	2.45	15	1
1:A:154:MET:HA	1:A:157:TYR:CE2	0.41	2.51	17	1
1:A:130:LEU:HD13	1:A:162:TYR:CZ	0.41	2.51	19	1
1:A:149:TYR:CD1	1:A:149:TYR:C	0.40	2.98	7	1
1:A:138:MET:HA	1:A:138:MET:HE3	0.40	1.94	5	2
1:A:192:THR:HG23	1:A:197:ASN:HA	0.40	1.93	10	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	105/114 (92%)	89±3 (84±3%)	14±3 (14±3%)	2±1 (2±1%)	9	52
All	All	2100/2280 (92%)	1774 (84%)	289 (14%)	37 (2%)	9	52

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	170	SER	15
1	A	141	PHE	6
1	A	167	ASP	5
1	A	131	GLY	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	132	SER	3
1	A	166	VAL	1
1	A	185	LYS	1
1	A	142	GLY	1
1	A	171	ASN	1
1	A	126	GLY	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	94/100 (94%)	77±3 (82±3%)	17±3 (18±3%)	3	36
All	All	1880/2000 (94%)	1539 (82%)	341 (18%)	3	36

All 60 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	166	VAL	20
1	A	182	ILE	20
1	A	209	VAL	19
1	A	129	MET	18
1	A	223	GLN	18
1	A	138	MET	15
1	A	132	SER	13
1	A	189	VAL	12
1	A	136	ARG	12
1	A	174	ASN	11
1	A	193	THR	11
1	A	187	HIS	11
1	A	217	GLN	10
1	A	159	ASN	9
1	A	139	ILE	8
1	A	214	CYS	7
1	A	173	ASN	7
1	A	196	GLU	6
1	A	197	ASN	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	190	THR	6
1	A	167	ASP	6
1	A	130	LEU	5
1	A	202	ASP	5
1	A	170	SER	5
1	A	143	ASN	5
1	A	155	TYR	4
1	A	168	GLN	4
1	A	180	VAL	4
1	A	212	GLN	4
1	A	211	GLU	4
1	A	201	THR	4
1	A	208	ARG	3
1	A	147	ASP	3
1	A	215	VAL	3
1	A	135	SER	3
1	A	210	VAL	3
1	A	229	ARG	2
1	A	161	VAL	2
1	A	192	THR	2
1	A	199	THR	2
1	A	171	ASN	2
1	A	227	ASP	2
1	A	179	CYS	2
1	A	185	LYS	2
1	A	222	SER	2
1	A	186	GLN	2
1	A	221	GLU	2
1	A	188	THR	2
1	A	216	THR	2
1	A	153	ASN	1
1	A	184	ILE	1
1	A	200	GLU	1
1	A	148	ARG	1
1	A	178	ASP	1
1	A	207	GLU	1
1	A	144	ASP	1
1	A	146	GLU	1
1	A	154	MET	1
1	A	204	LYS	1
1	A	125	LEU	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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided