



Full wwPDB NMR Structure Validation Report ⓘ

Mar 1, 2026 – 03:05 PM UTC

PDB ID : 1XYW / pdb_00001xyw
Title : elk prion protein
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Deposited on : 2004-11-11

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

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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

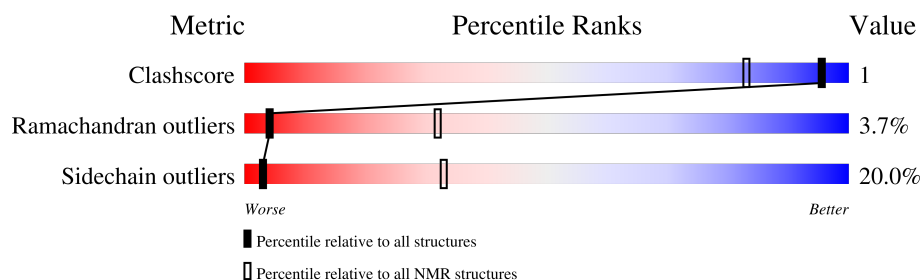
1 Overall quality at a glance

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	73% 19% • 7%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:124-A:226 (103)	0.71	4

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 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1776 atoms, of which 858 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

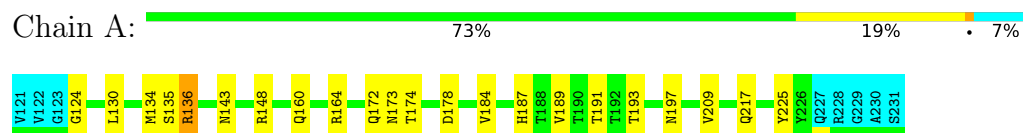
Mol	Chain	Residues	Atoms						Trace
1	A	111	Total	C	H	N	O	S	0
			1776	571	858	160	179	8	

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

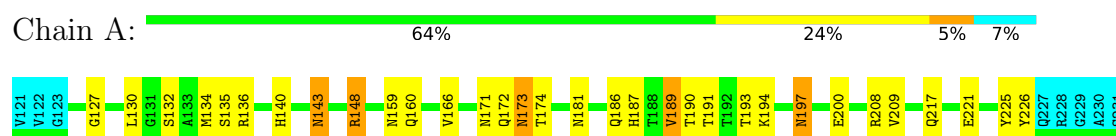


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

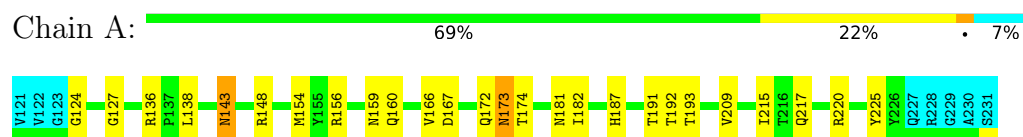
4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



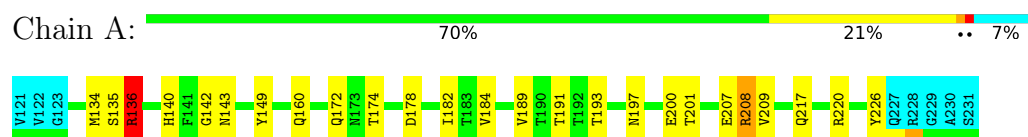
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



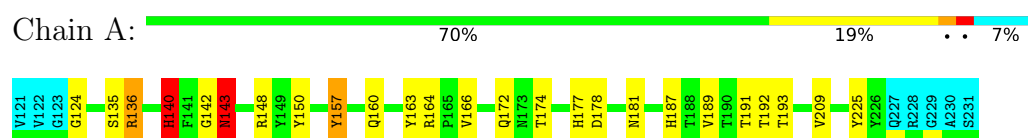
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



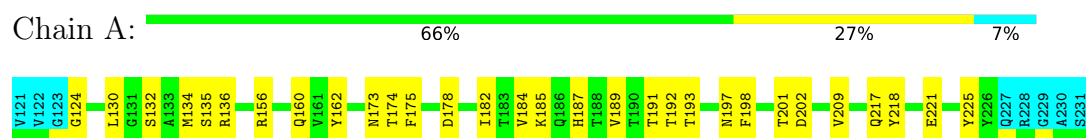
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Major prion protein



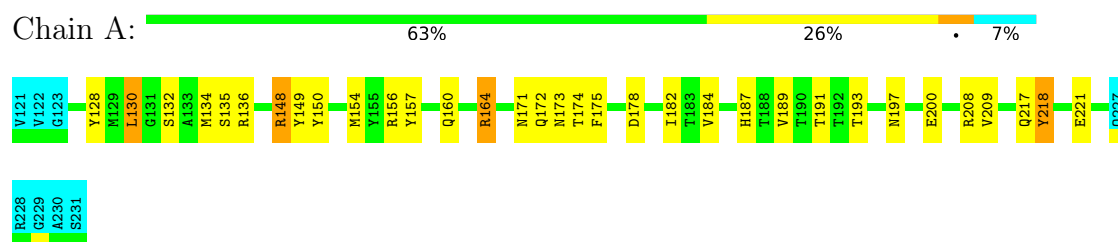
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



4.2.6 Score per residue for model 6

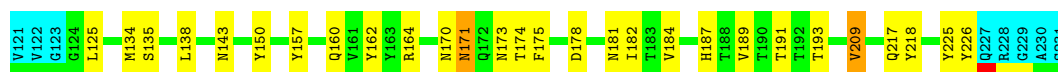
- Molecule 1: Major prion protein



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

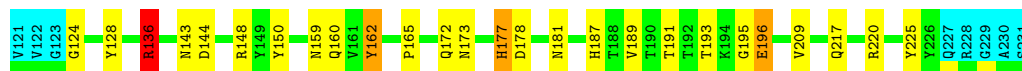
Chain A: 63% 27% 7%



4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein

Chain A: 69% 20% 7%



4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein

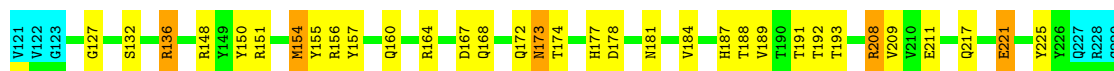
Chain A: 70% 21% 7%



4.2.11 Score per residue for model 11

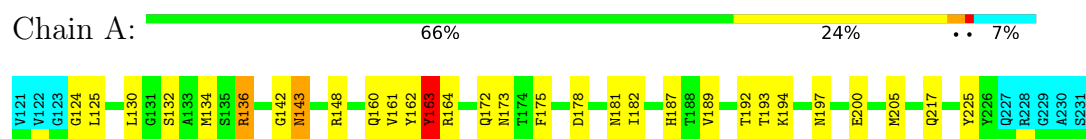
- Molecule 1: Major prion protein

Chain A: 63% 25% 5% 7%



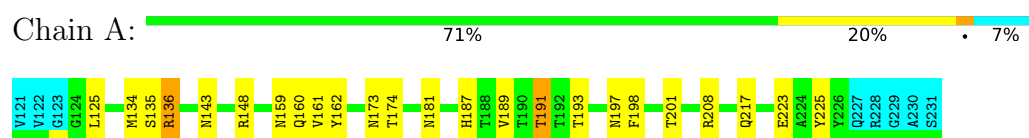
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



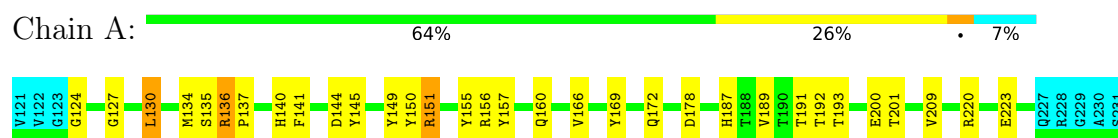
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



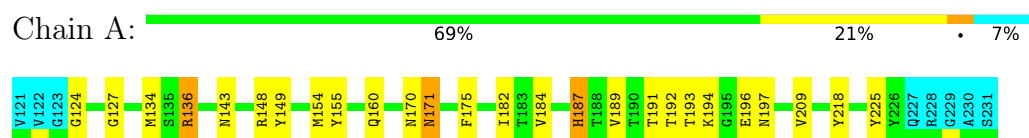
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



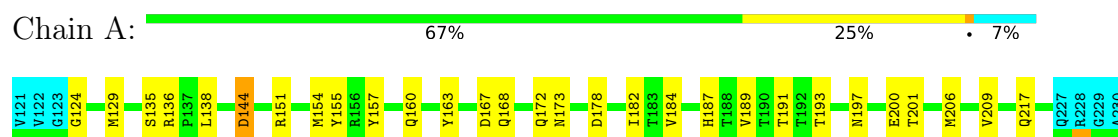
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



S231

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

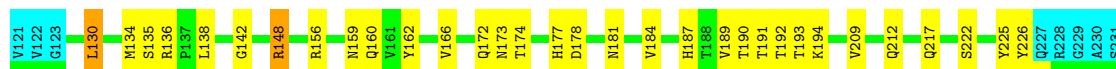
Chain A: 



4.2.19 Score per residue for model 19

- Molecule 1: Major prion protein

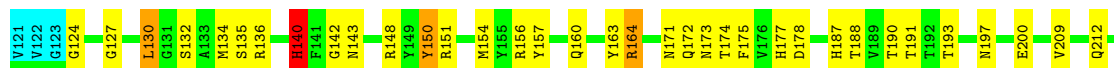
Chain A: 



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

6.1 Standard geometry

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±0.02	0±0/886 (0.0± 0.1%)	1.51±0.03	6±3/1200 (0.5± 0.3%)
All	All	0.71	6/17720 (0.0%)	1.51	126/24000 (0.5%)

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	3.1±1.6
All	All	0	63

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	184	VAL	N-CA	-5.96	1.39	1.46	19	6

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	184	VAL	N-CA-CB	-10.00	99.72	110.62	5	10
1	A	184	VAL	CA-CB-CG2	9.62	126.76	110.40	11	10
1	A	130	LEU	CA-C-N	7.78	127.39	119.92	20	3
1	A	130	LEU	C-N-CA	7.78	127.39	119.92	20	3
1	A	226	TYR	CA-C-N	6.76	134.45	121.54	7	5
1	A	226	TYR	C-N-CA	6.76	134.45	121.54	7	5
1	A	166	VAL	CA-C-N	6.61	134.17	121.54	2	2
1	A	166	VAL	C-N-CA	6.61	134.17	121.54	2	2
1	A	140	HIS	CB-CG-CD2	-6.52	122.72	131.20	20	3
1	A	173	ASN	CA-CB-CG	-6.45	106.15	112.60	2	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	171	ASN	CA-CB-CG	6.42	119.02	112.60	7	3
1	A	190	THR	N-CA-C	-6.25	107.49	114.62	17	1
1	A	140	HIS	CA-C-N	6.16	133.31	121.54	14	3
1	A	140	HIS	C-N-CA	6.16	133.31	121.54	14	3
1	A	178	ASP	CA-C-N	6.10	128.74	120.38	14	14
1	A	178	ASP	C-N-CA	6.10	128.74	120.38	14	14
1	A	143	ASN	CA-CB-CG	6.02	118.62	112.60	2	1
1	A	221	GLU	CA-C-N	5.99	128.22	120.44	11	3
1	A	221	GLU	C-N-CA	5.99	128.22	120.44	11	3
1	A	189	VAL	CB-CA-C	5.91	120.98	111.29	18	1
1	A	159	ASN	CA-CB-CG	5.85	118.45	112.60	9	1
1	A	196	GLU	CA-C-N	5.81	132.64	121.54	15	1
1	A	196	GLU	C-N-CA	5.81	132.64	121.54	15	1
1	A	178	ASP	CA-CB-CG	5.80	118.40	112.60	7	1
1	A	198	PHE	CA-CB-CG	5.61	119.41	113.80	5	1
1	A	143	ASN	CA-C-N	5.52	132.08	121.54	9	1
1	A	143	ASN	C-N-CA	5.52	132.08	121.54	9	1
1	A	209	VAL	CB-CA-C	5.48	116.56	111.30	8	1
1	A	149	TYR	N-CA-C	-5.40	105.08	110.97	15	1
1	A	165	PRO	CA-C-N	5.38	128.11	120.53	9	1
1	A	165	PRO	C-N-CA	5.38	128.11	120.53	9	1
1	A	154	MET	CA-C-N	5.33	128.42	120.31	15	1
1	A	154	MET	C-N-CA	5.33	128.42	120.31	15	1
1	A	191	THR	CB-CA-C	5.33	119.17	110.17	18	1
1	A	190	THR	CB-CA-C	5.27	116.29	109.28	17	1
1	A	205	MET	CA-C-N	5.25	127.62	120.54	17	1
1	A	205	MET	C-N-CA	5.25	127.62	120.54	17	1
1	A	197	ASN	CA-CB-CG	-5.25	107.35	112.60	1	1
1	A	177	HIS	CB-CG-CD2	-5.23	124.41	131.20	11	2
1	A	149	TYR	CA-C-N	5.21	127.52	120.65	3	1
1	A	149	TYR	C-N-CA	5.21	127.52	120.65	3	1
1	A	159	ASN	CA-C-N	5.20	129.02	122.16	19	1
1	A	159	ASN	C-N-CA	5.20	129.02	122.16	19	1
1	A	187	HIS	CB-CG-CD2	-5.13	124.52	131.20	15	3
1	A	135	SER	N-CA-CB	-5.10	102.94	110.49	14	1
1	A	137	PRO	N-CA-CB	5.03	105.73	102.92	14	1
1	A	209	VAL	CA-CB-CG1	5.02	118.93	110.40	7	1
1	A	215	ILE	CA-C-N	5.00	127.48	120.28	2	1
1	A	215	ILE	C-N-CA	5.00	127.48	120.28	2	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	148	ARG	Sidechain	8
1	A	136	ARG	Sidechain,Peptide	7
1	A	150	TYR	Sidechain	6
1	A	151	ARG	Sidechain	5
1	A	208	ARG	Sidechain	4
1	A	220	ARG	Sidechain	4
1	A	157	TYR	Sidechain	4
1	A	162	TYR	Sidechain	4
1	A	155	TYR	Sidechain	4
1	A	156	ARG	Sidechain	3
1	A	164	ARG	Sidechain	3
1	A	149	TYR	Sidechain	2
1	A	169	TYR	Sidechain	2
1	A	226	TYR	Sidechain	2
1	A	142	GLY	Peptide	1
1	A	218	TYR	Sidechain	1
1	A	195	GLY	Peptide	1
1	A	175	PHE	Sidechain	1
1	A	163	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	865	803	803	2±1
All	All	17300	16060	16060	34

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:184:VAL:HG22	1:A:206:MET:SD	0.54	2.43	8	1
1:A:128:TYR:CE2	1:A:164:ARG:CZ	0.50	2.94	18	1
1:A:191:THR:HG21	1:A:198:PHE:CE2	0.48	2.44	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:MET:HE3	1:A:165:PRO:CD	0.47	2.39	10	1
1:A:154:MET:HA	1:A:157:TYR:CD2	0.47	2.44	6	2
1:A:175:PHE:CE2	1:A:218:TYR:HB2	0.46	2.46	18	6
1:A:206:MET:O	1:A:210:VAL:HG23	0.46	2.11	17	1
1:A:150:TYR:CE1	1:A:157:TYR:CD2	0.46	3.04	20	1
1:A:150:TYR:CE1	1:A:157:TYR:CE2	0.45	3.04	14	3
1:A:129:MET:HE3	1:A:165:PRO:HD3	0.45	1.89	10	1
1:A:128:TYR:CE1	1:A:164:ARG:HD2	0.45	2.46	6	1
1:A:130:LEU:HD13	1:A:130:LEU:C	0.44	2.37	12	4
1:A:139:ILE:HD11	1:A:212:GLN:HG3	0.44	1.89	8	1
1:A:125:LEU:CD1	1:A:162:TYR:CE1	0.44	3.01	13	2
1:A:163:TYR:CD2	1:A:164:ARG:O	0.43	2.72	4	1
1:A:186:GLN:HA	1:A:189:VAL:HG22	0.42	1.92	1	1
1:A:140:HIS:CD2	1:A:143:ASN:C	0.42	2.97	4	1
1:A:163:TYR:CD2	1:A:175:PHE:CE1	0.42	3.08	12	1
1:A:206:MET:HA	1:A:209:VAL:CG2	0.41	2.46	17	1
1:A:130:LEU:C	1:A:130:LEU:HD13	0.41	2.41	20	1
1:A:140:HIS:CD2	1:A:143:ASN:HA	0.40	2.51	20	1
1:A:157:TYR:CD1	1:A:206:MET:HG3	0.40	2.51	8	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	103/111 (93%)	89±2 (87±2%)	10±2 (10±2%)	4±1 (4±1%)	4	32
All	All	2060/2220 (93%)	1784 (87%)	199 (10%)	77 (4%)	4	32

All 15 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	136	ARG	16
1	A	189	VAL	16
1	A	124	GLY	12

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Mol	Chain	Res	Type	Models (Total)
1	A	127	GLY	6
1	A	197	ASN	5
1	A	167	ASP	4
1	A	142	GLY	4
1	A	143	ASN	3
1	A	144	ASP	3
1	A	196	GLU	2
1	A	154	MET	2
1	A	145	TYR	1
1	A	125	LEU	1
1	A	141	PHE	1
1	A	190	THR	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	95/100 (95%)	76±3 (80±3%)	19±3 (20±3%)	3	33
All	All	1900/2000 (95%)	1520 (80%)	380 (20%)	3	33

All 64 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	160	GLN	20
1	A	193	THR	20
1	A	191	THR	17
1	A	209	VAL	17
1	A	187	HIS	16
1	A	134	MET	15
1	A	173	ASN	15
1	A	217	GLN	15
1	A	172	GLN	14
1	A	174	THR	14
1	A	225	TYR	14
1	A	135	SER	13
1	A	148	ARG	10

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Mol	Chain	Res	Type	Models (Total)
1	A	181	ASN	10
1	A	200	GLU	10
1	A	182	ILE	9
1	A	192	THR	9
1	A	143	ASN	8
1	A	136	ARG	8
1	A	132	SER	7
1	A	130	LEU	6
1	A	171	ASN	6
1	A	208	ARG	6
1	A	190	THR	5
1	A	138	LEU	5
1	A	201	THR	5
1	A	177	HIS	5
1	A	197	ASN	5
1	A	164	ARG	5
1	A	194	LYS	4
1	A	154	MET	4
1	A	156	ARG	4
1	A	140	HIS	3
1	A	159	ASN	3
1	A	166	VAL	3
1	A	220	ARG	3
1	A	221	GLU	3
1	A	161	VAL	3
1	A	163	TYR	3
1	A	207	GLU	2
1	A	185	LYS	2
1	A	170	ASN	2
1	A	129	MET	2
1	A	189	VAL	2
1	A	199	THR	2
1	A	162	TYR	2
1	A	196	GLU	2
1	A	168	GLN	2
1	A	188	THR	2
1	A	223	GLU	2
1	A	144	ASP	2
1	A	212	GLN	2
1	A	202	ASP	1
1	A	152	GLU	1
1	A	175	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	214	CYS	1
1	A	128	TYR	1
1	A	211	GLU	1
1	A	205	MET	1
1	A	145	TYR	1
1	A	151	ARG	1
1	A	206	MET	1
1	A	155	TYR	1
1	A	222	SER	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