W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB NMR Structure Validation Report ⓘ

Nov 9, 2024 – 09:55 PM EST

PDB ID	:	2L1D
Title	:	Mouse prion protein (121-231) containing the substitution Y169G
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:

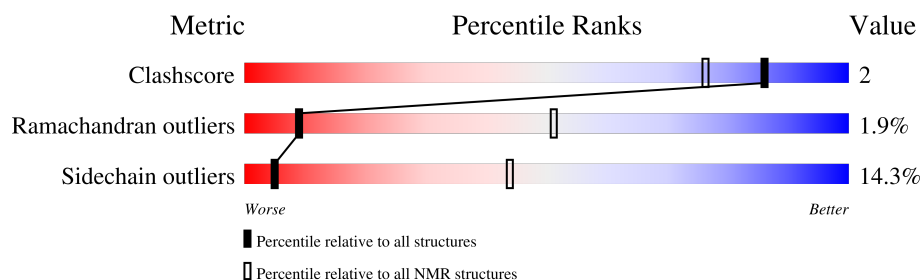| MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		1.9%
Sidechain outliers		14.3%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	114	80% 13% • 6%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 12 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:120-A:226 (107)	0.55	12

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 1 single-model cluster was found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 1795 atoms, of which 866 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	114	1795	573	866	165	182	9	0

There are 3 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	GLY	TYR	engineered mutation	UNP Q4FJQ7

4 Residue-property plots (i)

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.
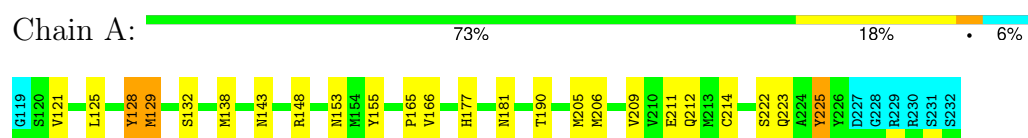
- Molecule 1: Major prion protein

Chain A:
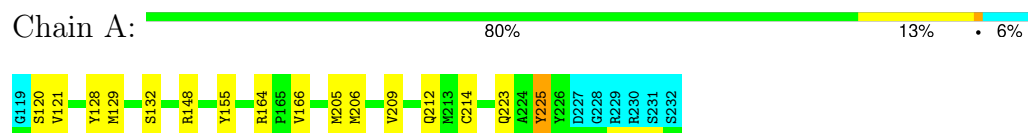
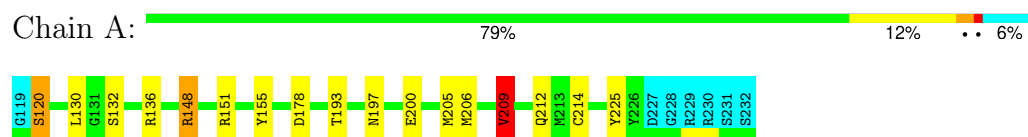## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1
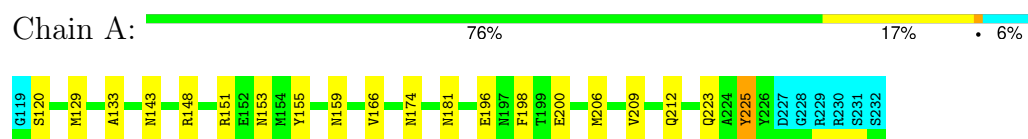
- Molecule 1: Major prion protein

Chain A:

4.2.2 Score per residue for model 2

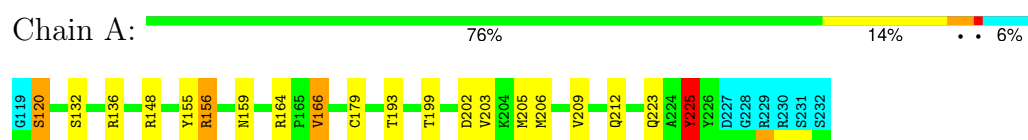- Molecule 1: Major prion protein

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:
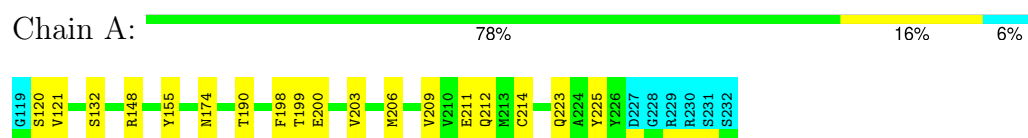

4.2.6　Score per residue for model 6

• 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:

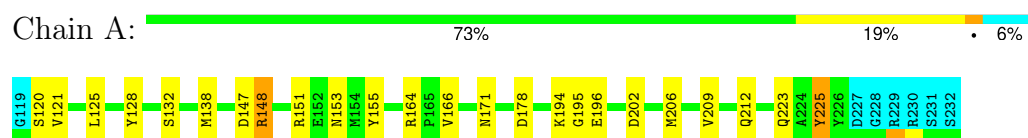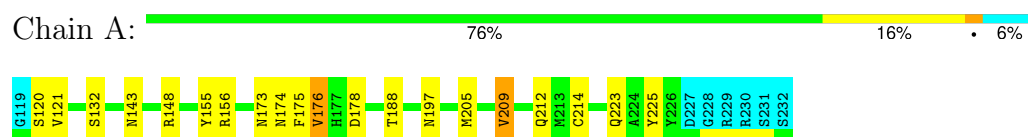### 4.2.10 Score per residue for model 10

• 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 (medoid)

• Molecule 1: Major prion protein

Chain A:

4.2.13 Score per residue for model 13

• Molecule 1: Major prion protein

Chain A:
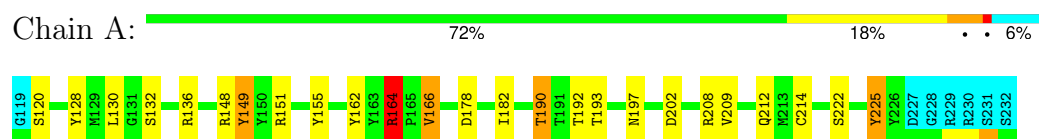
4.2.14 Score per residue for model 14

• Molecule 1: Major prion protein

Chain A:
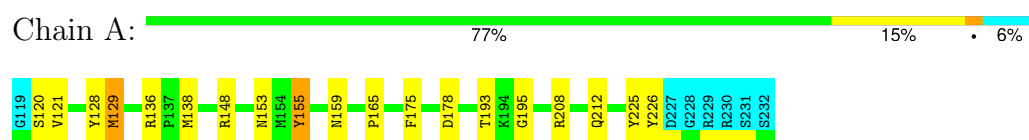
4.2.15 Score per residue for model 15

• Molecule 1: Major prion protein

Chain A:
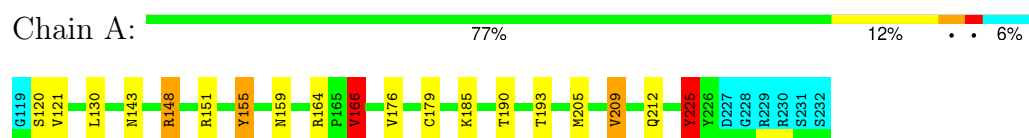
4.2.16 Score per residue for model 16
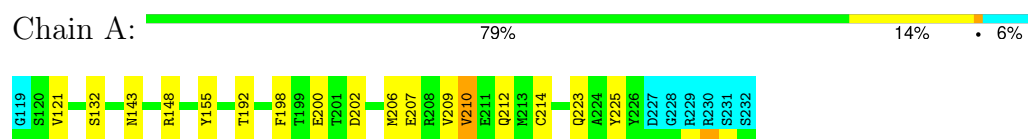
• Molecule 1: Major prion protein

Chain A:
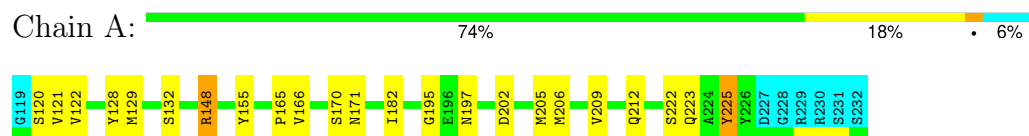
4.2.17 Score per residue for model 17

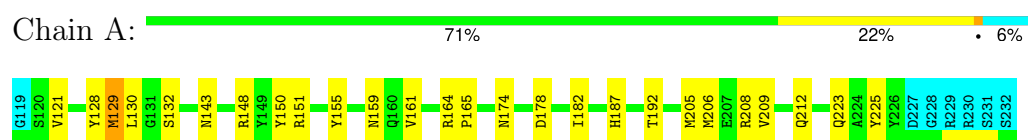• Molecule 1: Major prion protein

Chain A:
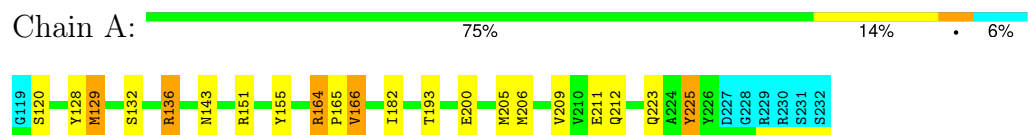
4.2.18 Score per residue for model 18

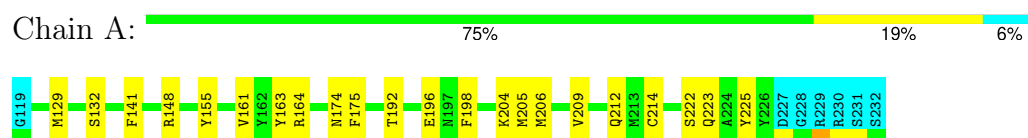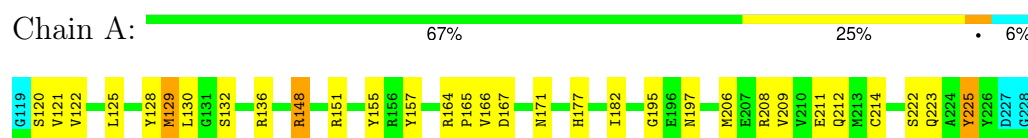• Molecule 1: Major prion protein

Chain A:
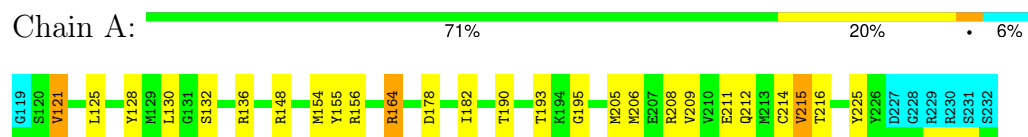
4.2.19 Score per residue for model 19

• Molecule 1: Major prion protein

Chain A:

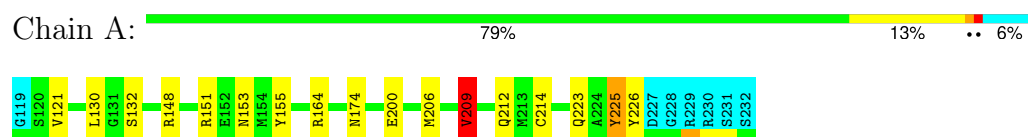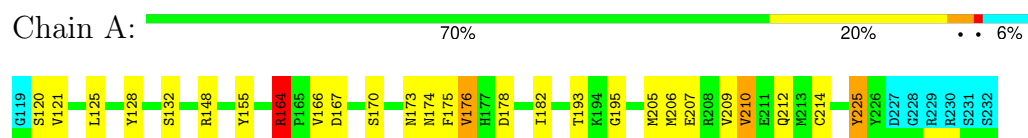#### 4.2.20 Score per residue for model 20

• Molecule 1: Major prion protein

Chain A:
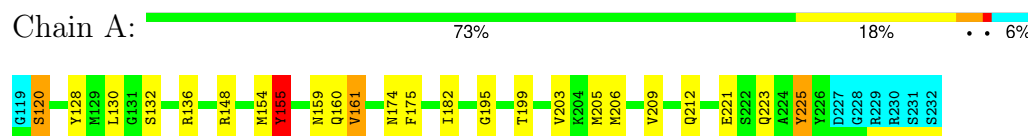
5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics.*

Of the 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 ⓘ

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	0.66±0.00	0±0/900 (0.0± 0.0%)	1.10±0.03	1±1/1218 (0.1± 0.1%)
All	All	0.66	0/18000 (0.0%)	1.10	26/24360 (0.1%)

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	2.2±1.4
All	All	0	44

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	178	ASP	CB-CG-OD1	-9.55	109.71	118.30	7	1
1	A	176	VAL	CA-CB-CG2	9.41	125.01	110.90	19	2
1	A	190	THR	CA-CB-CG2	8.23	123.92	112.40	1	3
1	A	136	ARG	CD-NE-CZ	7.83	134.57	123.60	17	1
1	A	209	VAL	CA-CB-CG1	6.92	121.28	110.90	12	5
1	A	136	ARG	NE-CZ-NH1	6.85	123.73	120.30	17	1
1	A	208	ARG	NE-CZ-NH2	-6.55	117.03	120.30	9	2
1	A	136	ARG	NE-CZ-NH2	-6.31	117.14	120.30	11	2
1	A	215	VAL	CA-CB-CG1	5.87	119.70	110.90	18	1
1	A	166	VAL	CA-CB-CG2	5.69	119.43	110.90	15	1
1	A	209	VAL	CA-CB-CG2	5.68	119.43	110.90	13	1
1	A	161	VAL	CA-CB-CG2	5.68	119.42	110.90	20	1
1	A	210	VAL	CA-CB-CG1	5.56	119.24	110.90	19	1
1	A	215	VAL	CA-CB-CG2	5.34	118.91	110.90	18	1
1	A	148	ARG	NE-CZ-NH2	-5.30	117.65	120.30	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
1	A	156	ARG	NE-CZ-NH2	-5.10	117.75	120.30	4	1
1	A	188	THR	CA-CB-CG2	5.01	119.42	112.40	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	225	TYR	Sidechain	5
1	A	148	ARG	Sidechain	4
1	A	175	PHE	Sidechain	4
1	A	164	ARG	Sidechain	4
1	A	156	ARG	Sidechain	3
1	A	155	TYR	Sidechain	3
1	A	128	TYR	Sidechain	2
1	A	136	ARG	Sidechain	2
1	A	226	TYR	Sidechain	2
1	A	208	ARG	Sidechain	2
1	A	190	THR	Peptide	2
1	A	195	GLY	Peptide	1
1	A	150	TYR	Sidechain	1
1	A	163	TYR	Sidechain	1
1	A	157	TYR	Sidechain	1
1	A	149	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	879	820	820	3±2
All	All	17580	16400	16400	67

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:176:VAL:HG12	1:A:214:CYS:HB2	0.65	1.69	7	2
1:A:206:MET:HA	1:A:209:VAL:HG22	0.56	1.77	10	13
1:A:129:MET:SD	1:A:165:PRO:HD3	0.54	2.43	11	3
1:A:166:VAL:HG22	1:A:225:TYR:CD2	0.53	2.39	4	8
1:A:128:TYR:CE2	1:A:182:ILE:HG13	0.52	2.40	18	8
1:A:176:VAL:HG12	1:A:214:CYS:CB	0.52	2.35	19	2
1:A:129:MET:CE	1:A:165:PRO:HD3	0.50	2.37	1	3
1:A:211:GLU:O	1:A:215:VAL:HG13	0.50	2.06	18	1
1:A:173:ASN:HA	1:A:176:VAL:HG22	0.49	1.85	19	2
1:A:206:MET:O	1:A:210:VAL:HG13	0.49	2.08	8	1
1:A:130:LEU:HD21	1:A:160:GLN:HB3	0.48	1.86	20	1
1:A:128:TYR:CE2	1:A:164:ARG:HG2	0.47	2.44	13	3
1:A:125:LEU:HD13	1:A:128:TYR:HB2	0.47	1.86	11	4
1:A:129:MET:SD	1:A:129:MET:N	0.44	2.90	11	1
1:A:199:THR:O	1:A:203:VAL:HG23	0.44	2.12	4	3
1:A:176:VAL:HA	1:A:179:CYS:SG	0.44	2.53	15	1
1:A:192:THR:HG23	1:A:197:ASN:HA	0.43	1.90	13	1
1:A:206:MET:HA	1:A:209:VAL:HG12	0.43	1.90	12	2
1:A:133:ALA:HB1	1:A:159:ASN:HD21	0.43	1.73	3	1
1:A:130:LEU:HD23	1:A:162:TYR:CE2	0.43	2.49	13	1
1:A:225:TYR:CD1	1:A:225:TYR:C	0.42	2.92	4	3
1:A:173:ASN:HA	1:A:176:VAL:CG2	0.42	2.44	19	1
1:A:166:VAL:CG2	1:A:225:TYR:CD2	0.41	3.03	15	1
1:A:121:VAL:HG23	1:A:125:LEU:O	0.40	2.17	18	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	107/114 (94%)	93±3 (87±3%)	12±3 (11±3%)	2±1 (2±1%)	9	51
All	All	2140/2280 (94%)	1869 (87%)	230 (11%)	41 (2%)	9	51

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	121	VAL	13
1	A	120	SER	11
1	A	195	GLY	6
1	A	198	PHE	4
1	A	122	VAL	2
1	A	194	LYS	1
1	A	141	PHE	1
1	A	132	SER	1
1	A	207	GLU	1
1	A	155	TYR	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	97/102 (95%)	83±2 (86±2%)	14±2 (14±2%)	5	44
All	All	1940/2040 (95%)	1662 (86%)	278 (14%)	5	44

All 50 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	155	TYR	20
1	A	212	GLN	20
1	A	225	TYR	20
1	A	148	ARG	19
1	A	132	SER	16
1	A	223	GLN	14
1	A	205	MET	12
1	A	164	ARG	10
1	A	214	CYS	9
1	A	193	THR	8
1	A	174	ASN	8
1	A	129	MET	7
1	A	143	ASN	7
1	A	178	ASP	7
1	A	120	SER	6
1	A	130	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	200	GLU	6
1	A	153	ASN	5
1	A	222	SER	5
1	A	159	ASN	5
1	A	166	VAL	5
1	A	202	ASP	5
1	A	211	GLU	4
1	A	197	ASN	4
1	A	209	VAL	4
1	A	136	ARG	4
1	A	138	MET	3
1	A	196	GLU	3
1	A	171	ASN	3
1	A	192	THR	3
1	A	151	ARG	3
1	A	161	VAL	3
1	A	177	HIS	2
1	A	181	ASN	2
1	A	210	VAL	2
1	A	167	ASP	2
1	A	170	SER	2
1	A	154	MET	2
1	A	179	CYS	1
1	A	147	ASP	1
1	A	207	GLU	1
1	A	187	HIS	1
1	A	204	LYS	1
1	A	208	ARG	1
1	A	149	TYR	1
1	A	190	THR	1
1	A	175	PHE	1
1	A	185	LYS	1
1	A	216	THR	1
1	A	221	GLU	1

6.3.3   RNA ⓘ

There are no RNA molecules in this entry.

6.4   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides 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 (i)

No chemical shift data were provided