



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:01 AM BST

PDB ID : 2L1E
Title : Mouse prion protein (121-231) containing the substitution F175A
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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

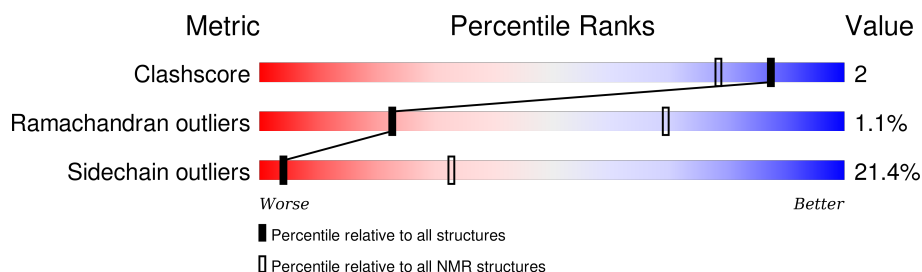
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	 68% 19% • 12%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 9 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:128-A:227 (100)	0.34	9

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1799 atoms, of which 868 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
			1799	574	868	165	183	9	

There are 3 discrepancies between the modelled and reference sequences:

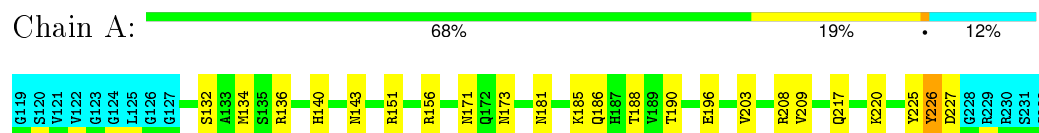
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	EXPRESSION TAG	UNP Q4FJQ7
A	120	SER	-	EXPRESSION TAG	UNP Q4FJQ7
A	175	ALA	PHE	ENGINEERED MUTATION	UNP Q4FJQ7

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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

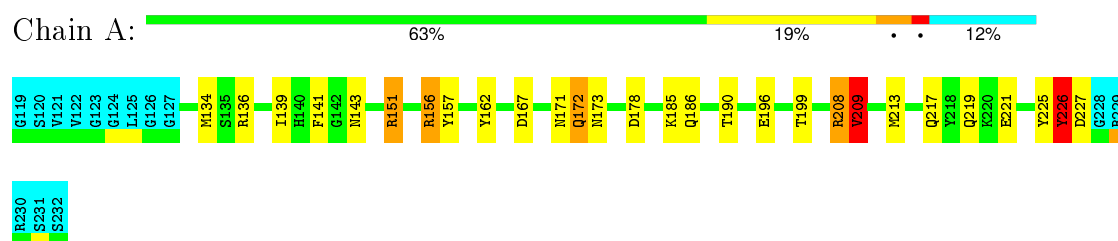


4.2 Scores per residue for each member of the ensemble

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

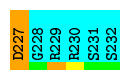
- Molecule 1: Major prion protein





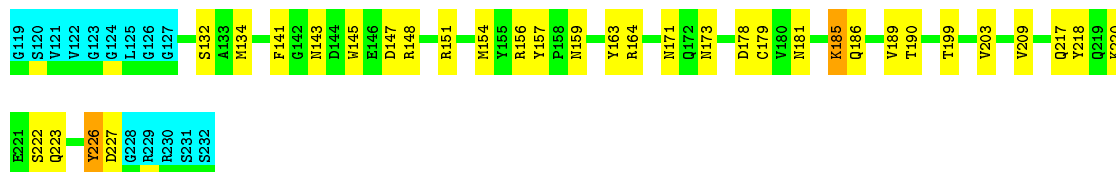
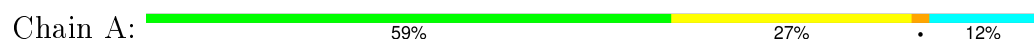
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



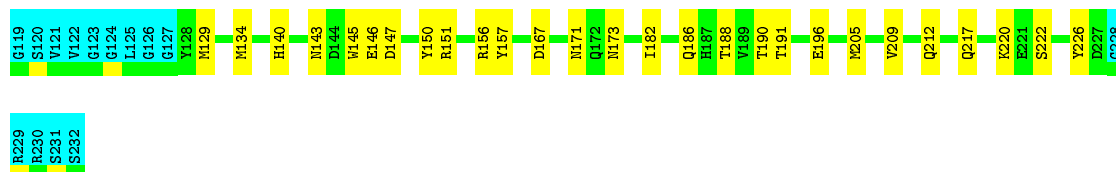
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



4.2.5 Score per residue for model 5

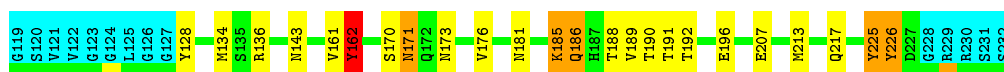
- Molecule 1: Major prion protein



4.2.6 Score per residue for model 6

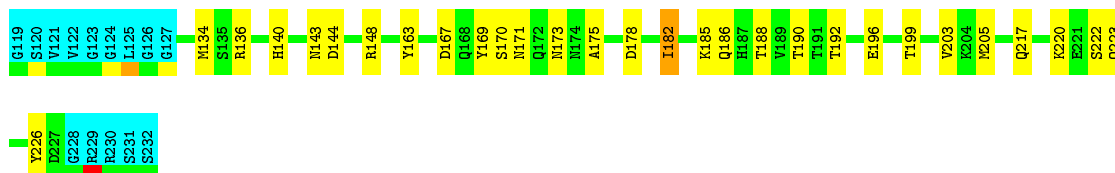
- Molecule 1: Major prion protein





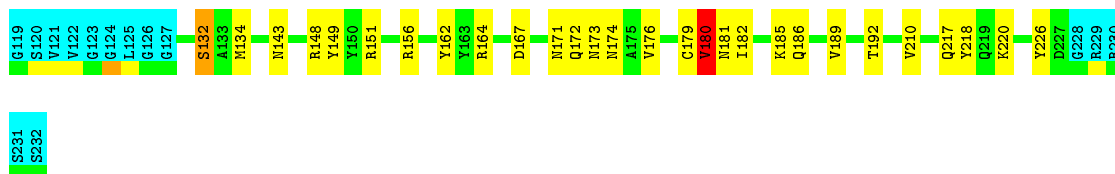
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



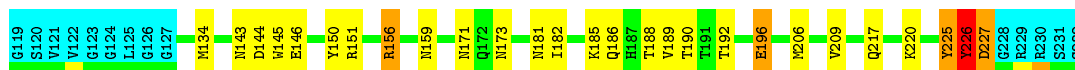
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Major prion protein



4.2.10 Score per residue for model 10

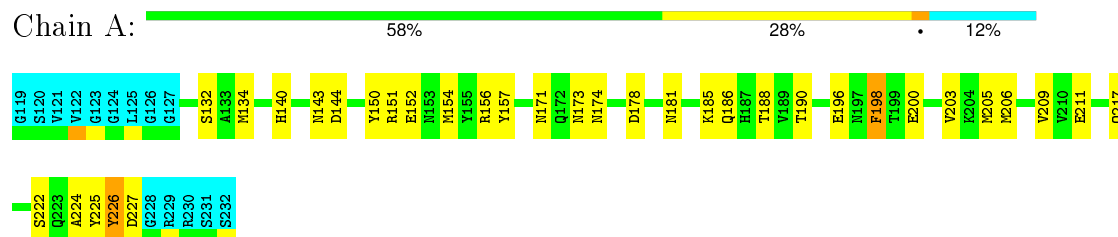
- Molecule 1: Major prion protein





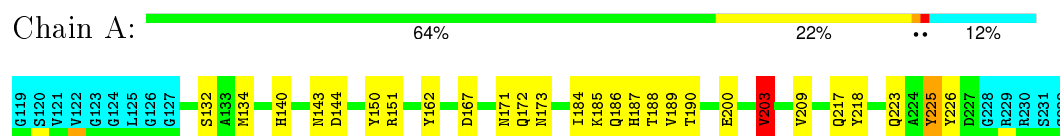
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



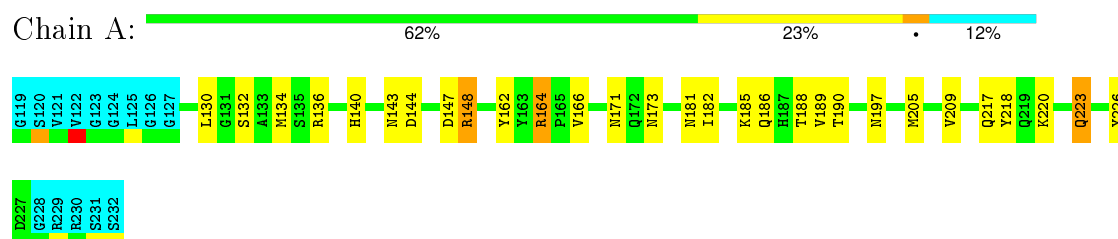
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



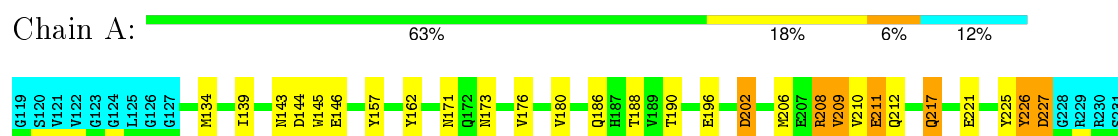
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



4.2.14 Score per residue for model 14

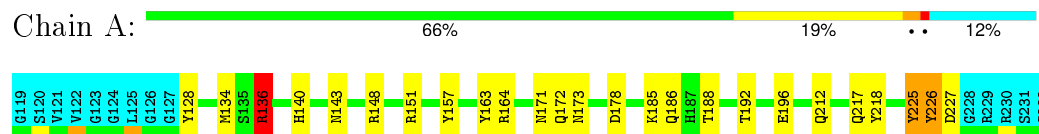
- Molecule 1: Major prion protein



S232

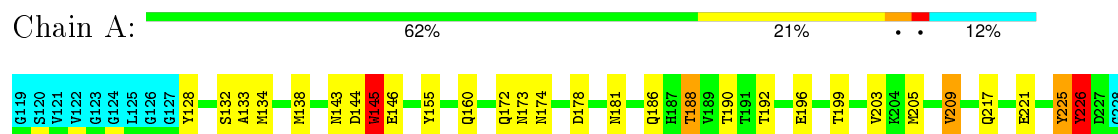
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



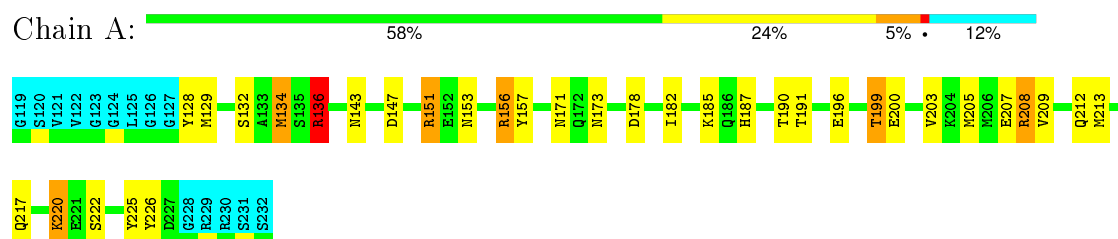
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein

R229
R230
S231
S232

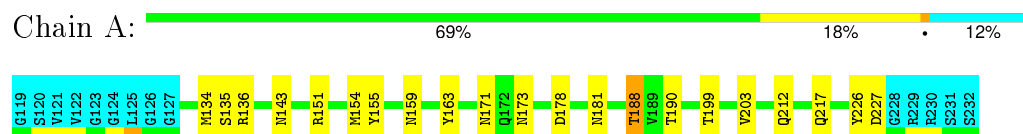
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein

Q217
R220
E221
S222
Y225
Y226
D227
G228
R229
R230
S231
S232

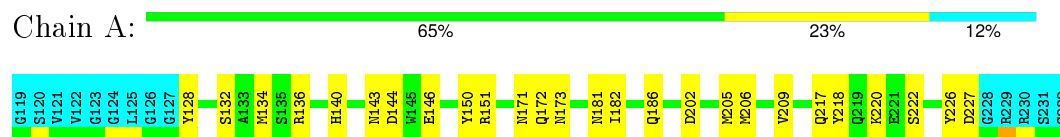
4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



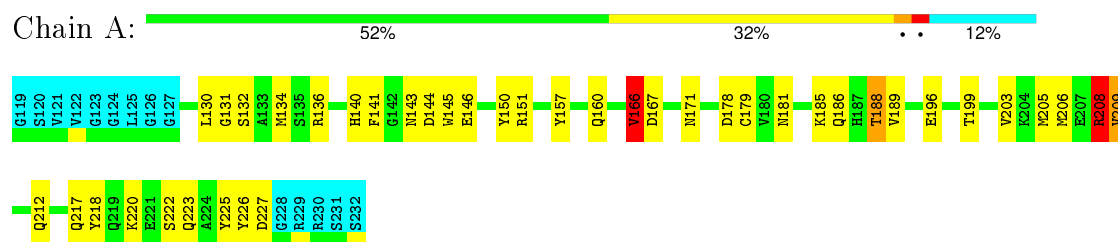
4.2.19 Score per residue for model 19

- 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	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 17082
Number of chemical shift lists	1
Total number of shifts	1411
Number of shifts mapped to atoms	1411
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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	0.69±0.01	0±0/866 (0.0±0.0%)	1.16±0.03	2±1/1174 (0.2±0.1%)
All	All	0.69	0/17320 (0.0%)	1.16	43/23480 (0.2%)

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	2.8±1.2
All	All	0	55

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	209	VAL	CA-CB-CG2	9.66	125.39	110.90	10	5
1	A	203	VAL	CA-CB-CG1	7.71	122.46	110.90	12	2
1	A	166	VAL	CG1-CB-CG2	7.20	122.41	110.90	20	1
1	A	156	ARG	NE-CZ-NH2	-7.10	116.75	120.30	1	2
1	A	156	ARG	NE-CZ-NH1	7.04	123.82	120.30	9	1
1	A	188	THR	CA-CB-CG2	6.76	121.86	112.40	18	3
1	A	151	ARG	NE-CZ-NH1	6.67	123.63	120.30	2	2
1	A	210	VAL	CA-CB-CG2	6.46	120.59	110.90	14	1
1	A	136	ARG	NE-CZ-NH2	-6.45	117.07	120.30	15	1
1	A	164	ARG	NE-CZ-NH1	6.39	123.50	120.30	15	3
1	A	148	ARG	NE-CZ-NH1	6.38	123.49	120.30	3	1
1	A	209	VAL	CA-CB-CG1	6.15	120.12	110.90	20	2
1	A	132	SER	N-CA-CB	-6.09	101.36	110.50	17	3
1	A	163	TYR	CB-CG-CD2	-6.09	117.34	121.00	7	1
1	A	180	VAL	CA-CB-CG1	5.89	119.73	110.90	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	162	TYR	CB-CG-CD2	-5.85	117.49	121.00	6	1
1	A	136	ARG	CD-NE-CZ	5.82	131.75	123.60	2	1
1	A	176	VAL	CA-CB-CG1	5.64	119.35	110.90	6	1
1	A	190	THR	CA-CB-CG2	5.56	120.18	112.40	13	1
1	A	218	TYR	CB-CG-CD1	-5.50	117.70	121.00	12	2
1	A	199	THR	CA-CB-CG2	-5.41	104.83	112.40	17	1
1	A	202	ASP	CB-CG-OD2	-5.33	113.51	118.30	14	1
1	A	157	TYR	CB-CG-CD2	-5.28	117.83	121.00	17	1
1	A	135	SER	C-N-CA	5.26	134.86	121.70	10	1
1	A	164	ARG	CD-NE-CZ	5.25	130.95	123.60	8	1
1	A	164	ARG	NE-CZ-NH2	-5.20	117.70	120.30	8	1
1	A	226	TYR	CB-CG-CD2	-5.12	117.93	121.00	16	1
1	A	136	ARG	NE-CZ-NH1	5.08	122.84	120.30	18	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	150	TYR	Sidechain	8
1	A	162	TYR	Sidechain	7
1	A	128	TYR	Sidechain	4
1	A	157	TYR	Sidechain	4
1	A	156	ARG	Sidechain	4
1	A	163	TYR	Sidechain	3
1	A	218	TYR	Sidechain	3
1	A	151	ARG	Sidechain	3
1	A	208	ARG	Sidechain	3
1	A	136	ARG	Sidechain	3
1	A	148	ARG	Sidechain	3
1	A	226	TYR	Sidechain	2
1	A	141	PHE	Sidechain	1
1	A	164	ARG	Sidechain	1
1	A	169	TYR	Sidechain	1
1	A	155	TYR	Sidechain	1
1	A	149	TYR	Sidechain	1
1	A	196	GLU	Peptide	1
1	A	198	PHE	Sidechain	1
1	A	225	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	845	780	780	4±2
All	All	16900	15600	15600	81

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:206:MET:HA	1:A:209:VAL:HG22	0.76	1.55	10	4
1:A:191:THR:HG22	1:A:196:GLU:HB3	0.63	1.69	17	5
1:A:185:LYS:O	1:A:189:VAL:HG23	0.61	1.94	13	3
1:A:199:THR:O	1:A:203:VAL:HG23	0.57	1.99	4	6
1:A:184:ILE:HG21	1:A:203:VAL:HG23	0.57	1.76	12	1
1:A:141:PHE:CE1	1:A:208:ARG:CZ	0.56	2.89	20	2
1:A:169:TYR:CD2	1:A:175:ALA:HB2	0.54	2.37	7	1
1:A:200:GLU:HA	1:A:203:VAL:HG12	0.54	1.79	11	4
1:A:200:GLU:HA	1:A:203:VAL:CG1	0.54	2.33	12	2
1:A:162:TYR:CE2	1:A:186:GLN:HG2	0.54	2.37	6	1
1:A:172:GLN:NE2	1:A:219:GLN:HE21	0.50	2.04	1	1
1:A:133:ALA:HB2	1:A:160:GLN:CD	0.50	2.26	16	1
1:A:191:THR:HG22	1:A:196:GLU:CB	0.49	2.37	17	2
1:A:145:TRP:CG	1:A:146:GLU:N	0.49	2.81	16	3
1:A:206:MET:HA	1:A:209:VAL:CG2	0.47	2.39	19	2
1:A:141:PHE:CE1	1:A:208:ARG:NH2	0.47	2.83	20	2
1:A:136:ARG:HH12	1:A:209:VAL:HG11	0.46	1.69	17	1
1:A:226:TYR:CD1	1:A:227:ASP:N	0.45	2.84	9	5
1:A:130:LEU:HD11	1:A:160:GLN:NE2	0.45	2.27	20	1
1:A:198:PHE:CD2	1:A:206:MET:CE	0.45	2.98	11	1
1:A:134:MET:SD	1:A:220:LYS:HE3	0.45	2.51	17	1
1:A:225:TYR:CE1	1:A:226:TYR:HB3	0.45	2.46	15	4
1:A:185:LYS:O	1:A:189:VAL:HG12	0.45	2.12	9	3
1:A:223:GLN:HE21	1:A:223:GLN:HA	0.45	1.72	13	1
1:A:180:VAL:HG22	1:A:211:GLU:HA	0.45	1.89	14	1
1:A:161:VAL:HG11	1:A:213:MET:HB2	0.44	1.88	6	1
1:A:166:VAL:CG1	1:A:218:TYR:CE1	0.44	3.01	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:ASN:HD21	1:A:174:ASN:ND2	0.43	2.12	10	1
1:A:176:VAL:HG22	1:A:218:TYR:CD2	0.43	2.49	8	2
1:A:217:GLN:HE22	1:A:221:GLU:HG3	0.43	1.73	14	1
1:A:186:GLN:HA	1:A:189:VAL:HG12	0.42	1.91	20	2
1:A:154:MET:HA	1:A:157:TYR:CD2	0.42	2.50	11	2
1:A:150:TYR:CG	1:A:208:ARG:CZ	0.42	3.03	20	1
1:A:191:THR:HG21	1:A:198:PHE:CZ	0.42	2.50	3	1
1:A:225:TYR:CE1	1:A:226:TYR:CD1	0.41	3.08	10	2
1:A:209:VAL:HB	1:A:213:MET:SD	0.41	2.55	1	1
1:A:145:TRP:CE2	1:A:146:GLU:HG2	0.41	2.50	9	2
1:A:130:LEU:C	1:A:130:LEU:HD13	0.41	2.36	10	1
1:A:180:VAL:HA	1:A:210:VAL:HG12	0.41	1.93	8	1
1:A:145:TRP:CZ2	1:A:146:GLU:CD	0.41	2.94	14	1
1:A:139:ILE:HG21	1:A:208:ARG:HD3	0.41	1.92	3	1
1:A:157:TYR:CE1	1:A:206:MET:SD	0.40	3.14	20	1
1:A:176:VAL:O	1:A:180:VAL:HG23	0.40	2.16	14	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	100/114 (88%)	88±2 (88±2%)	11±3 (11±3%)	1±1 (1±1%)	23	69
All	All	2000/2280 (88%)	1751 (88%)	228 (11%)	21 (1%)	23	69

All 14 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	227	ASP	4
1	A	132	SER	2
1	A	159	ASN	2
1	A	136	ARG	2
1	A	187	HIS	2
1	A	131	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	166	VAL	1
1	A	171	ASN	1
1	A	185	LYS	1
1	A	145	TRP	1
1	A	144	ASP	1
1	A	163	TYR	1
1	A	170	SER	1
1	A	224	ALA	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	94/102 (92%)	74±3 (79±3%)	20±3 (21±3%)	4	33
All	All	1880/2040 (92%)	1478 (79%)	402 (21%)	4	33

All 61 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	226	TYR	20
1	A	134	MET	20
1	A	217	GLN	20
1	A	143	ASN	20
1	A	173	ASN	19
1	A	171	ASN	18
1	A	190	THR	14
1	A	188	THR	13
1	A	181	ASN	13
1	A	220	LYS	12
1	A	186	GLN	11
1	A	225	TYR	11
1	A	140	HIS	11
1	A	151	ARG	11
1	A	178	ASP	9
1	A	182	ILE	9
1	A	185	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	144	ASP	9
1	A	222	SER	8
1	A	136	ARG	8
1	A	209	VAL	8
1	A	132	SER	8
1	A	205	MET	8
1	A	192	THR	8
1	A	196	GLU	8
1	A	212	GLN	7
1	A	172	GLN	7
1	A	156	ARG	6
1	A	167	ASP	6
1	A	227	ASP	6
1	A	147	ASP	5
1	A	223	GLN	5
1	A	179	CYS	5
1	A	129	MET	4
1	A	208	ARG	4
1	A	145	TRP	3
1	A	148	ARG	3
1	A	164	ARG	3
1	A	174	ASN	3
1	A	221	GLU	3
1	A	211	GLU	2
1	A	202	ASP	2
1	A	199	THR	2
1	A	139	ILE	2
1	A	207	GLU	2
1	A	170	SER	2
1	A	203	VAL	1
1	A	135	SER	1
1	A	153	ASN	1
1	A	152	GLU	1
1	A	180	VAL	1
1	A	146	GLU	1
1	A	155	TYR	1
1	A	197	ASN	1
1	A	154	MET	1
1	A	166	VAL	1
1	A	213	MET	1
1	A	130	LEU	1
1	A	138	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	159	ASN	1
1	A	214	CYS	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 carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17082

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1411
Number of shifts mapped to atoms	1411
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	114	0.16 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	105	0.68 ± 0.11	Should be applied
$^{13}\text{C}'$	113	2.42 ± 0.12	Should be applied
^{15}N	110	-0.10 ± 0.19	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1163 atoms were assigned a chemical shift out of a possible 1286. 10 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	490/494 (99%)	194/197 (98%)	199/200 (100%)	97/97 (100%)
Sidechain	570/653 (87%)	362/385 (94%)	186/230 (81%)	22/38 (58%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	103/139 (74%)	65/72 (90%)	37/63 (59%)	1/4 (25%)
Overall	1163/1286 (90%)	621/654 (95%)	422/493 (86%)	120/139 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1280 atoms were assigned a chemical shift out of a possible 1422. 13 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	555/564 (98%)	218/225 (97%)	227/228 (100%)	110/111 (99%)
Sidechain	622/719 (87%)	393/424 (93%)	205/251 (82%)	24/44 (55%)
Aromatic	103/139 (74%)	65/72 (90%)	37/63 (59%)	1/4 (25%)
Overall	1280/1422 (90%)	676/721 (94%)	469/542 (87%)	135/159 (85%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	217	GLN	HG3	0.83	3.75 – 0.85	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

