



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1DX0
Title : BOVINE PRION PROTEIN RESIDUES 23-230
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This is a wwPDB NMR Structure Validation Summary 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
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

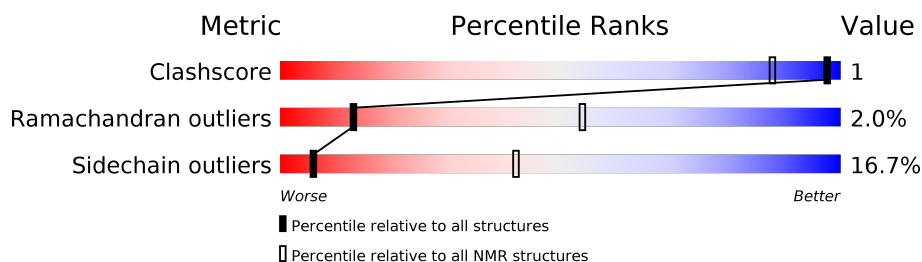
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	219	 37% 8% .. 53%

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1675 atoms, of which 806 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRION PROTEIN.

Mol	Chain	Residues	Atoms							Trace
1	A	104	Total	C	H	N	O	S		0
			1675	540	806	151	170	8		

- Molecule 1: PRION PROTEIN

D147	R148	Y149	R156	Y157	P158	N159	Y162	Q168	N173	N174	F175	H187	T190	T191	F198	T199	M205	V209	S222	Y225	Y226	Q227	ARG	GLY	ALA	
GLY	TRP	GLN	PRO	HIS	GLY	GLY	TRP	GLN	PRO	HIS	GLY	GLY	TRP	GLN	GLN	THR	HIS	GLY	ASN	LYS	PRO	SER	LYS	ASN	THR	ALA
GLY	SER	LYS	ARG	PRO	LYS	PRO	GLY	TRP	ASN	GLY	SER	ARG	TYR	PRO	GLN	SER	PRO	GLY	ASN	TYR	PRO	PRO	GLN	GLY	GLY	

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 50 calculated structures, 1 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
OPALP	refinement	
DYANA	structure solution	

No chemical shift data was provided. 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	0.68	0/889 (0.0%)	1.16	6/1201 (0.5%)
All	All	0.68	0/889 (0.0%)	1.16	6/1201 (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	5
All	All	0	5

There are no bond-length outliers.

5 of 6 angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	TYR	CB-CG-CD1	-7.23	116.66	121.00
1	A	156	ARG	CD-NE-CZ	6.79	133.10	123.60
1	A	156	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	190	THR	CA-CB-CG2	-5.23	105.08	112.40
1	A	191	THR	CA-CB-OG1	5.15	119.82	109.00

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	128	TYR	Sidechain
1	A	149	TYR	Sidechain
1	A	162	TYR	Sidechain
1	A	225	TYR	Sidechain
1	A	157	TYR	Sidechain

6.2 Too-close contacts [i](#)

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	869	806	805	1
All	All	869	806	805	1

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 clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:191:THR:HG21	1:A:198:PHE:CE2	0.48	2.43

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	102/219 (47%)	89 (87%)	11 (11%)	2 (2%)	13	54
All	All	102/219 (47%)	89 (87%)	11 (11%)	2 (2%)	13	54

All 2 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	168	GLN
1	A	128	TYR

6.3.2 Protein sidechains [i](#)

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	96/161 (60%)	80 (83%)	16 (17%)	6	42
All	All	96/161 (60%)	80 (83%)	16 (17%)	6	42

5 of 16 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	222	SER
1	A	159	ASN
1	A	187	HIS
1	A	191	THR
1	A	209	VAL

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

No chemical shift data were provided