



wwPDB NMR Structure Validation Summary Report ⓘ

Feb 12, 2017 – 07:33 pm GMT

PDB ID : 1QLX
Title : HUMAN PRION PROTEIN
Authors : Zahn, R.; Liu, A.; Luhrs, T.; Wuthrich, K.
Deposited on : 1999-09-17

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

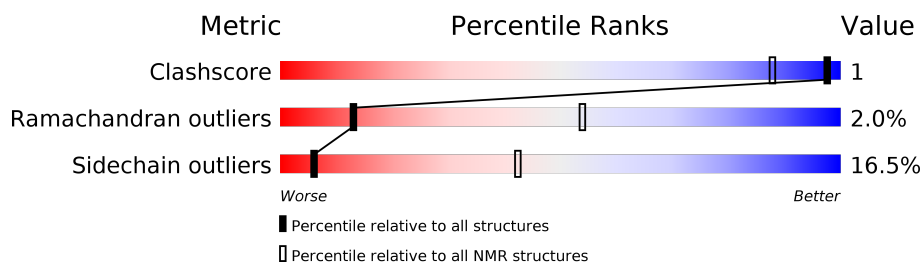
1 Overall quality at a glance

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	210	

2 Ensemble composition and analysis ⓘ

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1688 atoms, of which 811 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
			1688	544	811	153	171	9	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	CLONING ARTIFACT	UNP P04156
A	22	SER	-	CLONING ARTIFACT	UNP P04156

- Molecule 1: PRION PROTEIN

GLY	S170	TRP	GLY	SER
LYS	M171	GLN	GLY	LYS
ARG	Q172	PRO	PRO	ARG
PRO	M173	GLY	GLY	PRO
LYS	D178	GLY	GLY	LYS
PRO	H187	TRP	TRP	PRO
GLY	M197	GLN	GLY	GLY
TRP	M206	GLY	GLY	ASN
GLY	E207	THR	GLY	THR
GLY	R208	THR	GLY	GLY
SER	E211	HIS	SER	SER
ARG	Q217	SER	GLN	ARG
TYR	Q217	GLN	TRP	TYR
PRO	Q227	TRP	ASN	PRO
GLY	R228	LYS	GLY	PRO
SER	GLY	PRO	LYS	GLN
PRO	SER	LYS	SER	GLY
GLY	GLY	PRO	PRO	GLY
GLY	GLY	THR	THR	ASN
ASN	ASN	ASN	ASN	ARG
TYR	TYR	MET	MET	TYR
PRO	LYS	LYS	LYS	PRO
PRO	HIS	HIS	HIS	PRO
GLN	ALA	ALA	ALA	GLN
GLY	GLY	GLY	GLY	GLY
GLY	ALA	ALA	ALA	GLY
GLY	ALA	ALA	ALA	GLY
PRO	ALA	ALA	ALA	PRO
HIS	VAL	VAL	VAL	HIS
GLY	VAL	VAL	VAL	GLY
GLY	GLY	GLY	GLY	GLY
GLY	GLY	GLY	GLY	GLY
TRP	L125	GLY	TRP	TRP
GLY	L130	GLY	GLN	GLY
GLN	G131	GLY	PRO	GLN
PRO	S132	GLY	HIS	PRO
HIS	S135	GLY	GLY	HIS
GLY	S135	GLY	GLY	GLY
GLY	Y145	GLY	TRP	GLY
TRP	Y145	GLY	TRP	TRP
GLY	R148	GLY	GLN	GLY
GLN	Y149	GLY	GLN	GLN
PRO	Y150	GLY	PRO	PRO
HIS	Y150	GLY	HIS	HIS
GLY	GLY	GLY	GLY	GLY
GLY	N159	GLY	GLY	GLY
TYR	G159	GLY	GLY	TYR

5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 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 [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

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	2
All	All	0	2

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	228	ARG	Sidechain
1	A	145	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	877	811	813	1
All	All	877	811	813	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:130:LEU:HD11	1:A:160:GLN:HB2	0.48	1.85

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	102/210 (49%)	94 (92%)	6 (6%)	2 (2%)	13	54
All	All	102/210 (49%)	94 (92%)	6 (6%)	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	171	ASN
1	A	170	SER

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	97/159 (61%)	81 (84%)	16 (16%)	6	42
All	All	97/159 (61%)	81 (84%)	16 (16%)	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	227	GLN
1	A	217	GLN
1	A	132	SER
1	A	135	SER
1	A	197	ASN

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 carbohydrates 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

No chemical shift data were provided