W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 08:45 PM GMT

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PDB ID	:	4YXH
Title	:	Crystal structure of Deer prion protein complexed with POM1 FAB
Authors	:	Baral, P.K.; Swayampakula, M.; James, M.N.G.
Deposited on	:	2015-03-23
Resolution	:	2.70 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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
Rfree		0.313
Clashscore		31
Ramachandran outliers		1.7%
Sidechain outliers		4.9%
RSRZ outliers		18.8%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
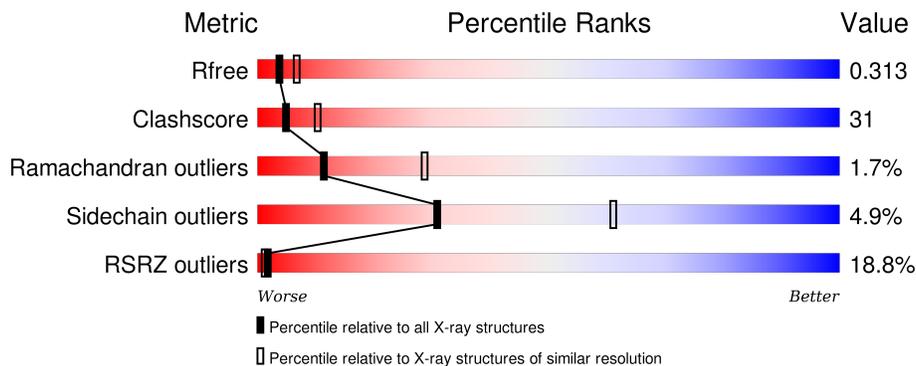
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	4% 52% 21% • 25%
2	H	218	16% 68% 27% 5%
3	L	213	28% 56% 33% 9% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	L	301	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4223 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	101	851	530	148	165	8	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	MET	-	expression tag	UNP P47852
A	87	GLY	-	expression tag	UNP P47852
A	88	SER	-	expression tag	UNP P47852
A	89	SER	-	expression tag	UNP P47852
A	90	HIS	-	expression tag	UNP P47852
A	91	HIS	-	expression tag	UNP P47852
A	92	HIS	-	expression tag	UNP P47852
A	93	HIS	-	expression tag	UNP P47852
A	94	HIS	-	expression tag	UNP P47852
A	95	HIS	-	expression tag	UNP P47852
A	96	SER	-	expression tag	UNP P47852
A	97	SER	-	expression tag	UNP P47852
A	98	GLY	-	expression tag	UNP P47852
A	99	LEU	-	expression tag	UNP P47852
A	100	VAL	-	expression tag	UNP P47852
A	101	PRO	-	expression tag	UNP P47852
A	102	ARG	-	expression tag	UNP P47852
A	103	GLY	-	expression tag	UNP P47852
A	104	SER	-	expression tag	UNP P47852
A	105	HIS	-	expression tag	UNP P47852
A	106	MET	-	expression tag	UNP P47852
A	107	LEU	-	expression tag	UNP P47852
A	108	GLU	-	expression tag	UNP P47852
A	109	ASP	-	expression tag	UNP P47852
A	110	PRO	-	expression tag	UNP P47852
A	111	HIS	-	expression tag	UNP P47852
A	112	MET	-	expression tag	UNP P47852

- Molecule 2 is a protein called POM1 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1642	1037	265	330	10	0	0	0

- Molecule 3 is a protein called POM1 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	1652	1022	280	345	5	0	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	L	1	1	1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total 18	O 18	0	0
5	H	30	Total 30	O 30	0	0
5	L	29	Total 29	O 29	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Major prion protein
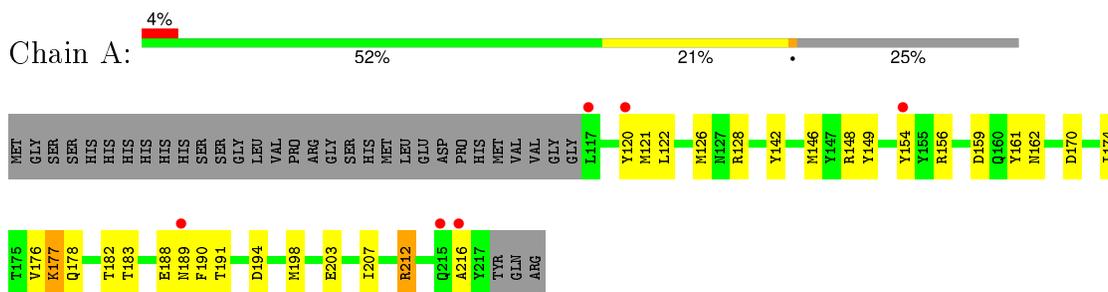
- Molecule 2: POM1 FAB HEAVY CHAIN
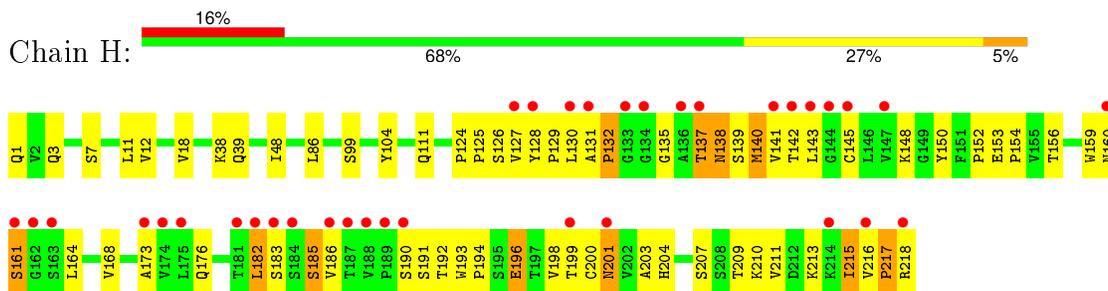
- Molecule 3: POM1 FAB LIGHT CHAIN
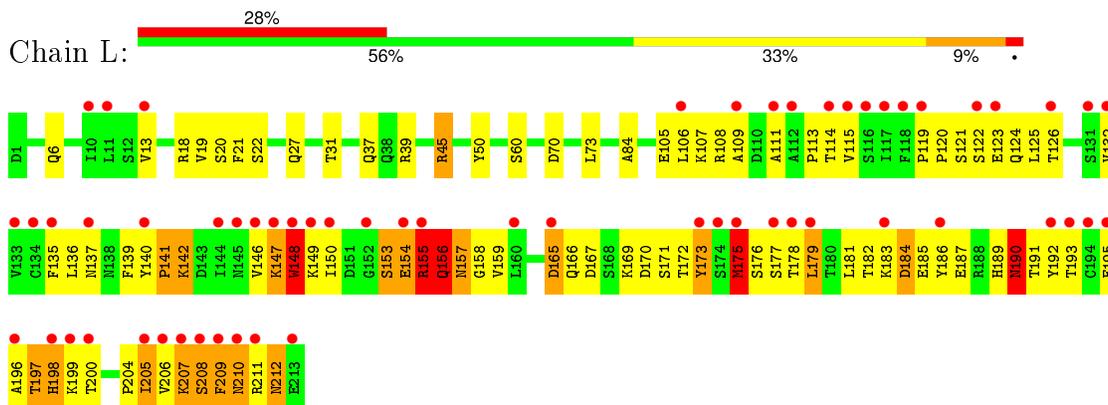
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.28Å 106.58Å 75.78Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	38.33 – 2.70 47.77 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.33-2.70) 91.4 (47.77-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$<I/\sigma(I)>$ [1]	1.78 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.242 , 0.288 0.273 , 0.313	Depositor DCC
R_{free} test set	870 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 51.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 18203 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4223	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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 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	0/870	0.95	3/1177 (0.3%)
2	H	0.72	0/1688	0.96	4/2306 (0.2%)
3	L	0.81	2/1687 (0.1%)	1.38	25/2291 (1.1%)
All	All	0.76	2/4245 (0.0%)	1.14	32/5774 (0.6%)

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 outliers	#Planarity outliers
1	A	0	1
3	L	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	141	PRO	N-CD	5.91	1.56	1.47
3	L	153	SER	CA-CB	5.29	1.60	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	179	LEU	CA-CB-CG	15.16	150.16	115.30
3	L	141	PRO	CA-N-CD	-10.43	96.90	111.50
3	L	173	TYR	CB-CG-CD2	-8.44	115.94	121.00
3	L	210	ASN	N-CA-C	8.20	133.13	111.00
3	L	148	TRP	CA-C-N	8.04	134.88	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	ASN	Sidechain
3	L	148	TRP	Mainchain
3	L	155	ARG	Mainchain
3	L	45	ARG	Sidechain

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	851	0	793	23	0
2	H	1642	0	1580	81	0
3	L	1652	0	1573	155	0
4	L	1	0	0	0	0
5	A	18	0	0	5	0
5	H	30	0	0	2	0
5	L	29	0	0	4	0
All	All	4223	0	3946	252	0

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 31.

The worst 5 of 252 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:141:PRO:HG2	3:L:199:LYS:NZ	1.42	1.31
3:L:154:GLU:O	3:L:155:ARG:HG3	1.37	1.23
3:L:150:ILE:HG13	3:L:154:GLU:OE2	1.40	1.21
3:L:198:HIS:CE1	3:L:205:ILE:HD11	1.81	1.16
2:H:138:ASN:HB2	2:H:140:MET:HG3	1.31	1.13

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	99/135 (73%)	97 (98%)	2 (2%)	0	100	100
2	H	216/218 (99%)	207 (96%)	6 (3%)	3 (1%)	14	35
3	L	211/213 (99%)	192 (91%)	13 (6%)	6 (3%)	6	15
All	All	526/566 (93%)	496 (94%)	21 (4%)	9 (2%)	11	29

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	135	GLY
3	L	154	GLU
3	L	198	HIS
2	H	138	ASN
3	L	155	ARG

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	94/123 (76%)	92 (98%)	2 (2%)	61	87
2	H	187/187 (100%)	175 (94%)	12 (6%)	22	47
3	L	191/191 (100%)	182 (95%)	9 (5%)	32	63
All	All	472/501 (94%)	449 (95%)	23 (5%)	31	61

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	191	SER
2	H	201	ASN
3	L	190	ASN
2	H	196	GLU
2	H	215	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
2	H	201	ASN
3	L	189	HIS
3	L	198	HIS
3	L	212	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	101/135 (74%)	0.38	6 (5%)	26	24	45, 65, 95, 107	0
2	H	218/218 (100%)	0.76	35 (16%)	3	2	39, 61, 132, 146	0
3	L	213/213 (100%)	1.20	59 (27%)	1	1	43, 78, 147, 155	0
All	All	532/566 (93%)	0.86	100 (18%)	2	1	39, 68, 140, 155	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	116	SER	8.5
3	L	206	VAL	7.7
2	H	134	GLY	7.5
2	H	130	LEU	6.8
3	L	194	CYS	6.4

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NA	L	301	1/1	0.65	0.38	2.76	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.