Full wwPDB X-ray Structure Validation Report (i)

Jan 24, 2017 – 02:48 PM EST

PDB ID	:	3DXD
Title	:	Crystal structure of the intracellular domain of human APP (T668E mutant) in complex with Fe65-PTB2
Authors	:	Radzimanowski, J.; Sinning, I.; Wild, K.
Deposited on	:	2008-07-24
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

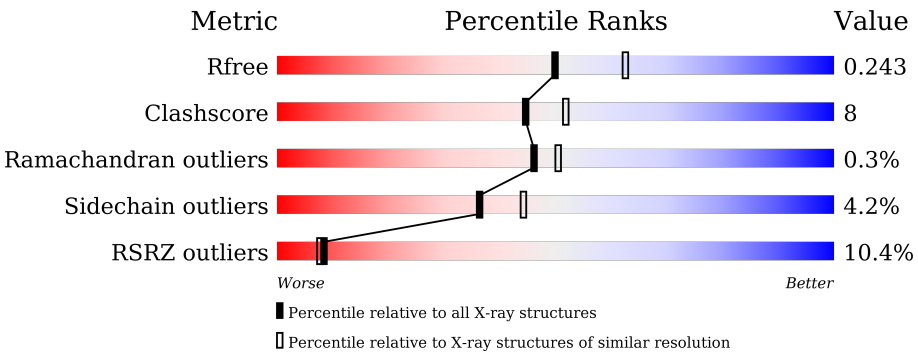
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	140	10%, 74%, 19%, • 6%
1	C	140	4%, 79%, 9%, 12%
2	B	35	14%, 51%, 20%, 6%, 23%
2	D	35	20%, 63%, 9%, •, 26%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2569 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 Amyloid beta A4 protein-binding family B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	131	1003	637	174	183	9	0	0	0
1	C	123	938	598	162	169	9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	HIS	-	EXPRESSION TAG	UNP O00213
A	669	HIS	-	EXPRESSION TAG	UNP O00213
A	670	HIS	-	EXPRESSION TAG	UNP O00213
A	671	HIS	-	EXPRESSION TAG	UNP O00213
A	672	HIS	-	EXPRESSION TAG	UNP O00213
A	673	HIS	-	EXPRESSION TAG	UNP O00213
C	668	HIS	-	EXPRESSION TAG	UNP O00213
C	669	HIS	-	EXPRESSION TAG	UNP O00213
C	670	HIS	-	EXPRESSION TAG	UNP O00213
C	671	HIS	-	EXPRESSION TAG	UNP O00213
C	672	HIS	-	EXPRESSION TAG	UNP O00213
C	673	HIS	-	EXPRESSION TAG	UNP O00213

- Molecule 2 is a protein called Amyloid beta A4 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	27	254	159	43	50	2	0	2	0
2	D	26	246	154	42	49	1	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	661	GLY	-	EXPRESSION TAG	UNP P05067
B	662	ALA	-	EXPRESSION TAG	UNP P05067
B	663	MET	-	EXPRESSION TAG	UNP P05067
B	668	GLU	THR	ENGINEERED	UNP P05067
D	661	GLY	-	EXPRESSION TAG	UNP P05067
D	662	ALA	-	EXPRESSION TAG	UNP P05067
D	663	MET	-	EXPRESSION TAG	UNP P05067
D	668	GLU	THR	ENGINEERED	UNP P05067

- Molecule 3 is water.

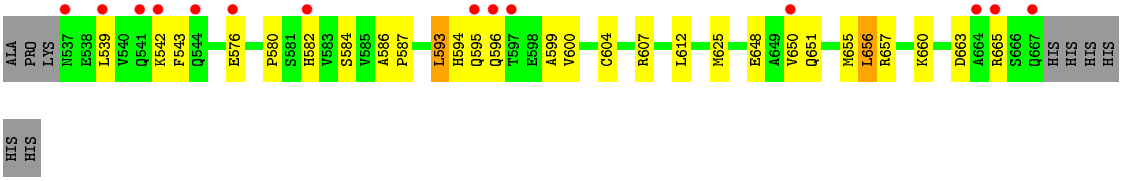
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	46	46	46	0	0
			Total	O		
3	B	12	12	12	0	0
			Total	O		
3	C	57	57	57	0	0
			Total	O		
3	D	13	13	13	0	0

3 Residue-property plots (i)

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: Amyloid beta A4 protein-binding family B member 1

Chain A:

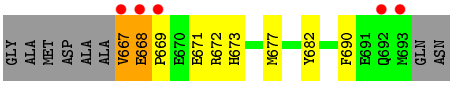


- Molecule 1: Amyloid beta A4 protein-binding family B member 1

Chain C:

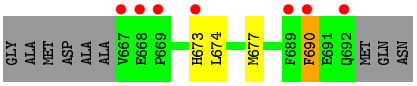
- Molecule 2: Amyloid beta A4 protein

Chain B:



- Molecule 2: Amyloid beta A4 protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	115.11Å 115.11Å 75.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.69 – 2.20 37.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.69-2.20) 99.3 (37.68-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.247 0.200 , 0.243	Depositor DCC
R_{free} test set	1464 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.069 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2569	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.73	0/1026	0.68	0/1396
1	C	0.74	0/961	0.65	0/1309
2	B	0.69	0/261	0.62	0/349
2	D	0.64	0/253	0.61	0/339
All	All	0.72	0/2501	0.65	0/3393

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	594	HIS	Peptide

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	1003	0	988	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	938	0	922	8	0
2	B	254	0	225	12	0
2	D	246	0	216	3	0
3	A	46	0	0	2	0
3	B	12	0	0	0	0
3	C	57	0	0	6	0
3	D	13	0	0	0	0
All	All	2569	0	2351	38	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 8.

All (38) 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)
1:A:543:PHE:O	1:A:582:HIS:HA	1.70	0.91
2:B:668:GLU:HG2	2:B:669:PRO:HD2	1.76	0.67
1:A:542:LYS:HB3	1:A:582:HIS:HB2	1.76	0.66
3:C:25:HOH:O	2:D:690:PHE:HB3	1.99	0.61
2:B:667:VAL:HG23	2:B:671[A]:GLU:HG2	1.83	0.60
2:B:671[B]:GLU:HA	2:B:671[B]:GLU:OE1	2.01	0.59
1:A:648:GLU:HG3	2:B:673[B]:HIS:CE1	2.37	0.59
1:C:648:GLU:OE2	3:C:43:HOH:O	2.18	0.57
1:A:543:PHE:O	1:A:582:HIS:CA	2.49	0.57
1:A:586:ALA:HB1	1:A:587:PRO:HD2	1.87	0.57
1:A:604:CYS:HB3	1:A:625:MET:CE	2.36	0.55
1:A:542:LYS:HD3	1:A:582:HIS:CD2	2.41	0.55
2:B:668:GLU:HG2	2:B:669:PRO:CD	2.36	0.54
1:C:648:GLU:HG2	2:D:673[A]:HIS:CE1	2.42	0.53
1:A:604:CYS:HB3	1:A:625:MET:SD	2.49	0.53
1:A:580:PRO:HB2	1:A:595:GLN:HG3	1.93	0.51
1:C:660:LYS:NZ	3:C:57:HOH:O	2.44	0.50
1:A:607:ARG:HD2	3:A:8:HOH:O	2.12	0.50
1:A:655:MET:HG2	2:B:682:TYR:OH	2.12	0.49
1:A:539:LEU:HG	1:A:587:PRO:HD3	1.95	0.48
3:C:43:HOH:O	2:D:677:MET:HG3	2.12	0.48
2:B:667:VAL:HG22	2:B:672:ARG:HH21	1.79	0.47
1:A:612:LEU:HD22	1:A:650:VAL:HG12	1.97	0.46
2:B:671[B]:GLU:CA	2:B:671[B]:GLU:OE1	2.64	0.46
1:C:543:PHE:CE1	3:C:24:HOH:O	2.56	0.46
1:A:665:ARG:HH21	2:B:690:PHE:HE1	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:GLN:OE1	2:B:673[A]:HIS:CE1	2.70	0.45
1:C:543:PHE:N	3:C:74:HOH:O	2.50	0.44
2:B:673[B]:HIS:CE1	2:B:677:MET:HG2	2.54	0.43
1:C:556:PRO:HB3	1:C:632:PHE:CE1	2.53	0.43
2:B:668:GLU:HB3	2:B:671[B]:GLU:HG2	2.00	0.42
1:A:542:LYS:HG2	1:A:584:SER:HB2	2.01	0.42
1:A:657:ARG:NH1	3:A:54:HOH:O	2.37	0.42
1:C:550:ASN:HA	1:C:634:CYS:O	2.19	0.42
1:A:656:LEU:HD22	1:A:660:LYS:HE3	2.02	0.41
1:A:593:LEU:HD23	1:A:600:VAL:HG22	2.02	0.41
1:C:581:SER:HB2	1:C:593:LEU:O	2.21	0.41
1:A:593:LEU:HA	1:A:599:ALA:O	2.22	0.40

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	129/140 (92%)	127 (98%)	2 (2%)	0	100 100
1	C	121/140 (86%)	120 (99%)	1 (1%)	0	100 100
2	B	27/35 (77%)	25 (93%)	2 (7%)	0	100 100
2	D	26/35 (74%)	23 (88%)	2 (8%)	1 (4%)	4 1
All	All	303/350 (87%)	295 (97%)	7 (2%)	1 (0%)	46 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	690	PHE

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	109/117 (93%)	104 (95%)	5 (5%)	33	40
1	C	101/117 (86%)	98 (97%)	3 (3%)	48	60
2	B	28/30 (93%)	26 (93%)	2 (7%)	18	19
2	D	27/30 (90%)	26 (96%)	1 (4%)	41	50
All	All	265/294 (90%)	254 (96%)	11 (4%)	36	44

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	576	GLU
1	A	593	LEU
1	A	596	GLN
1	A	656	LEU
1	A	663	ASP
2	B	667	VAL
2	B	668	GLU
1	C	596	GLN
1	C	618	VAL
1	C	661	CYS
2	D	674	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	GLN
1	A	544	GLN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	131/140 (93%)	0.28	14 (10%)	8	7	31, 45, 82, 93	0
1	C	123/140 (87%)	0.03	6 (4%)	33	33	31, 42, 63, 86	0
2	B	27/35 (77%)	1.03	5 (18%)	2	1	41, 58, 85, 91	0
2	D	26/35 (74%)	1.16	7 (26%)	1	1	39, 50, 84, 91	0
All	All	307/350 (87%)	0.32	32 (10%)	8	8	31, 44, 82, 93	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	667	VAL	6.8
2	D	667	VAL	6.7
1	A	541	GLN	5.3
1	A	667	GLN	4.9
2	D	668	GLU	4.9
1	C	665	ARG	4.8
2	D	690	PHE	4.4
2	B	693	MET	4.4
1	A	596	GLN	4.4
1	A	537	ASN	4.2
2	B	668	GLU	4.2
2	D	669	PRO	3.9
1	A	576	GLU	3.4
1	C	596	GLN	3.3
1	A	595	GLN	3.2
2	B	692	GLN	3.2
2	B	669	PRO	3.0
1	A	665	ARG	3.0
2	D	689	PHE	2.9
2	D	692	GLN	2.8
1	A	582	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	542	LYS	2.7
1	C	543	PHE	2.6
2	D	673[A]	HIS	2.6
1	A	664	ALA	2.5
1	A	597	THR	2.4
1	C	652	ALA	2.4
1	A	650	VAL	2.4
1	C	650	VAL	2.4
1	A	539	LEU	2.3
1	C	595	GLN	2.1
1	A	544	GLN	2.0

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.