



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3DXC / pdb_00003dxc
Title : Crystal structure of the intracellular domain of human APP in complex with Fe65-PTB2
Authors : Radzimanowski, J.; Sinning, I.; Wild, K.
Deposited on : 2008-07-24
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

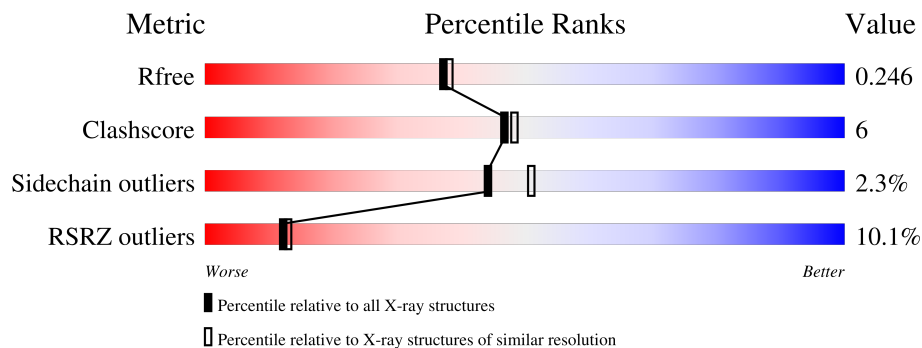
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	 11% 81% 9% • 7%
1	C	140	 3% 81% 6% • 12%
2	B	35	 20% 66% 11% • 20%
2	D	35	 11% 60% 14% 26%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 2651 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	130	994	632	172	181	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	28	248	156	43	47	2	0	1	0
2	D	26	235	148	41	45	1	0	1	0

There are 6 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
D	661	GLY	-	expression tag	UNP P05067
D	662	ALA	-	expression tag	UNP P05067
D	663	MET	-	expression tag	UNP P05067

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	85	Total O 85 85	0	0
3	B	24	Total O 24 24	0	0
3	C	94	Total O 94 94	0	0
3	D	33	Total O 33 33	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	114.32Å 114.32Å 74.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.00 – 2.10 33.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.00-2.10) 99.9 (33.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.202 , 0.238 (Not available) , 0.246	Depositor DCC
R_{free} test set	1997 reflections (6.13%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2651	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.80	0/1017	0.93	1/1384 (0.1%)
1	C	0.79	0/961	0.83	1/1309 (0.1%)
2	B	0.71	0/255	0.94	0/342
2	D	0.72	0/242	0.86	0/325
All	All	0.78	0/2475	0.89	2/3360 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	GLN	N-CA-C	6.64	119.08	111.11
1	C	581	SER	N-CA-C	5.07	115.22	108.38

There are no chirality outliers.

There are no planarity outliers.

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	994	0	980	13	0
1	C	938	0	922	6	0
2	B	248	0	226	8	0
2	D	235	0	212	5	0
3	A	85	0	0	2	0
3	B	24	0	0	0	0
3	C	94	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	33	0	0	0	0
All	All	2651	0	2340	27	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 6.

The worst 5 of 27 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	1.59	1.03
1:A:542:LYS:HB3	1:A:582:HIS:HB2	1.58	0.84
1:C:612:LEU:HD12	2:D:677:MET:HE1	1.60	0.81
1:A:659:GLN:HG3	3:A:188:HOH:O	1.94	0.67
2:B:677:MET:HA	2:B:677:MET:HE2	1.77	0.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	108/117 (92%)	104 (96%)	4 (4%)	30	33
1	C	101/117 (86%)	100 (99%)	1 (1%)	68	76
2	B	27/30 (90%)	26 (96%)	1 (4%)	30	33
2	D	26/30 (87%)	26 (100%)	0	100	100
All	All	262/294 (89%)	256 (98%)	6 (2%)	44	51

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	663	ASP
2	B	667	VAL
1	C	663	ASP
1	A	593	LEU
1	A	582	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	595	GLN
1	C	596	GLN
2	D	678	GLN
1	A	550	ASN
1	A	541	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 oligosaccharides 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

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	130/140 (92%)	0.53	16 (12%) 8 8	25, 36, 69, 79	0
1	C	123/140 (87%)	0.09	4 (3%) 49 51	23, 33, 55, 75	0
2	B	28/35 (80%)	1.16	7 (25%) 2 2	23, 44, 69, 77	1 (3%)
2	D	26/35 (74%)	0.86	4 (15%) 5 5	20, 40, 65, 74	1 (3%)
All	All	307/350 (87%)	0.44	31 (10%) 12 13	20, 36, 68, 79	2 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	VAL	6.2
2	D	673[A]	HIS	4.2
1	A	599	ALA	4.2
2	B	666	ALA	3.9
2	D	667	VAL	3.7

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 oligosaccharides 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.