



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:55 pm GMT

PDB ID : 4PQE
Title : Crystal Structure of Human Acetylcholinesterase
Authors : Dym, O.; Unger, T.; Toker, L.; Silman, I.; Sussman, J.L.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2014-03-02
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

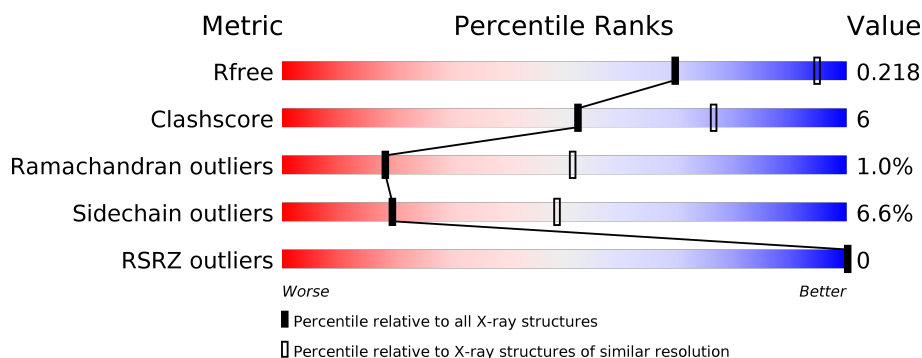
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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 $\leq 5\%$. 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	543	 78% 17% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4099 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	0	0
			4087	2630	712	732	13			

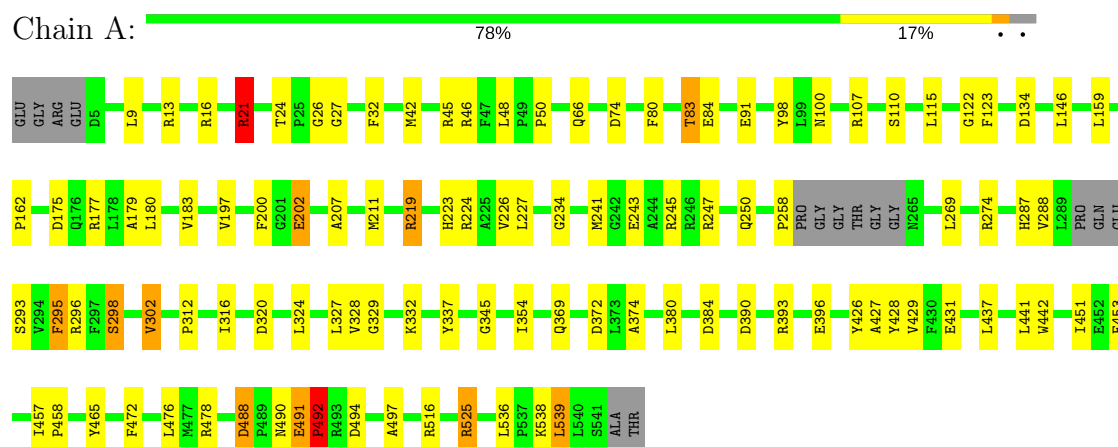
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		

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 the various outlier classes 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: Acetylcholinesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	125.31Å 125.31Å 131.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 41.84 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.90) 99.7 (41.84-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.28 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.185 , 0.218 0.185 , 0.218	Depositor DCC
R_{free} test set	1287 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4099	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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

5.1 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 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	0.96	2/4212 (0.0%)	1.10	19/5760 (0.3%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	GLU	CD-OE2	5.62	1.31	1.25
1	A	442	TRP	CG-CD1	5.43	1.44	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	ASP	CB-CG-OD1	9.39	126.75	118.30
1	A	302	VAL	CB-CA-C	-7.62	96.92	111.40
1	A	224	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	539	LEU	CA-CB-CG	6.58	130.43	115.30
1	A	219	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	224	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	134	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	525	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	74	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	A	245	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	488	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	21	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	241	MET	CG-SD-CE	5.42	108.88	100.20
1	A	320	ASP	CB-CG-OD1	5.35	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	320	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	332	LYS	CD-CE-NZ	-5.14	99.88	111.70
1	A	13	ARG	CG-CD-NE	-5.09	101.10	111.80
1	A	525	ARG	CG-CD-NE	-5.03	101.24	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	ASP	Peptide

5.2 Too-close contacts

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	4087	0	3962	51	0
2	A	12	0	0	0	0
All	All	4099	0	3962	51	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.

All (51) 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:24:THR:HG22	1:A:26:GLY:H	1.32	0.93
1:A:478:ARG:HD3	1:A:491:GLU:OE1	1.74	0.87
1:A:197:VAL:H	1:A:223:HIS:HD2	1.21	0.83
1:A:24:THR:HG22	1:A:26:GLY:N	2.10	0.65
1:A:80:PHE:HD2	1:A:83:THR:HB	1.62	0.65
1:A:478:ARG:CD	1:A:491:GLU:OE1	2.47	0.63
1:A:429:VAL:HG12	1:A:431:GLU:HG3	1.80	0.62
1:A:24:THR:HB	1:A:27:GLY:O	2.02	0.60
1:A:488:ASP:OD1	1:A:490:ASN:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ALA:O	1:A:211:MET:HG3	2.05	0.57
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.40	0.56
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.40	0.56
1:A:491:GLU:OE2	1:A:492:PRO:HD2	2.05	0.56
1:A:258:PRO:HD3	1:A:269:LEU:CD1	2.36	0.55
1:A:312:PRO:O	1:A:316:ILE:HG13	2.08	0.54
1:A:50:PRO:HG3	1:A:175:ASP:OD1	2.10	0.52
1:A:46:ARG:O	1:A:274:ARG:NH1	2.45	0.50
1:A:32:PHE:CD1	1:A:32:PHE:N	2.79	0.49
1:A:243:GLU:OE1	1:A:247:ARG:NE	2.42	0.48
1:A:329:GLY:HA3	1:A:428:TYR:CZ	2.48	0.48
1:A:45:ARG:HA	1:A:48:LEU:HD12	1.96	0.48
1:A:226:VAL:HA	1:A:327:LEU:O	2.15	0.47
1:A:536:LEU:HA	1:A:536:LEU:HD12	1.72	0.47
1:A:295:PHE:O	1:A:296:ARG:HD3	2.15	0.47
1:A:288:VAL:CG2	1:A:298:SER:HB3	2.45	0.46
1:A:374:ALA:HA	1:A:539:LEU:HD21	1.99	0.45
1:A:202:GLU:CG	1:A:451:ILE:HD11	2.47	0.45
1:A:453:PHE:HB3	1:A:476:LEU:HD12	1.98	0.45
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.52	0.45
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.52	0.45
1:A:177:ARG:O	1:A:180:LEU:N	2.51	0.43
1:A:258:PRO:HD3	1:A:269:LEU:HD13	2.00	0.43
1:A:327:LEU:HD12	1:A:327:LEU:HA	1.61	0.43
1:A:345:GLY:HA3	1:A:354:ILE:HG22	2.01	0.43
1:A:457:ILE:N	1:A:458:PRO:CD	2.82	0.43
1:A:16:ARG:HG3	1:A:16:ARG:HH11	1.84	0.42
1:A:179:ALA:O	1:A:183:VAL:HG23	2.18	0.42
1:A:227:LEU:N	1:A:227:LEU:HD12	2.35	0.42
1:A:429:VAL:HG12	1:A:431:GLU:CG	2.48	0.42
1:A:269:LEU:HD12	1:A:269:LEU:HA	1.79	0.41
1:A:80:PHE:CD2	1:A:83:THR:HB	2.50	0.41
1:A:122:GLY:O	1:A:123:PHE:HB2	2.20	0.41
1:A:83:THR:CG2	1:A:84:GLU:N	2.84	0.41
1:A:328:VAL:O	1:A:427:ALA:HA	2.21	0.41
1:A:197:VAL:H	1:A:223:HIS:CD2	2.14	0.41
1:A:115:LEU:O	1:A:146:LEU:HD12	2.21	0.41
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.86	0.41
1:A:384:ASP:C	1:A:384:ASP:OD1	2.59	0.41
1:A:390:ASP:HB3	1:A:393:ARG:HB2	2.03	0.41
1:A:202:GLU:HG3	1:A:451:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LEU:CD1	1:A:426:TYR:HB2	2.51	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	522/543 (96%)	488 (94%)	29 (6%)	5 (1%)	18 51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	GLY
1	A	492	PRO
1	A	538	LYS
1	A	497	ALA
1	A	491	GLU

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	423/438 (97%)	395 (93%)	28 (7%)	19 49

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	21	ARG
1	A	42	MET
1	A	83	THR
1	A	91	GLU
1	A	100	ASN
1	A	107	ARG
1	A	110	SER
1	A	159	LEU
1	A	162	PRO
1	A	200	PHE
1	A	219	ARG
1	A	250	GLN
1	A	287	HIS
1	A	293	SER
1	A	295	PHE
1	A	298	SER
1	A	302	VAL
1	A	324	LEU
1	A	337	TYR
1	A	369	GLN
1	A	372	ASP
1	A	380	LEU
1	A	396	GLU
1	A	437	LEU
1	A	441	LEU
1	A	492	PRO
1	A	525	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	369	GLN
1	A	413	GLN

5.3.3 RNA ⓘ

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	528/543 (97%)	-0.78	0 100 100	14, 27, 49, 118	0

There are no RSRZ outliers to report.

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.