



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 07:45 AM EDT

PDB ID : 1QIE
Title : SPECIFIC CHEMICAL AND STRUCTURAL DAMAGE AT NINE TIME POINTS (POINT B) CAUSED BY INTENSE SYNCHROTRON RADIATION TO TORPEDO CALIFORNICA ACETYLCHOLINESTERASE
Authors : Kryger, G.; Weik, M.; Ravelli, R.B.G.
Deposited on : unknown
Resolution : 2.10 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 : rb-20030345
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) : rb-20030345

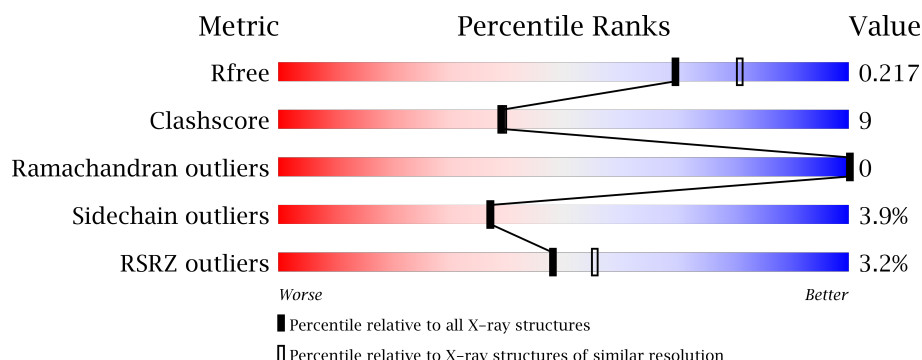
1 Overall quality at a glance

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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 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	537	<div> <div>3%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4558 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	532	Total	C	N	O	S	0	0	0
			4238	2721	720	781	16			

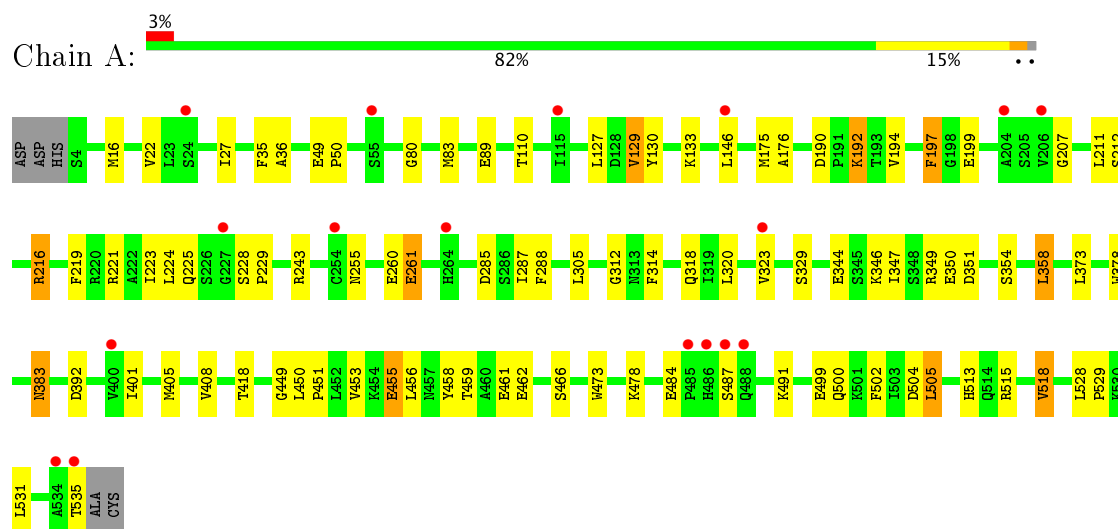
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	320	Total	O	0	0
			320	320		

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 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 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.97Å 111.97Å 137.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.47 – 2.10 35.47 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (35.47-2.10) 96.1 (35.47-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.10Å)	Xtriage
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.214 , 0.230 0.214 , 0.217	Depositor DCC
R_{free} test set	2871 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4558	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	0.39	0/4361	0.63	1/5923 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASP	N-CA-C	-5.26	96.79	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4238	0	4086	71	1
2	A	320	0	0	3	0
All	All	4558	0	4086	71	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 9.

All (71) 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:50:PRO:HA	1:A:175:MET:HE3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLU:CD	1:A:455:GLU:H	1.86	0.77
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.88	0.73
1:A:484:GLU:HB2	1:A:487:SER:HB2	1.71	0.72
1:A:255:ASN:CG	1:A:261:GLU:HG2	2.10	0.72
1:A:450:LEU:O	1:A:453:VAL:HG12	1.92	0.69
1:A:110:THR:OG1	1:A:478:LYS:HG2	1.92	0.69
1:A:49:GLU:O	1:A:175:MET:HE1	1.93	0.69
1:A:383:ASN:HD22	1:A:383:ASN:C	1.97	0.68
1:A:221:ARG:HD3	1:A:318:GLN:OE1	1.96	0.66
1:A:194:VAL:HG13	1:A:219:PHE:HA	1.81	0.63
1:A:50:PRO:HA	1:A:175:MET:CE	2.29	0.62
1:A:515:ARG:HB3	1:A:518:VAL:CG1	2.30	0.61
1:A:127:LEU:HD12	1:A:130:TYR:CE2	2.38	0.59
1:A:212:SER:O	1:A:216:ARG:HG2	2.03	0.59
1:A:36:ALA:HB2	1:A:175:MET:HE2	1.85	0.58
1:A:500:GLN:NE2	1:A:515:ARG:HG2	2.19	0.57
1:A:515:ARG:HB3	1:A:518:VAL:HG13	1.86	0.57
1:A:27:ILE:HD11	1:A:133:LYS:HB2	1.85	0.57
1:A:344:GLU:OE1	1:A:346:LYS:HE3	2.06	0.56
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.89	0.55
1:A:197:PHE:CB	1:A:223:ILE:HB	2.37	0.55
1:A:35:PHE:O	1:A:175:MET:HE2	2.07	0.55
1:A:405:MET:HA	1:A:408:VAL:HG12	1.88	0.54
1:A:323:VAL:HG21	1:A:401:ILE:HG12	1.90	0.54
1:A:211:LEU:HD13	1:A:305:LEU:HD22	1.91	0.53
1:A:504:ASP:OD2	1:A:513:HIS:NE2	2.41	0.53
1:A:449:GLY:HA2	1:A:466:SER:OG	2.11	0.51
1:A:531:LEU:HD23	1:A:531:LEU:C	2.31	0.51
1:A:484:GLU:O	1:A:491:LYS:NZ	2.44	0.51
1:A:80:GLY:HA2	1:A:83:MET:HE3	1.93	0.49
1:A:287:ILE:HG22	1:A:358:LEU:O	2.12	0.49
1:A:194:VAL:CG1	1:A:219:PHE:HA	2.43	0.49
1:A:36:ALA:HA	1:A:175:MET:CE	2.43	0.49
1:A:223:ILE:HA	1:A:320:LEU:O	2.13	0.48
1:A:487:SER:HB3	1:A:491:LYS:NZ	2.28	0.48
1:A:373:LEU:HD12	1:A:378:TRP:HE1	1.78	0.48
1:A:450:LEU:N	1:A:451:PRO:CD	2.77	0.47
1:A:35:PHE:O	1:A:175:MET:CE	2.63	0.47
1:A:197:PHE:HB2	1:A:223:ILE:HB	1.97	0.46
1:A:450:LEU:O	1:A:453:VAL:CG1	2.62	0.46
1:A:408:VAL:HG23	1:A:418:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.15	0.45
1:A:455:GLU:N	1:A:455:GLU:OE1	2.49	0.45
1:A:228:SER:HB2	1:A:229:PRO:HD2	1.99	0.45
1:A:146:LEU:HD12	1:A:146:LEU:C	2.36	0.45
1:A:499:GLU:HB2	2:A:1024:HOH:O	2.16	0.45
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.98	0.45
1:A:453:VAL:CG2	1:A:455:GLU:HG2	2.47	0.44
1:A:146:LEU:HD22	1:A:176:ALA:HB3	1.98	0.44
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.53	0.44
1:A:505:LEU:HD12	1:A:505:LEU:HA	1.90	0.43
1:A:515:ARG:O	1:A:518:VAL:HG22	2.19	0.43
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.99	0.43
1:A:383:ASN:C	1:A:383:ASN:ND2	2.70	0.43
1:A:224:LEU:N	1:A:224:LEU:HD12	2.33	0.42
1:A:199:GLU:HA	1:A:225:GLN:O	2.20	0.42
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.54	0.42
1:A:129:VAL:HG22	2:A:1027:HOH:O	2.18	0.42
1:A:453:VAL:HG22	1:A:455:GLU:HG2	2.01	0.42
1:A:373:LEU:CD1	1:A:378:TRP:HE1	2.33	0.42
1:A:22:VAL:HG13	1:A:22:VAL:O	2.19	0.42
1:A:453:VAL:CG1	1:A:456:LEU:HD12	2.51	0.41
1:A:450:LEU:HD22	1:A:450:LEU:N	2.36	0.41
1:A:461:GLU:CD	1:A:461:GLU:H	2.23	0.41
1:A:36:ALA:CB	1:A:175:MET:HE2	2.50	0.40
1:A:329:SER:HB3	1:A:392:ASP:OD2	2.22	0.40
1:A:347:ILE:HG23	1:A:351:ASP:HB2	2.02	0.40
1:A:358:LEU:HD13	2:A:1158:HOH:O	2.21	0.40
1:A:260:GLU:H	1:A:260:GLU:CD	2.25	0.40
1:A:502:PHE:CE1	1:A:513:HIS:HB2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:THR:CG2	1:A:535:THR:CG2[4_556]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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	530/537 (99%)	501 (94%)	29 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	459/469 (98%)	441 (96%)	18 (4%)	37	37

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	89	GLU
1	A	129	VAL
1	A	192	LYS
1	A	197	PHE
1	A	216	ARG
1	A	243	ARG
1	A	261	GLU
1	A	288	PHE
1	A	349	ARG
1	A	350	GLU
1	A	354	SER
1	A	358	LEU

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Mol	Chain	Res	Type
1	A	383	ASN
1	A	455	GLU
1	A	473	TRP
1	A	505	LEU
1	A	518	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	74	GLN
1	A	181	HIS
1	A	383	ASN
1	A	500	GLN
1	A	526	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

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	532/537 (99%)	0.05	17 (3%) 48 55	21, 31, 51, 72	5 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	HIS	5.2
1	A	535	THR	4.6
1	A	485	PRO	3.7
1	A	488	GLN	3.2
1	A	115	ILE	3.2
1	A	55	SER	2.9
1	A	206	VAL	2.4
1	A	204	ALA	2.4
1	A	534	ALA	2.3
1	A	227	GLY	2.3
1	A	264	HIS	2.2
1	A	323	VAL	2.2
1	A	254	CYS	2.2
1	A	24	SER	2.2
1	A	146	LEU	2.1
1	A	400	VAL	2.1
1	A	487	SER	2.1

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.