



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6O52  
Title : Room temperature structure of binary complex of native hAChE with BW284c51  
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Deposited on : 2019-03-01  
Resolution : 3.20 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

PERCENTILES INFOmissingINFO

# 1 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8466 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.

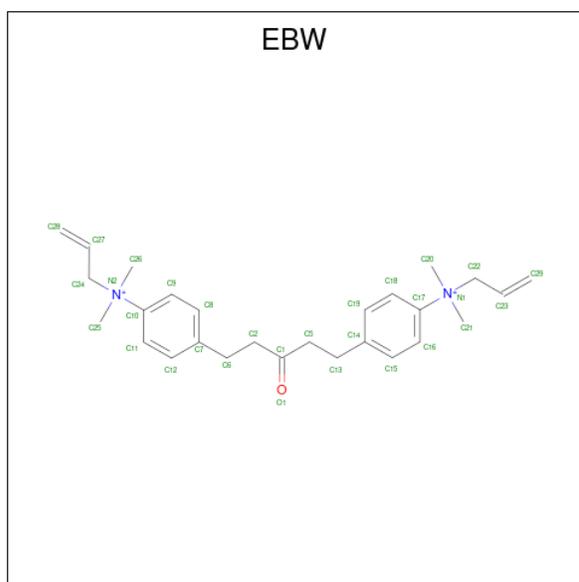
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	540	4188	2686	732	757	13	0	0	0
1	B	540	4188	2686	732	757	13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P22303
A	-1	PRO	-	expression tag	UNP P22303
A	0	LEU	-	expression tag	UNP P22303
B	-2	GLY	-	expression tag	UNP P22303
B	-1	PRO	-	expression tag	UNP P22303
B	0	LEU	-	expression tag	UNP P22303

- Molecule 2 is 4-(5-{4-[DIMETHYL(PROP-2-ENYL)AMMONIO]PHENYL}-3-OXOPEN TYL)-N,N-DIMETHYL-N-PROP-2-ENYLBENZENAMINIUM (three-letter code: EBW) (formula: C<sub>27</sub>H<sub>38</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	30	27	2	1	0	0
2	B	1	30	27	2	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	13	13	13	0	0
3	B	17	17	17	0	0

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.43Å 125.43Å 130.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.17 – 3.20	Depositor
% Data completeness (in resolution range)	77.5 (39.17-3.20)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 3.18Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.153 , 0.189	Depositor
Wilson B-factor (Å <sup>2</sup> )	74.7	Xtrriage
Anisotropy	0.061	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.046 for -h,-k,l 0.056 for h,-h-k,-l 0.417 for -k,-h,-l	Xtrriage
Total number of atoms	8466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

### 3 Model quality [i](#)

#### 3.1 Standard geometry [i](#)

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

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	0.28	1/4317 (0.0%)	0.41	0/5903
1	B	0.27	1/4317 (0.0%)	0.42	0/5903
All	All	0.27	2/8634 (0.0%)	0.42	0/11806

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	PRO	C-N	8.21	1.49	1.34
1	B	40	PRO	C-N	7.52	1.48	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

#### 3.2 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	4188	0	4068	36	0
1	B	4188	0	4068	39	0
2	A	30	0	38	1	0
2	B	30	0	38	1	0
3	A	13	0	0	0	0
3	B	17	0	0	0	0
All	All	8466	0	8212	75	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 5.

The worst 5 of 75 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:113:PRO:HG3	1:A:485:ARG:HG2	1.73	0.71
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.74	0.67
1:B:408:VAL:HG11	1:B:525:ARG:HD3	1.81	0.62
1:A:258:PRO:HB2	1:A:262:THR:HG22	1.81	0.61
1:B:115:LEU:HD23	1:B:198:THR:HB	1.84	0.60

There are no symmetry-related clashes.

### 3.3 Torsion angles [i](#)

#### 3.3.1 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	538/550 (98%)	514 (96%)	23 (4%)	1 (0%)	47 79
1	B	538/550 (98%)	516 (96%)	22 (4%)	0	100 100
All	All	1076/1100 (98%)	1030 (96%)	45 (4%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLY

#### 3.3.2 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	436/444 (98%)	432 (99%)	4 (1%)	78	91
1	B	436/444 (98%)	433 (99%)	3 (1%)	84	94
All	All	872/888 (98%)	865 (99%)	7 (1%)	81	93

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	LEU
1	B	70	TYR
1	B	295	PHE
1	B	200	PHE
1	A	490	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 3.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 3.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 3.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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.

### 3.7 Other polymers

There are no such residues in this entry.

### 3.8 Polymer linkage issues

There are no chain breaks in this entry.

## 4 Fit of model and data

### 4.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

### 4.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

### 4.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 4.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 4.5 Other polymers

EDS failed to run properly - this section is therefore empty.