

wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2021 – 03:18 pm BST

PDB ID	:	7AIV
Title	:	Crystal structure of Torpedo Californica acetylcholinesterase in complex with
		4-{[(3-Chloro-6,7,10,11-tetrahydro-9-methyl-7,11-methanocycloocta[b]quinoli
		n-12-yl)amino]methyl}-N-(4-hydroxy-3-methoxybenzyl)benzamide
Authors	:	Coquelle, N.; Colletier, J.P.
Deposited on	:	2020-09-28
Resolution	:	2.55 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 (i) symbol.

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

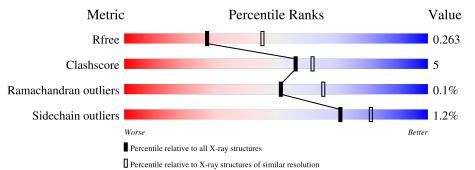
MolProbity Mogul Xtriage (Phenix) EDS buster-report	: : :	1.8.5 (274361), CSD as541be (2020) 1.13 2.23.2
		20191225.v01 (using entries in the PDB archive December 25th 2019)
		5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)		
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.55 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	$1284 \ (2.56-2.52)$
Clashscore	141614	1332(2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)

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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	586	79%	11%	9%
1	В	586	78%	12%	9%



2 Entry composition (i)

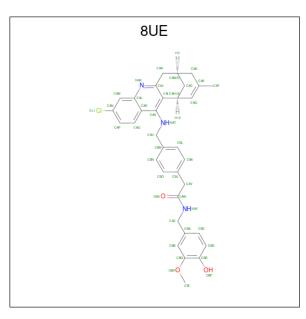
There are 3 unique types of molecules in this entry. The entry contains 8848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	А	532	Total 4283	C 2750	N 724	0 786	S 23	0	8	0
1	В	532	Total 4283	С	N 724	0	S	0	8	0

• Molecule 2 is 4-{[(3-Chloro-6,7,10,11-tetrahydro-9-methyl-7,11-methanocycloocta[b]quinolin -12-yl)amino]methyl}-N-(4-hydroxy-3-methoxybenzyl)benzamide (three-letter code: 8UE) (formula: C₃₄H₃₄ClN₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	В	1	Total 41	C 34		N 3	0 3	0	0

• Molecule 3 is water.

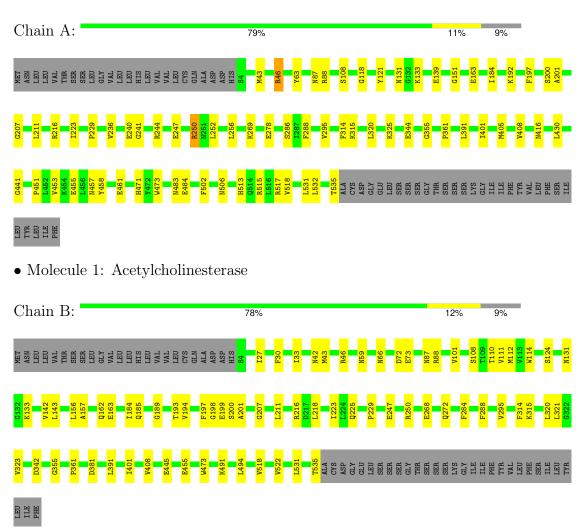


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	117	Total O 117 117	0	0
3	В	124	Total O 124 124	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	92.03Å 106.66Å 151.47Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 - 2.55	Depositor
Resolution (A)	19.98 - 2.55	EDS
% Data completeness	98.3 (19.98-2.55)	Depositor
(in resolution range)	98.5(19.98-2.55)	EDS
R _{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.13 (at 2.56 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
D D.	0.208 , 0.262	Depositor
R, R_{free}	0.208 , 0.263	DCC
R_{free} test set	2292 reflections (4.73%)	wwPDB-VP
Wilson B-factor $(Å^2)$	35.9	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ L > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8848	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 39.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0100e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: $8\mathrm{UE}$

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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.35	0/4430	0.54	2/6014~(0.0%)	
1	В	0.36	2/4430~(0.0%)	0.52	1/6014~(0.0%)	
All	All	0.35	2/8860~(0.0%)	0.53	3/12028~(0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	В	268	GLU	CD-OE1	-5.90	1.19	1.25
1	В	268	GLU	CD-OE2	-5.27	1.19	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	46	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	В	494	LEU	CA-CB-CG	6.43	130.08	115.30
1	А	46	ARG	NE-CZ-NH2	6.06	123.33	120.30

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	А	4283	0	4149	43	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes				
1	В	4283	0	4149	42	1				
2	В	41	0	0	0	0				
3	А	117	0	0	9	0				
3	В	124	0	0	9	0				
All	All	8848	0	8298	85	1				

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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 85 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:B:162:GLN:NE2	3:B:702:HOH:O	1.91	0.96
1:B:42:ASN:OD1	3:B:701:HOH:O	1.89	0.91
1:B:43[B]:MET:SD	1:B:46:ARG:NH1	2.52	0.82
1:A:43[A]:MET:HA	1:A:46:ARG:HG3	1.61	0.82
1:A:43[B]:MET:HA	1:A:46:ARG:HG3	1.61	0.80

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:192:LYS:NZ	1:B:73[A]:GLU:OE2[4_576]	2.19	0.01

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	А	538/586~(92%)	513 (95%)	24 (4%)	1 (0%)	47 6	0
1	В	538/586~(92%)	515 (96%)	23 (4%)	0	100 1	00

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Mol	Chain	Analysed Favoured		Allowed Outliers		Percentiles	
All	All	1076/1172~(92%)	1028 (96%)	47 (4%)	1 (0%)	51 65	

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	118	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	470/513~(92%)	463~(98%)	7(2%)	65 77
1	В	470/513~(92%)	466 (99%)	4 (1%)	78 86
All	All	940/1026~(92%)	929~(99%)	11 (1%)	71 81

5 of 11 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	108	SER
1	В	288	PHE
1	В	473	TRP
1	В	445	GLU
1	А	344	GLU

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

Mol	Chain	Res	Type
1	А	131	ASN
1	В	253	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	B	ond leng	gths	B	ond ang	les
WIOI	rybe	Ullaili	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	8UE	В	601	-	45,46,46	2.95	12 (26%)	58,66,66	1.91	9 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8UE	В	601	-	-	5/16/36/36	0/6/6/6

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	В	601	8UE	CAA-CAJ	-8.91	1.41	1.51
2	В	601	8UE	CAH-CAG	-7.94	1.41	1.50
2	В	601	8UE	CAI-CAH	-7.32	1.41	1.52
2	В	601	8UE	CAV-CBJ	-6.24	1.41	1.51
2	В	601	8UE	CAZ-CBA	-5.24	1.40	1.51

The worst 5 of 9 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	601	8UE	CAI-CAJ-NAK	-6.44	120.78	123.66
2	В	601	8UE	CBI-OBH-CBG	4.64	124.54	117.53
2	В	601	8UE	CAJ-NAK-CAL	4.54	123.27	117.67
2	В	601	8UE	CAJ-CAI-CAH	-4.53	118.13	120.04
2	В	601	8UE	OBH-CBG-CBE	4.20	120.66	114.57

There are no chirality outliers.

All (5) torsion outliers are listed below:

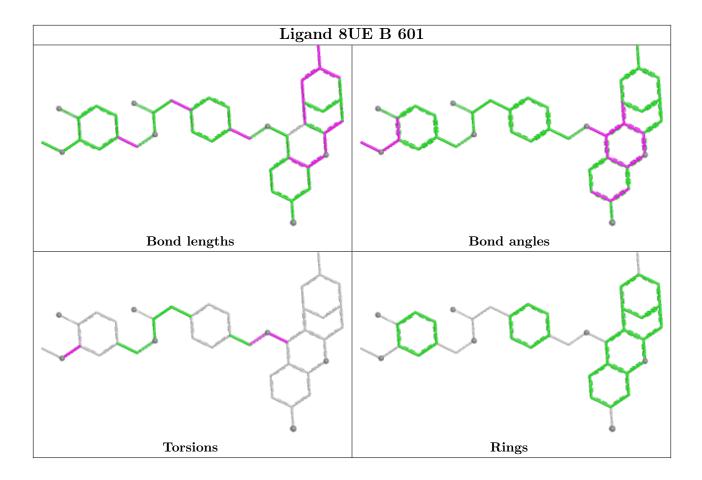
Mol	Chain	Res	Type	Atoms
2	В	601	8UE	CBB-CBG-OBH-CBI
2	В	601	8UE	CBE-CBG-OBH-CBI
2	В	601	8UE	CAR-CAS-NAT-CAU
2	В	601	8UE	CAI-CAS-NAT-CAU
2	В	601	8UE	CBM-CAU-NAT-CAS

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and similar rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

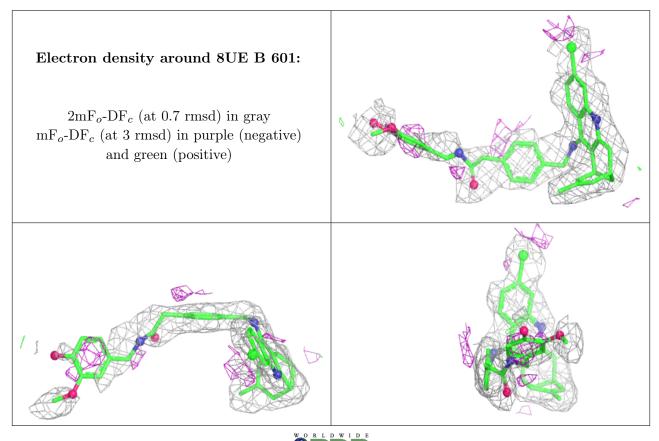
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

