



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 9, 2019 – 02:28 AM EST

PDB ID : 6I2T
EMDB ID: : EMD-4400
Title : CryoEM reconstruction of full-length, fully-glycosylated human butyrylcholinesterase tetramer
Authors : Leung, M.R.; van Bezouwen, L.S.; Schopfer, L.M.; Sussman, J.L.; Silman, I.; Lockridge, O.; Zeev-Ben-Mordehai, T.
Deposited on : 2018-11-01
Resolution : 5.70 Å (reported)
Based on PDB ID : 1VZJ, 4AQD

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

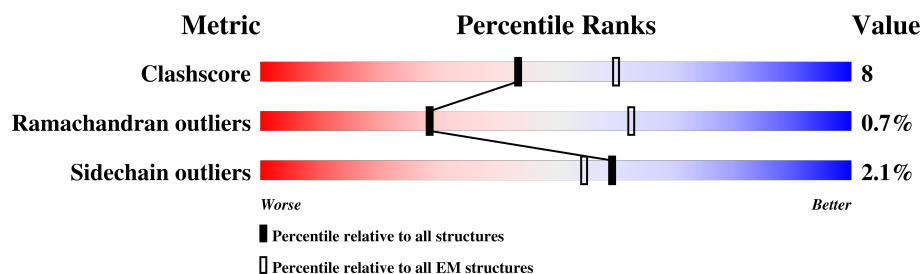
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	574	75% 21% ..
1	B	574	78% 19% .
1	C	574	76% 20% ..
1	D	574	77% 20% .
2	J	12	92% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 18174 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

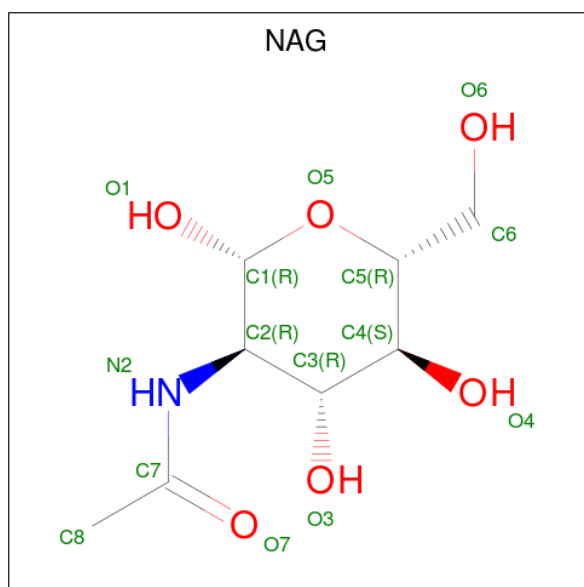
- Molecule 1 is a protein called Cholinesterase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	562	Total	C	N	O	S	0	0
			4512	2910	758	826	18		
1	A	558	Total	C	N	O	S	0	0
			4477	2889	753	817	18		
1	C	558	Total	C	N	O	S	0	0
			4477	2889	753	817	18		
1	D	562	Total	C	N	O	S	0	0
			4512	2910	758	826	18		

- Molecule 2 is a protein called lamellipodin-derived polyproline peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	12	Total	C	N	O	0	0
			84	60	12	12		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

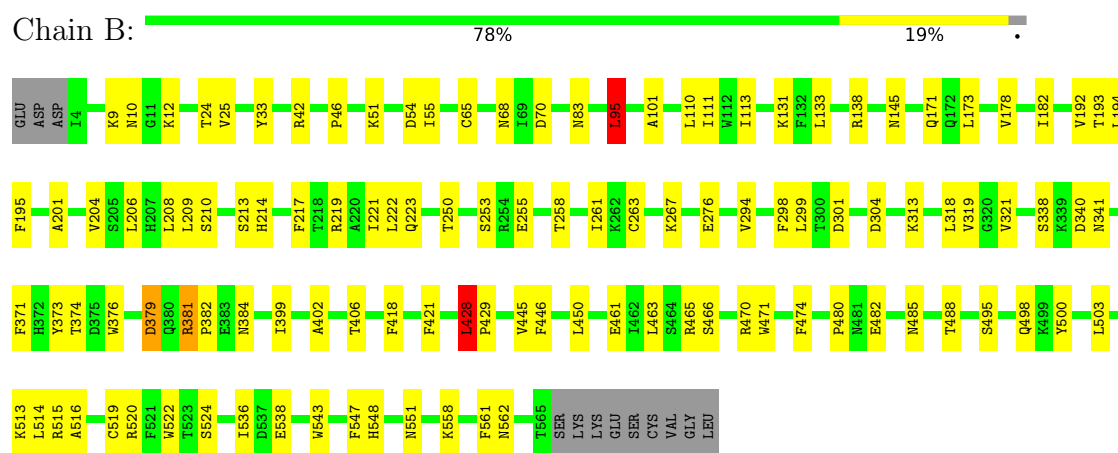


Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total 14	C 8	N 1	O 5	0
3	A	1	Total 42	C 24	N 3	O 15	0
3	A	1	Total 42	C 24	N 3	O 15	0
3	A	1	Total 42	C 24	N 3	O 15	0
3	C	1	Total 42	C 24	N 3	O 15	0
3	C	1	Total 42	C 24	N 3	O 15	0
3	C	1	Total 42	C 24	N 3	O 15	0
3	D	1	Total 14	C 8	N 1	O 5	0

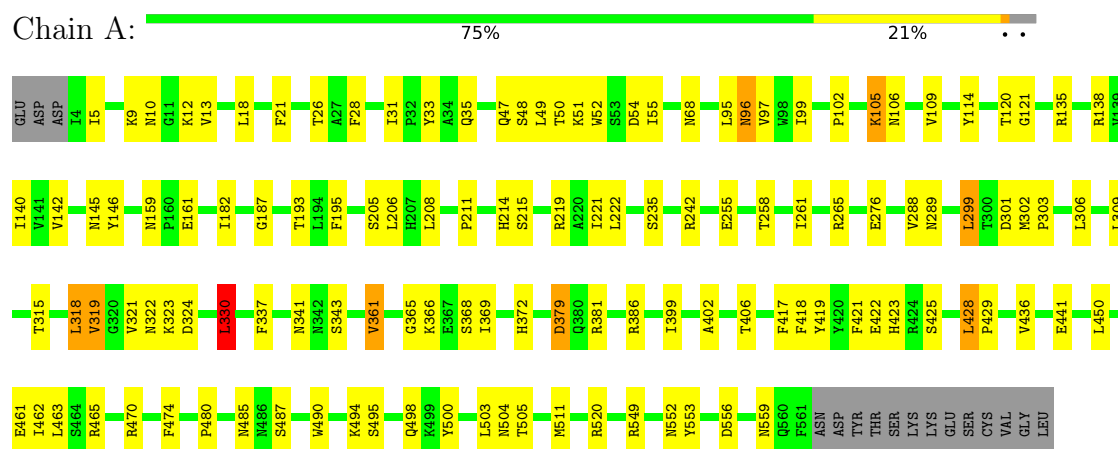
3 Residue-property plots

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. 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.

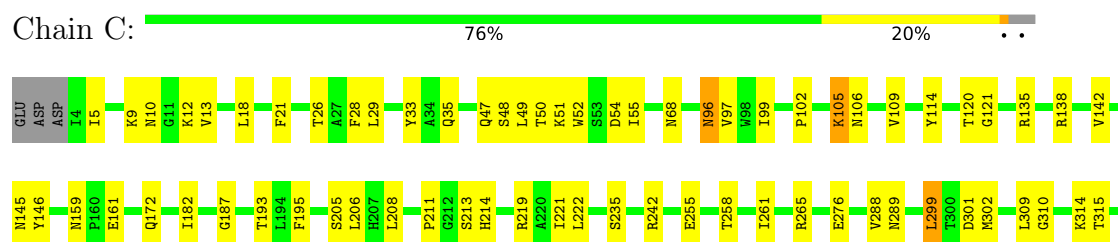
• Molecule 1: Cholinesterase

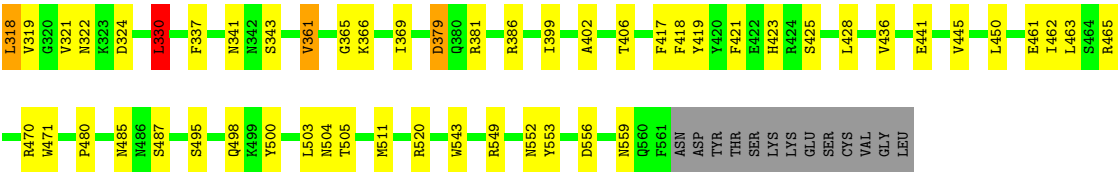


• Molecule 1: Cholinesterase

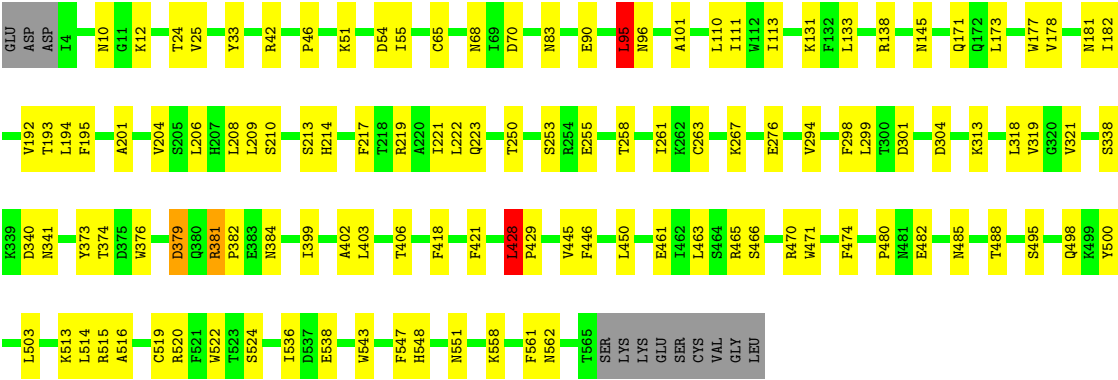
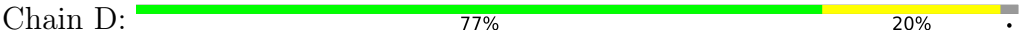


• Molecule 1: Cholinesterase

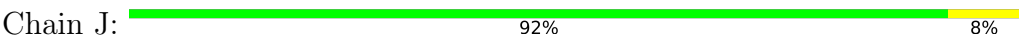




• Molecule 1: Cholinesterase



• Molecule 2: lamellipodin-derived polyproline peptide



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	111986	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.5	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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:
NAG

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.41	0/4608	0.72	4/6257 (0.1%)
1	B	0.41	0/4644	0.71	5/6307 (0.1%)
1	C	0.41	0/4608	0.72	3/6257 (0.0%)
1	D	0.41	0/4644	0.71	5/6307 (0.1%)
2	J	0.54	0/95	0.53	0/140
All	All	0.41	0/18599	0.71	17/25268 (0.1%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	263	CYS	CA-CB-SG	7.47	127.45	114.00
1	B	263	CYS	CA-CB-SG	7.46	127.44	114.00
1	C	330	LEU	CA-CB-CG	6.90	131.17	115.30
1	A	330	LEU	CA-CB-CG	6.88	131.12	115.30
1	A	318	LEU	CA-CB-CG	6.59	130.47	115.30

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	A	4477	0	4341	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4512	0	4369	64	0
1	C	4477	0	4341	71	0
1	D	4512	0	4369	64	0
2	J	84	0	84	2	0
3	A	42	0	39	0	0
3	B	14	0	13	0	0
3	C	42	0	39	0	0
3	D	14	0	13	0	0
All	All	18174	0	17608	270	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 8.

The worst 5 of 270 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:C:222:LEU:HB2	1:C:319:VAL:HG12	1.65	0.79
1:A:222:LEU:HB2	1:A:319:VAL:HG12	1.65	0.79
1:B:373:TYR:HH	1:B:522:TRP:HE1	1.32	0.77
1:C:379:ASP:N	1:C:379:ASP:OD1	2.23	0.70
1:A:379:ASP:N	1:A:379:ASP:OD1	2.23	0.70

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 PDB entries followed by that with respect to all EM entries.

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	556/574 (97%)	527 (95%)	25 (4%)	4 (1%)	24 67
1	B	560/574 (98%)	532 (95%)	24 (4%)	4 (1%)	24 67
1	C	556/574 (97%)	527 (95%)	25 (4%)	4 (1%)	24 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	560/574 (98%)	532 (95%)	24 (4%)	4 (1%)	24 67
2	J	10/12 (83%)	6 (60%)	4 (40%)	0	100 100
All	All	2242/2308 (97%)	2124 (95%)	102 (4%)	16 (1%)	28 67

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	ASP
1	A	54	ASP
1	C	54	ASP
1	D	54	ASP
1	B	255	GLU

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 PDB entries followed by that with respect to all EM entries.

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	479/494 (97%)	468 (98%)	11 (2%)	53 76
1	B	483/494 (98%)	474 (98%)	9 (2%)	60 80
1	C	479/494 (97%)	468 (98%)	11 (2%)	53 76
1	D	483/494 (98%)	473 (98%)	10 (2%)	56 78
2	J	12/12 (100%)	12 (100%)	0	100 100
All	All	1936/1988 (97%)	1895 (98%)	41 (2%)	59 78

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	425	SER
1	C	195	PHE
1	D	253	SER
1	A	428	LEU
1	C	96	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	C	119	GLN
1	D	171	GLN
1	B	551	ASN
1	D	119	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	601	1	14,14,15	0.23	0	17,19,21	0.65	0
3	NAG	A	602	1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	A	603	1	14,14,15	0.88	1 (7%)	17,19,21	0.78	1 (5%)
3	NAG	B	601	1	14,14,15	0.92	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	C	601	1	14,14,15	0.23	0	17,19,21	0.64	0
3	NAG	C	602	1	14,14,15	0.22	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	603	1	14,14,15	0.88	1 (7%)	17,19,21	0.77	1 (5%)
3	NAG	D	601	1	14,14,15	0.92	1 (7%)	17,19,21	0.73	1 (5%)

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
3	NAG	A	601	1	-	4/6/23/26	0/1/1/1
3	NAG	A	602	1	-	4/6/23/26	0/1/1/1
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	C	601	1	-	4/6/23/26	0/1/1/1
3	NAG	C	602	1	-	4/6/23/26	0/1/1/1
3	NAG	C	603	1	-	2/6/23/26	0/1/1/1
3	NAG	D	601	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	NAG	C1-C2	2.89	1.56	1.52
3	B	601	NAG	C1-C2	2.87	1.56	1.52
3	A	603	NAG	C1-C2	2.79	1.56	1.52
3	C	603	NAG	C1-C2	2.74	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	NAG	C1-O5-C5	2.69	115.86	112.20
3	C	603	NAG	C1-O5-C5	2.65	115.80	112.20
3	D	601	NAG	C1-O5-C5	2.27	115.29	112.20
3	B	601	NAG	C1-O5-C5	2.27	115.29	112.20

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	601	NAG	C4-C5-C6-O6
3	C	602	NAG	O5-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.