

wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 03:02 AM EDT

PDB ID : 6OL9

Title : Structure of the M5 muscarinic acetylcholine receptor (M5-T4L) bound to

tiotropium

Authors: Vuckovic, Z.; Christopoulos, A.; Thal, D.M.

Deposited on : 2019-04-16

Resolution : 2.54 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

buster-report : 1.1.7 (2018)

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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3279 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 Muscarinic acetylcholine receptor M5, T4 Lysozyme fusion.

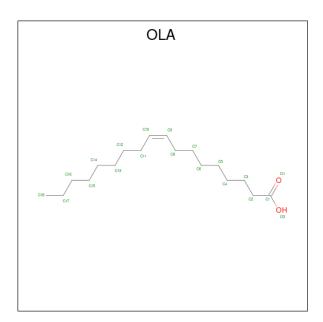
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	416	Total	С	N	О	S	0	0	0
1	A	410	3167	2072	521	552	22	U	U	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	=	expression tag	UNP P08912
A	20	ALA	=	expression tag	UNP P08912
A	117	ARG	SER	conflict	UNP P08912
A	1096	ALA	CYS	conflict	UNP D9IEF7
A	533	SER	-	expression tag	UNP P08912
A	534	SER	ı	expression tag	UNP P08912
A	535	HIS	-	expression tag	UNP P08912
A	536	HIS	-	expression tag	UNP P08912
A	537	HIS	ı	expression tag	UNP P08912
A	538	HIS	-	expression tag	UNP P08912
A	539	HIS	ı	expression tag	UNP P08912
A	540	HIS	-	expression tag	UNP P08912
A	541	HIS	-	expression tag	UNP P08912
A	542	HIS		expression tag	UNP P08912
A	543	HIS	-	expression tag	UNP P08912
A	544	HIS	-	expression tag	UNP P08912

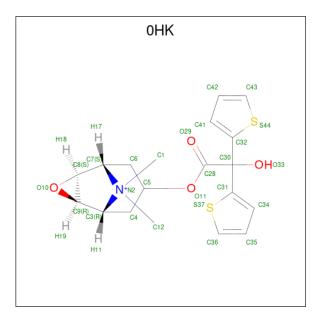
• Molecule 2 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	A	1	Total C O	0	0	
		_	12 10 2			
9	Λ	1	Total C O	0	0	
2	Λ	1	20 18 2	0	0	

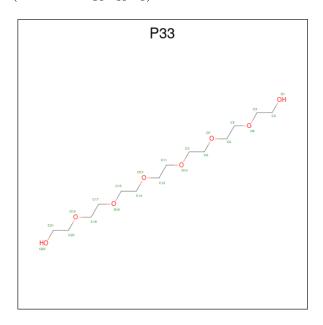
• Molecule 3 is (1R,2R,4S,5S,7S)-7-{[hydroxy(dithiophen-2-yl)acetyl]oxy}-9,9-dimethyl-3-oxa-9-azoniatricyclo[3.3.1.0 2,4]nonane (three-letter code: 0HK) (formula: $C_{19}H_{22}NO_4S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	Λ	1	Total	С	N	О	S	0	0
)	Λ	1	26	19	1	4	2	0	0

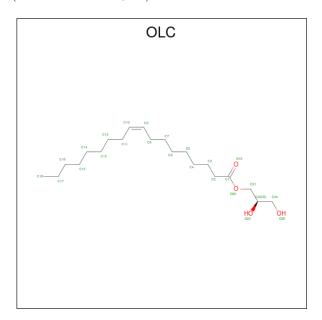


• Molecule 4 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 22	C 14	O 8	0	0

• Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 25	C 21	O 4	0	0



• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0

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



3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	97.06Å 63.31Å 91.62Å	Depositor
a, b, c, α , β , γ	90.00° 102.11° 90.00°	Depositor
Resolution (Å)	47.90 - 2.54	Depositor
% Data completeness	99.2 (47.90-2.54)	Depositor
(in resolution range)	33.2 (41.30 2.04)	_
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.29 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.236 , 0.257	Depositor
Wilson B-factor (A^2)	66.7	Xtriage
Anisotropy	0.126	Xtriage
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3279	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.90% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ 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.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

5 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	Trino	Chain	Res	Link	Bo	ond leng	ths	Bond angles		les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLC	A	1205	-	24,24,24	0.68	1 (4%)	25,25,25	0.93	1 (4%)
4	P33	A	1204	-	21,21,21	0.46	0	20,20,20	0.30	0
2	OLA	A	1201	-	11,11,19	0.64	0	11,11,19	0.99	0
2	OLA	A	1202	-	19,19,19	0.47	0	19,19,19	0.84	0
3	0HK	A	1203	-	28,30,30	0.49	0	38,48,48	1.11	4 (10%)

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
5	OLC	A	1205	-	-	10/24/24/24	-
4	P33	A	1204	-	-	5/19/19/19	-
2	OLA	A	1201	-	-	3/9/9/17	-
2	OLA	A	1202	-	-	5/17/17/17	-
3	0HK	A	1203	-	-	0/10/55/55	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
5	A	1205	OLC	O20-C1	2.67	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	1203	0HK	C12-N2-C3	2.66	116.80	113.03
3	A	1203	0HK	C1-N2-C7	2.53	116.62	113.03
5	A	1205	OLC	O20-C1-C2	2.33	119.21	111.91
3	A	1203	0HK	C12-N2-C7	2.12	116.03	113.03
3	A	1203	0HK	O10-C9-C3	2.05	119.03	117.11

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

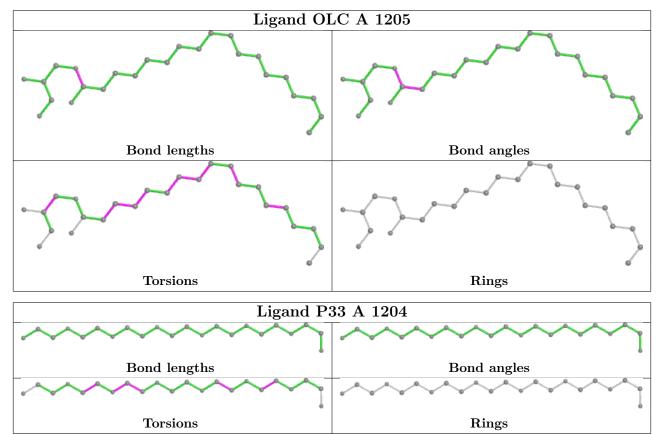


Mol	Chain	Res	Type	Atoms
5	A	1205	OLC	O20-C21-C22-O23
5	A	1205	OLC	O20-C21-C22-C24
5	A	1205	OLC	C1-C2-C3-C4
5	A	1205	OLC	C2-C3-C4-C5
5	A	1205	OLC	C3-C4-C5-C6

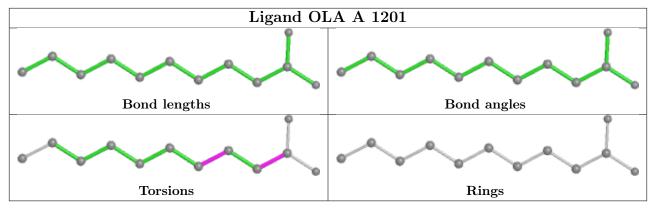
There are no ring outliers.

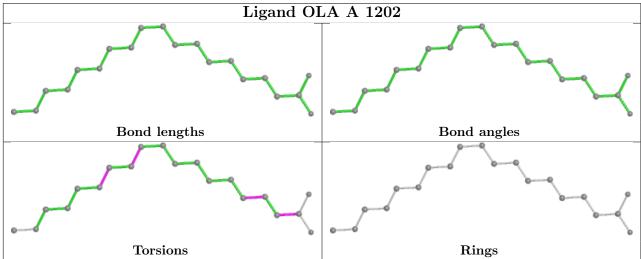
No monomer is involved in short contacts.

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 any Mogul-identified 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.

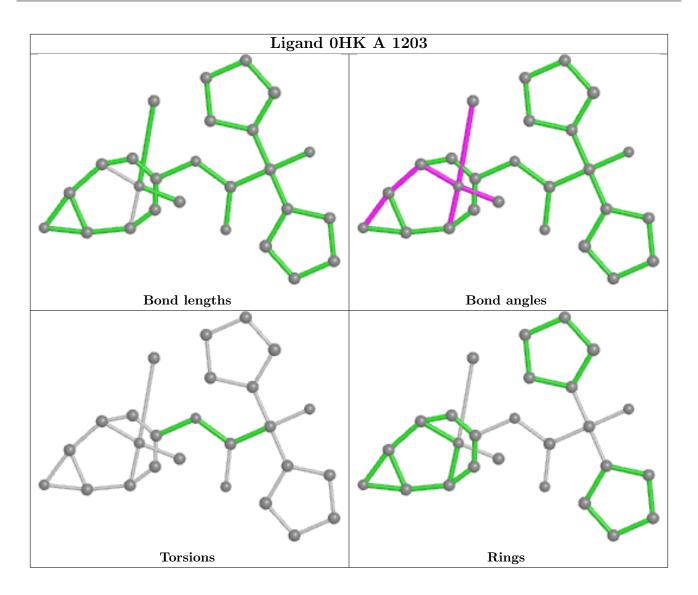












4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

