



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2021 – 12:12 pm GMT

PDB ID : 6ZFZ
Title : Structure of M1-StaR-T4L in complex with 77-LH-28-1 at 2.17Å
Authors : Rucktooa, P.; Cooke, R.M.
Deposited on : 2020-06-18
Resolution : 2.17 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

<https://www.wwpdb.org/validation/2017/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
Mogul : 1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

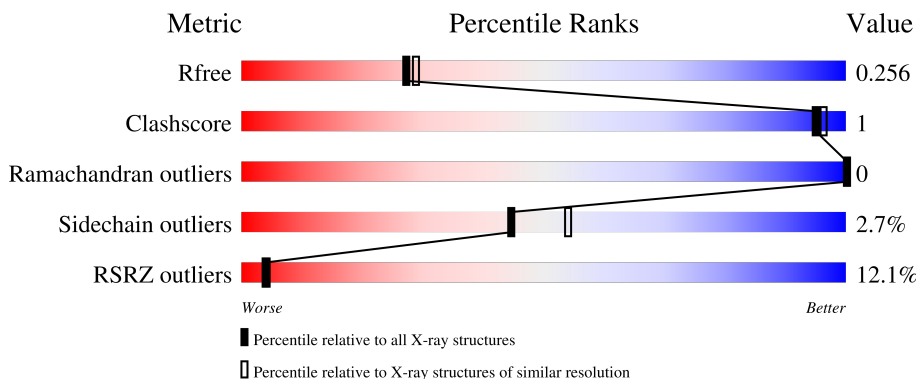
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 $\leq 5\%$. 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	455	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	OLC	A	1211	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EPE	A	1212	-	-	-	X
7	PGE	A	1214	-	-	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 3855 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 M1,Endolysin,Muscarinic acetylcholine receptor M1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3573	2325	601	623	24	0	2	0

There are 49 discrepancies between the modelled and reference sequences:

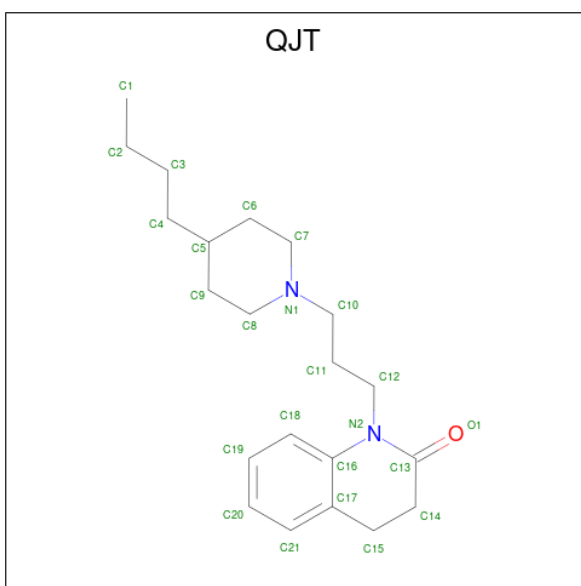
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP P11229
A	21	GLU	-	expression tag	UNP P11229
A	22	THR	-	expression tag	UNP P11229
A	23	VAL	-	expression tag	UNP P11229
A	24	GLU	-	expression tag	UNP P11229
A	25	MET	-	expression tag	UNP P11229
A	26	VAL	-	expression tag	UNP P11229
A	27	ALA	PHE	engineered mutation	UNP P11229
A	29	ALA	GLY	conflict	UNP P11229
A	30	THR	ILE	conflict	UNP P11229
A	31	VAL	THR	conflict	UNP P11229
A	32	ALA	THR	engineered mutation	UNP P11229
A	44	ILE	LEU	engineered mutation	UNP P11229
A	46	LEU	VAL	engineered mutation	UNP P11229
A	47	MET	LEU	conflict	UNP P11229
A	48	LEU	ILE	conflict	UNP P11229
A	50	ILE	PHE	conflict	UNP P11229
A	54	ARG	THR	conflict	UNP P11229
A	55	GLN	GLU	conflict	UNP P11229
A	57	GLN	LYS	conflict	UNP P11229
A	64	ALA	LEU	engineered mutation	UNP P11229
A	65	PHE	LEU	conflict	UNP P11229
A	76	ALA	THR	engineered mutation	UNP P11229
A	84	VAL	THR	engineered mutation	UNP P11229
A	86	ILE	LEU	conflict	UNP P11229
A	87	ILE	LEU	conflict	UNP P11229

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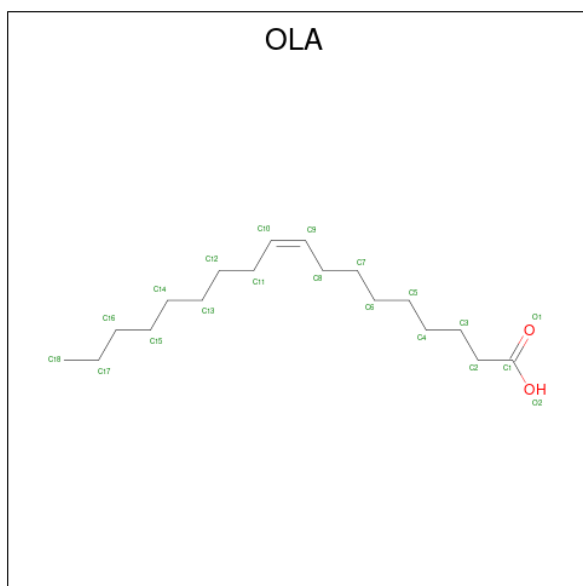
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ALA	THR	engineered mutation	UNP P11229
A	101	ALA	TRP	engineered mutation	UNP P11229
A	112	ALA	SER	engineered mutation	UNP P11229
A	143	LEU	ALA	engineered mutation	UNP P11229
A	196	THR	ALA	engineered mutation	UNP P11229
A	1012	GLY	ARG	conflict	UNP P00720
A	1054	THR	CYS	conflict	UNP P00720
A	1097	ALA	CYS	conflict	UNP P00720
A	1137	ARG	ILE	conflict	UNP P00720
A	362	ALA	LYS	engineered mutation	UNP P11229
A	364	LEU	ALA	engineered mutation	UNP P11229
A	411	ALA	SER	engineered mutation	UNP P11229
A	435	ALA	CYS	conflict	UNP P11229
A	439	HIS	-	expression tag	UNP P11229
A	440	HIS	-	expression tag	UNP P11229
A	441	HIS	-	expression tag	UNP P11229
A	442	HIS	-	expression tag	UNP P11229
A	443	HIS	-	expression tag	UNP P11229
A	444	HIS	-	expression tag	UNP P11229
A	445	HIS	-	expression tag	UNP P11229
A	446	HIS	-	expression tag	UNP P11229
A	447	HIS	-	expression tag	UNP P11229
A	448	HIS	-	expression tag	UNP P11229

- Molecule 2 is 1-[3-(4-butylpiperidin-1-yl)propyl]-3,4-dihydroquinolin-2-one (three-letter code: QJT) (formula: C₂₁H₃₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	24	21	2	1	0	0

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



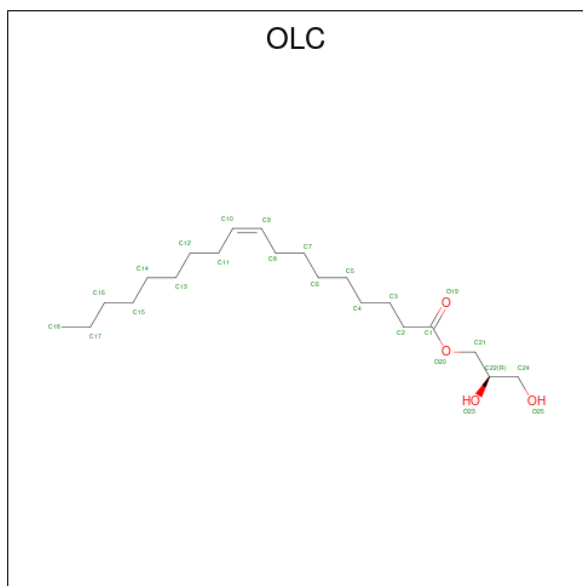
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	20	18	2	0	0
3	A	1	20	18	2	0	0
3	A	1	20	18	2	0	0
3	A	1	20	18	2	0	0
3	A	1	20	18	2	0	0
3	A	1	20	18	2	0	0
3	A	1	20	18	2	0	0
3	A	1	20	18	2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



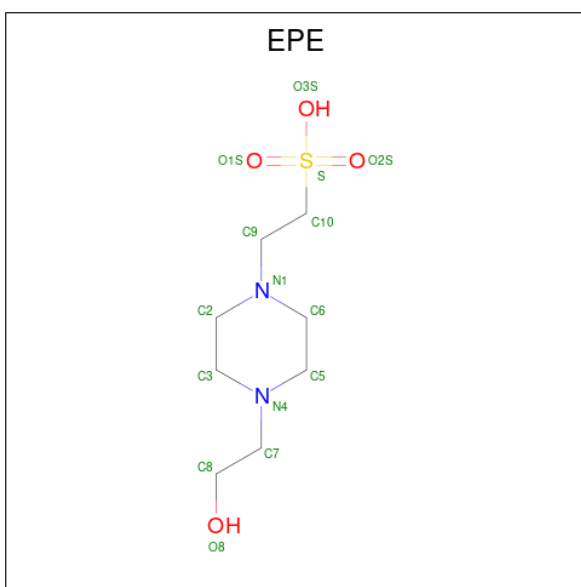
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

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



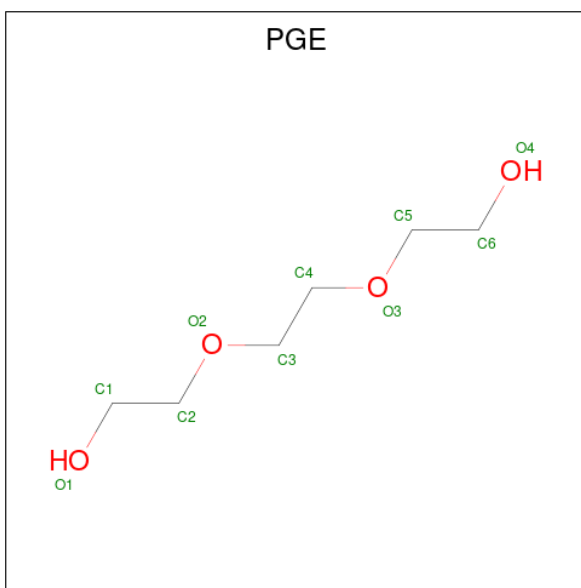
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	15	8	2	4	1	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	10	6	4	0	0
7	A	1	10	6	4	0	0

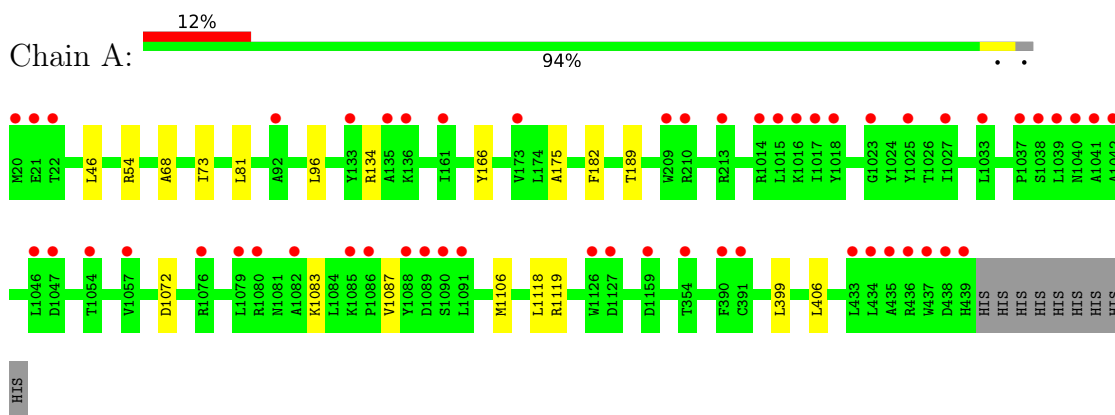
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	33	Total 33	O 33	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 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: Muscarinic acetylcholine receptor M1,Endolysin,Muscarinic acetylcholine receptor M1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.34Å 65.63Å 156.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.30 – 2.17 50.30 – 2.17	Depositor EDS
% Data completeness (in resolution range)	72.3 (50.30-2.17) 72.3 (50.30-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.16Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.214 , 0.242 0.226 , 0.256	Depositor DCC
R_{free} test set	1194 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for k,h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3855	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, PO4, EPE, PGE, OLC, QJT

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	0.42	0/3659	0.57	0/4977

There are no bond length outliers.

There are no bond angle outliers.

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	3573	0	3652	9	0
2	A	24	0	0	0	0
3	A	160	0	264	2	0
4	A	5	0	0	0	0
5	A	25	0	40	0	0
6	A	15	0	18	3	0
7	A	20	0	28	2	0
8	A	33	0	0	0	0
All	All	3855	0	4002	9	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 1.

All (9) 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:166:TYR:HA	6:A:1212:EPE:H32	1.80	0.62
1:A:46:LEU:HD23	1:A:68:ALA:HB2	1.87	0.56
1:A:166:TYR:HD1	6:A:1212:EPE:H52	1.70	0.55
1:A:73:ILE:HD11	3:A:1202:OLA:H162	1.90	0.53
1:A:175:ALA:HA	7:A:1214:PGE:H5	1.91	0.52
1:A:189:THR:HG21	7:A:1213:PGE:H6	1.92	0.51
1:A:166:TYR:CD1	6:A:1212:EPE:H52	2.48	0.48
1:A:81:LEU:HD11	3:A:1205:OLA:H81	2.00	0.42
1:A:1087:VAL:HG11	1:A:1118:LEU:HD22	2.01	0.42

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 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	446/455 (98%)	438 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 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	378/385 (98%)	368 (97%)	10 (3%)	46 55

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	96	LEU
1	A	134	ARG
1	A	182	PHE
1	A	1072	ASP
1	A	1083	LYS
1	A	1106	MET
1	A	1119	ARG
1	A	399	LEU
1	A	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	115	ASN
1	A	177	GLN
1	A	1002	ASN
1	A	414	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](#)

14 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

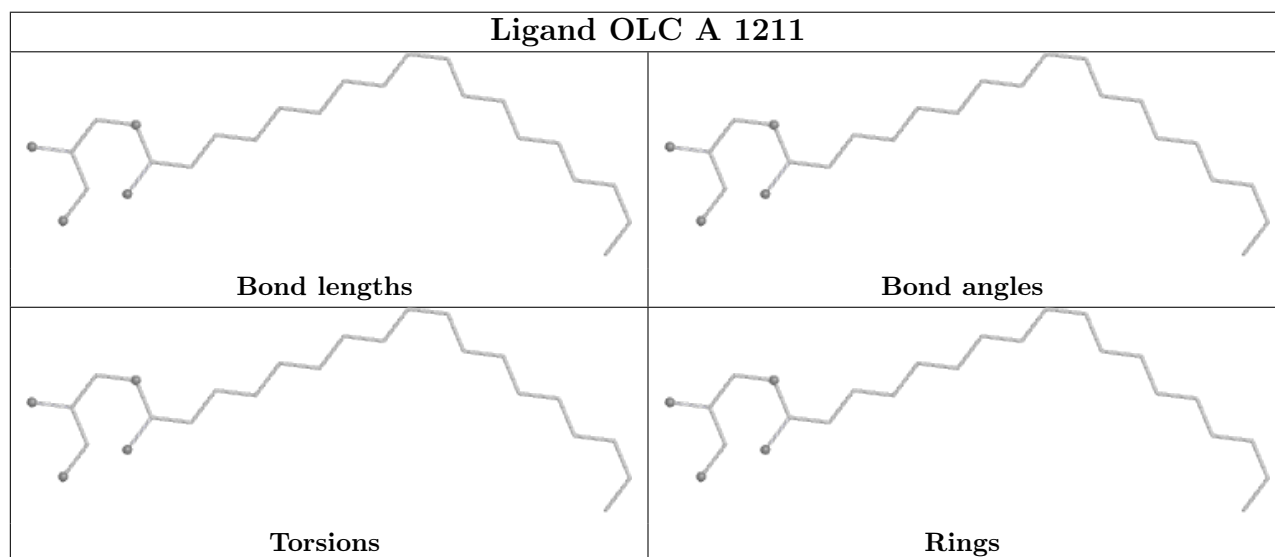
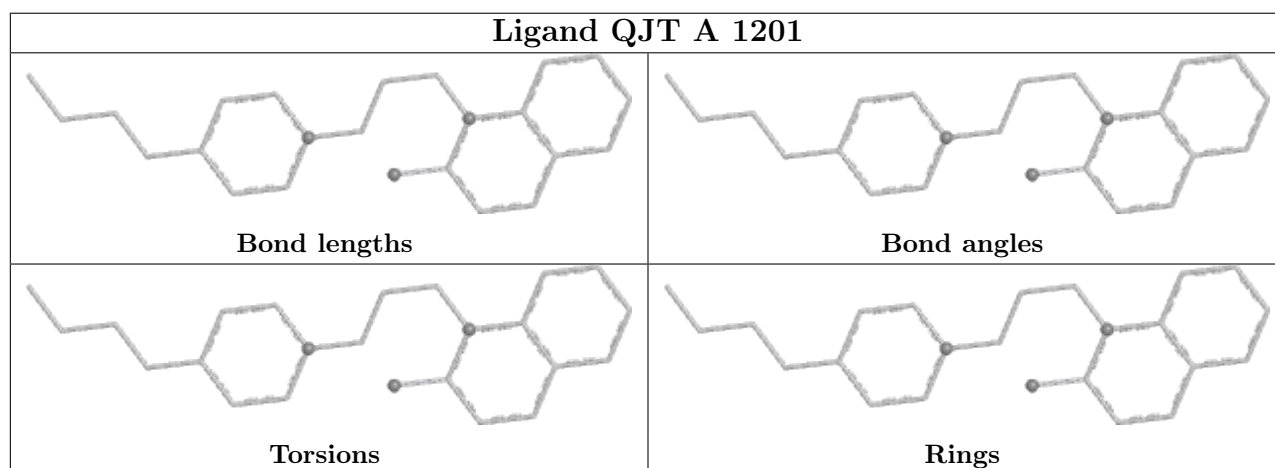
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



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](#)

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	446/455 (98%)	0.81	54 (12%) 4 4	20, 41, 76, 138	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	TRP	14.5
1	A	438	ASP	8.2
1	A	439	HIS	6.7
1	A	209[A]	TRP	5.4
1	A	1017	ILE	5.2
1	A	436	ARG	4.9
1	A	435	ALA	4.8
1	A	354	THR	4.5
1	A	434	LEU	4.4
1	A	1057	VAL	4.4
1	A	1082	ALA	4.1
1	A	1046	LEU	4.0
1	A	1047	ASP	3.8
1	A	1126	TRP	3.8
1	A	21	GLU	3.6
1	A	1016	LYS	3.5
1	A	1079	LEU	3.4
1	A	1042	ALA	3.4
1	A	1039	LEU	3.3
1	A	1038	SER	3.3
1	A	1025	TYR	3.3
1	A	1040	ASN	3.3
1	A	20	MET	3.1
1	A	391	CYS	3.0
1	A	1023	GLY	3.0
1	A	1085	LYS	2.9
1	A	1014	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1076	ARG	2.8
1	A	210	ARG	2.7
1	A	133	TYR	2.7
1	A	1090	SER	2.7
1	A	1088	TYR	2.7
1	A	22	THR	2.6
1	A	136	LYS	2.5
1	A	1080	ARG	2.5
1	A	1086	PRO	2.4
1	A	213	ARG	2.4
1	A	1037	PRO	2.4
1	A	1033	LEU	2.4
1	A	1041	ALA	2.4
1	A	1091	LEU	2.4
1	A	433	LEU	2.4
1	A	1127	ASP	2.4
1	A	92	ALA	2.3
1	A	1027	ILE	2.3
1	A	1015	LEU	2.3
1	A	1089	ASP	2.3
1	A	173	VAL	2.2
1	A	1054	THR	2.2
1	A	390	PHE	2.1
1	A	135	ALA	2.1
1	A	1018	TYR	2.1
1	A	1159	ASP	2.0
1	A	161	ILE	2.0

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 monosaccharides in this entry.

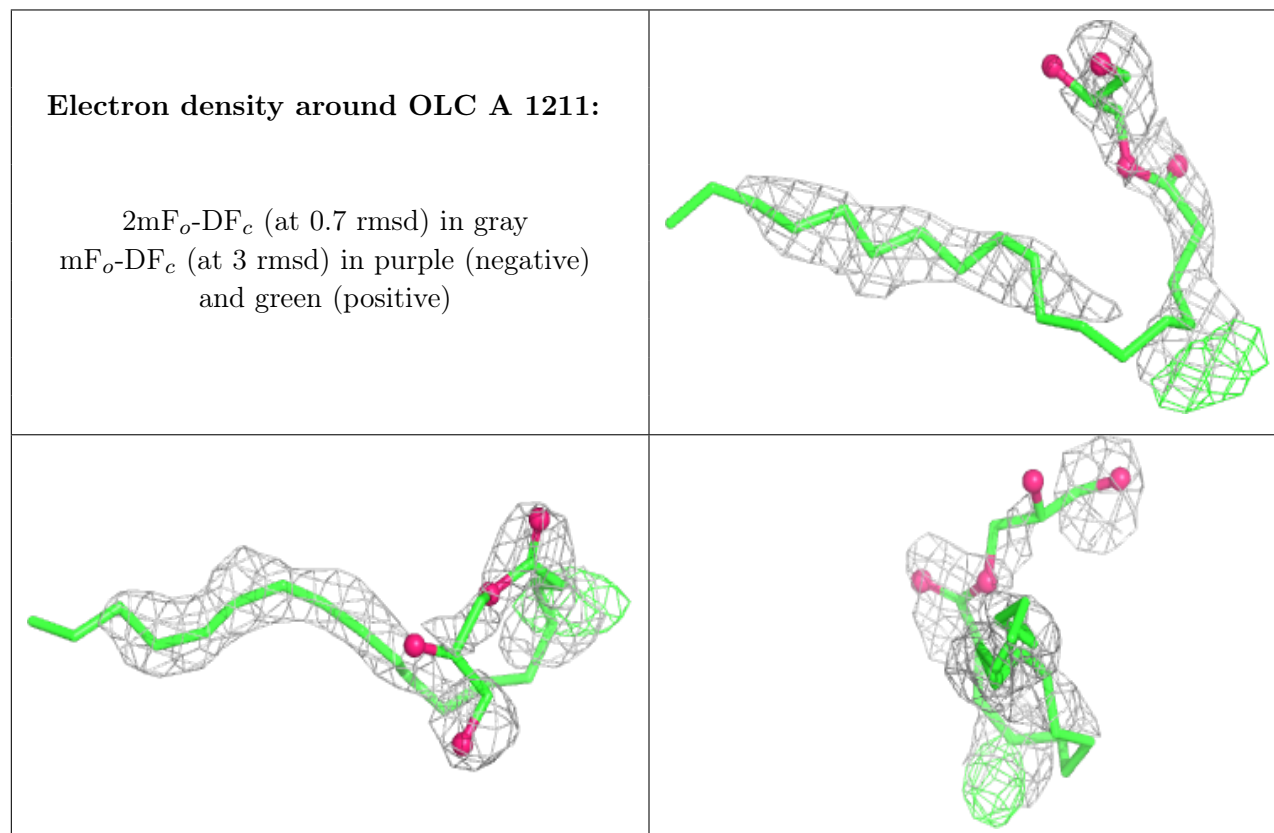
6.4 Ligands [i](#)

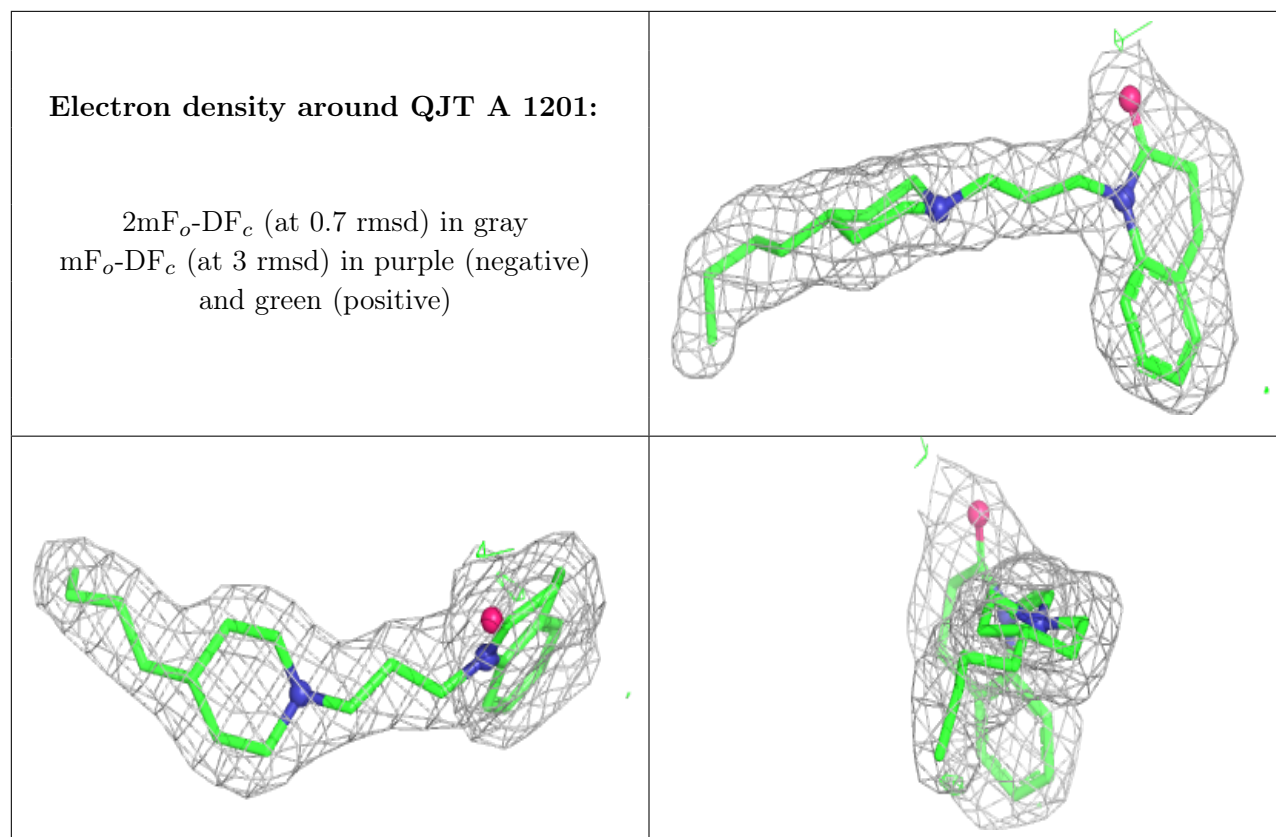
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PGE	A	1214	10/10	0.39	0.42	61,70,78,78	0
3	OLA	A	1208	20/20	0.47	0.36	57,63,74,74	0
6	EPE	A	1212	15/15	0.49	0.43	83,85,91,93	0
3	OLA	A	1205	20/20	0.51	0.38	65,73,85,85	0
5	OLC	A	1211	25/25	0.57	0.45	68,76,82,82	0
3	OLA	A	1210	20/20	0.59	0.33	83,84,85,85	0
3	OLA	A	1202	20/20	0.60	0.35	54,58,69,70	0
7	PGE	A	1213	10/10	0.63	0.24	54,62,67,67	0
3	OLA	A	1209	20/20	0.65	0.32	50,65,67,67	0
3	OLA	A	1204	20/20	0.67	0.24	47,58,79,79	0
3	OLA	A	1207	20/20	0.71	0.21	65,70,79,80	0
3	OLA	A	1203	20/20	0.75	0.37	51,55,64,64	0
4	PO4	A	1206	5/5	0.86	0.24	102,103,103,103	0
2	QJT	A	1201	24/24	0.91	0.17	27,31,37,39	0

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](#)

There are no such residues in this entry.