

wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2021 – 09:03 am GMT

PDB ID : 6Z70

Title: Structure of the MATE family multidrug resistance transporter Aq. 128 from

Aquifex aeolicus in the outward-facing state

Authors: Zhao, J.; Safarian, S.; Thielmann, Y.; Xie, H.; Wang, J.; Michel, H.

Deposited on : 2020-05-29

Resolution : 2.00 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: 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)

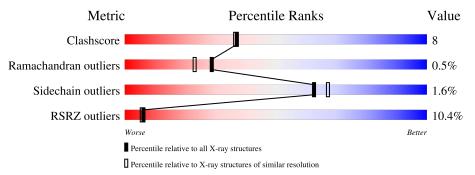
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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% 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	496	74%	14% • 10%					
1	В	496	9%	9% • 10%					



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7154 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 Aq128.

\mathbf{Mol}	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf	Trace		
1	Λ	444	Total	С	Ν	О	S	0	0	0	
1	Λ	444	3486	2348	544	579	15	0	0		
1	B	444	Total	С	N	О	S	0	0	0	
1	D	444	3487	2349	544	579	15				

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	473	ARG	-	expression tag	UNP O66528
A	474	ASN	-	expression tag	UNP O66528
A	475	SER	-	expression tag	UNP O66528
A	476	GLU	-	expression tag	UNP O66528
A	477	ASN	-	expression tag	UNP O66528
A	478	LEU	-	expression tag	UNP O66528
A	479	TYR	-	expression tag	UNP O66528
A	480	PHE	-	expression tag	UNP O66528
A	481	GLN	-	expression tag	UNP O66528
A	482	GLY	-	expression tag	UNP O66528
A	483	GLY	-	expression tag	UNP O66528
A	484	ARG	-	expression tag	UNP O66528
A	485	GLY	-	expression tag	UNP O66528
A	486	SER	-	expression tag	UNP O66528
A	487	HIS	-	expression tag	UNP O66528
A	488	HIS	-	expression tag	UNP O66528
A	489	HIS	-	expression tag	UNP O66528
A	490	HIS	-	expression tag	UNP O66528
A	491	HIS	-	expression tag	UNP O66528
A	492	HIS	-	expression tag	UNP O66528
A	493	HIS	-	expression tag	UNP O66528
A	494	HIS	-	expression tag	UNP O66528
A	495	HIS	-	expression tag	UNP O66528
A	496	HIS	-	expression tag	UNP O66528
В	473	ARG	-	expression tag	UNP O66528

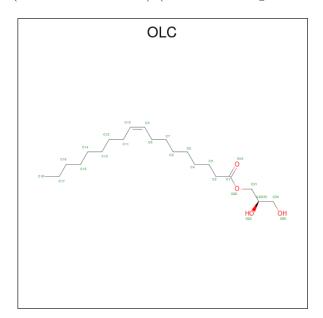
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Chain	Residue	Modelled	Actual	Comment	Reference
В	474	ASN	-	expression tag	UNP O66528
В	475	SER	-	expression tag	UNP O66528
В	476	GLU	-	expression tag	UNP O66528
В	477	ASN	-	expression tag	UNP O66528
В	478	LEU	-	expression tag	UNP O66528
В	479	TYR	-	expression tag	UNP O66528
В	480	PHE	-	expression tag	UNP O66528
В	481	GLN	-	expression tag	UNP O66528
В	482	GLY	-	expression tag	UNP O66528
В	483	GLY	-	expression tag	UNP O66528
В	484	ARG	-	expression tag	UNP O66528
В	485	GLY	-	expression tag	UNP O66528
В	486	SER	-	expression tag	UNP O66528
В	487	HIS	-	expression tag	UNP O66528
В	488	HIS	-	expression tag	UNP O66528
В	489	HIS	-	expression tag	UNP O66528
В	490	HIS	-	expression tag	UNP O66528
В	491	HIS	-	expression tag	UNP O66528
В	492	HIS	-	expression tag	UNP O66528
В	493	HIS	=	expression tag	UNP O66528
В	494	HIS	=	expression tag	UNP O66528
В	495	HIS	-	expression tag	UNP O66528
В	496	HIS	=	expression tag	UNP O66528

• Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).





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

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	В	3	Total O 3 3	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: Aq128 Chain A: | Coling | C • Molecule 1: Aq128 Chain B: 80% 10% SER HIS HIS HIS HIS HIS



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	72.10Å 116.10Å 137.60Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 - 2.00	Depositor
Resolution (A)	19.99 - 2.00	EDS
% Data completeness	98.9 (19.99-2.00)	Depositor
(in resolution range)	99.1 (19.99-2.00)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.54 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D D.	0.266 , 0.284	Depositor
R, R_{free}	0.266 , (Not available)	DCC
R_{free} test set	748 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ < L > = 0.57, < L^2> = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7154	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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 59.92 % 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 1.6430e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.

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: OLC

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		nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.45	$2/3585 \ (0.1\%)$	0.54	1/4875 (0.0%)	
1	В	0.44	1/3586 (0.0%)	0.56	1/4876 (0.0%)	
All	All	0.45	3/7171 (0.0%)	0.55	2/9751 (0.0%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
1	В	157	TYR	CB-CG	-6.64	1.41	1.51
1	A	350	GLU	CB-CG	5.71	1.62	1.52
1	A	157	TYR	CD1-CE1	-5.18	1.31	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	248	LEU	CA-CB-CG	-8.30	96.22	115.30
1	A	248	LEU	CA-CB-CG	-5.67	102.26	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	3486	0	3643	65	0

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	.,	10	1

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	3487	0	3648	48	0
2	A	100	0	160	23	0
2	В	75	0	120	13	0
3	A	3	0	0	1	0
3	В	3	0	0	1	0
All	All	7154	0	7571	115	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 115 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$	
1:B:157:TYR:OH	1:B:223:LYS:NZ	1.73	1.22	
1:A:223:LYS:HG3	1:A:224:PRO:HD2	1.18	1.16	
1:B:223:LYS:HG3	1:B:224:PRO:HD2	1.31	1.06	
1:A:107:PRO:HG2	2:A:501:OLC:H13	1.54	0.86	
1:A:37:ASN:HD21	2:A:504:OLC:H24A	1.40	0.86	

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	Perce	entiles
1	A	442/496 (89%)	432 (98%)	9 (2%)	1 (0%)	47	44
1	В	442/496 (89%)	429 (97%)	10 (2%)	3 (1%)	22	16
All	All	884/992 (89%)	861 (97%)	19 (2%)	4 (0%)	29	23

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	223	LYS
1	В	121	LYS
1	В	122	VAL
1	В	223	LYS

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	376/424 (89%)	371 (99%)	5 (1%)	69	74	
1	В	376/424 (89%)	369 (98%)	7 (2%)	57	61	
All	All	752/848 (89%)	740 (98%)	12 (2%)	62	67	

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	238	LYS
1	В	280	ARG
1	В	431	PHE
1	В	357	TYR
1	A	431	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	177	HIS
1	В	37	ASN
1	В	177	HIS

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)

7 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

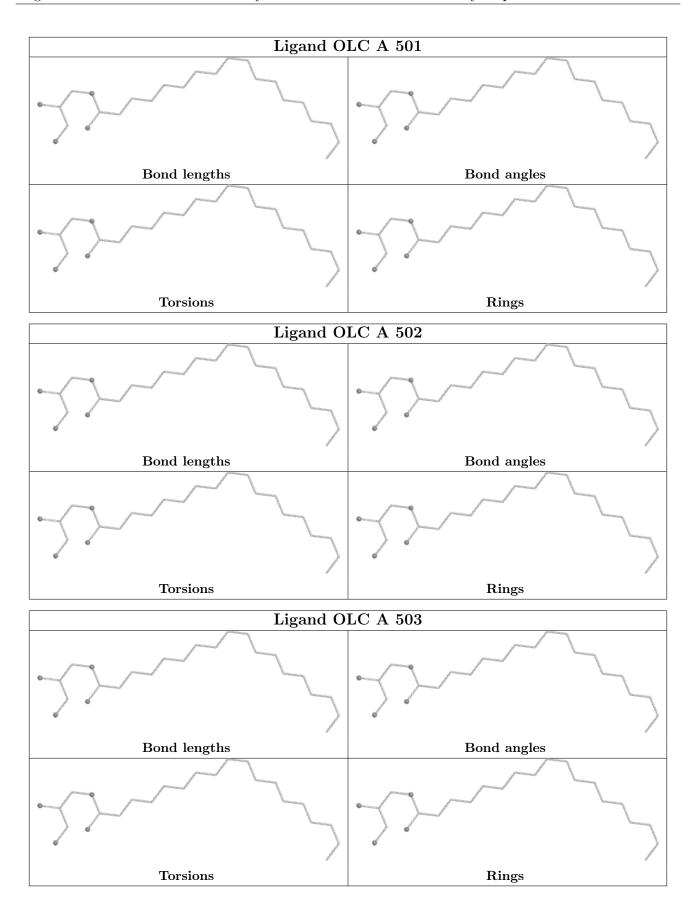
There are no torsion outliers.

There are no ring outliers.

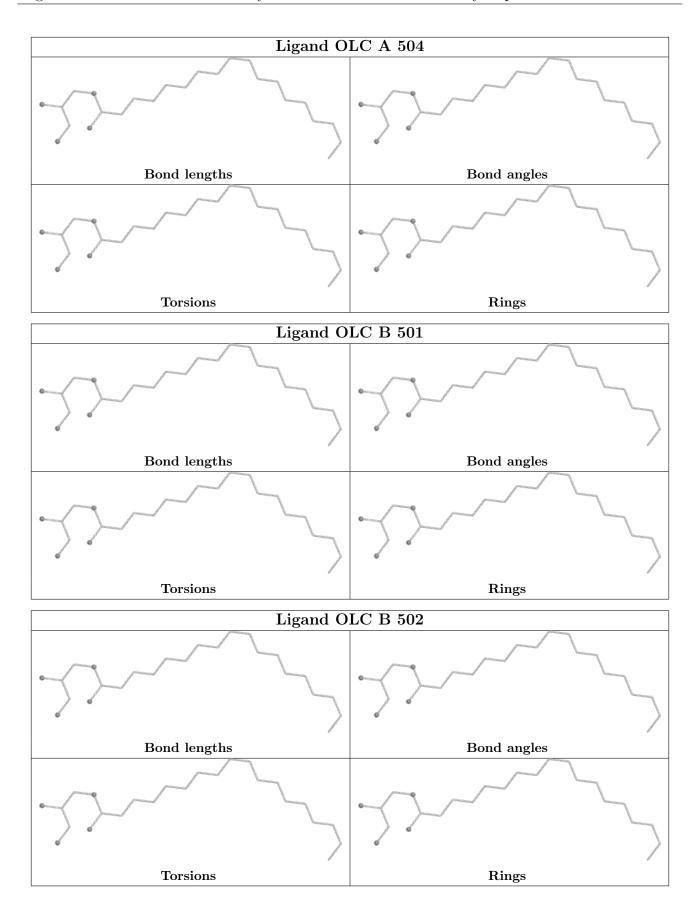
No monomer is involved in short contacts.

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 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.

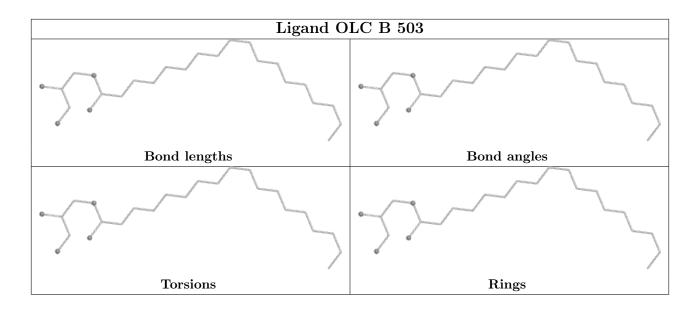












5.7 Other polymers (i)

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	# RSRZ > 2		$OWAB(A^2)$	Q<0.9	
1	A	444/496 (89%)	0.74	48 (10%)	5	5	27, 39, 60, 70	0
1	В	444/496 (89%)	0.55	44 (9%)	7	6	26, 38, 58, 73	0
All	All	888/992 (89%)	0.64	92 (10%)	6	5	26, 39, 60, 73	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	PHE	7.3
1	В	357	TYR	6.9
1	В	189	PHE	5.9
1	В	124	GLY	5.3
1	В	190	GLY	5.2

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.

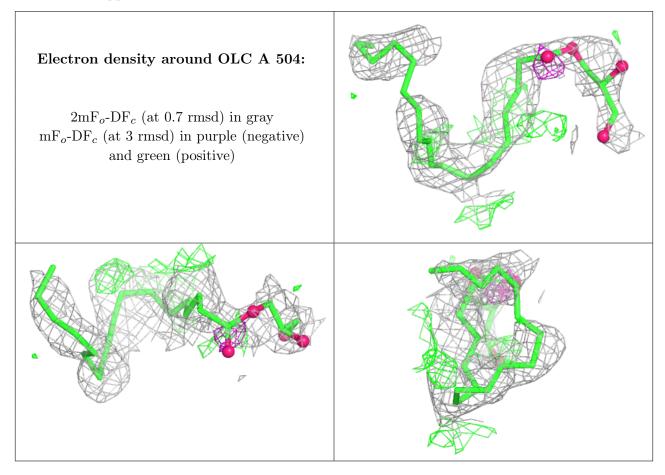
6.4 Ligands (i)

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	OLC	A	504	25/25	0.48	0.36	51,64,70,75	0
2	OLC	В	502	25/25	0.60	0.29	35,45,68,72	0
2	OLC	A	502	25/25	0.65	0.29	31,43,67,70	0
2	OLC	A	503	25/25	0.68	0.35	46,53,59,63	0
2	OLC	В	503	25/25	0.68	0.29	44,54,63,64	0
2	OLC	В	501	25/25	0.70	0.28	35,48,65,68	0
2	OLC	A	501	25/25	0.72	0.29	30,50,65,72	0

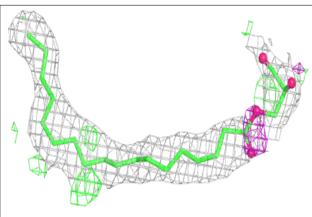
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

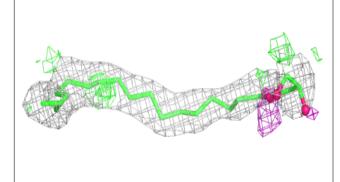


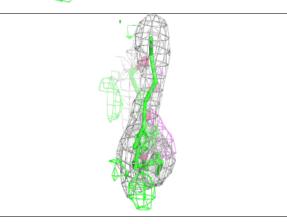


Electron density around OLC B 502:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

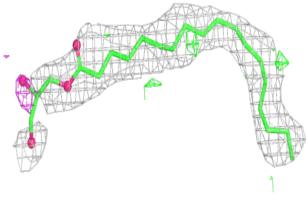


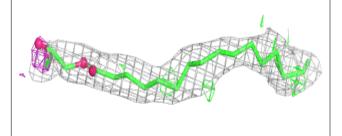


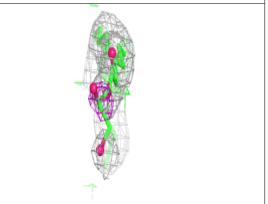


Electron density around OLC A 502:

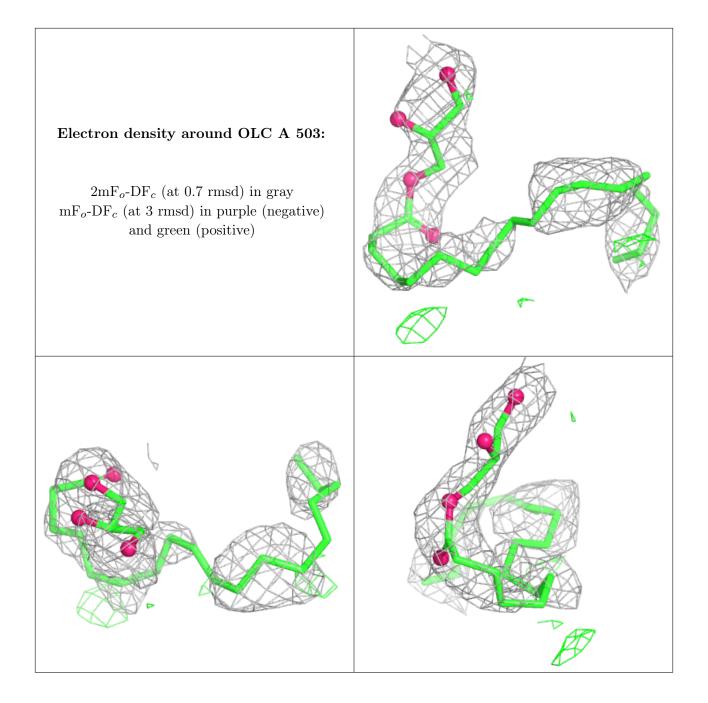
 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



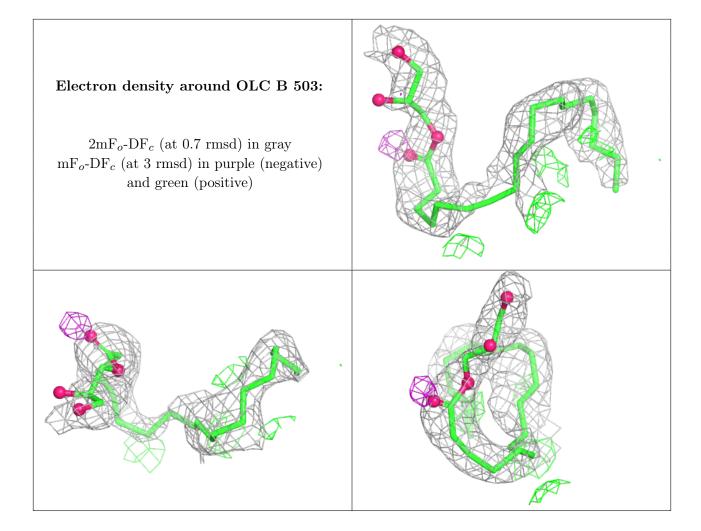








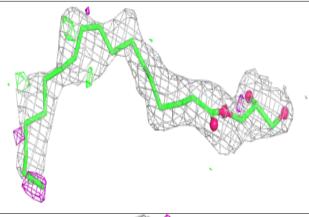


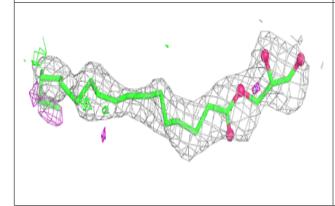


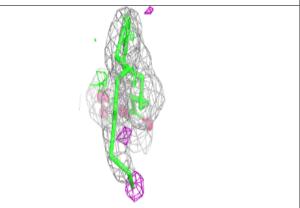


Electron density around OLC B 501:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

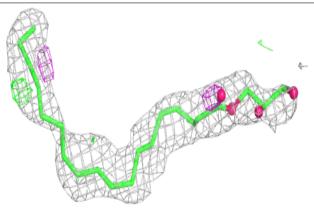


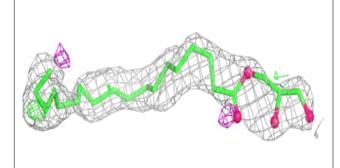


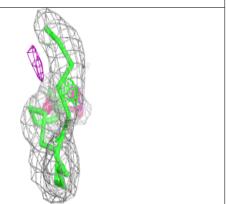


Electron density around OLC A 501:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

