Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 03:47 AM EDT

PDB ID	:	6EID
Title	:	Crystal structure of wild-type Channelrhodopsin 2
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Deposited on	:	2017-09-19
Resolution	:	2.39 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 (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 (i)) were used in the production of this report:

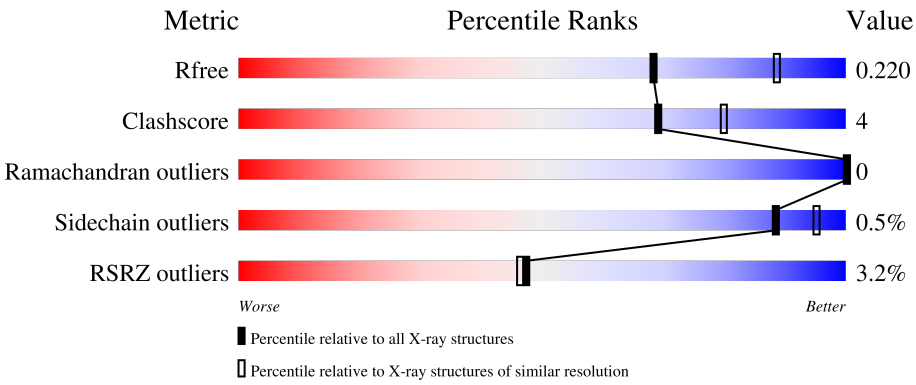
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	315	2% 75% • 22%
1	B	315	3% 76% • 20%

2 Entry composition (i)

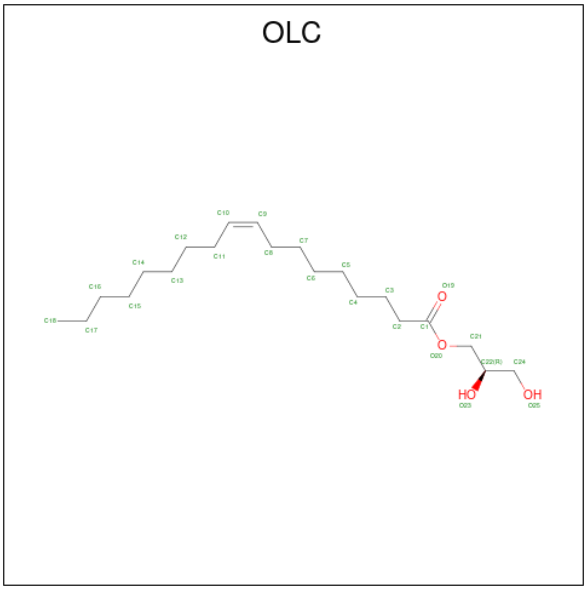
There are 5 unique types of molecules in this entry. The entry contains 4265 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Archaeal-type opsin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	247	1965	1313	310	325	17	0	1	0
1	B	251	2012	1343	317	335	17	0	1	0

- Molecule 2 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
			Total	C	O		
2	A	1	16	12	4	0	0
2	A	1	18	15	3	0	0
2	A	1	18	14	4	0	0
2	A	1	15	14	1	0	0

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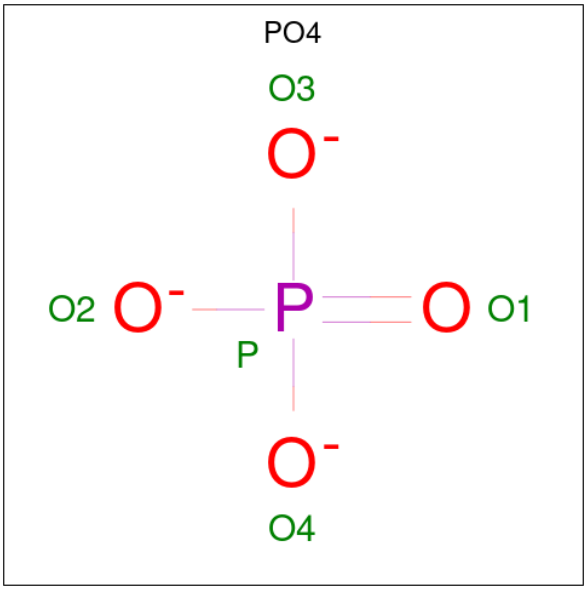
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 18 18	0	0
2	A	1	Total C O 8 6 2	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C O 12 11 1	0	0
2	B	1	Total C 13 13	0	0
2	B	1	Total C O 21 17 4	0	0
2	B	1	Total C O 19 15 4	0	0
2	B	1	Total C O 18 14 4	0	0
2	B	1	Total C 18 18	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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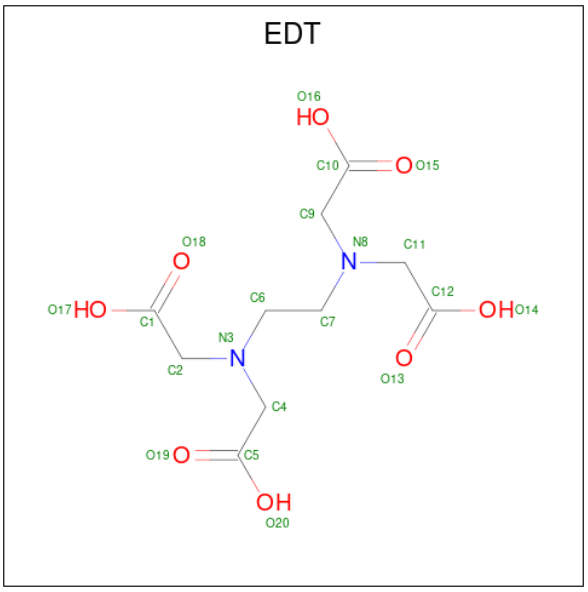
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	B	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0

- Molecule 4 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (three-letter code: EDT) (formula: $C_{10}H_{16}N_2O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	20	10	2	8	0	0

- Molecule 5 is water.

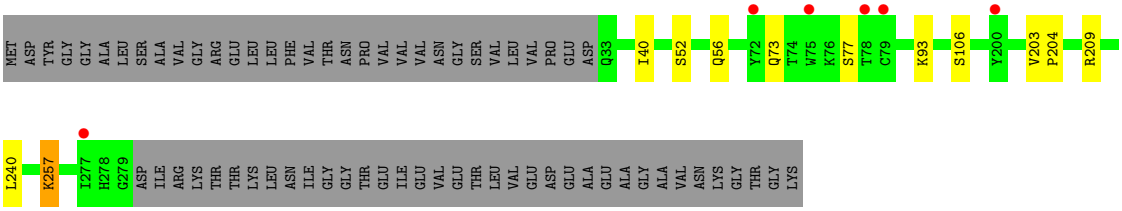
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	26	26	26	0	0
			Total	O		
5	B	24	24	24	0	0

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.

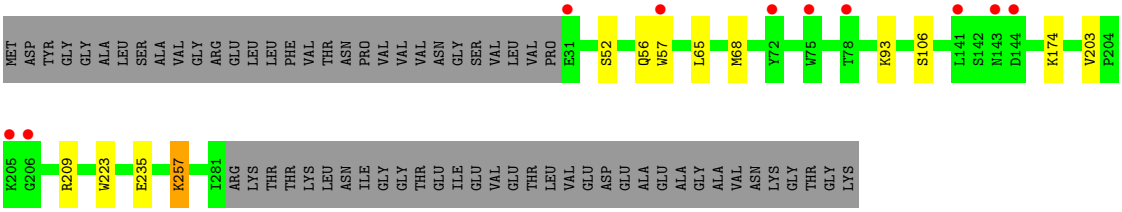
• Molecule 1: Archaeal-type opsin 2

Chain A:



• Molecule 1: Archaeal-type opsin 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	62.78Å 135.77Å 78.12Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.39 19.72 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.39) 100.0 (19.72-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.8.0158, BUSTER	Depositor
R, R_{free}	0.209 , 0.219 0.209 , 0.220	Depositor DCC
R_{free} test set	1281 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.168 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4265	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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, LYR, PO4, EDT

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	0.47	0/1964	0.56	0/2676
1	B	0.46	0/2014	0.56	0/2743
All	All	0.46	0/3978	0.56	0/5419

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	1965	0	1931	15	0
1	B	2012	0	1971	16	0
2	A	109	0	150	0	0
2	B	89	0	130	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	20	0	12	0	0
5	A	26	0	0	1	0
5	B	24	0	0	1	0
All	All	4265	0	4194	31	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 4.

All (31) 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:257[B]:LYR:H192	1:B:257[B]:LYR:H9	1.19	1.13
1:A:257[B]:LYR:H192	1:A:257[B]:LYR:H9	1.36	1.04
1:B:257[B]:LYR:H192	1:B:257[B]:LYR:C9	1.94	0.91
1:A:257[B]:LYR:H192	1:A:257[B]:LYR:C9	2.08	0.83
1:B:174:LYS:HE2	1:B:235:GLU:O	1.82	0.79
1:B:257[B]:LYR:H9	1:B:257[B]:LYR:C19	2.03	0.75
1:B:257[A]:LYR:H192	1:B:257[A]:LYR:H9	1.74	0.69
1:A:257[A]:LYR:H192	1:A:257[A]:LYR:H9	1.74	0.68
1:B:257[B]:LYR:C9	1:B:257[B]:LYR:C19	2.68	0.66
1:B:93:LYS:HD2	5:B:1204:HOH:O	1.98	0.63
1:A:73:GLN:O	1:A:77:SER:N	2.41	0.52
1:A:257[A]:LYR:H192	1:A:257[A]:LYR:C9	2.42	0.50
1:A:203:VAL:HG23	1:A:209:ARG:HG2	1.94	0.49
1:B:257[A]:LYR:H192	1:B:257[A]:LYR:C9	2.42	0.49
1:A:93:LYS:HD2	5:A:1207:HOH:O	2.12	0.49
1:A:257[B]:LYR:C9	1:A:257[B]:LYR:C19	2.81	0.49
1:B:52:SER:O	1:B:56:GLN:HG2	2.13	0.49
1:A:52:SER:O	1:A:56:GLN:HG2	2.13	0.48
1:B:57:TRP:HA	1:B:57:TRP:CE3	2.48	0.48
1:B:203:VAL:HG23	1:B:209:ARG:HG2	1.96	0.47
1:B:65:LEU:HA	1:B:68:MET:HE2	1.97	0.47
1:A:240:LEU:HD21	2:B:1105:OLC:H18A	1.96	0.46
1:B:174:LYS:CE	1:B:235:GLU:O	2.57	0.46
1:B:257[B]:LYR:H6	1:B:257[B]:LYR:H41	1.48	0.45
1:B:257[B]:LYR:H81	1:B:257[B]:LYR:H10	1.79	0.45
1:B:223:TRP:CE2	1:B:257[B]:LYR:C4	3.01	0.44
1:A:257[B]:LYR:H41	1:A:257[B]:LYR:H6	1.65	0.44
1:A:203:VAL:HB	1:A:204:PRO:HD2	2.01	0.42
1:A:257[A]:LYR:H6	1:A:257[A]:LYR:H41	1.84	0.42
1:A:257[A]:LYR:H10	1:A:257[A]:LYR:H81	1.86	0.42
1:A:40:ILE:O	1:A:40:ILE:HG22	2.20	0.41

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	244/315 (78%)	242 (99%)	2 (1%)	0	100	100
1	B	248/315 (79%)	244 (98%)	4 (2%)	0	100	100
All	All	492/630 (78%)	486 (99%)	6 (1%)	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	194/258 (75%)	193 (100%)	1 (0%)	88	95
1	B	200/258 (78%)	199 (100%)	1 (0%)	88	95
All	All	394/516 (76%)	392 (100%)	2 (0%)	88	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	B	106	SER

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	134	HIS

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Mol	Chain	Res	Type
1	A	258	ASN
1	B	46	ASN
1	B	49	GLN
1	B	134	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LYR	A	257[A]	1	27,29,30	0.61	0	30,37,39	1.60	7 (23%)
1	LYR	B	257[A]	1	27,29,30	0.63	0	30,37,39	1.59	6 (20%)
1	LYR	A	257[B]	1	27,29,30	0.84	1 (3%)	30,37,39	2.90	10 (33%)
1	LYR	B	257[B]	1	27,29,30	0.66	0	30,37,39	2.20	9 (30%)

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
1	LYR	A	257[A]	1	-	4/22/40/42	0/1/1/1
1	LYR	B	257[A]	1	-	4/22/40/42	0/1/1/1
1	LYR	A	257[B]	1	-	4/22/40/42	0/1/1/1
1	LYR	B	257[B]	1	-	5/22/40/42	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257[B]	LYR	C4-C3	-2.26	1.46	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257[B]	LYR	C1-NZ-CE	9.86	128.96	113.33
1	A	257[B]	LYR	C4-C3-C2	-7.02	109.82	123.59
1	B	257[B]	LYR	C1-NZ-CE	5.75	122.44	113.33
1	A	257[B]	LYR	C13-C12-C11	-5.68	118.15	124.53
1	B	257[B]	LYR	C13-C12-C11	-4.75	119.20	124.53
1	B	257[B]	LYR	C6-C7-C80	-4.27	121.22	127.31
1	B	257[B]	LYR	C10-C9-C80	-3.78	120.52	126.23
1	A	257[B]	LYR	C10-C9-C80	-3.65	120.72	126.23
1	A	257[A]	LYR	C1-NZ-CE	3.46	118.82	113.33
1	B	257[B]	LYR	C6-C5-C3	-3.40	116.85	126.42
1	B	257[B]	LYR	C4-C3-C2	-3.35	117.01	123.59
1	A	257[A]	LYR	C9-C80-C7	-3.35	113.81	118.94
1	B	257[A]	LYR	C1-NZ-CE	3.28	118.53	113.33
1	B	257[A]	LYR	C9-C80-C7	-3.24	113.97	118.94
1	B	257[A]	LYR	C1-C2-C3	-3.01	121.19	126.97
1	A	257[B]	LYR	C13-C12-C14	2.90	119.18	113.62
1	A	257[B]	LYR	C8-C80-C9	2.79	122.48	118.08
1	B	257[A]	LYR	C6-C7-C80	-2.69	123.47	127.31
1	A	257[A]	LYR	C1-C2-C3	-2.67	121.85	126.97
1	A	257[A]	LYR	C6-C7-C80	-2.51	123.73	127.31
1	A	257[B]	LYR	C6-C5-C3	-2.43	119.58	126.42
1	A	257[B]	LYR	C8-C80-C7	-2.41	119.55	122.92
1	B	257[B]	LYR	C15-C14-C12	-2.37	109.84	114.08
1	B	257[B]	LYR	C9-C10-C11	-2.29	120.77	127.20
1	B	257[B]	LYR	C13-C12-C14	2.25	117.93	113.62
1	A	257[B]	LYR	C6-C7-C80	-2.24	124.12	127.31
1	B	257[A]	LYR	C8-C80-C7	2.20	126.00	122.92
1	A	257[A]	LYR	C15-C14-C12	-2.18	110.18	114.08
1	B	257[A]	LYR	C15-C14-C12	-2.16	110.22	114.08
1	A	257[A]	LYR	C8-C80-C7	2.11	125.88	122.92
1	A	257[A]	LYR	C10-C9-C80	-2.11	123.05	126.23
1	A	257[B]	LYR	C10-C11-C12	-2.01	116.58	121.46

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	257[A]	LYR	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	257[A]	LYR	CD-CE-NZ-C1
1	A	257[B]	LYR	C-CA-CB-CG
1	B	257[A]	LYR	C-CA-CB-CG
1	B	257[A]	LYR	CD-CE-NZ-C1
1	B	257[B]	LYR	C-CA-CB-CG
1	A	257[B]	LYR	C2-C1-NZ-CE
1	A	257[B]	LYR	CG-CD-CE-NZ
1	B	257[B]	LYR	CG-CD-CE-NZ
1	A	257[A]	LYR	CE-CD-CG-CB
1	B	257[A]	LYR	CE-CD-CG-CB
1	B	257[B]	LYR	C2-C1-NZ-CE
1	B	257[B]	LYR	CE-CD-CG-CB
1	A	257[B]	LYR	CD-CE-NZ-C1
1	B	257[B]	LYR	CD-CE-NZ-C1
1	A	257[A]	LYR	N-CA-CB-CG
1	B	257[A]	LYR	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	257[A]	LYR	4	0
1	B	257[A]	LYR	2	0
1	A	257[B]	LYR	4	0
1	B	257[B]	LYR	7	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	PO4	A	1109	-	4,4,4	0.93	0	6,6,6	0.87	0
2	OLC	A	1105	-	17,17,24	0.46	0	16,16,25	0.32	0
4	EDT	A	1111	-	19,19,19	1.02	0	24,24,24	1.19	2 (8%)
2	OLC	A	1102	-	17,17,24	0.70	0	16,17,25	0.99	2 (12%)
2	OLC	B	1103	-	18,18,24	1.18	1 (5%)	18,19,25	1.26	2 (11%)
3	PO4	A	1110	-	4,4,4	0.90	0	6,6,6	0.44	0
2	OLC	A	1106	-	7,7,24	2.89	2 (28%)	7,7,25	1.27	1 (14%)
2	OLC	B	1105	-	17,17,24	0.45	0	16,16,25	0.22	0
3	PO4	B	1106	-	4,4,4	0.99	0	6,6,6	0.30	0
3	PO4	B	1107	-	4,4,4	0.93	0	6,6,6	0.42	0
2	OLC	A	1101	-	15,15,24	1.40	1 (6%)	16,16,25	1.19	2 (12%)
2	OLC	B	1102	-	20,20,24	1.10	1 (5%)	21,21,25	1.03	2 (9%)
2	OLC	A	1103	-	17,17,24	1.28	1 (5%)	18,18,25	1.04	2 (11%)
2	OLC	A	1107	-	3,3,24	0.47	0	2,2,25	0.60	0
2	OLC	A	1104	-	14,14,24	0.57	0	12,13,25	1.00	1 (8%)
2	OLC	B	1104	-	17,17,24	1.39	1 (5%)	18,18,25	1.12	2 (11%)
2	OLC	B	1101	-	12,12,24	0.50	0	11,11,25	0.24	0
2	OLC	A	1108	-	11,11,24	0.58	0	10,10,25	1.13	1 (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
2	OLC	A	1105	-	-	5/15/15/24	-
4	EDT	A	1111	-	-	10/21/21/21	-
2	OLC	A	1102	-	-	10/16/16/24	-
2	OLC	B	1103	-	-	10/18/18/24	-
2	OLC	A	1106	-	-	3/5/5/24	-
2	OLC	B	1105	-	-	8/15/15/24	-
2	OLC	A	1101	-	-	7/15/15/24	-
2	OLC	B	1102	-	-	10/20/20/24	-
2	OLC	A	1103	-	-	8/17/17/24	-
2	OLC	A	1107	-	-	0/1/1/24	-
2	OLC	A	1104	-	-	4/12/12/24	-
2	OLC	B	1104	-	-	4/17/17/24	-
2	OLC	B	1101	-	-	2/10/10/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	1108	-	-	1/9/9/24	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1106	OLC	O19-C1	7.11	1.45	1.22
2	B	1104	OLC	O20-C1	5.20	1.48	1.33
2	A	1101	OLC	O20-C1	4.99	1.47	1.33
2	A	1103	OLC	O20-C1	4.80	1.47	1.33
2	B	1103	OLC	O20-C1	4.67	1.47	1.33
2	B	1102	OLC	O20-C1	4.46	1.46	1.33
2	A	1106	OLC	O20-C1	-2.55	1.22	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1103	OLC	O20-C1-C2	3.76	123.72	111.91
2	B	1102	OLC	O20-C1-C2	3.09	121.59	111.91
2	A	1108	OLC	C21-O20-C1	3.08	123.94	112.90
2	A	1101	OLC	O20-C1-C2	2.99	121.28	111.91
2	B	1104	OLC	O20-C1-C2	2.81	120.74	111.91
2	A	1103	OLC	O20-C1-C2	2.76	120.58	111.91
2	B	1103	OLC	O20-C1-O19	-2.76	116.62	123.59
2	B	1102	OLC	O20-C1-O19	-2.74	116.68	123.59
2	A	1104	OLC	C21-O20-C1	2.63	122.31	112.90
2	A	1101	OLC	O20-C1-O19	-2.63	116.97	123.59
2	A	1106	OLC	O20-C1-C2	2.48	121.99	114.03
2	B	1104	OLC	C21-O20-C1	2.47	126.28	117.12
2	A	1102	OLC	O20-C1-C2	2.41	122.91	110.26
4	A	1111	EDT	C4-N3-C6	-2.17	106.67	111.94
4	A	1111	EDT	O17-C1-C2	2.15	121.91	113.45
2	A	1103	OLC	C21-O20-C1	2.06	124.75	117.12
2	A	1102	OLC	C1-O20-C21	2.01	122.62	113.61

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	OLC	O20-C21-C22-O23
2	B	1103	OLC	C9-C10-C11-C12
2	B	1103	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
2	B	1104	OLC	C21-C22-C24-O25
4	A	1111	EDT	N3-C4-C5-O20
4	A	1111	EDT	N3-C4-C5-O19
4	A	1111	EDT	O16-C10-C9-N8
4	A	1111	EDT	O15-C10-C9-N8
2	B	1102	OLC	O19-C1-O20-C21
2	B	1102	OLC	C2-C1-O20-C21
4	A	1111	EDT	C5-C4-N3-C2
2	A	1101	OLC	C2-C1-O20-C21
2	A	1101	OLC	O19-C1-O20-C21
2	B	1103	OLC	C2-C1-O20-C21
2	B	1103	OLC	O23-C22-C24-O25
2	A	1103	OLC	C1-C2-C3-C4
2	B	1103	OLC	O19-C1-O20-C21
2	A	1103	OLC	O20-C21-C22-O23
2	B	1102	OLC	O20-C21-C22-O23
2	A	1102	OLC	C5-C6-C7-C8
2	A	1103	OLC	O20-C21-C22-C24
2	B	1102	OLC	O20-C21-C22-C24
2	B	1103	OLC	C2-C3-C4-C5
2	A	1101	OLC	C4-C5-C6-C7
2	B	1105	OLC	C12-C13-C14-C15
2	A	1102	OLC	C21-C22-C24-O25
2	B	1102	OLC	C21-C22-C24-O25
2	B	1105	OLC	C3-C4-C5-C6
2	B	1104	OLC	O23-C22-C24-O25
2	A	1103	OLC	C6-C7-C8-C9
2	A	1104	OLC	C6-C7-C8-C9
2	A	1102	OLC	C4-C5-C6-C7
2	A	1102	OLC	C6-C7-C8-C9
2	A	1105	OLC	C14-C15-C16-C17
2	A	1101	OLC	C5-C6-C7-C8
4	A	1111	EDT	C1-C2-N3-C4
2	B	1103	OLC	C4-C5-C6-C7
2	B	1101	OLC	C1-C2-C3-C4
2	B	1103	OLC	C6-C7-C8-C9
2	A	1103	OLC	C5-C6-C7-C8
2	A	1105	OLC	C3-C4-C5-C6
2	A	1108	OLC	C5-C6-C7-C8
2	A	1103	OLC	C2-C1-O20-C21
2	B	1104	OLC	C4-C5-C6-C7
2	A	1103	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	1104	OLC	C22-C21-O20-C1
2	A	1105	OLC	C2-C3-C4-C5
2	B	1105	OLC	C11-C12-C13-C14
4	A	1111	EDT	C6-C7-N8-C11
2	A	1102	OLC	O20-C1-C2-C3
2	A	1103	OLC	O19-C1-O20-C21
2	A	1101	OLC	O20-C21-C22-C24
2	A	1102	OLC	O23-C22-C24-O25
2	A	1101	OLC	C2-C3-C4-C5
2	B	1103	OLC	C3-C4-C5-C6
2	B	1105	OLC	C14-C15-C16-C17
2	A	1104	OLC	C9-C10-C11-C12
2	A	1102	OLC	O20-C21-C22-C24
2	A	1102	OLC	C22-C21-O20-C1
2	B	1102	OLC	O23-C22-C24-O25
2	B	1105	OLC	C1-C2-C3-C4
4	A	1111	EDT	N3-C6-C7-N8
2	B	1105	OLC	C4-C5-C6-C7
2	A	1105	OLC	C4-C5-C6-C7
4	A	1111	EDT	C6-C7-N8-C9
2	B	1102	OLC	C1-C2-C3-C4
2	A	1104	OLC	C1-C2-C3-C4
2	B	1101	OLC	C10-C11-C12-C13
2	B	1105	OLC	C13-C14-C15-C16
2	B	1105	OLC	C9-C10-C11-C12
2	A	1105	OLC	C1-C2-C3-C4
2	B	1102	OLC	C3-C4-C5-C6
2	A	1106	OLC	O19-C1-C2-C3
2	A	1106	OLC	C1-C2-C3-C4
2	A	1102	OLC	C2-C1-O20-C21
2	A	1106	OLC	O20-C1-C2-C3
2	A	1102	OLC	C7-C8-C9-C10
4	A	1111	EDT	C10-C9-N8-C11
2	B	1104	OLC	C7-C8-C9-C10
2	B	1102	OLC	C11-C12-C13-C14
2	B	1102	OLC	C2-C3-C4-C5
2	B	1103	OLC	O20-C21-C22-O23

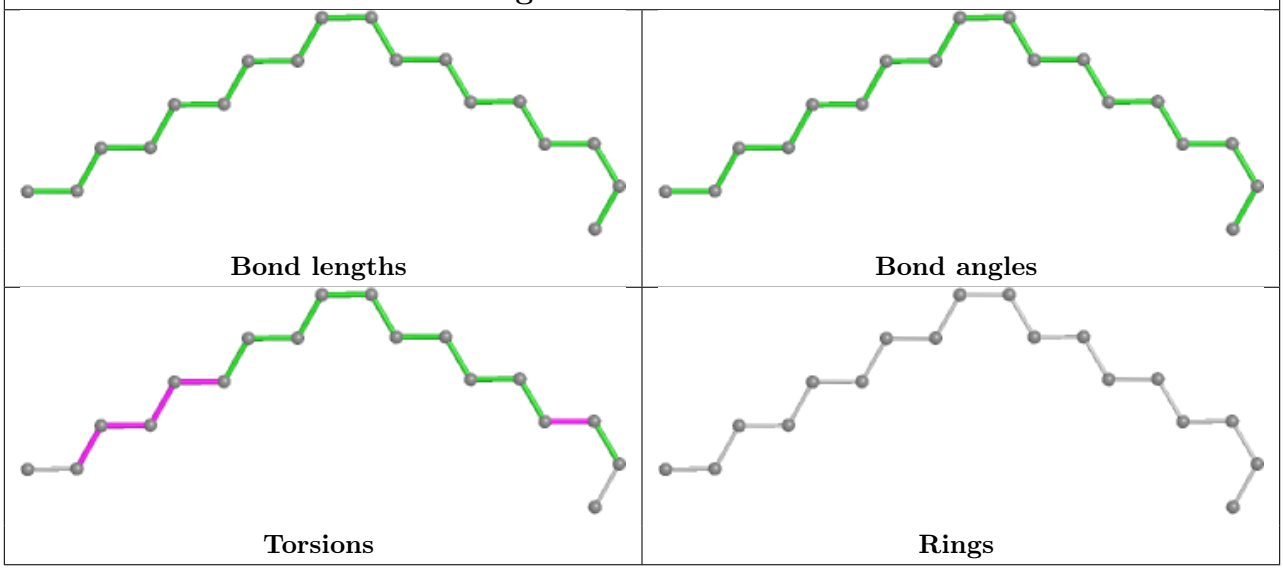
There are no ring outliers.

1 monomer is involved in 1 short contact:

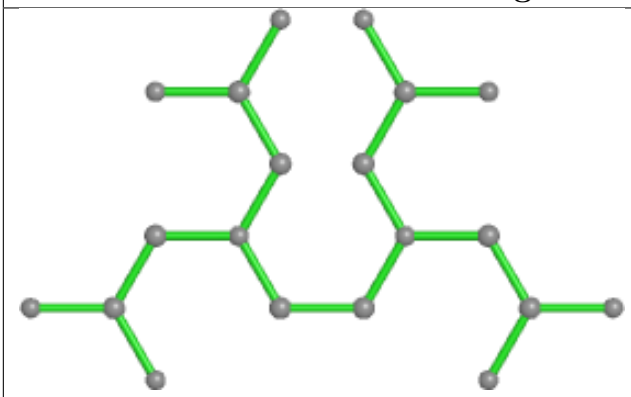
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1105	OLC	1	0

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.

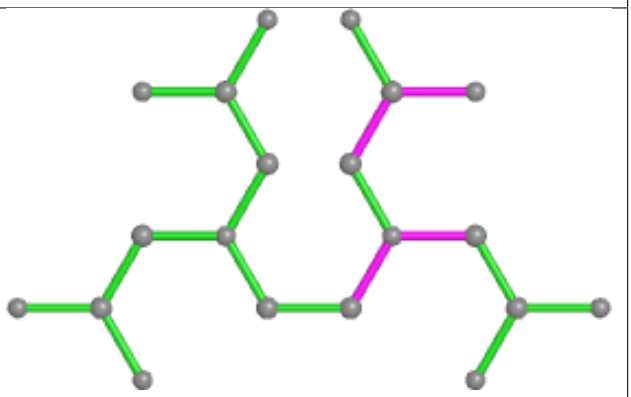
Ligand OLC A 1105



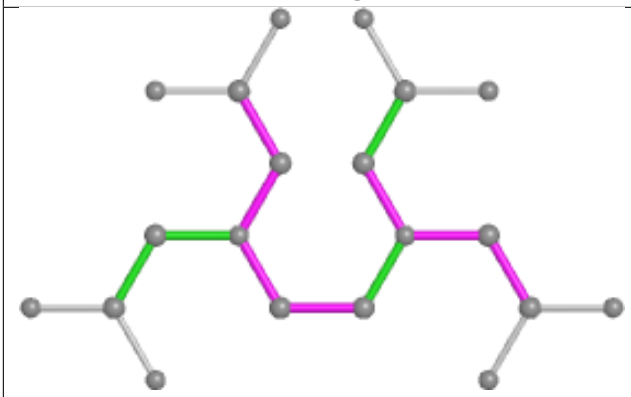
Ligand EDT A 1111



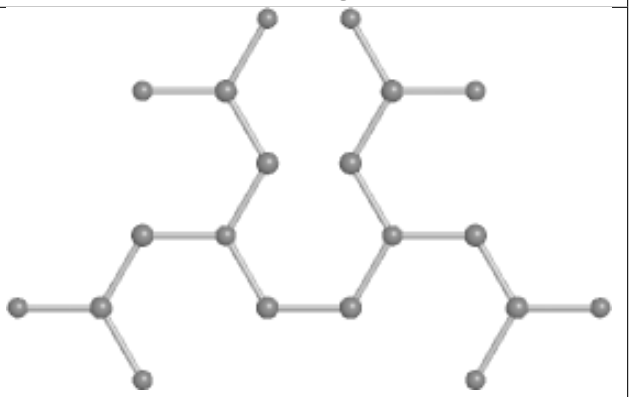
Bond lengths



Bond angles

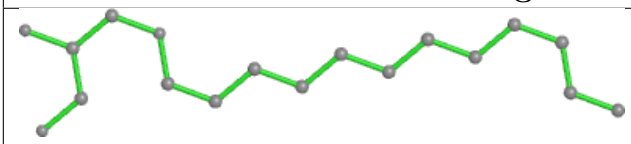


Torsions



Rings

Ligand OLC A 1102



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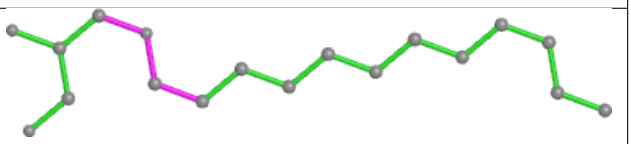

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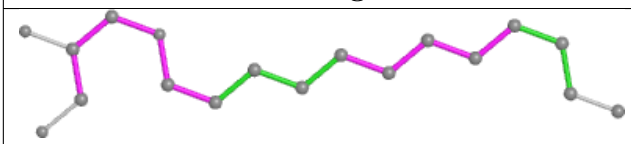

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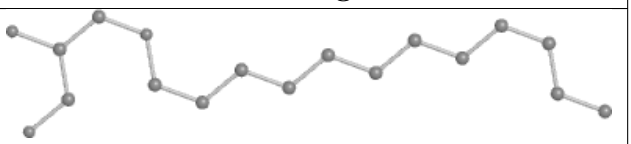
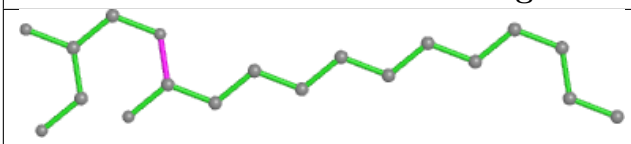
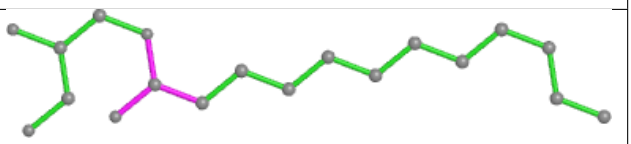


Rings

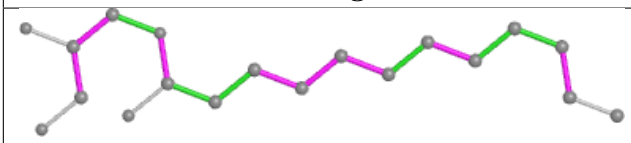
Ligand OLC B 1103



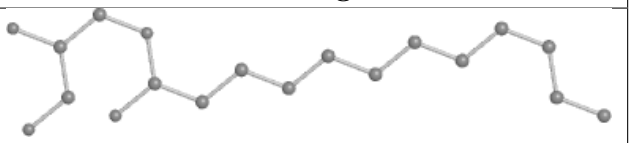
Bond lengths



Bond angles

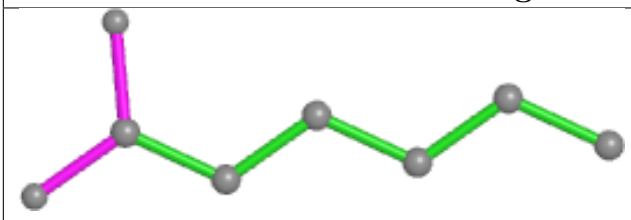


Torsions

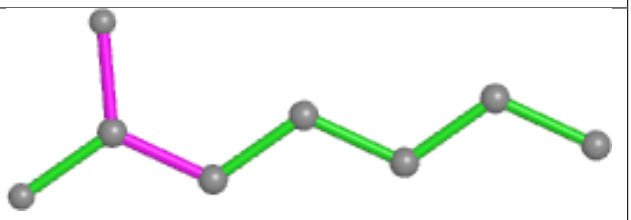


Rings

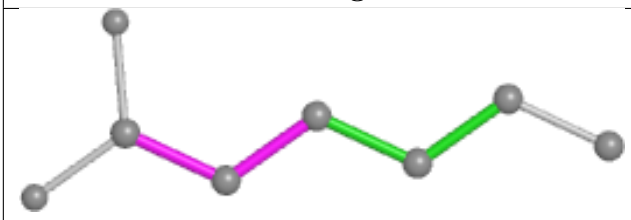
Ligand OLC A 1106



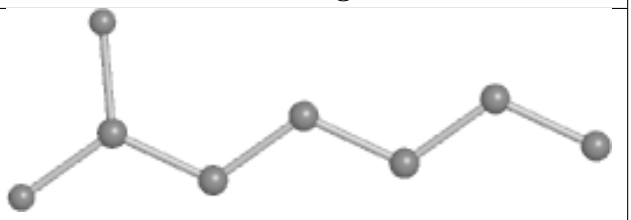
Bond lengths



Bond angles

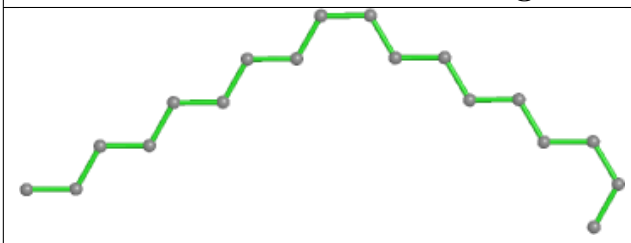


Torsions

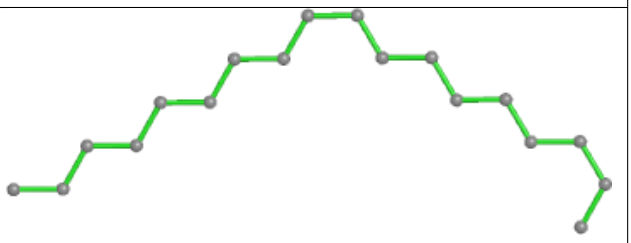


Rings

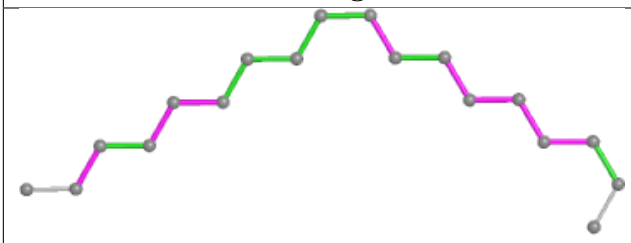
Ligand OLC B 1105



Bond lengths



Bond angles



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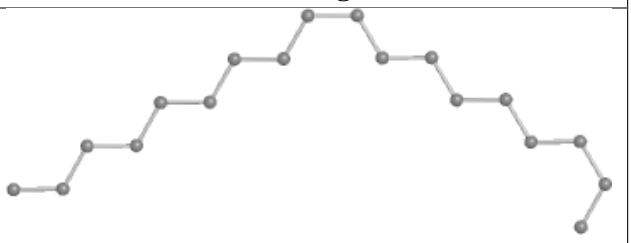
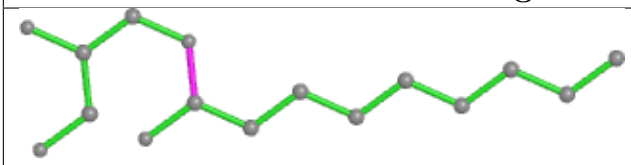
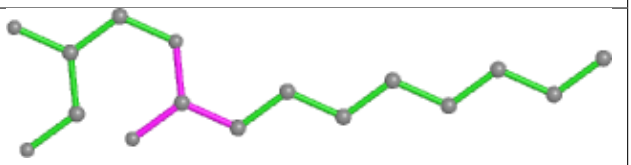


Rings

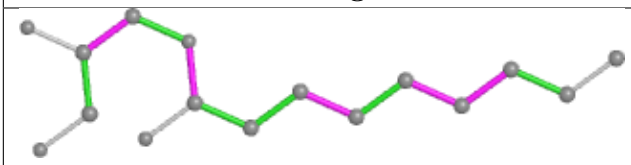
Ligand OLC A 1101



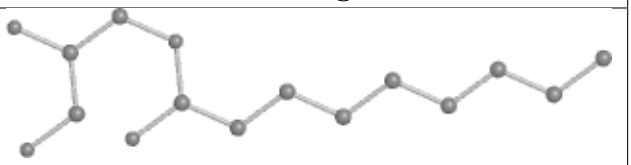
Bond lengths



Bond angles

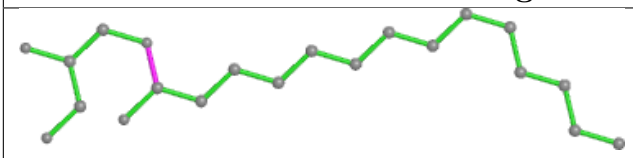


Torsions

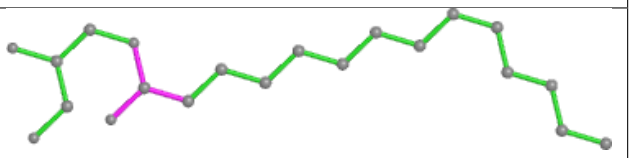


Rings

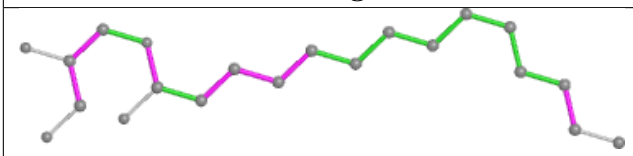
Ligand OLC B 1102



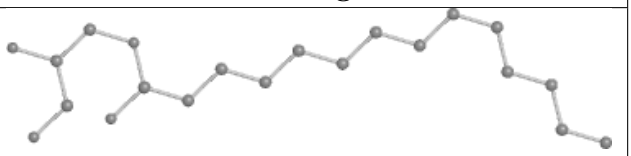
Bond lengths



Bond angles

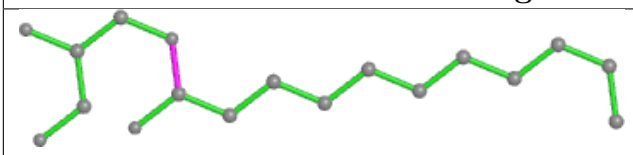


Torsions

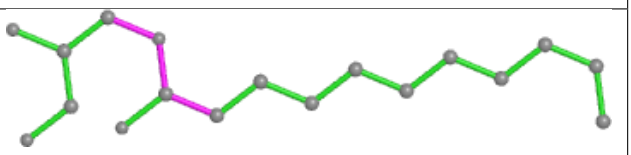


Rings

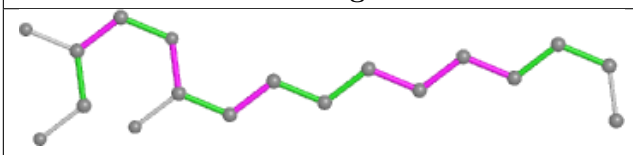
Ligand OLC A 1103



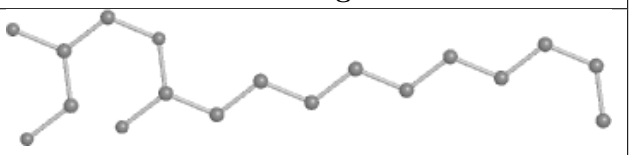
Bond lengths



Bond angles

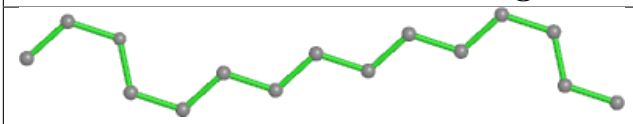


Torsions

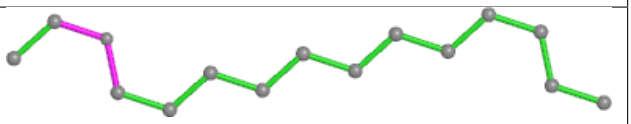


Rings

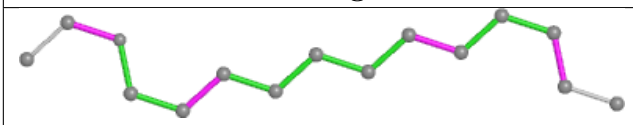
Ligand OLC A 1104



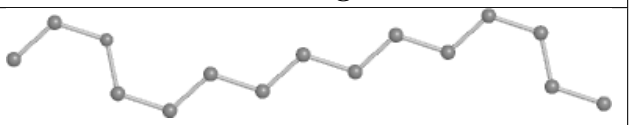
Bond lengths



Bond angles

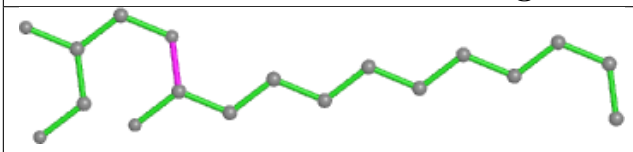


Torsions

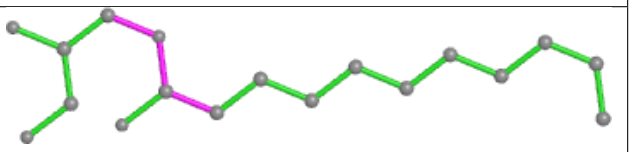


Rings

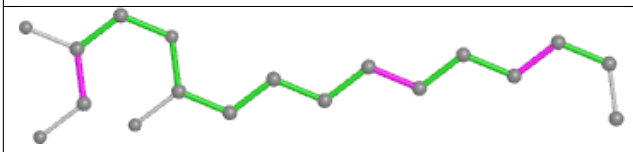
Ligand OLC B 1104



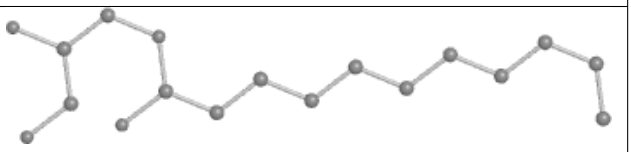
Bond lengths



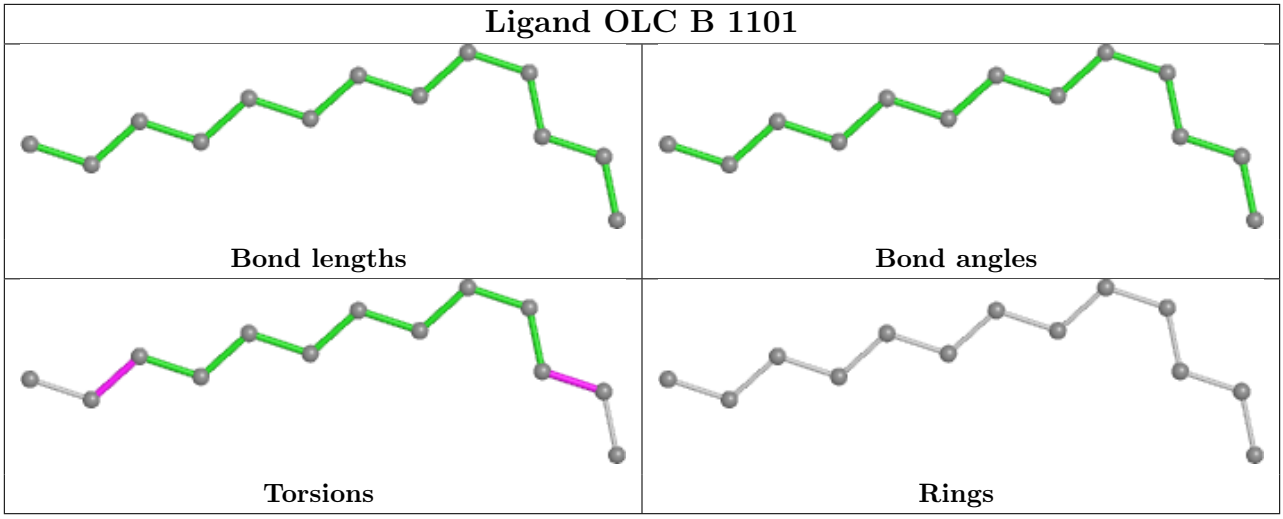
Bond angles

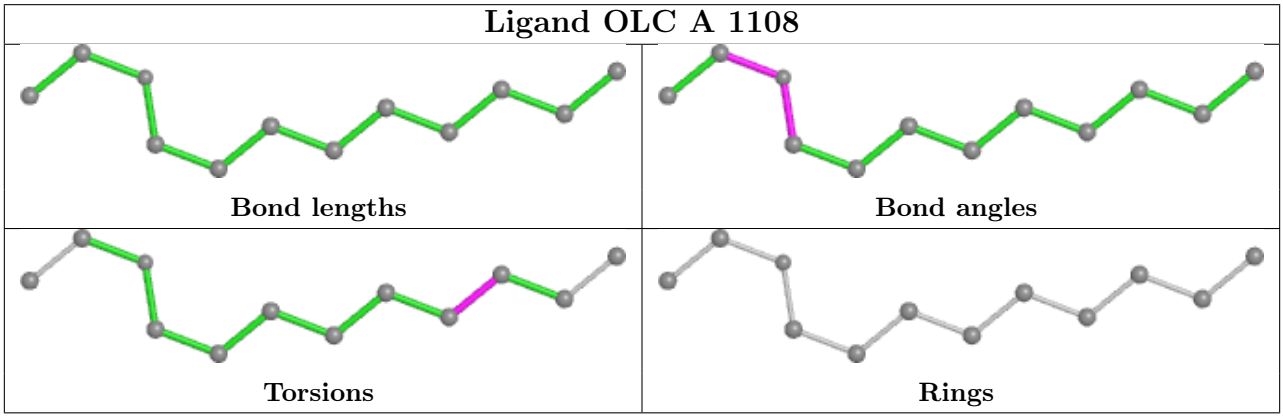


Torsions



Rings





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	246/315 (78%)	0.21	6 (2%)	59	57	41, 59, 96, 140	0
1	B	250/315 (79%)	0.26	10 (4%)	38	37	43, 64, 105, 132	0
All	All	496/630 (78%)	0.23	16 (3%)	47	46	41, 62, 101, 140	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	CYS	5.0
1	A	75	TRP	4.7
1	B	72	TYR	4.3
1	A	78	THR	3.5
1	B	141	LEU	3.3
1	A	72	TYR	3.1
1	B	57	TRP	2.5
1	B	78	THR	2.3
1	B	206	GLY	2.3
1	B	31	GLU	2.2
1	B	143	ASN	2.2
1	B	75	TRP	2.2
1	A	200	TYR	2.1
1	B	205	LYS	2.0
1	A	277	ILE	2.0
1	B	144	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	LYR	B	257[A]	29/30	0.94	0.24	52,60,65,68	29
1	LYR	B	257[B]	29/30	0.94	0.24	54,59,63,64	29
1	LYR	A	257[A]	29/30	0.96	0.21	55,60,65,66	29
1	LYR	A	257[B]	29/30	0.96	0.21	56,61,64,65	29

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

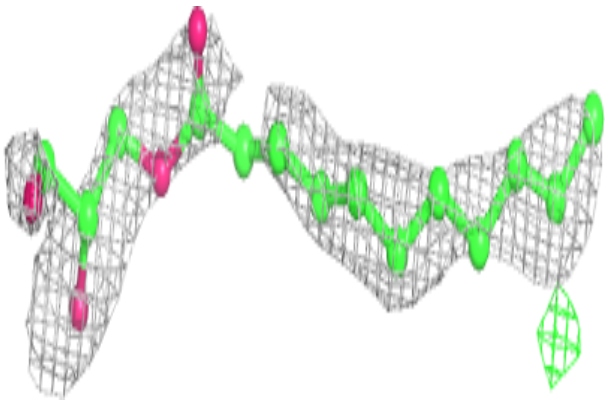
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

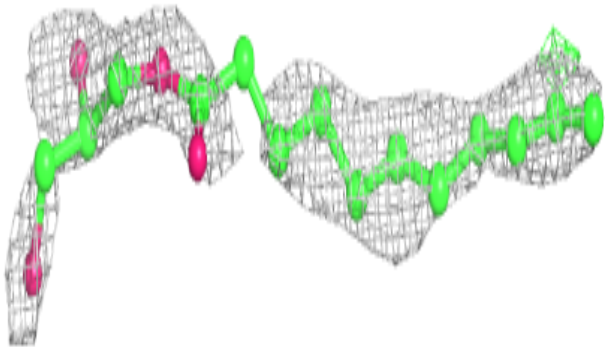
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OLC	B	1104	18/25	0.68	0.39	71,96,110,113	0
2	OLC	A	1103	18/25	0.70	0.31	77,94,105,108	0
2	OLC	A	1106	8/25	0.76	0.23	78,91,96,96	0
2	OLC	A	1101	16/25	0.79	0.23	53,65,97,98	0
2	OLC	A	1105	18/25	0.79	0.34	68,83,88,91	0
4	EDT	A	1111	20/20	0.83	0.16	89,98,113,115	0
3	PO4	B	1107	5/5	0.84	0.18	125,128,133,134	0
2	OLC	B	1101	13/25	0.84	0.18	60,64,75,76	0
2	OLC	A	1102	18/25	0.85	0.27	68,74,82,83	0
2	OLC	B	1103	19/25	0.87	0.34	65,72,104,109	0
2	OLC	A	1104	15/25	0.87	0.27	61,69,74,76	0
3	PO4	A	1110	5/5	0.88	0.13	132,139,142,142	0
2	OLC	A	1108	12/25	0.89	0.34	58,66,75,76	0
2	OLC	B	1105	18/25	0.90	0.28	52,75,89,89	0
2	OLC	B	1102	21/25	0.90	0.33	81,86,91,100	0
3	PO4	A	1109	5/5	0.91	0.20	80,89,92,99	0
2	OLC	A	1107	4/25	0.94	0.11	60,60,61,61	0
3	PO4	B	1106	5/5	0.96	0.10	88,92,94,96	0

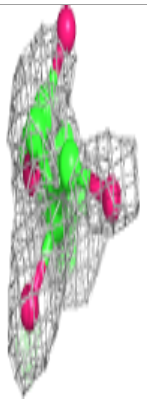
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC B 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

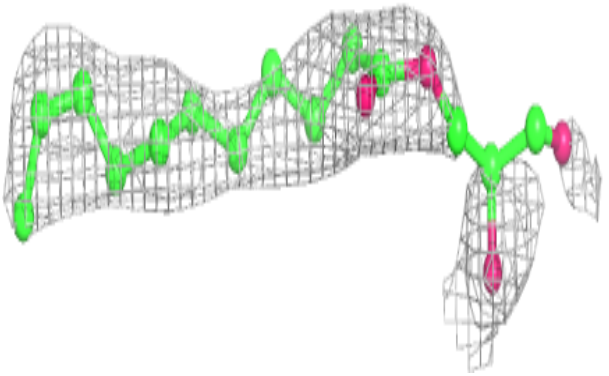


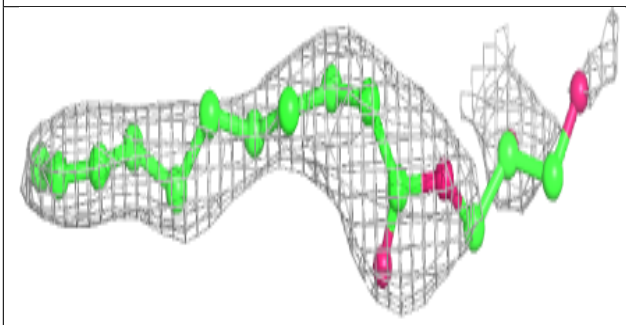


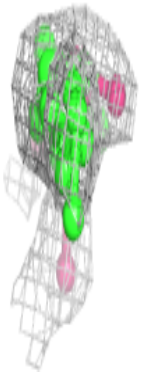


Electron density around OLC A 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around OLC A 1106:

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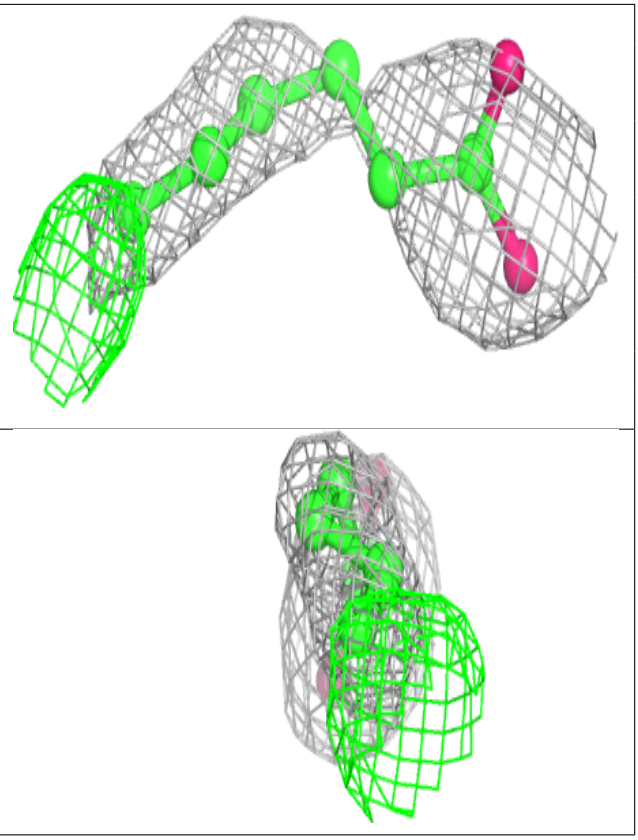
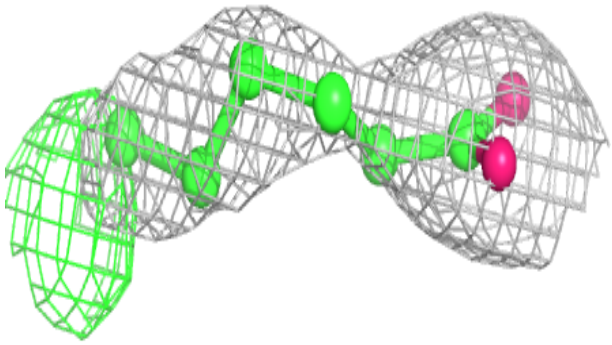
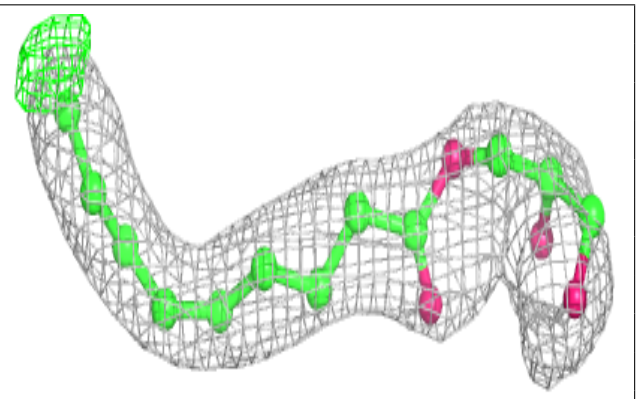
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

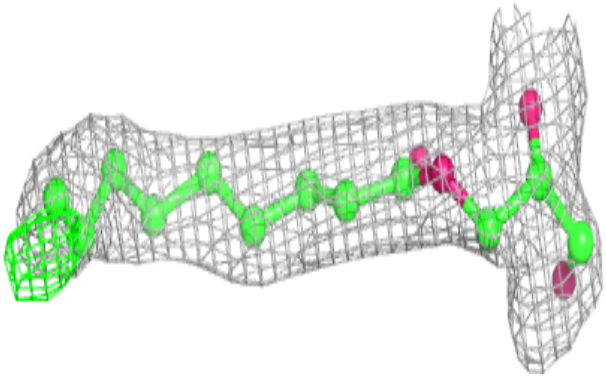


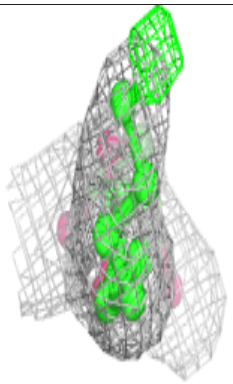


Electron density around OLC A 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

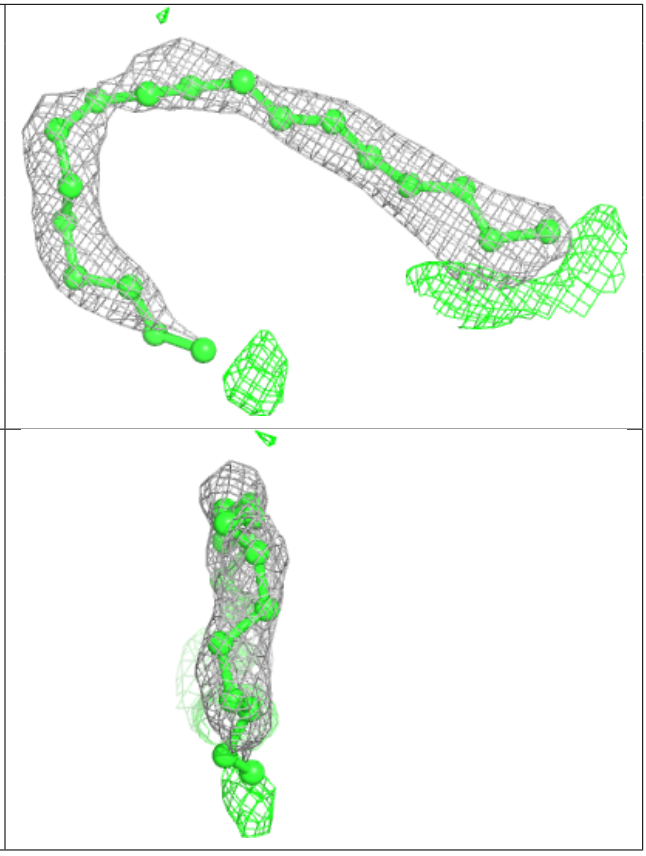


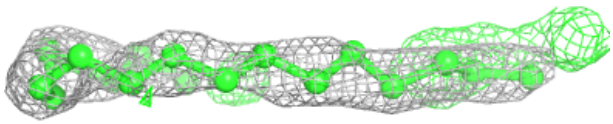




Electron density around OLC A 1105:

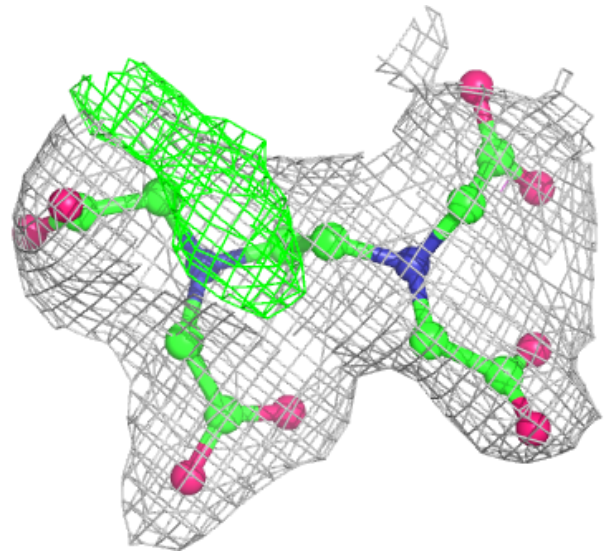
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

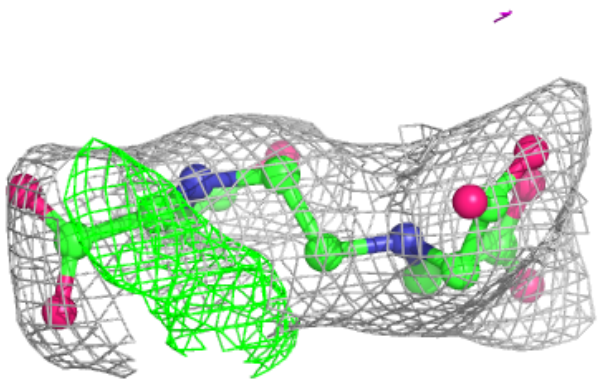


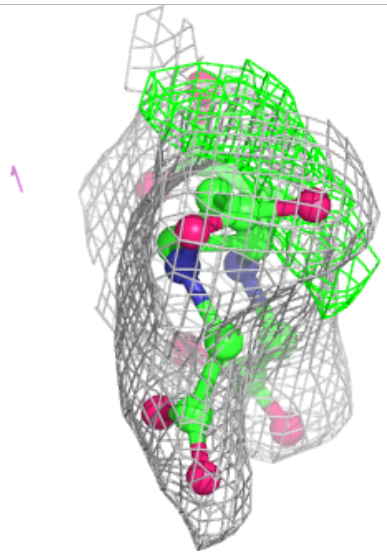


Electron density around EDT A 1111:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

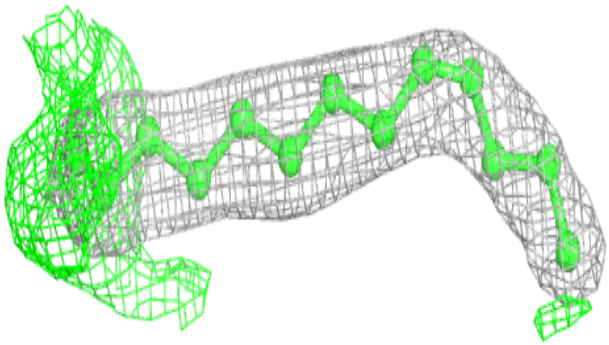


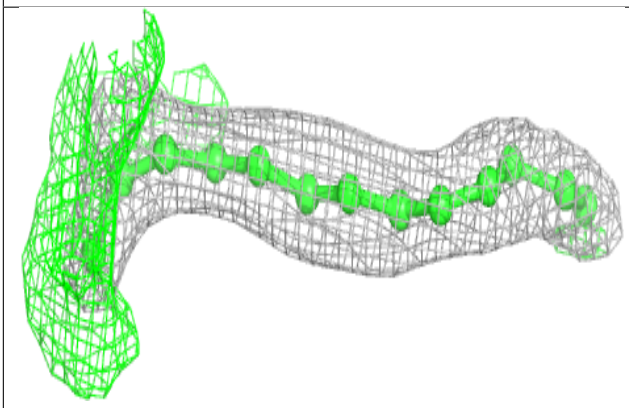


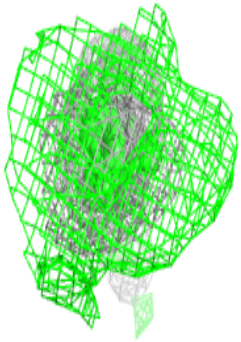


Electron density around OLC B 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

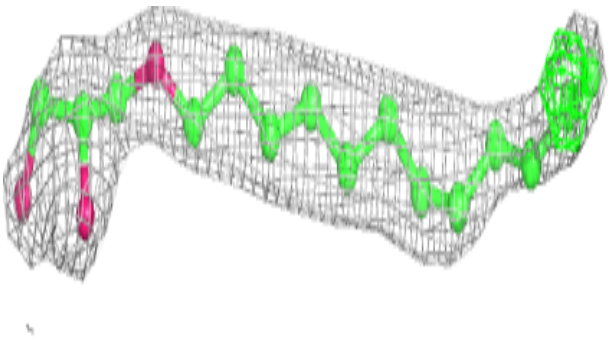


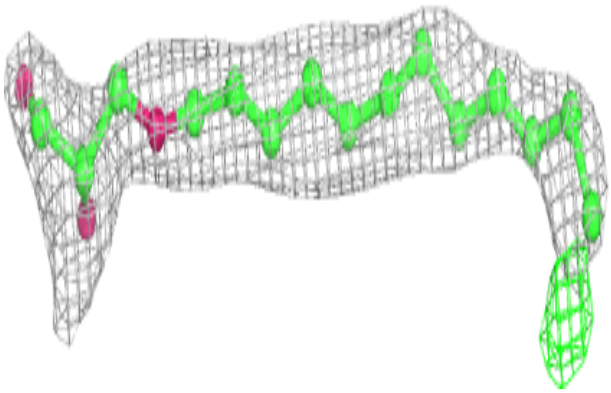


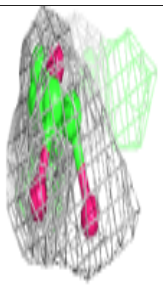


Electron density around OLC A 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

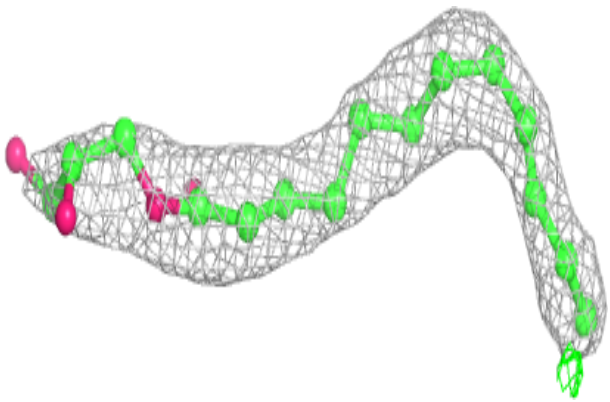


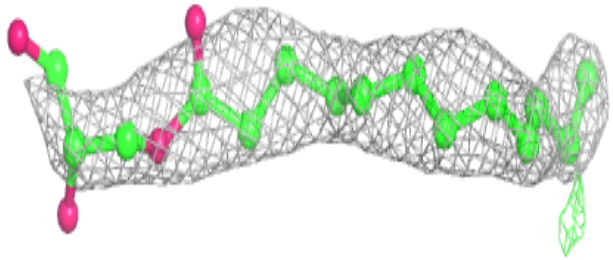


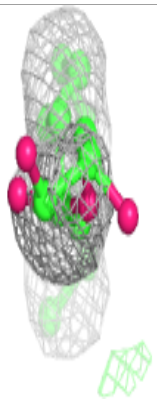


Electron density around OLC B 1103:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

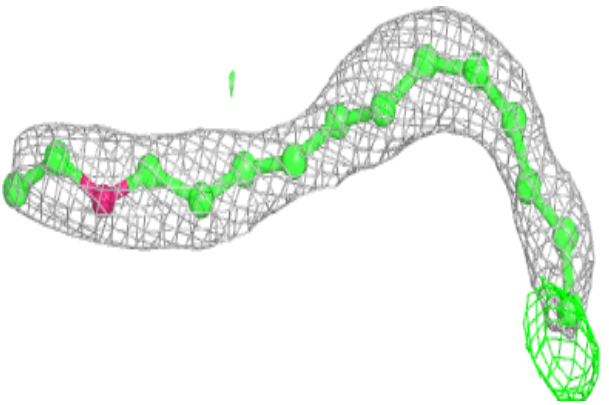


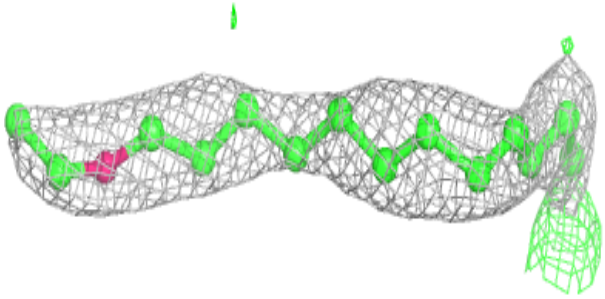


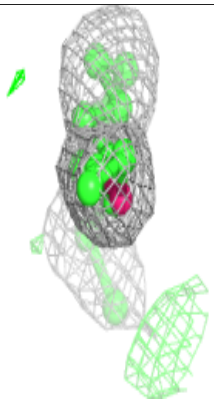


Electron density around OLC A 1104:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

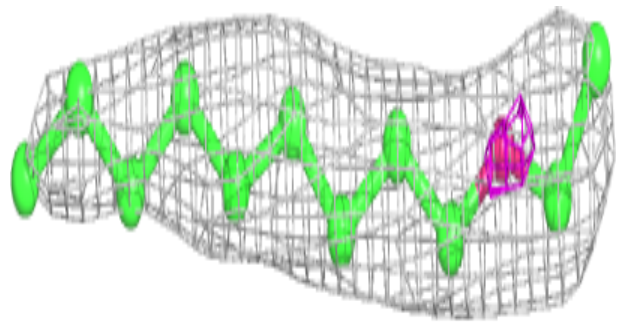


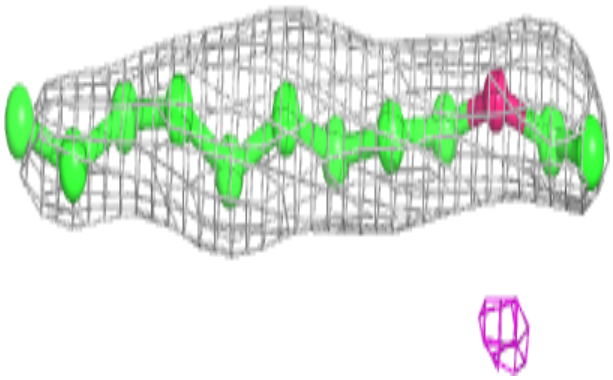


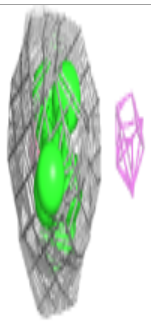


Electron density around OLC A 1108:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

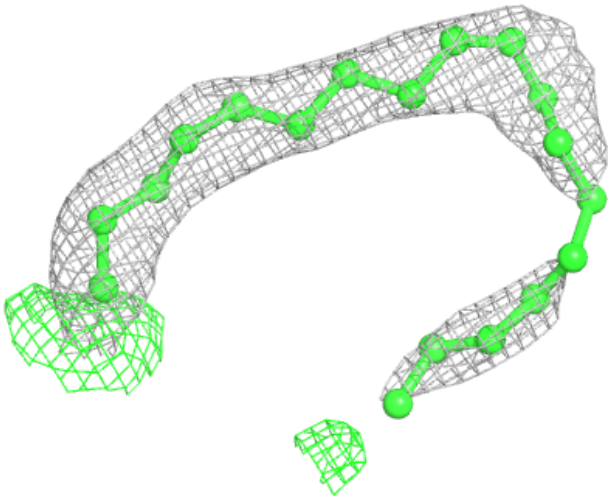


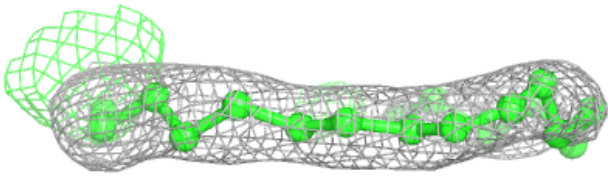


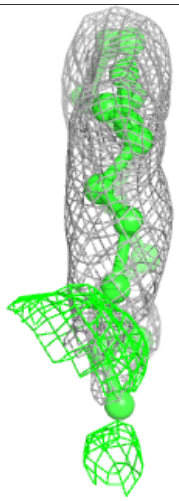


Electron density around OLC B 1105:

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

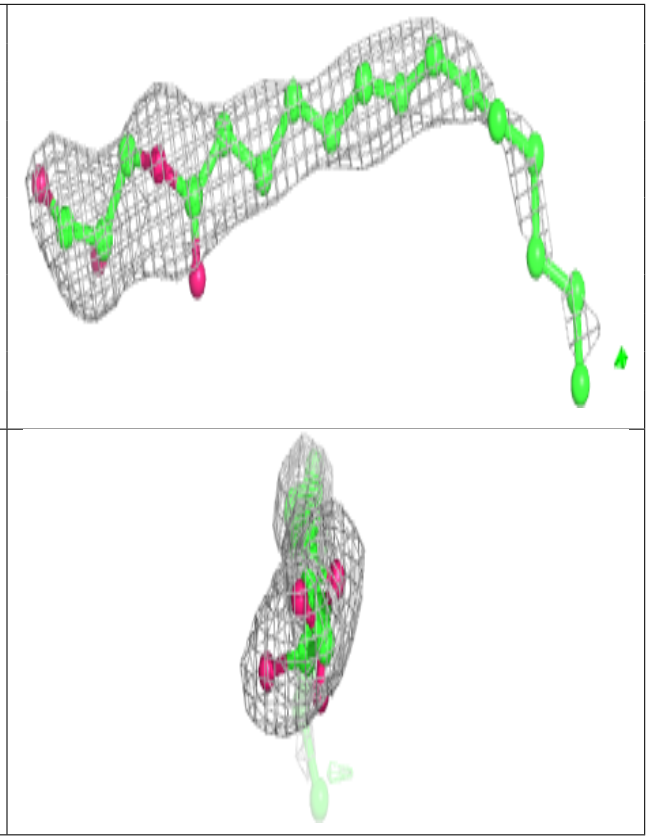






Electron density around OLC B 1102:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.