wwPDB X-ray Structure Validation Summary Report (i)

Mar 24, 2022 – 03:34 pm GMT

PDB ID	:	6RZ9
Title	:	Crystal structure of the human cysteinyl leukotriene receptor 2 in complex with ONO-2770372
Authors	:	Gusach, A.; Luginina, A.; Marin, E.; Brouillette, R.L.; Besserer-Offroy, E.; Longpre, J.M.; Ishchenko, A.; Popov, P.; Fujimoto, T.; Maruyama, T.; Stauch, B.; Ergasheva, M.; Romanovskaya, D.; Stepko, A.; Kovalev, K.; Shevtsov, M.; Gordeliy, V.; Han, G.W.; Sarret, P.; Katritch, V.; Borshchevskiy, V.; Mishin, A.; Cherezov, V.
Deposited on	:	2019-06-12
Resolution	:	2.73 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 (i)) were used in the production of this report:

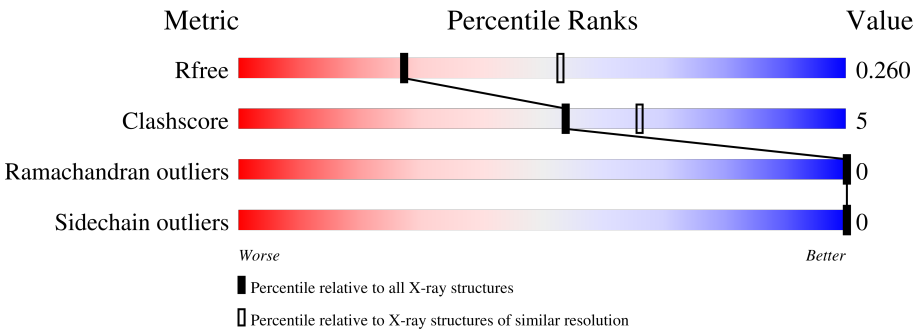
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)

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%

Mol	Chain	Length	Quality of chain
1	A	405	79% 11% 10%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3106 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.

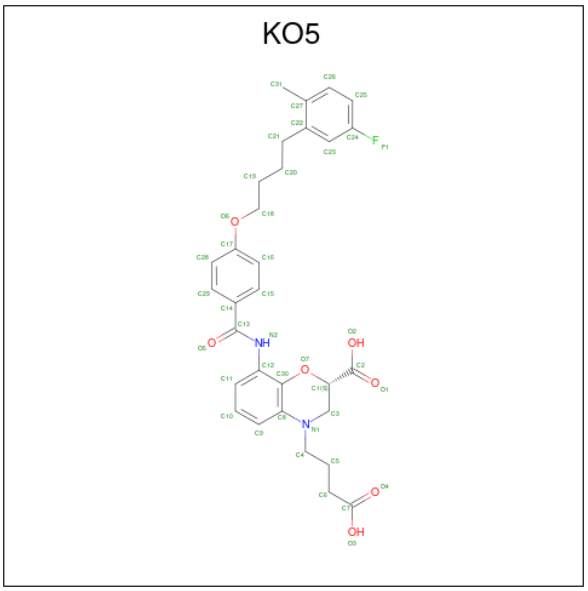
- Molecule 1 is a protein called Cysteinyl leukotriene receptor 2,Soluble cytochrome b562,Cysteinyl leukotriene receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2740	1816	441	466	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

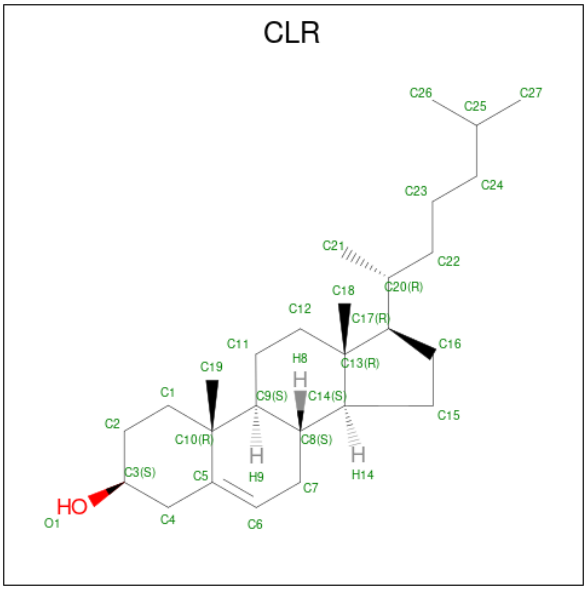
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	VAL	TRP	engineered mutation	UNP Q9NS75
A	84	ASN	ASP	engineered mutation	UNP Q9NS75
A	137	TYR	PHE	engineered mutation	UNP Q9NS75
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7

- Molecule 2 is (2 {S})-8-[[4-[4-(5-fluoranyl-2-methyl-phenyl)butoxy]phenyl]carbonylamino]-4-(4-oxidanyl-4-oxidanylidene-butyl)-2,3-dih ydro-1,4-benzoxazine-2-carboxylic acid (three-letter code: KO5) (formula: $C_{31}H_{33}FN_2O_7$) (labeled as "Ligand of Interest" by depositor).



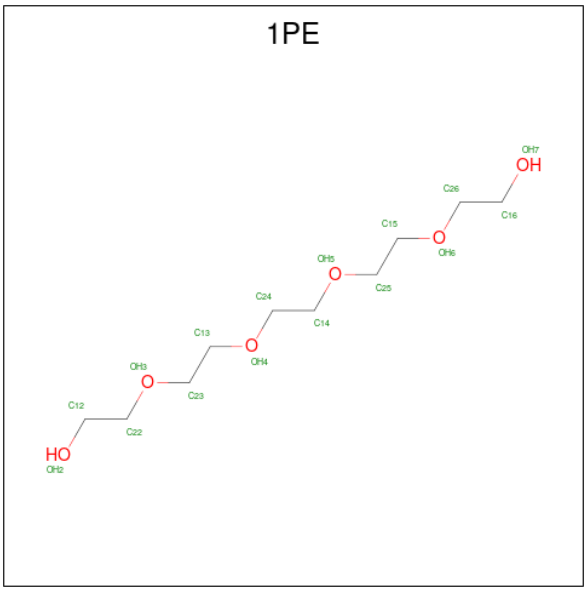
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	41	31	1	2	7	0	0

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



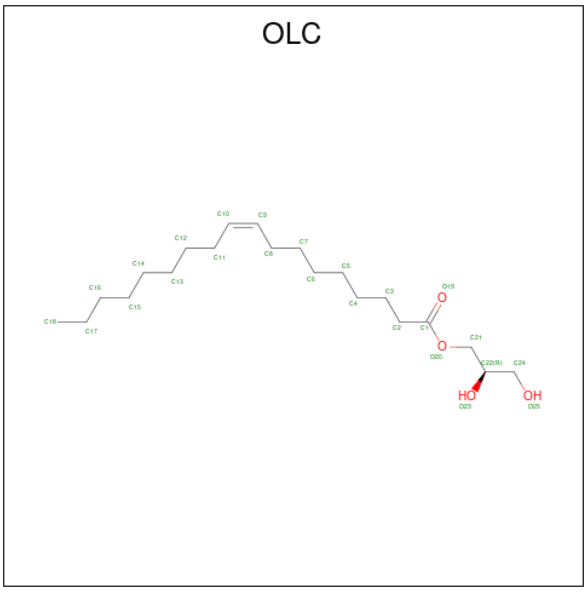
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	28	27	1	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	9	4	0	0

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



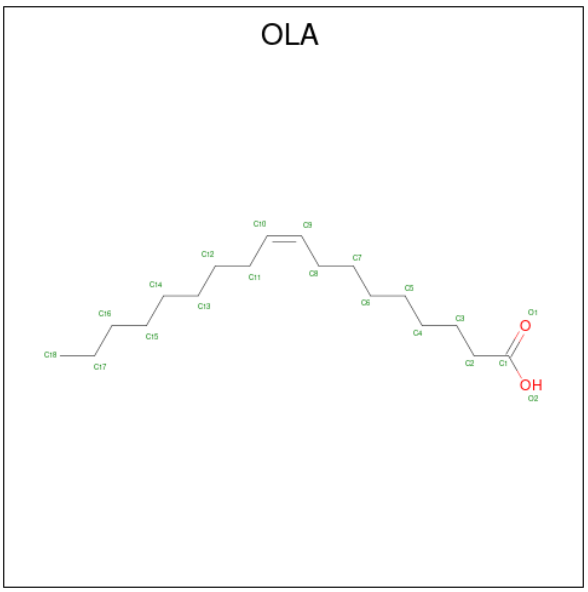
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	13	9	4	0	0
			Total	C	O		
5	A	1	14	10	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 17 13 4	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C O 22 18 4	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 10 10	0	0
5	A	1	Total C O 17 13 4	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 11 11	0	0
5	A	1	Total C O 10 6 4	0	0
5	A	1	Total C 14 14	0	0

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 16 14 2	0	0
6	A	1	Total C O 17 15 2	0	0
6	A	1	Total C 9 9	0	0
6	A	1	Total C O 20 18 2	0	0
6	A	1	Total C O 19 17 2	0	0
6	A	1	Total C O 20 18 2	0	0
6	A	1	Total C O 13 11 2	0	0

- Molecule 7 is water.

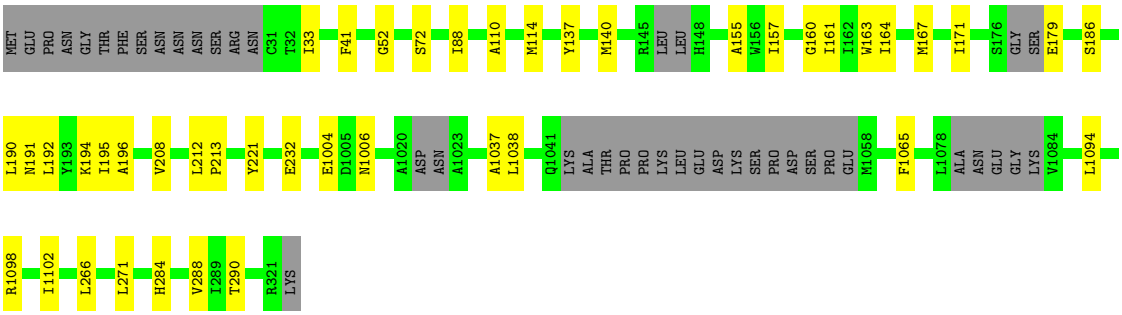
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	12	Total O 12 12	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cysteinyl leukotriene receptor 2,Soluble cytochrome b562,Cysteinyl leukotriene receptor 2

Chain A: 79% 11% 10%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	69.63Å 170.21Å 85.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 – 2.73 28.81 – 2.72	Depositor EDS
% Data completeness (in resolution range)	97.1 (28.80-2.73) 86.3 (28.81-2.72)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.12-2829, BUSTER 2.10.3	Depositor
R, R_{free}	0.217 , 0.254 0.232 , 0.260	Depositor DCC
R_{free} test set	680 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	62.3	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3106	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.19% 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: OLA, OLC, CLR, 1PE, KO5

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	0.29	0/2794	0.46	0/3810

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	2740	0	2702	28	0
2	A	41	0	0	2	0
3	A	28	0	46	0	0
4	A	13	0	14	1	0
5	A	158	0	209	7	0
6	A	114	0	169	5	0
7	A	12	0	0	0	0
All	All	3106	0	3140	33	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 5.

The worst 5 of 33 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)
5:A:2012:OLC:H8	6:A:2023:OLA:H41	1.68	0.75
1:A:1006:ASN:OD1	1:A:1098:ARG:NH1	2.29	0.66
1:A:33:ILE:HD13	1:A:284:HIS:CG	2.34	0.61
5:A:2012:OLC:H6	6:A:2023:OLA:H21	1.82	0.60
1:A:179:GLU:N	1:A:186:SER:O	2.35	0.60

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	351/405 (87%)	347 (99%)	4 (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	271/356 (76%)	271 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

23 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	$\#\|Z\| > 2$
6	OLA	A	2019	-	8,8,19	0.35	0	7,7,19	0.70	0
5	OLC	A	2016	-	13,13,24	0.33	0	12,12,25	0.73	0
5	OLC	A	2011	-	9,9,24	0.36	0	8,8,25	0.58	0
5	OLC	A	2012	-	16,16,24	0.97	2 (12%)	17,17,25	1.08	1 (5%)
6	OLA	A	2023	-	9,12,19	0.29	0	8,12,19	0.83	0
4	1PE	A	2003	-	12,12,15	0.48	0	11,11,14	0.38	0
6	OLA	A	2021	-	15,18,19	0.20	0	14,18,19	0.71	0
3	CLR	A	2002	-	31,31,31	0.65	0	48,48,48	1.07	4 (8%)
5	OLC	A	2006	-	16,16,24	0.98	2 (12%)	17,17,25	1.07	1 (5%)
5	OLC	A	2013	-	7,7,24	0.44	0	6,6,25	0.94	0
5	OLC	A	2010	-	5,5,24	0.31	0	4,4,25	0.58	0
5	OLC	A	2015	-	9,9,24	1.23	2 (22%)	10,10,25	1.31	1 (10%)
5	OLC	A	2005	-	13,13,24	1.05	2 (15%)	14,14,25	1.04	1 (7%)
2	KO5	A	2001	-	38,44,44	0.46	1 (2%)	48,60,60	0.61	1 (2%)
6	OLA	A	2020	-	16,19,19	0.24	0	15,19,19	0.55	0
5	OLC	A	2007	-	7,7,24	0.42	0	5,6,25	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	OLA	A	2018	-	13,16,19	0.24	0	12,16,19	0.58	0
5	OLC	A	2014	-	10,10,24	0.39	0	9,9,25	0.90	0
5	OLC	A	2008	-	7,7,24	0.46	0	6,6,25	0.81	0
5	OLC	A	2004	-	12,12,24	1.11	2 (16%)	13,13,25	1.13	1 (7%)
6	OLA	A	2017	-	12,15,19	0.25	0	11,15,19	0.60	0
6	OLA	A	2022	-	16,19,19	0.21	0	15,19,19	0.67	0
5	OLC	A	2009	-	21,21,24	0.85	2 (9%)	22,22,25	0.95	1 (4%)

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
6	OLA	A	2019	-	-	2/6/6/17	-
5	OLC	A	2016	-	-	3/11/11/24	-
5	OLC	A	2011	-	-	3/7/7/24	-
5	OLC	A	2012	-	-	6/16/16/24	-
6	OLA	A	2023	-	-	2/8/10/17	-
4	1PE	A	2003	-	-	4/10/10/13	-
6	OLA	A	2021	-	-	3/14/16/17	-
3	CLR	A	2002	-	-	6/10/68/68	0/4/4/4
5	OLC	A	2006	-	-	9/16/16/24	-
5	OLC	A	2013	-	-	0/5/5/24	-
5	OLC	A	2010	-	-	0/3/3/24	-
5	OLC	A	2015	-	-	6/9/9/24	-
5	OLC	A	2005	-	-	5/13/13/24	-
2	KO5	A	2001	-	-	0/20/38/38	0/4/4/4
6	OLA	A	2020	-	-	6/15/17/17	-
5	OLC	A	2007	-	-	3/5/5/24	-
6	OLA	A	2018	-	-	5/12/14/17	-
5	OLC	A	2014	-	-	4/8/8/24	-
5	OLC	A	2008	-	-	2/5/5/24	-
5	OLC	A	2004	-	-	1/12/12/24	-
6	OLA	A	2017	-	-	8/11/13/17	-
6	OLA	A	2022	-	-	9/15/17/17	-
5	OLC	A	2009	-	-	5/21/21/24	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2004	OLC	O20-C1	2.50	1.40	1.33
5	A	2009	OLC	O20-C1	2.41	1.40	1.33
5	A	2006	OLC	O20-C1	2.40	1.40	1.33
5	A	2005	OLC	O20-C1	2.38	1.40	1.33
5	A	2015	OLC	O20-C1	2.37	1.40	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2015	OLC	O20-C1-C2	3.38	120.24	111.38
5	A	2004	OLC	O20-C1-C2	2.84	120.82	111.91
3	A	2002	CLR	C21-C20-C22	-2.79	105.98	110.36
5	A	2012	OLC	O20-C1-C2	2.62	120.11	111.91
5	A	2006	OLC	O20-C1-C2	2.61	120.11	111.91

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2005	OLC	C21-C22-C24-O25
5	A	2009	OLC	C21-C22-C24-O25
5	A	2011	OLC	C10-C11-C12-C13
5	A	2015	OLC	C21-C22-C24-O25
5	A	2015	OLC	O23-C22-C24-O25

There are no ring outliers.

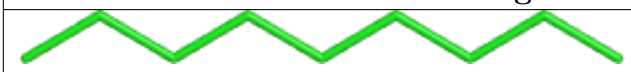
9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2012	OLC	2	0
6	A	2023	OLA	2	0
4	A	2003	1PE	1	0
5	A	2013	OLC	1	0
2	A	2001	KO5	2	0
5	A	2014	OLC	3	0
6	A	2017	OLA	1	0
6	A	2022	OLA	2	0
5	A	2009	OLC	1	0

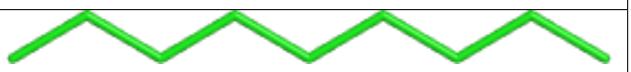
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

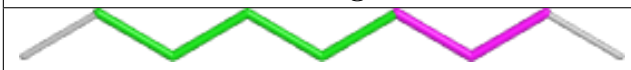
Ligand OLA A 2019



Bond lengths



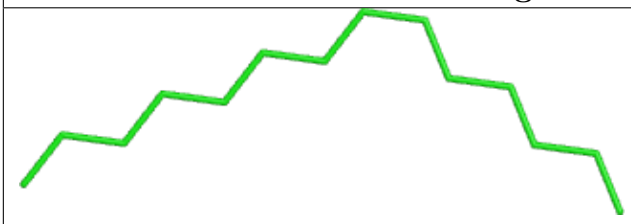
Bond angles



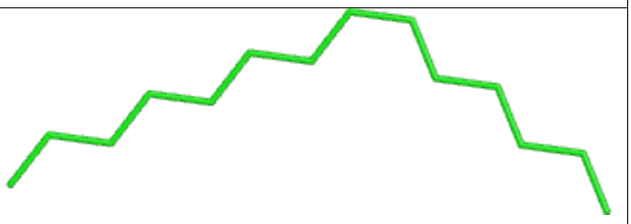
Torsions

Rings

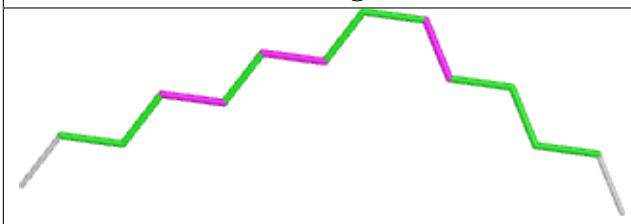
Ligand OLC A 2016



Bond lengths



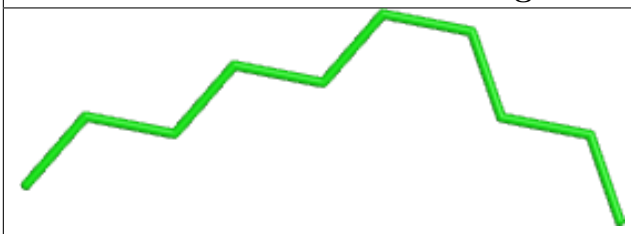
Bond angles



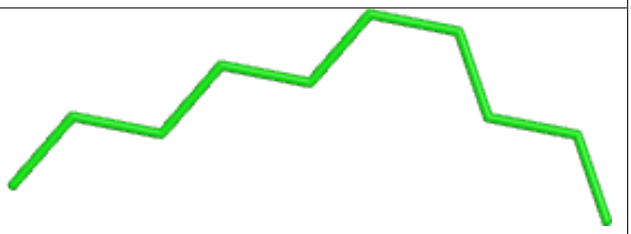
Torsions

Rings

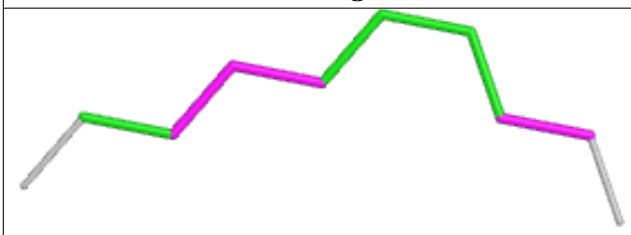
Ligand OLC A 2011



Bond lengths



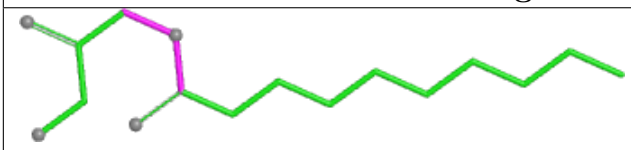
Bond angles



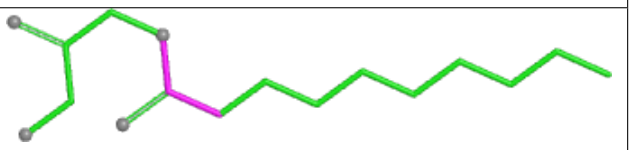
Torsions

Rings

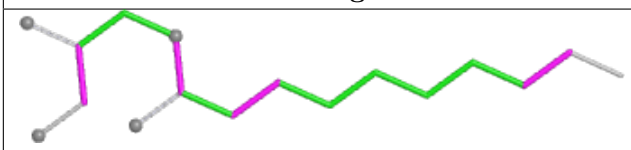
Ligand OLC A 2012



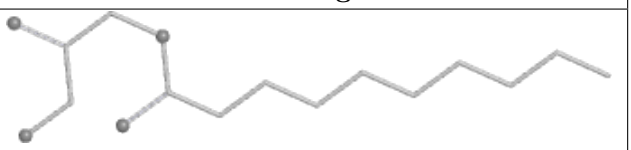
Bond lengths



Bond angles

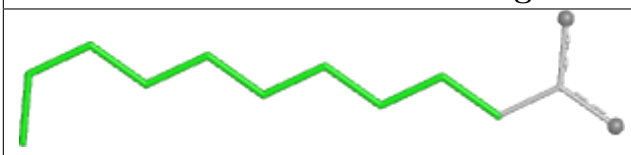


Torsions

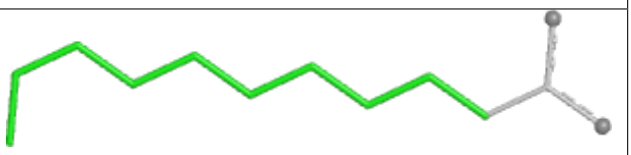


Rings

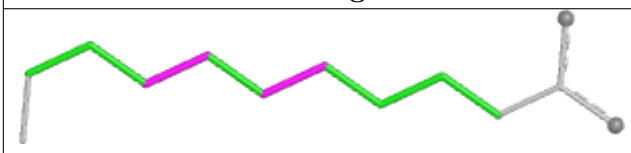
Ligand OLA A 2023



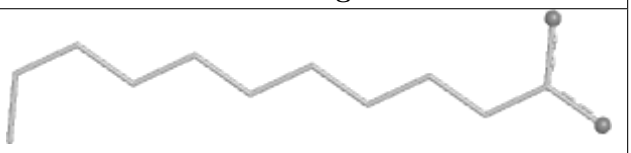
Bond lengths



Bond angles

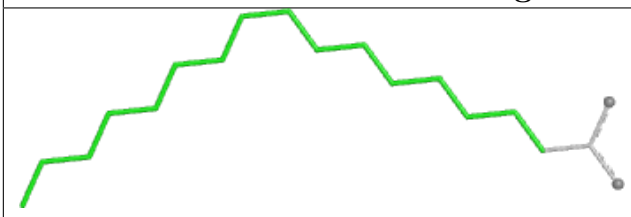


Torsions

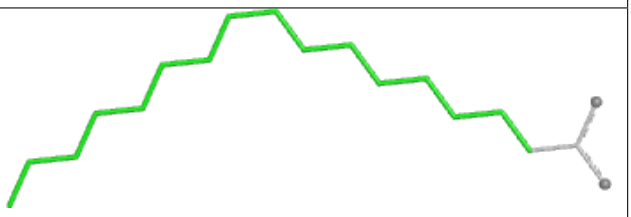


Rings

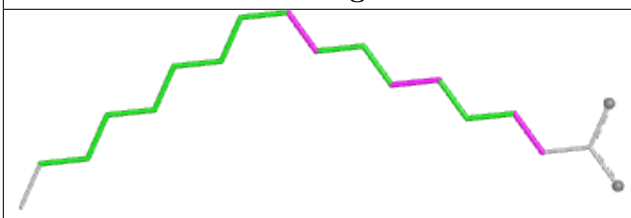
Ligand OLA A 2021



Bond lengths



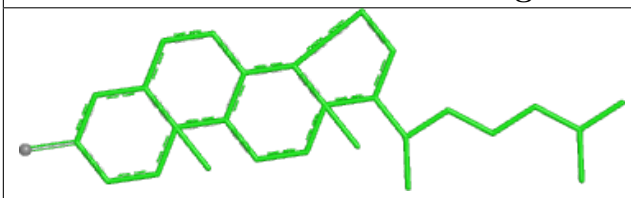
Bond angles



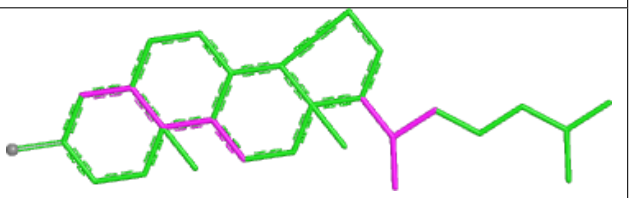
Torsions

Rings

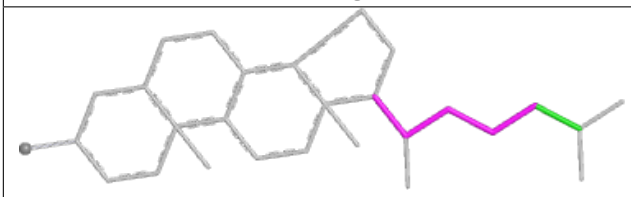
Ligand CLR A 2002



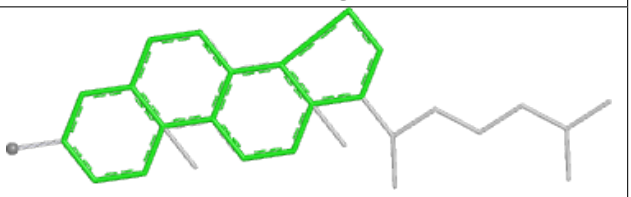
Bond lengths



Bond angles

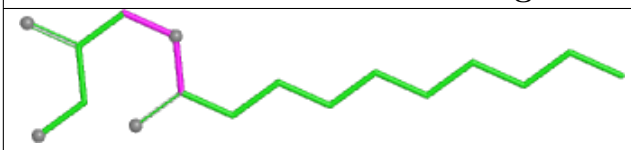


Torsions

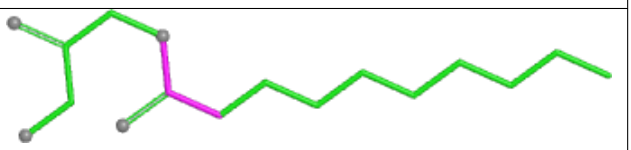


Rings

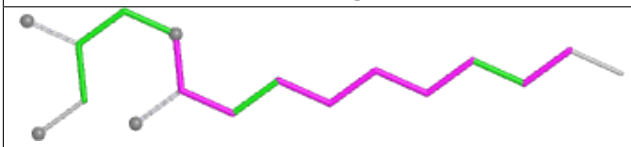
Ligand OLC A 2006



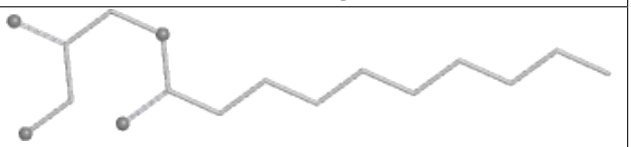
Bond lengths



Bond angles

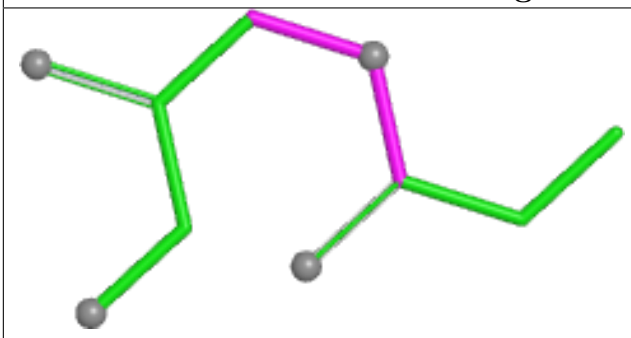


Torsions

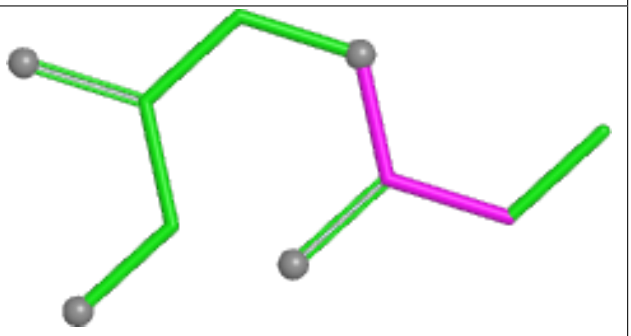


Rings

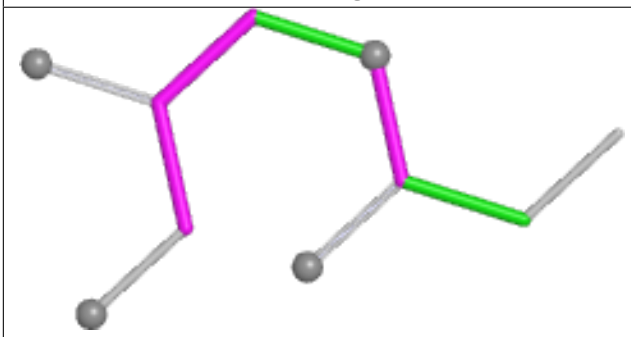
Ligand OLC A 2015



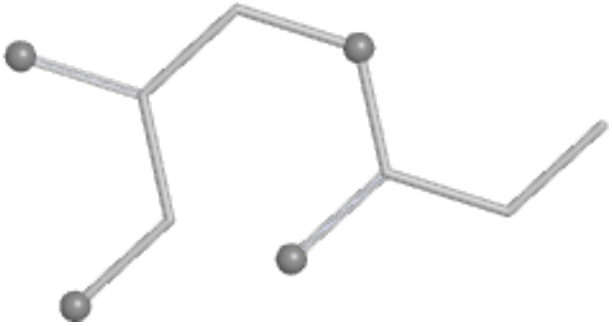
Bond lengths



Bond angles

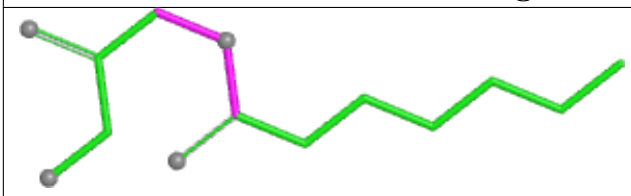


Torsions

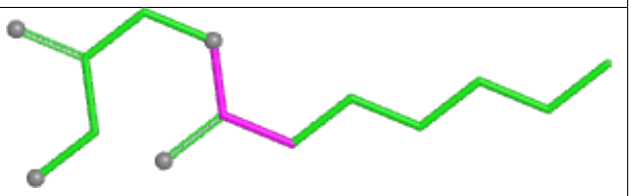


Rings

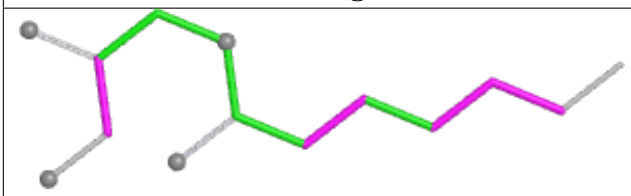
Ligand OLC A 2005



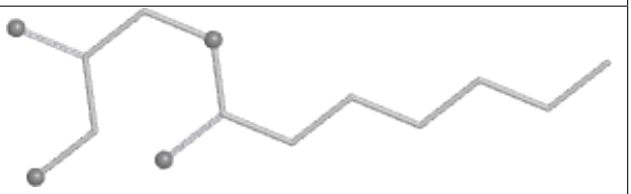
Bond lengths



Bond angles

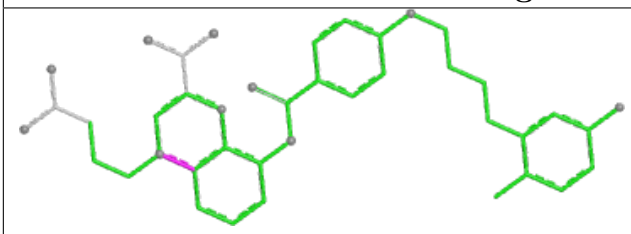


Torsions

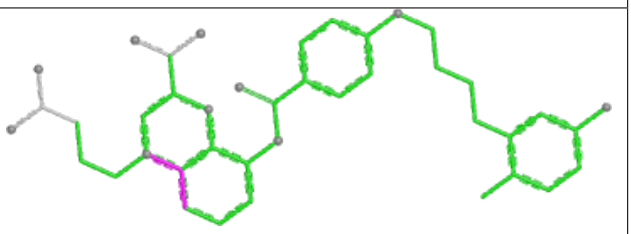


Rings

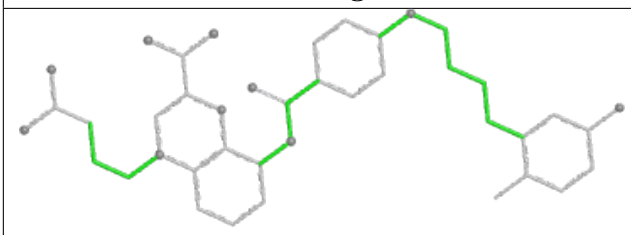
Ligand KO5 A 2001



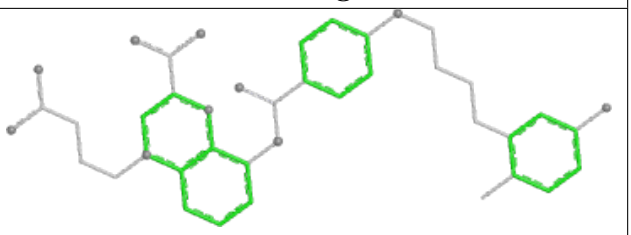
Bond lengths



Bond angles

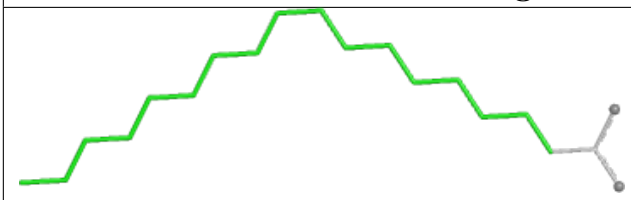


Torsions

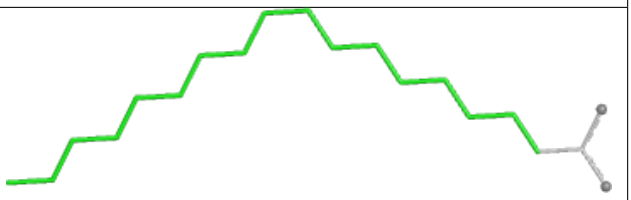


Rings

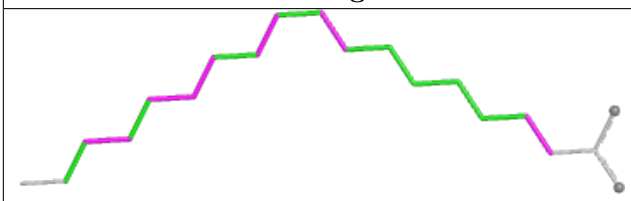
Ligand OLA A 2020



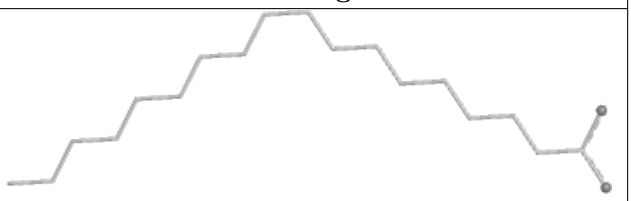
Bond lengths



Bond angles

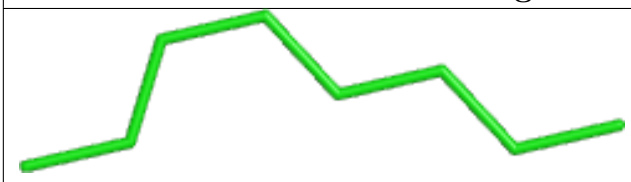


Torsions

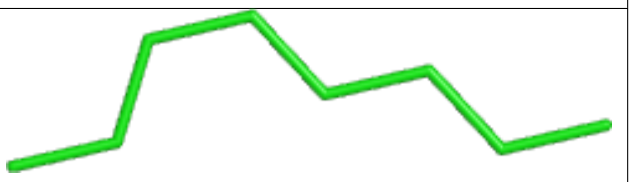


Rings

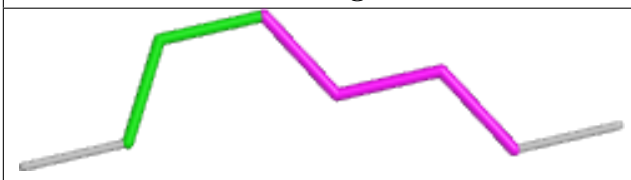
Ligand OLC A 2007



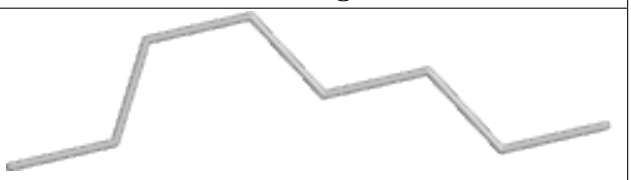
Bond lengths



Bond angles

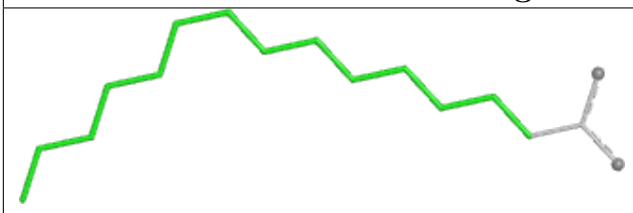


Torsions

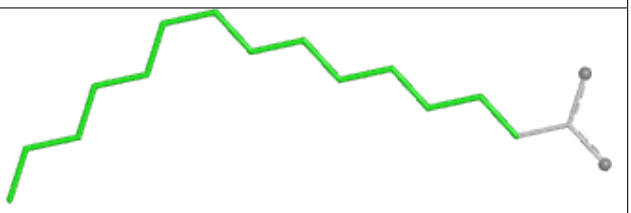


Rings

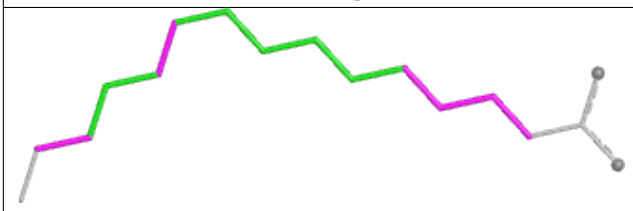
Ligand OLA A 2018



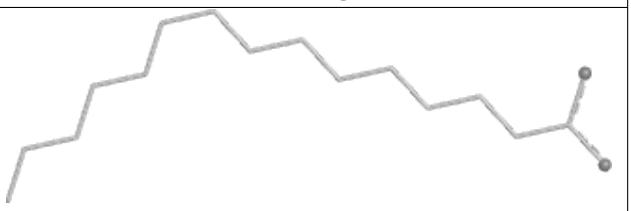
Bond lengths



Bond angles

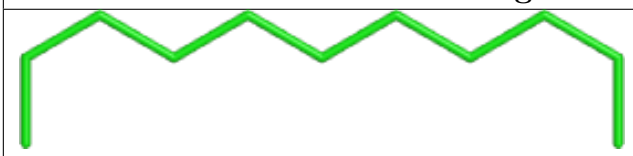


Torsions

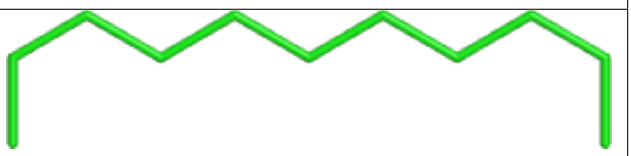


Rings

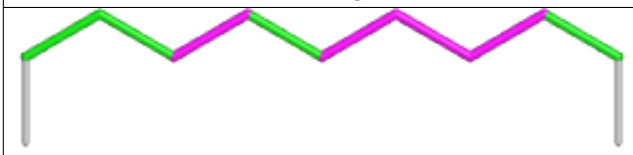
Ligand OLC A 2014



Bond lengths



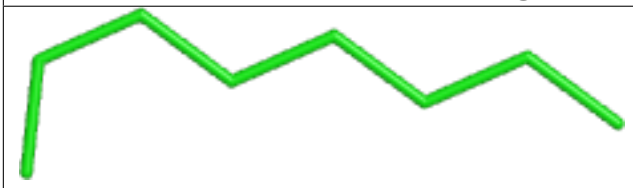
Bond angles



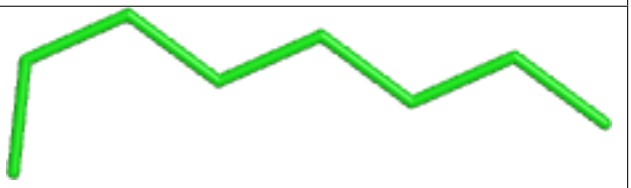
Torsions

Rings

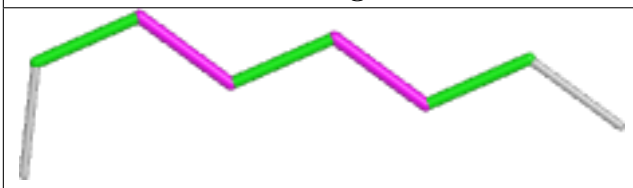
Ligand OLC A 2008



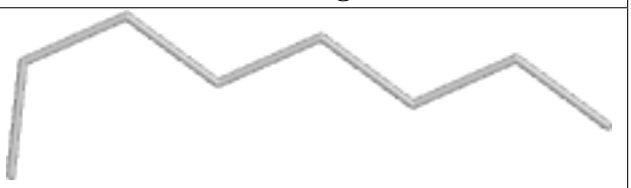
Bond lengths



Bond angles

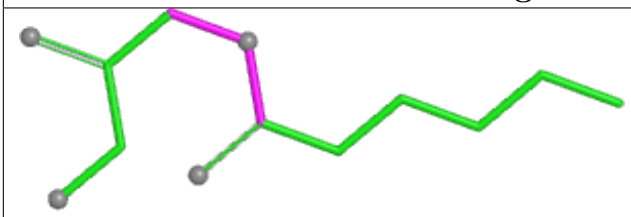


Torsions

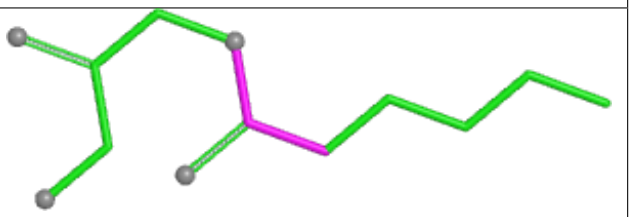


Rings

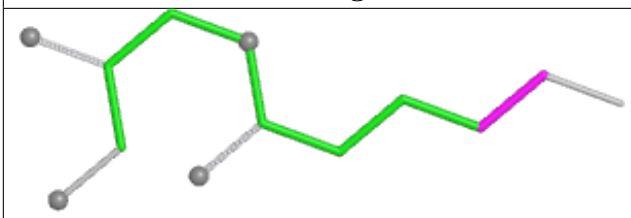
Ligand OLC A 2004



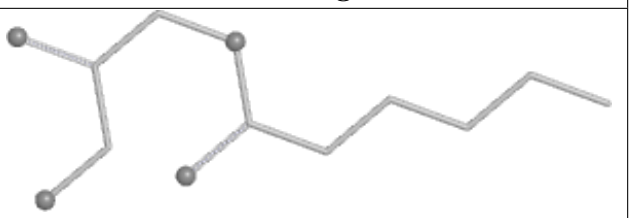
Bond lengths



Bond angles

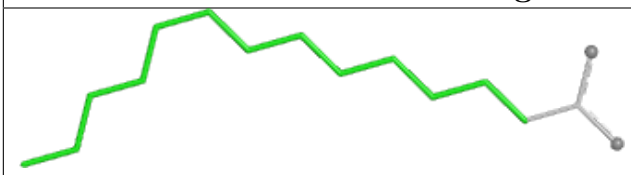


Torsions

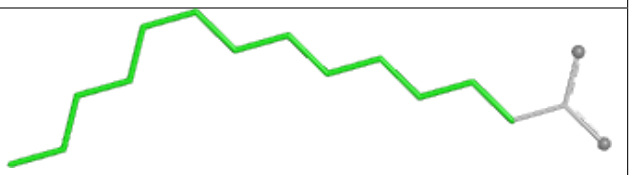


Rings

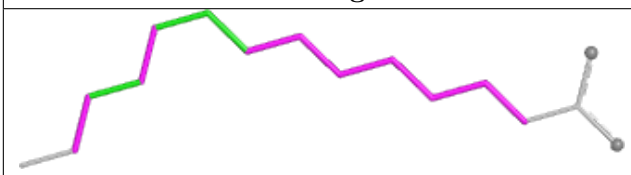
Ligand OLA A 2017



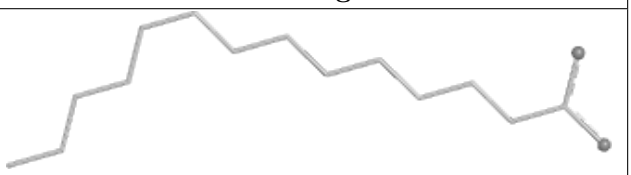
Bond lengths



Bond angles

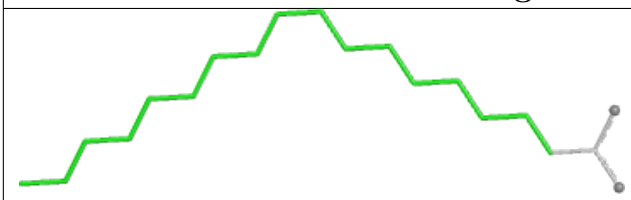


Torsions

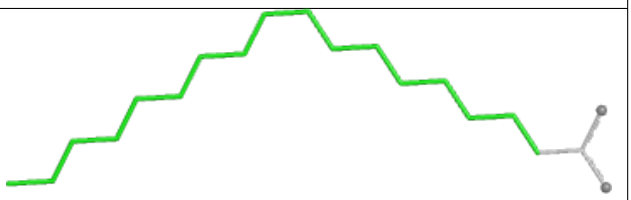


Rings

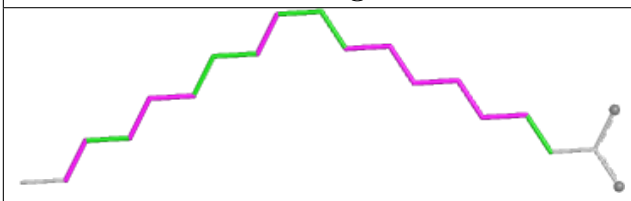
Ligand OLA A 2022



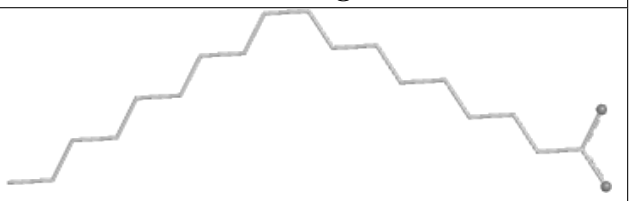
Bond lengths



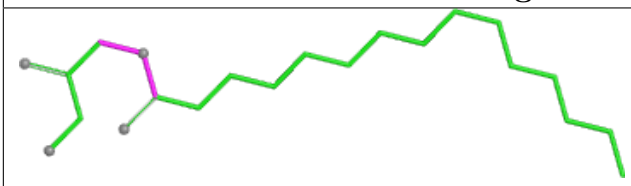
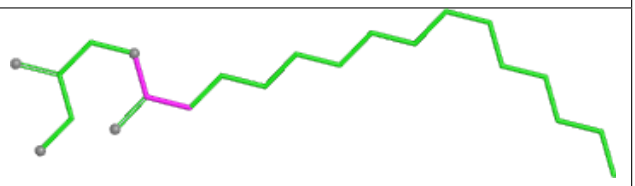
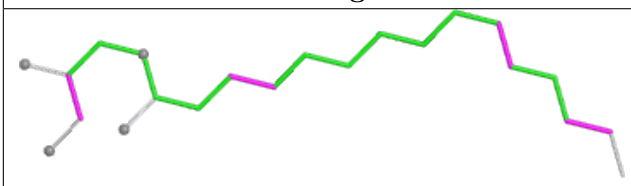
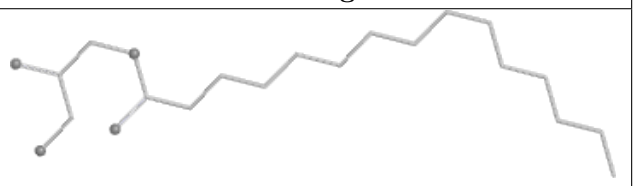
Bond angles



Torsions



Rings

Ligand OLC A 2009	
 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

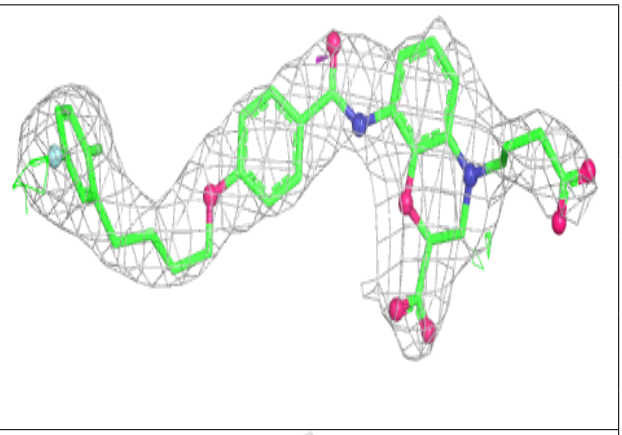
6.4 Ligands (i)

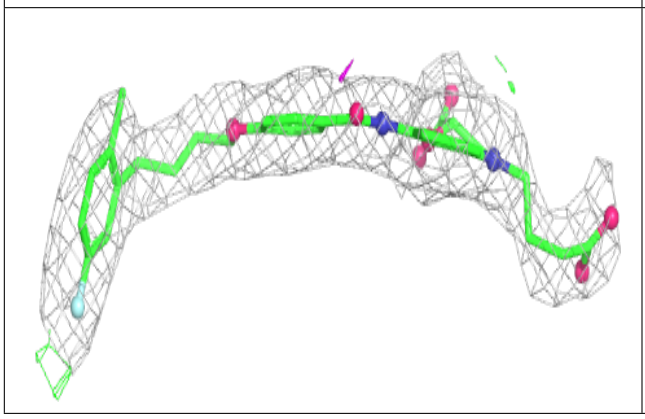
Unable to reproduce the depositors R factor - this section is therefore empty.

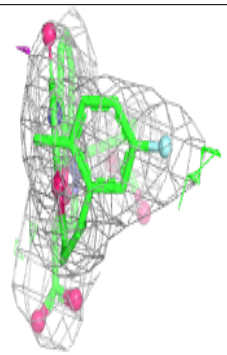
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KO5 A 2001:

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

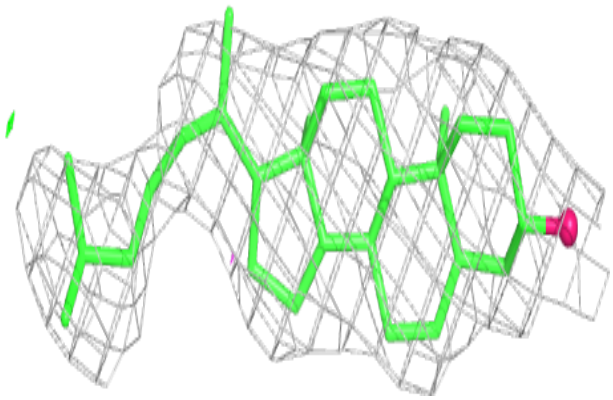


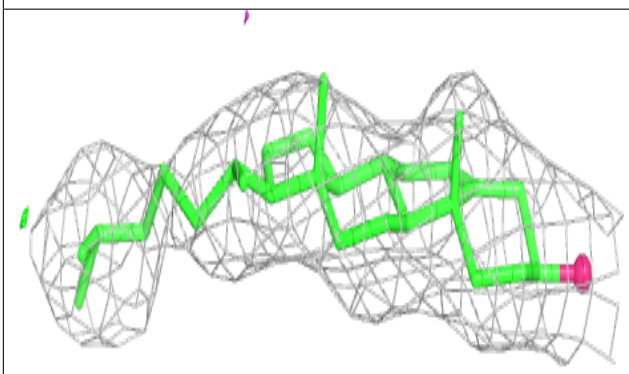


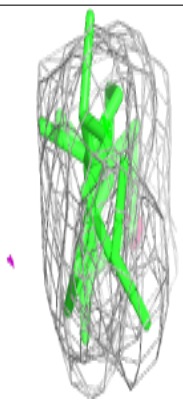


Electron density around CLR A 2002:

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

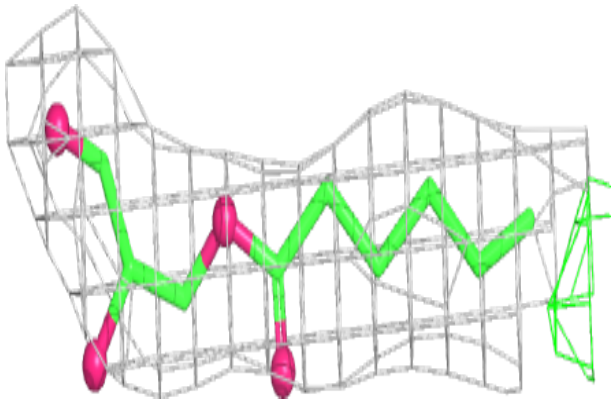


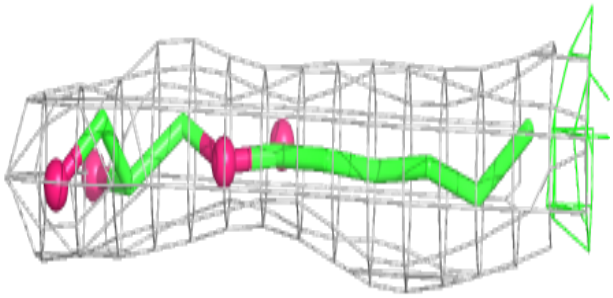


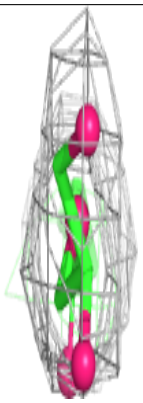


Electron density around OLC A 2004:

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

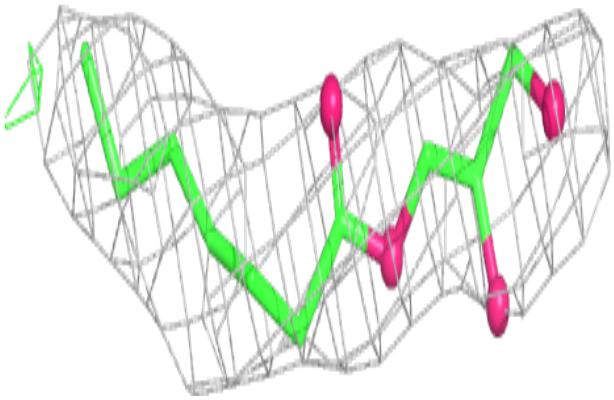


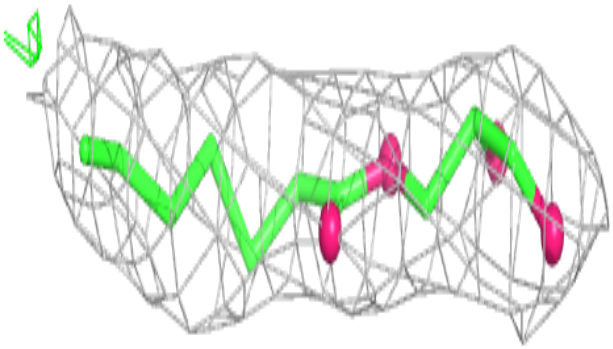




Electron density around OLC A 2005:

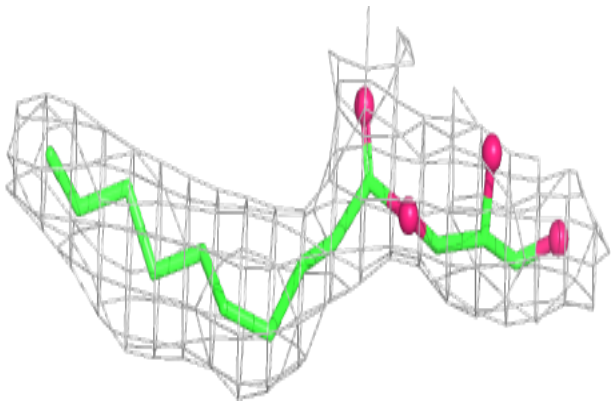
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

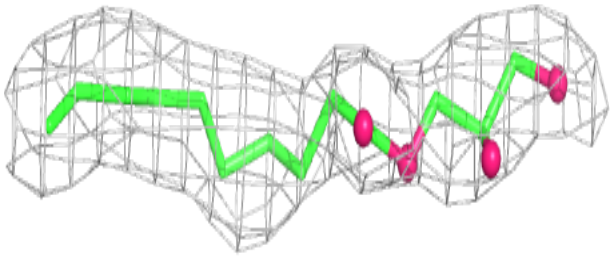


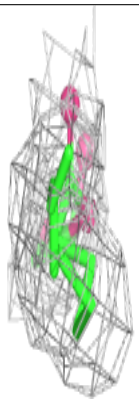


Electron density around OLC A 2006:

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

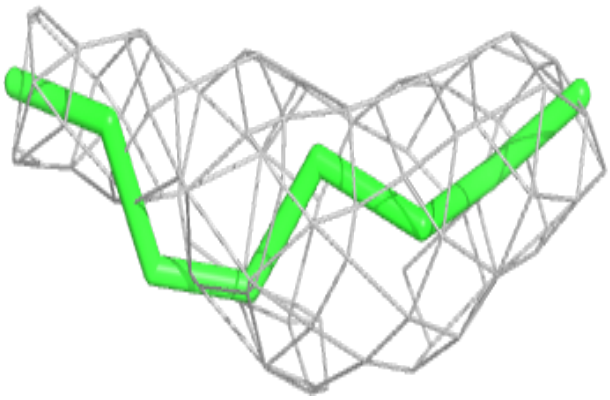


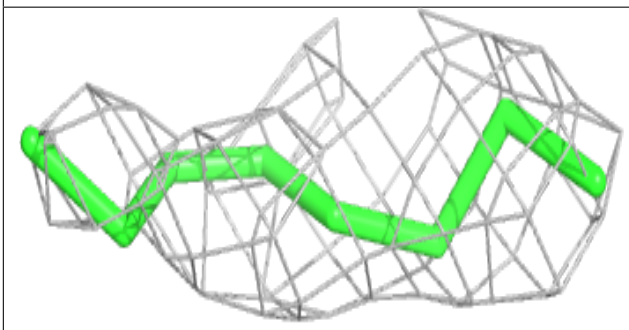


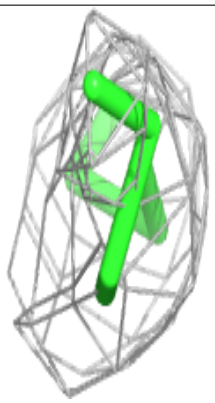


Electron density around OLC A 2007:

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

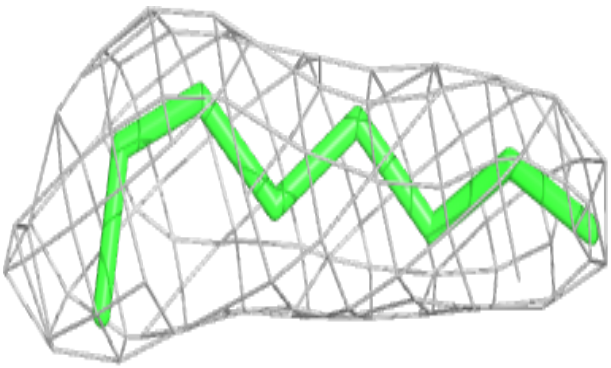


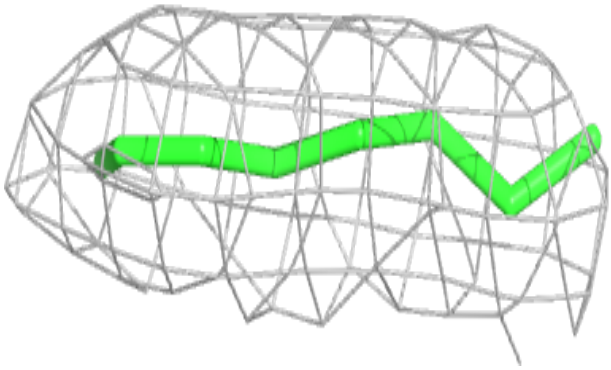


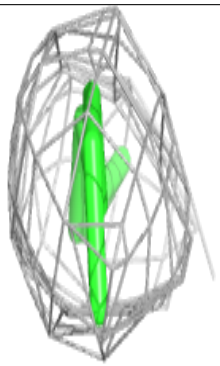


Electron density around OLC A 2008:

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

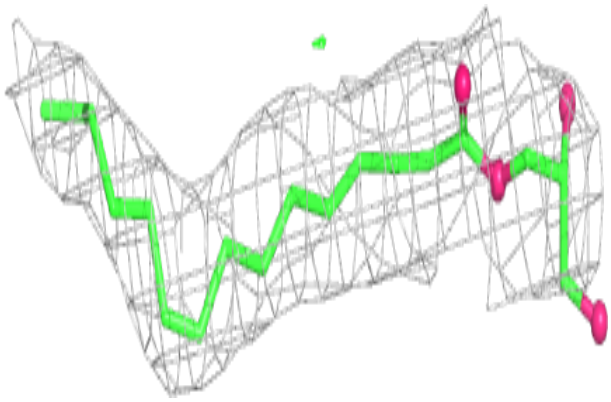


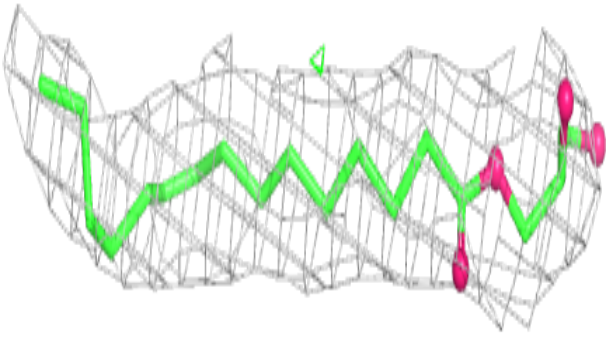


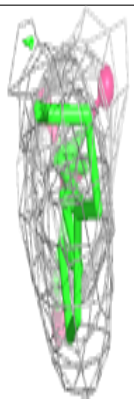


Electron density around OLC A 2009:

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

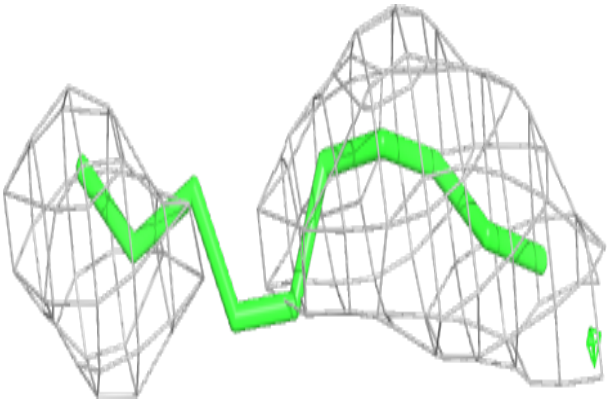


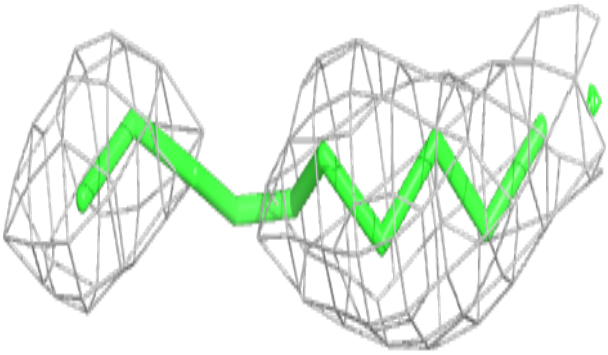


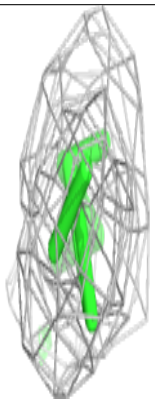


Electron density around OLC A 2011:

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

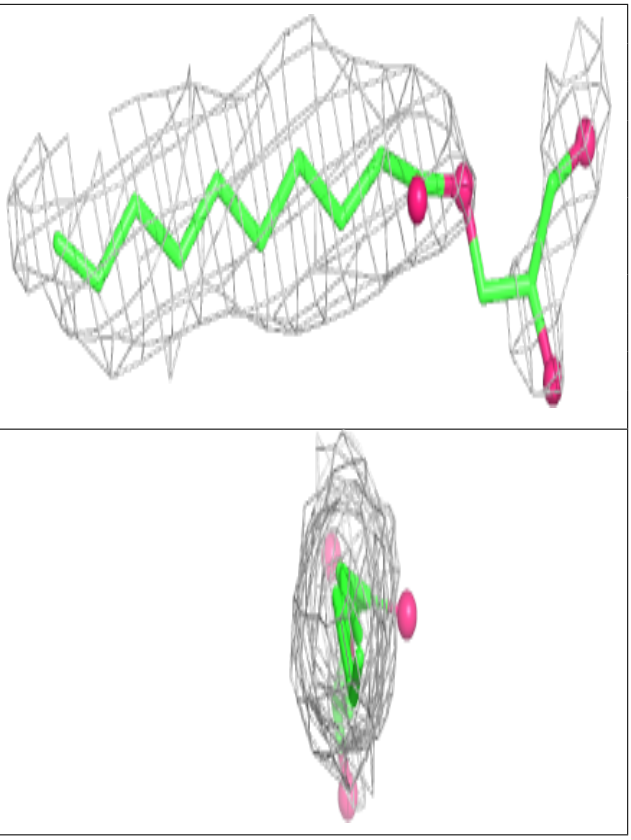


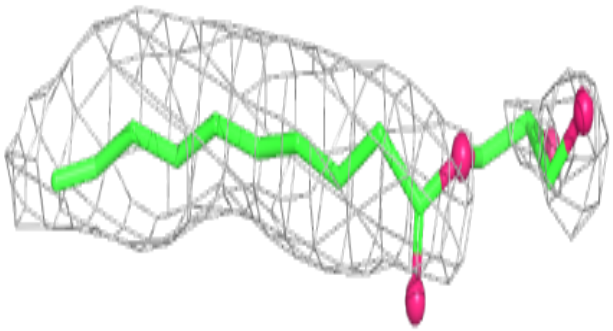




Electron density around OLC A 2012:

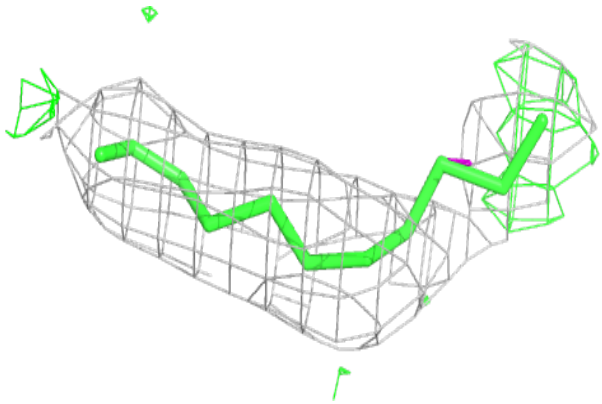
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

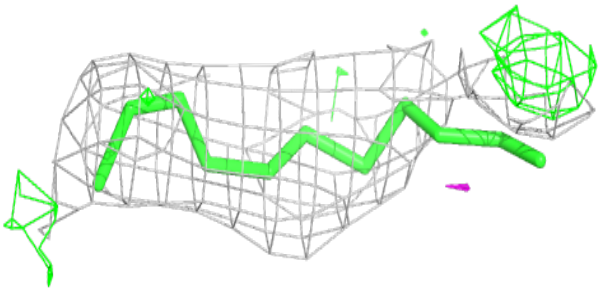


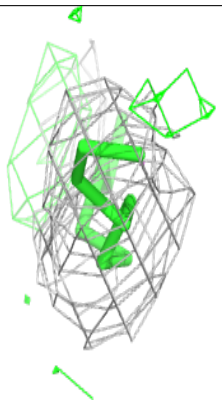


Electron density around OLC A 2014:

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

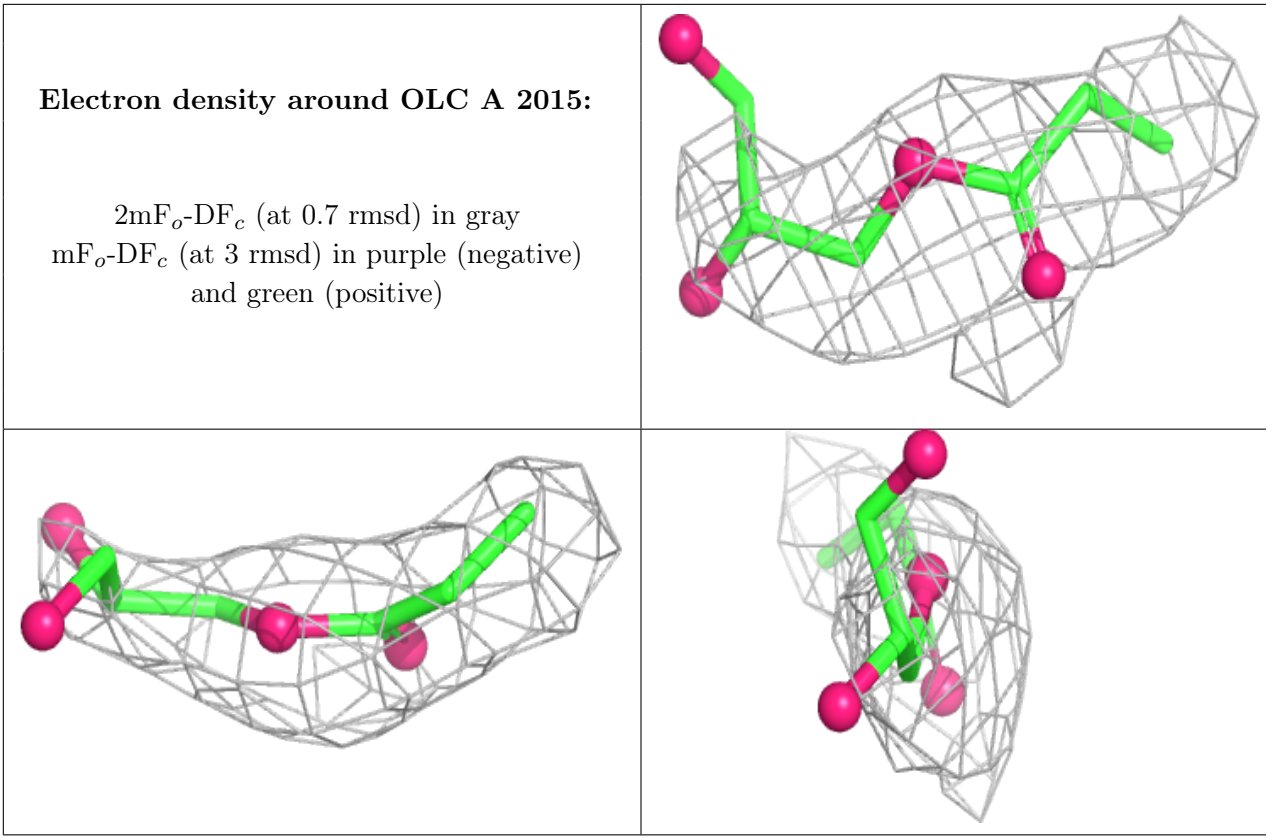






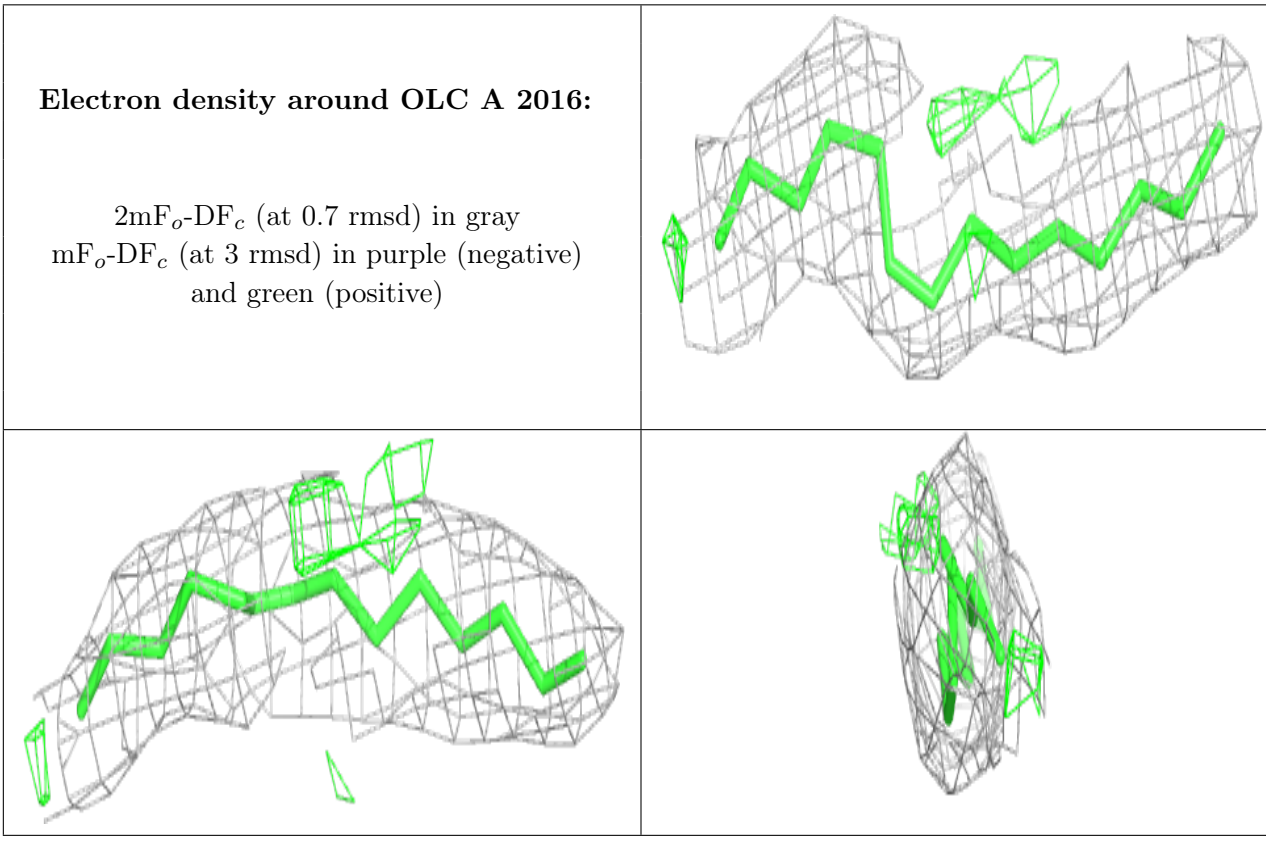
Electron density around OLC A 2015:

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



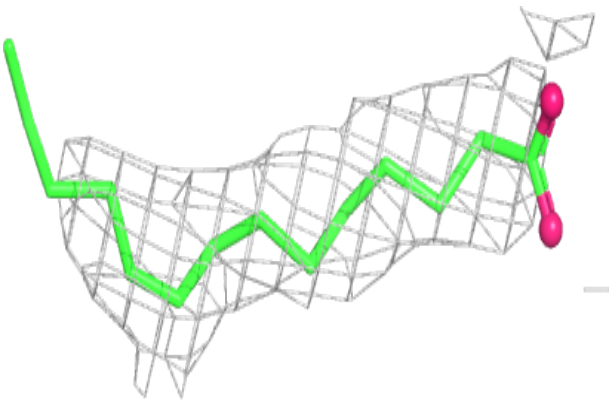
Electron density around OLC A 2016:

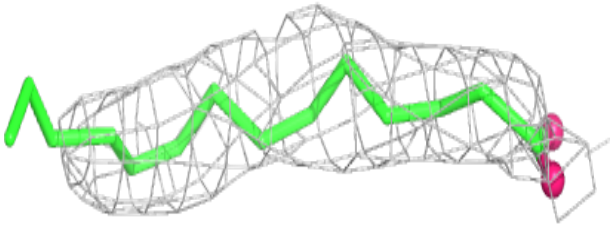
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

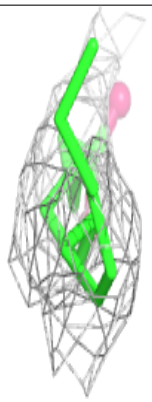


Electron density around OLA A 2017:

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

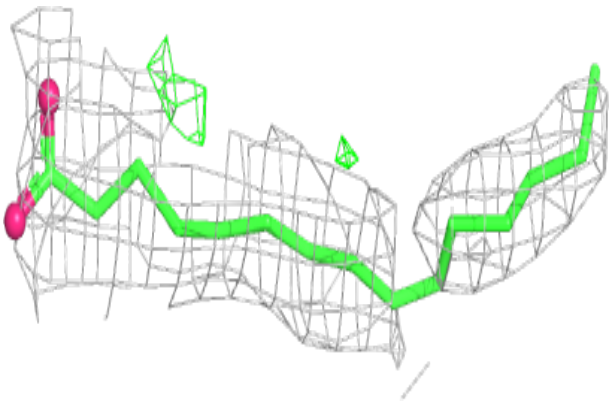


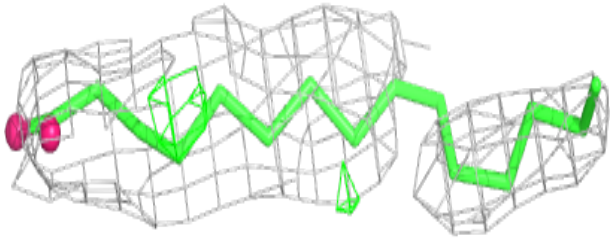


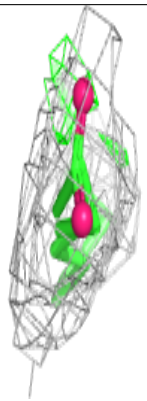


Electron density around OLA A 2018:

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

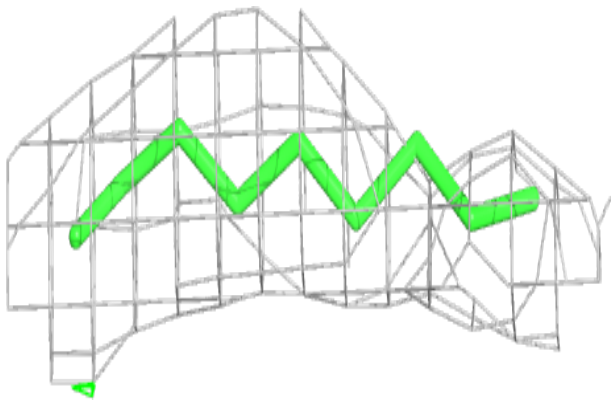


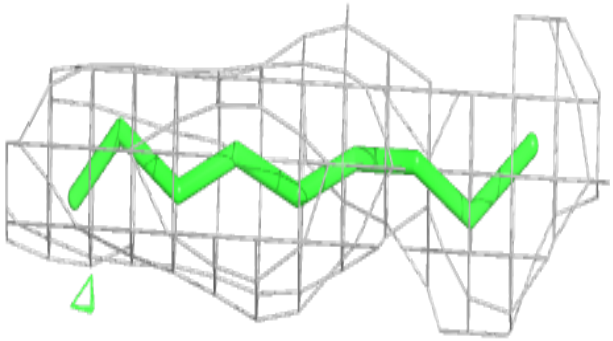


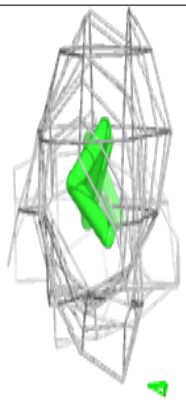


Electron density around OLA A 2019:

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

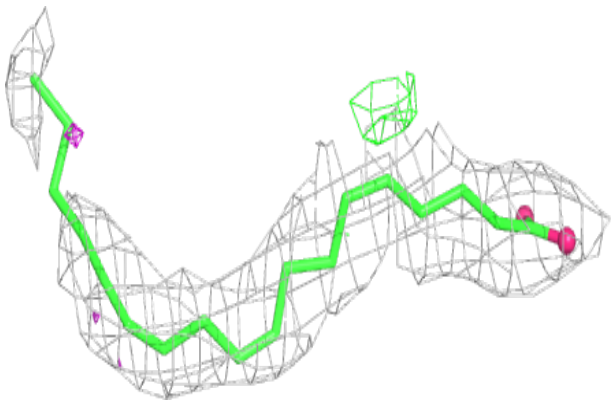


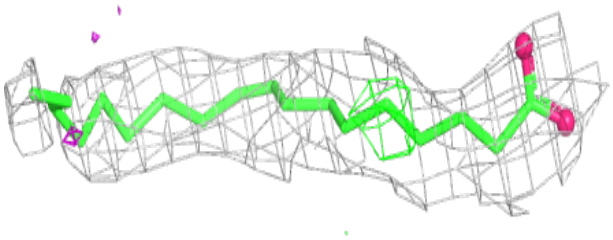


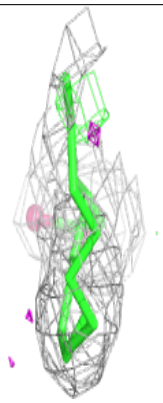


Electron density around OLA A 2020:

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

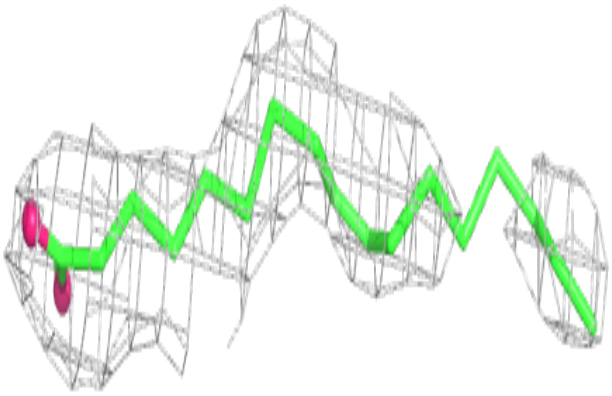


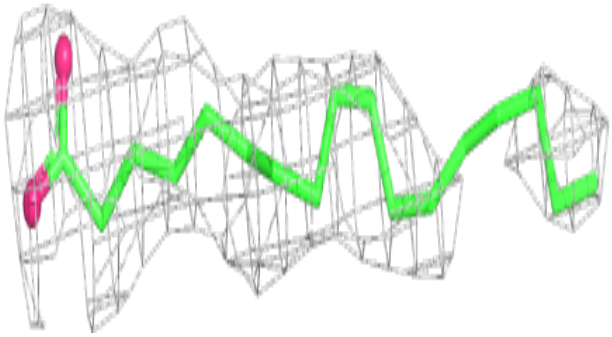


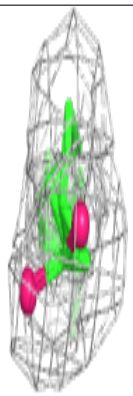


Electron density around OLA A 2021:

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

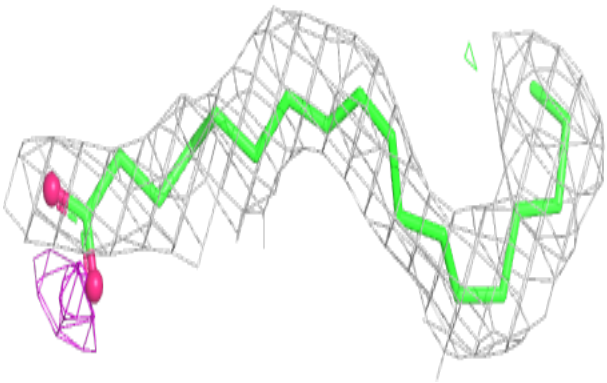


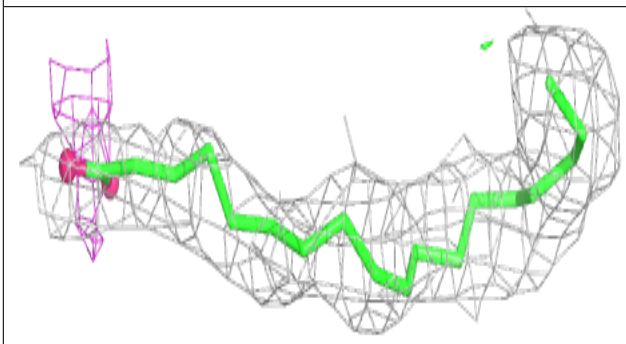


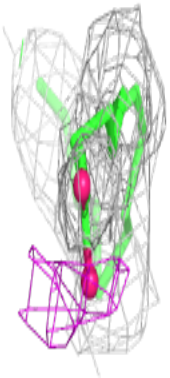


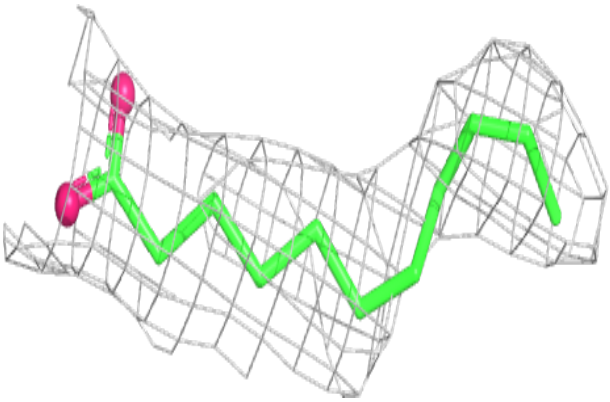
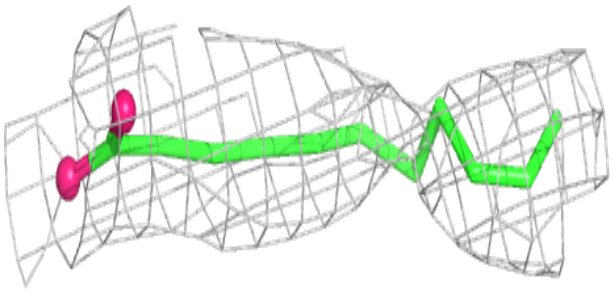
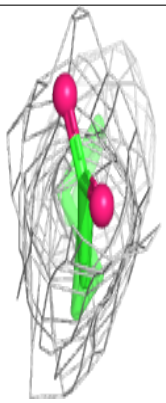
Electron density around OLA A 2022:

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







Electron density around OLA A 2023: 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)

Unable to reproduce the depositors R factor - this section is therefore empty.