Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2022 – 03:36 pm GMT

PDB ID	:	6RZ7
Title	:	Crystal structure of the human cysteinyl leukotriene receptor 2 in complex with ONO-2570366 (F222 space group)
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	:	2.43 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 following versions of software and data (see references (1)) were used in the production of this report:

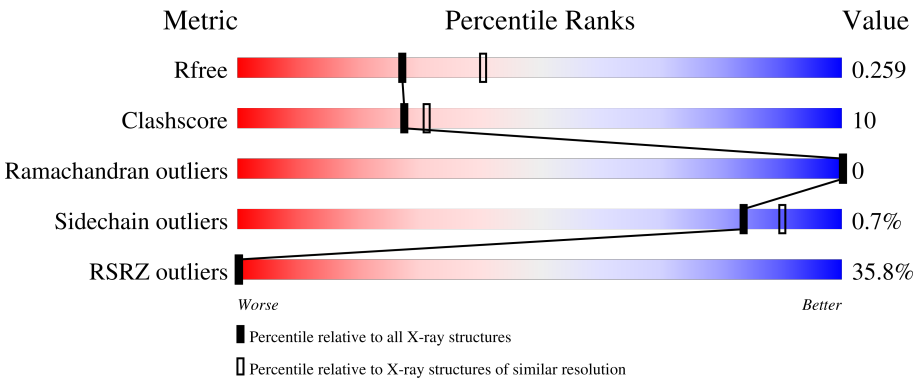
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	405	32% 74% 15% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLC	A	2004	-	-	-	X
5	OLA	A	2009	-	-	-	X
5	OLA	A	2015	-	-	-	X
5	OLA	A	2016	-	-	-	X
5	OLA	A	2019	-	-	-	X
5	OLA	A	2020	-	-	-	X
5	OLA	A	2022	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3142 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.

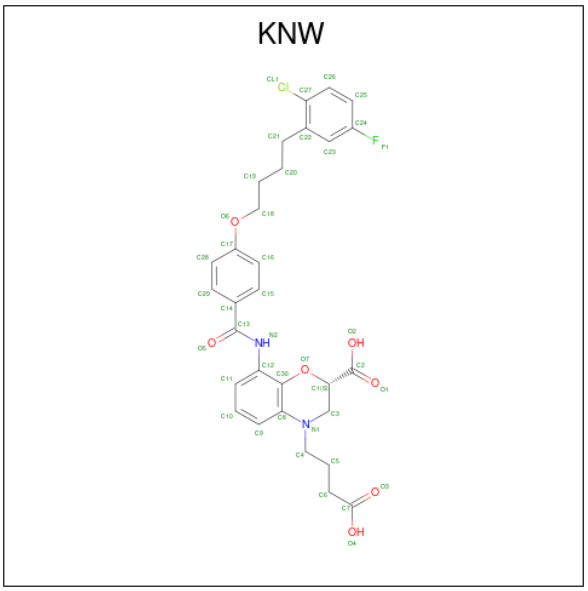
- Molecule 1 is a protein called Cysteinyl leukotriene receptor 2,Soluble cytochrome b562,Cysteinyl leukotriene receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2740	1810	431	481	18	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

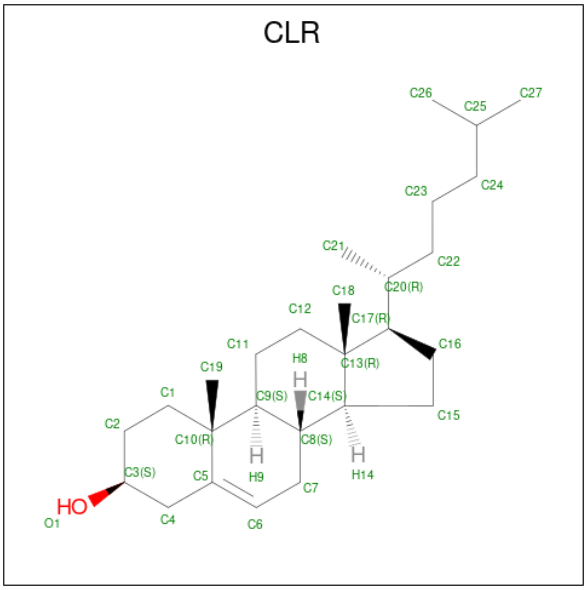
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	VAL	TRP	engineered mutation	UNP Q9NS75
A	84	ASN	ASP	engineered mutation	UNP Q9NS75
A	137	TYR	PHE	engineered mutation	UNP Q9NS75
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation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

- Molecule 2 is (2 {S})-8-[[4-[4-(2-chloranyl-5-fluoranyl-phenyl)butoxy]phenyl]carbonylamino]-4-(4-oxidanyl-4-oxidanylidene-butyl)-2,3- dihydro-1,4-benzoxazine-2-carboxylic acid (three-letter code: KNW) (formula: $C_{30}H_{30}ClFN_2O_7$) (labeled as "Ligand of Interest" by depositor).



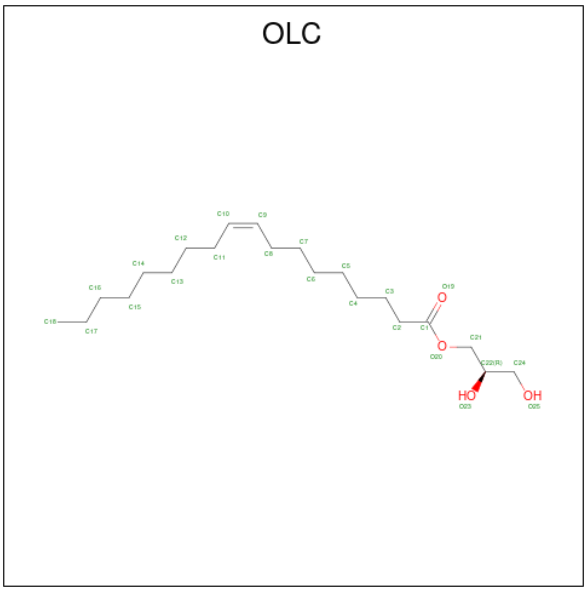
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
2	A	1	41	30	1	1	2	7	0	0

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



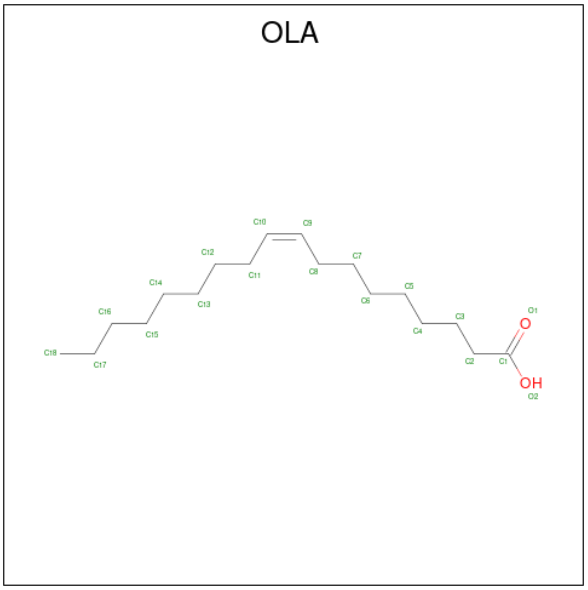
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	28	27	1	0	0

- Molecule 4 is (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
4	A	1	Total C 9 9	0	0
4	A	1	Total C O 25 21 4	0	0

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 17 15 2	0	0
5	A	1	Total C O 15 13 2	0	0

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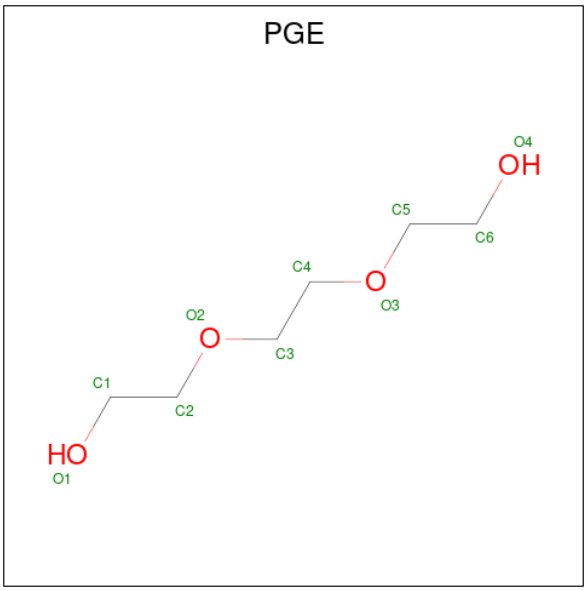
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 14 14	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 18 16 2	0	0
5	A	1	Total C O 19 17 2	0	0
5	A	1	Total C O 10 8 2	0	0
5	A	1	Total C O 9 7 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C 11 11	0	0
5	A	1	Total C O 7 5 2	0	0
5	A	1	Total C O 9 7 2	0	0
5	A	1	Total C O 9 7 2	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C O 17 15 2	0	0
5	A	1	Total C O 6 4 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 17 15 2	0	0
5	A	1	Total C 14 14	0	0
5	A	1	Total C 10 10	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 7 is water.

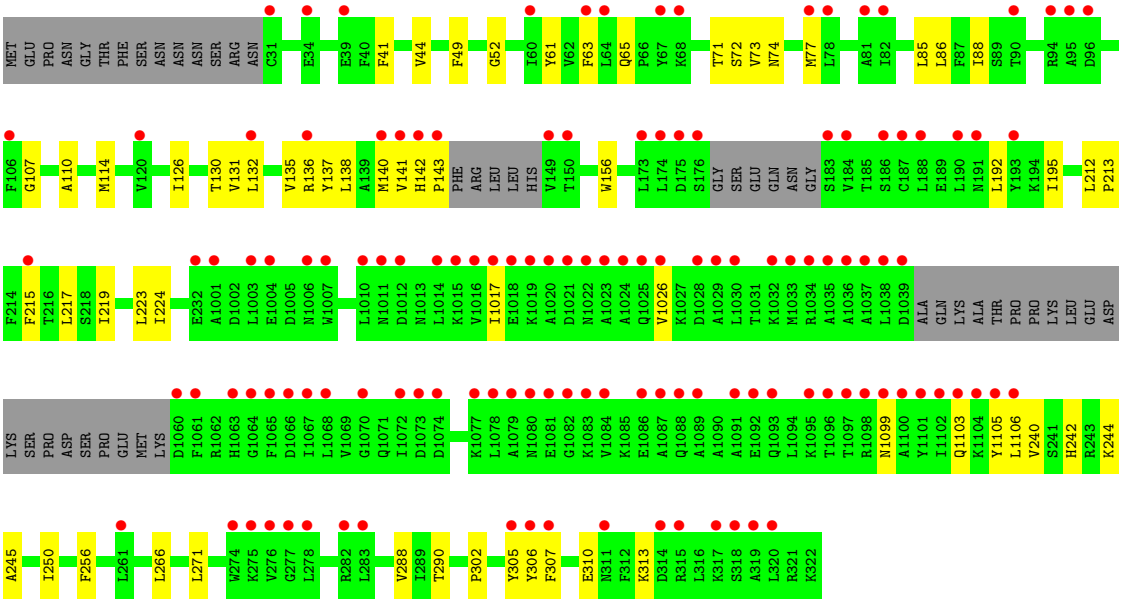
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	20	20	20	0	0

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: Cysteinyl leukotriene receptor 2,Soluble cytochrome b562,Cysteinyl leukotriene receptor 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	81.83Å 142.07Å 171.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.43 19.93 – 2.43	Depositor EDS
% Data completeness (in resolution range)	92.6 (19.93-2.43) 82.9 (19.93-2.43)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 2.44Å)	Xtriage
Refinement program	PHENIX 1.12-2829, BUSTER 2.10.3	Depositor
R, R_{free}	0.229 , 0.259 0.229 , 0.259	Depositor DCC
R_{free} test set	890 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3142	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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: CLR, KNW, OLA, OLC, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.42	0/2794	0.60	0/3811

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	47	0
2	A	41	0	0	1	0
3	A	28	0	46	3	0
4	A	34	0	57	5	0
5	A	269	0	373	17	0
6	A	10	0	14	0	0
7	A	20	0	0	1	0
All	All	3142	0	3192	63	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 10.

All (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:HB2	5:A:2006:OLA:H122	1.72	0.71
1:A:73:VAL:HG13	1:A:132:LEU:HD11	1.74	0.70
1:A:71:THR:HB	1:A:310:GLU:OE2	1.95	0.65
1:A:141:VAL:HG23	1:A:143:PRO:HD3	1.79	0.65
1:A:107:GLY:HA3	5:A:2012:OLA:C1	2.28	0.64
1:A:73:VAL:HB	1:A:310:GLU:OE2	1.98	0.63
5:A:2012:OLA:H21	5:A:2016:OLA:H22	1.82	0.62
1:A:61:TYR:O	1:A:65:GLN:HG2	1.98	0.62
1:A:41:PHE:CZ	1:A:288:VAL:HG13	2.36	0.60
1:A:52:GLY:HA3	1:A:88:ILE:HD13	1.85	0.59
5:A:2009:OLA:H131	5:A:2022:OLA:H121	1.84	0.59
1:A:140:MET:HE3	1:A:224:ILE:HG23	1.86	0.57
1:A:140:MET:HE3	1:A:245:ALA:HB3	1.86	0.57
1:A:140:MET:HE2	1:A:242:HIS:HA	1.86	0.56
1:A:215:PHE:CE2	1:A:219:ILE:HD11	2.40	0.55
4:A:2004:OLC:H4A	5:A:2010:OLA:H9	1.88	0.55
1:A:85:LEU:HD22	4:A:2004:OLC:H12	1.88	0.55
1:A:140:MET:CE	1:A:245:ALA:HB3	2.38	0.54
1:A:73:VAL:HG11	1:A:136:ARG:NH2	2.23	0.54
1:A:240:VAL:O	1:A:244:LYS:HG2	2.09	0.53
1:A:71:THR:HG22	1:A:72:SER:H	1.74	0.53
1:A:306:TYR:CE1	1:A:313:LYS:HG2	2.45	0.51
5:A:2005:OLA:H81	5:A:2006:OLA:H52	1.91	0.51
5:A:2007:OLA:H9	5:A:2010:OLA:H142	1.93	0.50
1:A:86:LEU:HD23	4:A:2004:OLC:H15A	1.94	0.49
1:A:71:THR:HG22	1:A:72:SER:N	2.27	0.49
1:A:49:PHE:HA	1:A:88:ILE:HG23	1.94	0.49
5:A:2012:OLA:H32	5:A:2020:OLA:O2	2.13	0.49
5:A:2007:OLA:H71	5:A:2010:OLA:H111	1.95	0.49
1:A:302:PRO:HA	1:A:305:TYR:CD2	2.48	0.48
1:A:138:LEU:O	1:A:142:HIS:N	2.31	0.48
1:A:250:ILE:HG21	5:A:2019:OLA:H122	1.96	0.47
1:A:85:LEU:CD2	4:A:2004:OLC:H14	2.45	0.47
5:A:2010:OLA:H41	5:A:2014:OLA:H71	1.96	0.47
1:A:126:ILE:HG23	1:A:256:PHE:HZ	1.80	0.47
1:A:110:ALA:O	1:A:114:MET:HG2	2.15	0.46
3:A:2002:CLR:H272	3:A:2002:CLR:H231	1.66	0.46
1:A:140:MET:CE	1:A:242:HIS:HA	2.46	0.45
3:A:2002:CLR:O1	7:A:2101:HOH:O	2.21	0.45
5:A:2007:OLA:H122	5:A:2007:OLA:H152	1.62	0.45
1:A:302:PRO:HA	1:A:305:TYR:CG	2.52	0.45
1:A:192:LEU:O	1:A:195:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD12	1:A:290:THR:HG21	1.97	0.45
1:A:137:TYR:CE1	1:A:223:LEU:HB3	2.52	0.44
5:A:2016:OLA:H51	5:A:2017:OLA:H52	1.98	0.44
1:A:307:PHE:CG	5:A:2019:OLA:H51	2.52	0.44
1:A:212:LEU:HB3	1:A:213:PRO:HD3	1.99	0.44
1:A:271:LEU:HD11	2:A:2001:KNW:O5	2.18	0.44
1:A:63:PHE:CZ	1:A:77:MET:HB3	2.54	0.43
1:A:137:TYR:O	1:A:141:VAL:HG22	2.18	0.43
1:A:1017:ILE:HG23	1:A:1026:VAL:HG13	2.01	0.43
1:A:1106:LEU:HD13	1:A:1106:LEU:O	2.19	0.42
1:A:1103:GLN:O	1:A:240:VAL:HG13	2.19	0.42
5:A:2011:OLA:H41	5:A:2011:OLA:H72	1.67	0.42
5:A:2008:OLA:H22	5:A:2013:OLA:O2	2.20	0.42
5:A:2023:OLA:H82	5:A:2023:OLA:H112	1.59	0.42
1:A:156:TRP:HZ2	4:A:2004:OLC:H21A	1.85	0.42
1:A:130:THR:HA	1:A:217:LEU:HD21	2.02	0.41
3:A:2002:CLR:H183	3:A:2002:CLR:H20	1.80	0.41
1:A:41:PHE:HA	1:A:44:VAL:HG22	2.03	0.41
1:A:136:ARG:HG2	1:A:245:ALA:HA	2.04	0.40
1:A:1105:TYR:CE2	1:A:242:HIS:HE1	2.39	0.40
1:A:131:VAL:O	1:A:135:VAL:HG23	2.22	0.40

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	353/405 (87%)	345 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	277/356 (78%)	275 (99%)	2 (1%)	84 90

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

Mol	Chain	Res	Type
1	A	74	ASN
1	A	1099	ASN

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)

26 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	$\#\|Z\| > 2$
5	OLA	A	2011	-	6,9,19	0.23	0	5,9,19	0.64	0
5	OLA	A	2005	-	13,16,19	0.24	0	12,16,19	0.70	0
6	PGE	A	2026	-	9,9,9	0.32	0	8,8,8	0.39	0
5	OLA	A	2017	-	5,8,19	0.23	0	4,8,19	0.55	0
5	OLA	A	2012	-	5,8,19	0.27	0	4,8,19	0.46	0
3	CLR	A	2002	-	31,31,31	0.67	0	48,48,48	1.36	9 (18%)
5	OLA	A	2019	-	13,16,19	0.28	0	12,16,19	0.50	0
5	OLA	A	2023	-	13,16,19	0.24	0	12,16,19	0.59	0
5	OLA	A	2010	-	15,18,19	0.23	0	14,18,19	0.60	0
5	OLA	A	2013	-	7,10,19	0.20	0	6,10,19	0.61	0
5	OLA	A	2021	-	4,7,19	0.28	0	3,7,19	0.35	0
5	OLA	A	2008	-	16,19,19	0.23	0	15,19,19	0.61	0
5	OLA	A	2018	-	7,7,19	0.31	0	6,6,19	0.32	0
4	OLC	A	2003	-	8,8,24	0.30	0	7,7,25	0.83	0
5	OLA	A	2020	-	2,5,19	0.36	0	2,5,19	0.72	0
2	KNW	A	2001	-	38,44,44	0.46	1 (2%)	48,60,60	0.73	1 (2%)
5	OLA	A	2015	-	3,6,19	0.25	0	2,6,19	0.42	0
5	OLA	A	2016	-	5,8,19	0.22	0	4,8,19	0.55	0
5	OLA	A	2025	-	9,9,19	0.25	0	8,8,19	0.55	0
4	OLC	A	2004	-	24,24,24	0.57	0	25,25,25	1.01	1 (4%)
5	OLA	A	2014	-	10,10,19	0.30	0	9,9,19	0.40	0
5	OLA	A	2024	-	13,13,19	0.21	0	12,12,19	0.53	0
5	OLA	A	2009	-	14,17,19	0.22	0	13,17,19	0.63	0
5	OLA	A	2007	-	13,13,19	0.26	0	12,12,19	0.61	0
5	OLA	A	2022	-	16,19,19	0.25	0	15,19,19	0.52	0
5	OLA	A	2006	-	11,14,19	0.27	0	10,14,19	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	2011	-	-	0/5/7/17	-
5	OLA	A	2005	-	-	2/12/14/17	-
6	PGE	A	2026	-	-	4/7/7/7	-
5	OLA	A	2017	-	-	0/4/6/17	-
5	OLA	A	2012	-	-	2/4/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	A	2002	-	-	6/10/68/68	0/4/4/4
5	OLA	A	2019	-	-	7/12/14/17	-
5	OLA	A	2023	-	-	2/12/14/17	-
5	OLA	A	2010	-	-	11/14/16/17	-
5	OLA	A	2013	-	-	1/6/8/17	-
5	OLA	A	2021	-	-	3/3/5/17	-
5	OLA	A	2008	-	-	3/15/17/17	-
5	OLA	A	2018	-	-	0/5/5/17	-
4	OLC	A	2003	-	-	2/6/6/24	-
5	OLA	A	2020	-	-	0/1/3/17	-
2	KNW	A	2001	-	-	0/20/38/38	0/4/4/4
5	OLA	A	2015	-	-	1/2/4/17	-
5	OLA	A	2016	-	-	1/4/6/17	-
5	OLA	A	2025	-	-	1/7/7/17	-
4	OLC	A	2004	-	-	10/24/24/24	-
5	OLA	A	2014	-	-	4/8/8/17	-
5	OLA	A	2024	-	-	5/11/11/17	-
5	OLA	A	2009	-	-	7/13/15/17	-
5	OLA	A	2007	-	-	5/11/11/17	-
5	OLA	A	2022	-	-	9/15/17/17	-
5	OLA	A	2006	-	-	4/10/12/17	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	KNW	C8-N1	-2.13	1.38	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2002	CLR	C4-C5-C10	3.63	121.24	116.42
3	A	2002	CLR	C13-C17-C20	-3.14	114.57	119.49
3	A	2002	CLR	C19-C10-C9	-2.89	108.24	111.68
3	A	2002	CLR	C4-C5-C6	-2.80	116.58	120.61
3	A	2002	CLR	C18-C13-C17	-2.74	106.60	111.71
3	A	2002	CLR	C2-C3-C4	-2.74	106.55	110.31
4	A	2004	OLC	O20-C1-C2	2.71	120.41	111.91
2	A	2001	KNW	C9-C8-N1	2.45	122.15	118.87
3	A	2002	CLR	C17-C13-C14	2.30	102.80	100.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2002	CLR	C19-C10-C5	2.15	111.83	108.34
3	A	2002	CLR	C11-C12-C13	-2.04	109.29	112.78

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2009	OLA	C1-C2-C3-C4
5	A	2010	OLA	C1-C2-C3-C4
5	A	2021	OLA	C1-C2-C3-C4
5	A	2022	OLA	C1-C2-C3-C4
4	A	2004	OLC	O19-C1-O20-C21
4	A	2004	OLC	C2-C1-O20-C21
5	A	2007	OLA	C12-C13-C14-C15
3	A	2002	CLR	C22-C23-C24-C25
5	A	2008	OLA	C11-C12-C13-C14
5	A	2019	OLA	C11-C12-C13-C14
4	A	2003	OLC	C14-C15-C16-C17
5	A	2014	OLA	C4-C5-C6-C7
5	A	2010	OLA	C10-C11-C12-C13
5	A	2010	OLA	C2-C3-C4-C5
4	A	2004	OLC	C12-C13-C14-C15
5	A	2019	OLA	C3-C4-C5-C6
5	A	2022	OLA	C13-C14-C15-C16
5	A	2024	OLA	C11-C12-C13-C14
5	A	2014	OLA	C6-C7-C8-C9
5	A	2022	OLA	C5-C6-C7-C8
5	A	2007	OLA	C13-C14-C15-C16
5	A	2023	OLA	C11-C12-C13-C14
5	A	2009	OLA	C6-C7-C8-C9
5	A	2019	OLA	C6-C7-C8-C9
4	A	2004	OLC	C5-C6-C7-C8
5	A	2010	OLA	C4-C5-C6-C7
5	A	2005	OLA	C4-C5-C6-C7
5	A	2009	OLA	C3-C4-C5-C6
5	A	2019	OLA	C2-C3-C4-C5
5	A	2010	OLA	C6-C7-C8-C9
5	A	2010	OLA	C14-C15-C16-C17
5	A	2006	OLA	C4-C5-C6-C7
5	A	2015	OLA	C2-C3-C4-C5
5	A	2024	OLA	C4-C5-C6-C7
5	A	2010	OLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	A	2004	OLC	C1-C2-C3-C4
5	A	2022	OLA	C12-C13-C14-C15
5	A	2024	OLA	C14-C15-C16-C17
5	A	2012	OLA	C4-C5-C6-C7
5	A	2010	OLA	C3-C4-C5-C6
5	A	2021	OLA	C3-C4-C5-C6
4	A	2003	OLC	C11-C12-C13-C14
5	A	2012	OLA	C3-C4-C5-C6
5	A	2007	OLA	C14-C15-C16-C17
5	A	2025	OLA	C11-C12-C13-C14
4	A	2004	OLC	C13-C14-C15-C16
3	A	2002	CLR	C20-C22-C23-C24
6	A	2026	PGE	C1-C2-O2-C3
5	A	2019	OLA	C12-C13-C14-C15
5	A	2021	OLA	C2-C3-C4-C5
3	A	2002	CLR	C13-C17-C20-C22
5	A	2013	OLA	C4-C5-C6-C7
5	A	2023	OLA	C1-C2-C3-C4
3	A	2002	CLR	C13-C17-C20-C21
5	A	2022	OLA	C14-C15-C16-C17
5	A	2019	OLA	C5-C6-C7-C8
3	A	2002	CLR	C23-C24-C25-C27
5	A	2007	OLA	C6-C7-C8-C9
5	A	2022	OLA	C4-C5-C6-C7
5	A	2008	OLA	C15-C16-C17-C18
5	A	2009	OLA	C7-C8-C9-C10
5	A	2024	OLA	C12-C13-C14-C15
6	A	2026	PGE	C4-C3-O2-C2
5	A	2010	OLA	C12-C13-C14-C15
5	A	2009	OLA	C11-C12-C13-C14
5	A	2010	OLA	C13-C14-C15-C16
5	A	2010	OLA	C7-C8-C9-C10
4	A	2004	OLC	C9-C10-C11-C12
5	A	2007	OLA	C7-C8-C9-C10
5	A	2009	OLA	C13-C14-C15-C16
5	A	2014	OLA	C10-C11-C12-C13
5	A	2006	OLA	C9-C10-C11-C12
5	A	2009	OLA	C9-C10-C11-C12
5	A	2022	OLA	C7-C8-C9-C10
5	A	2016	OLA	C4-C5-C6-C7
4	A	2004	OLC	C7-C8-C9-C10
5	A	2024	OLA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
4	A	2004	OLC	O20-C1-C2-C3
5	A	2019	OLA	C9-C10-C11-C12
5	A	2006	OLA	C3-C4-C5-C6
5	A	2008	OLA	C9-C10-C11-C12
5	A	2014	OLA	C7-C8-C9-C10
5	A	2022	OLA	C9-C10-C11-C12
3	A	2002	CLR	C17-C20-C22-C23
6	A	2026	PGE	O2-C3-C4-O3
6	A	2026	PGE	C3-C4-O3-C5
4	A	2004	OLC	O19-C1-C2-C3
5	A	2005	OLA	C5-C6-C7-C8
5	A	2022	OLA	C11-C12-C13-C14
5	A	2006	OLA	C10-C11-C12-C13

There are no ring outliers.

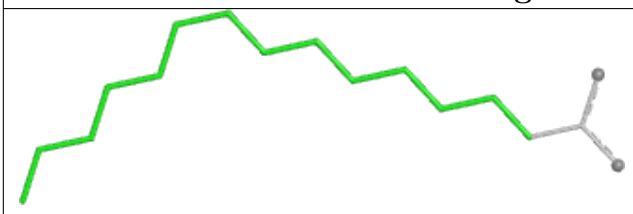
19 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2011	OLA	1	0
5	A	2005	OLA	1	0
5	A	2017	OLA	1	0
5	A	2012	OLA	3	0
3	A	2002	CLR	3	0
5	A	2019	OLA	2	0
5	A	2023	OLA	1	0
5	A	2010	OLA	4	0
5	A	2013	OLA	1	0
5	A	2008	OLA	1	0
5	A	2020	OLA	1	0
2	A	2001	KNW	1	0
5	A	2016	OLA	2	0
4	A	2004	OLC	5	0
5	A	2014	OLA	1	0
5	A	2009	OLA	1	0
5	A	2007	OLA	3	0
5	A	2022	OLA	1	0
5	A	2006	OLA	2	0

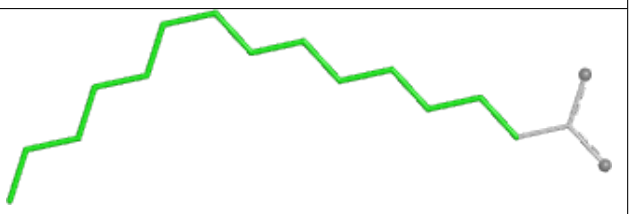
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

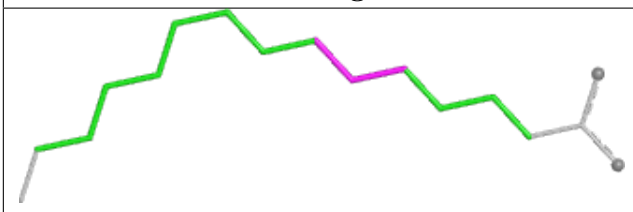
Ligand OLA A 2005



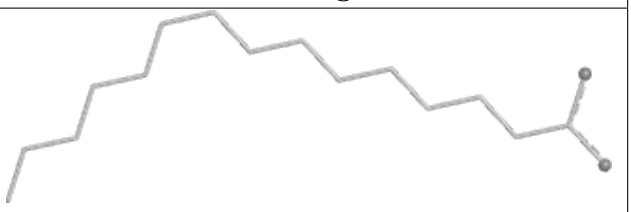
Bond lengths



Bond angles

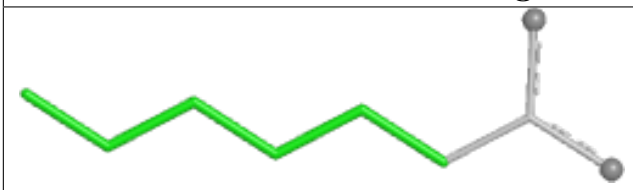


Torsions



Rings

Ligand OLA A 2012



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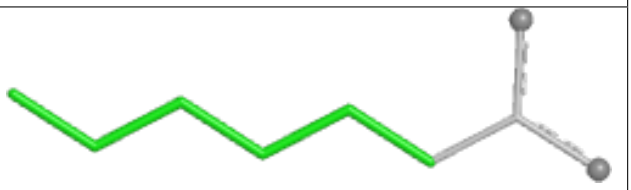

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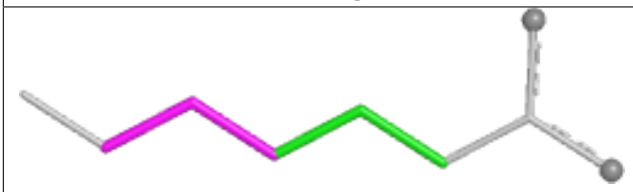

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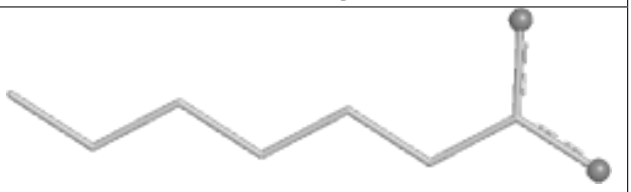
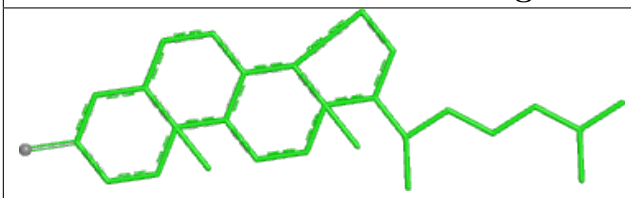
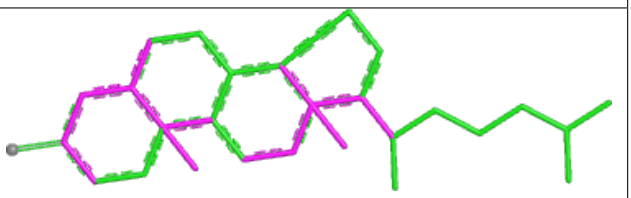


Rings

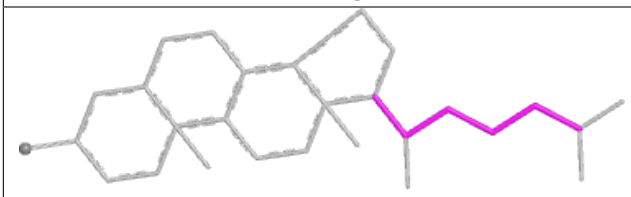
Ligand CLR A 2002



Bond lengths



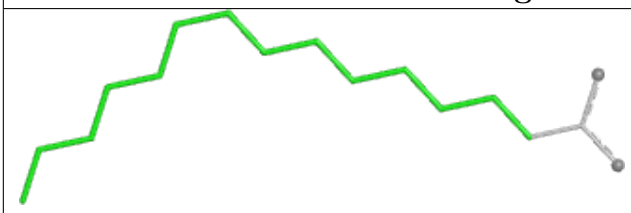
Bond angles



Torsions

Rings

Ligand OLA A 2019



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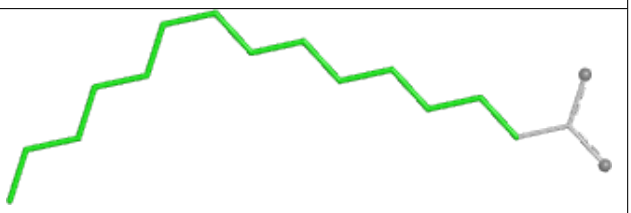
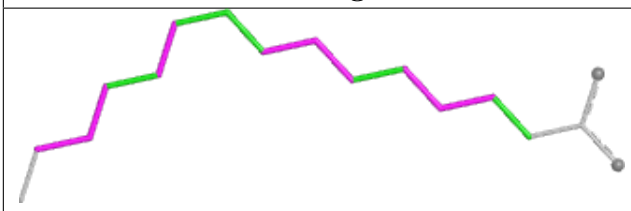


Bond angles



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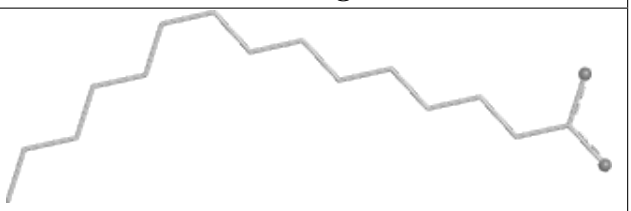
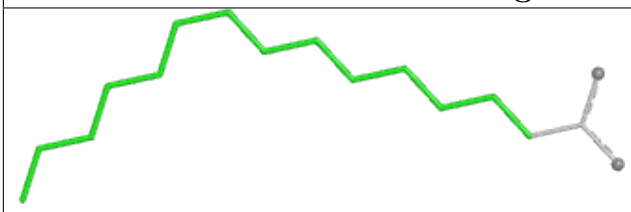


Rings

Ligand OLA A 2023



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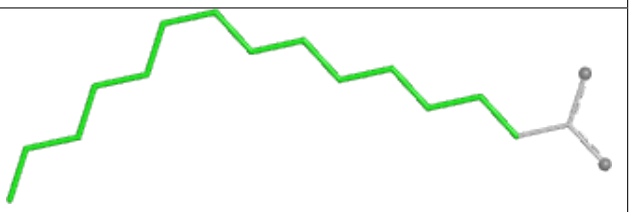

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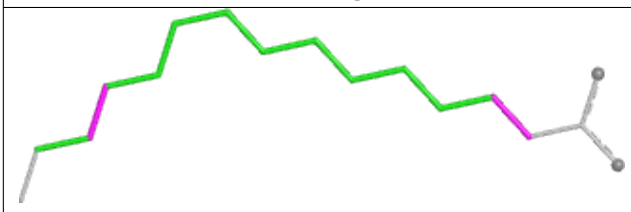
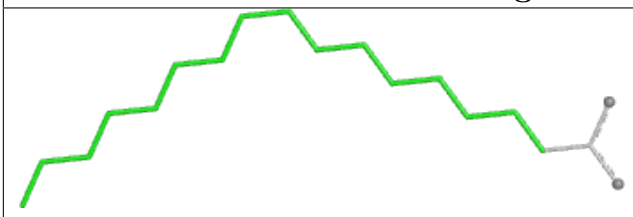


Torsions

Rings

Ligand OLA A 2010



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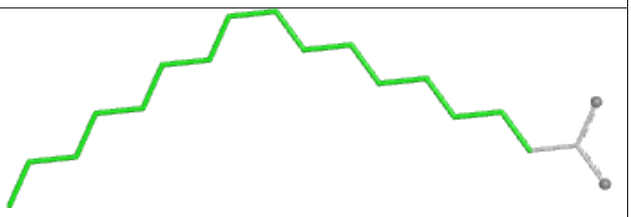

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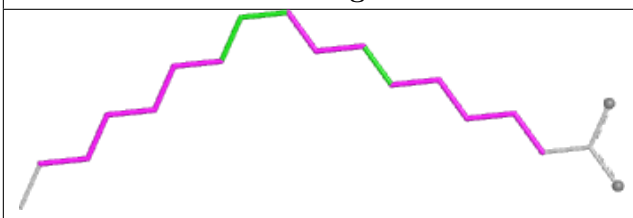
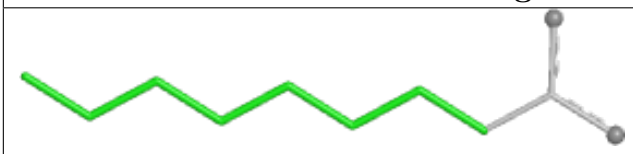


Torsions

Rings

Ligand OLA A 2013



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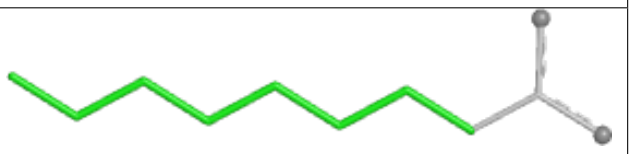
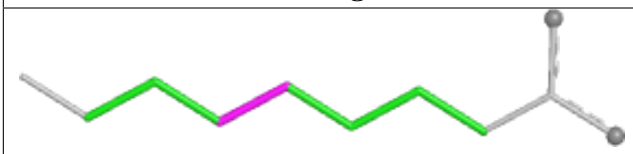
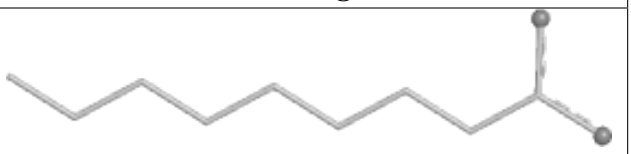


Bond angles

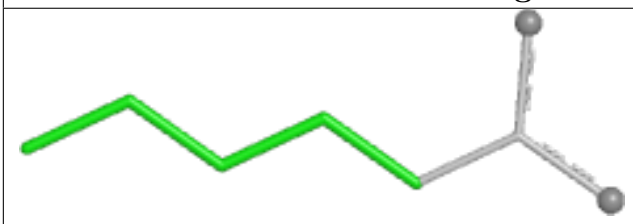


Torsions

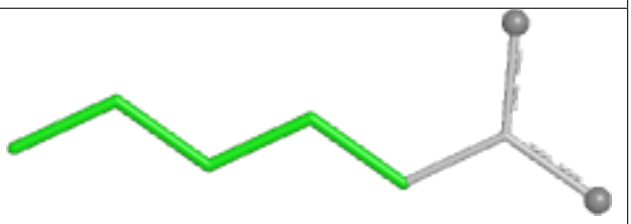


Rings

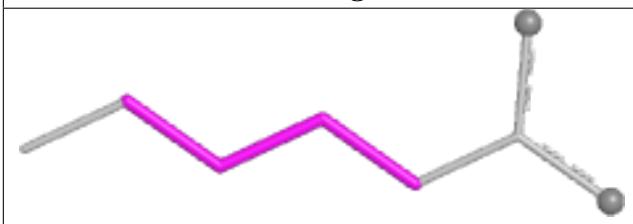
Ligand OLA A 2021



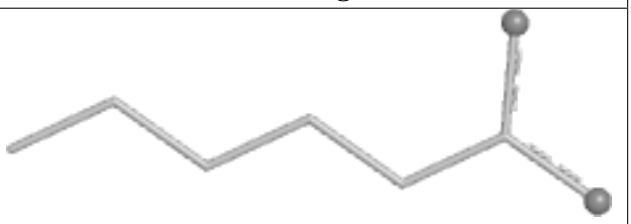
Bond lengths



Bond angles

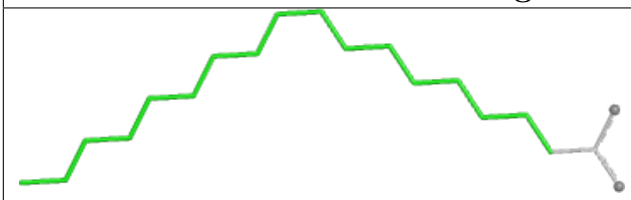


Torsions



Rings

Ligand OLA A 2008



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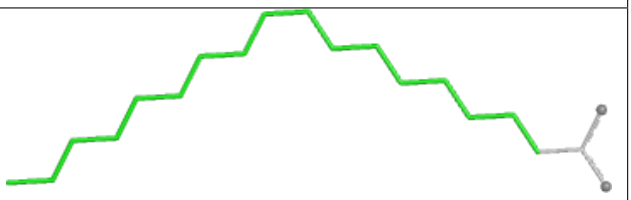
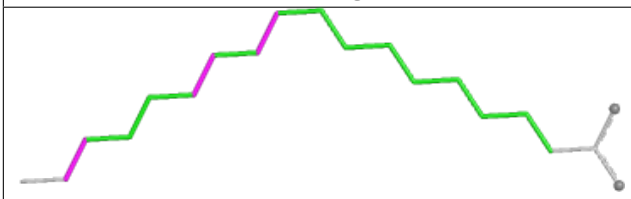


Bond angles



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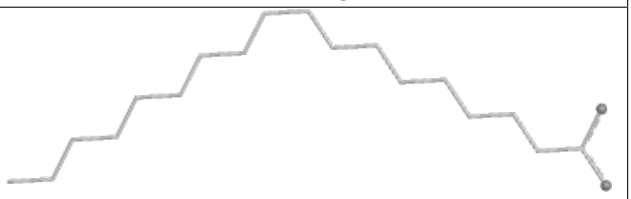
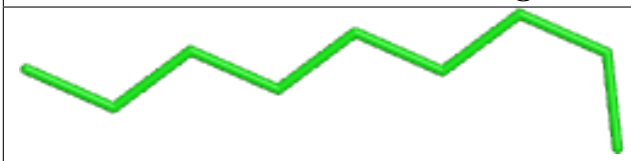


Rings

Ligand OLC A 2003



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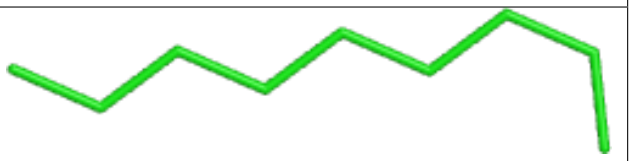
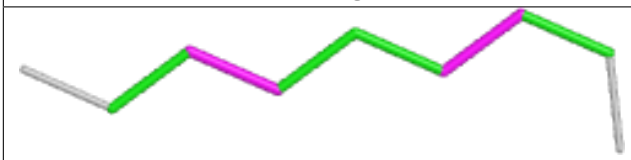
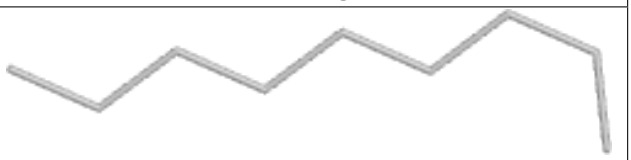


Bond angles

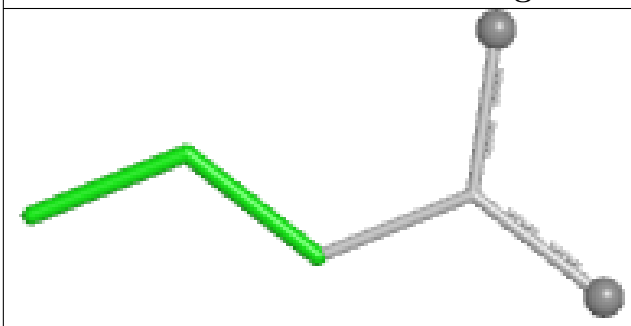


Torsions



Rings

Ligand OLA A 2020



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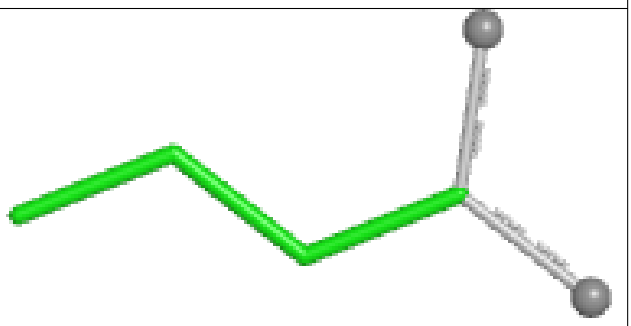
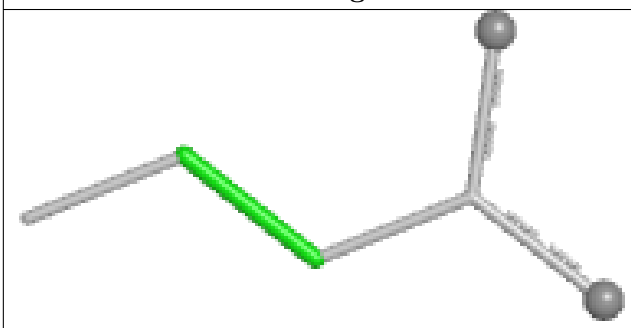
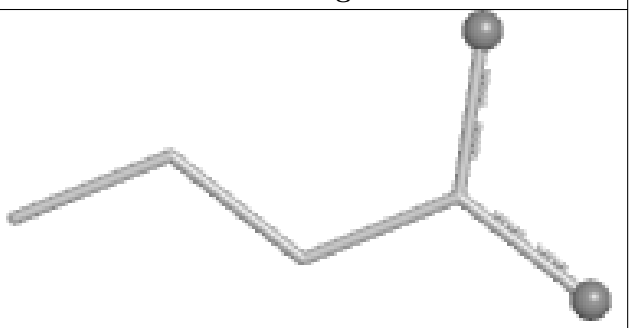


Bond angles

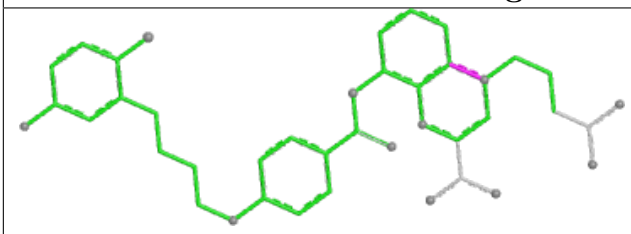


Torsions



Rings

Ligand KNW A 2001



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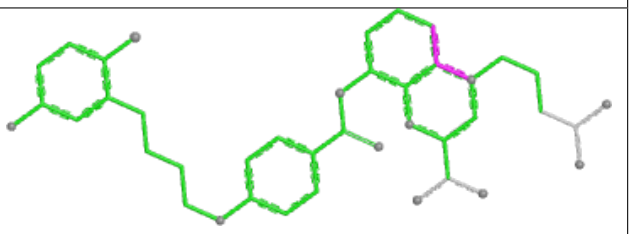
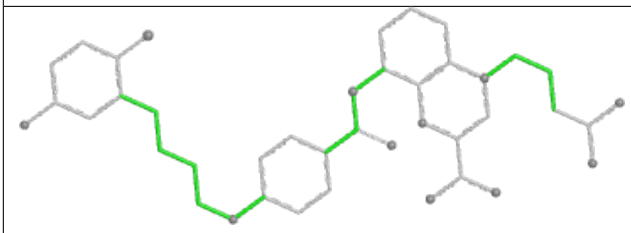


Bond angles



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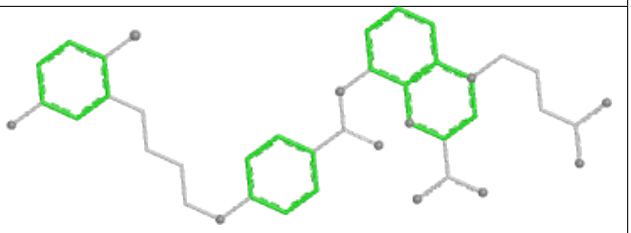
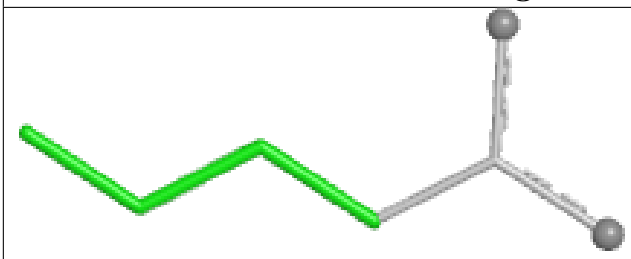


Rings

Ligand OLA A 2015



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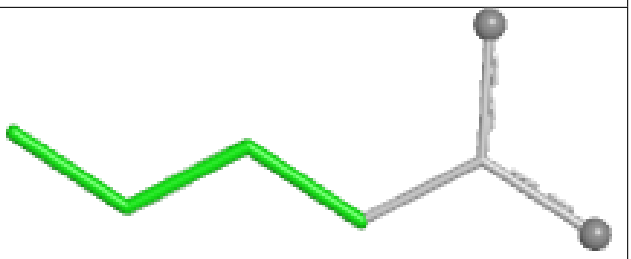
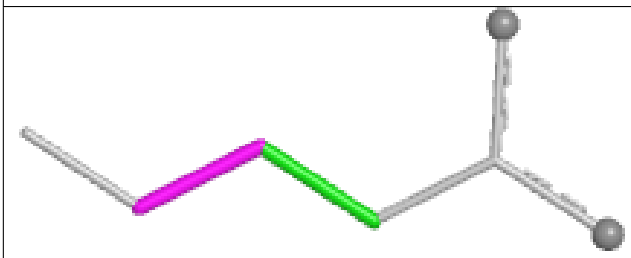
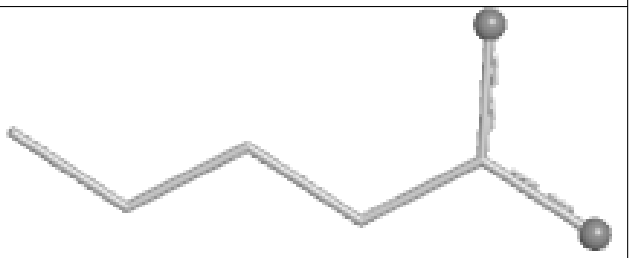


Bond angles

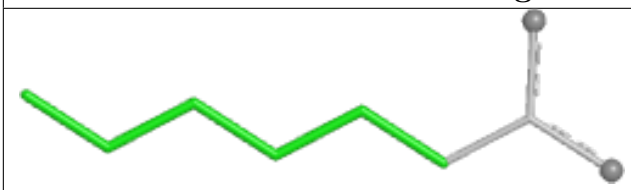


Torsions



Rings

Ligand OLA A 2016



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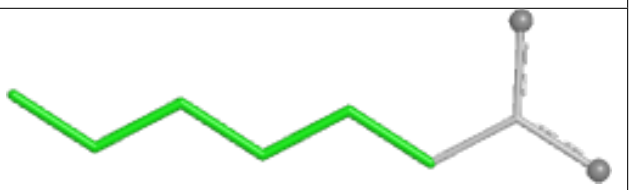
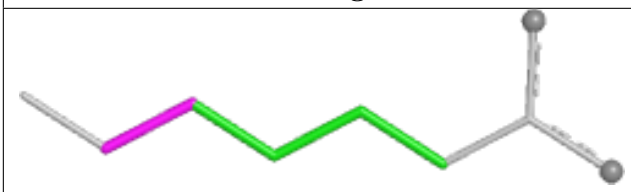


Bond angles



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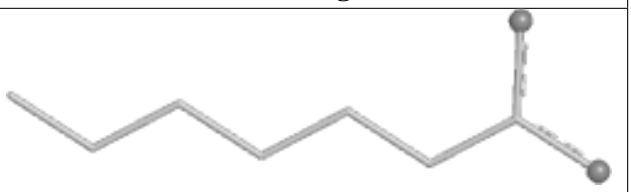
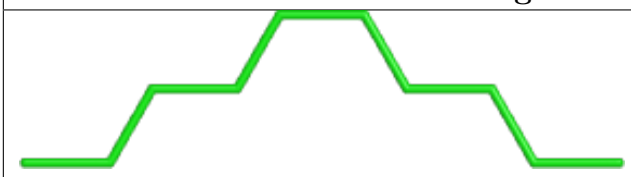


Rings

Ligand OLA A 2025



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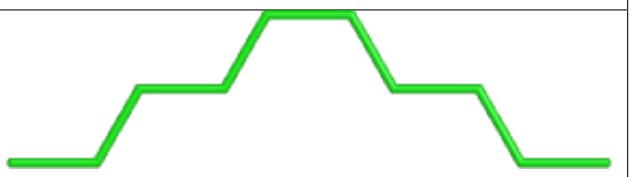
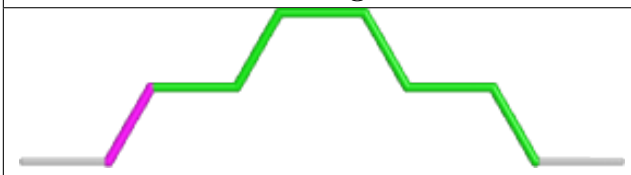
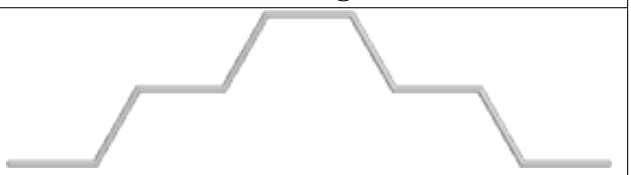


Bond angles

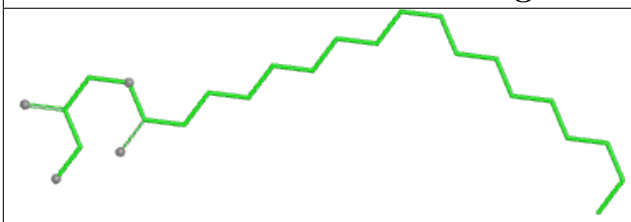


Torsions



Rings

Ligand OLC A 2004



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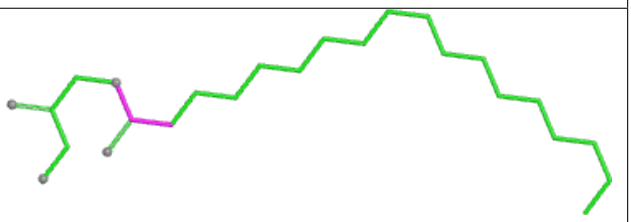
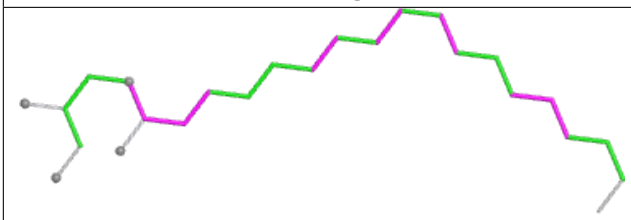
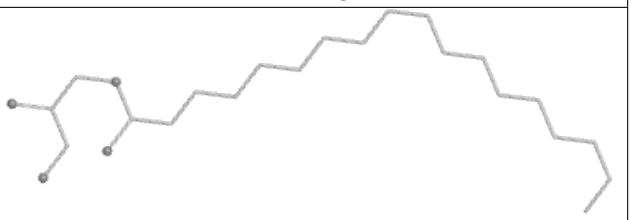


Bond angles

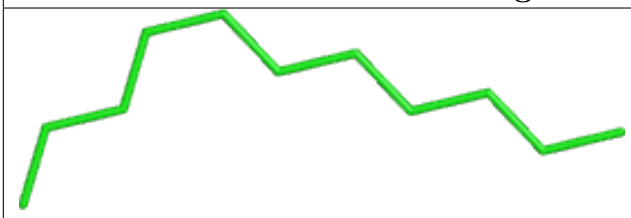


Torsions



Rings

Ligand OLA A 2014



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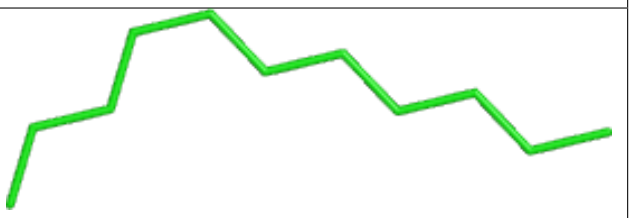
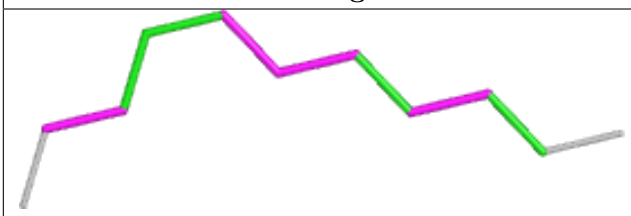


Bond angles



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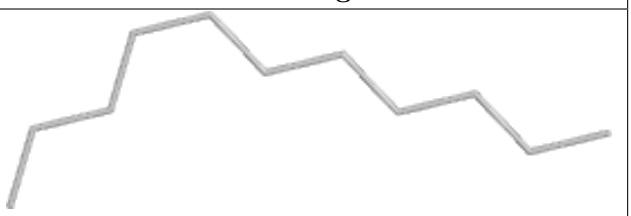
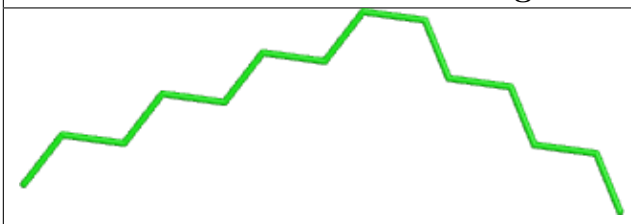


Rings

Ligand OLA A 2024



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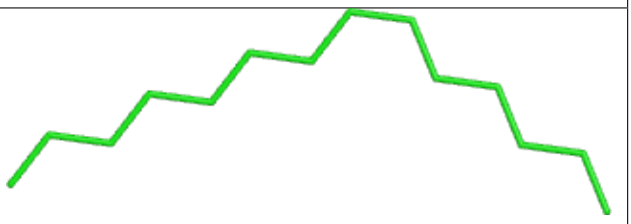
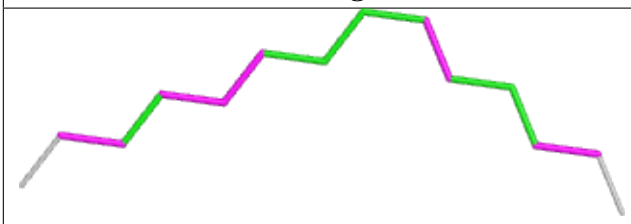


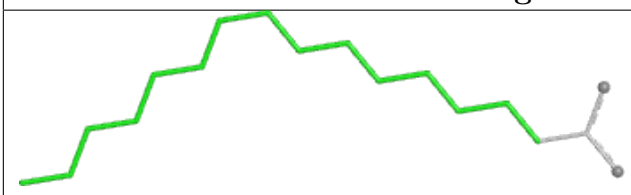
Bond angles



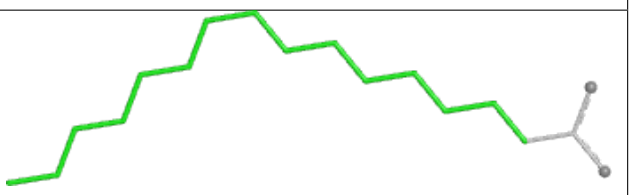
Torsions

Rings

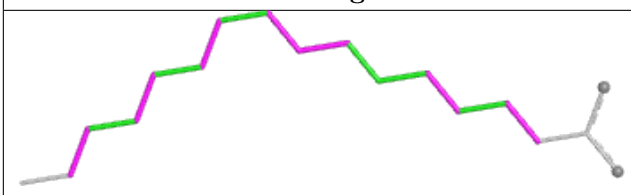
Ligand OLA A 2009



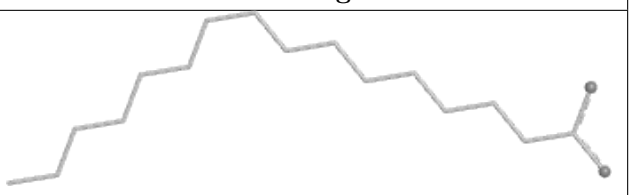
Bond lengths



Bond angles

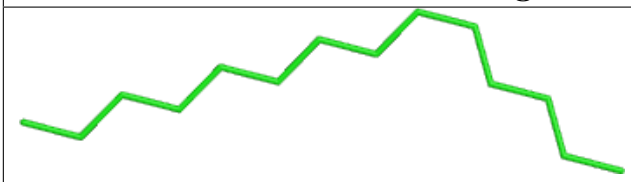


Torsions

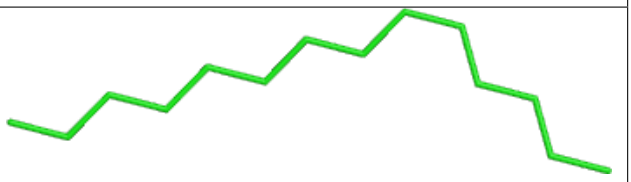


Rings

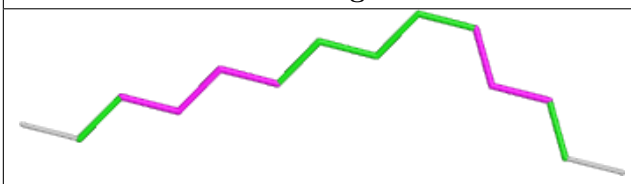
Ligand OLA A 2007



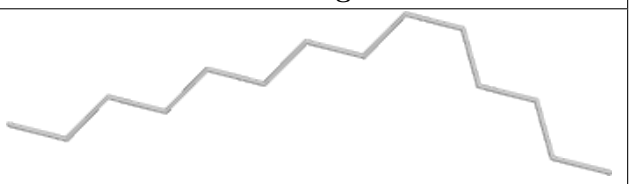
Bond lengths



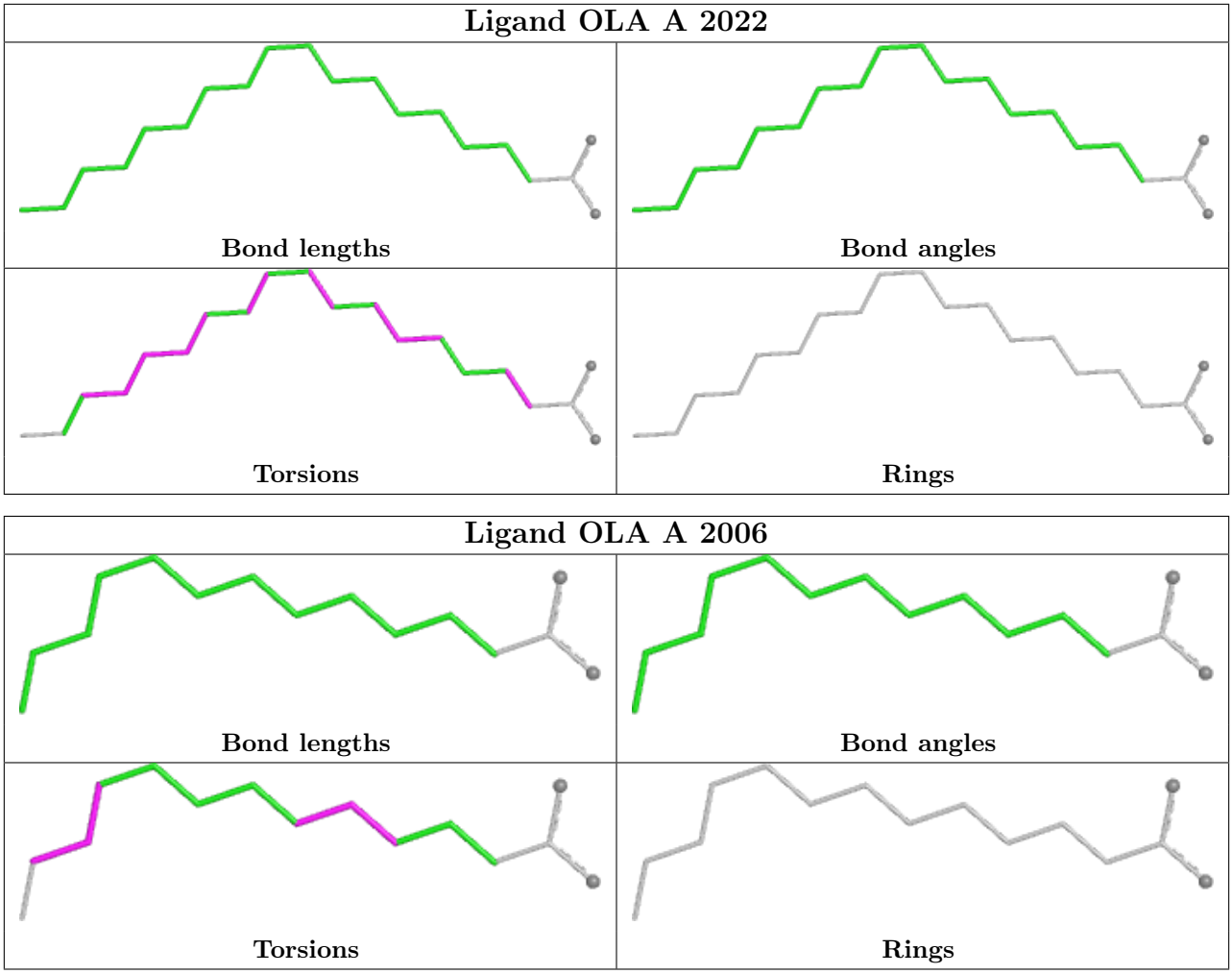
Bond angles



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	360/405 (88%)	1.94	129 (35%) 0 0	36, 56, 131, 154	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1065	PHE	17.5
1	A	143	PRO	16.3
1	A	1036	ALA	11.8
1	A	1037	ALA	11.2
1	A	1067	ILE	9.5
1	A	1099	ASN	8.8
1	A	1021	ASP	8.4
1	A	1105	TYR	8.1
1	A	193	TYR	7.2
1	A	1038	LEU	6.8
1	A	175	ASP	6.6
1	A	1064	GLY	6.5
1	A	149	VAL	6.5
1	A	142	HIS	6.5
1	A	1016	VAL	6.3
1	A	1101	TYR	6.0
1	A	67	TYR	5.8
1	A	1100	ALA	5.6
1	A	319	ALA	5.5
1	A	1104	LYS	5.3
1	A	183	SER	5.3
1	A	1096	THR	5.2
1	A	1098	ARG	5.2
1	A	314	ASP	5.2
1	A	1020	ALA	5.0
1	A	1039	ASP	4.9
1	A	1066	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	276	VAL	4.7
1	A	1023	ALA	4.7
1	A	176	SER	4.5
1	A	1010	LEU	4.4
1	A	150	THR	4.3
1	A	1093	GLN	4.3
1	A	1035	ALA	4.3
1	A	1026	VAL	4.1
1	A	275	LYS	4.1
1	A	1086	GLU	4.0
1	A	1083	LYS	3.9
1	A	1024	ALA	3.9
1	A	1012	ASP	3.9
1	A	1097	THR	3.9
1	A	78	LEU	3.8
1	A	1033	MET	3.7
1	A	1074	ASP	3.6
1	A	1078	LEU	3.6
1	A	278	LEU	3.6
1	A	184	VAL	3.6
1	A	1072	ILE	3.5
1	A	1029	ALA	3.5
1	A	31	CYS	3.5
1	A	317	LYS	3.5
1	A	1034	ARG	3.4
1	A	188	LEU	3.4
1	A	315	ARG	3.4
1	A	120	VAL	3.3
1	A	1022	ASN	3.3
1	A	1017	ILE	3.3
1	A	1028	ASP	3.3
1	A	1061	PHE	3.3
1	A	1070	GLY	3.3
1	A	187	CYS	3.3
1	A	1015	LYS	3.3
1	A	1006	ASN	3.2
1	A	1014	LEU	3.1
1	A	1092	GLU	3.1
1	A	274	TRP	3.1
1	A	1073	ASP	3.1
1	A	68	LYS	3.0
1	A	1003	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	311	ASN	3.0
1	A	63	PHE	2.9
1	A	1079	ALA	2.9
1	A	261	LEU	2.9
1	A	1018	GLU	2.9
1	A	1019	LYS	2.8
1	A	81	ALA	2.8
1	A	1084	VAL	2.8
1	A	1032	LYS	2.8
1	A	1102	ILE	2.8
1	A	1011	ASN	2.8
1	A	174	LEU	2.8
1	A	1080	ASN	2.8
1	A	320	LEU	2.8
1	A	1060	ASP	2.8
1	A	1091	ALA	2.7
1	A	282	ARG	2.7
1	A	140	MET	2.7
1	A	106	PHE	2.7
1	A	141	VAL	2.6
1	A	277	GLY	2.5
1	A	1025	GLN	2.5
1	A	1089	ALA	2.5
1	A	1001	ALA	2.5
1	A	64	LEU	2.5
1	A	82	ILE	2.5
1	A	34	GLU	2.4
1	A	215	PHE	2.4
1	A	136	ARG	2.4
1	A	307	PHE	2.4
1	A	318	SER	2.4
1	A	232	GLU	2.4
1	A	1030	LEU	2.3
1	A	1068	LEU	2.3
1	A	1004	GLU	2.3
1	A	94	ARG	2.3
1	A	1106	LEU	2.3
1	A	60	ILE	2.3
1	A	1063	HIS	2.3
1	A	1095	LYS	2.3
1	A	1088	GLN	2.3
1	A	90	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1103	GLN	2.2
1	A	1087	ALA	2.2
1	A	190	LEU	2.1
1	A	305	TYR	2.1
1	A	1007	TRP	2.1
1	A	132	LEU	2.1
1	A	306	TYR	2.1
1	A	283	LEU	2.1
1	A	1081	GLU	2.1
1	A	96	ASP	2.1
1	A	1077	LYS	2.1
1	A	39	GLU	2.1
1	A	77	MET	2.1
1	A	186	SER	2.1
1	A	1082	GLY	2.1
1	A	95	ALA	2.0
1	A	173	LEU	2.0
1	A	191	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	OLA	A	2019	17/20	0.24	0.44	85,93,103,104	0
5	OLA	A	2021	8/20	0.30	0.33	110,116,117,118	0
4	OLC	A	2004	25/25	0.37	0.42	80,86,111,112	0
5	OLA	A	2012	9/20	0.40	0.38	89,92,93,94	0
5	OLA	A	2022	20/20	0.40	0.42	103,108,111,112	0

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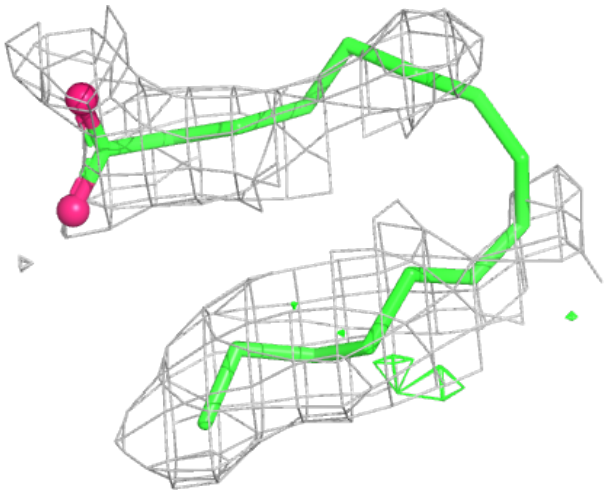
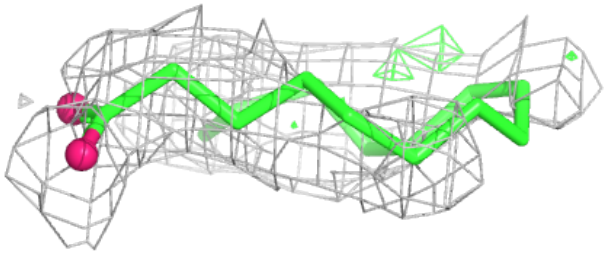
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PGE	A	2026	10/10	0.45	0.37	68,71,72,72	0
5	OLA	A	2010	19/20	0.46	0.37	91,100,103,104	0
5	OLA	A	2016	9/20	0.46	0.44	91,92,99,99	0
5	OLA	A	2009	18/20	0.47	0.42	84,89,97,98	0
5	OLA	A	2017	9/20	0.47	0.36	91,96,100,102	0
5	OLA	A	2007	14/20	0.51	0.39	61,67,71,71	0
5	OLA	A	2024	14/20	0.52	0.29	84,91,97,97	0
5	OLA	A	2006	15/20	0.55	0.39	64,74,92,94	0
5	OLA	A	2020	6/20	0.55	0.40	103,104,104,104	0
5	OLA	A	2008	20/20	0.58	0.34	65,76,117,119	0
5	OLA	A	2025	10/20	0.61	0.22	75,76,76,76	0
5	OLA	A	2015	7/20	0.62	0.43	108,108,110,110	0
5	OLA	A	2005	17/20	0.62	0.33	81,82,84,85	0
5	OLA	A	2013	11/20	0.66	0.29	76,81,96,98	0
5	OLA	A	2018	8/20	0.74	0.28	62,62,66,67	0
5	OLA	A	2023	17/20	0.76	0.25	63,74,96,97	0
3	CLR	A	2002	28/28	0.77	0.24	49,52,61,62	0
5	OLA	A	2014	11/20	0.77	0.21	63,64,66,66	0
4	OLC	A	2003	9/25	0.82	0.40	60,61,65,65	0
2	KNW	A	2001	41/41	0.82	0.24	44,48,50,51	0
5	OLA	A	2011	10/20	0.82	0.29	82,88,92,95	0

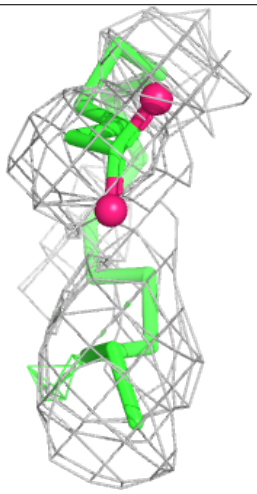
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

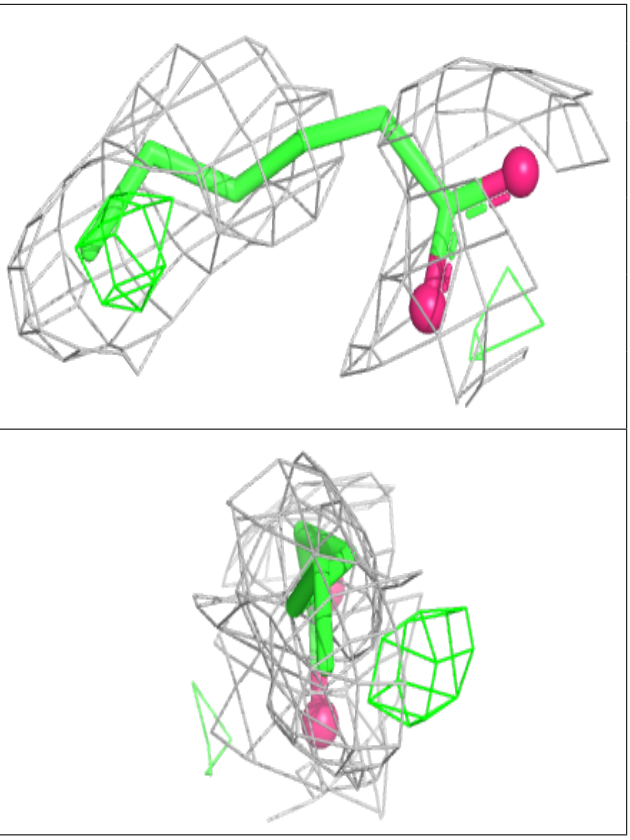


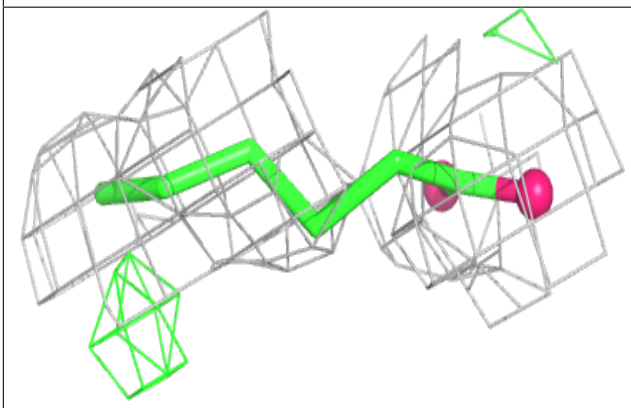




Electron density around OLA A 2021:

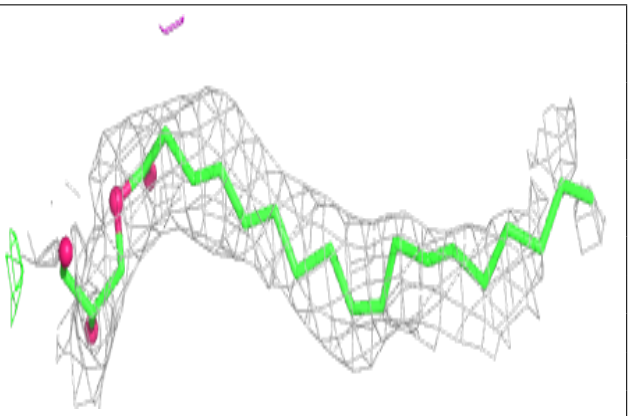
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

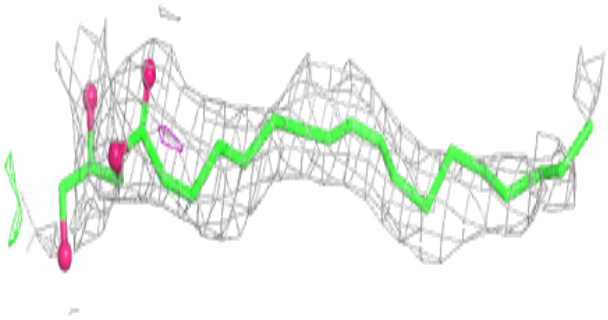


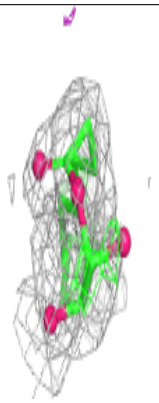


Electron density around OLC A 2004:

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

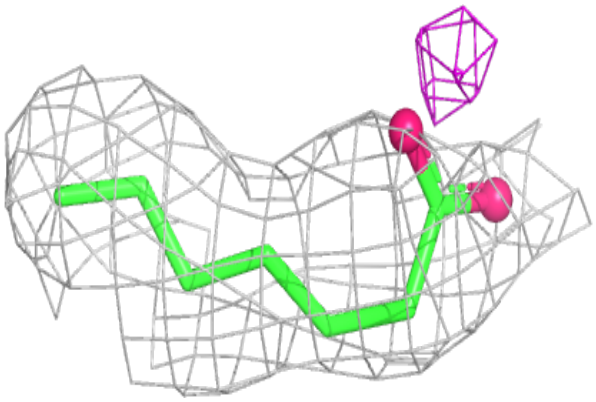


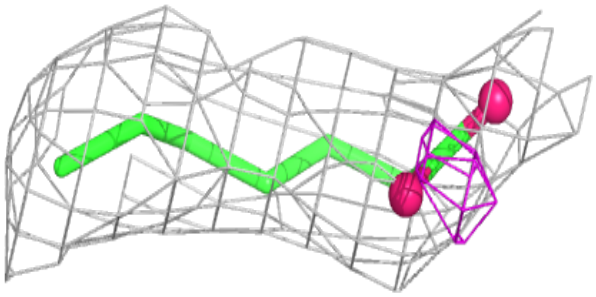


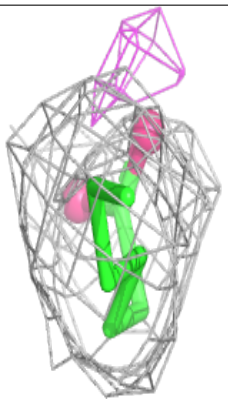


Electron density around OLA A 2012:

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

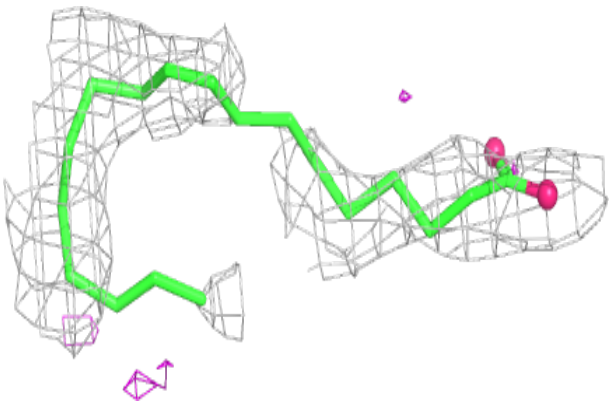


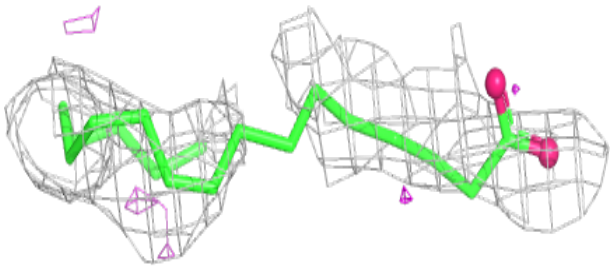


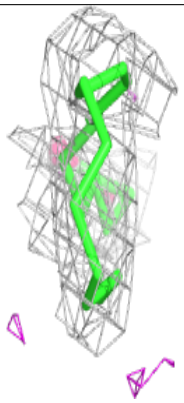


Electron density around OLA A 2022:

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

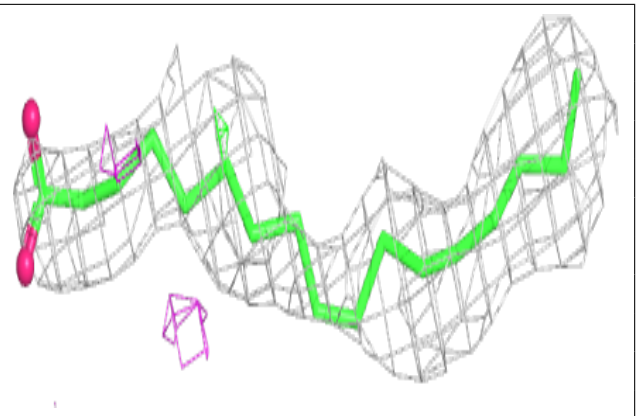


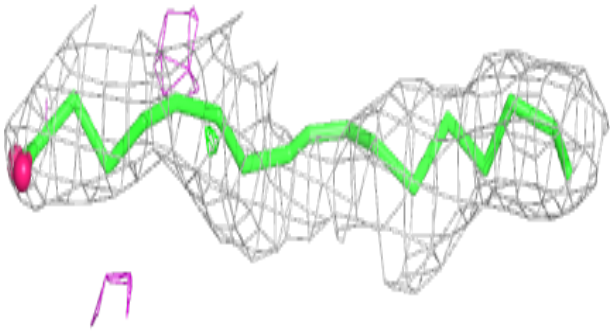


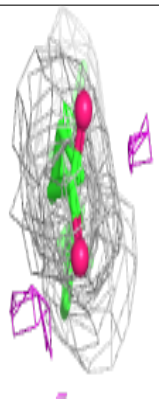


Electron density around OLA A 2010:

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

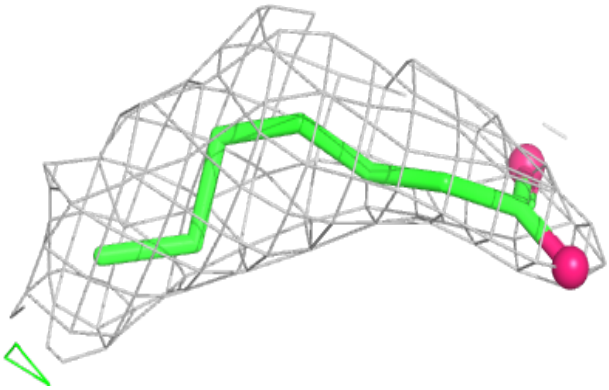


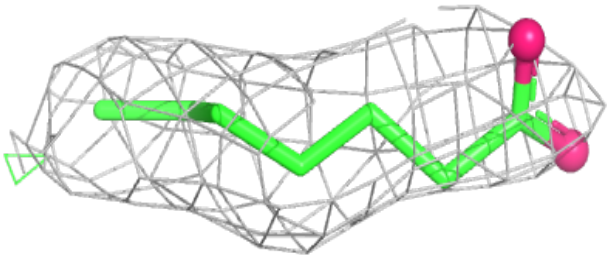


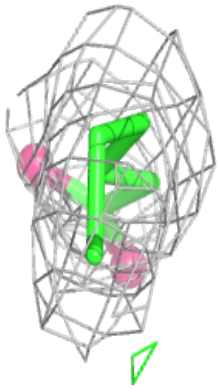


Electron density around OLA A 2016:

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

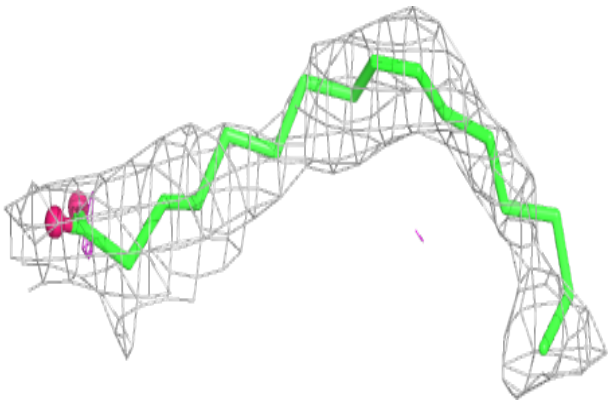


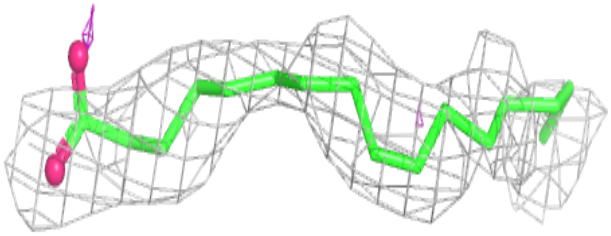


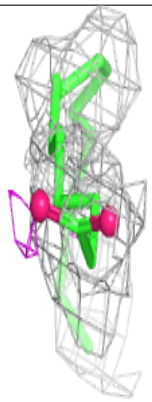


Electron density around OLA A 2009:

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

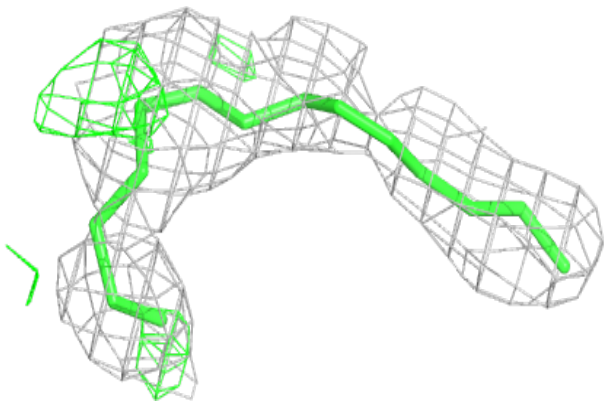


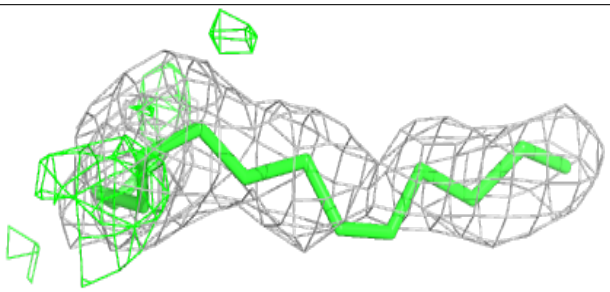


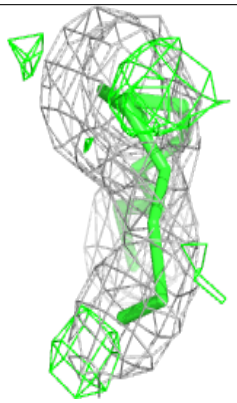


Electron density around OLA A 2007:

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

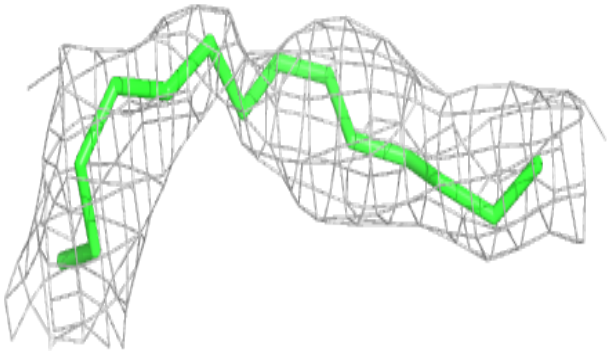


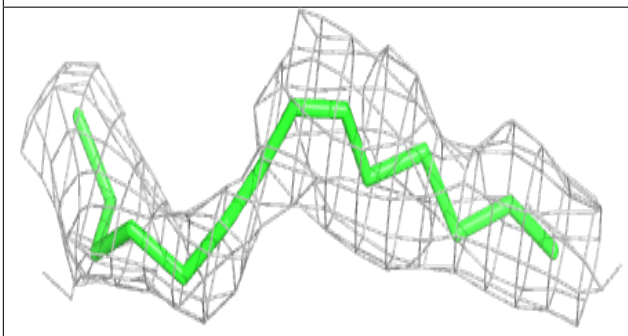


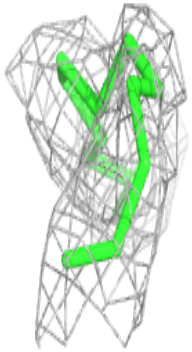


Electron density around OLA A 2024:

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

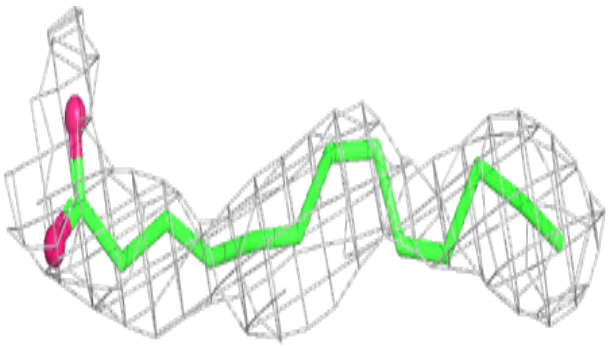


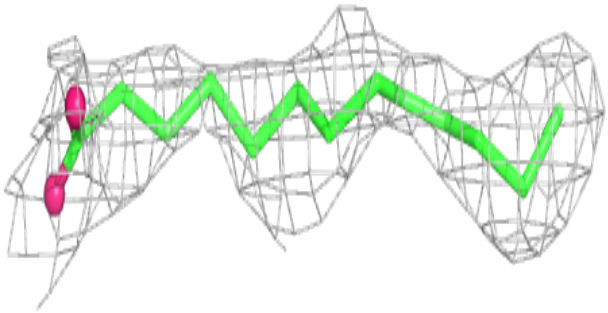


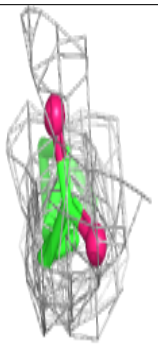


Electron density around OLA A 2006:

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

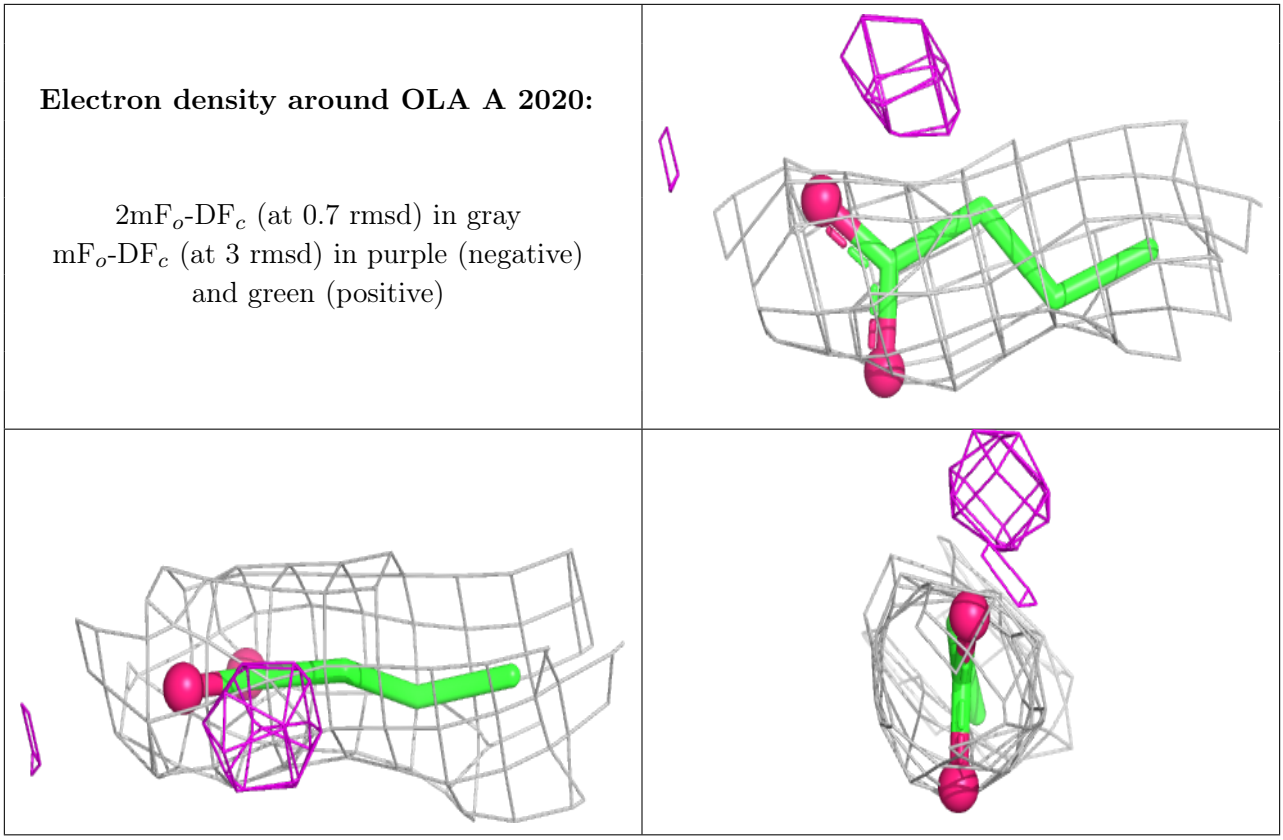






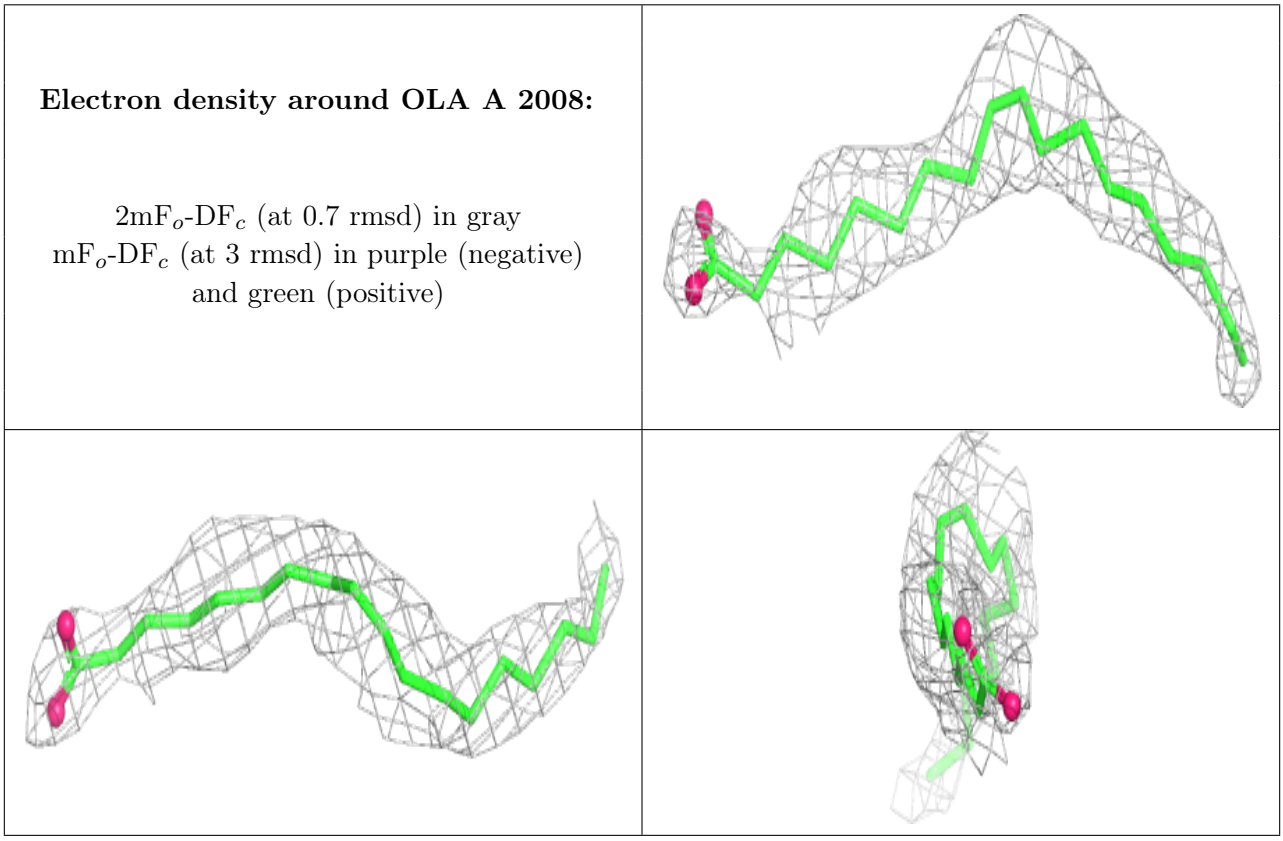
Electron density around OLA A 2020:

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



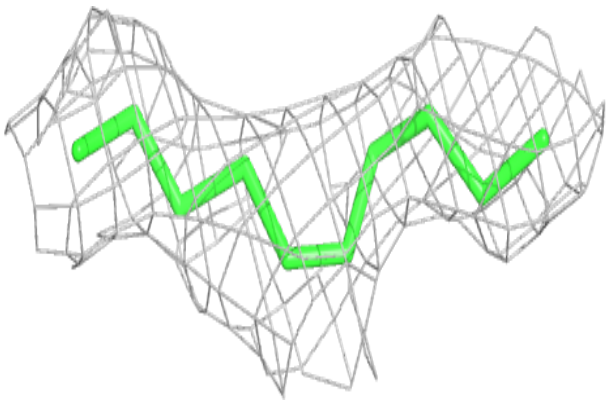
Electron density around OLA A 2008:

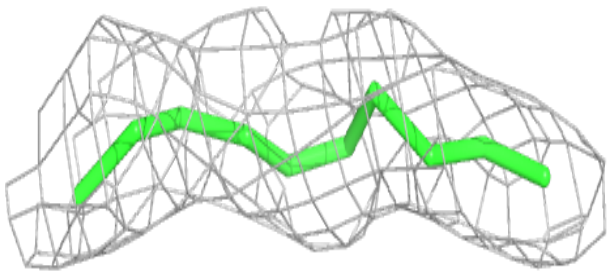
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

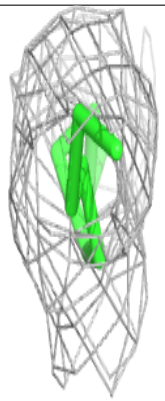


Electron density around OLA A 2025:

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

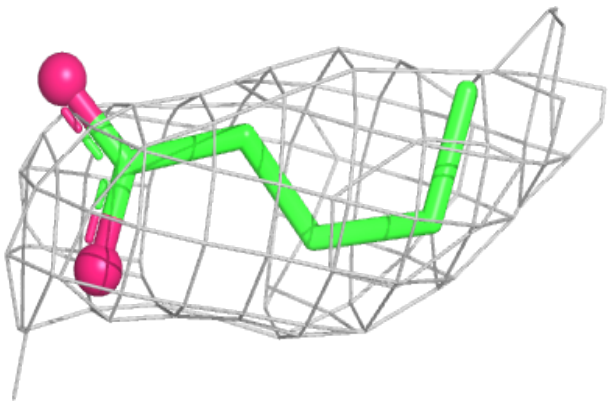


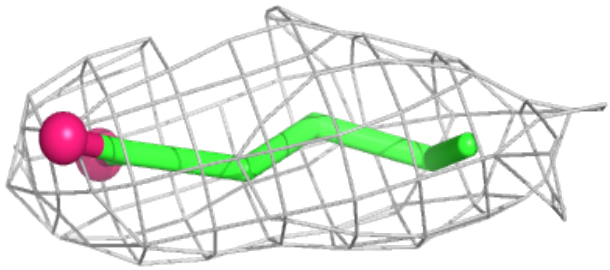


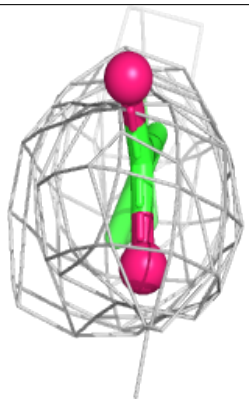


Electron density around OLA A 2015:

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

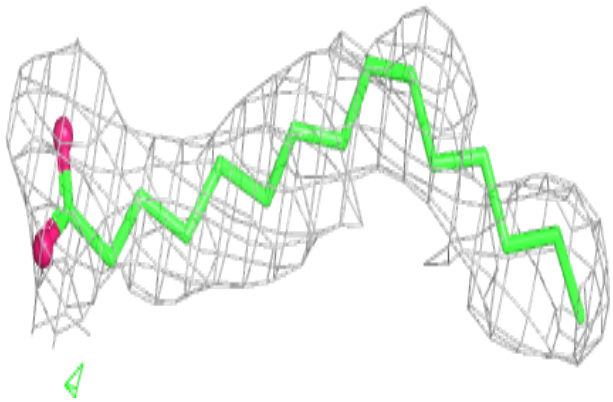


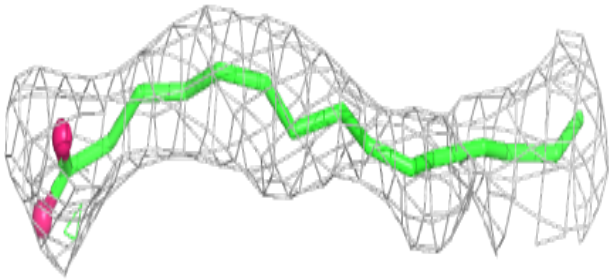


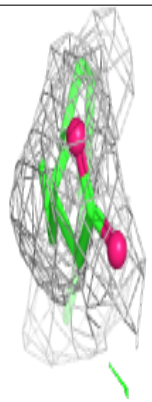


Electron density around OLA A 2005:

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

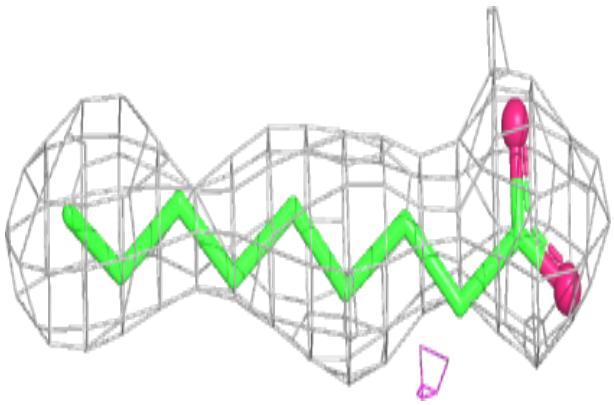


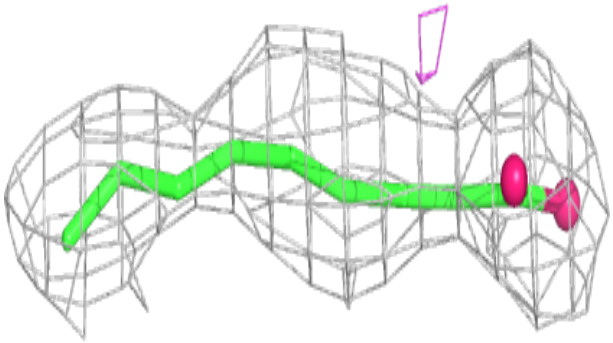


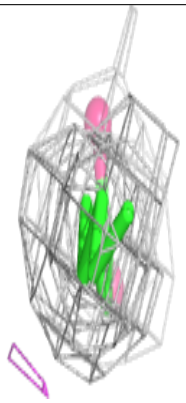


Electron density around OLA A 2013:

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

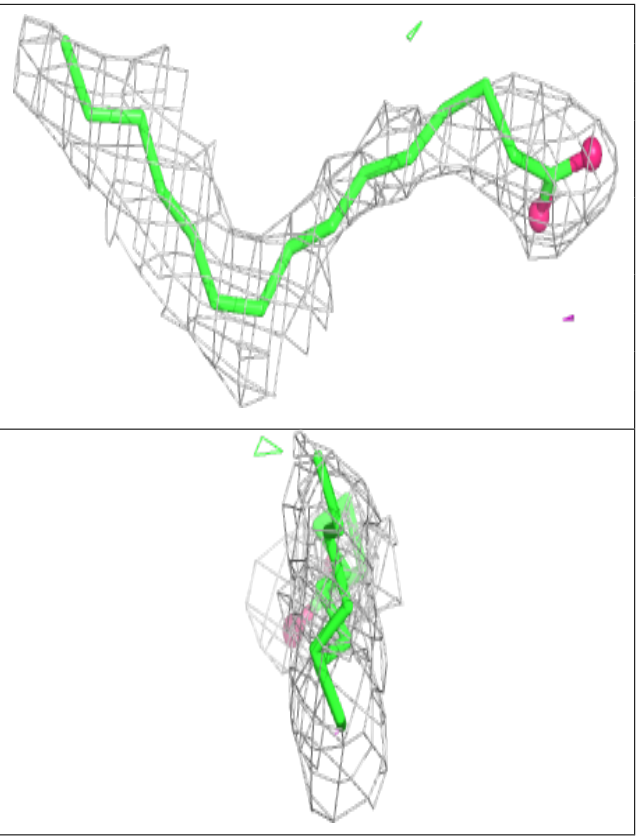


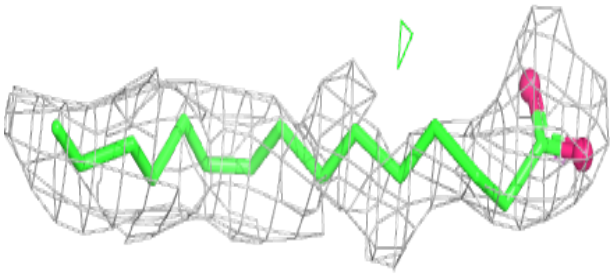




Electron density around OLA A 2023:

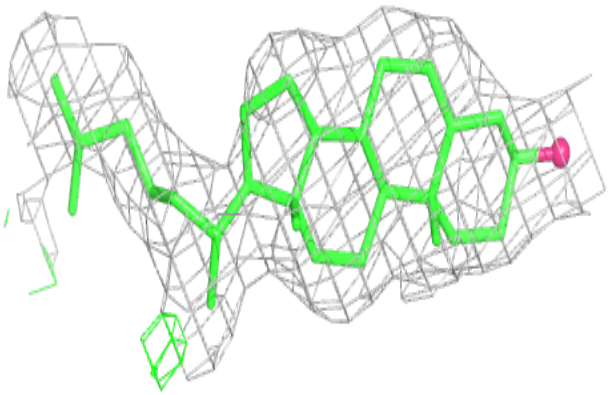
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

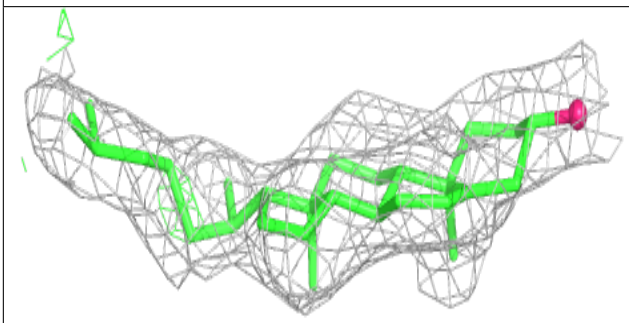


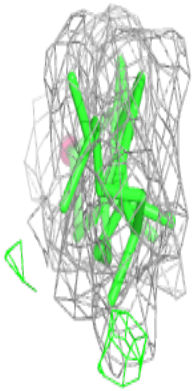


Electron density around CLR A 2002:

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

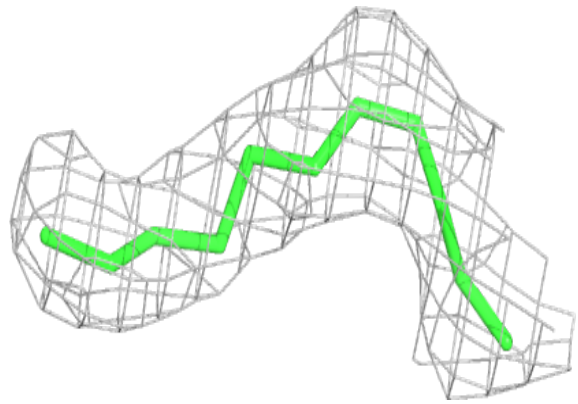


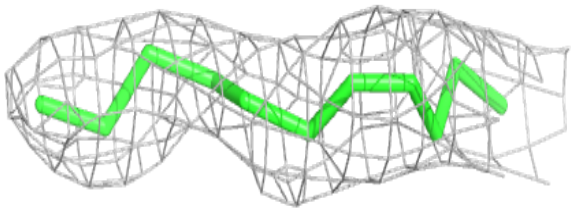


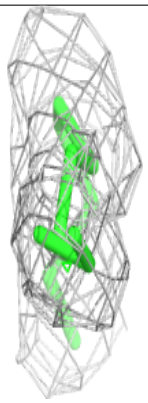


Electron density around OLA A 2014:

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

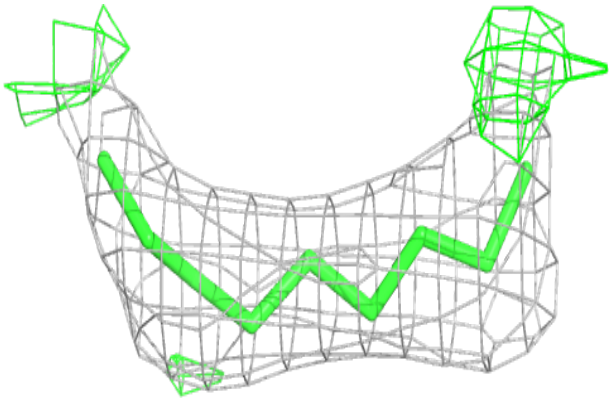


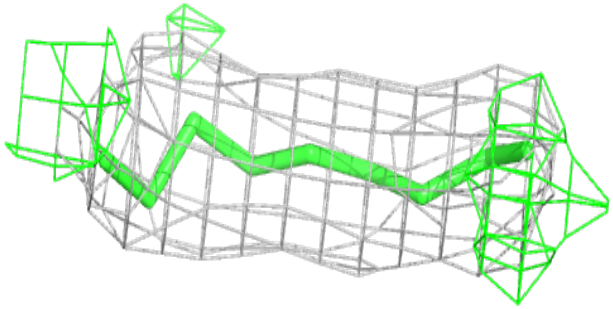


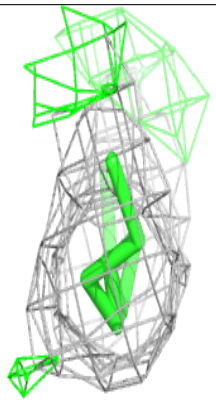


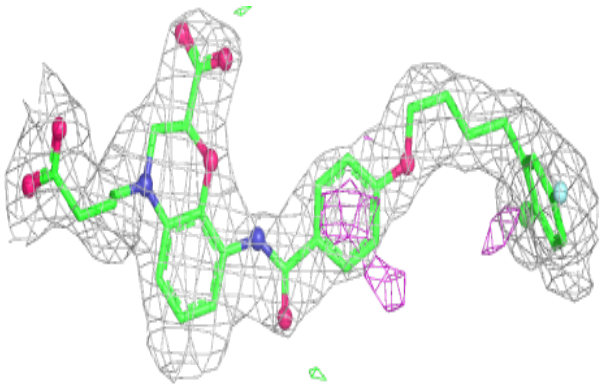
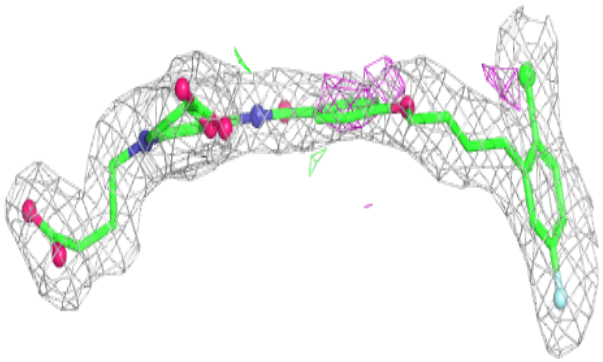
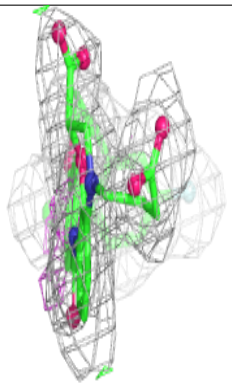
Electron density around OLC A 2003:

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







Electron density around KNW 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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.