wwPDB X-ray Structure Validation Summary Report (i)

Mar 24, 2022 – 03:45 pm GMT

PDB ID	:	6RZ5
Title	:	XFEL crystal structure of the human cysteinyl leukotriene receptor 1 in complex with zafirlukast
Authors	:	Luginina, A.; Gusach, A.; Marin, E.; Mishin, A.; Brouillette, R.; Popov, P.; Shiryaeva, A.; Besserer-Offroy, E.; Longpre, J.M.; Lyapina, E.; Ishchenko, A.; Patel, N.; Polovinkin, V.; Safronova, N.; Bogorodskiy, A.; Edelweiss, E.; Liu, W.; Batyuk, A.; Gordeliy, V.; Han, G.W.; Sarret, P.; Katritch, V.; Borshchevskiy, V.; Cherezov, V.
Deposited on	:	2019-06-12
Resolution	:	2.53 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:

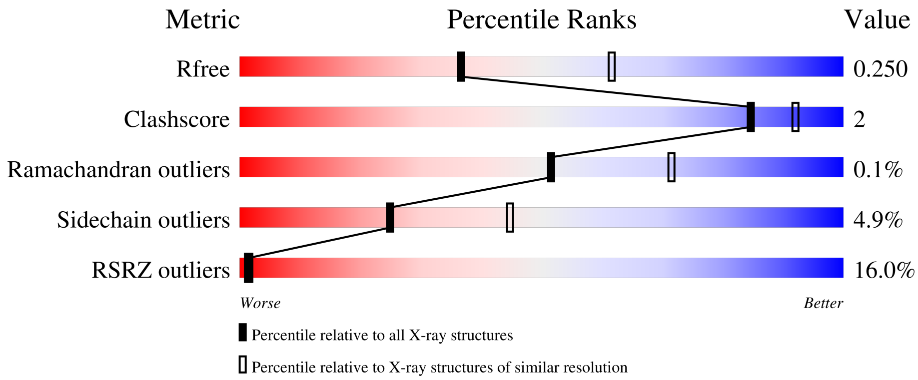
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	423	12% 81% 5% • 13%
1	B	423	17% 84% 6% • 9%

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	OLA	B	2013	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6138 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.

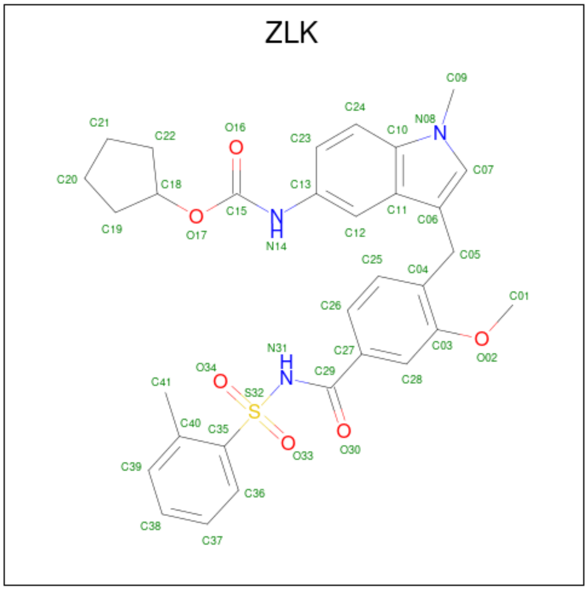
- Molecule 1 is a protein called Cysteinyl leukotriene receptor 1,Soluble cytochrome b562,Cysteinyl leukotriene receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total 2719	C 1781	N 437	O 477	S 24	0	1	0
1	B	385	Total 2837	C 1851	N 462	O 499	S 25	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

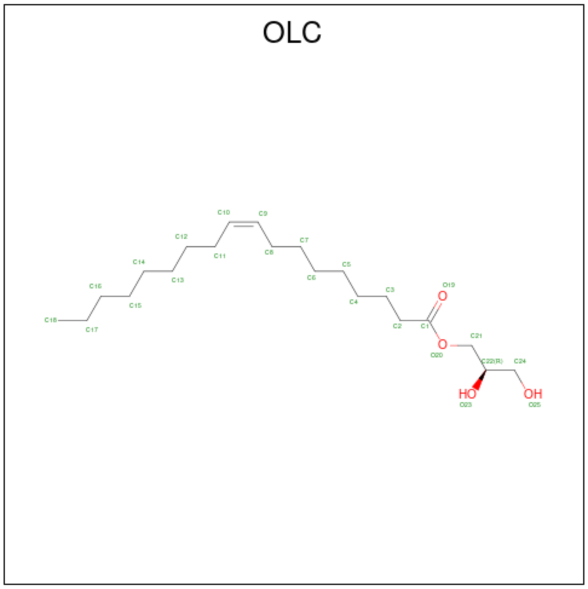
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9Y271
A	-1	GLY	-	expression tag	UNP Q9Y271
A	0	THR	-	expression tag	UNP Q9Y271
A	1000	SER	-	linker	UNP Q9Y271
A	1007	TRP	MET	conflict	UNP P0ABE7
A	1102	ILE	HIS	conflict	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	?	SER	-	linker	UNP P0ABE7
A	?	GLY	-	linker	UNP P0ABE7
B	-2	GLY	-	expression tag	UNP Q9Y271
B	-1	GLY	-	expression tag	UNP Q9Y271
B	0	THR	-	expression tag	UNP Q9Y271
B	1000	SER	-	linker	UNP Q9Y271
B	1007	TRP	MET	conflict	UNP P0ABE7
B	1102	ILE	HIS	conflict	UNP P0ABE7
B	1106	LEU	-	linker	UNP P0ABE7
B	?	SER	-	linker	UNP P0ABE7
B	?	GLY	-	linker	UNP P0ABE7

- Molecule 2 is zafirlukast (three-letter code: ZLK) (formula: $C_{31}H_{33}N_3O_6S$) (labeled as "Ligand of Interest" by depositor).



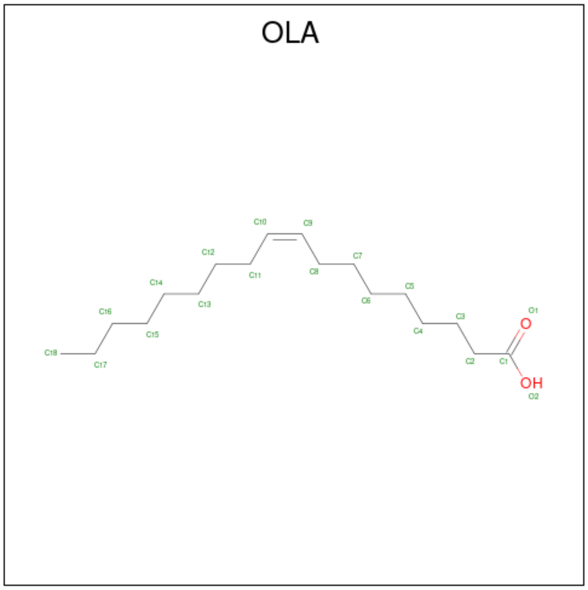
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 41 31 3 6 1	0	0
2	B	1	Total C N O S 41 31 3 6 1	0	0
2	B	1	Total C N O S 41 31 3 6 1	0	0

- Molecule 3 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
3	A	1	Total C 9 9	0	0
3	A	1	Total C 17 17	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C O 16 12 4	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 7 7	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C O 23 19 4	0	0
3	B	1	Total C O 7 5 2	0	0

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



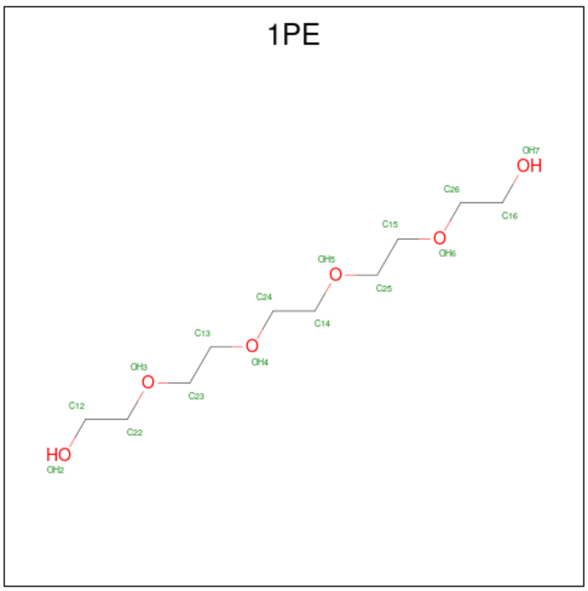
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 9 2	0	0
4	A	1	Total C O 13 11 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 19 17 2	0	0
4	A	1	Total C O 7 5 2	0	0
4	A	1	Total C O 7 5 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 13 11 2	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 14 12 2	0	0
4	B	1	Total C O 12 10 2	0	0
4	B	1	Total C O 10 8 2	0	0
4	B	1	Total C O 16 14 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 9 7 2	0	0
4	B	1	Total C O 11 9 2	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 18 16 2	0	0
4	B	1	Total C O 20 18 2	0	0

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0
6	B	1	Total Na 1 1	0	0

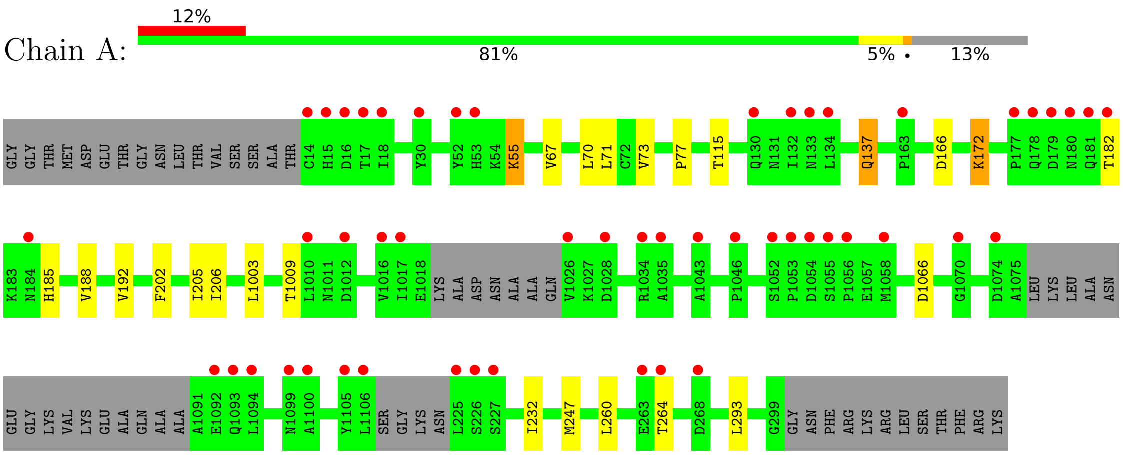
- Molecule 7 is water.

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

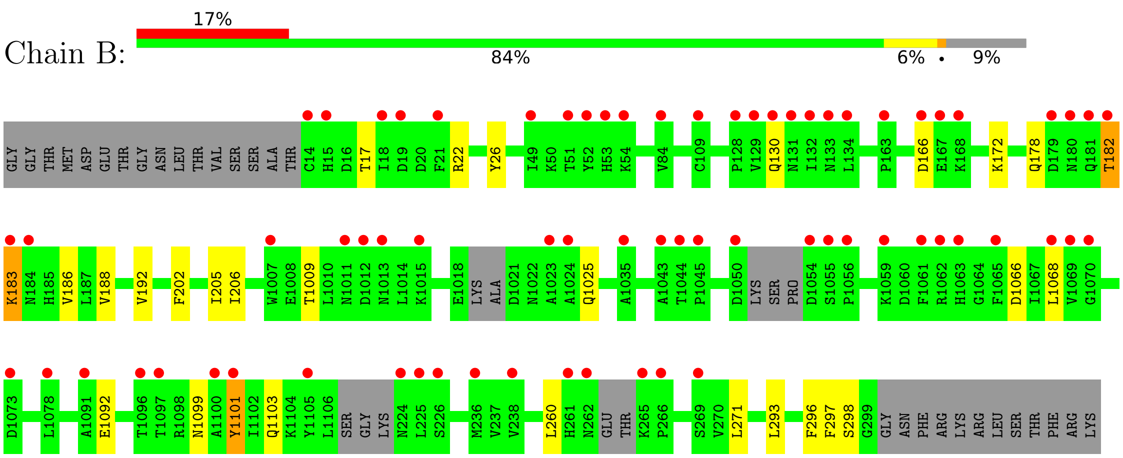
3 Residue-property plots

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 1,Soluble cytochrome b562,Cysteinyl leukotriene receptor 1



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



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.59Å 68.58Å 87.39Å 76.31° 76.68° 81.21°	Depositor
Resolution (Å)	19.84 – 2.53 19.84 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.84-2.53) 99.7 (19.84-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.53Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.189 , 0.223 0.215 , 0.250	Depositor DCC
R_{free} test set	1508 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.48, $< L^2 >$ = 0.31	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6138	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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: 1PE, OLC, NA, ZLK, OLA

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	0.51	0/2784	0.63	0/3807
1	B	0.52	0/2901	0.63	0/3960
All	All	0.51	0/5685	0.63	0/7767

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	2719	0	2514	13	0
1	B	2837	0	2602	10	0
2	A	41	0	0	0	0
2	B	82	0	0	0	0
3	A	89	0	130	0	0
3	B	94	0	129	2	0
4	A	138	0	184	6	0
4	B	116	0	165	3	0
5	A	10	0	13	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	5	0	0	0	0
7	B	5	0	0	0	0
All	All	6138	0	5737	27	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 2.

The worst 5 of 27 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:185[A]:HIS:HB2	4:A:2014:OLA:H32	1.68	0.76
1:A:55:LYS:O	1:A:137:GLN:HG2	1.92	0.70
1:B:182:THR:HG21	1:B:260:LEU:HD13	1.80	0.63
1:B:1099:ASN:HA	1:B:1103:GLN:HB2	1.83	0.60
1:B:296:PHE:HB3	4:B:2013:OLA:H41	1.84	0.59

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	362/423 (86%)	350 (97%)	12 (3%)	0	100	100
1	B	377/423 (89%)	368 (98%)	8 (2%)	1 (0%)	41	59
All	All	739/846 (87%)	718 (97%)	20 (3%)	1 (0%)	51	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/375 (71%)	254 (96%)	11 (4%)	30	51
1	B	269/375 (72%)	254 (94%)	15 (6%)	21	38
All	All	534/750 (71%)	508 (95%)	26 (5%)	25	45

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	182	THR
1	B	205	ILE
1	B	271	LEU
1	B	186	VAL
1	B	1009	THR

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

Mol	Chain	Res	Type
1	A	137	GLN
1	B	130	GLN
1	B	1041	GLN
1	B	1099	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 2 are monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OLC	B	2005	-	9,9,24	0.44	0	8,8,25	0.51	0
4	OLA	A	2013	-	15,18,19	0.27	0	14,18,19	0.51	0
2	ZLK	A	2001	-	41,45,45	2.32	23 (56%)	58,65,65	2.46	17 (29%)
4	OLA	A	2018	-	5,5,19	0.45	0	2,4,19	0.85	0
3	OLC	A	2003	-	16,16,24	0.43	0	15,15,25	0.59	0
3	OLC	B	2004	-	9,9,24	0.41	0	8,8,25	0.62	0
3	OLC	B	2002	-	7,7,24	0.37	0	6,6,25	0.62	0
3	OLC	B	2006	-	9,9,24	0.46	0	8,8,25	0.43	0
4	OLA	A	2017	-	9,12,19	0.37	0	8,12,19	0.58	0
4	OLA	B	2016	-	16,19,19	0.28	0	15,19,19	0.60	0
3	OLC	A	2005	-	7,7,24	0.45	0	6,6,25	0.39	0
4	OLA	B	2012	-	6,9,19	0.28	0	5,9,19	0.51	0
4	OLA	A	2019	-	16,19,19	0.31	0	15,19,19	0.42	0
4	OLA	A	2020	-	10,13,19	0.39	0	8,13,19	0.49	0
4	OLA	B	2018	-	16,19,19	0.31	0	15,19,19	0.44	0
4	OLA	B	2014	-	5,8,19	0.28	0	4,8,19	0.63	0
3	OLC	A	2007	-	15,15,24	0.74	0	16,16,25	1.00	1 (6%)
3	OLC	B	2008	-	6,6,24	0.34	0	5,5,25	0.72	0
4	OLA	A	2011	-	9,12,19	0.38	0	8,12,19	0.52	0
3	OLC	A	2006	-	11,11,24	0.46	0	9,10,25	0.69	0
4	OLA	A	2014	-	3,6,19	0.24	0	2,6,19	0.29	0
2	ZLK	B	2019	-	41,45,45	2.26	20 (48%)	58,65,65	2.50	13 (22%)
4	OLA	A	2015	-	3,6,19	0.30	0	2,6,19	0.28	0
4	OLA	A	2016	-	16,19,19	0.25	0	15,19,19	0.67	0
3	OLC	B	2003	-	8,8,24	0.53	0	7,7,25	0.64	0
4	OLA	A	2010	-	7,10,19	0.32	0	6,10,19	0.26	0
3	OLC	B	2010	-	3,6,24	0.30	0	2,6,25	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	OLC	B	2007	-	9,9,24	0.47	0	8,8,25	0.48	0
3	OLC	A	2008	-	8,8,24	0.44	0	7,7,25	0.46	0
4	OLA	B	2015	-	7,10,19	0.30	0	6,10,19	0.35	0
4	OLA	B	2011	-	8,11,19	0.39	0	7,11,19	0.72	0
4	OLA	B	2017	-	14,17,19	0.30	0	13,17,19	0.56	0
2	ZLK	B	2001	-	41,45,45	2.43	20 (48%)	58,65,65	2.44	16 (27%)
3	OLC	B	2009	-	22,22,24	0.68	1 (4%)	23,23,25	1.07	1 (4%)
5	1PE	A	2021	-	9,9,15	0.48	0	8,8,14	0.23	0
4	OLA	B	2013	-	12,15,19	0.31	0	11,15,19	0.44	0
4	OLA	A	2012	-	4,7,19	0.21	0	3,7,19	0.67	0
3	OLC	A	2004	-	10,10,24	0.41	0	9,9,25	0.50	0
3	OLC	A	2002	-	8,8,24	0.41	0	7,7,25	0.53	0
3	OLC	A	2009	-	6,6,24	0.30	0	5,5,25	0.66	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
3	OLC	B	2005	-	-	4/7/7/24	-
4	OLA	A	2013	-	-	9/14/16/17	-
2	ZLK	A	2001	-	-	2/29/36/36	0/5/5/5
4	OLA	A	2018	-	-	2/3/3/17	-
3	OLC	A	2003	-	-	9/14/14/24	-
3	OLC	B	2004	-	-	5/7/7/24	-
3	OLC	B	2002	-	-	1/5/5/24	-
3	OLC	B	2006	-	-	3/7/7/24	-
4	OLA	A	2017	-	-	5/8/10/17	-
4	OLA	B	2016	-	-	5/15/17/17	-
3	OLC	A	2005	-	-	2/5/5/24	-
4	OLA	B	2012	-	-	4/5/7/17	-
4	OLA	A	2019	-	-	10/15/17/17	-
4	OLA	A	2020	-	-	3/9/11/17	-
4	OLA	B	2018	-	-	10/15/17/17	-
4	OLA	B	2014	-	-	3/4/6/17	-
3	OLC	A	2007	-	-	11/15/15/24	-
3	OLC	B	2008	-	-	2/4/4/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	2011	-	-	4/8/10/17	-
3	OLC	A	2006	-	-	5/9/9/24	-
4	OLA	A	2014	-	-	1/2/4/17	-
2	ZLK	B	2019	-	-	9/29/36/36	0/5/5/5
4	OLA	A	2015	-	-	0/2/4/17	-
4	OLA	A	2016	-	-	9/15/17/17	-
3	OLC	B	2003	-	-	3/6/6/24	-
4	OLA	A	2010	-	-	4/6/8/17	-
3	OLC	B	2010	-	-	2/2/4/24	-
3	OLC	B	2007	-	-	4/7/7/24	-
3	OLC	A	2008	-	-	3/6/6/24	-
4	OLA	B	2015	-	-	3/6/8/17	-
4	OLA	B	2011	-	-	2/7/9/17	-
4	OLA	B	2017	-	-	8/13/15/17	-
2	ZLK	B	2001	-	-	1/29/36/36	0/5/5/5
3	OLC	B	2009	-	-	13/22/22/24	-
5	1PE	A	2021	-	-	4/7/7/13	-
4	OLA	B	2013	-	-	8/11/13/17	-
4	OLA	A	2012	-	-	3/3/5/17	-
3	OLC	A	2004	-	-	2/8/8/24	-
3	OLC	A	2002	-	-	4/6/6/24	-
3	OLC	A	2009	-	-	4/4/4/24	-

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	ZLK	C29-N31	5.63	1.45	1.39
2	B	2001	ZLK	C15-N14	5.50	1.47	1.36
2	A	2001	ZLK	C15-N14	5.32	1.47	1.36
2	B	2019	ZLK	C15-N14	4.78	1.45	1.36
2	A	2001	ZLK	C29-N31	4.71	1.44	1.39

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	ZLK	O34-S32-O33	-13.41	103.06	119.55
2	B	2019	ZLK	O34-S32-O33	-12.27	104.47	119.55
2	B	2001	ZLK	O34-S32-O33	-11.91	104.91	119.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2019	ZLK	O17-C15-N14	7.76	118.92	109.07
2	B	2001	ZLK	O17-C15-N14	6.47	117.28	109.07

There are no chirality outliers.

5 of 186 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2019	ZLK	N14-C15-O17-C18
2	B	2019	ZLK	O16-C15-O17-C18
2	B	2019	ZLK	C19-C18-O17-C15
3	A	2007	OLC	C21-C22-C24-O25
3	B	2007	OLC	C10-C11-C12-C13

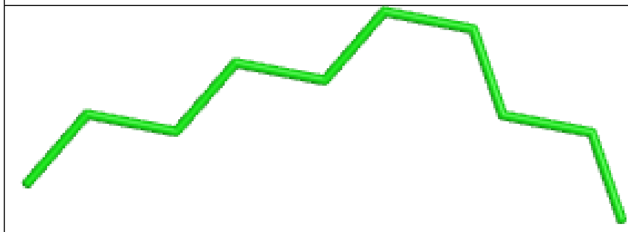
There are no ring outliers.

11 monomers are involved in 9 short contacts:

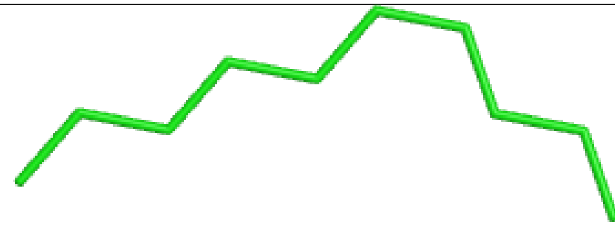
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2013	OLA	1	0
3	B	2004	OLC	1	0
3	B	2006	OLC	1	0
4	B	2016	OLA	1	0
4	A	2019	OLA	2	0
4	B	2014	OLA	1	0
4	A	2014	OLA	2	0
3	B	2010	OLC	1	0
4	B	2011	OLA	1	0
4	B	2013	OLA	1	0
4	A	2012	OLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

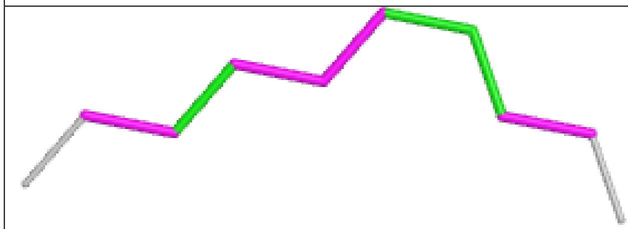
Ligand OLC B 2005



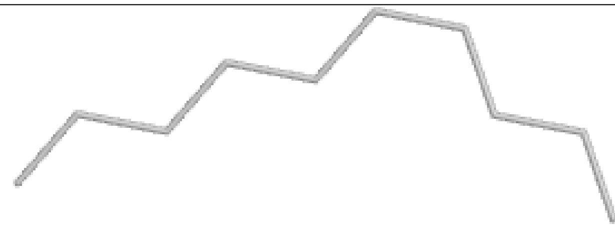
Bond lengths



Bond angles

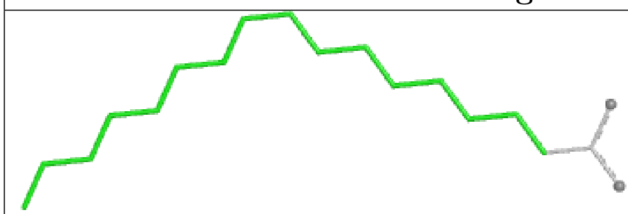


Torsions

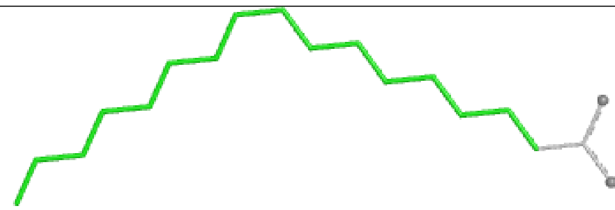


Rings

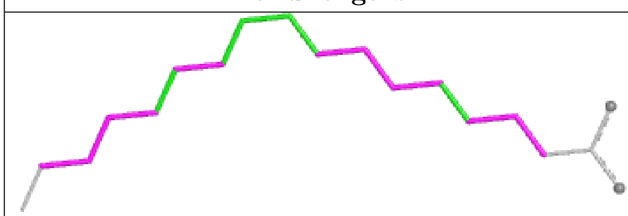
Ligand OLA A 2013



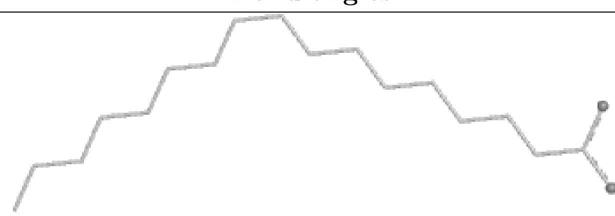
Bond lengths



Bond angles

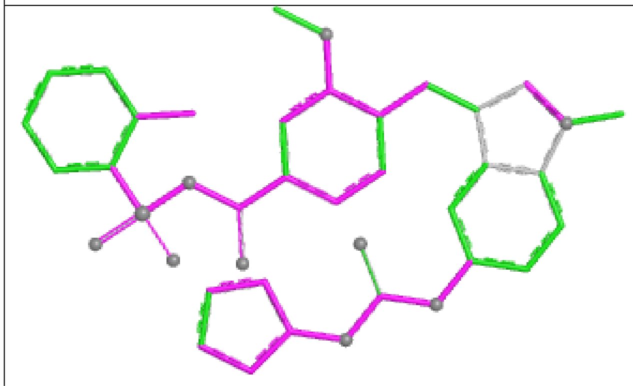


Torsions

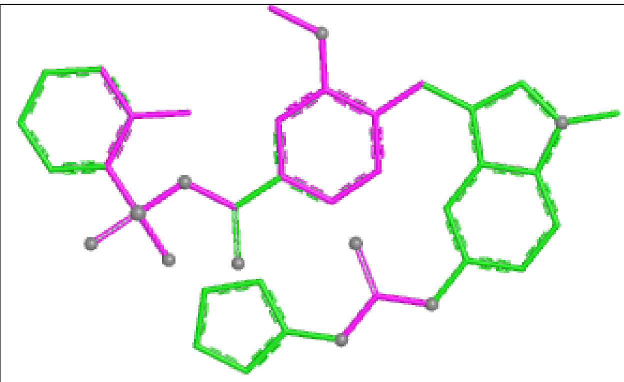


Rings

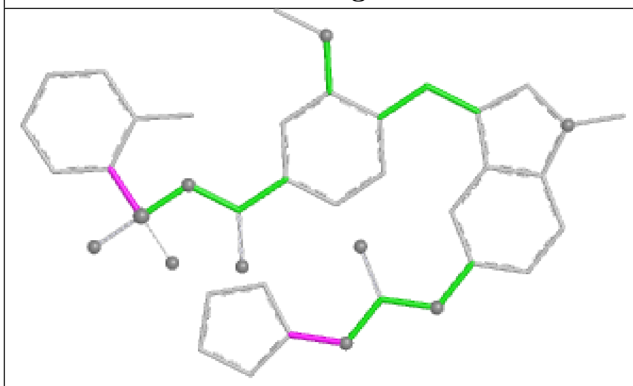
Ligand ZLK A 2001



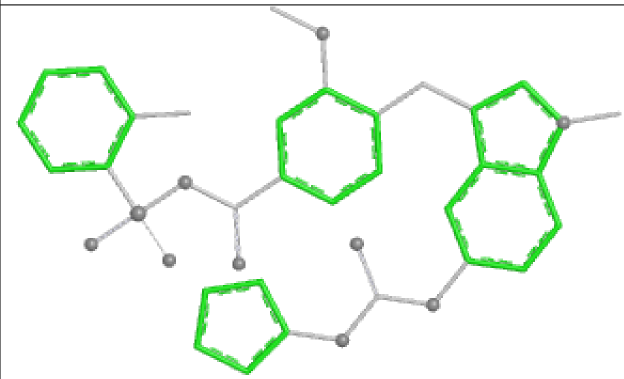
Bond lengths



Bond angles

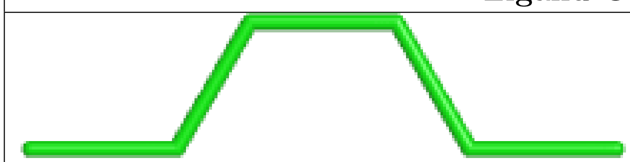


Torsions

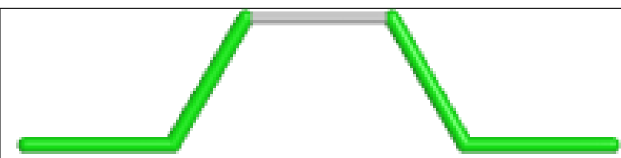


Rings

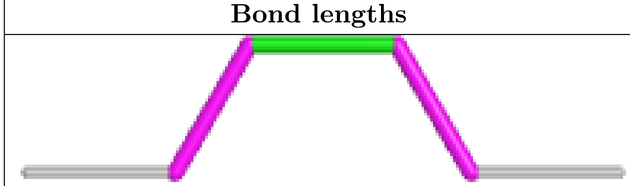
Ligand OLA A 2018



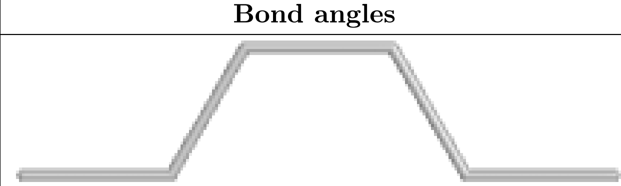
Bond lengths



Bond angles

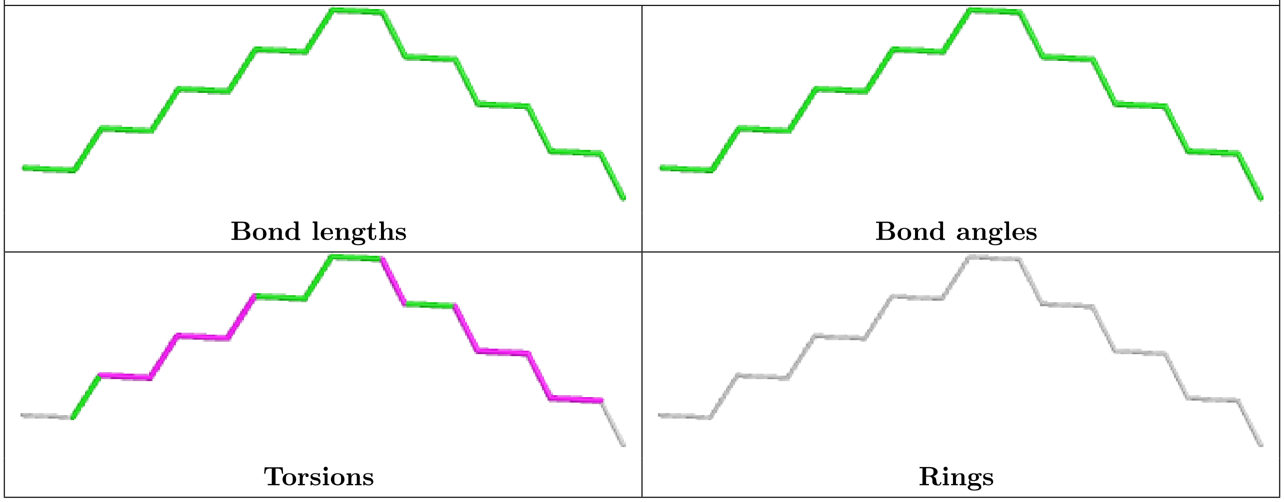


Torsions



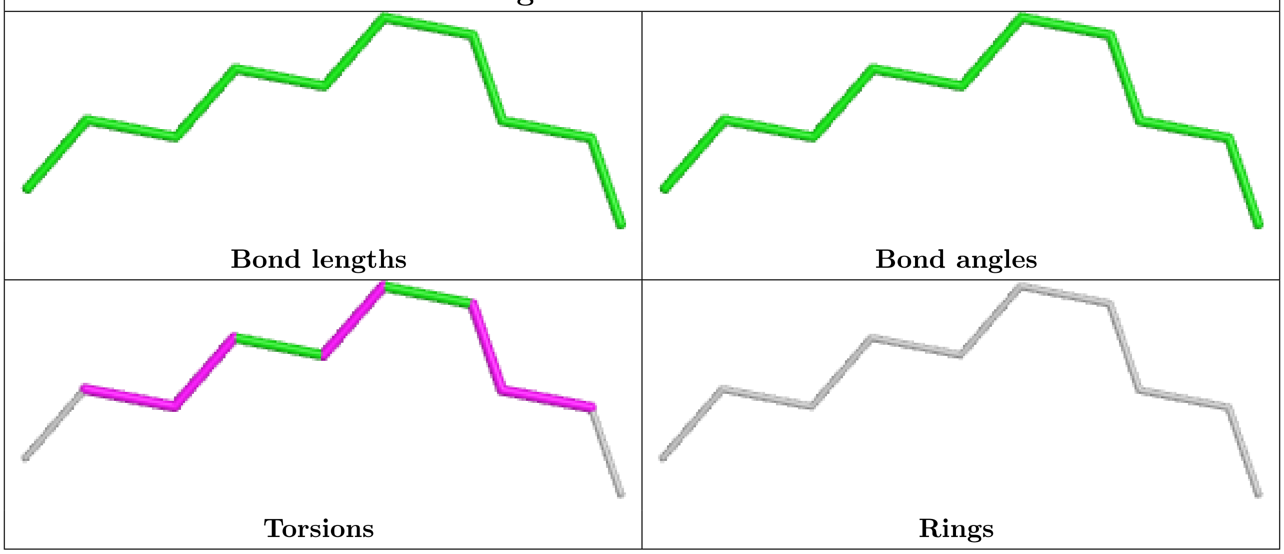
Rings

Ligand OLC A 2003



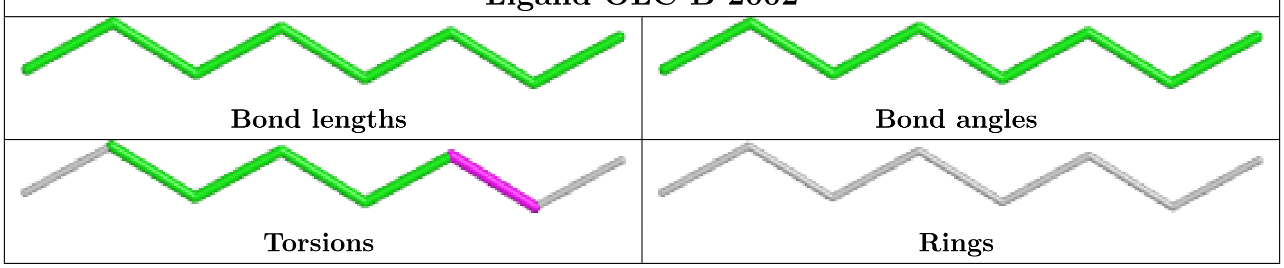
Bond lengths | Bond angles | Torsions | Rings

Ligand OLC B 2004



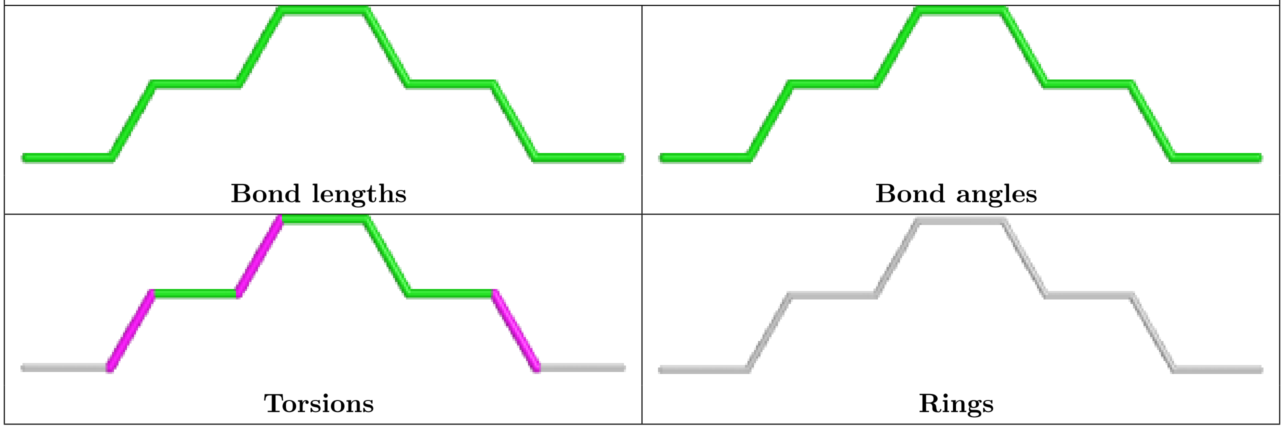
Bond lengths | Bond angles | Torsions | Rings

Ligand OLC B 2002

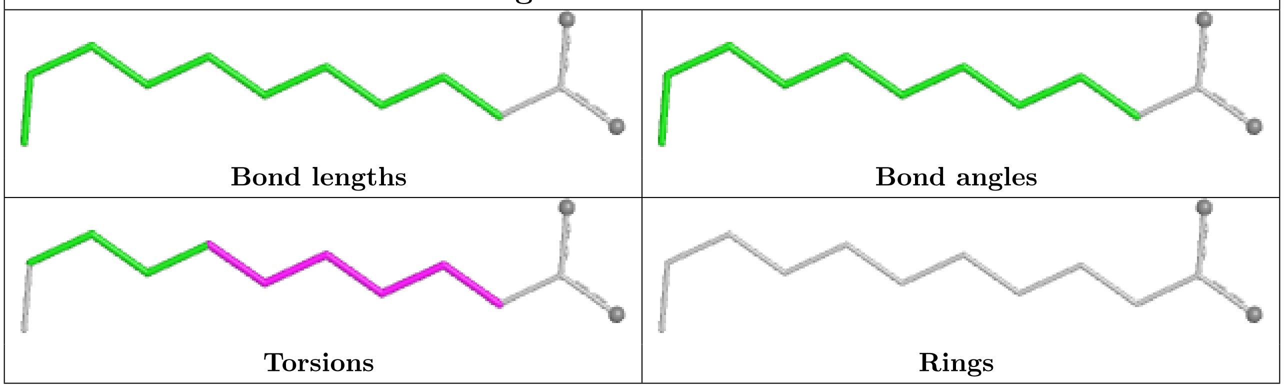


Bond lengths | Bond angles | Torsions | Rings

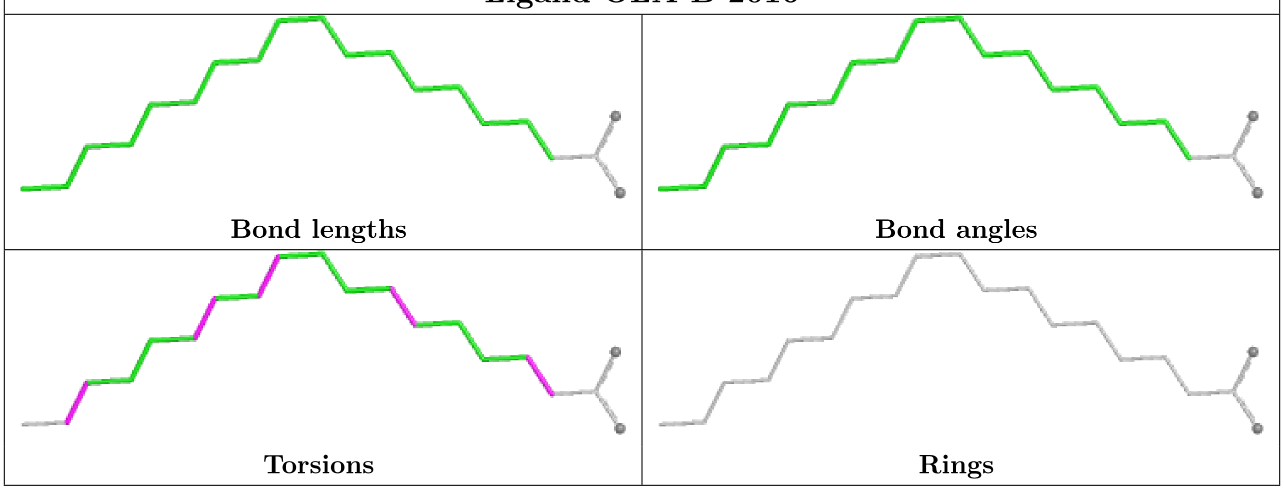
Ligand OLC B 2006



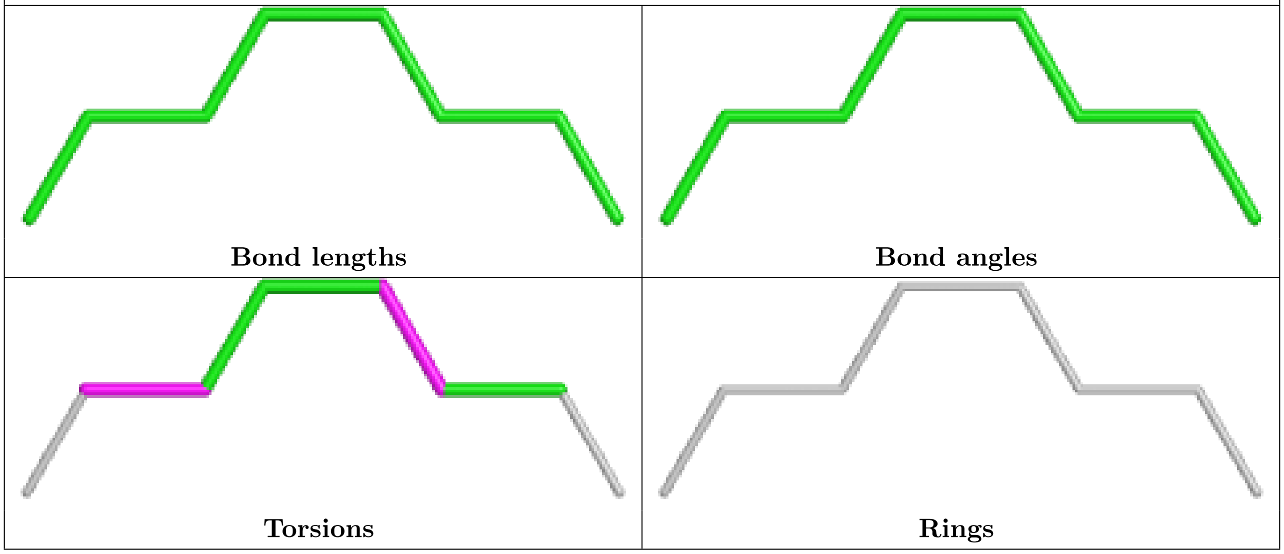
Ligand OLA A 2017



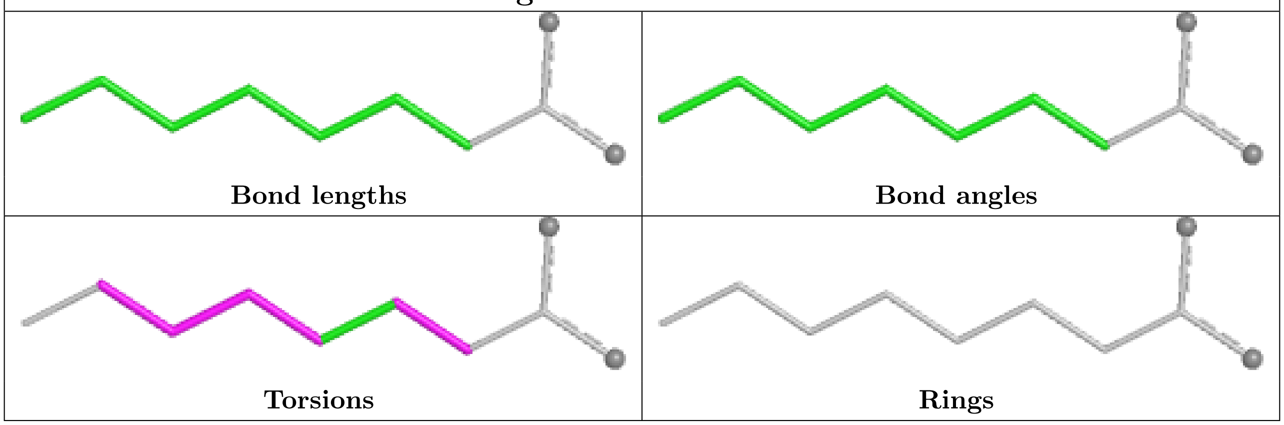
Ligand OLA B 2016



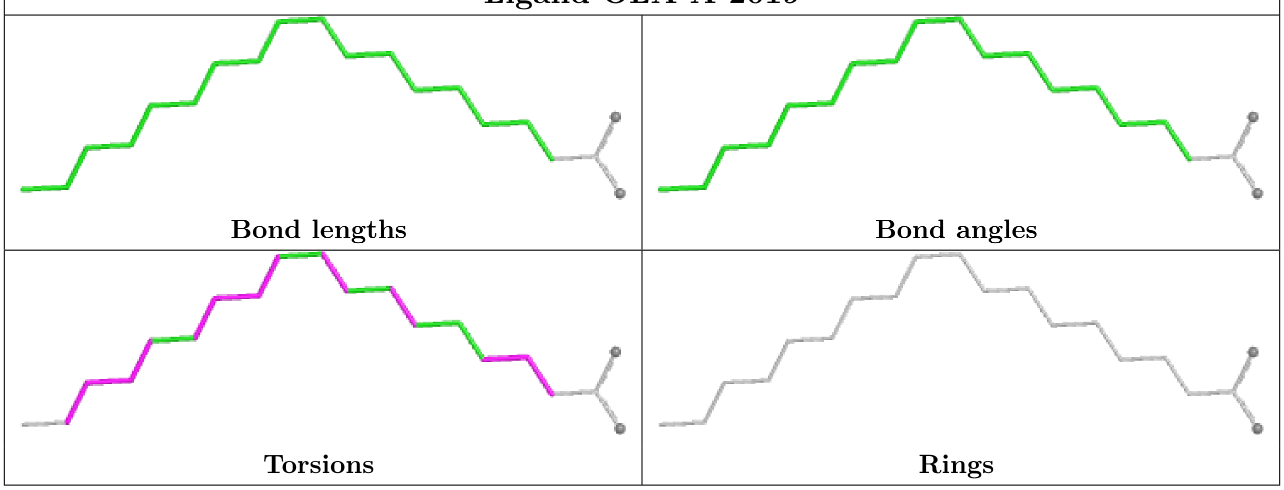
Ligand OLC A 2005



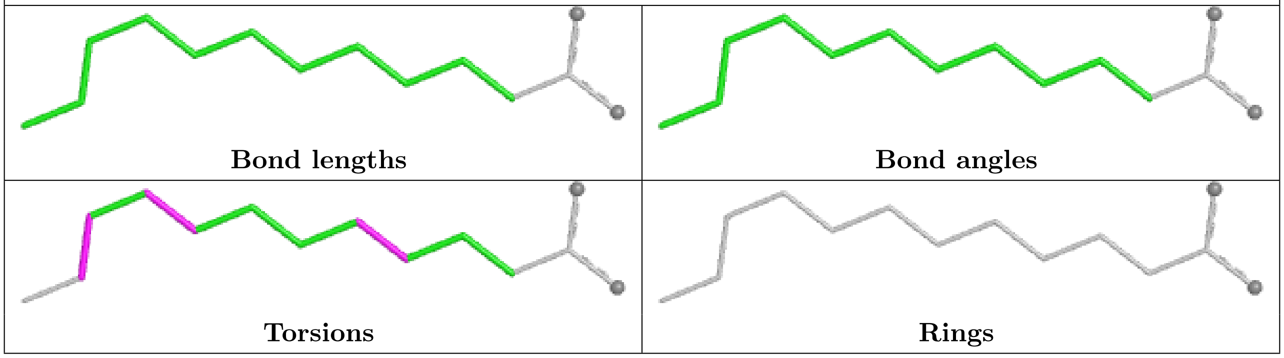
Ligand OLA B 2012



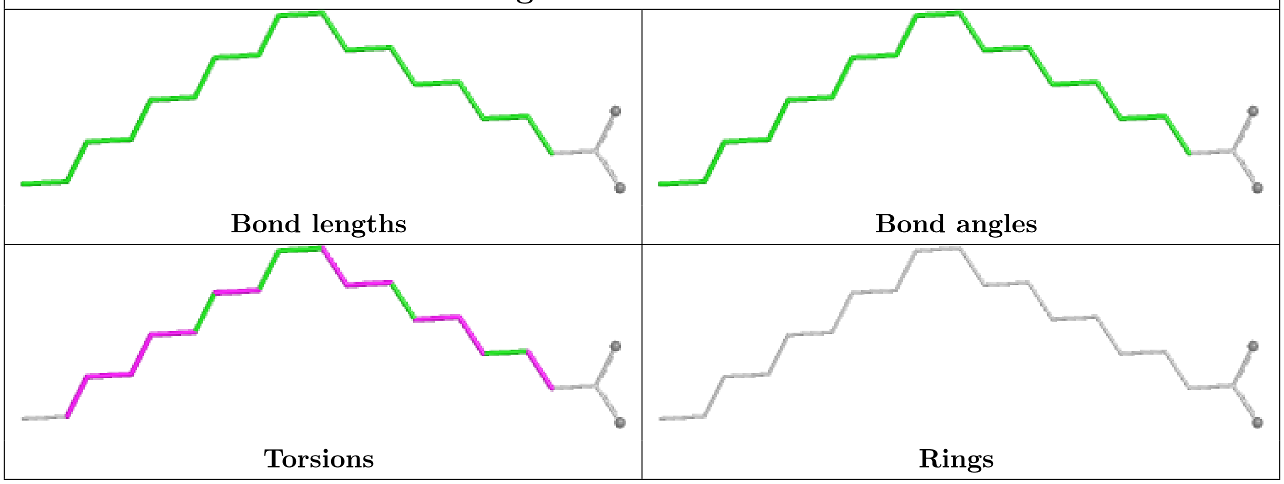
Ligand OLA A 2019



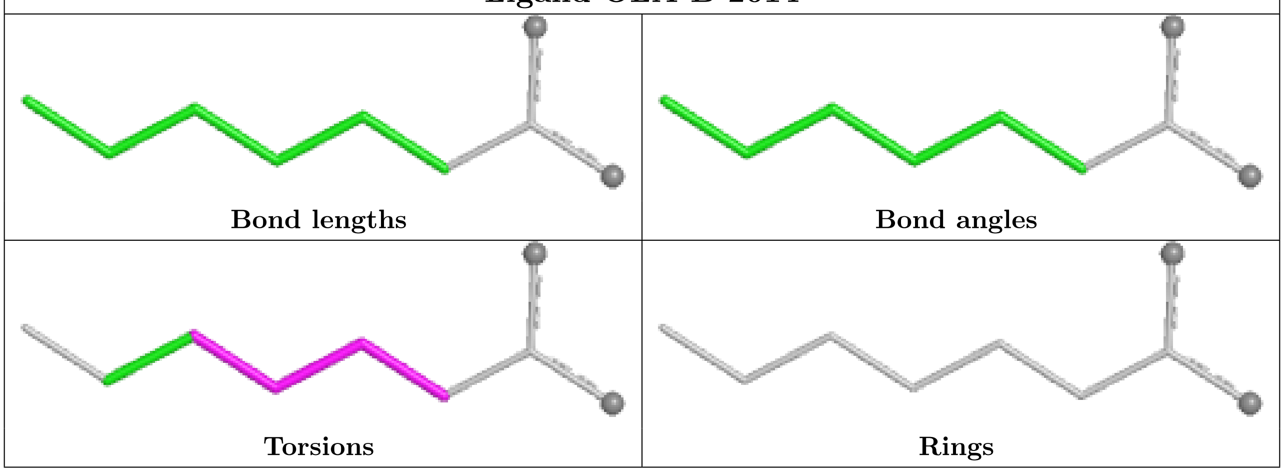
Ligand OLA A 2020



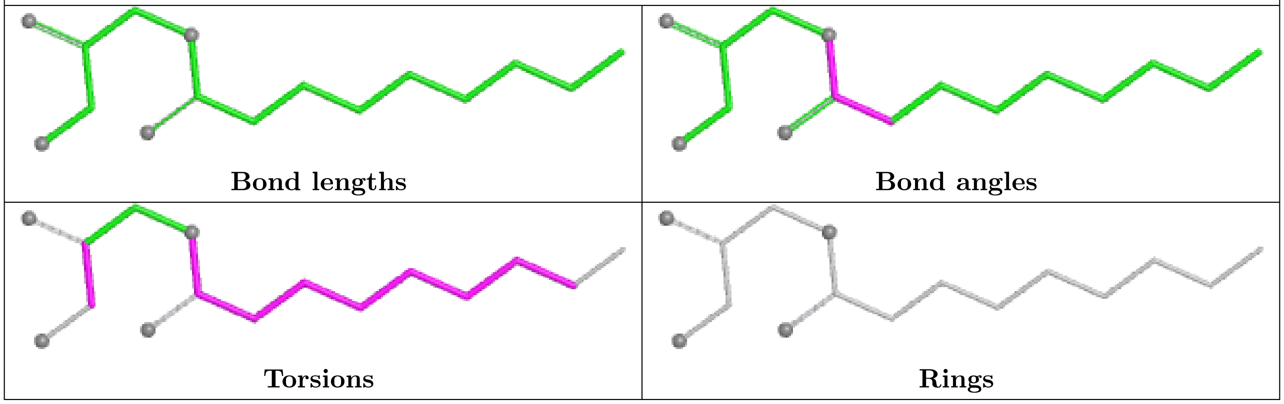
Ligand OLA B 2018



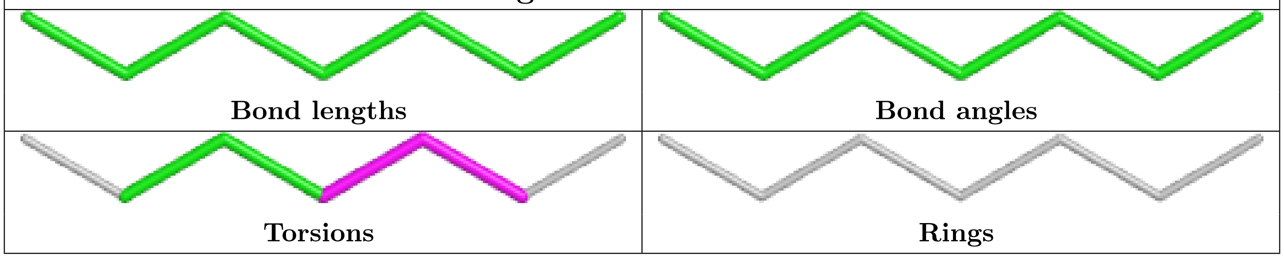
Ligand OLA B 2014



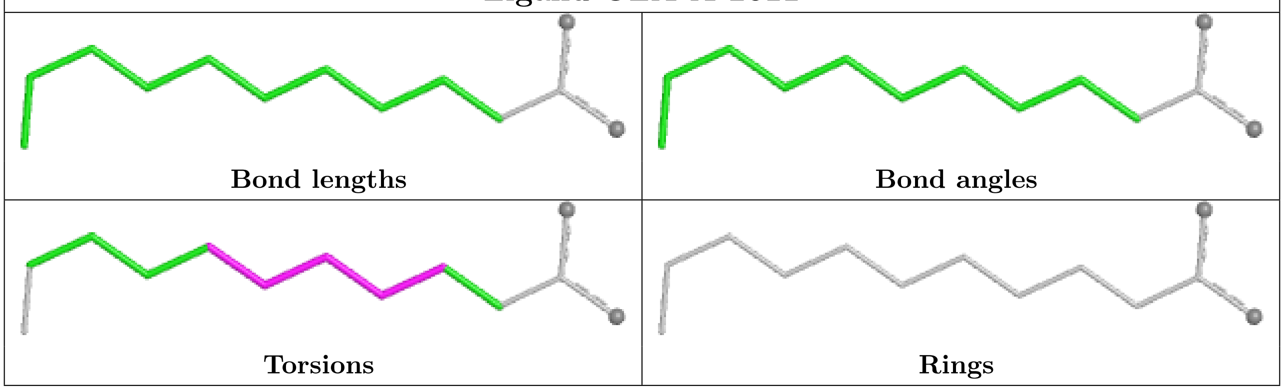
Ligand OLC A 2007



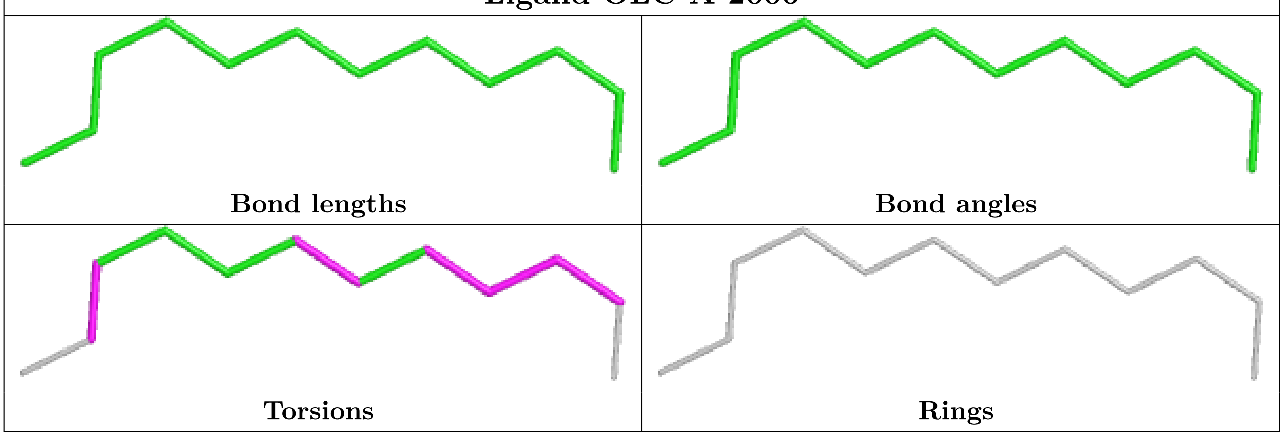
Ligand OLC B 2008



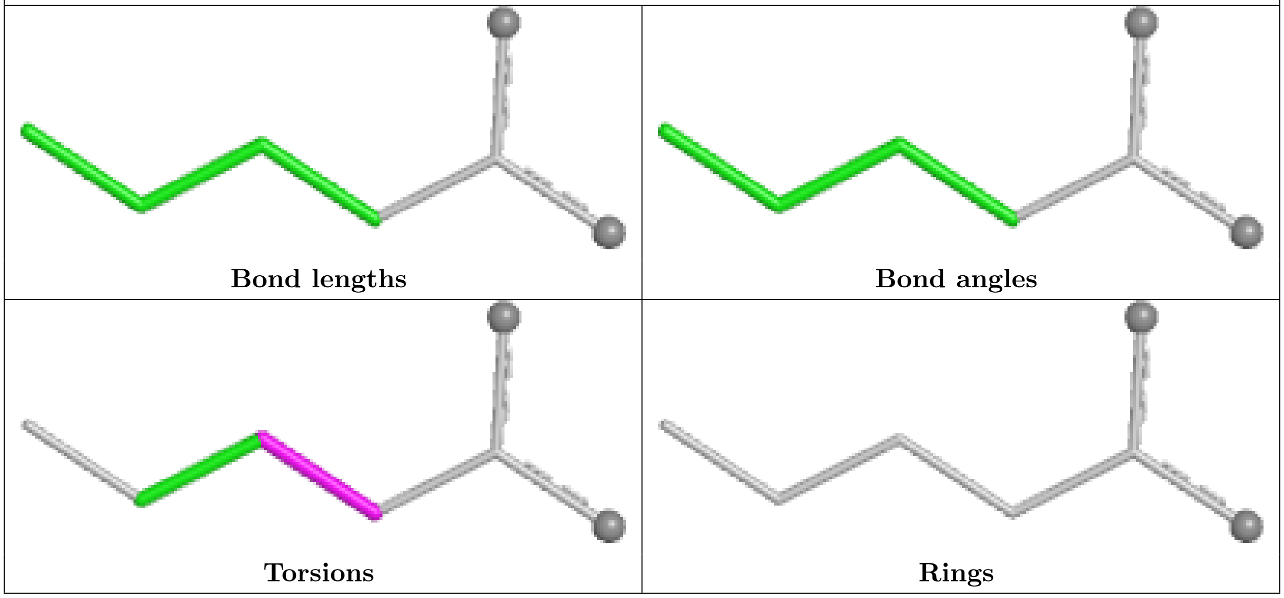
Ligand OLA A 2011



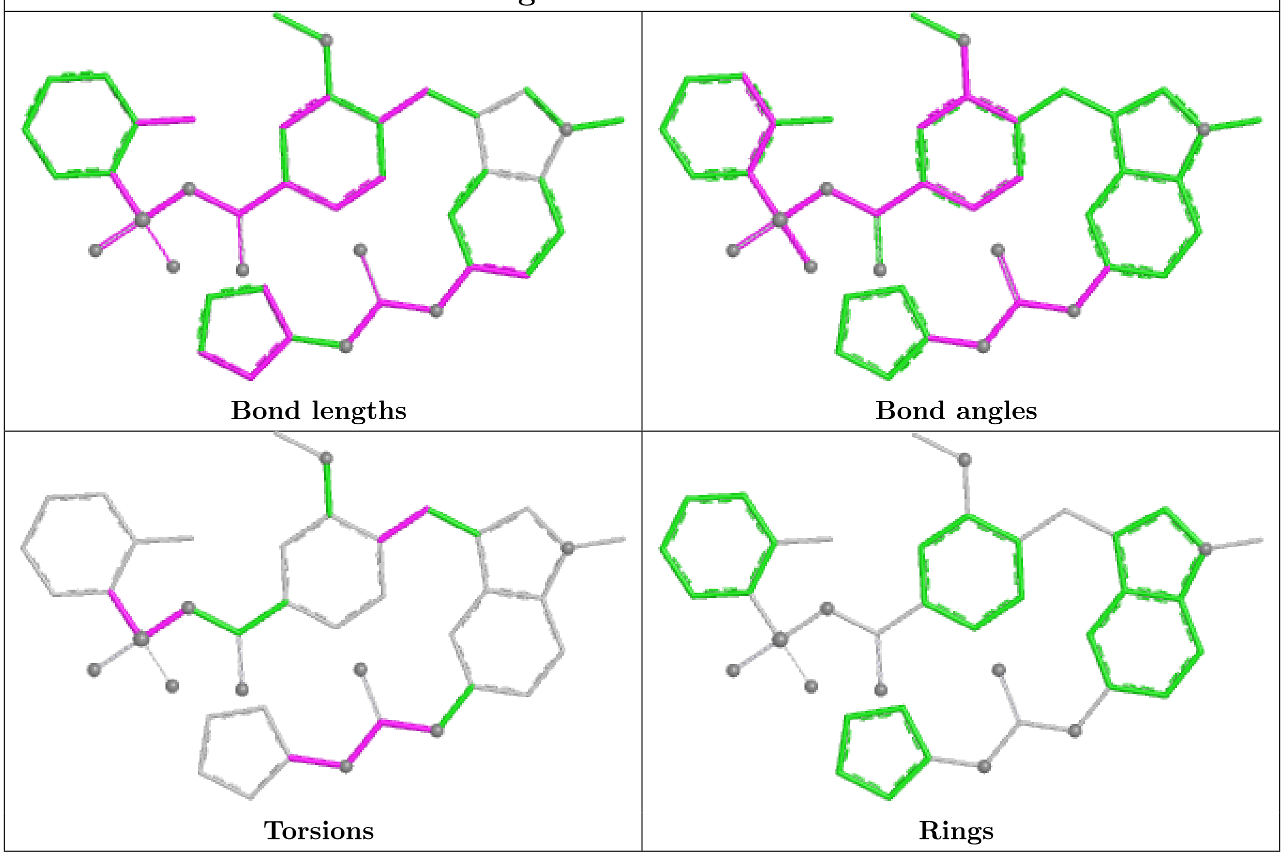
Ligand OLC A 2006



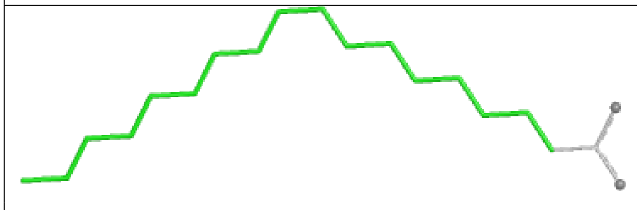
Ligand OLA A 2014

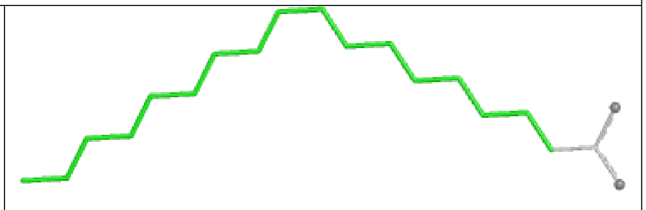


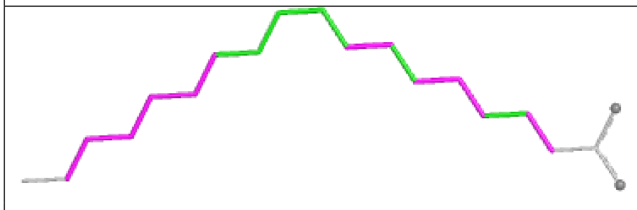
Ligand ZLK B 2019

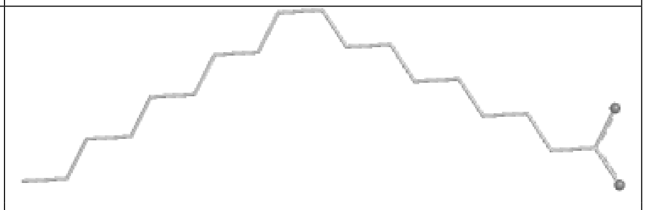


Ligand OLA A 2016

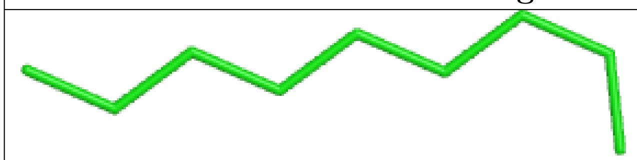

Bond lengths

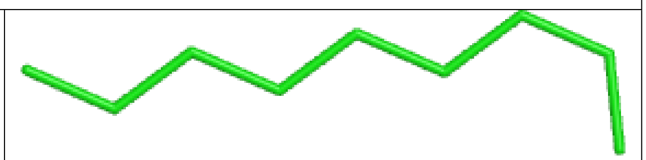

Bond angles

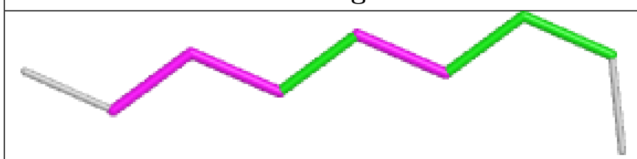

Torsions

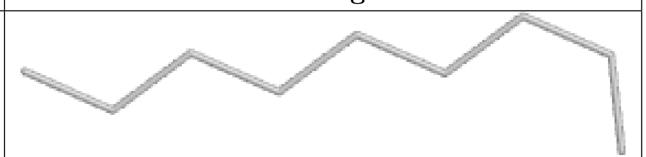

Rings

Ligand OLC B 2003

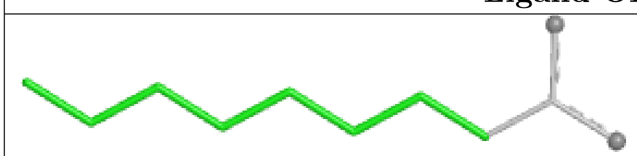

Bond lengths

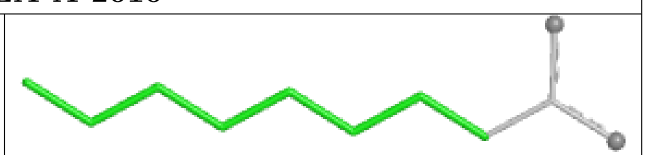

Bond angles

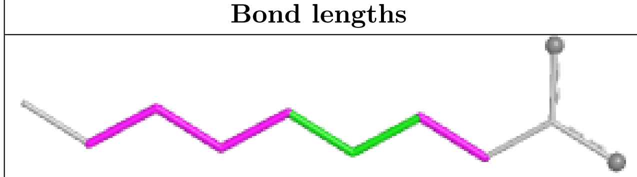

Torsions

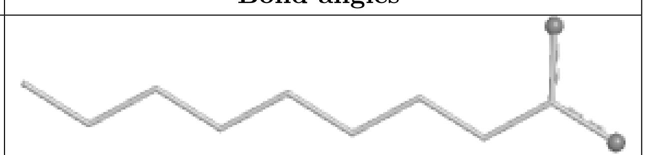

Rings

Ligand OLA A 2010

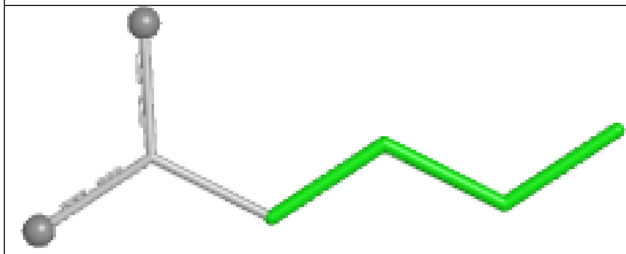

Bond lengths


Bond angles

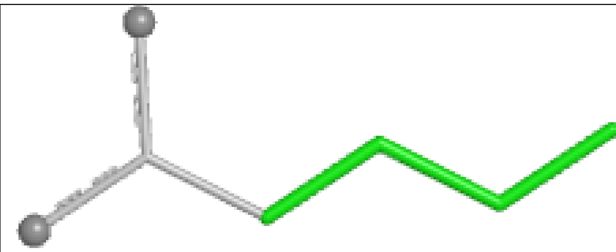

Torsions


Rings

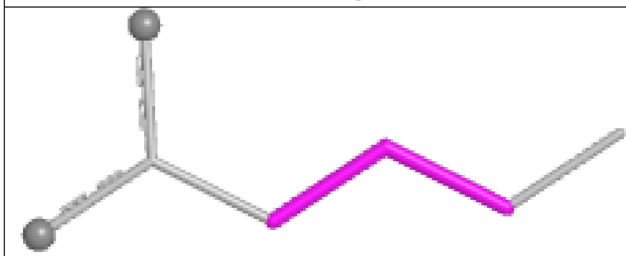
Ligand OLC B 2010



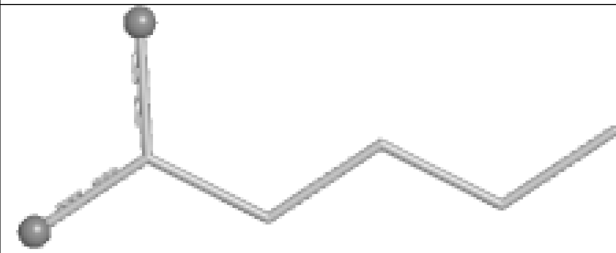
Bond lengths



Bond angles

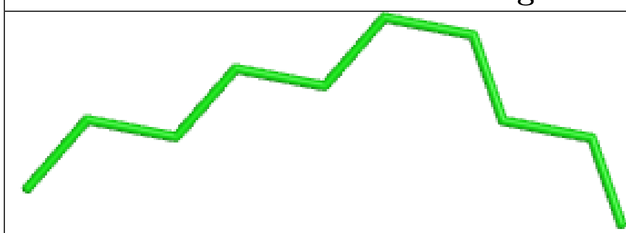


Torsions

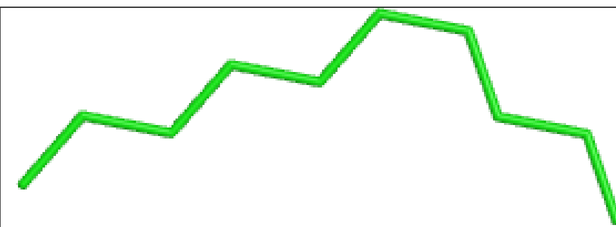


Rings

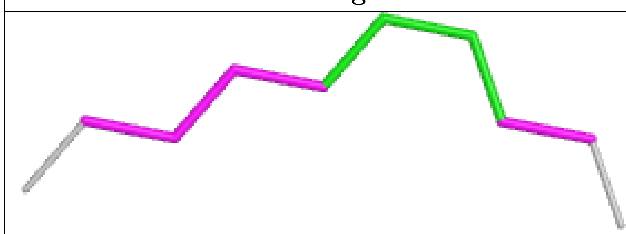
Ligand OLC B 2007



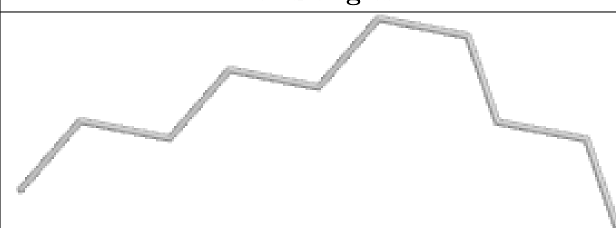
Bond lengths



Bond angles

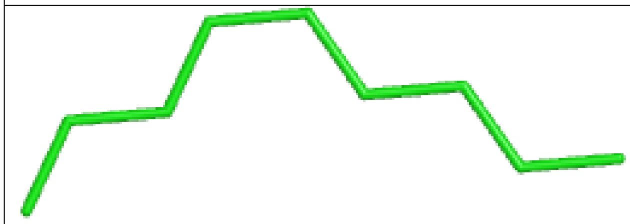


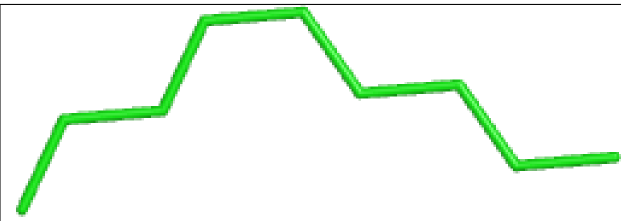
Torsions

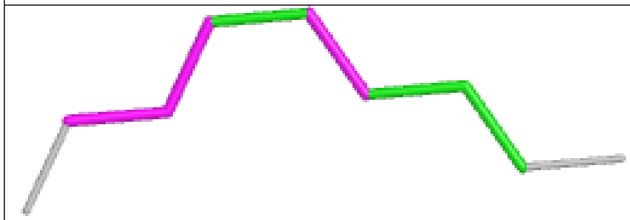


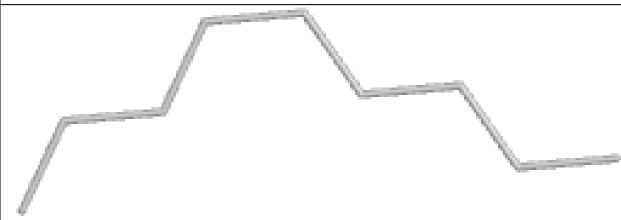
Rings

Ligand OLC A 2008

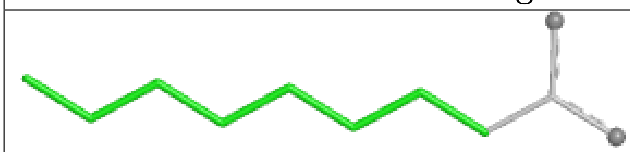

Bond lengths

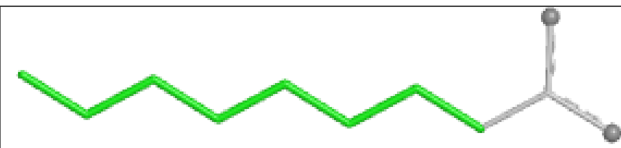

Bond angles

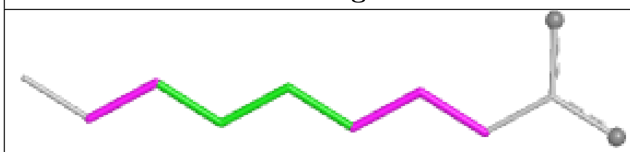

Torsions

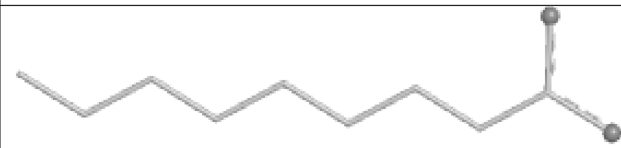

Rings

Ligand OLA B 2015

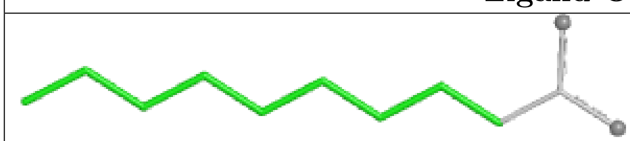

Bond lengths

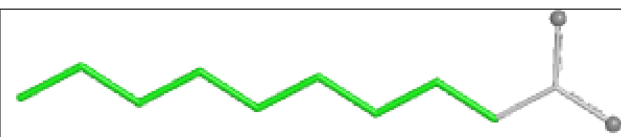

Bond angles

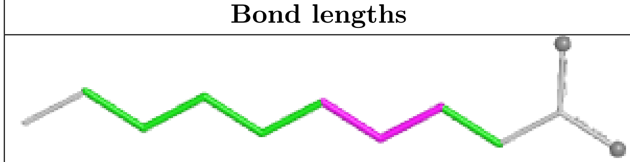

Torsions

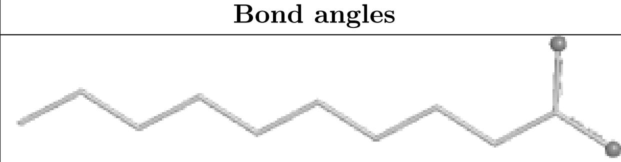

Rings

Ligand OLA B 2011

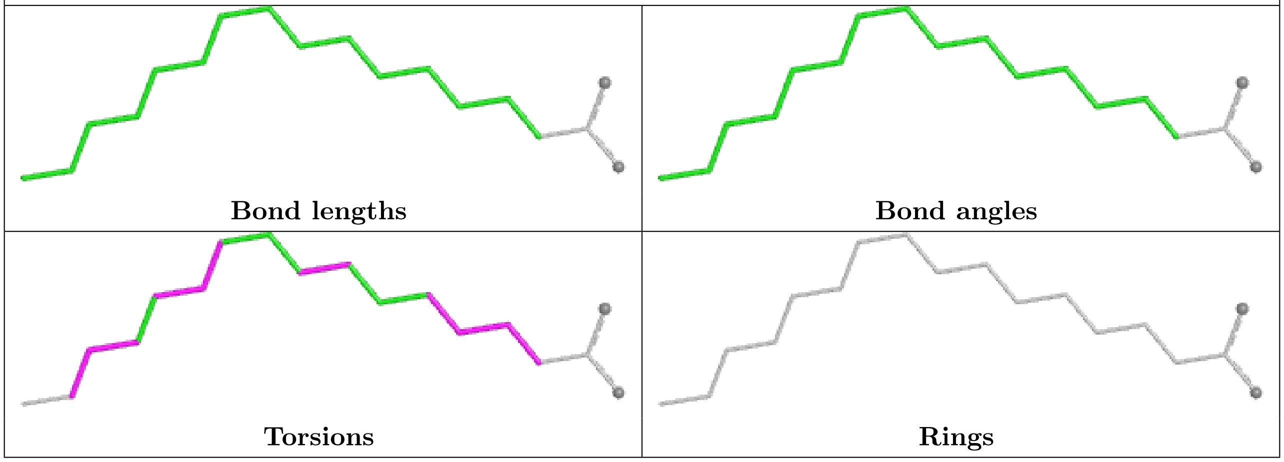

Bond lengths


Bond angles

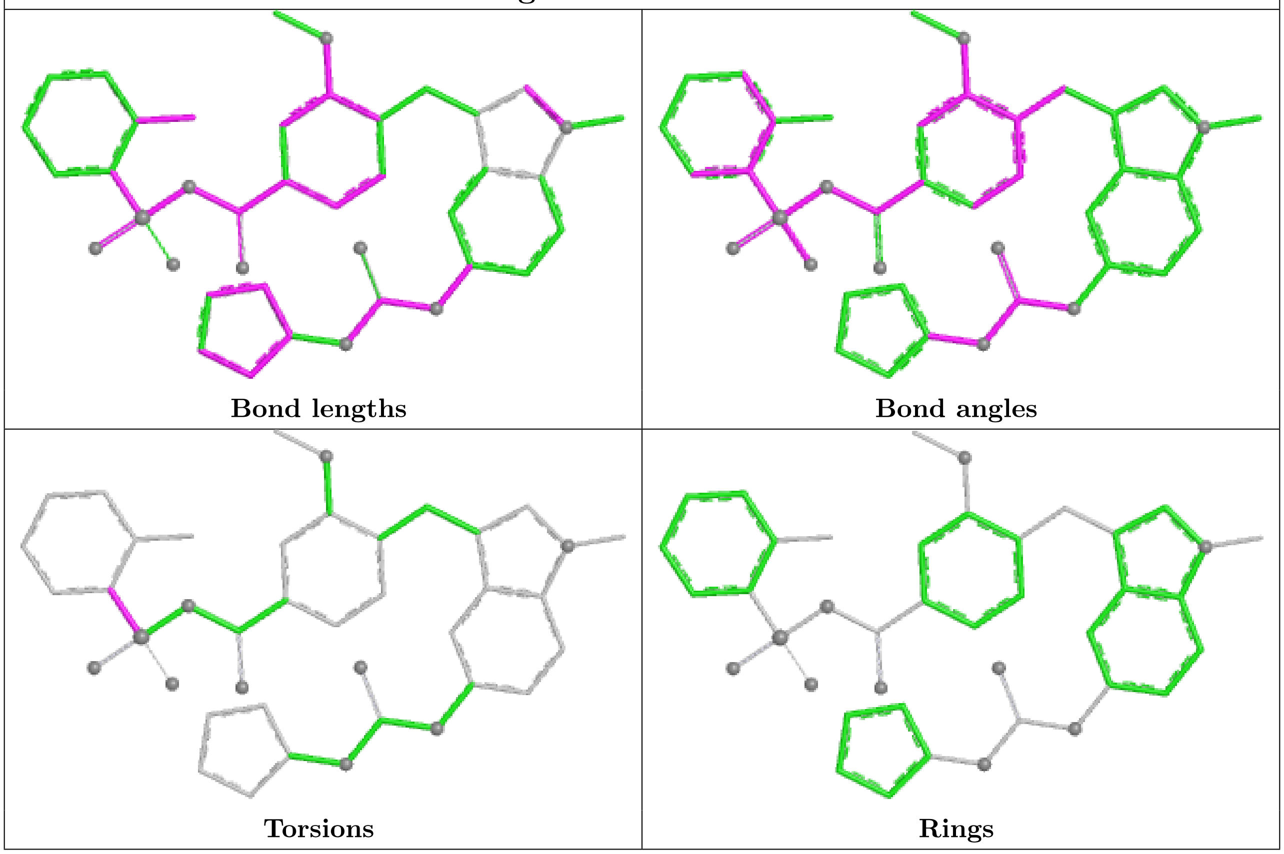

Torsions


Rings

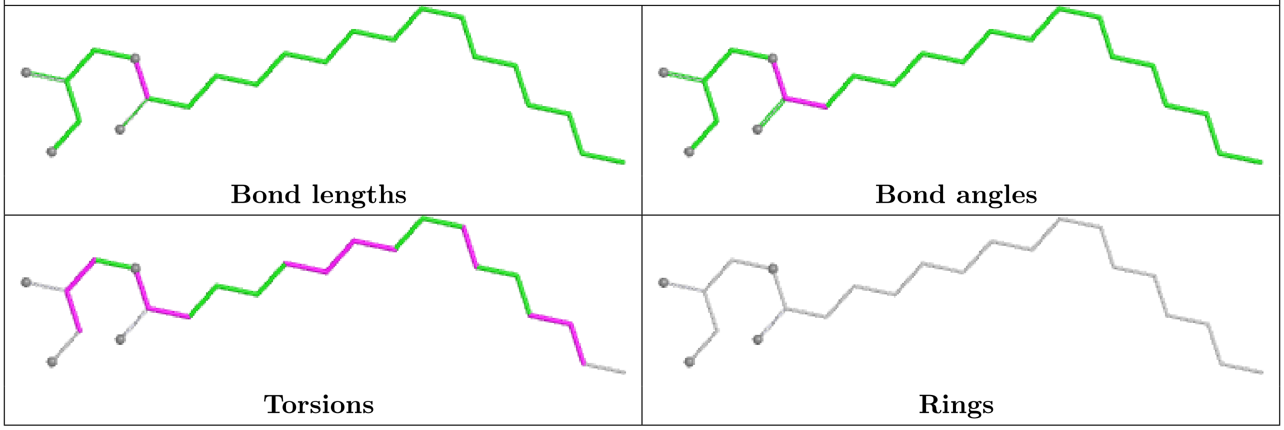
Ligand OLA B 2017



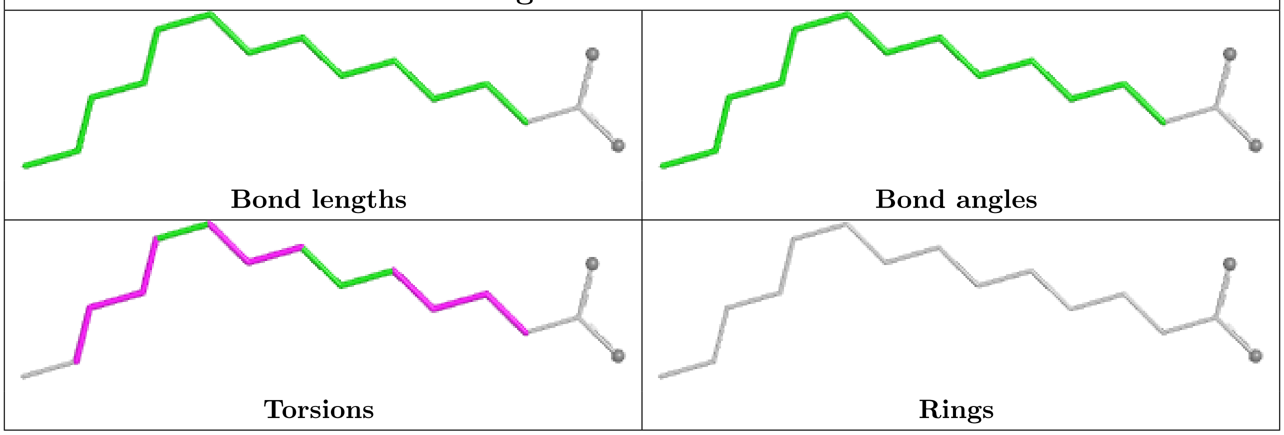
Ligand ZLK B 2001



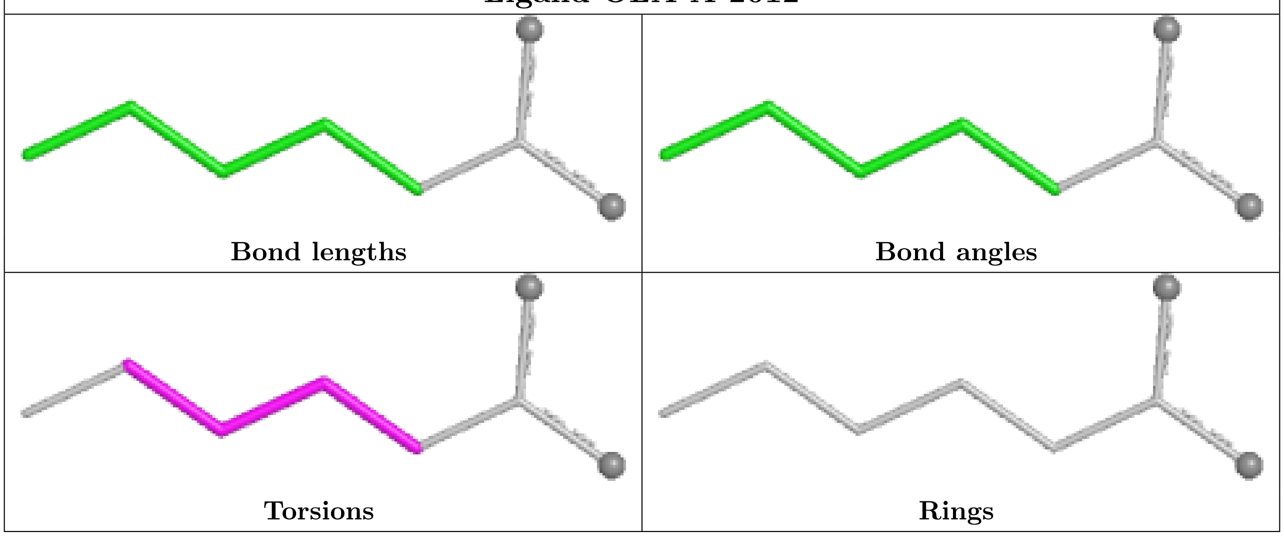
Ligand OLC B 2009



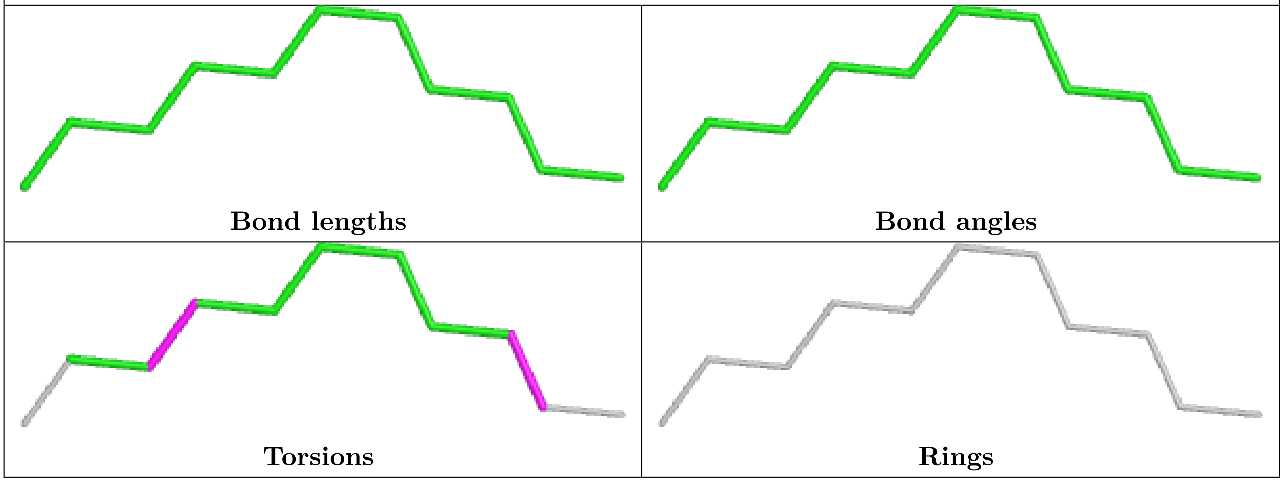
Ligand OLA B 2013



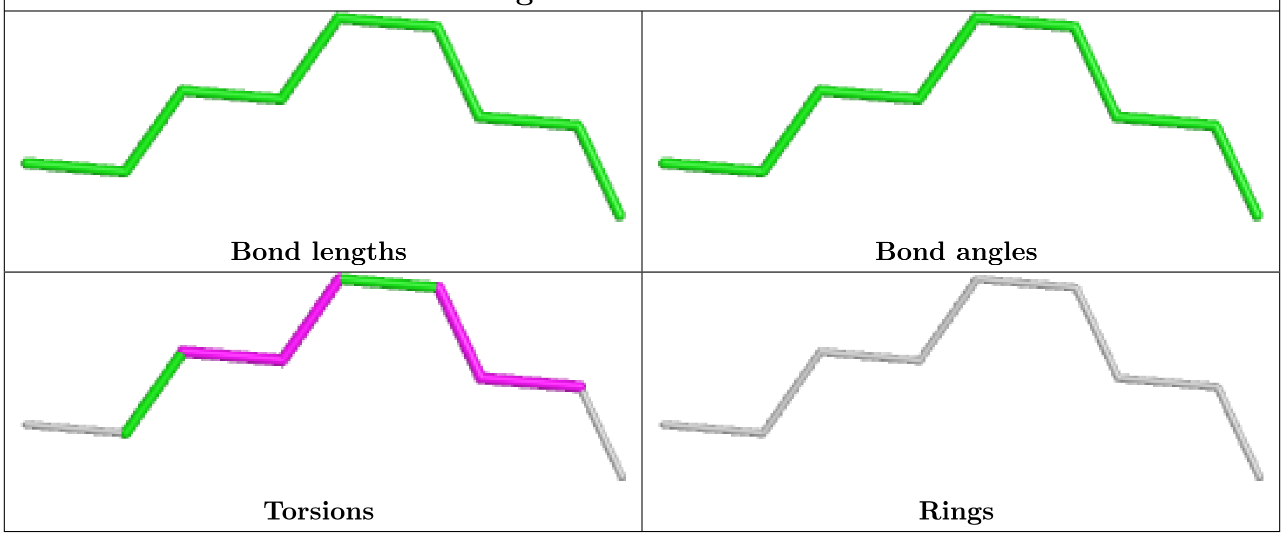
Ligand OLA A 2012



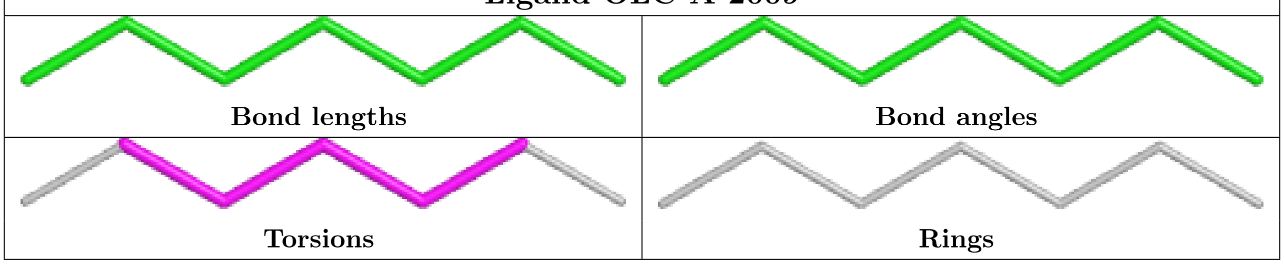
Ligand OLC A 2004



Ligand OLC A 2002



Ligand OLC A 2009



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	369/423 (87%)	0.69	51 (13%)	2	2	47, 81, 157, 171	0
1	B	385/423 (91%)	0.88	70 (18%)	1	1	49, 93, 154, 179	0
All	All	754/846 (89%)	0.79	121 (16%)	1	1	47, 87, 155, 179	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1056	PRO	6.8
1	B	131	ASN	6.7
1	B	132	ILE	6.5
1	A	1056	PRO	6.3
1	B	1011	ASN	6.0

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)

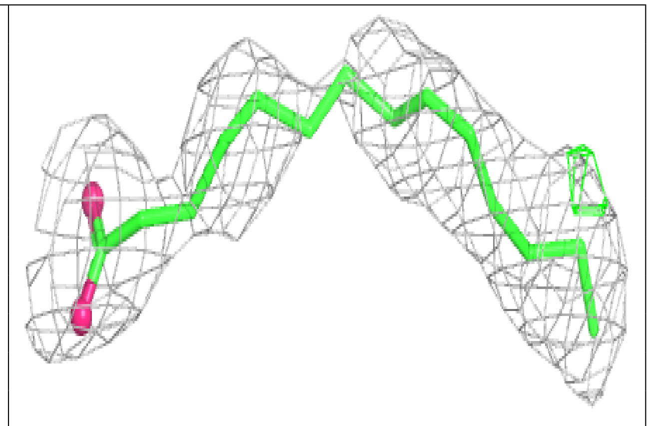
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

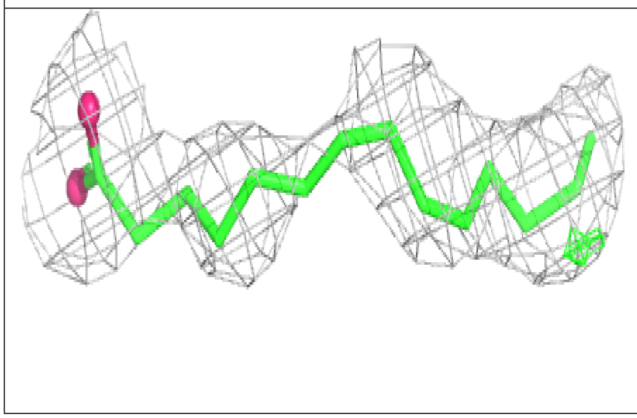
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLA	B	2013	16/20	0.61	0.41	109,114,120,121	0
3	OLC	A	2003	17/25	0.65	0.28	73,96,100,100	0
4	OLA	B	2016	20/20	0.66	0.32	80,87,106,106	0
4	OLA	A	2010	11/20	0.69	0.25	93,96,109,110	0
4	OLA	A	2012	8/20	0.72	0.30	85,88,98,100	0
3	OLC	B	2010	7/25	0.75	0.31	102,106,112,114	0
4	OLA	A	2019	20/20	0.75	0.21	97,104,120,121	0
4	OLA	A	2016	20/20	0.76	0.22	88,93,110,110	0
4	OLA	B	2015	11/20	0.78	0.26	95,101,110,112	0
4	OLA	A	2020	14/20	0.78	0.27	73,78,91,93	0
4	OLA	A	2013	19/20	0.79	0.26	86,95,101,101	0
4	OLA	A	2014	7/20	0.79	0.23	92,96,105,108	0
4	OLA	B	2017	18/20	0.79	0.27	79,98,112,114	0
4	OLA	A	2015	7/20	0.80	0.31	76,83,94,94	0
4	OLA	A	2011	13/20	0.80	0.19	102,112,120,121	0
3	OLC	B	2009	23/25	0.81	0.31	81,84,101,101	0
3	OLC	B	2002	8/25	0.82	0.15	79,80,82,82	0
4	OLA	B	2018	20/20	0.82	0.23	120,122,131,131	0
5	1PE	A	2021	10/16	0.83	0.30	111,112,114,114	0
3	OLC	A	2007	16/25	0.85	0.33	84,96,118,119	0
4	OLA	B	2011	12/20	0.85	0.17	90,94,103,104	0
4	OLA	A	2017	13/20	0.85	0.17	99,106,114,114	0
3	OLC	B	2005	10/25	0.85	0.21	90,95,97,97	0
3	OLC	A	2006	12/25	0.86	0.14	91,96,97,97	0
3	OLC	A	2002	9/25	0.86	0.22	80,81,84,84	0
3	OLC	A	2004	11/25	0.86	0.24	55,63,74,74	0
3	OLC	B	2004	10/25	0.86	0.23	87,89,91,91	0
3	OLC	A	2008	9/25	0.87	0.15	75,78,81,81	0
3	OLC	B	2006	10/25	0.88	0.16	111,112,114,115	0
3	OLC	B	2008	7/25	0.88	0.15	83,84,85,85	0
3	OLC	B	2003	9/25	0.88	0.17	95,95,97,97	0
4	OLA	B	2012	10/20	0.89	0.21	87,96,105,105	0
3	OLC	B	2007	10/25	0.91	0.17	75,76,79,79	0
3	OLC	A	2009	7/25	0.92	0.30	70,71,78,80	0
3	OLC	A	2005	8/25	0.92	0.15	77,77,78,78	0
4	OLA	B	2014	9/20	0.93	0.14	87,90,96,97	0
4	OLA	A	2018	6/20	0.93	0.22	69,70,72,72	0
2	ZLK	B	2019	41/41	0.93	0.25	53,63,72,77	41
2	ZLK	A	2001	41/41	0.98	0.14	41,55,65,69	0
2	ZLK	B	2001	41/41	0.98	0.18	48,56,61,63	0
6	NA	A	2022	1/1	0.99	0.25	54,54,54,54	0
6	NA	B	2020	1/1	0.99	0.13	53,53,53,53	0

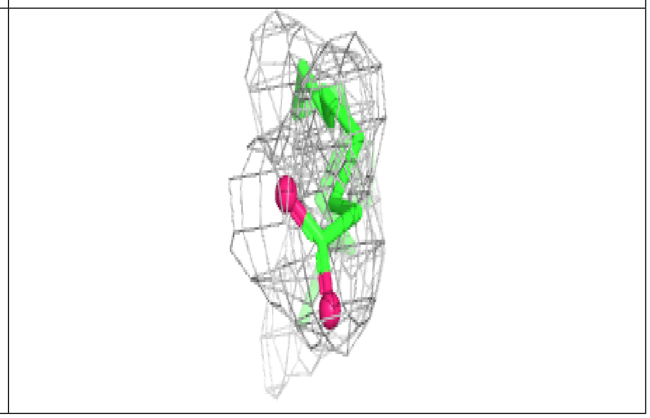
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA B 2013:

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

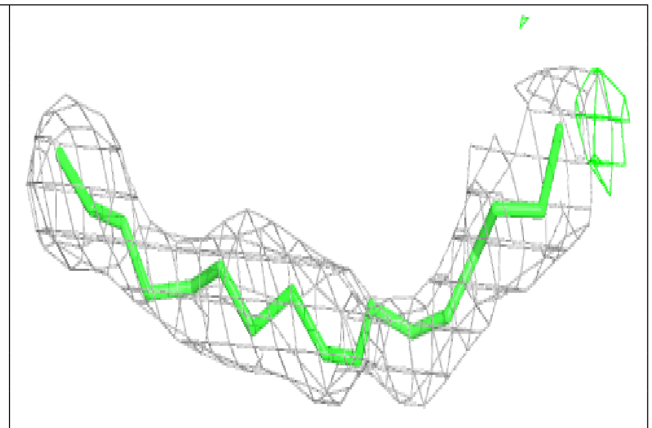


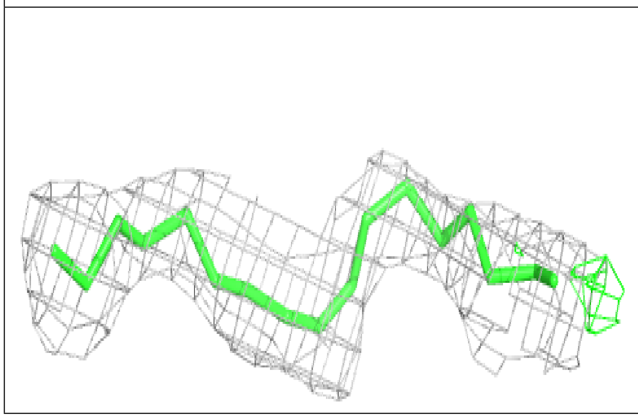


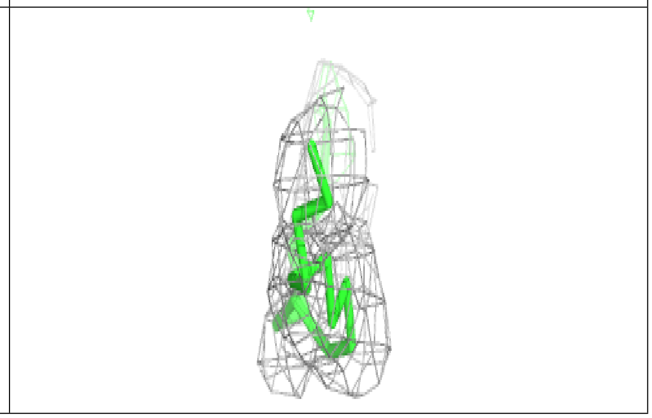


Electron density around OLC A 2003:

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

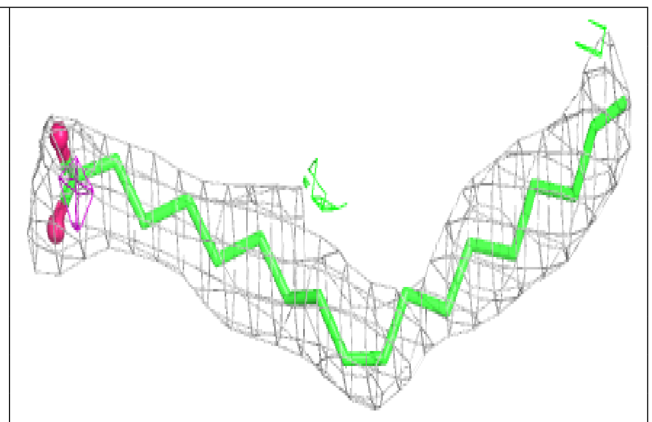


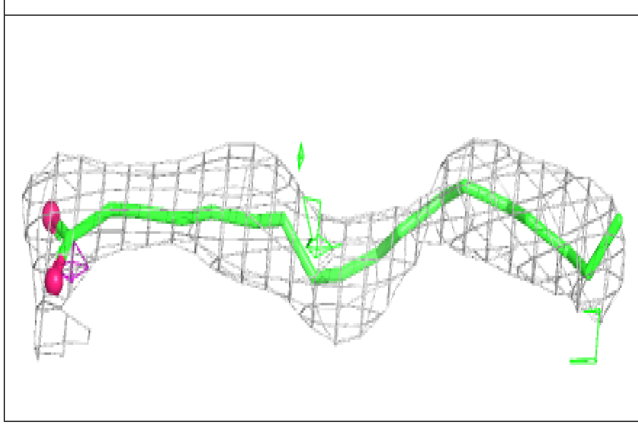


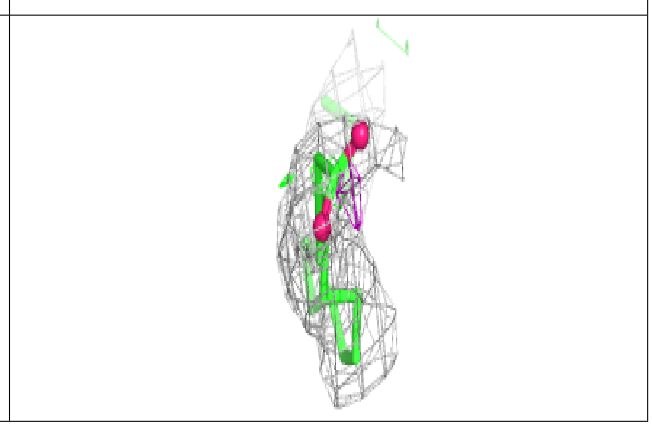


Electron density around OLA B 2016:

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

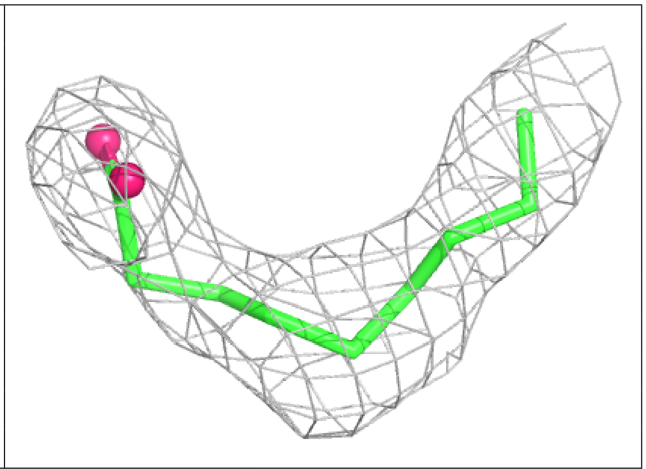


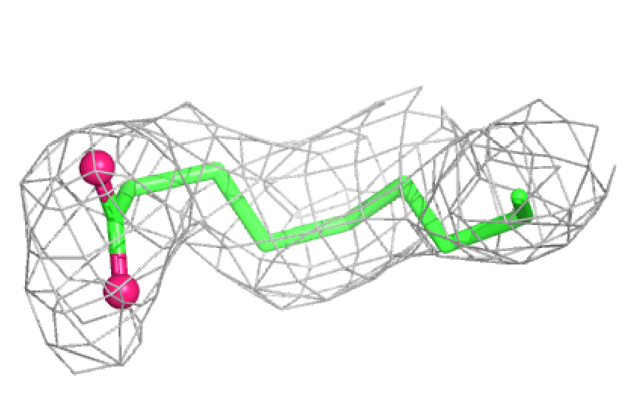


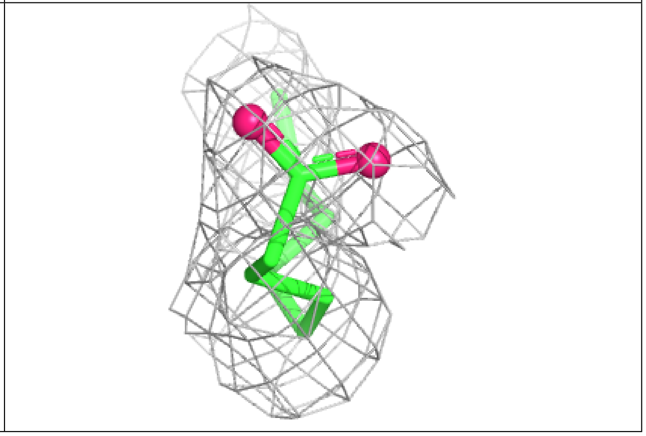


Electron density around OLA A 2010:

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

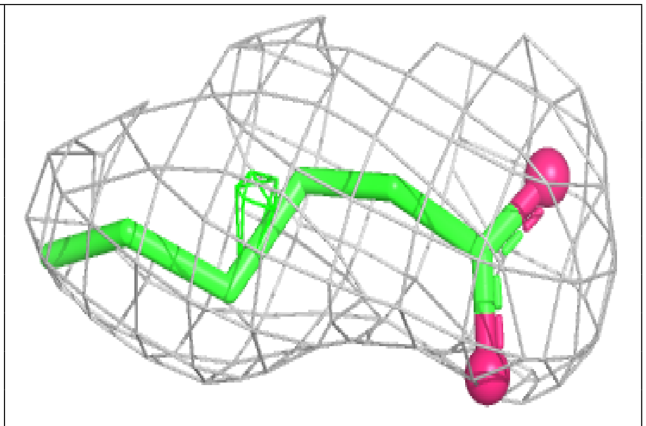


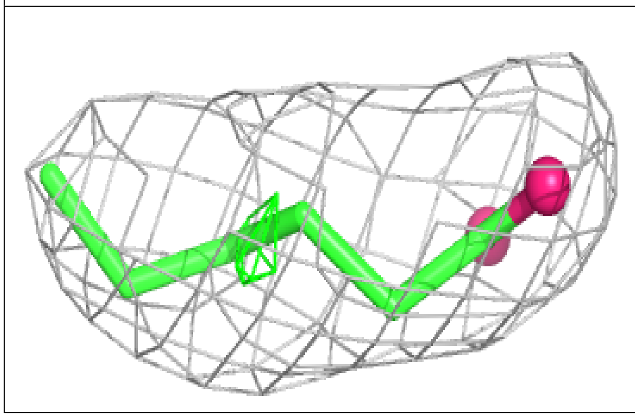


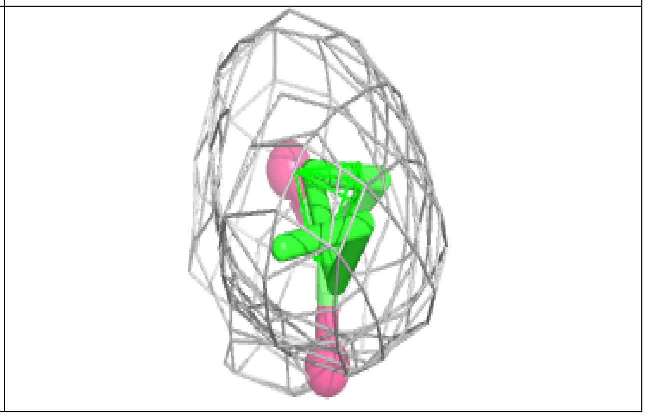


Electron density around OLA A 2012:

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

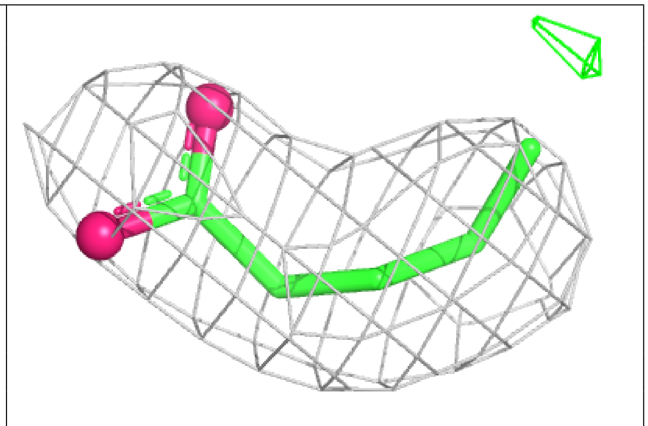


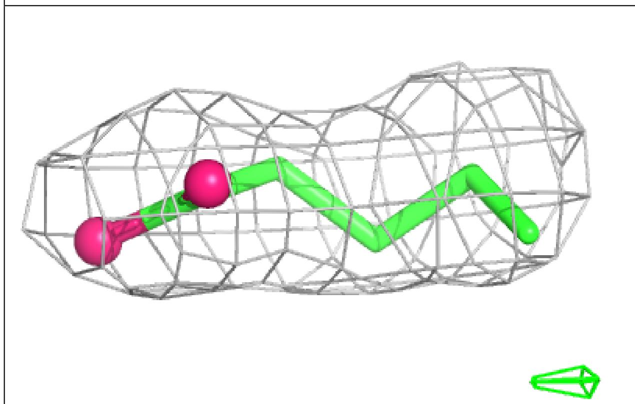


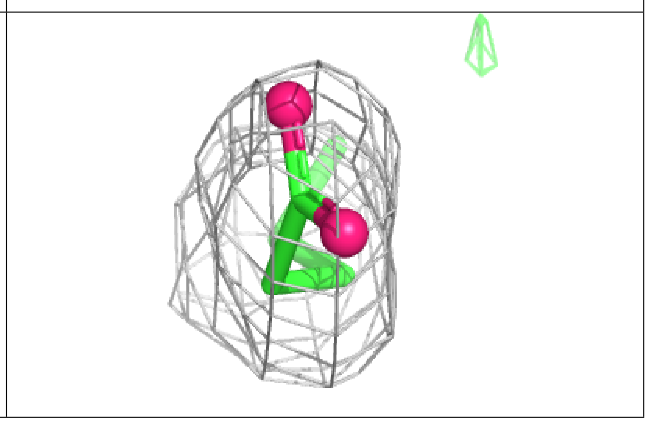


Electron density around OLC B 2010:

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

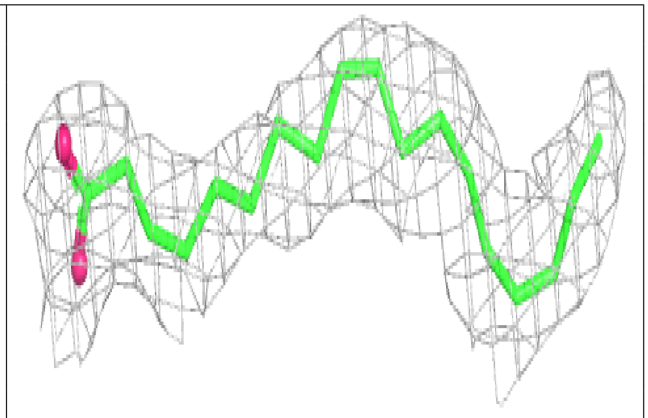


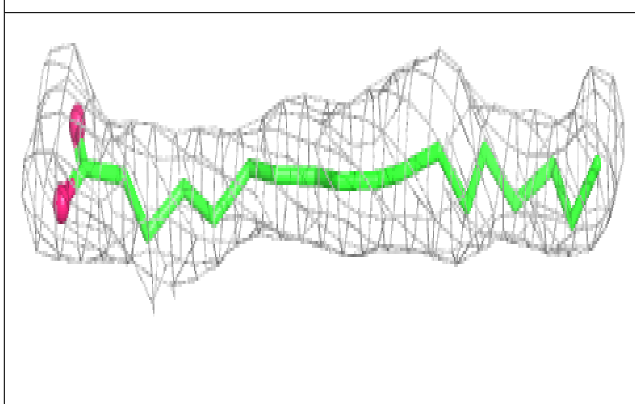


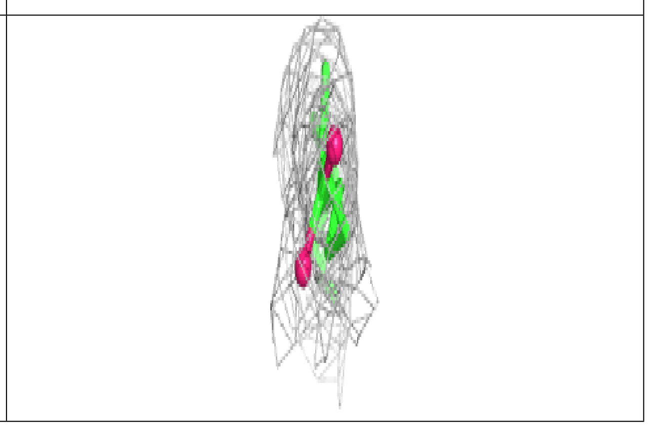


Electron density around OLA A 2019:

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

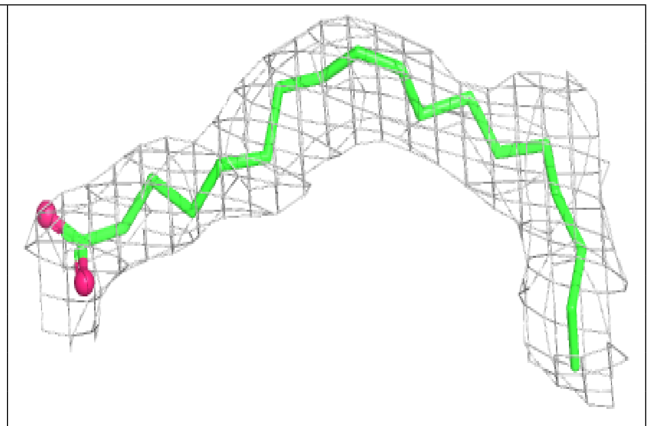


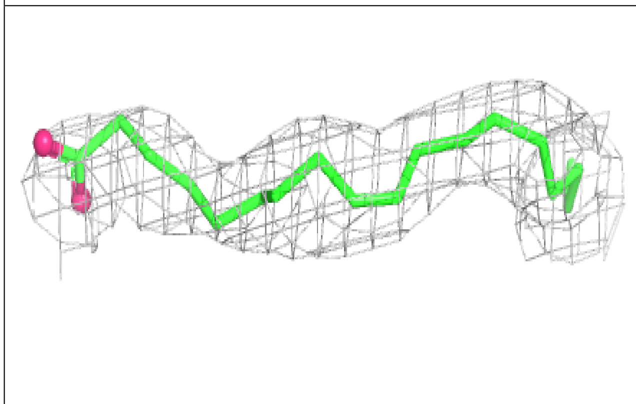


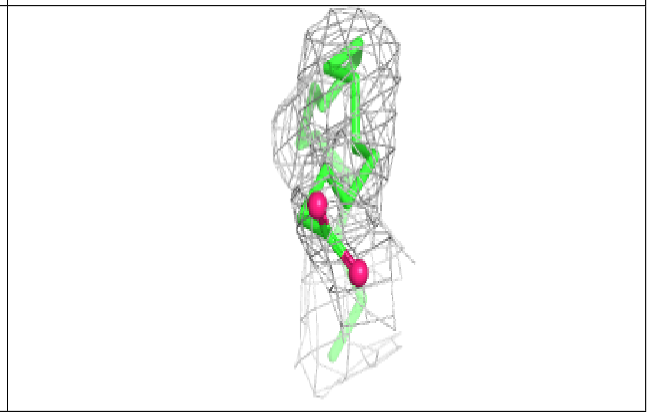


Electron density around OLA A 2016:

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

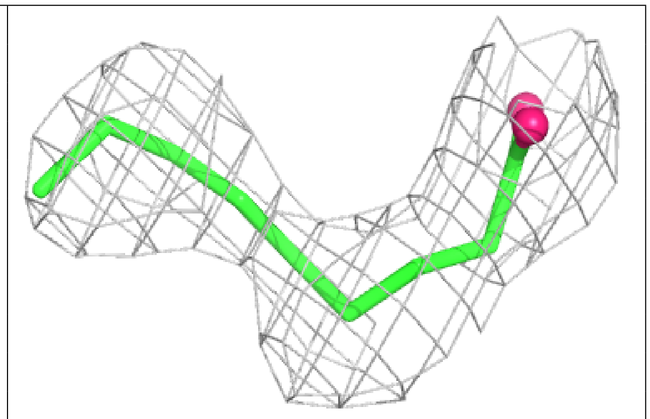


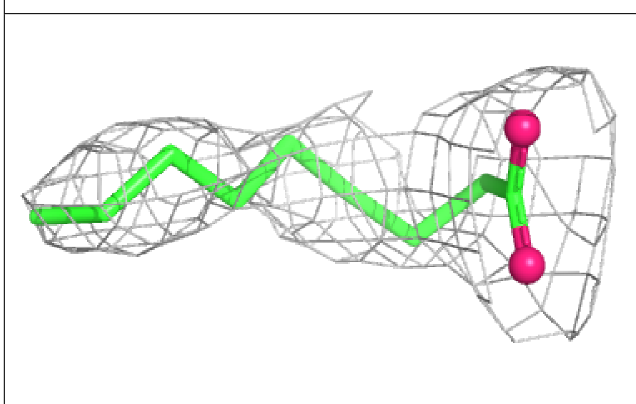


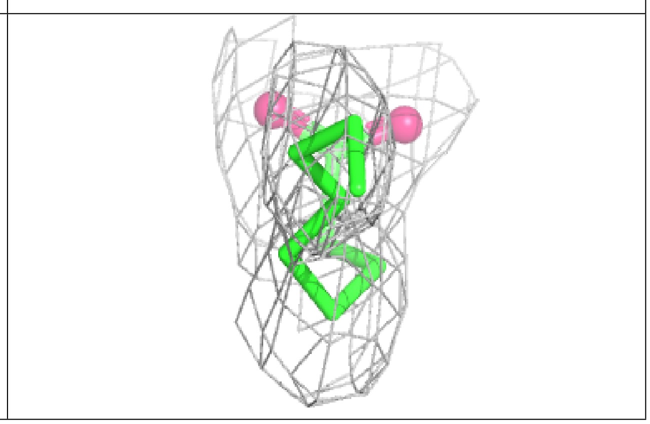


Electron density around OLA B 2015:

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

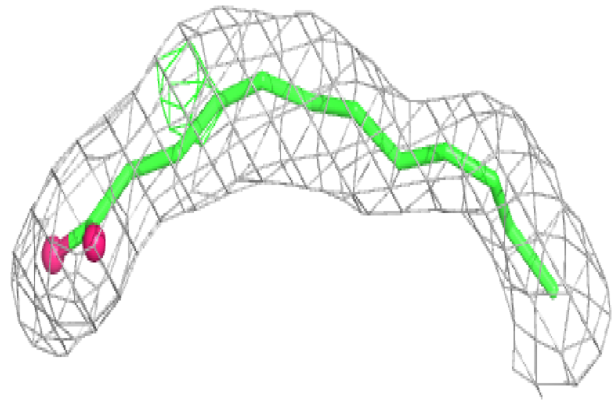


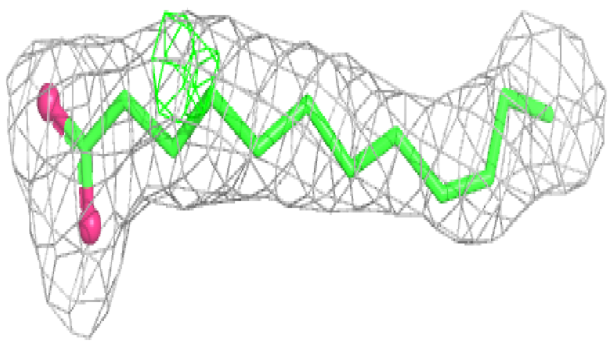


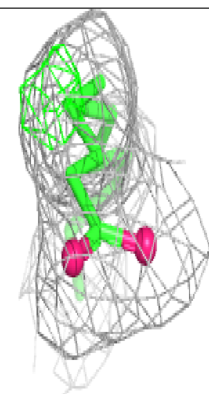


Electron density around OLA A 2020:

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

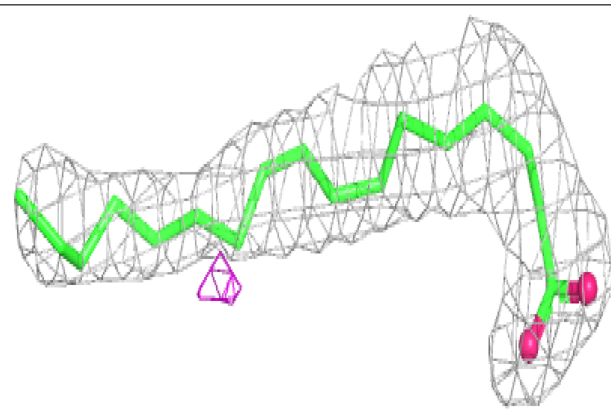


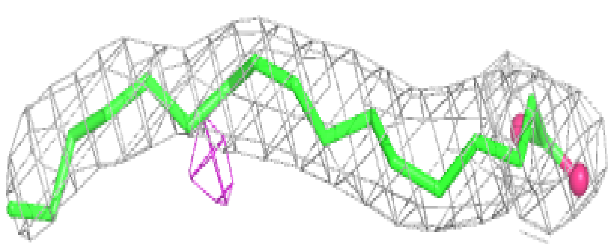


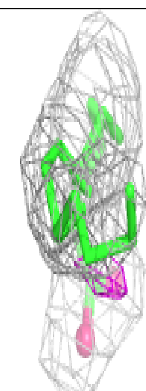


Electron density around OLA A 2013:

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

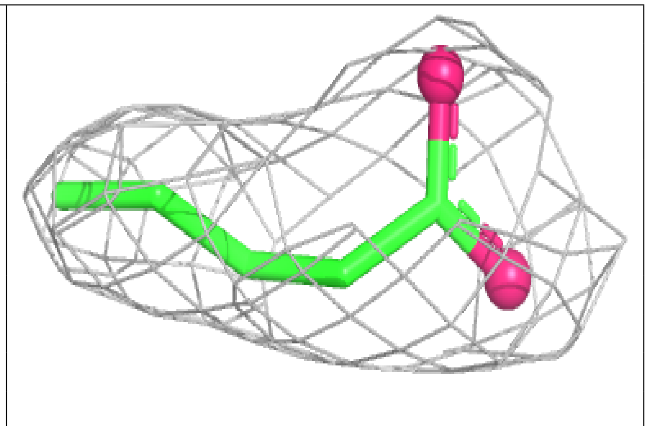


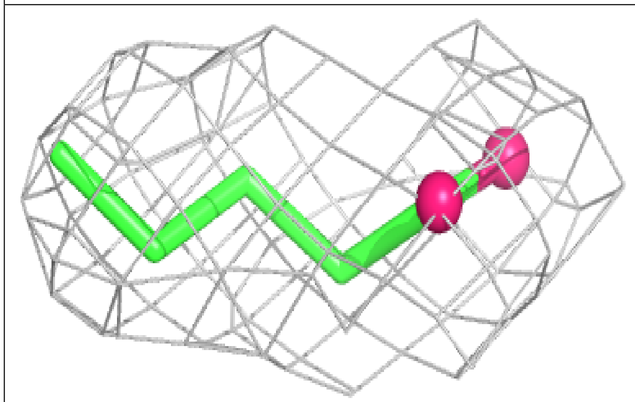


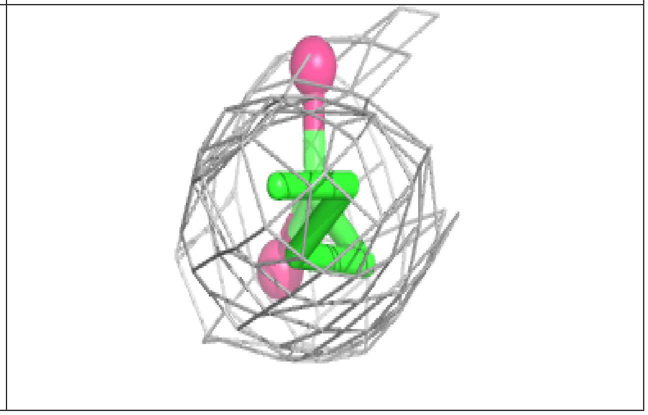


Electron density around OLA A 2014:

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

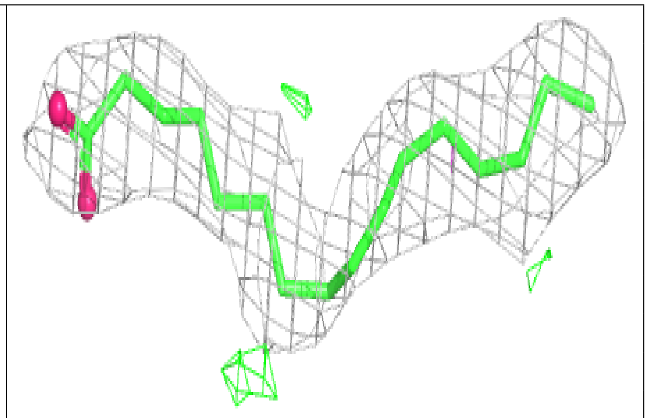


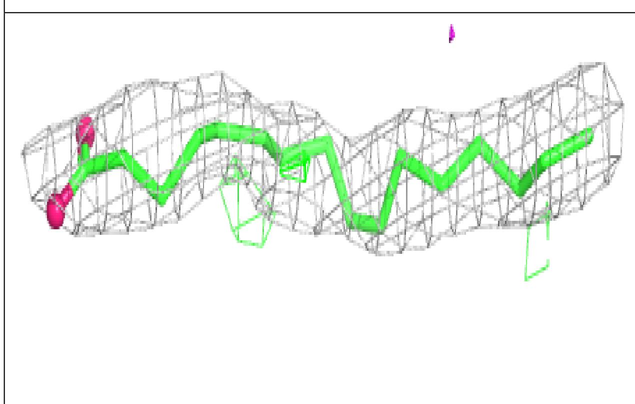


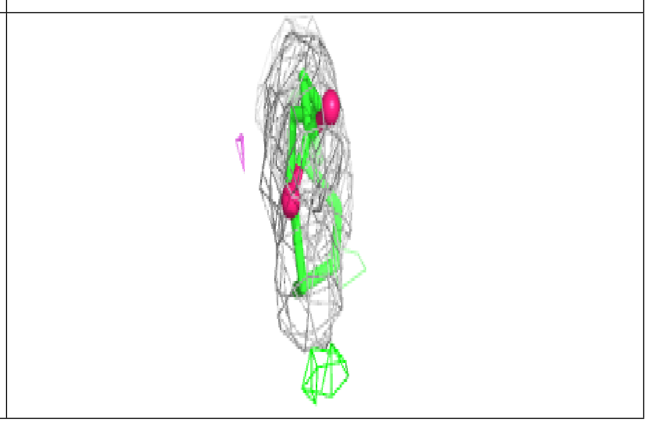


Electron density around OLA B 2017:

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

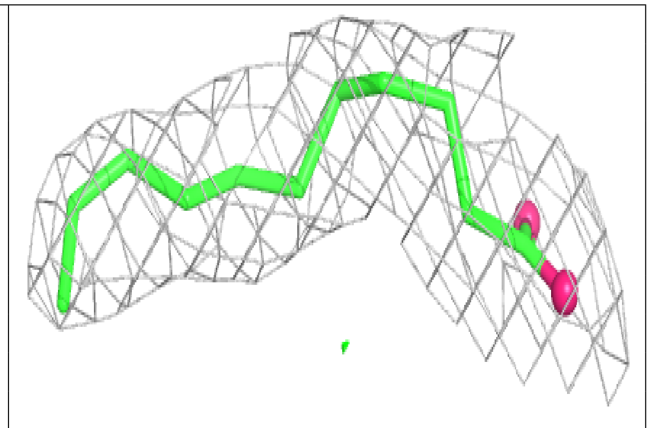


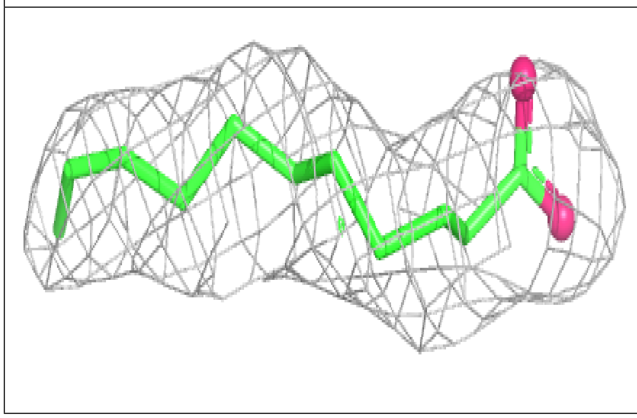


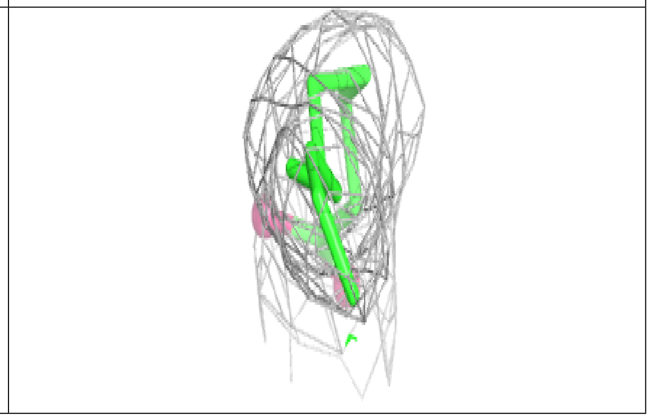


Electron density around OLA A 2011:

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

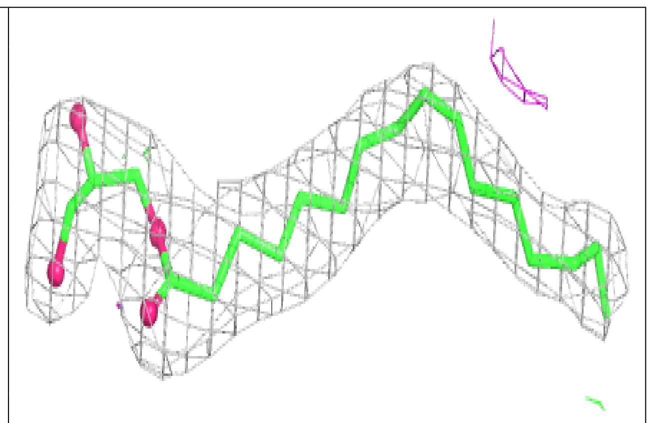


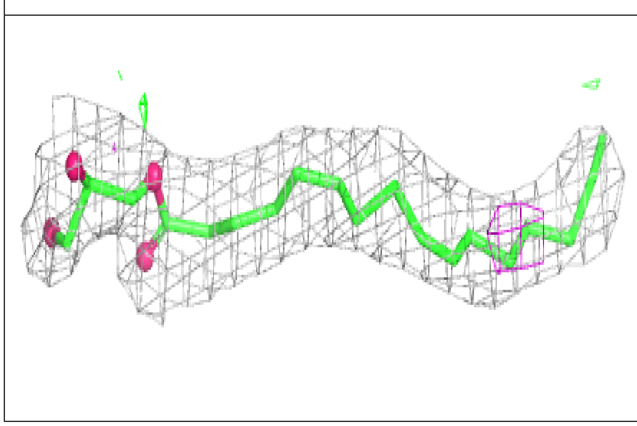


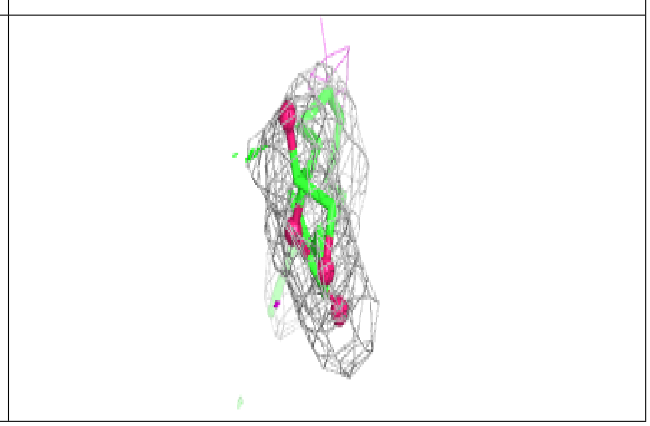


Electron density around OLC B 2009:

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

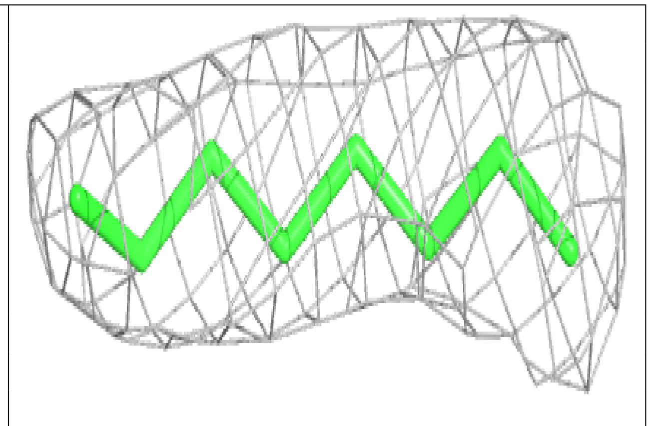


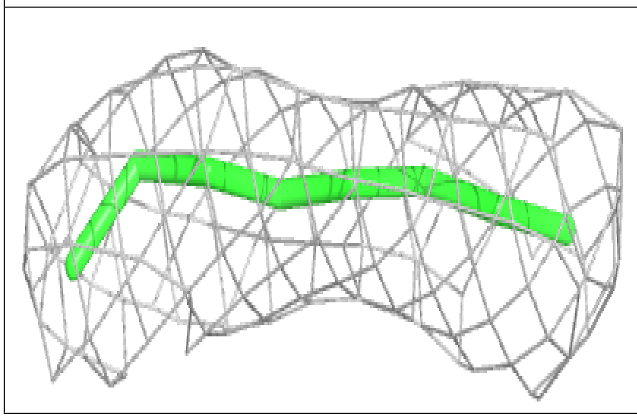


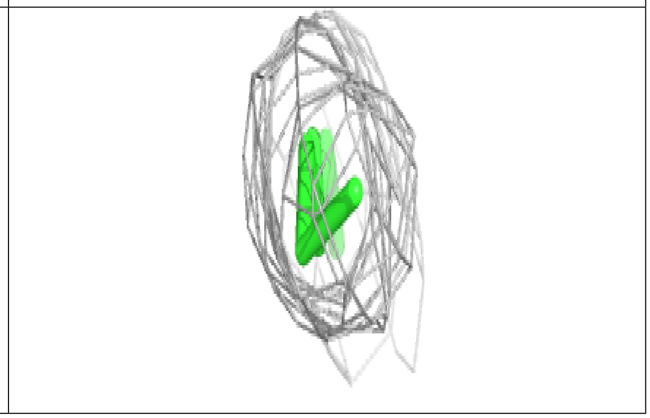


Electron density around OLC B 2002:

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

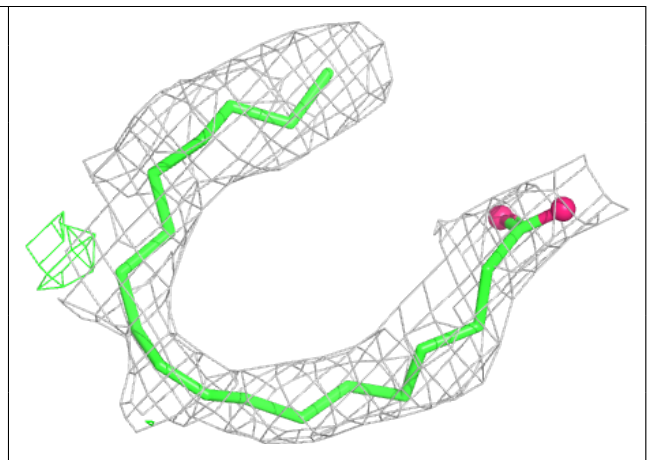


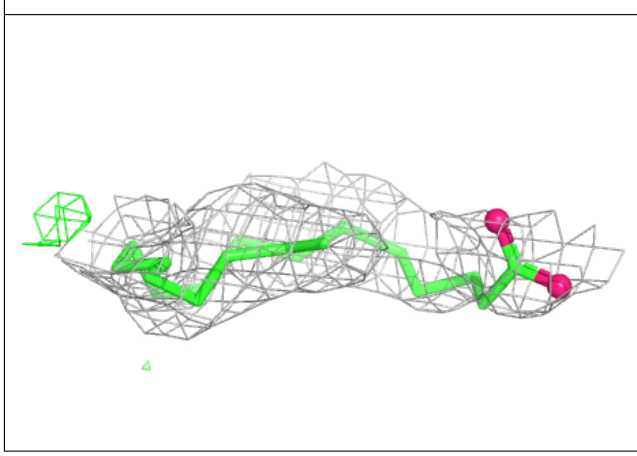


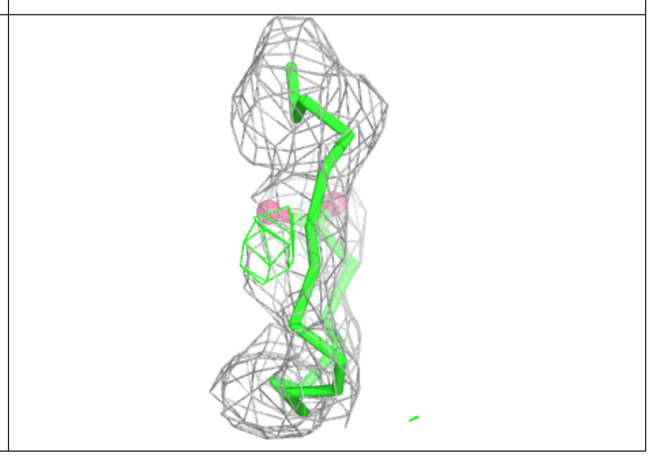


Electron density around OLA B 2018:

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

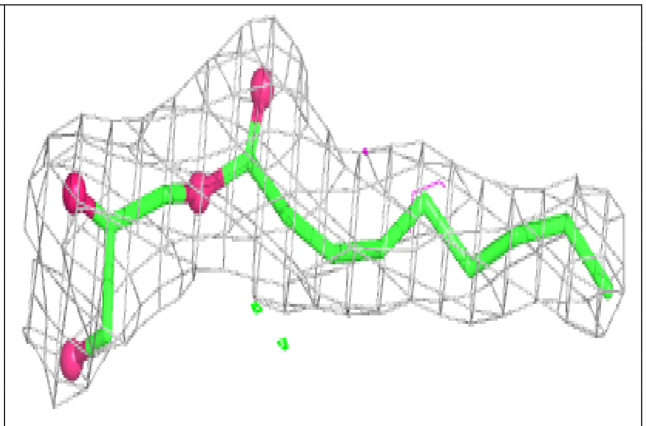


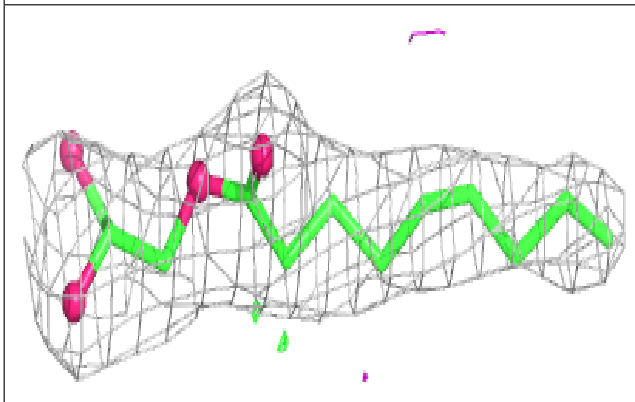


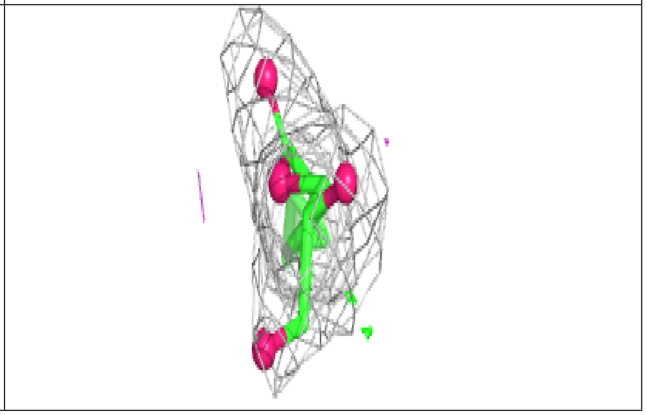


Electron density around OLC A 2007:

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

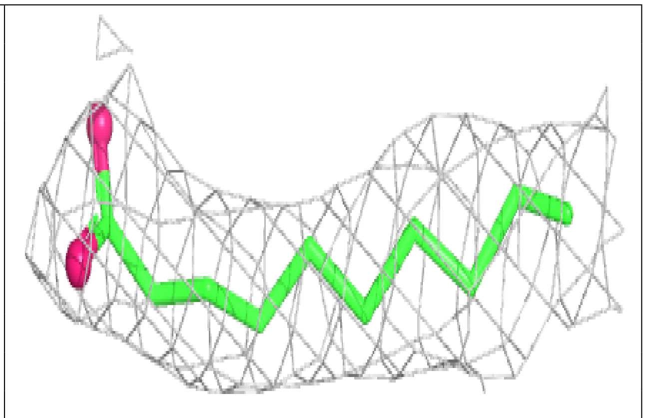


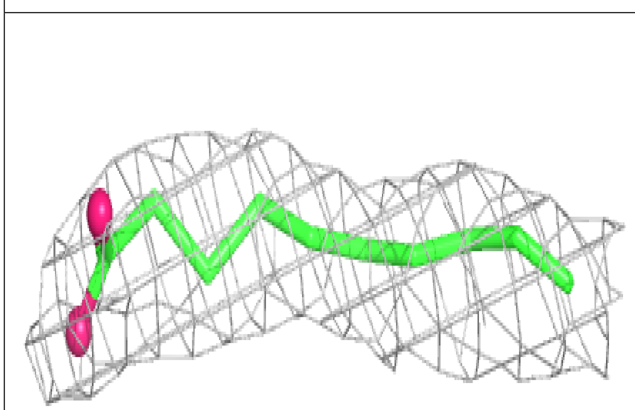


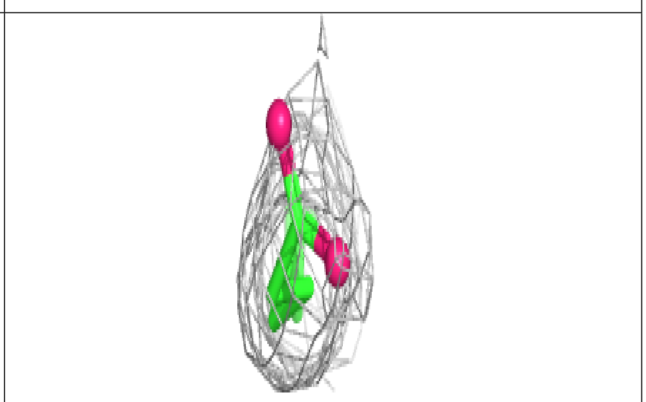


Electron density around OLA B 2011:

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

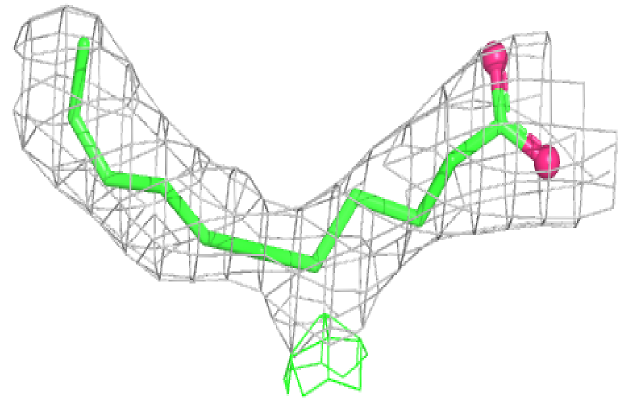


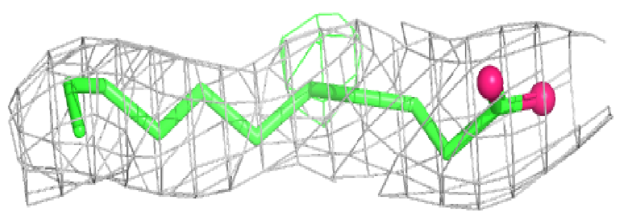


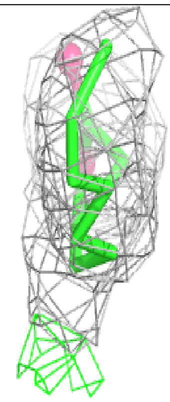


Electron density around OLA A 2017:

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

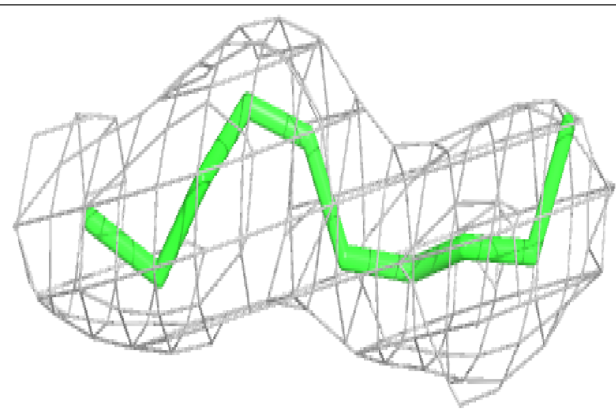


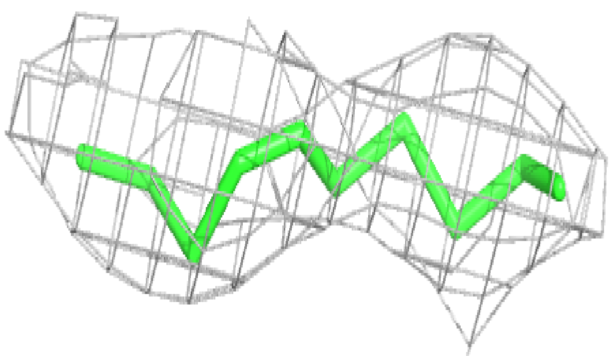


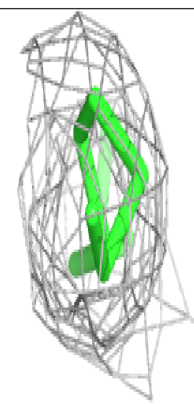


Electron density around OLC B 2005:

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

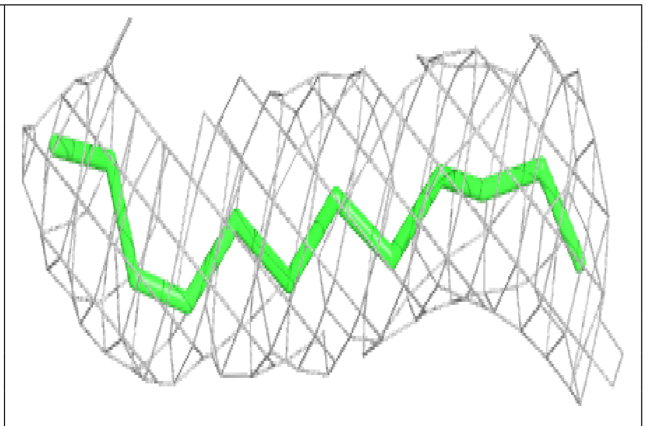


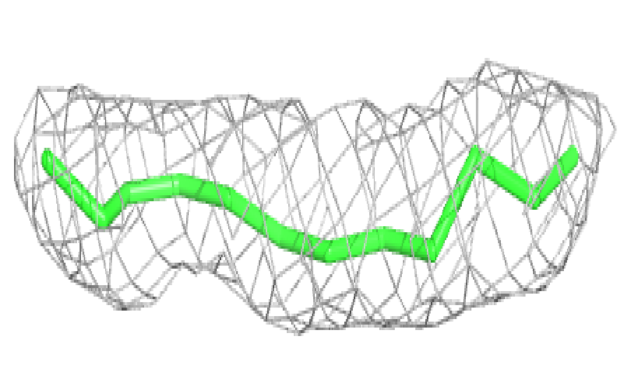


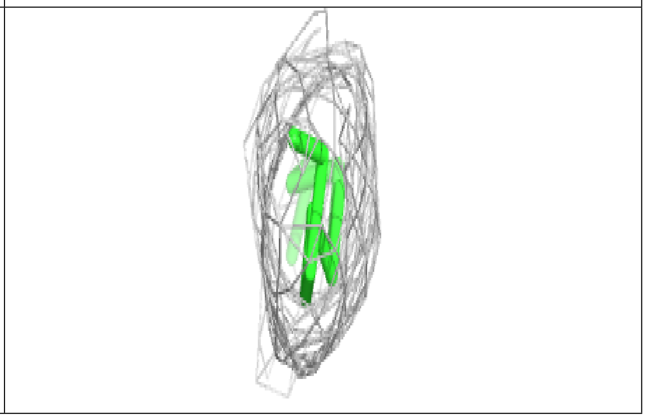


Electron density around OLC A 2006:

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

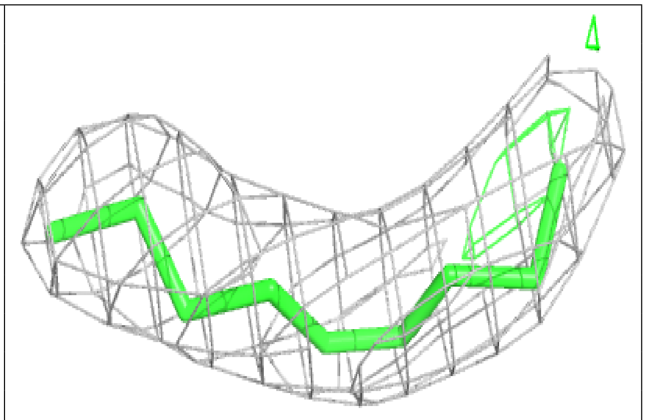


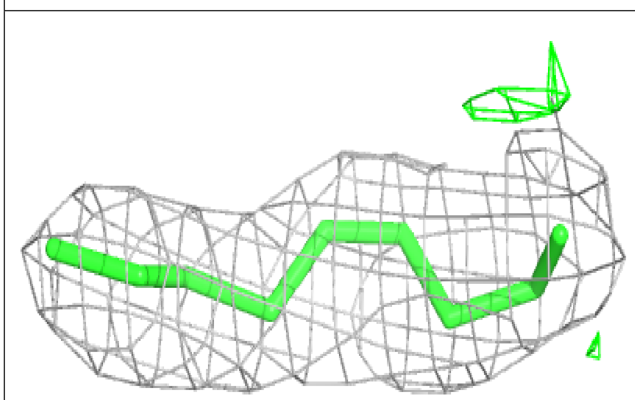


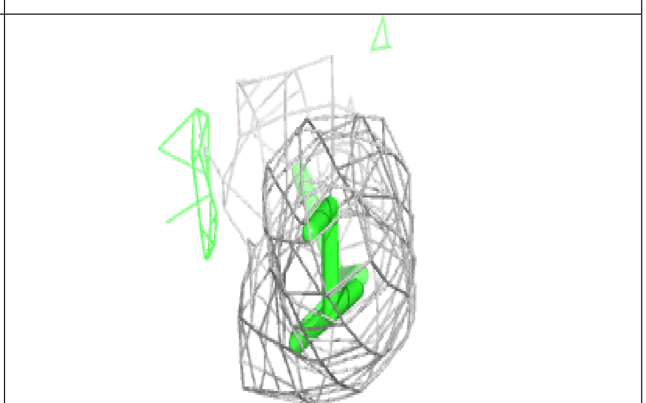


Electron density around OLC A 2002:

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

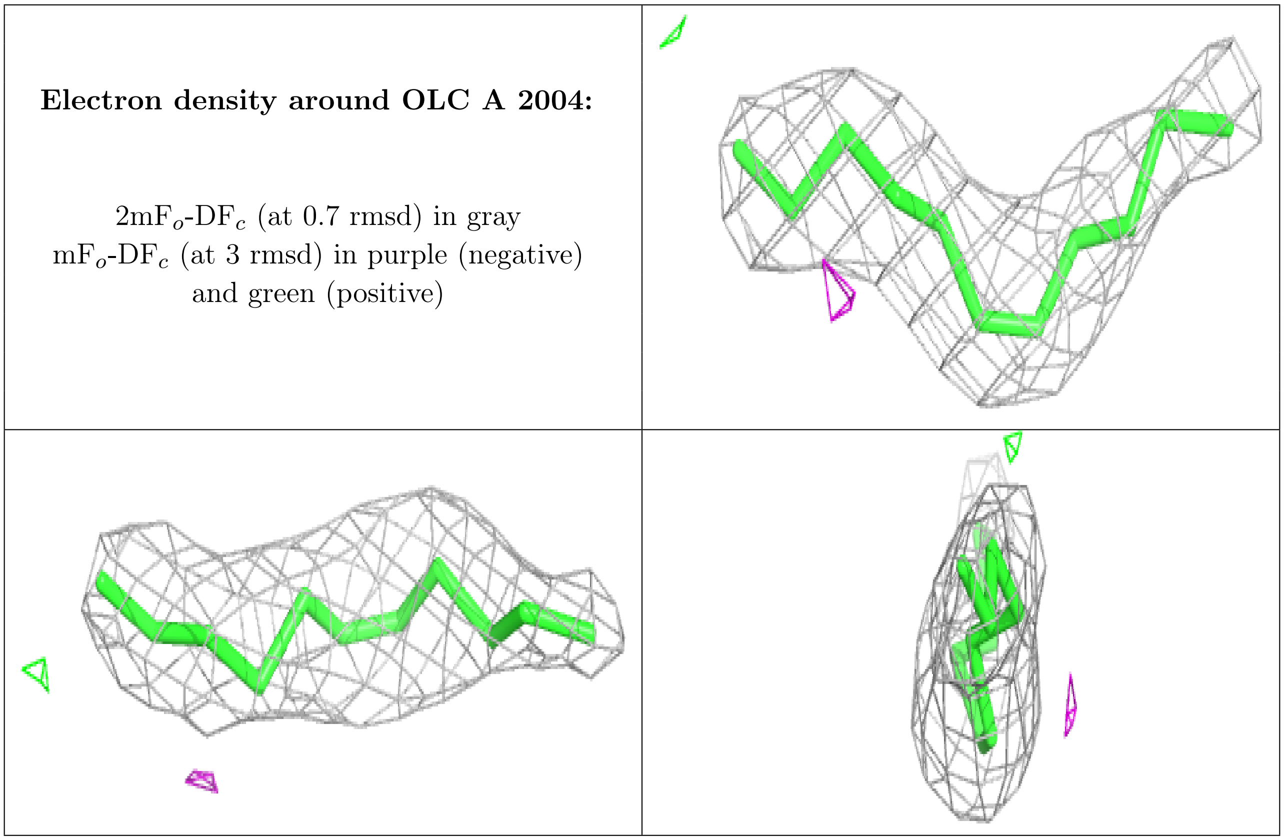






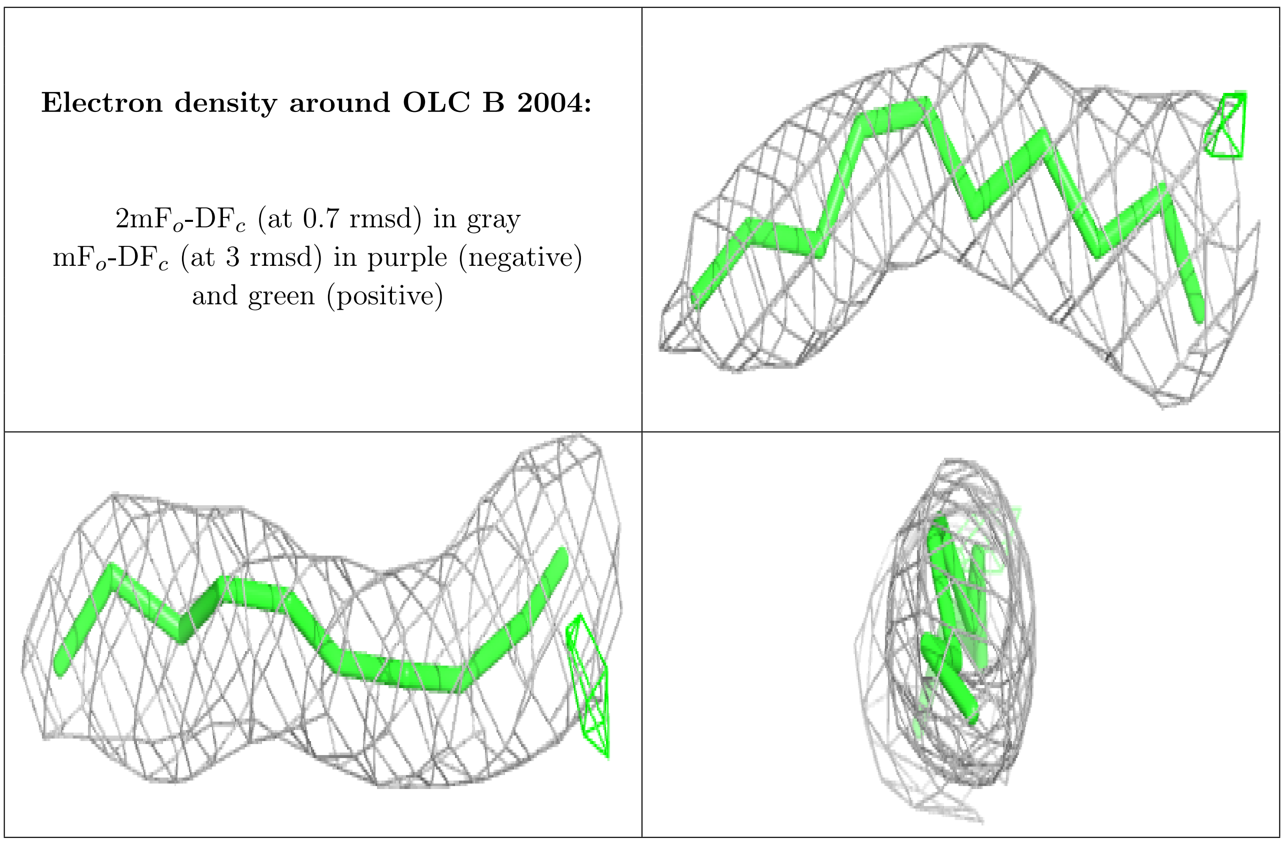
Electron density around OLC A 2004:

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



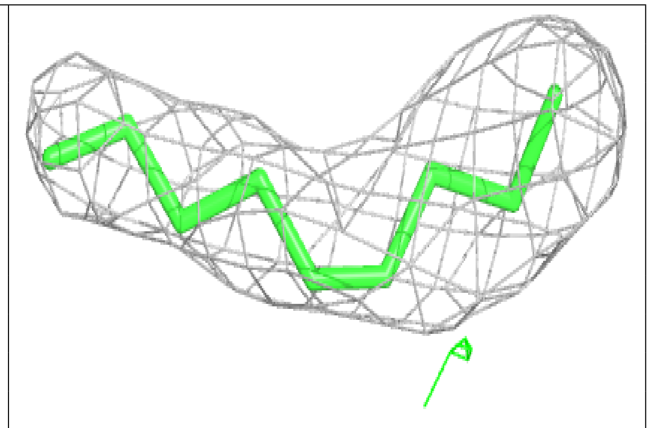
Electron density around OLC B 2004:

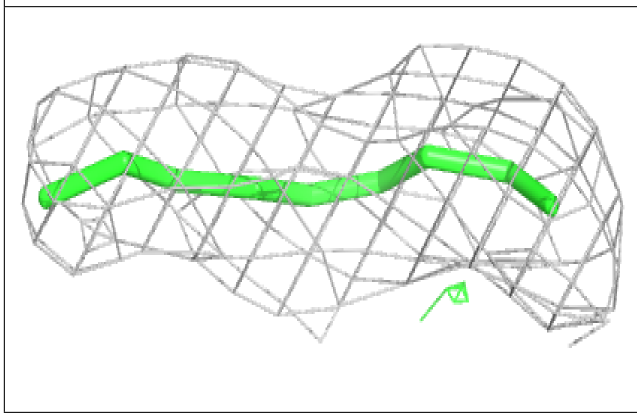
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

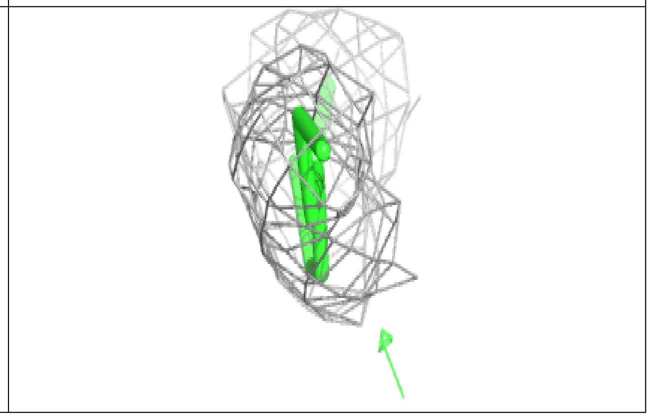


Electron density around OLC A 2008:

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

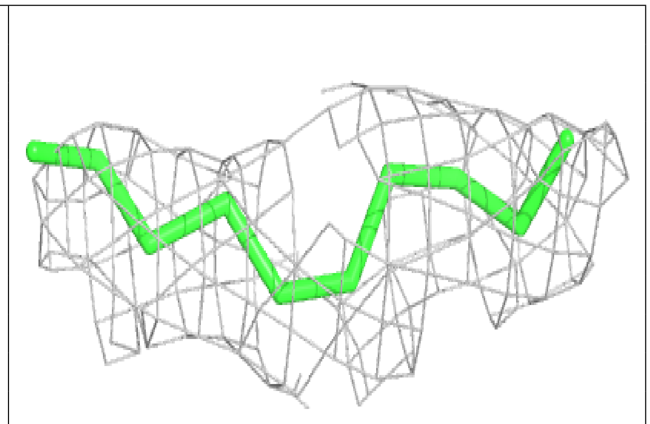


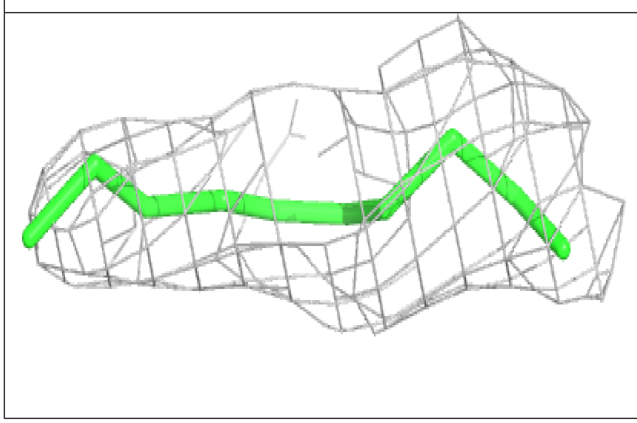


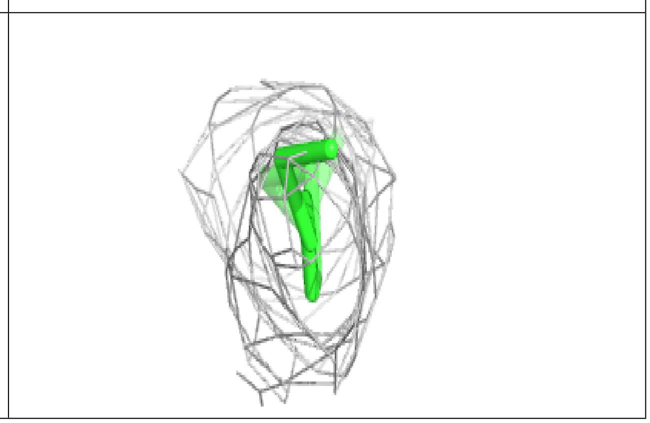


Electron density around OLC B 2006:

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

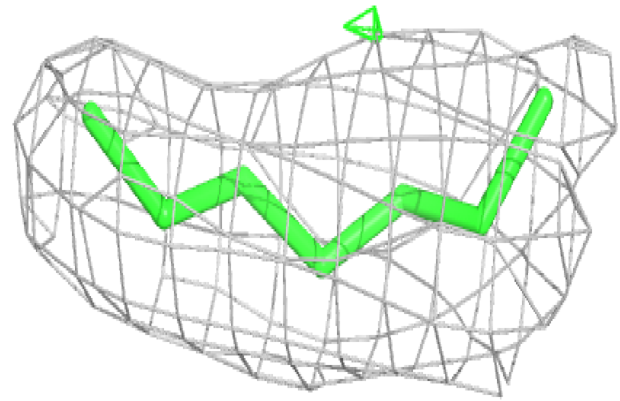


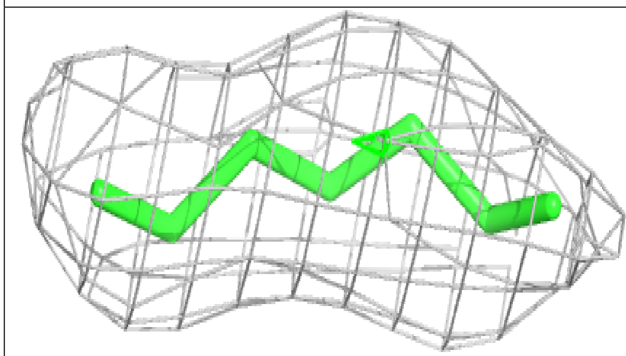


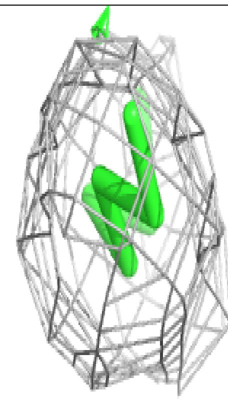


Electron density around OLC B 2008:

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

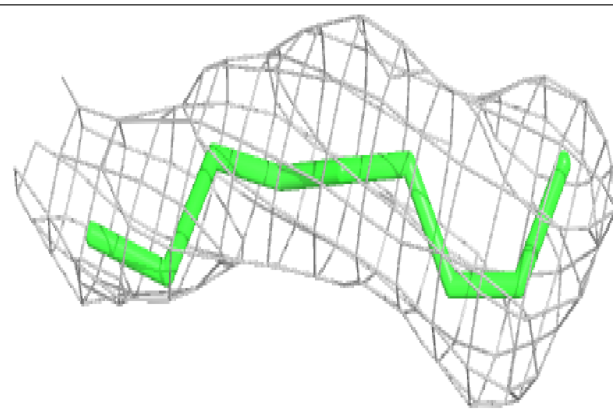


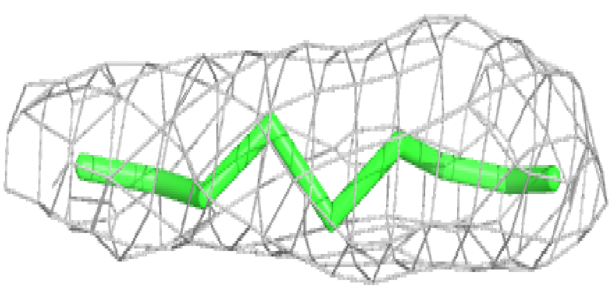


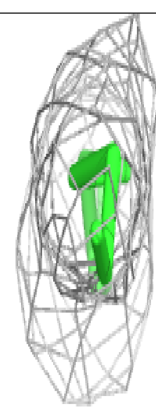


Electron density around OLC B 2003:

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

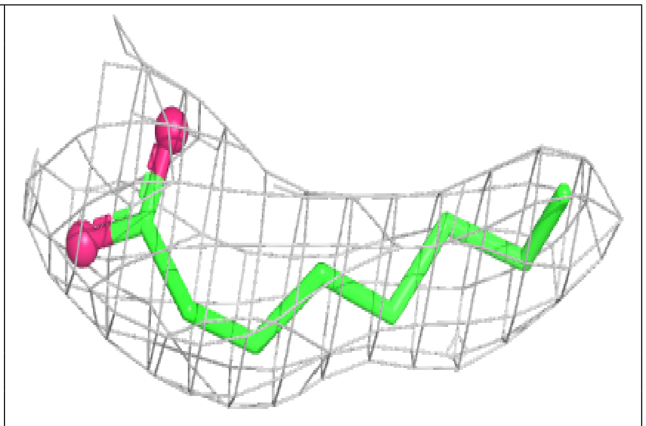


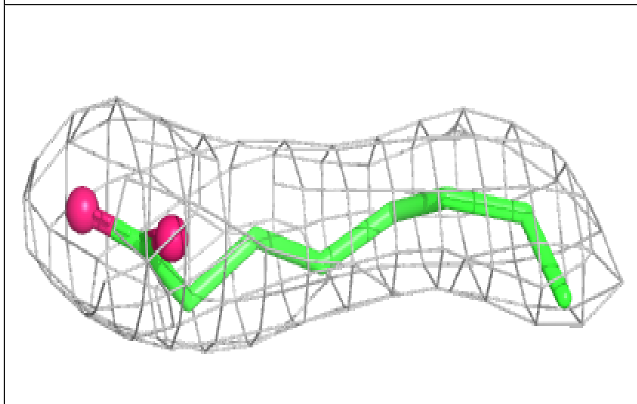


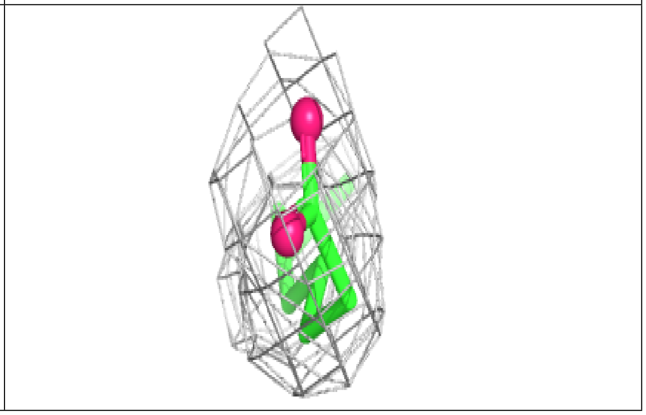


Electron density around OLA B 2012:

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

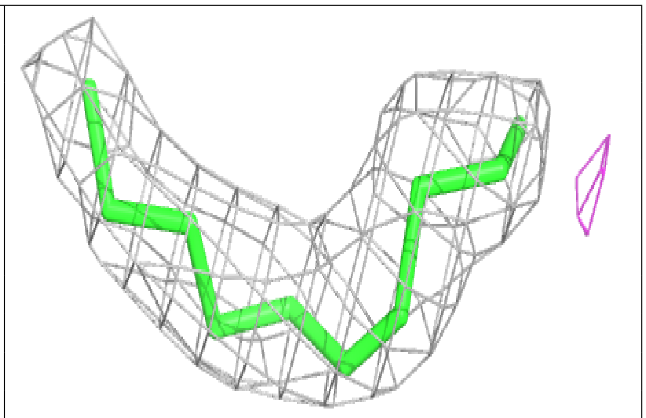


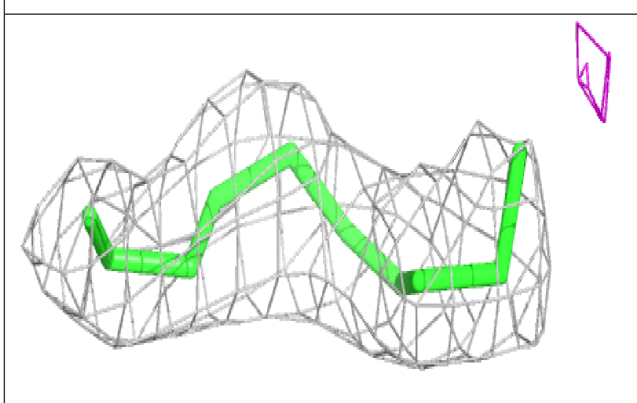


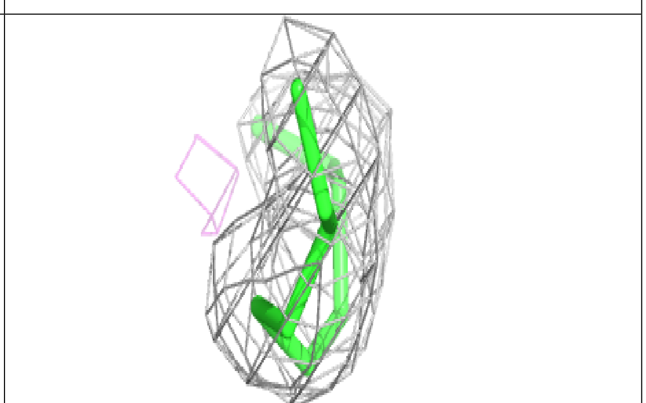


Electron density around OLC B 2007:

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

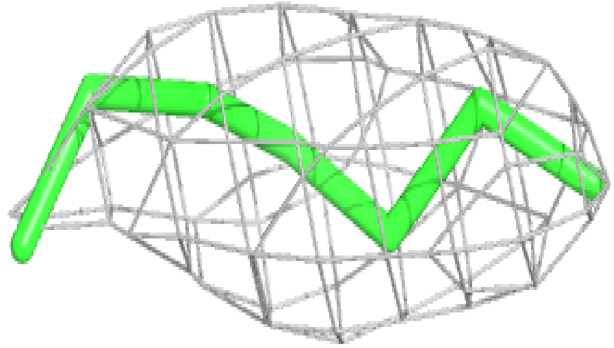


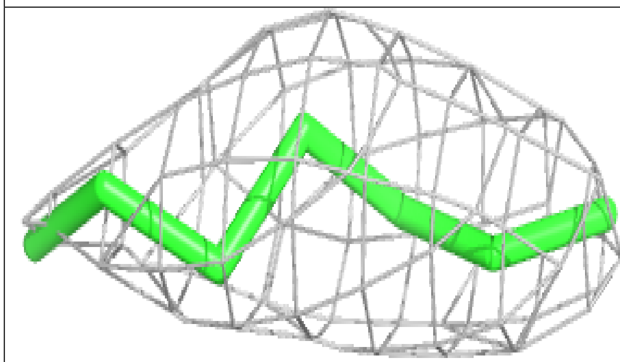


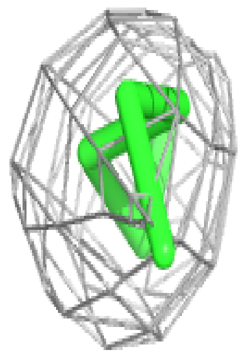


Electron density around OLC A 2009:

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

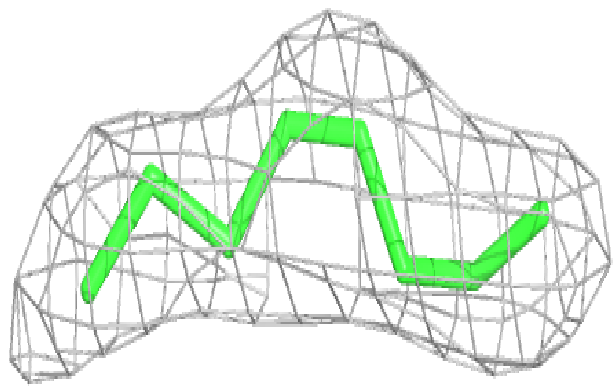


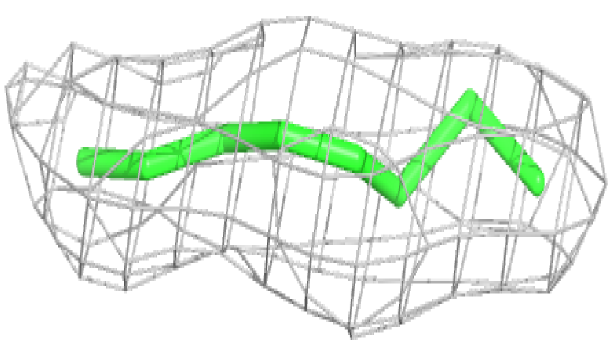


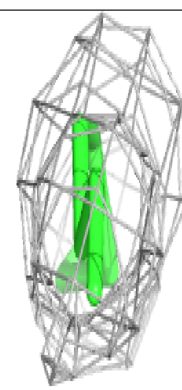


Electron density around OLC A 2005:

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

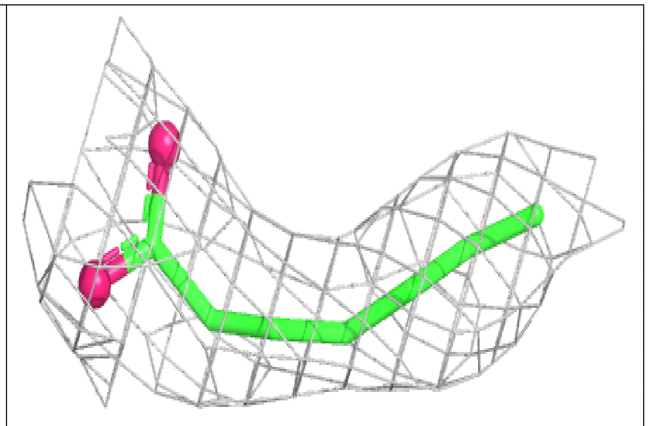


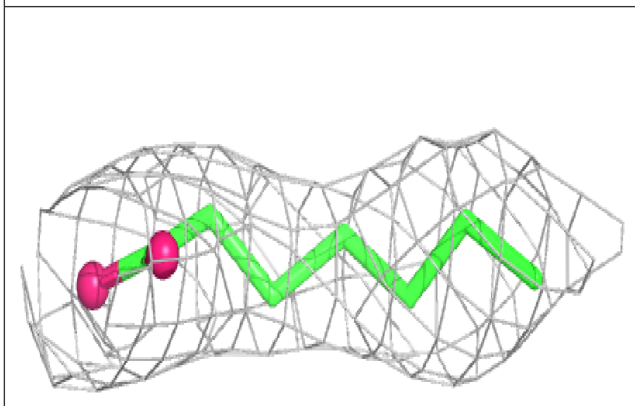


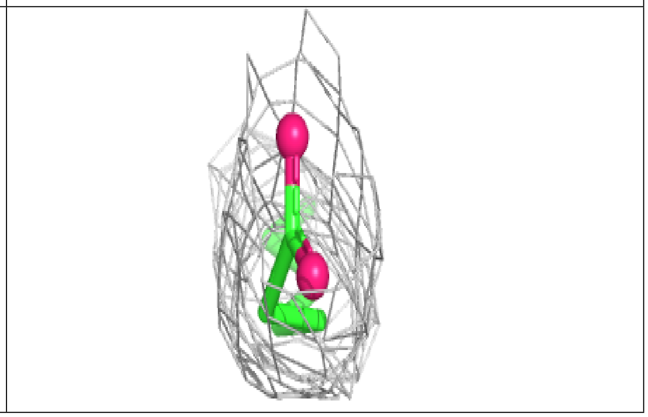


Electron density around OLA B 2014:

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

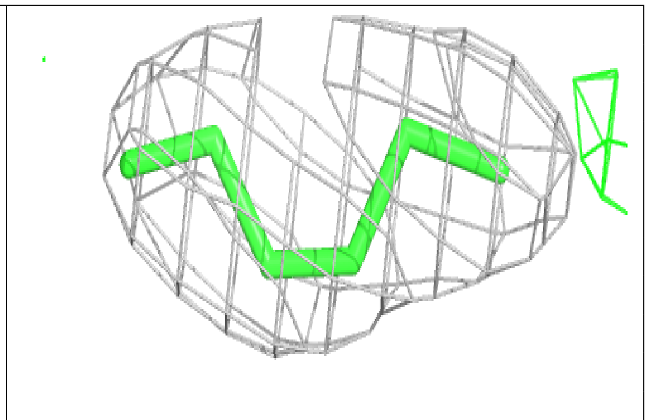


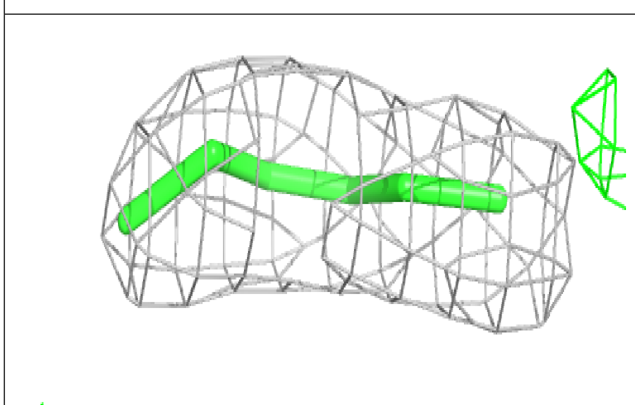


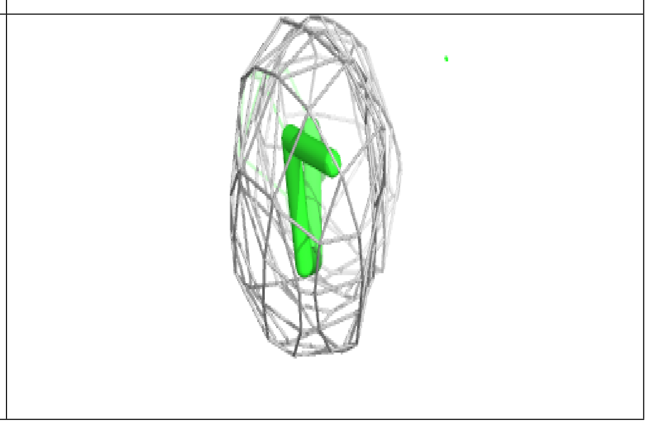


Electron density around OLA A 2018:

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

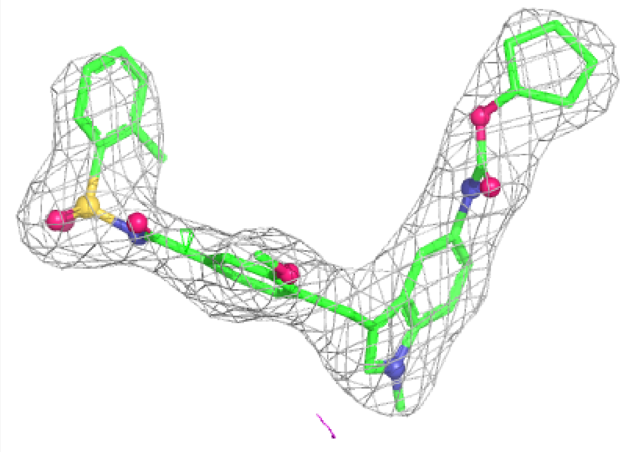


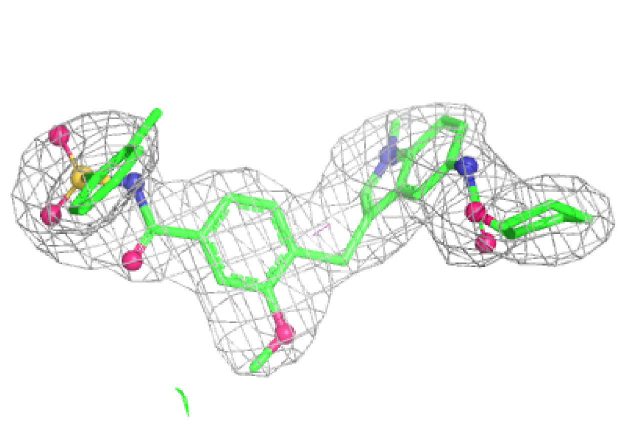


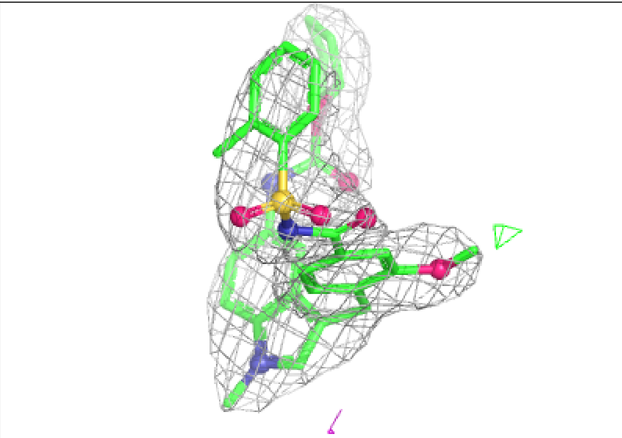


Electron density around ZLK B 2019:

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

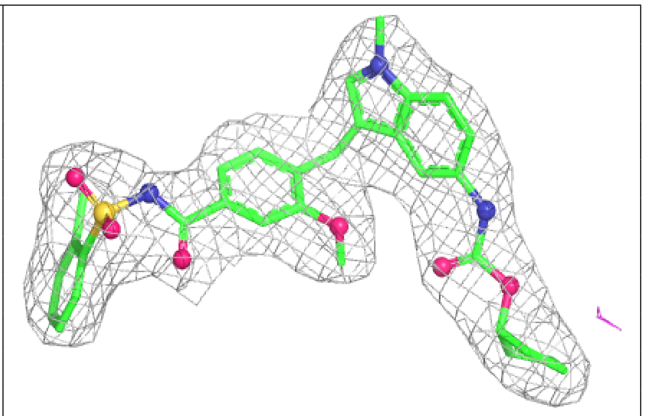


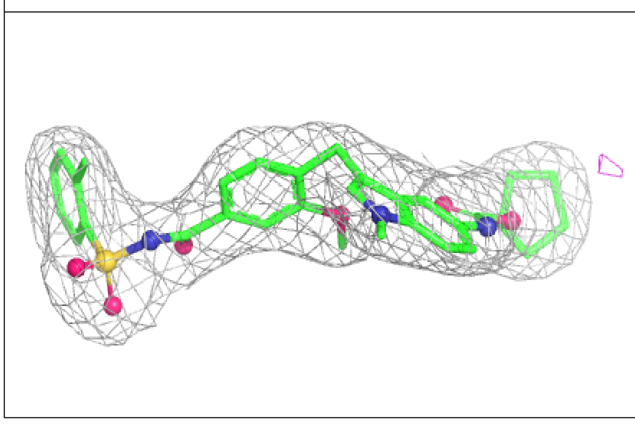


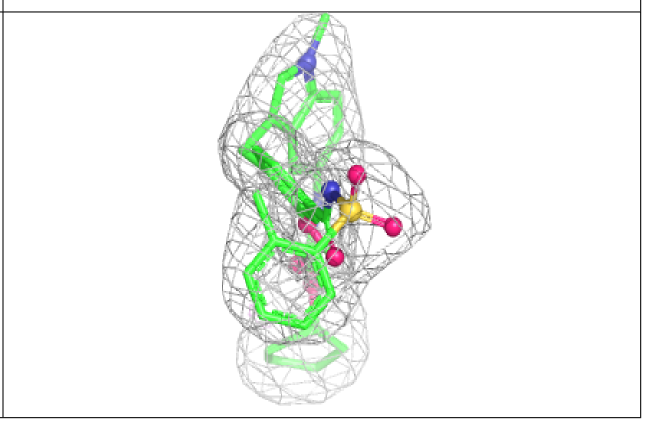


Electron density around ZLK A 2001:

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

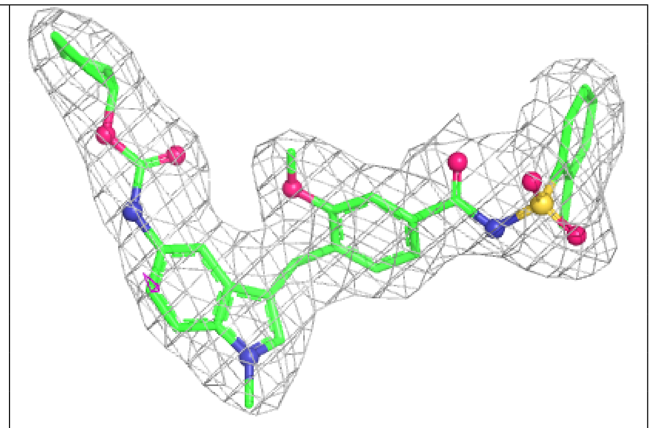


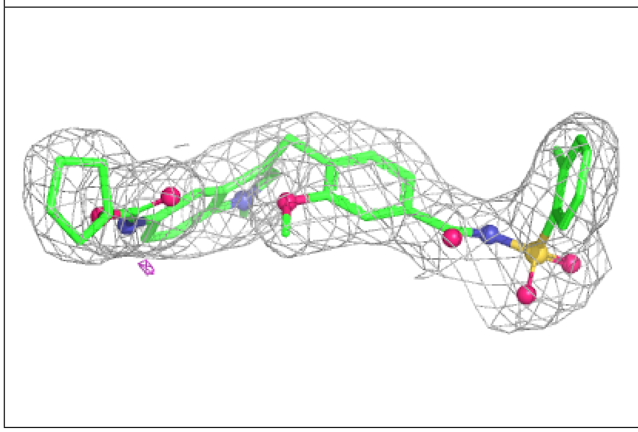


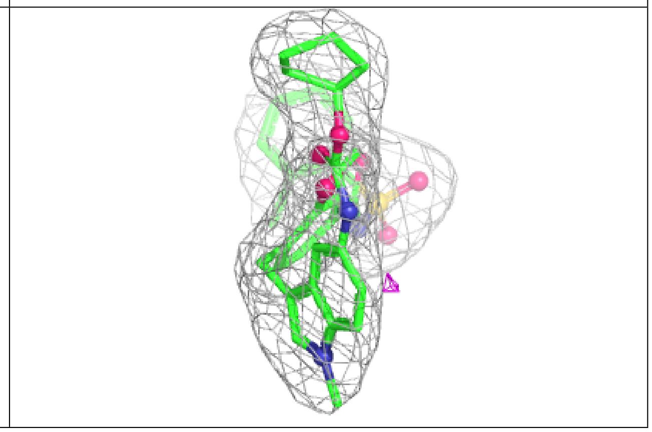


Electron density around ZLK B 2001:

$2mF_o$-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 ⓘ

There are no such residues in this entry.