wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 – 05:14 am GMT

PDB ID	:	6GT3
Title	:	Crystal Structure of the A2A-StaR2-bRIL562 in complex with AZD4635 at 2.0A resolution
Authors	:	Borodovsky, A.; Wang, Y.; Deng, N.; Ye, M.; Stephen, T.L.; Goodwin, K.; Goodwin, R.; Strittmatter, N.; Shaw, J.; Sachsenmeier, K.; Clarke, J.D.; Hay, C.; Reimer, C.; Andrews, S.P.; Brown, G.A.; Congreve, M.; Cheng, R.K.Y.; Dore, A.S.; Mason, J.S.; Marshall, F.H.; Weir, M.P.; Lyne, P.; Woessner, R.
Deposited on	:	2018-06-15
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

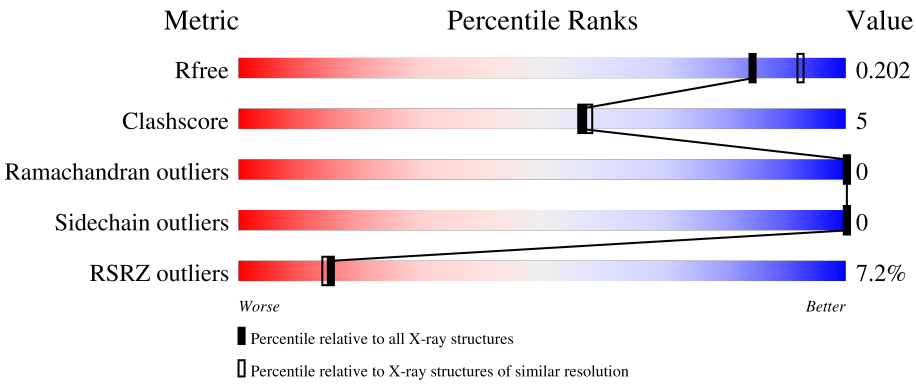
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

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

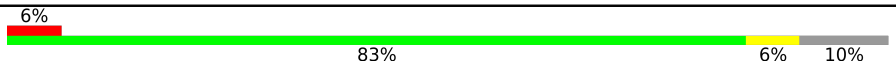
The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	

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:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	F9Q	A	2401	-	X	-	-
6	OLC	A	2420	X	-	-	-
6	OLC	A	2421	X	-	-	-
6	OLC	A	2422	X	-	-	-
6	OLC	A	2423	X	-	-	-
6	OLC	A	2424	X	-	-	-
6	OLC	A	2425	X	-	-	-
6	OLC	A	2426	X	-	-	-
6	OLC	A	2427	X	-	-	-
6	OLC	A	2428	X	-	-	-
6	OLC	A	2429	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3812 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 Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3165	2065	530	545	25	0	23	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274
A	54	LEU	ALA	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	318	ALA	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274

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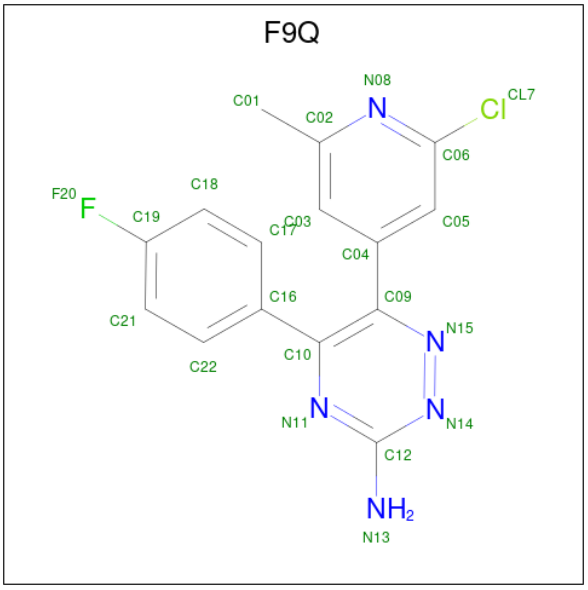
Chain	Residue	Modelled	Actual	Comment	Reference
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

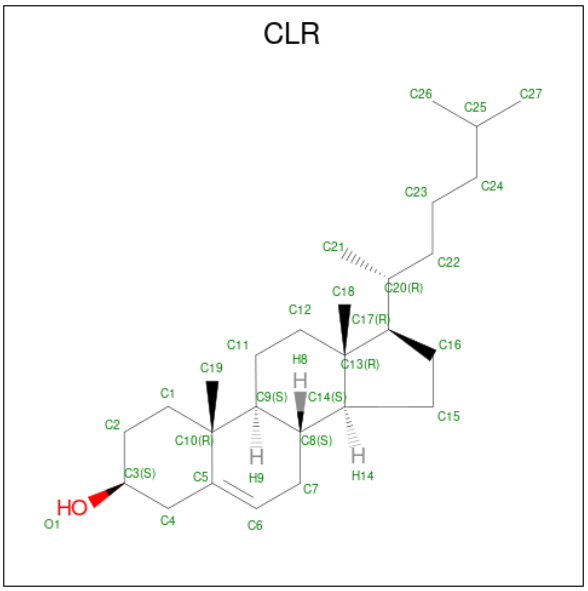
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0

- Molecule 3 is 6-(2-chloranyl-6-methyl-pyridin-4-yl)-5-(4-fluorophenyl)-1,2,4-triazin-3-amine (three-letter code: F9Q) (formula: $C_{15}H_{11}ClFN_5$) (labeled as "Ligand of Interest" by depositor).



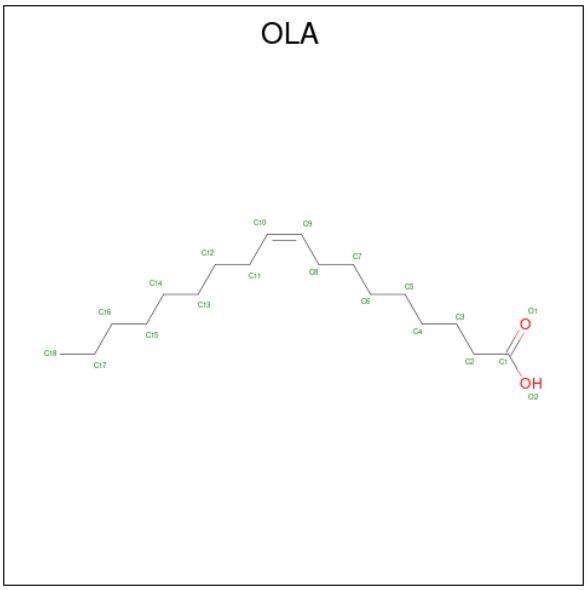
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	F	N		
3	A	1	22	15	1	1	5	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	20	18	2	0	0

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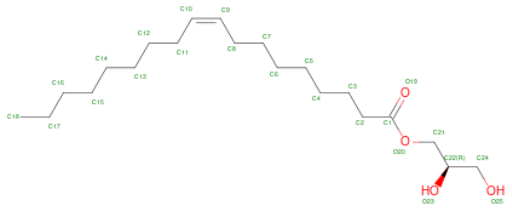
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	15	13	2	0	0
			Total	C	O		
5	A	1	9	7	2	0	0
			Total	C	O		
5	A	1	9	7	2	0	0
			Total	C	O		
5	A	1	9	7	2	0	0
			Total	C	O		
5	A	1	18	16	2	0	0
			Total	C	O		
5	A	1	20	18	2	0	0
			Total	C	O		
5	A	1	15	13	2	0	0
			Total	C	O		
5	A	1	12	10	2	0	0
			Total	C	O		
5	A	1	8	6	2	0	0
			Total	C	O		
5	A	1	11	9	2	0	0
			Total	C	O		
5	A	1	14	12	2	0	0
			Total	C	O		
5	A	1	13	11	2	0	0
			Total	C	O		
5	A	1	19	17	2	0	0
			Total	C	O		
5	A	1	9	7	2	0	0

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).

OLC



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	17	13	4	0	0
			Total	C	O		
6	A	1	23	19	4	0	0
			Total	C	O		
6	A	1	16	12	4	0	0
			Total	C	O		
6	A	1	14	10	4	0	0
			Total	C	O		
6	A	1	15	11	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	25	21	4	0	0
			Total	C	O		
6	A	1	25	21	4	0	0
			Total	C	O		
6	A	1	24	20	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0

- Molecule 7 is water.

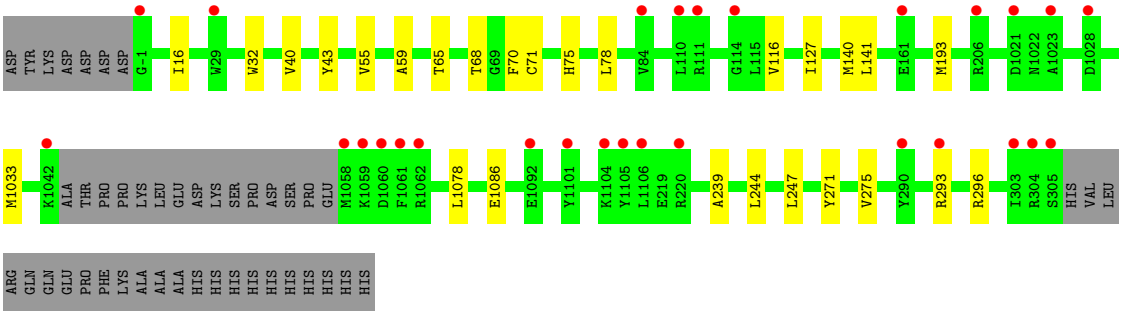
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	136	136	136	0	0

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: Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.55Å 179.71Å 140.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.80 – 2.00 33.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (33.80-2.00) 97.9 (33.86-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.183 , 0.201 0.184 , 0.202	Depositor DCC
R_{free} test set	1711 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.9	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	3812	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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, OLC, OLA, F9Q, NA

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	0.22	0/3235	0.35	0/4399

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	3165	0	3255	23	0
2	A	1	0	0	0	0
3	A	22	0	0	0	0
4	A	84	0	138	3	0
5	A	201	0	271	11	0
6	A	203	0	279	18	0
7	A	136	0	0	2	0
All	All	3812	0	3943	38	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 38 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)
6:A:2421:OLC:H3	6:A:2426:OLC:H24A	1.32	1.03
1:A:75:HIS:HB2	6:A:2424:OLC:H21A	1.60	0.81
1:A:1033:MET:O	7:A:2501:HOH:O	2.08	0.71
6:A:2428:OLC:H13	6:A:2429:OLC:C15	2.30	0.61
5:A:2411:OLA:H122	6:A:2421:OLC:C16	2.31	0.61

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	407/433 (94%)	405 (100%)	2 (0%)	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	335/353 (95%)	335 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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	$\#\|Z\| > 2$
6	OLC	A	2421	-	22,22,24	0.82	1 (4%)	23,23,25	1.86	5 (21%)
6	OLC	A	2427	-	24,24,24	0.79	1 (4%)	25,25,25	1.78	5 (20%)
6	OLC	A	2429	-	21,21,24	0.84	1 (4%)	22,22,25	1.90	5 (22%)
5	OLA	A	2418	-	18,18,19	0.67	0	18,18,19	0.78	1 (5%)
4	CLR	A	2402	-	31,31,31	0.65	0	48,48,48	1.05	2 (4%)
5	OLA	A	2410	-	17,17,19	0.68	0	17,17,19	0.80	1 (5%)
5	OLA	A	2405	-	19,19,19	0.67	0	19,19,19	0.75	1 (5%)
5	OLA	A	2416	-	13,13,19	0.58	0	12,13,19	1.06	2 (16%)
5	OLA	A	2408	-	8,8,19	0.86	0	8,8,19	1.12	1 (12%)
4	CLR	A	2403	-	31,31,31	0.70	0	48,48,48	0.90	0
5	OLA	A	2414	-	7,7,19	0.91	0	7,7,19	1.20	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CLR	A	2404	-	31,31,31	0.70	0	48,48,48	0.94	1 (2%)
5	OLA	A	2406	-	14,14,19	0.71	0	14,14,19	0.89	1 (7%)
5	OLA	A	2419	-	8,8,19	0.60	0	8,8,19	1.25	2 (25%)
5	OLA	A	2415	-	10,10,19	0.77	0	10,10,19	1.03	1 (10%)
6	OLC	A	2422	-	15,15,24	0.99	1 (6%)	16,16,25	2.24	5 (31%)
5	OLA	A	2417	-	12,12,19	0.76	0	12,12,19	0.97	1 (8%)
6	OLC	A	2423	-	13,13,24	1.06	1 (7%)	14,14,25	2.35	5 (35%)
5	OLA	A	2411	-	19,19,19	0.67	0	19,19,19	0.76	1 (5%)
3	F9Q	A	2401	-	24,24,24	5.26	21 (87%)	33,34,34	2.18	8 (24%)
5	OLA	A	2409	-	8,8,19	0.85	0	8,8,19	1.11	1 (12%)
5	OLA	A	2413	-	11,11,19	0.82	0	11,11,19	1.01	1 (9%)
5	OLA	A	2407	-	8,8,19	0.86	0	8,8,19	1.11	1 (12%)
6	OLC	A	2426	-	24,24,24	0.80	1 (4%)	25,25,25	1.80	5 (20%)
6	OLC	A	2428	-	23,23,24	0.82	1 (4%)	24,24,25	1.83	5 (20%)
6	OLC	A	2425	-	21,21,24	0.84	1 (4%)	22,22,25	1.89	5 (22%)
6	OLC	A	2420	-	16,16,24	0.97	1 (6%)	17,17,25	2.17	5 (29%)
5	OLA	A	2412	-	14,14,19	0.71	0	14,14,19	0.87	1 (7%)
6	OLC	A	2424	-	14,14,24	1.02	1 (7%)	15,15,25	2.28	5 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLC	A	2421	-	1/1/2/4	13/22/22/24	-
6	OLC	A	2427	-	1/1/2/4	14/24/24/24	-
6	OLC	A	2429	-	1/1/2/4	8/21/21/24	-
5	OLA	A	2418	-	-	6/16/16/17	-
4	CLR	A	2402	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2410	-	-	12/15/15/17	-
5	OLA	A	2405	-	-	11/17/17/17	-
5	OLA	A	2416	-	-	5/11/11/17	-
5	OLA	A	2408	-	-	1/6/6/17	-
4	CLR	A	2403	-	-	1/10/68/68	0/4/4/4
5	OLA	A	2414	-	-	1/5/5/17	-
4	CLR	A	2404	-	-	1/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	2406	-	-	9/12/12/17	-
5	OLA	A	2419	-	-	5/6/6/17	-
5	OLA	A	2415	-	-	5/8/8/17	-
6	OLC	A	2423	-	1/1/2/4	5/13/13/24	-
6	OLC	A	2422	-	1/1/2/4	4/15/15/24	-
5	OLA	A	2417	-	-	7/10/10/17	-
5	OLA	A	2411	-	-	9/17/17/17	-
3	F9Q	A	2401	-	-	0/8/8/8	0/3/3/3
5	OLA	A	2409	-	-	1/6/6/17	-
5	OLA	A	2413	-	-	4/9/9/17	-
5	OLA	A	2407	-	-	4/6/6/17	-
6	OLC	A	2426	-	1/1/2/4	14/24/24/24	-
6	OLC	A	2428	-	1/1/2/4	10/23/23/24	-
6	OLC	A	2425	-	1/1/2/4	8/21/21/24	-
6	OLC	A	2420	-	1/1/2/4	8/16/16/24	-
5	OLA	A	2412	-	-	2/12/12/17	-
6	OLC	A	2424	-	1/1/2/4	6/14/14/24	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2401	F9Q	C12-N14	8.55	1.45	1.35
3	A	2401	F9Q	C05-C06	7.73	1.51	1.38
3	A	2401	F9Q	C21-C19	7.54	1.51	1.37
3	A	2401	F9Q	C06-N08	7.49	1.46	1.33
3	A	2401	F9Q	C18-C19	7.49	1.51	1.37

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2401	F9Q	N11-C12-N14	-7.92	120.16	125.57
6	A	2422	OLC	O20-C1-C2	4.56	126.23	111.91
3	A	2401	F9Q	C05-C06-N08	-4.56	120.50	125.50
6	A	2428	OLC	O20-C1-C2	4.46	125.90	111.91
6	A	2421	OLC	O20-C1-C2	4.45	125.88	111.91

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	2420	OLC	C22
6	A	2421	OLC	C22
6	A	2422	OLC	C22
6	A	2423	OLC	C22
6	A	2424	OLC	C22

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2421	OLC	C21-C22-C24-O25
6	A	2422	OLC	O20-C21-C22-O23
6	A	2423	OLC	C21-C22-C24-O25
6	A	2423	OLC	O20-C21-C22-O23
6	A	2425	OLC	O20-C21-C22-O23

There are no ring outliers.

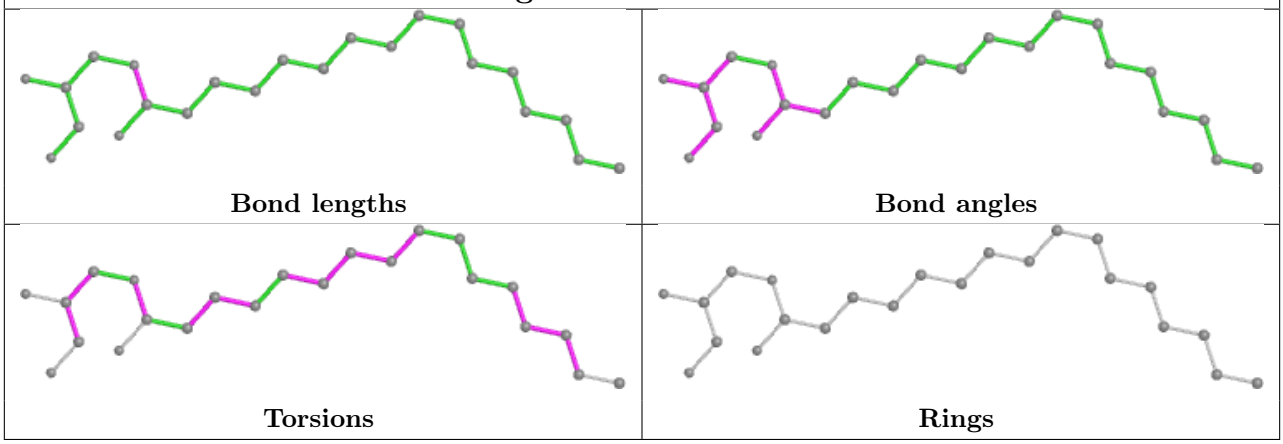
20 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2421	OLC	4	0
6	A	2427	OLC	4	0
6	A	2429	OLC	2	0
5	A	2418	OLA	1	0
4	A	2402	CLR	1	0
5	A	2410	OLA	3	0
5	A	2405	OLA	1	0
5	A	2416	OLA	1	0
4	A	2403	CLR	1	0
4	A	2404	CLR	1	0
6	A	2422	OLC	2	0
5	A	2417	OLA	1	0
5	A	2411	OLA	3	0
5	A	2407	OLA	1	0
6	A	2426	OLC	3	0
6	A	2428	OLC	3	0
6	A	2425	OLC	2	0
6	A	2420	OLC	2	0
5	A	2412	OLA	1	0
6	A	2424	OLC	1	0

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

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand OLC A 2421



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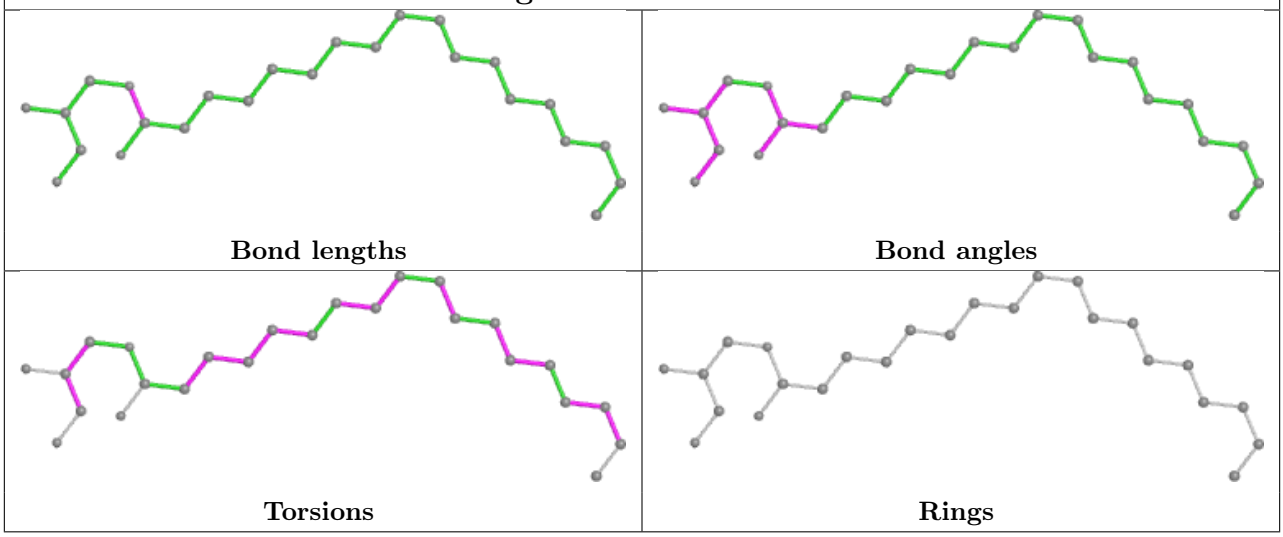

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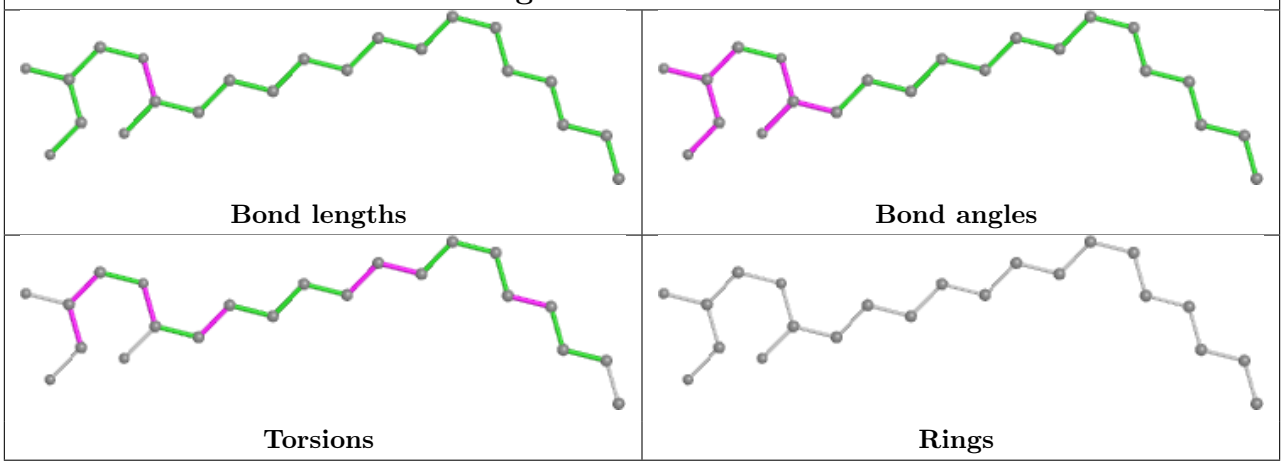

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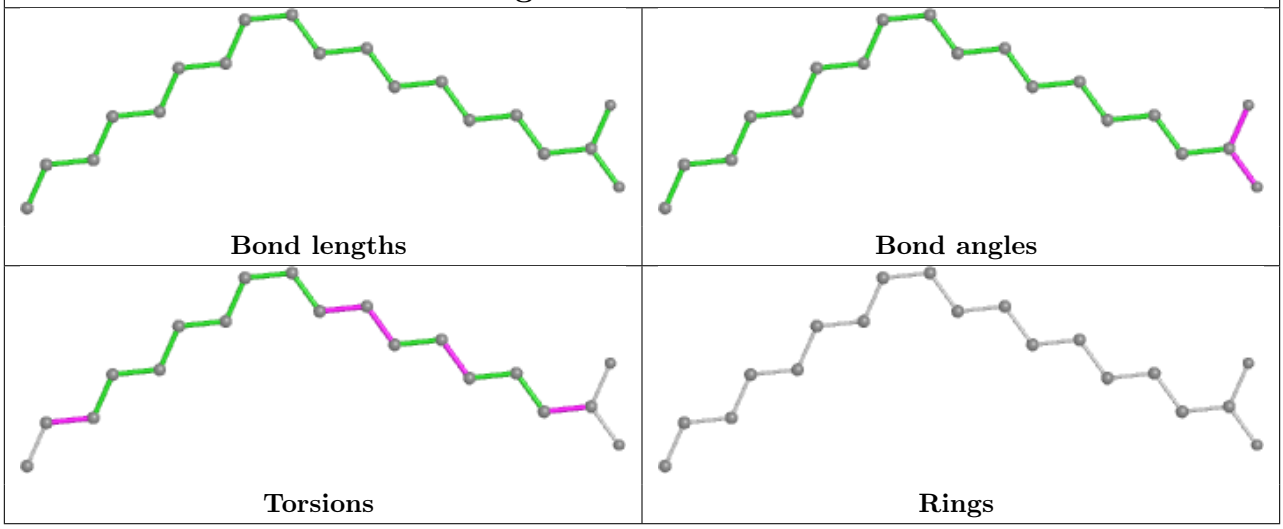

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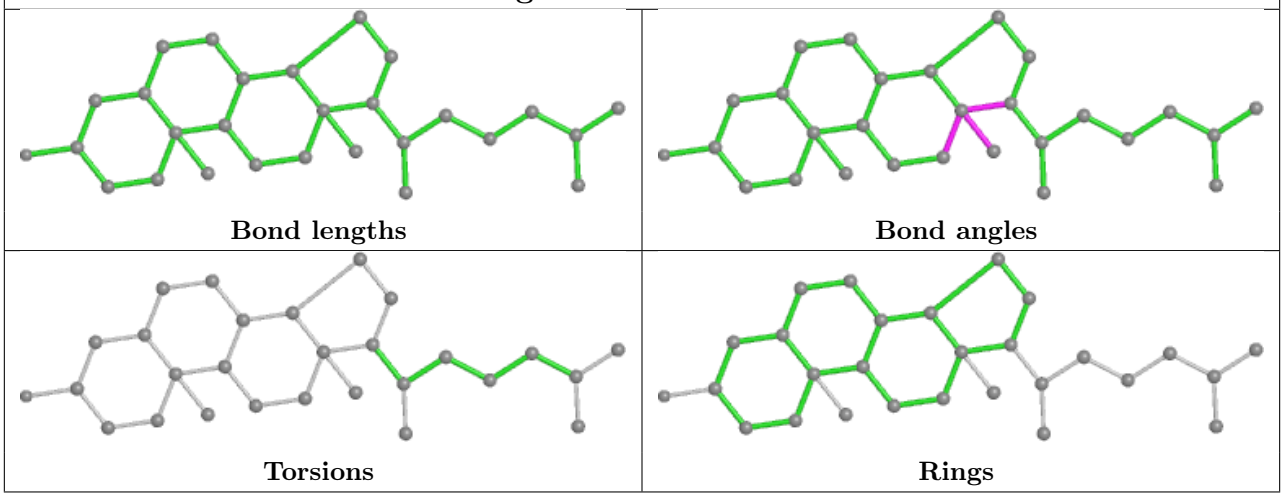

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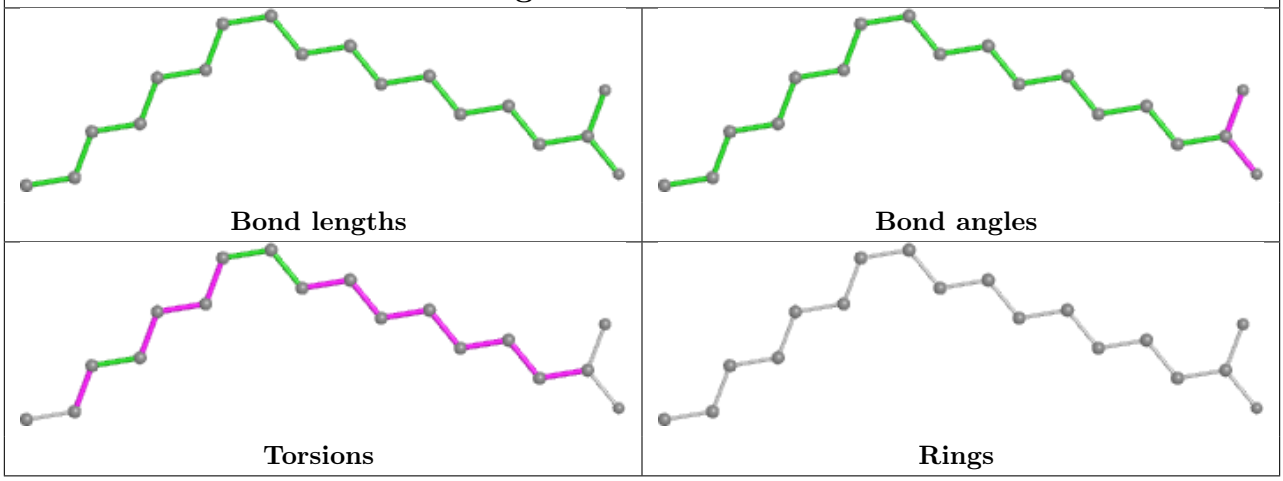

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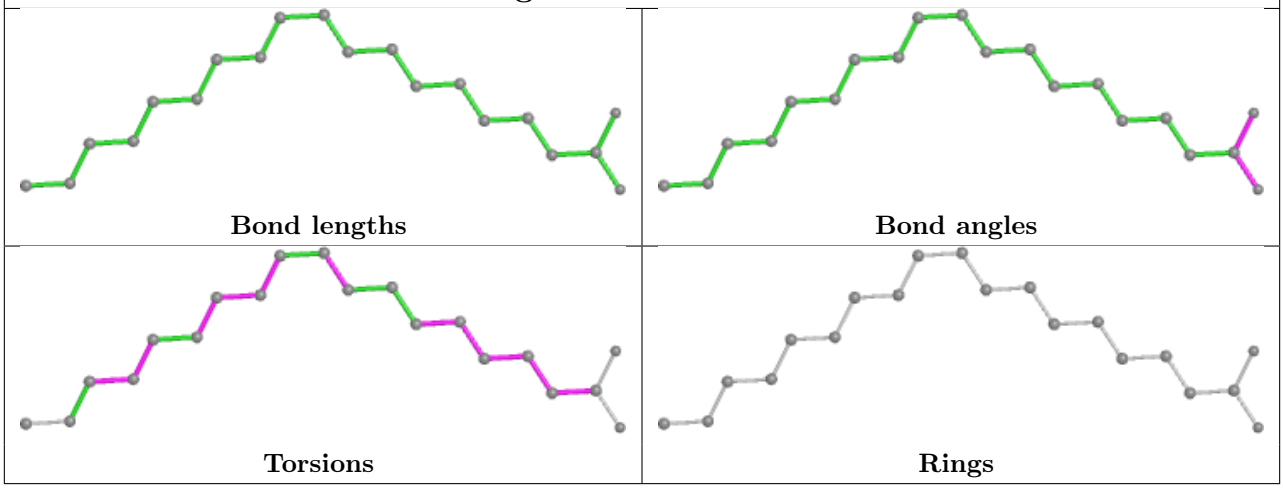

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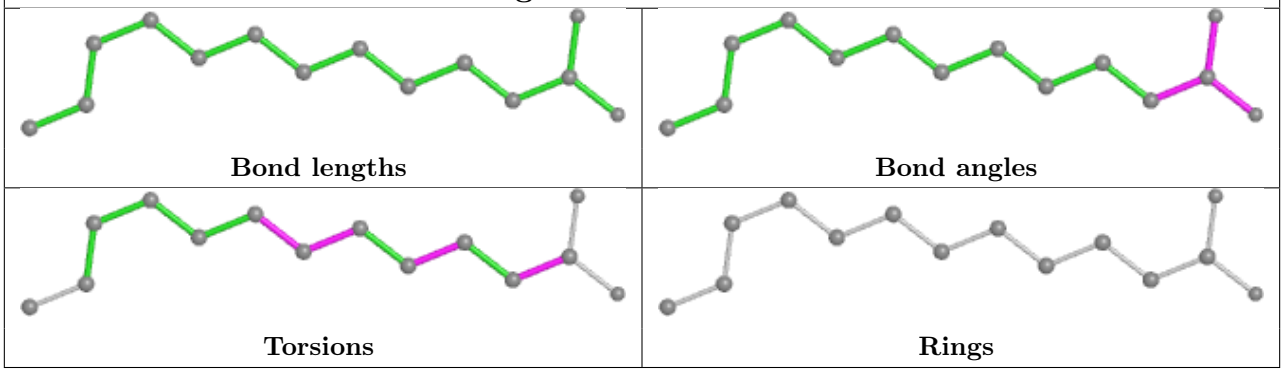

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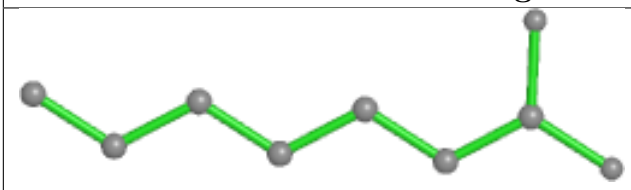

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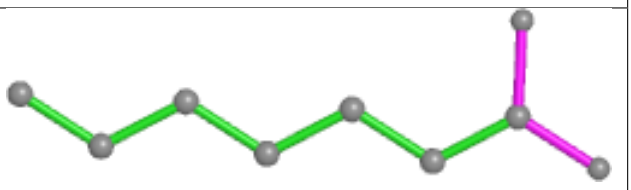
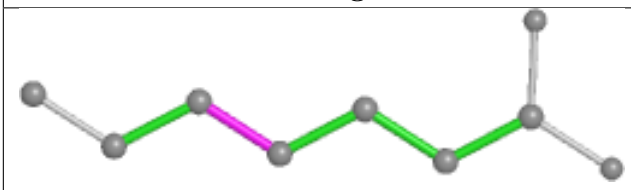
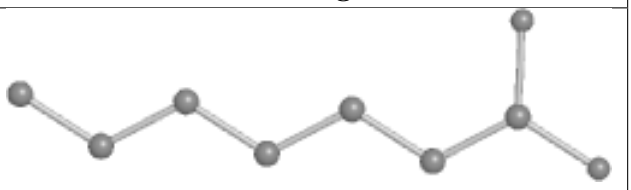


Bond angles

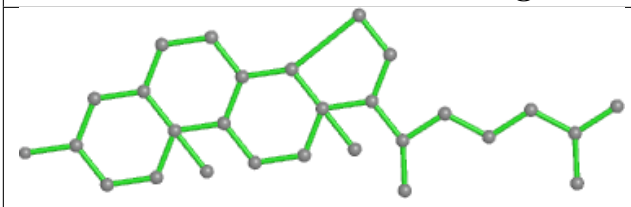


Torsions



Rings

Ligand CLR A 2403



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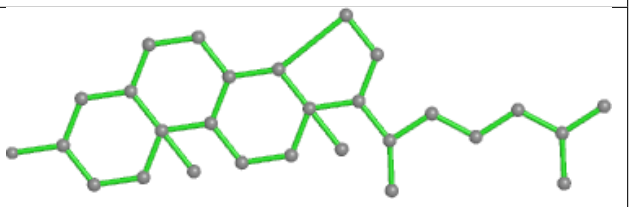

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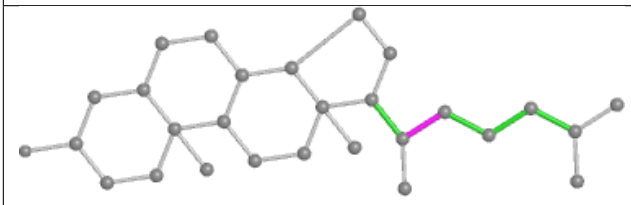

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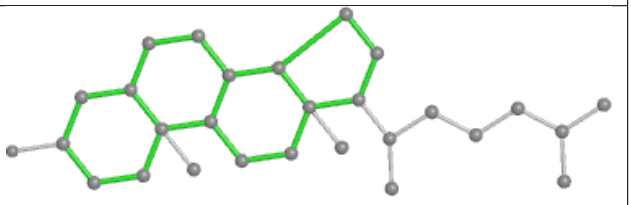
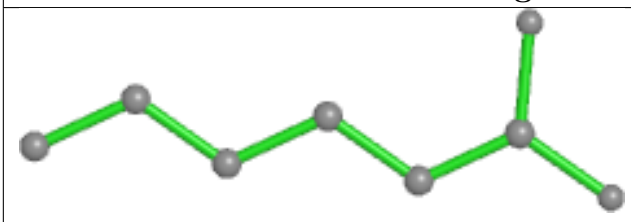


Rings

Ligand OLA A 2414



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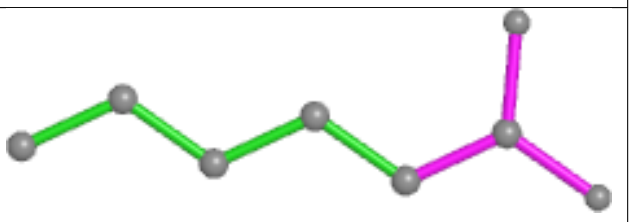

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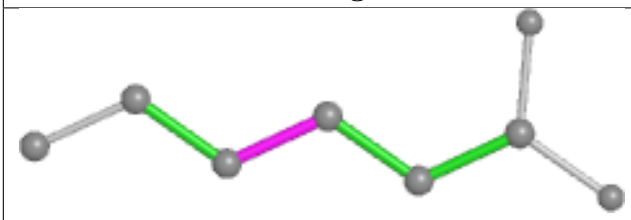

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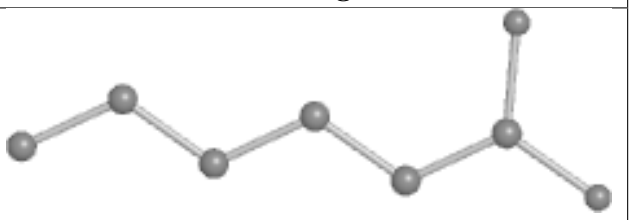

Rings

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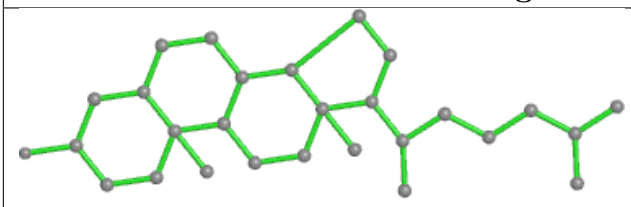

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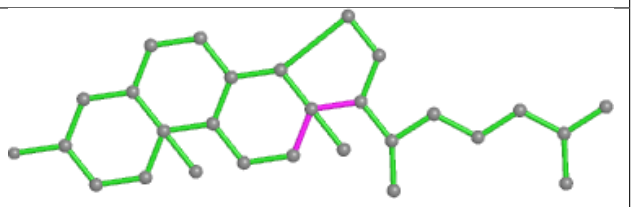

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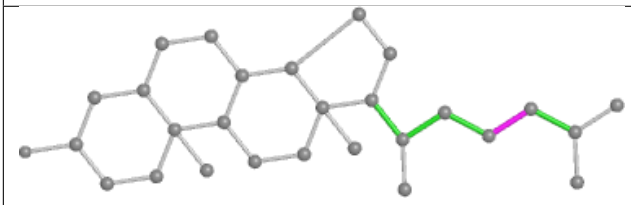

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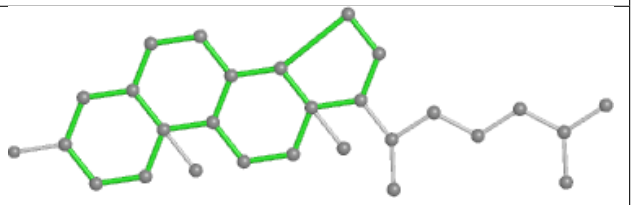

Rings

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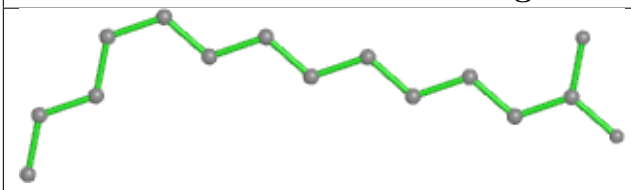

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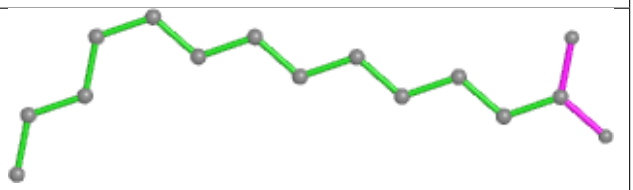

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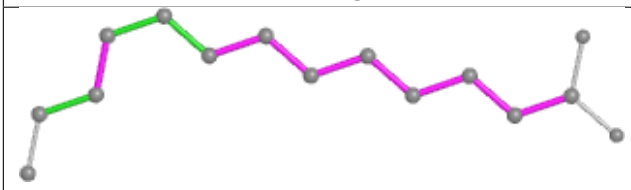

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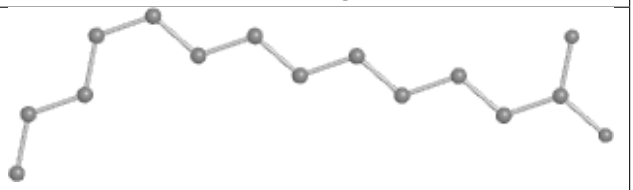
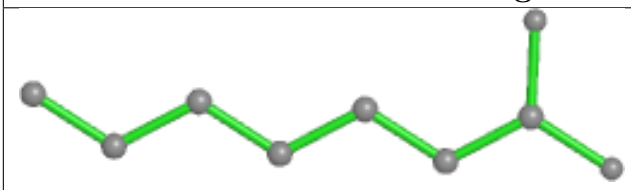


Rings

Ligand OLA A 2419



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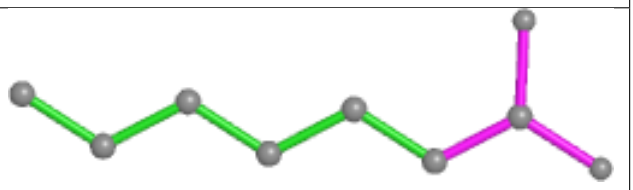

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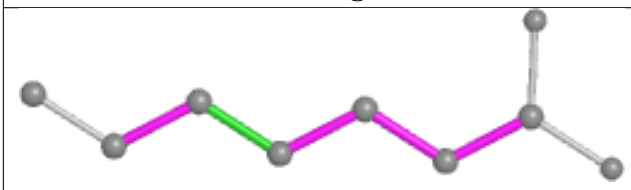

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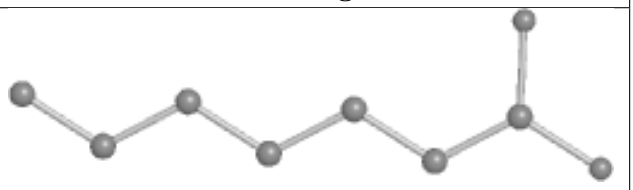
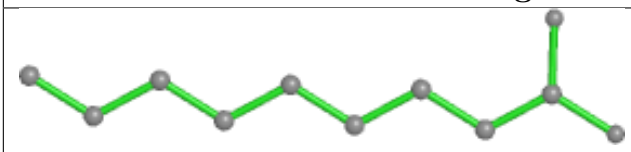


Rings

Ligand OLA A 2415



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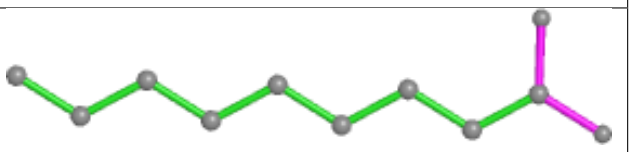

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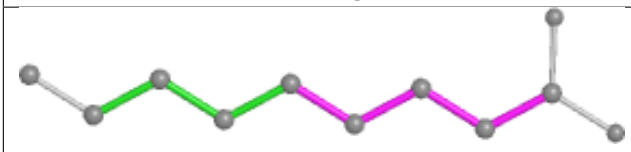

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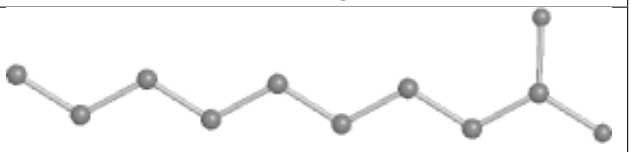

Rings

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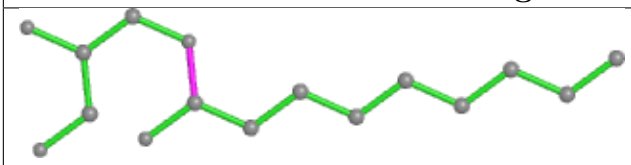

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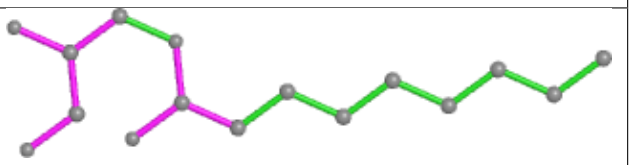
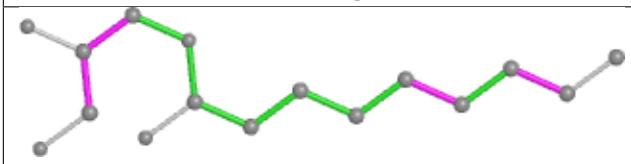
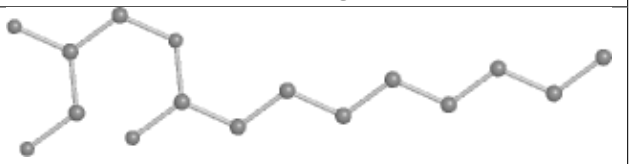


Bond angles

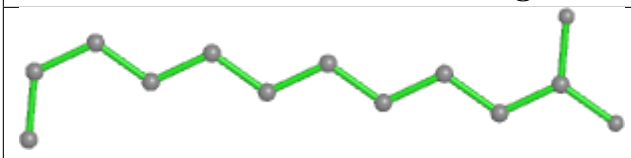


Torsions

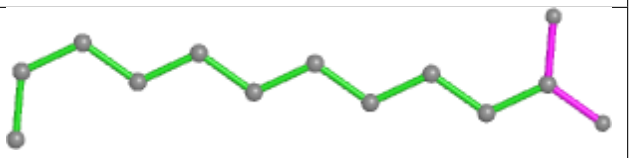


Rings

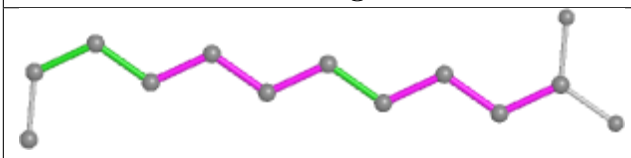
Ligand OLA A 2417



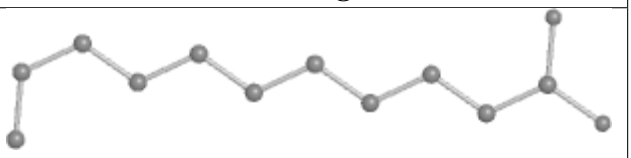
Bond lengths



Bond angles

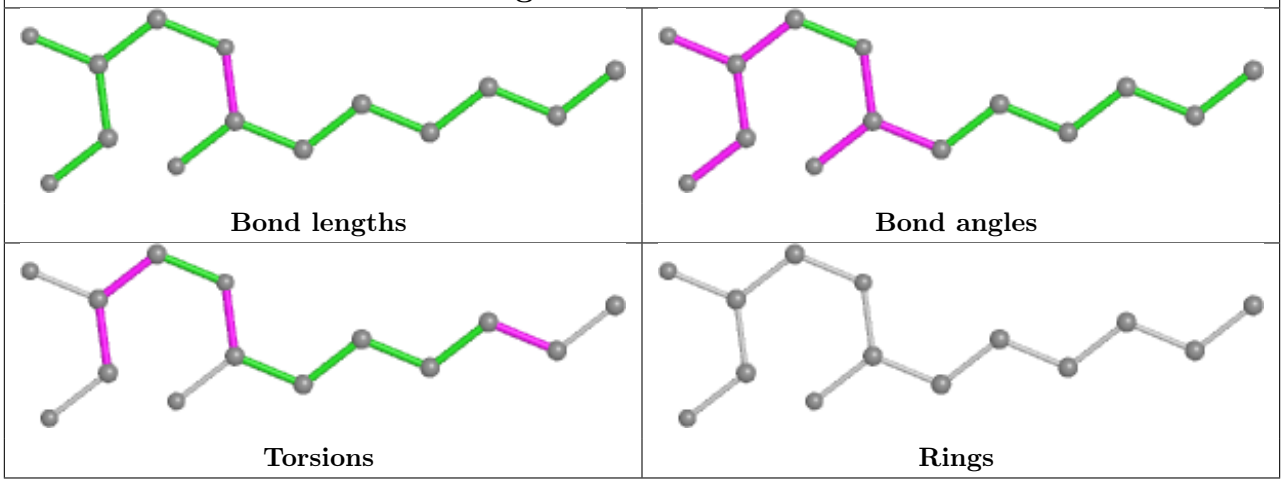


Torsions

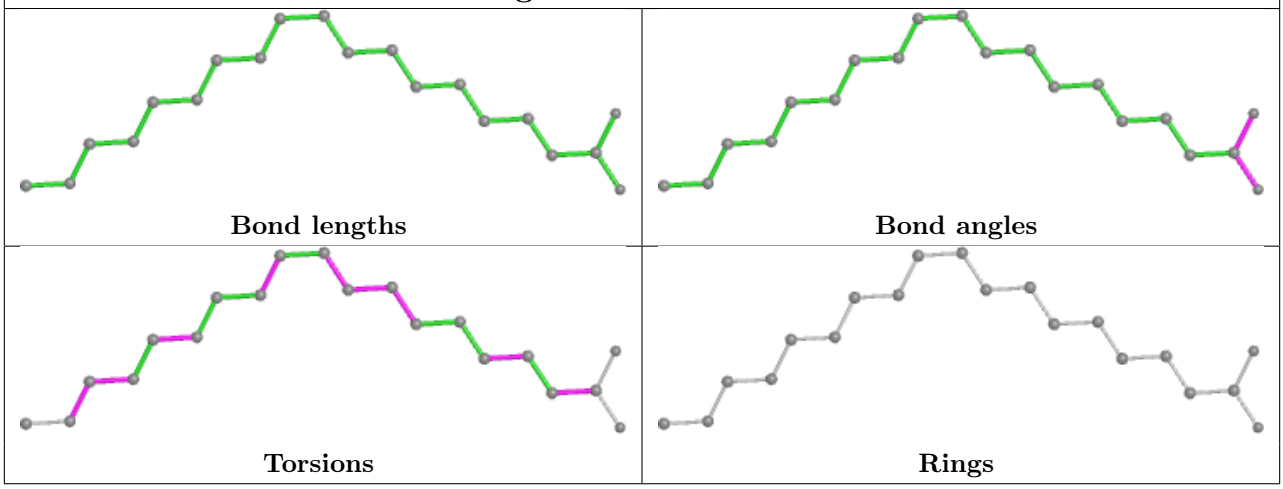


Rings

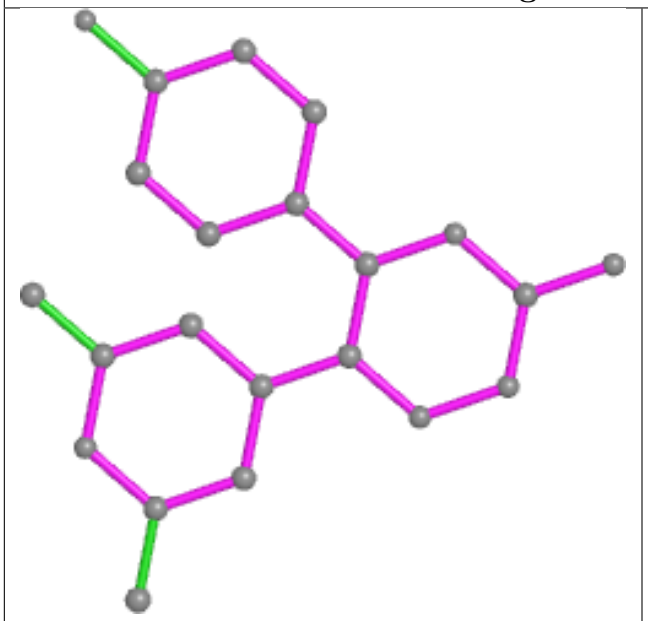
Ligand OLC A 2423



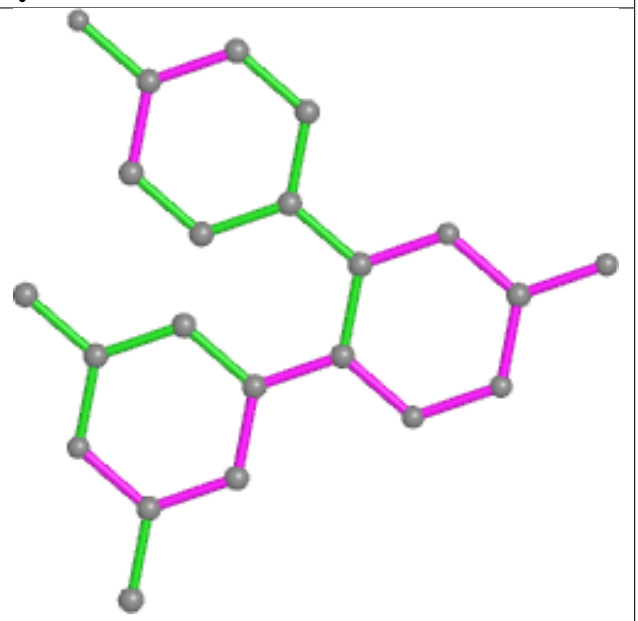
Ligand OLA A 2411



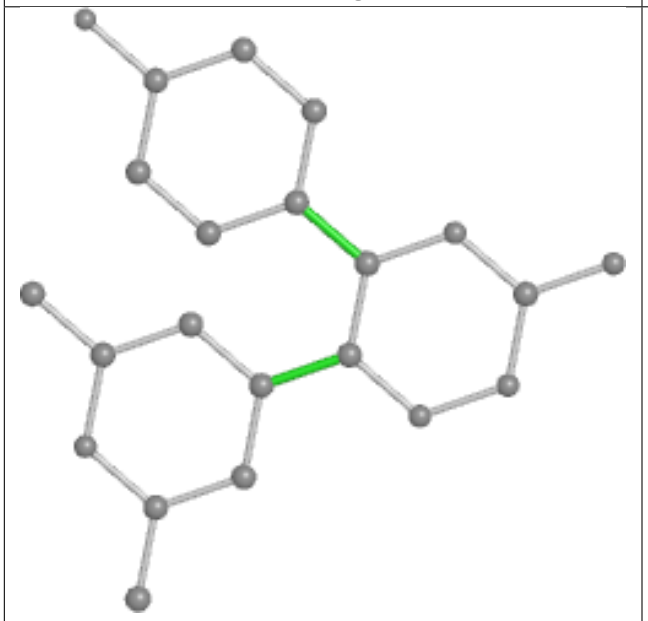
Ligand F9Q A 2401



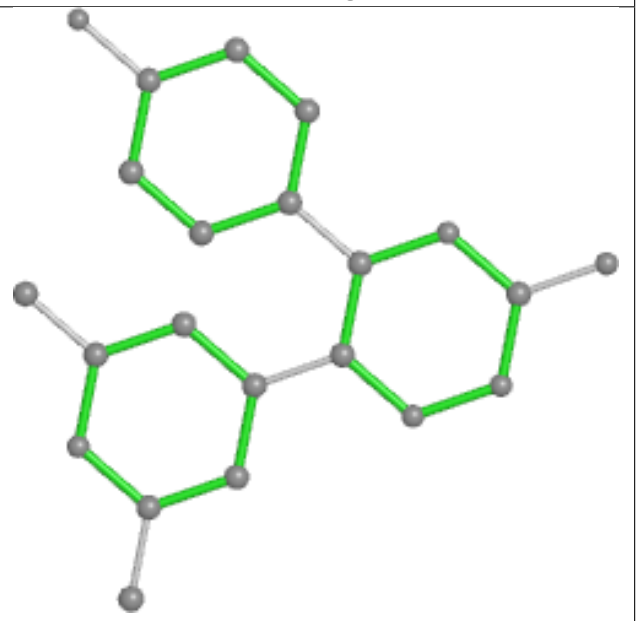
Bond lengths



Bond angles

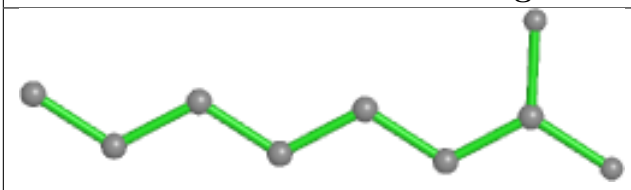


Torsions

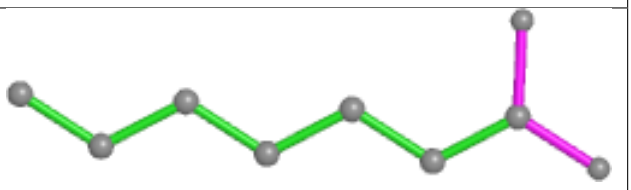


Rings

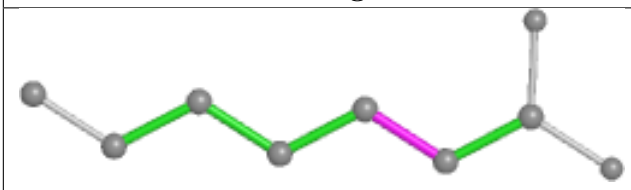
Ligand OLA A 2409



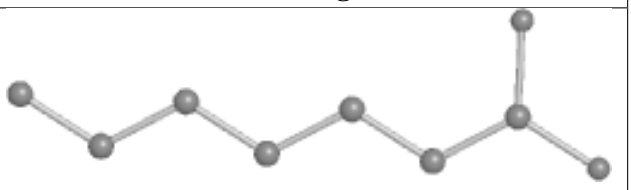
Bond lengths



Bond angles

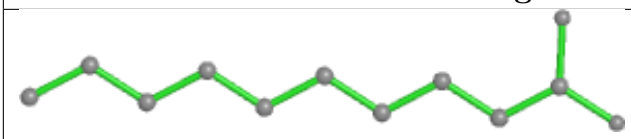


Torsions

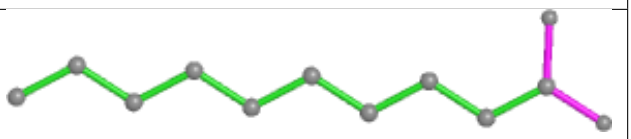


Rings

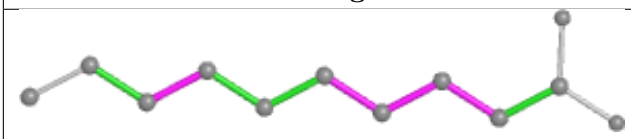
Ligand OLA A 2413



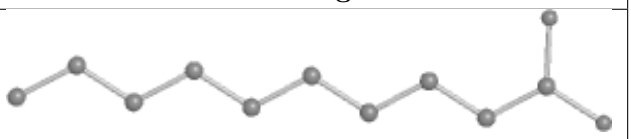
Bond lengths



Bond angles

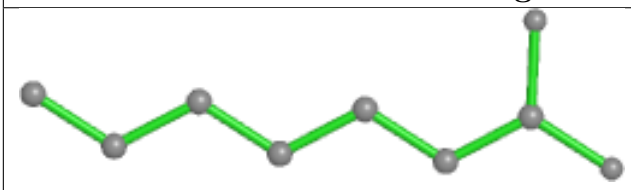


Torsions

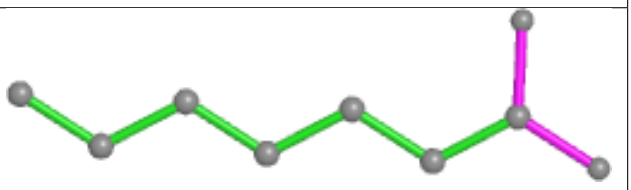


Rings

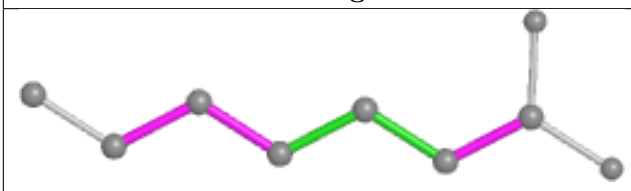
Ligand OLA A 2407



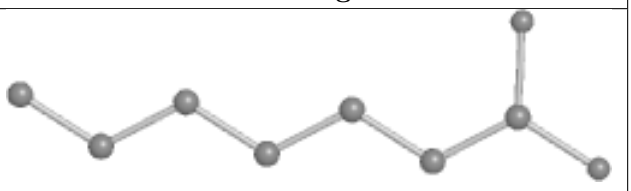
Bond lengths



Bond angles

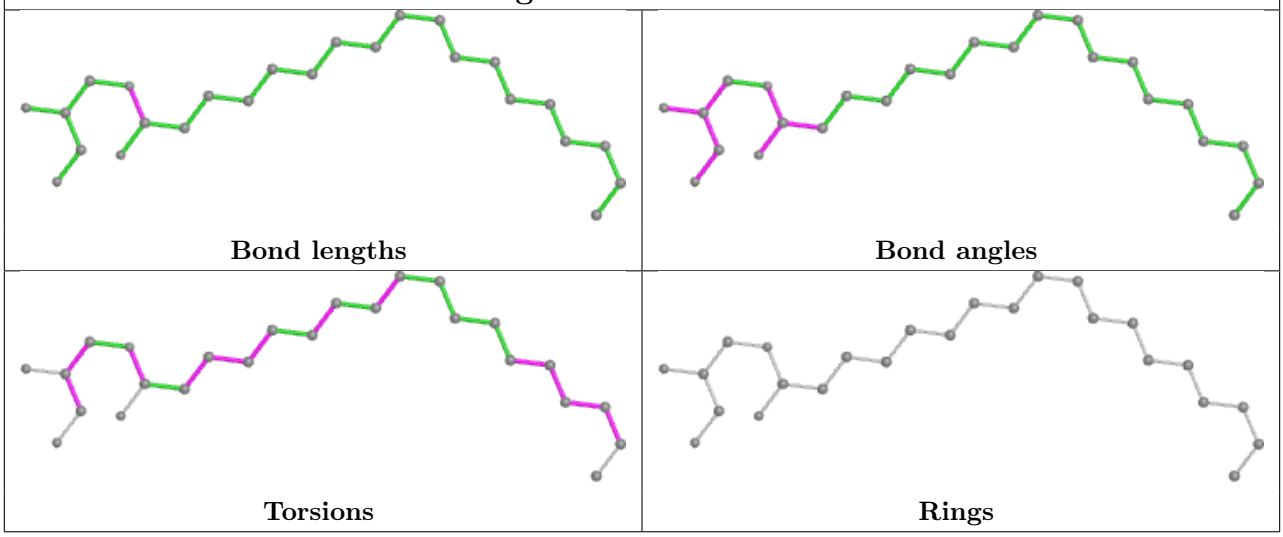


Torsions

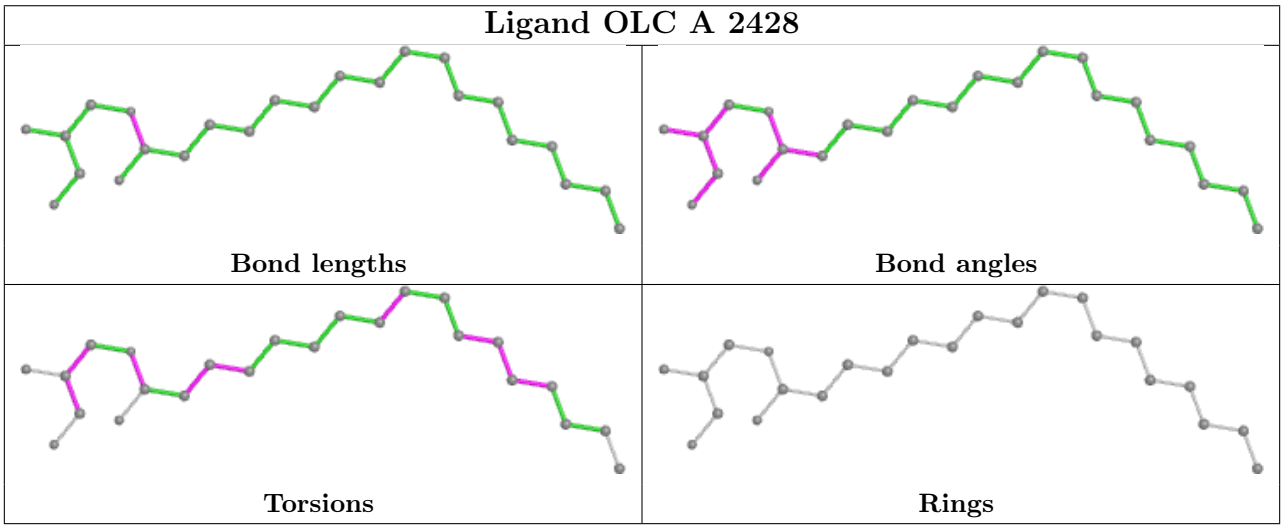


Rings

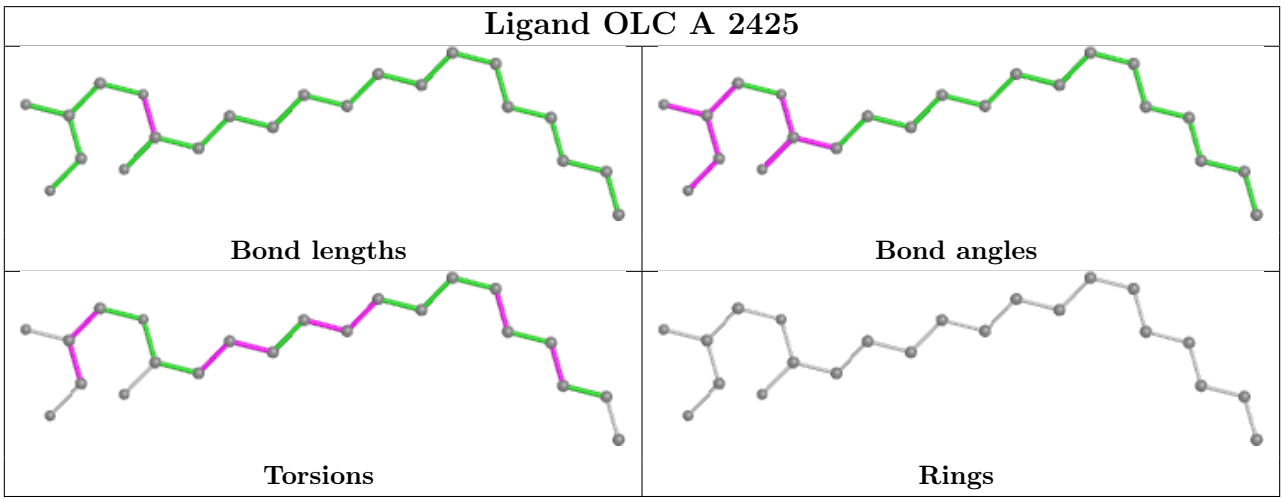
Ligand OLC A 2426



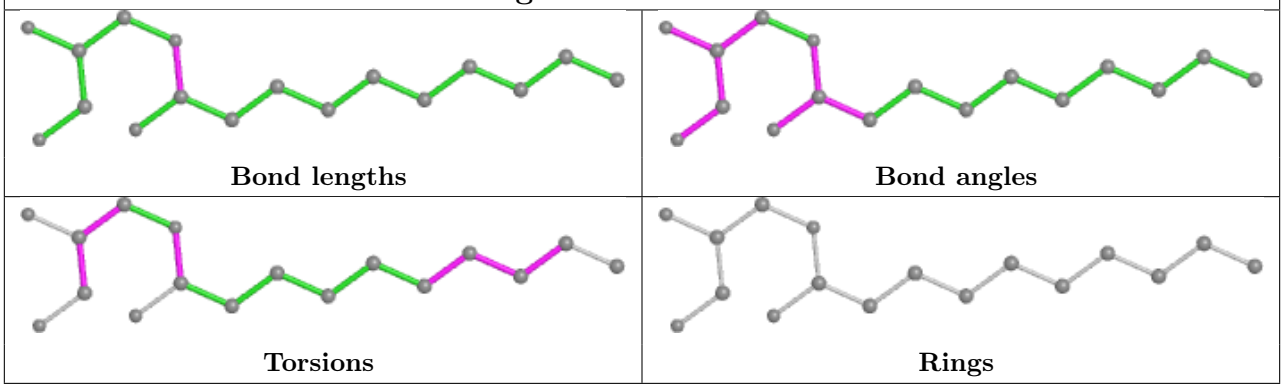
Ligand OLC A 2428



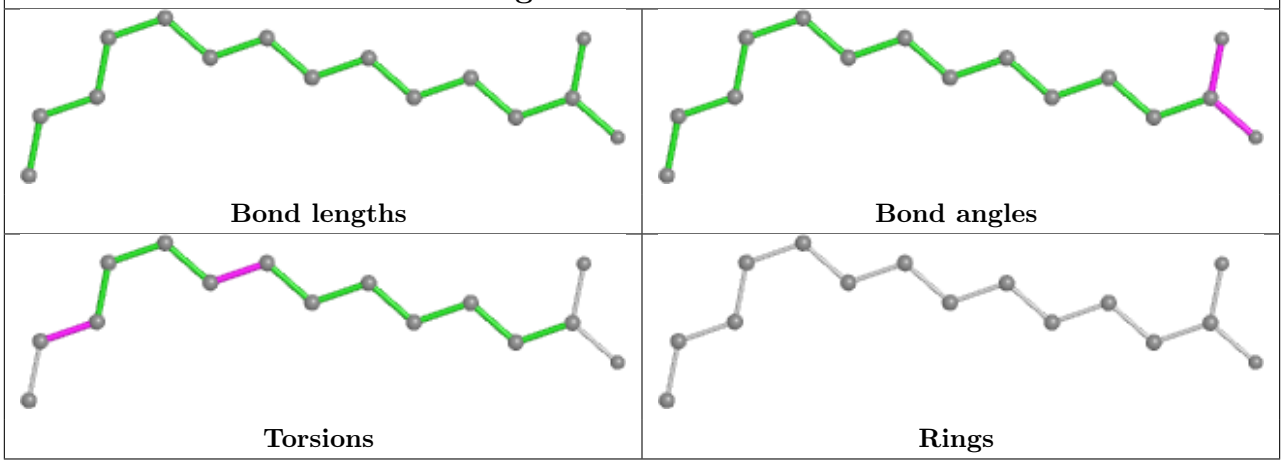
Ligand OLC A 2425



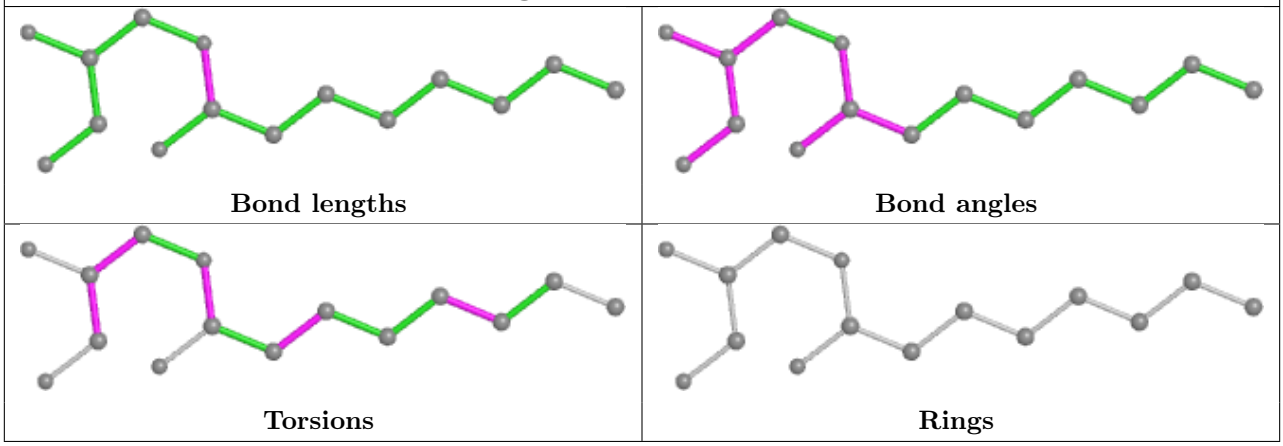
Ligand OLC A 2420



Ligand OLA A 2412



Ligand OLC A 2424



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	388/433 (89%)	0.37	28 (7%) 15 14	12, 30, 80, 126	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1058	MET	10.4
1	A	1061	PHE	6.7
1	A	-1	GLY	5.9
1	A	1059	LYS	5.2
1	A	305	SER	4.9

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	2414	8/20	0.61	0.19	57,60,66,68	0
5	OLA	A	2416	14/20	0.61	0.27	57,73,76,76	0

Continued on next page...

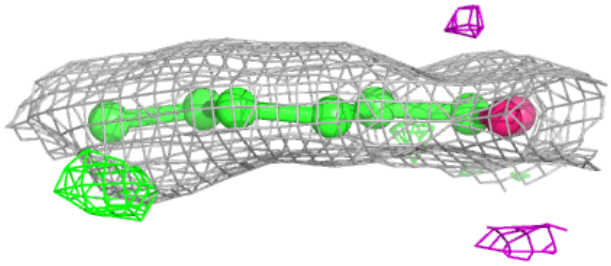
Continued from previous page...

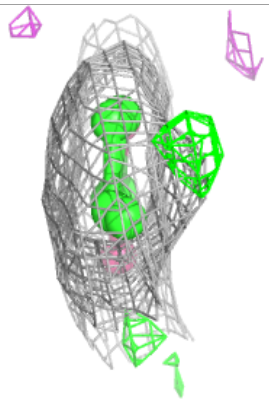
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OLC	A	2424	15/25	0.63	0.30	58,79,88,89	0
5	OLA	A	2413	12/20	0.70	0.34	47,65,81,84	0
6	OLC	A	2423	14/25	0.72	0.20	71,86,99,102	0
5	OLA	A	2412	15/20	0.72	0.24	65,68,89,90	0
5	OLA	A	2411	20/20	0.74	0.27	40,65,81,84	0
6	OLC	A	2426	25/25	0.74	0.25	49,53,77,82	0
5	OLA	A	2407	9/20	0.76	0.24	49,57,69,71	0
5	OLA	A	2418	19/20	0.77	0.23	55,63,69,73	0
6	OLC	A	2420	17/25	0.79	0.24	64,70,85,88	0
5	OLA	A	2415	11/20	0.79	0.30	57,73,97,100	0
5	OLA	A	2409	9/20	0.79	0.21	49,55,78,81	0
5	OLA	A	2410	18/20	0.79	0.22	49,65,88,88	0
6	OLC	A	2428	24/25	0.79	0.26	47,63,69,72	0
6	OLC	A	2429	22/25	0.80	0.28	48,64,79,81	0
5	OLA	A	2406	15/20	0.81	0.26	52,60,74,74	0
5	OLA	A	2417	13/20	0.85	0.24	58,68,82,83	0
5	OLA	A	2405	20/20	0.85	0.15	46,58,81,83	0
5	OLA	A	2419	9/20	0.85	0.21	48,52,59,61	0
6	OLC	A	2425	22/25	0.86	0.21	49,55,96,104	0
6	OLC	A	2421	23/25	0.87	0.22	42,55,68,71	0
6	OLC	A	2427	25/25	0.87	0.21	43,62,83,87	0
5	OLA	A	2408	9/20	0.89	0.16	41,43,58,61	0
4	CLR	A	2402	28/28	0.93	0.12	30,37,50,53	0
6	OLC	A	2422	16/25	0.93	0.17	36,45,54,56	0
4	CLR	A	2403	28/28	0.93	0.13	26,34,39,45	0
3	F9Q	A	2401	22/22	0.94	0.21	18,21,28,30	0
4	CLR	A	2404	28/28	0.94	0.11	27,34,50,56	0
2	NA	A	2400	1/1	0.94	0.26	44,44,44,44	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 2414:

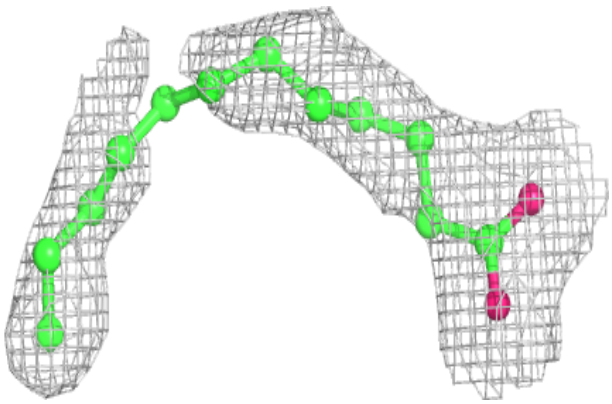
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

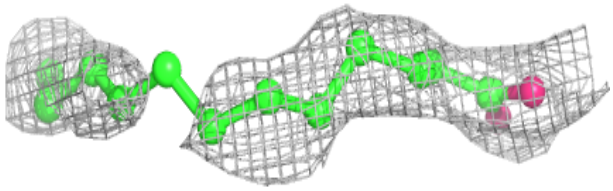


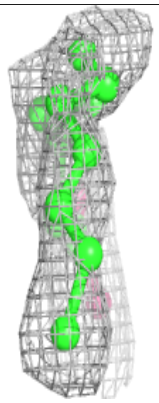


Electron density around OLA A 2416:

$2mF_o$-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 2424:

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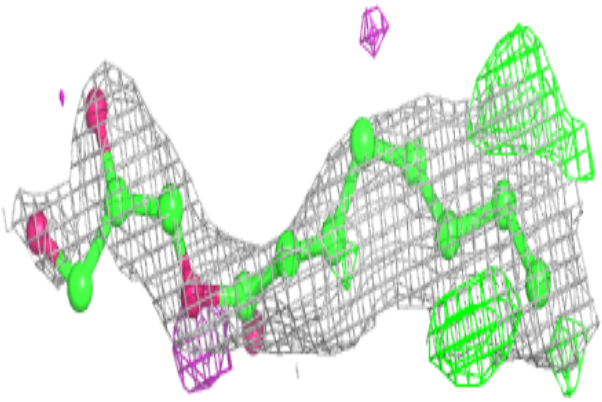
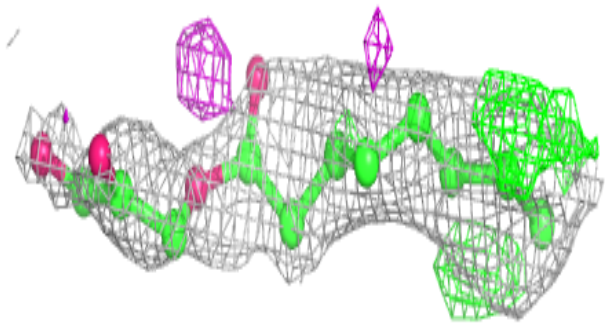
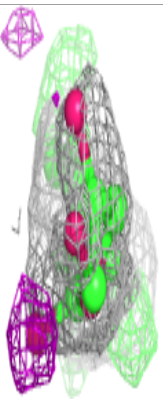
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

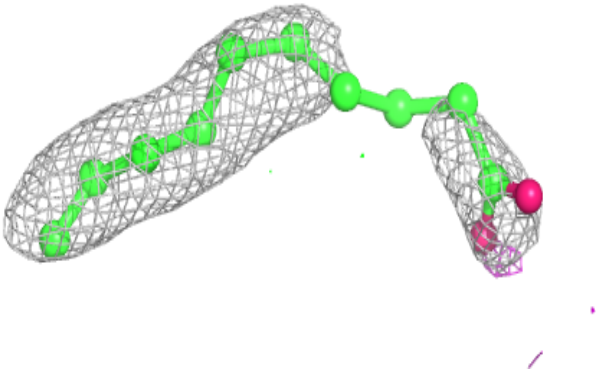


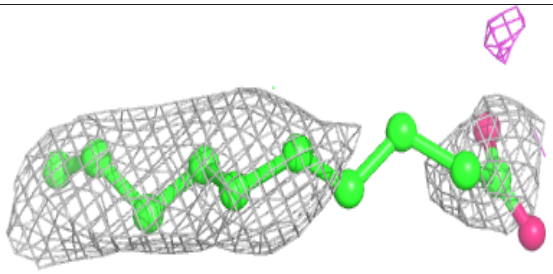


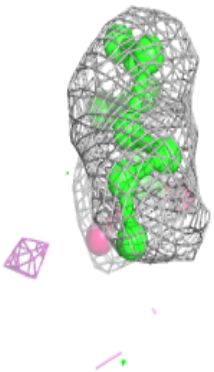


Electron density around OLA A 2413:

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

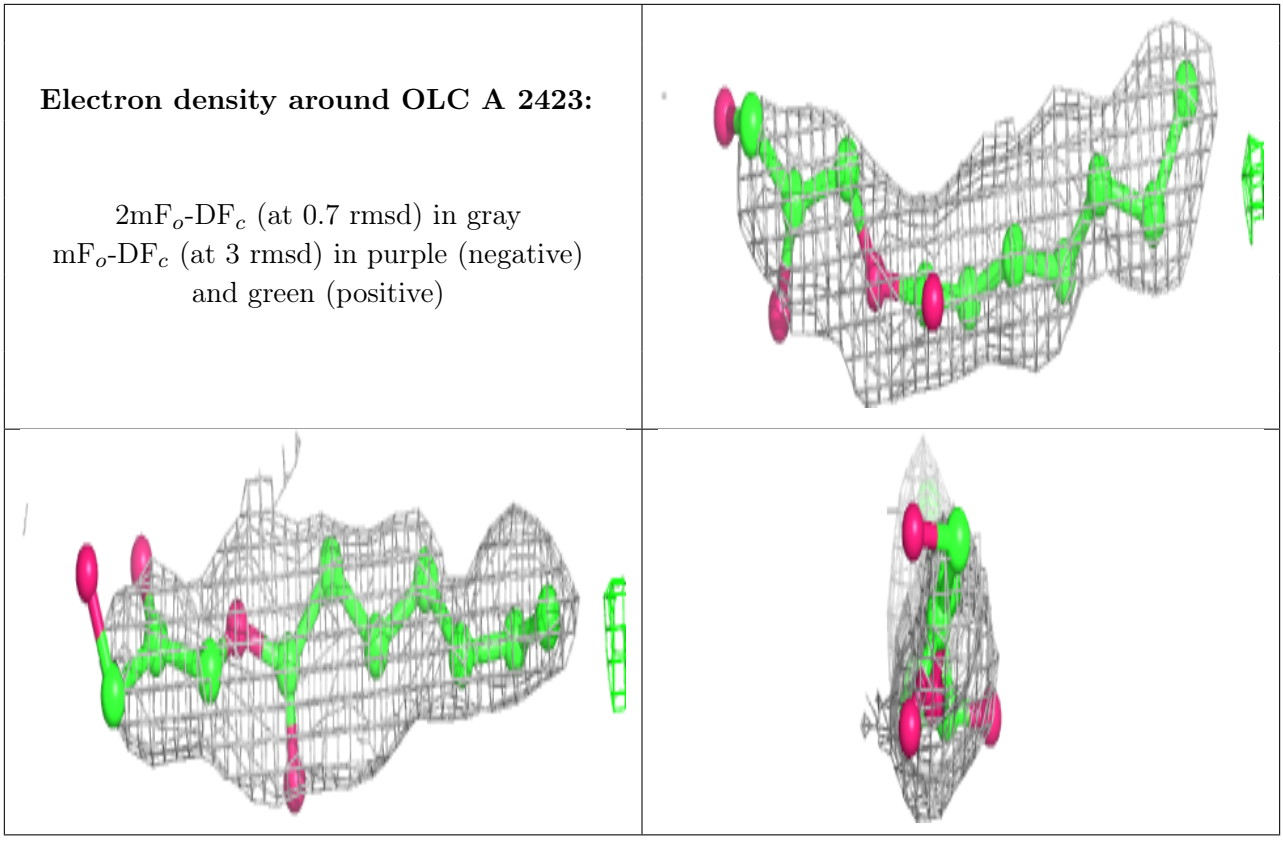






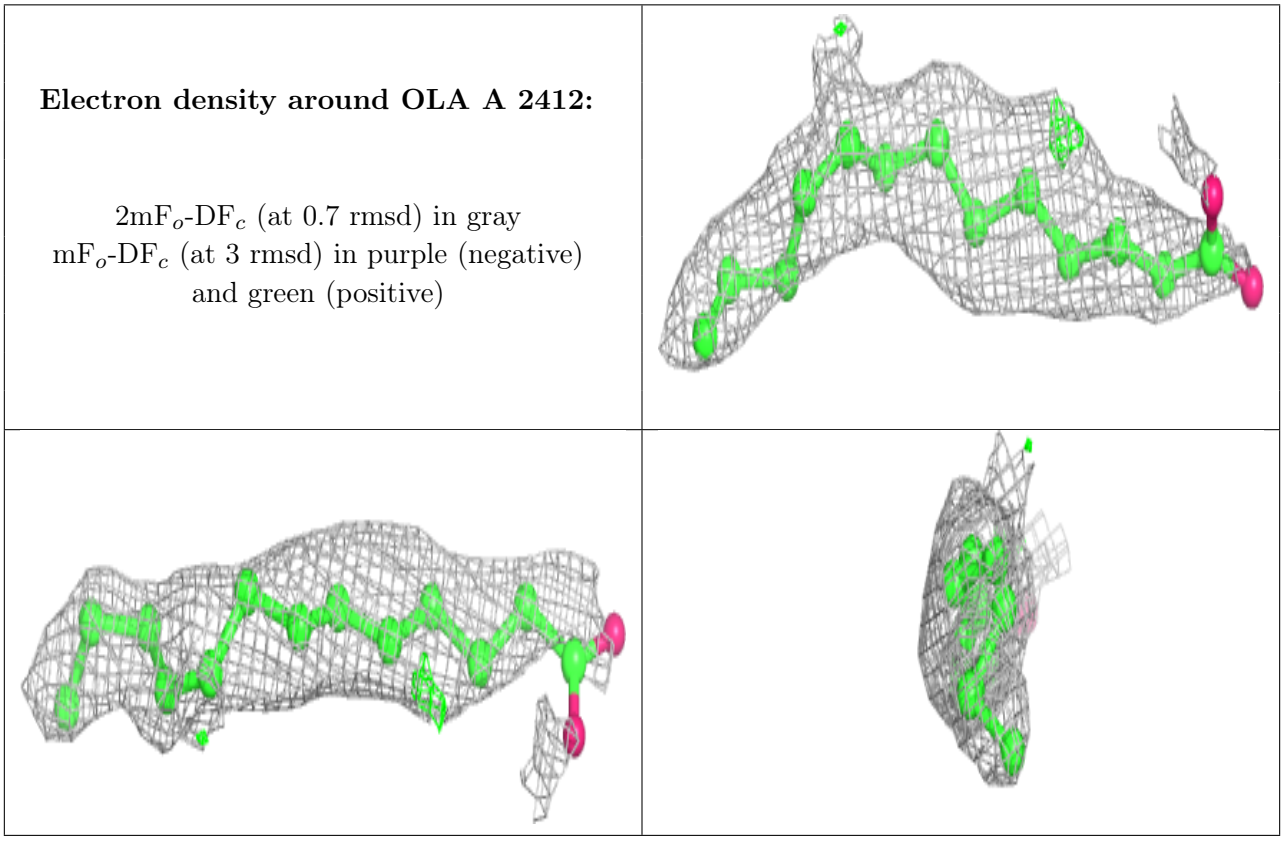
Electron density around OLC A 2423:

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



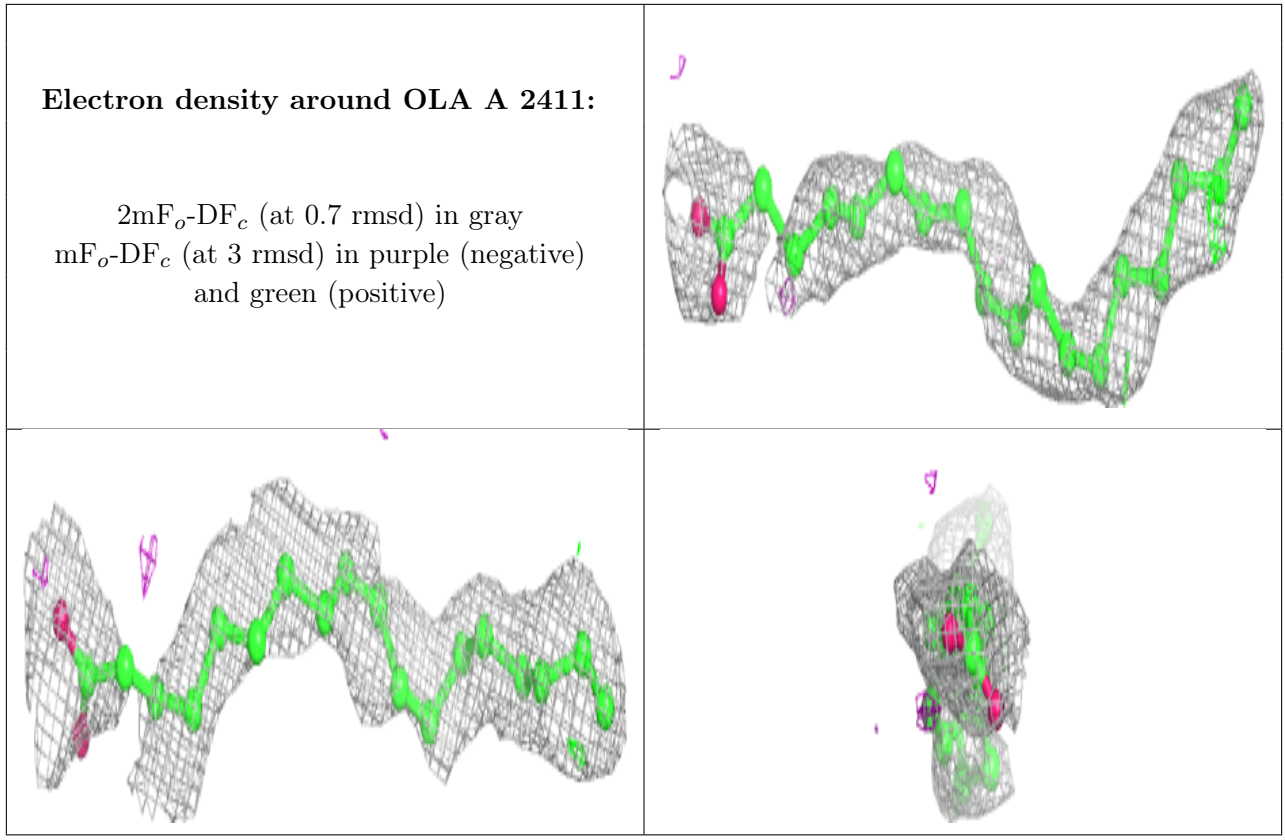
Electron density around OLA A 2412:

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



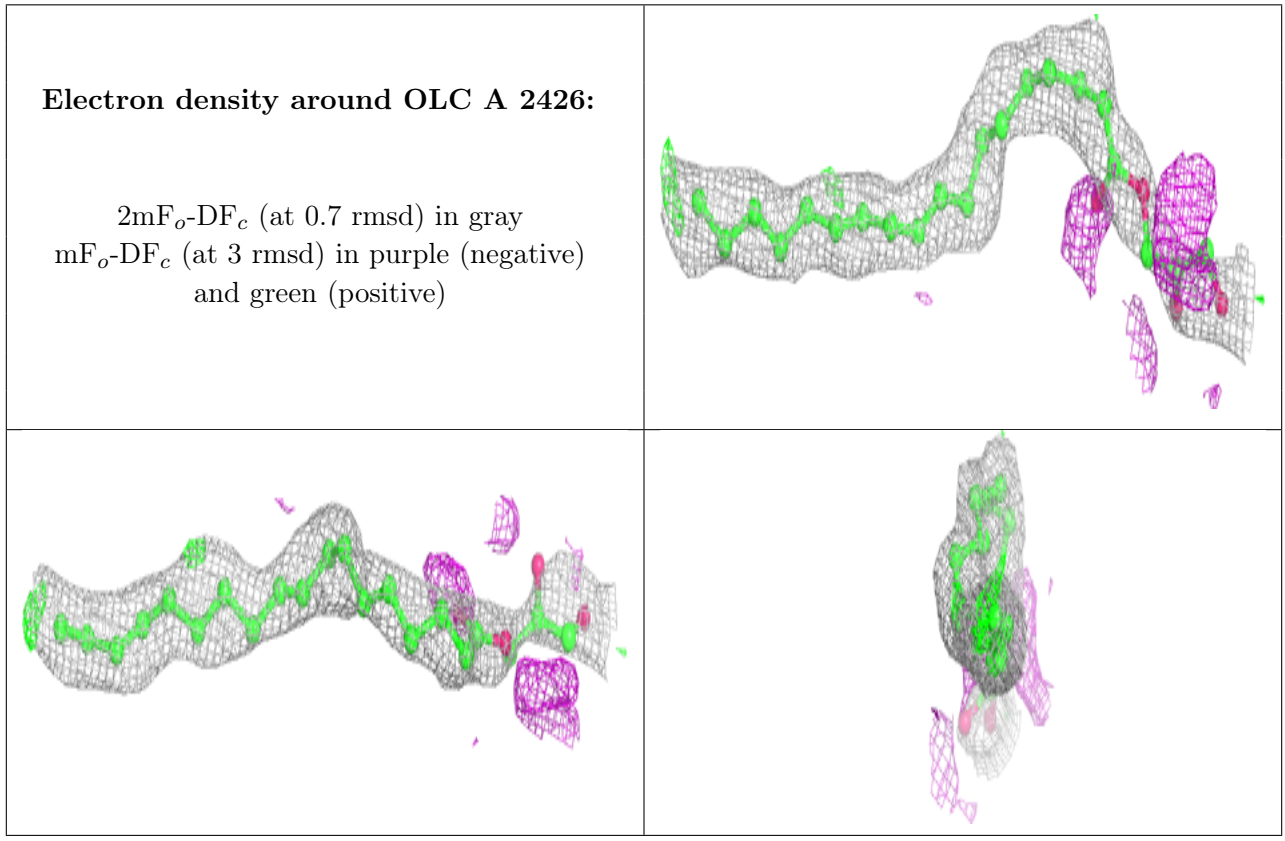
Electron density around OLA A 2411:

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



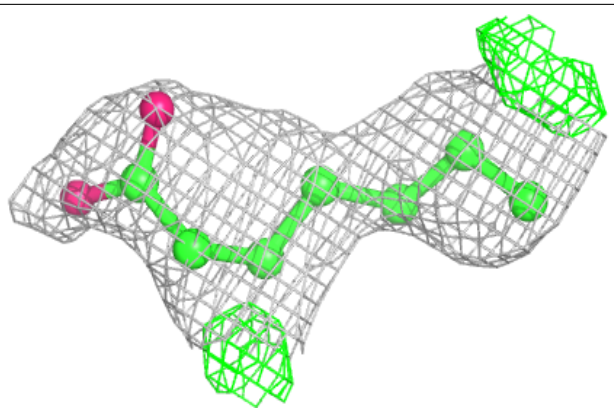
Electron density around OLC A 2426:

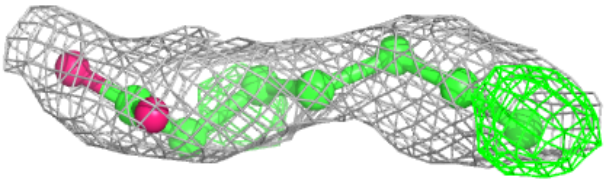
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

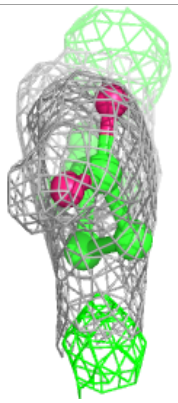


Electron density around OLA A 2407:

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

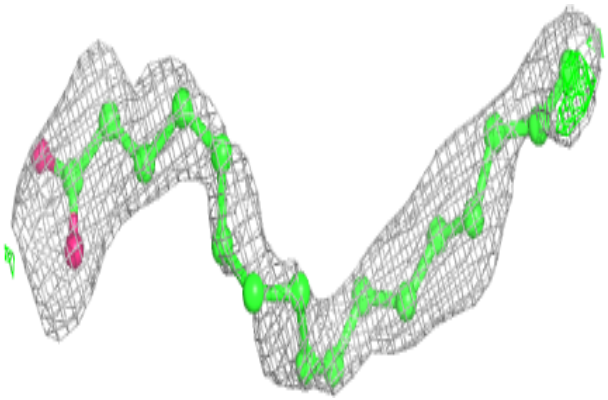


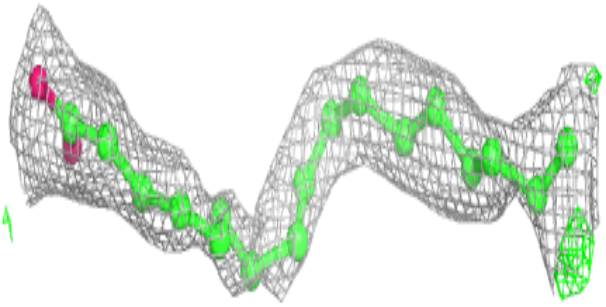


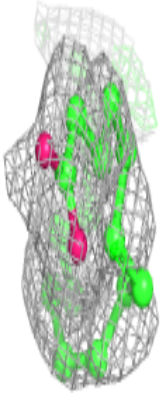


Electron density around OLA A 2418:

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

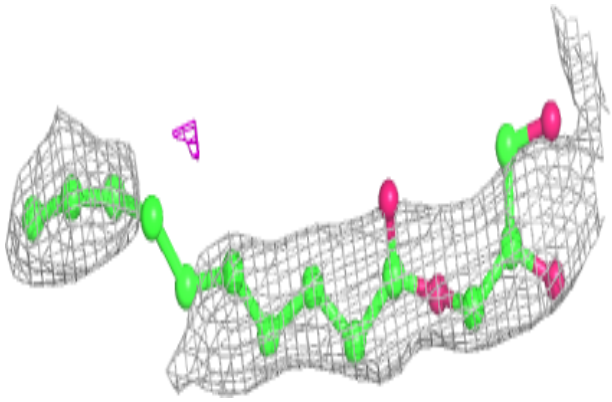


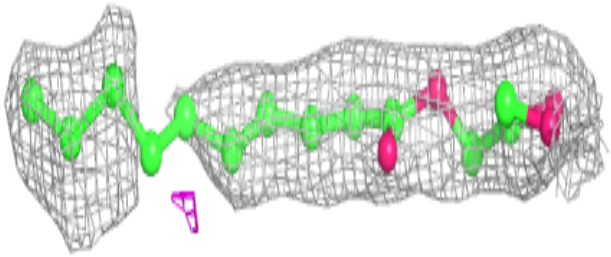


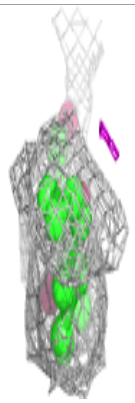


Electron density around OLC A 2420:

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

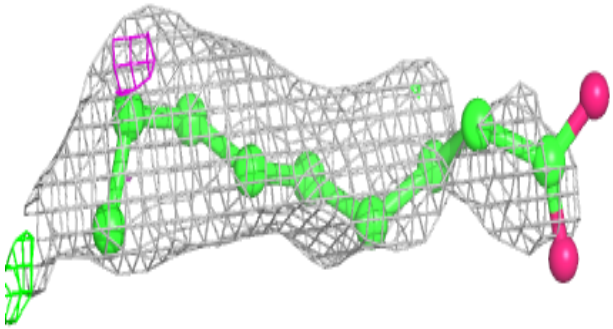


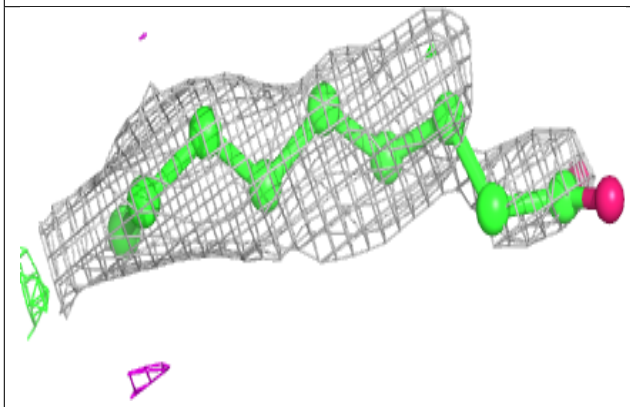


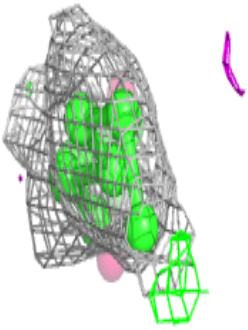


Electron density around OLA A 2415:

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

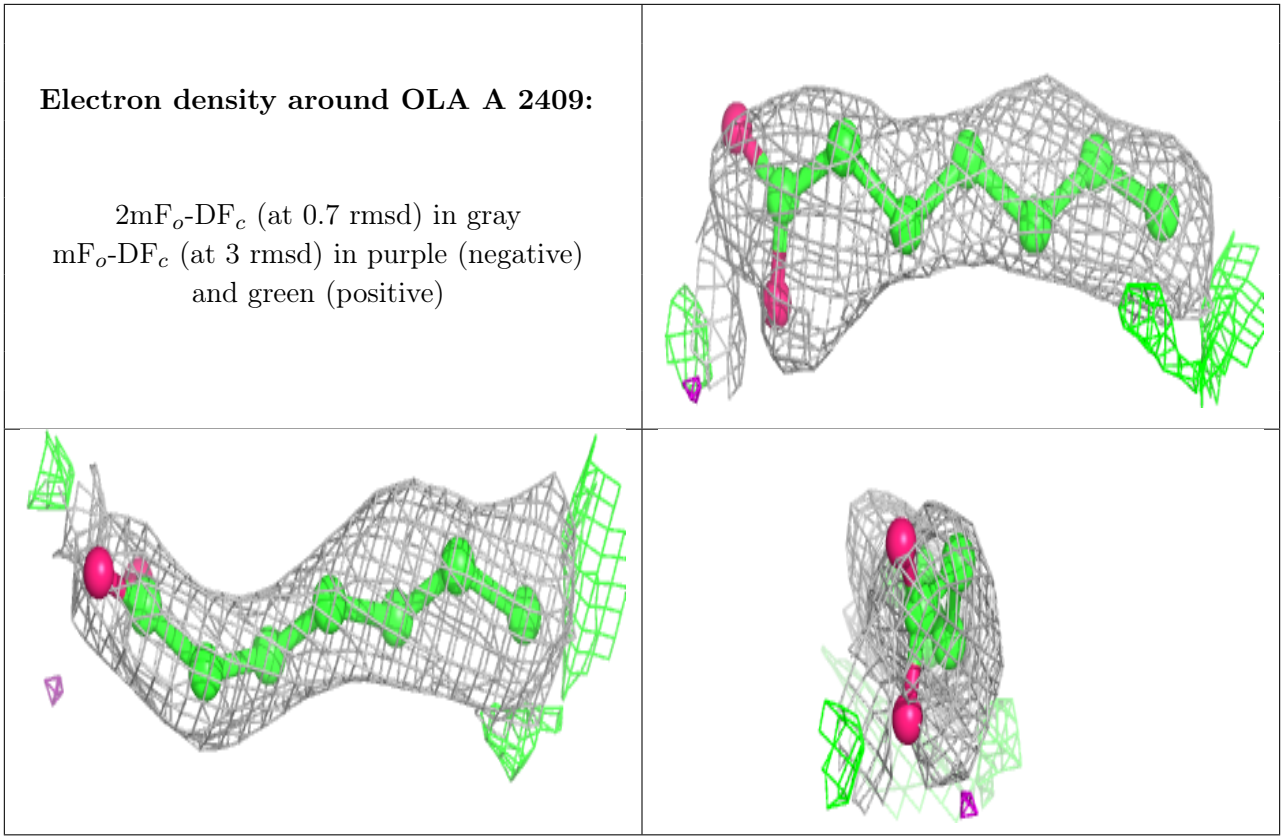






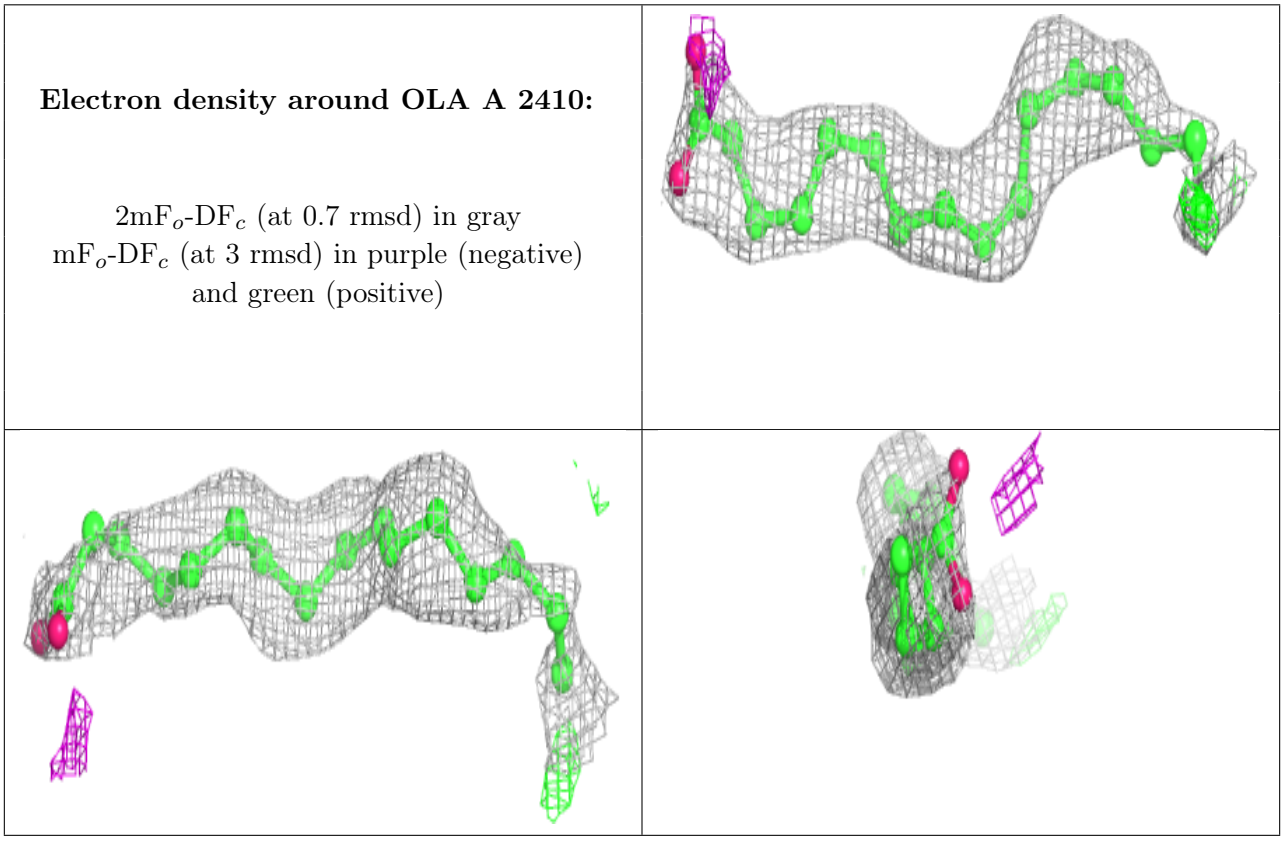
Electron density around OLA A 2409:

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



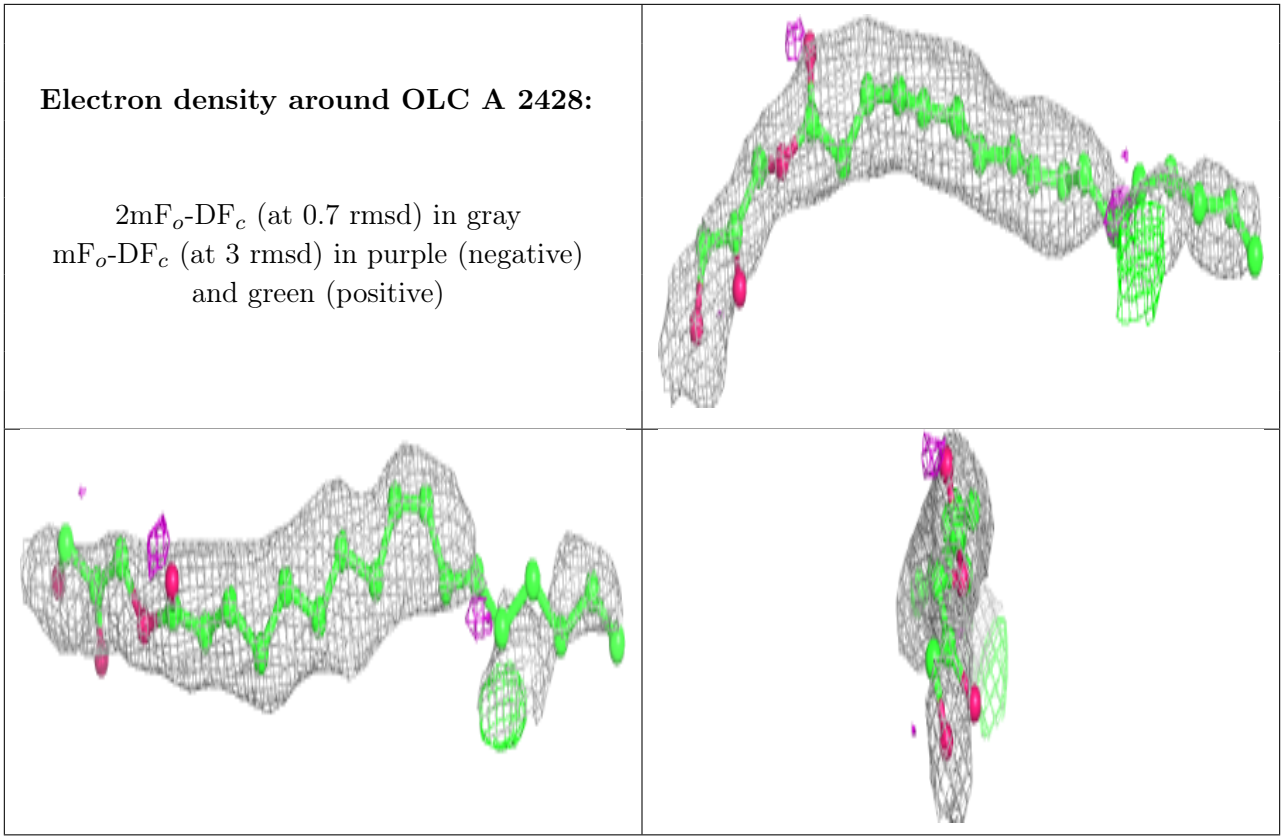
Electron density around OLA A 2410:

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



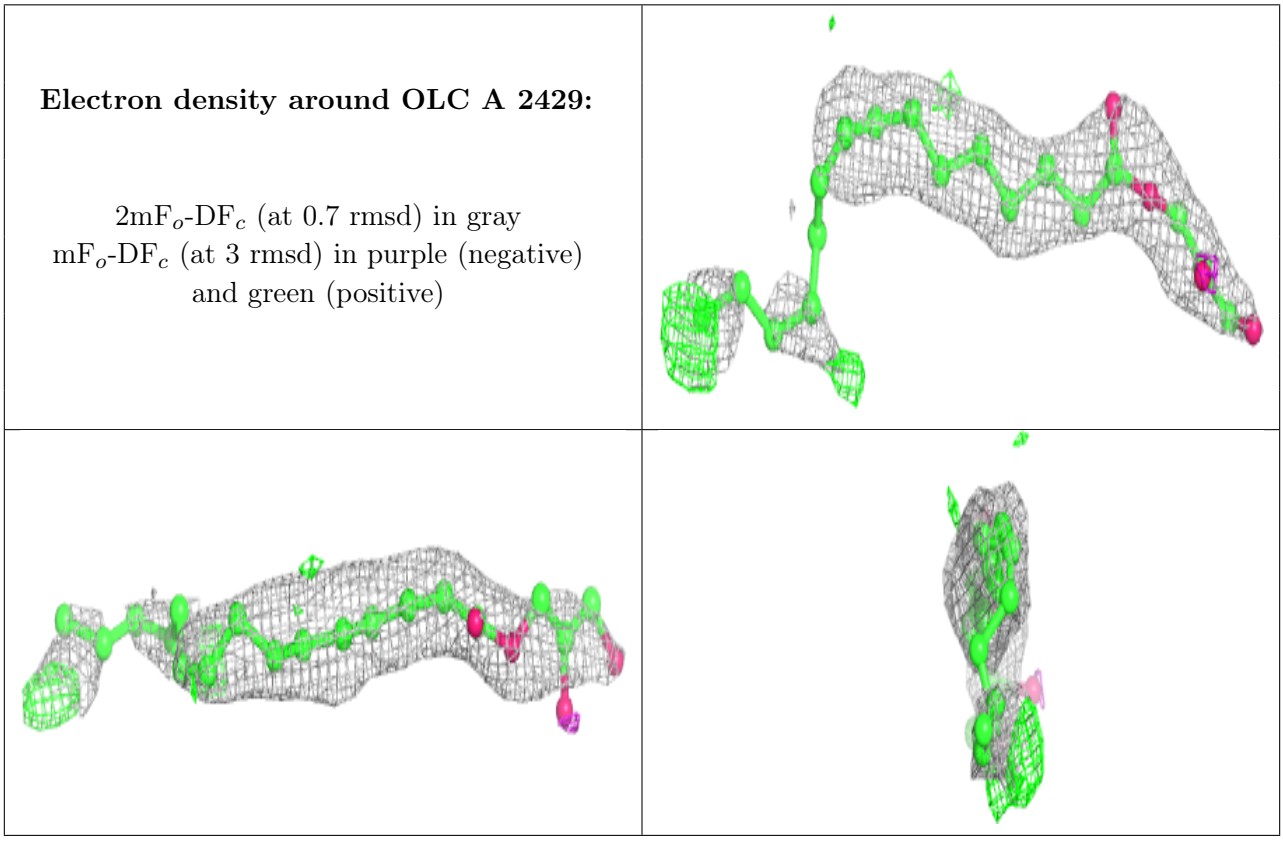
Electron density around OLC A 2428:

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



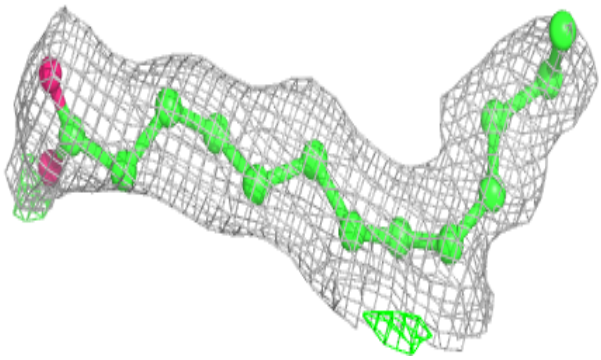
Electron density around OLC A 2429:

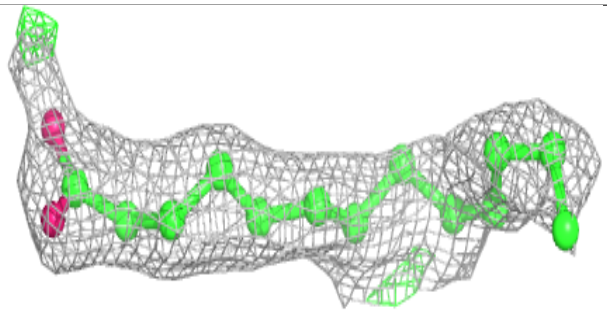
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

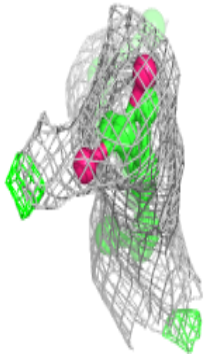


Electron density around OLA A 2406:

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

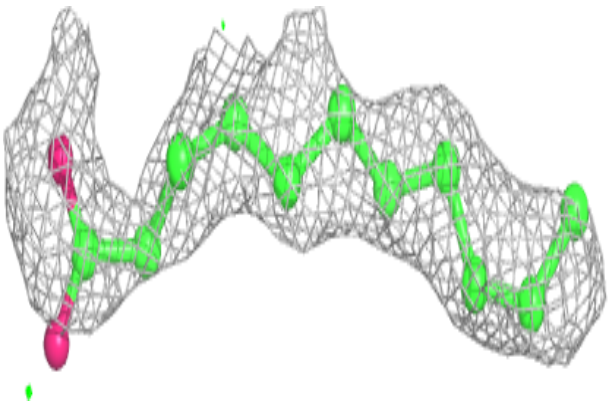


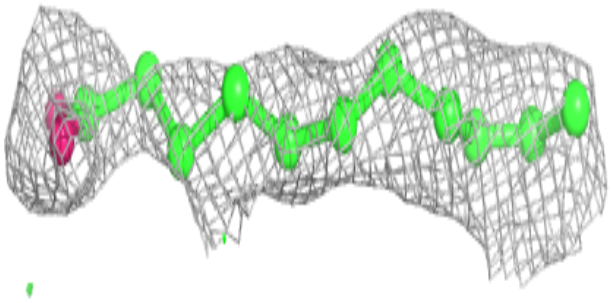


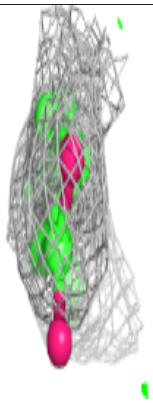


Electron density around OLA A 2417:

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

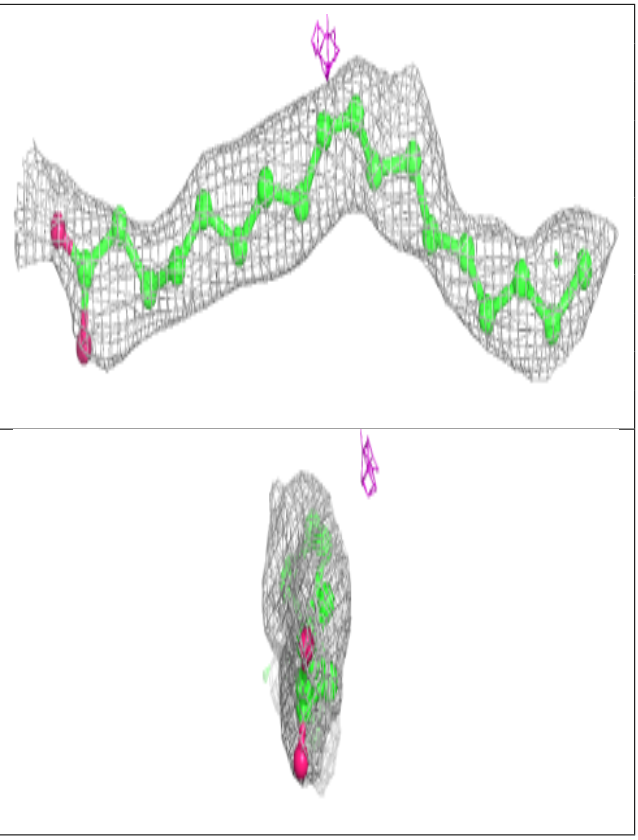






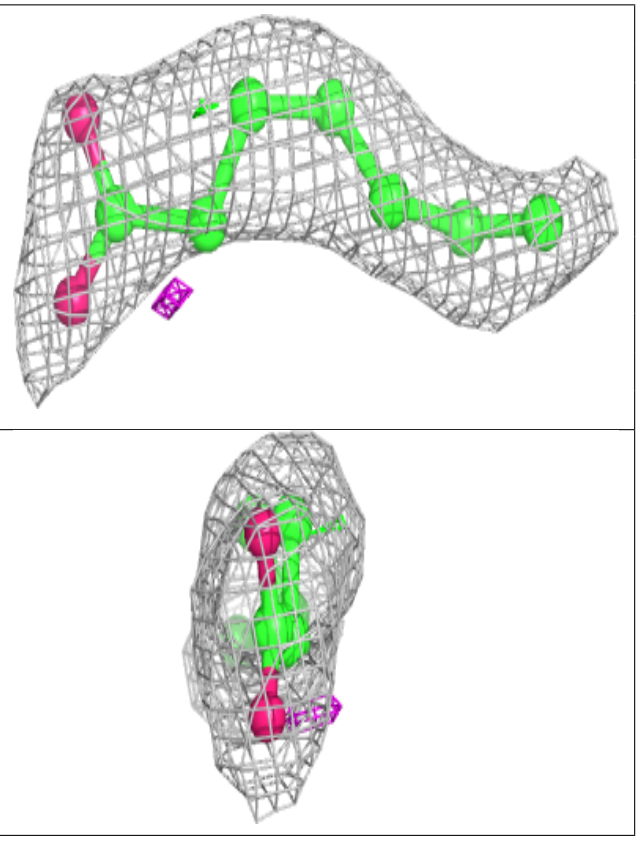
Electron density around OLA A 2405:

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



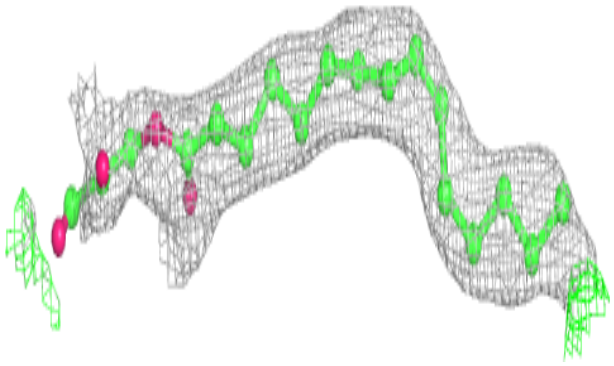
Electron density around OLA A 2419:

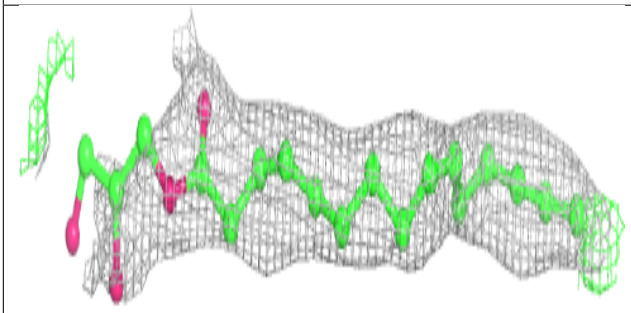
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

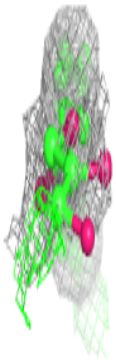


Electron density around OLC A 2425:

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

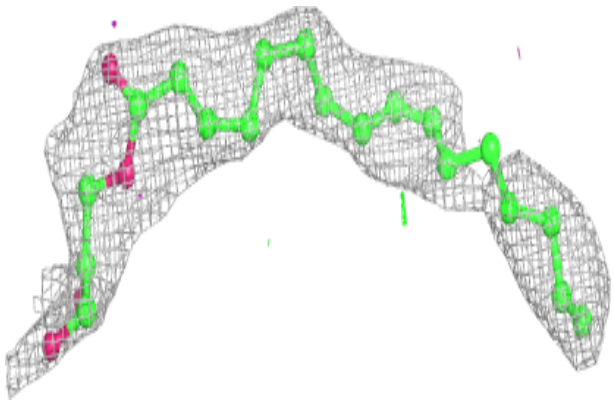


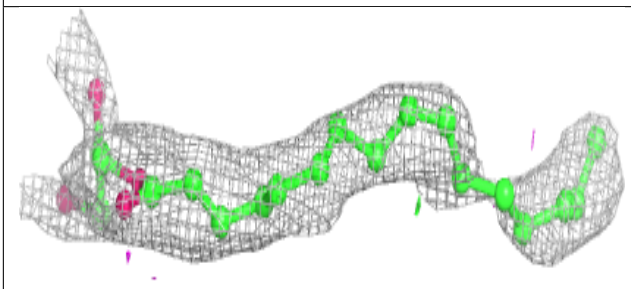


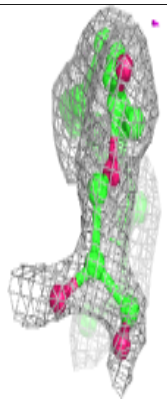


Electron density around OLC A 2421:

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

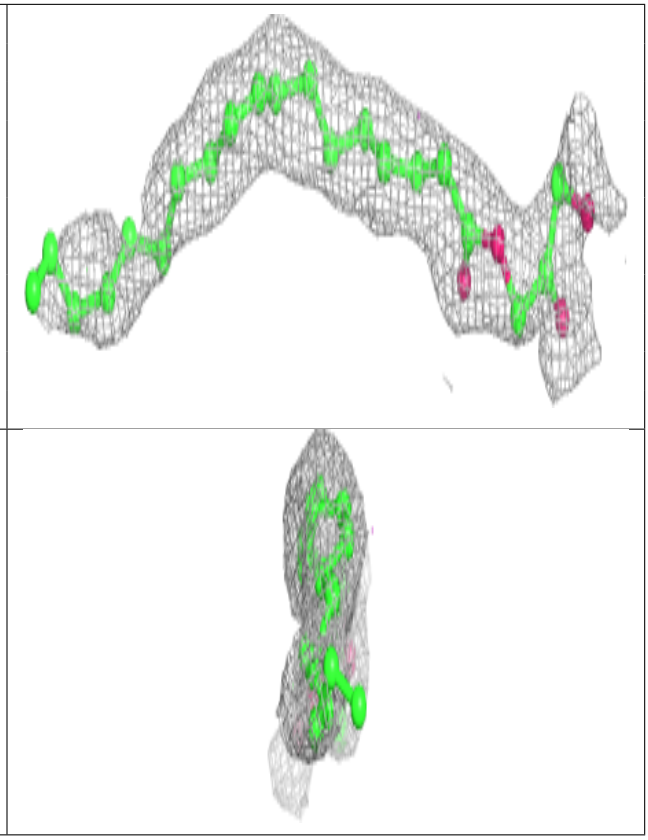






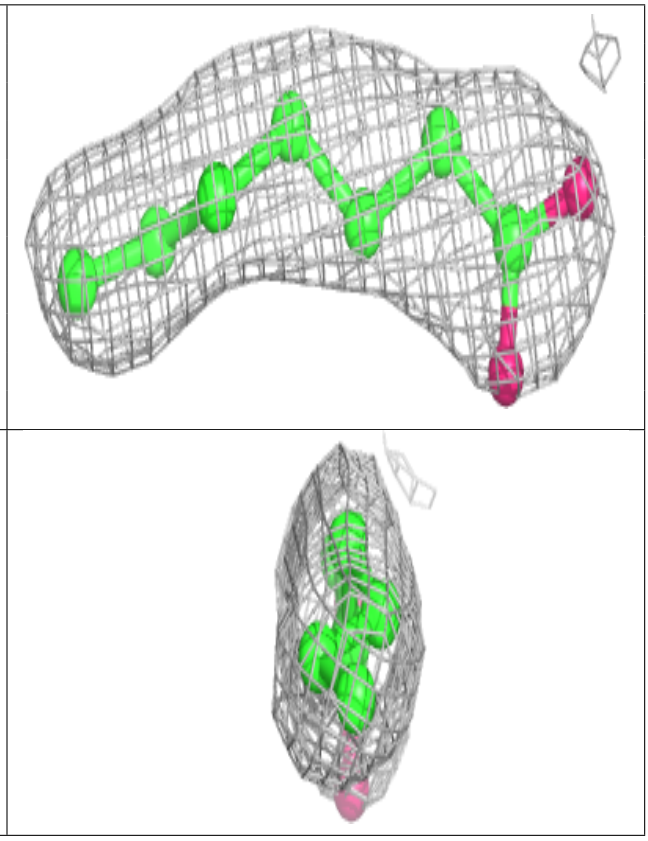
Electron density around OLC A 2427:

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



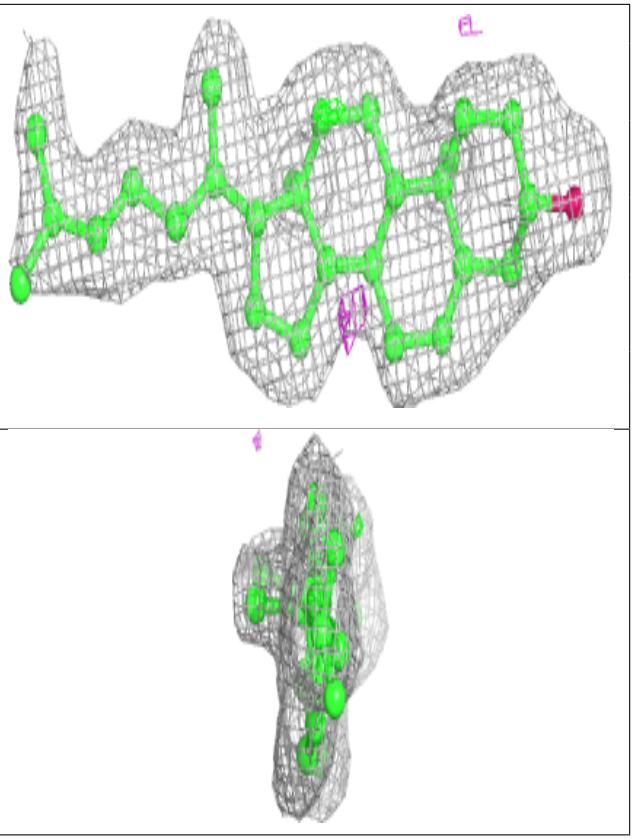
Electron density around OLA A 2408:

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



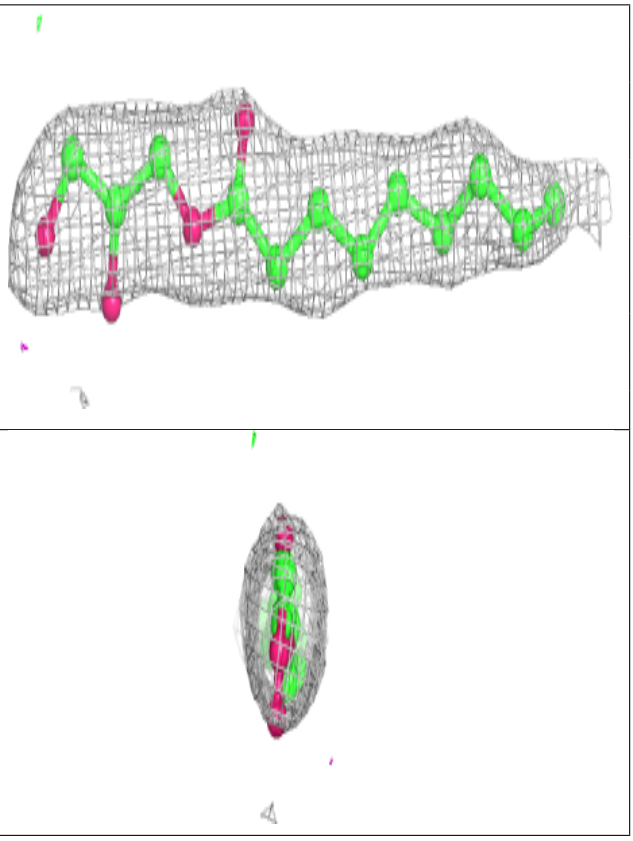
Electron density around CLR A 2402:

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



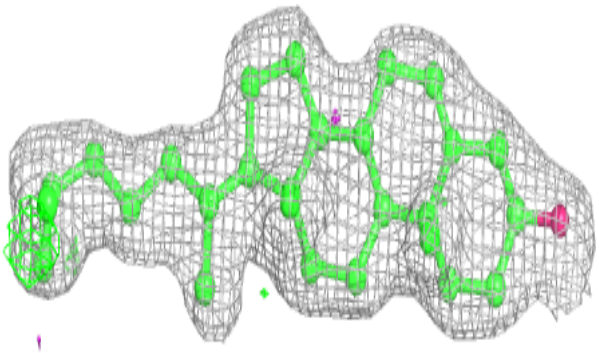
Electron density around OLC A 2422:

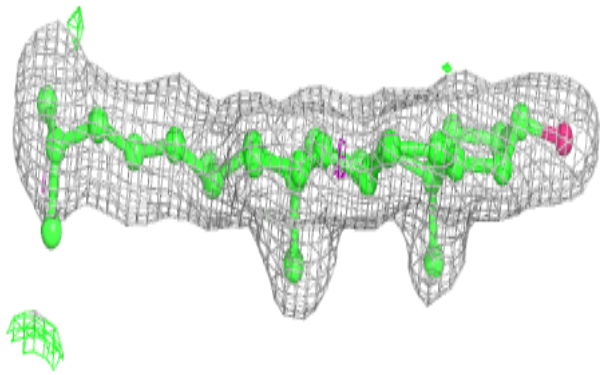
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

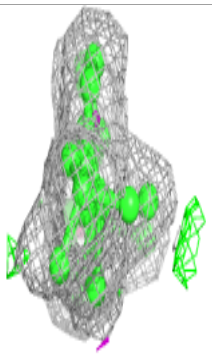


Electron density around CLR A 2403:

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

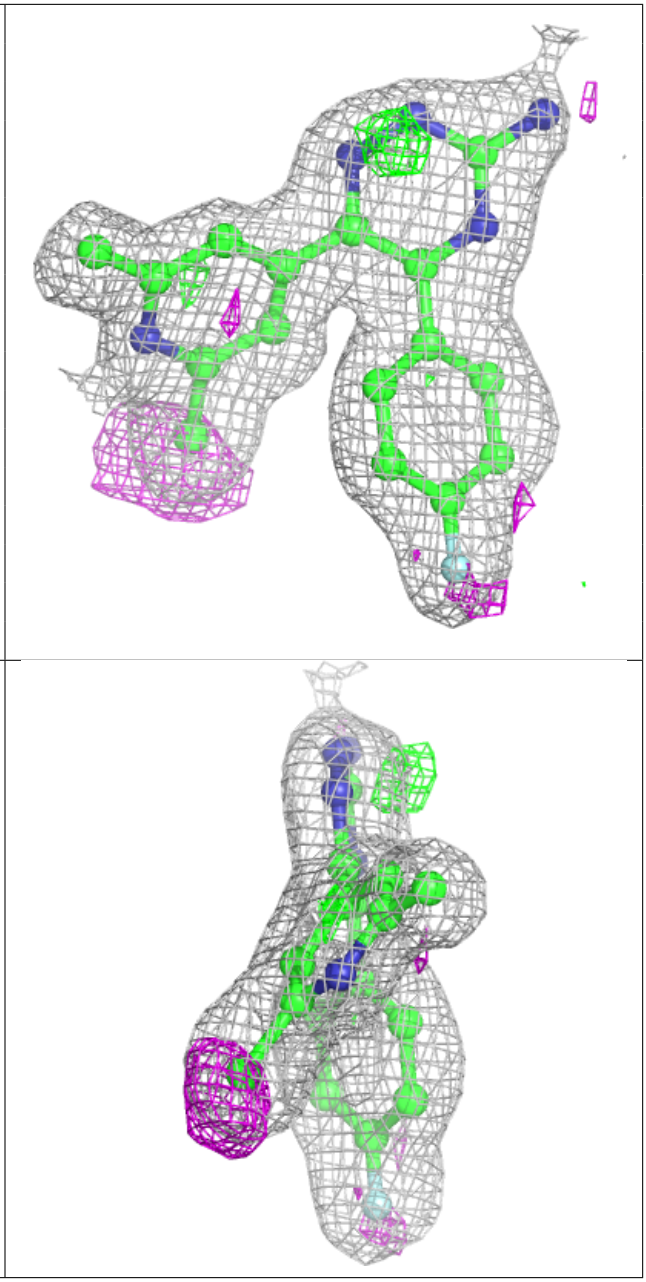






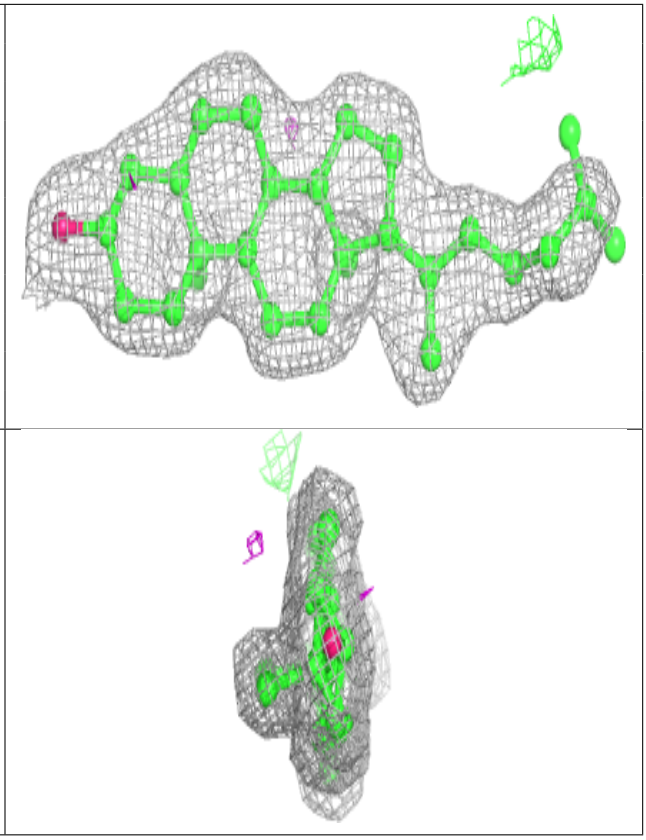
Electron density around F9Q A 2401:

$2mF_o$-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 2404:

$2mF_o$-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.