Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2022 – 02:34 pm GMT

PDB ID	:	7PX4
Title	:	Crystal structure of the adenosine A2A receptor (A2A-PSB1-bRIL) in complex with preladenant conjugate PSB-2113
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Deposited on	:	2021-10-07
Resolution	:	2.25 Å(reported)

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

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

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

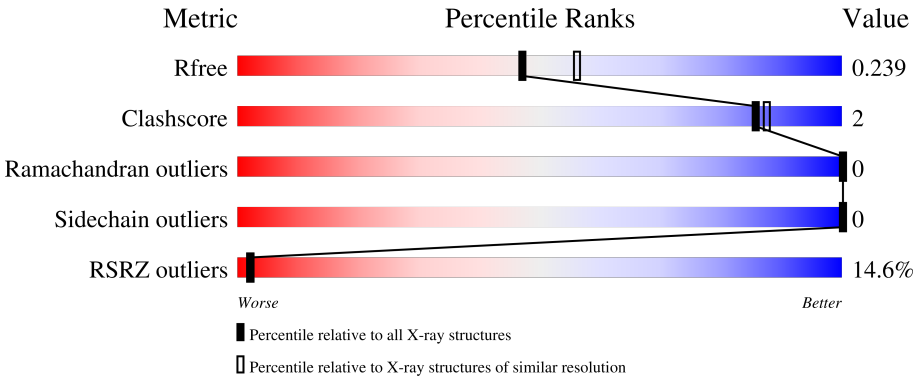
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance

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

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	447	13% 84% · 13%

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	A	2424	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3813 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	390	3004	1957	503	523	21	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
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

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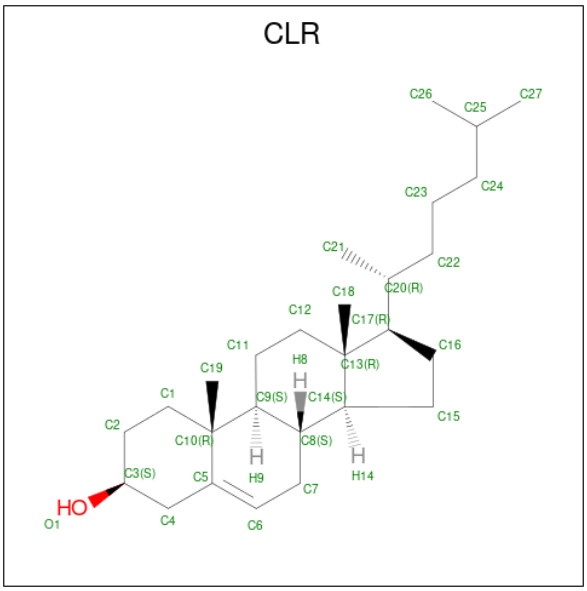
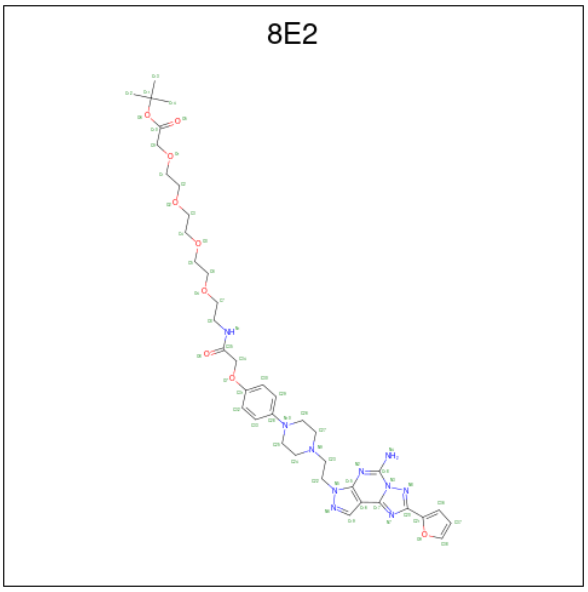
Chain	Residue	Modelled	Actual	Comment	Reference
A	91	LYS	SER	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
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

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



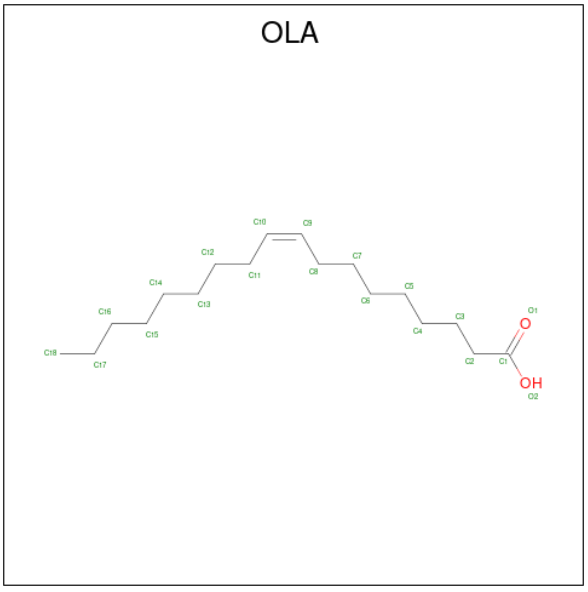
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 28 27 1	0	0
2	A	1	Total C O 28 27 1	0	0
2	A	1	Total C O 28 27 1	0	0

- Molecule 3 is Preladenant conjugate PSB-2113 (three-letter code: 8E2) (formula: $C_{38}H_{52}N_{10}O_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			50	33	10	7		

- 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	0	0
			9	7	2		
4	A	1	Total	C	O	0	0
			11	9	2		
4	A	1	Total	C	O	0	0
			20	18	2		

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

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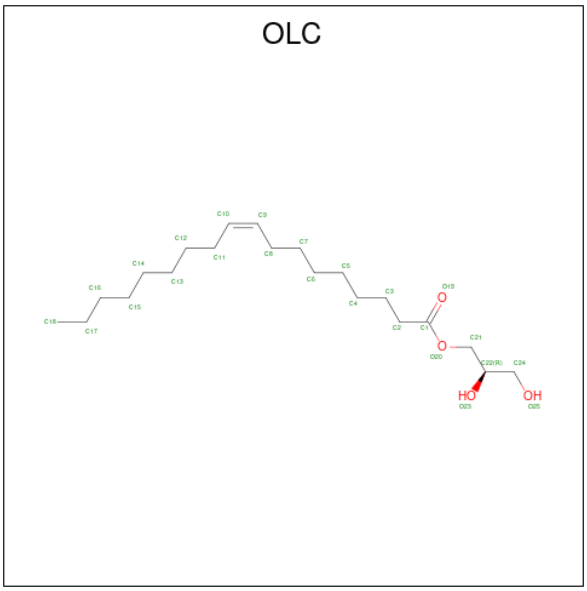
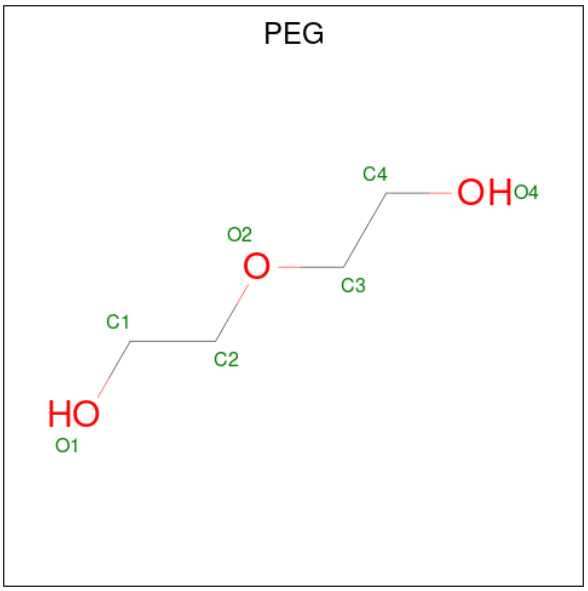
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C O 15 13 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C O 21 17 4	0	0
5	A	1	Total C O 19 15 4	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0

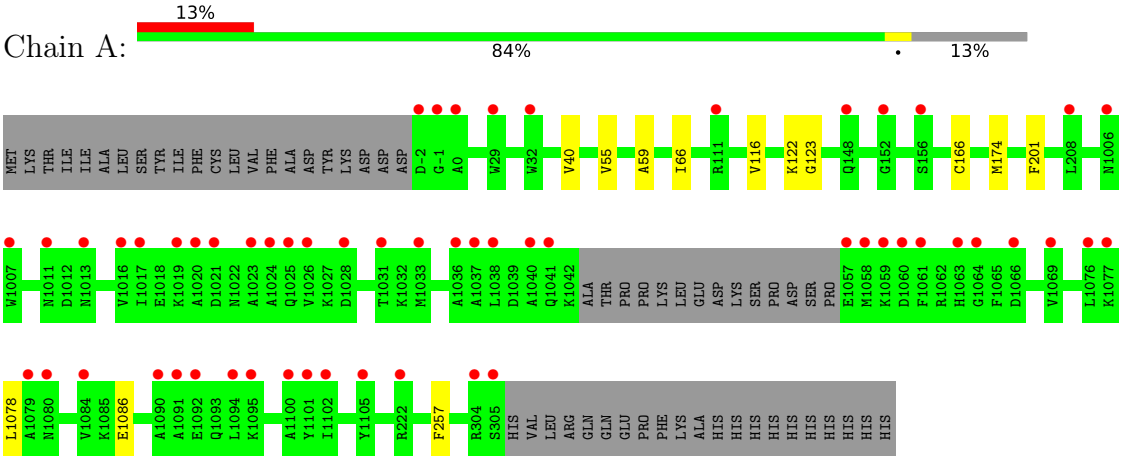
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	231	Total O 231 231	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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.60Å 180.26Å 139.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.88 – 2.25 42.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.88-2.25) 99.6 (42.88-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.240 0.195 , 0.239	Depositor DCC
R_{free} test set	1084 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3813	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, OLC, 8E2, PEG, 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	0.24	0/3067	0.41	0/4174

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

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	3004	0	3050	8	0
2	A	84	0	138	4	0
3	A	50	0	0	0	0
4	A	365	0	496	4	0
5	A	65	0	94	1	0
6	A	14	0	20	2	0
7	A	231	0	0	0	0
All	All	3813	0	3798	16	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.

All (16) 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:40:VAL:HG11	1:A:116:VAL:HG12	1.87	0.56
1:A:1078:LEU:HD13	1:A:1086:GLU:HG2	1.92	0.52
1:A:201:PHE:HB3	4:A:2410:OLA:H22	1.94	0.48
2:A:2402:CLR:H111	2:A:2402:CLR:H193	1.68	0.46
4:A:2427:OLA:H72	4:A:2427:OLA:H42	1.56	0.44
6:A:2434:PEG:H32	6:A:2434:PEG:H11	1.77	0.44
1:A:123:GLY:HA3	6:A:2435:PEG:H31	2.00	0.44
2:A:2401:CLR:H111	2:A:2401:CLR:H193	1.71	0.43
1:A:122:LYS:HG2	5:A:2432:OLC:H24	2.01	0.42
2:A:2401:CLR:H232	2:A:2401:CLR:H211	1.66	0.42
1:A:66:ILE:HG13	1:A:166:CYS:SG	2.60	0.42
2:A:2403:CLR:H111	2:A:2403:CLR:H193	1.73	0.41
1:A:55:VAL:HA	1:A:59:ALA:HB3	2.01	0.41
1:A:174:MET:HG3	1:A:257:PHE:HB2	2.03	0.41
4:A:2419:OLA:H9	4:A:2419:OLA:H62	1.85	0.41
4:A:2428:OLA:H41	4:A:2428:OLA:H72	1.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/447 (86%)	380 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	313/374 (84%)	313 (100%)	0	100 100

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	OLA	A	2408	-	15,18,19	0.73	1 (6%)	14,18,19	0.63	0
3	8E2	A	2404	-	46,55,62	2.25	14 (30%)	52,73,84	1.88	13 (25%)
2	CLR	A	2403	-	31,31,31	1.89	2 (6%)	48,48,48	3.32	23 (47%)
4	OLA	A	2411	-	15,18,19	0.73	1 (6%)	14,18,19	0.64	0
5	OLC	A	2433	-	18,18,24	0.80	0	18,19,25	0.69	0
4	OLA	A	2412	-	8,11,19	1.01	1 (12%)	7,11,19	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OLA	A	2414	-	8,11,19	1.01	1 (12%)	7,11,19	0.76	0
4	OLA	A	2420	-	10,13,19	0.89	1 (10%)	8,13,19	0.69	0
4	OLA	A	2429	-	12,15,19	0.83	1 (8%)	11,15,19	0.55	0
5	OLC	A	2432	-	20,20,24	0.79	0	21,21,25	0.70	0
4	OLA	A	2405	-	5,8,19	0.25	0	4,8,19	0.55	0
6	PEG	A	2435	-	6,6,6	0.43	0	5,5,5	0.31	0
4	OLA	A	2418	-	12,15,19	0.82	1 (8%)	11,15,19	0.58	0
4	OLA	A	2406	-	7,10,19	0.22	0	6,10,19	0.64	0
4	OLA	A	2419	-	13,16,19	0.77	1 (7%)	12,16,19	0.60	0
4	OLA	A	2417	-	7,10,19	0.20	0	6,10,19	0.62	0
4	OLA	A	2413	-	9,12,19	0.83	1 (11%)	8,12,19	0.79	0
4	OLA	A	2410	-	3,6,19	0.26	0	2,6,19	0.57	0
4	OLA	A	2426	-	10,13,19	0.90	1 (10%)	8,13,19	0.67	0
4	OLA	A	2430	-	11,14,19	0.87	1 (9%)	10,14,19	0.51	0
2	CLR	A	2402	-	31,31,31	1.92	2 (6%)	48,48,48	3.25	22 (45%)
4	OLA	A	2407	-	16,19,19	0.71	1 (6%)	15,19,19	0.62	0
4	OLA	A	2421	-	12,15,19	0.82	1 (8%)	11,15,19	0.51	0
4	OLA	A	2427	-	7,10,19	0.23	0	6,10,19	0.50	0
4	OLA	A	2416	-	5,8,19	0.24	0	4,8,19	0.51	0
2	CLR	A	2401	-	31,31,31	1.86	2 (6%)	48,48,48	3.19	24 (50%)
4	OLA	A	2428	-	7,10,19	0.23	0	6,10,19	0.56	0
4	OLA	A	2409	-	9,12,19	0.84	1 (11%)	8,12,19	0.74	0
5	OLC	A	2431	-	24,24,24	0.73	0	25,25,25	0.62	0
6	PEG	A	2434	-	6,6,6	0.43	0	5,5,5	0.31	0
4	OLA	A	2422	-	10,13,19	0.91	1 (10%)	8,13,19	0.58	0
4	OLA	A	2423	-	16,19,19	0.72	1 (6%)	15,19,19	0.57	0
4	OLA	A	2424	-	10,13,19	0.91	1 (10%)	8,13,19	0.61	0
4	OLA	A	2415	-	16,19,19	0.71	1 (6%)	15,19,19	0.59	0
4	OLA	A	2425	-	8,11,19	1.02	1 (12%)	7,11,19	0.67	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
4	OLA	A	2408	-	-	7/14/16/17	-
3	8E2	A	2404	-	-	13/28/42/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLR	A	2403	-	-	4/10/68/68	0/4/4/4
4	OLA	A	2411	-	-	7/14/16/17	-
5	OLC	A	2433	-	-	9/18/18/24	-
4	OLA	A	2412	-	-	4/7/9/17	-
4	OLA	A	2414	-	-	6/7/9/17	-
4	OLA	A	2420	-	-	5/9/11/17	-
4	OLA	A	2429	-	-	7/11/13/17	-
5	OLC	A	2432	-	-	11/20/20/24	-
4	OLA	A	2405	-	-	2/4/6/17	-
6	PEG	A	2435	-	-	3/4/4/4	-
4	OLA	A	2418	-	-	9/11/13/17	-
4	OLA	A	2406	-	-	4/6/8/17	-
4	OLA	A	2419	-	-	9/12/14/17	-
4	OLA	A	2417	-	-	3/6/8/17	-
4	OLA	A	2413	-	-	6/8/10/17	-
4	OLA	A	2410	-	-	2/2/4/17	-
4	OLA	A	2426	-	-	6/9/11/17	-
4	OLA	A	2430	-	-	7/10/12/17	-
2	CLR	A	2402	-	-	5/10/68/68	0/4/4/4
4	OLA	A	2407	-	-	9/15/17/17	-
4	OLA	A	2421	-	-	6/11/13/17	-
4	OLA	A	2427	-	-	3/6/8/17	-
4	OLA	A	2416	-	-	4/4/6/17	-
2	CLR	A	2401	-	-	7/10/68/68	0/4/4/4
4	OLA	A	2428	-	-	4/6/8/17	-
4	OLA	A	2409	-	-	6/8/10/17	-
5	OLC	A	2431	-	-	14/24/24/24	-
6	PEG	A	2434	-	-	3/4/4/4	-
4	OLA	A	2422	-	-	5/9/11/17	-
4	OLA	A	2423	-	-	8/15/17/17	-
4	OLA	A	2424	-	-	6/9/11/17	-
4	OLA	A	2415	-	-	9/15/17/17	-
4	OLA	A	2425	-	-	4/7/9/17	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2402	CLR	C6-C5	9.29	1.53	1.33
2	A	2403	CLR	C6-C5	9.08	1.53	1.33
2	A	2401	CLR	C6-C5	8.91	1.52	1.33
3	A	2404	8E2	C20-N7	6.07	1.43	1.35
3	A	2404	8E2	C34-C35	5.43	1.62	1.51
3	A	2404	8E2	C28-N10	4.76	1.51	1.38
3	A	2404	8E2	C35-N1	4.07	1.42	1.33
3	A	2404	8E2	C17-N7	3.97	1.37	1.33
3	A	2404	8E2	C15-N2	3.85	1.41	1.35
3	A	2404	8E2	C25-N10	3.09	1.51	1.46
3	A	2404	8E2	C16-C17	3.09	1.45	1.41
3	A	2404	8E2	C26-N10	3.08	1.51	1.46
2	A	2402	CLR	C10-C9	-2.81	1.51	1.56
4	A	2425	OLA	C10-C9	2.81	1.47	1.28
4	A	2412	OLA	C10-C9	2.79	1.47	1.28
4	A	2414	OLA	C10-C9	2.78	1.47	1.28
4	A	2430	OLA	C10-C9	2.76	1.47	1.31
4	A	2422	OLA	C10-C9	2.76	1.47	1.31
4	A	2429	OLA	C10-C9	2.74	1.47	1.31
4	A	2424	OLA	C10-C9	2.74	1.47	1.31
4	A	2421	OLA	C10-C9	2.74	1.47	1.31
4	A	2423	OLA	C10-C9	2.74	1.47	1.31
4	A	2418	OLA	C10-C9	2.72	1.47	1.31
4	A	2426	OLA	C10-C9	2.71	1.47	1.31
4	A	2408	OLA	C10-C9	2.71	1.47	1.31
4	A	2407	OLA	C10-C9	2.71	1.47	1.31
4	A	2420	OLA	C10-C9	2.70	1.47	1.31
4	A	2415	OLA	C10-C9	2.69	1.47	1.31
4	A	2411	OLA	C10-C9	2.69	1.47	1.31
4	A	2419	OLA	C10-C9	2.67	1.47	1.31
2	A	2401	CLR	C10-C9	-2.64	1.51	1.56
2	A	2403	CLR	C10-C9	-2.63	1.51	1.56
3	A	2404	8E2	C22-N5	2.42	1.52	1.47
4	A	2413	OLA	C9-C10	2.41	1.47	1.29
4	A	2409	OLA	C9-C10	2.41	1.47	1.29
3	A	2404	8E2	O8-C35	-2.32	1.18	1.23
3	A	2404	8E2	C8-C7	2.29	1.58	1.50
3	A	2404	8E2	C23-N9	2.12	1.52	1.47
3	A	2404	8E2	C8-N1	2.09	1.50	1.46

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2401	CLR	C4-C5-C6	-8.95	107.71	120.61
2	A	2402	CLR	C4-C5-C6	-8.82	107.90	120.61
2	A	2403	CLR	C4-C5-C6	-8.81	107.91	120.61
2	A	2402	CLR	C7-C6-C5	-8.54	109.31	125.06
2	A	2403	CLR	C7-C6-C5	-8.50	109.38	125.06
2	A	2401	CLR	C7-C6-C5	-8.22	109.90	125.06
2	A	2401	CLR	C4-C5-C10	-7.71	106.17	116.42
2	A	2403	CLR	C4-C5-C10	-7.10	106.99	116.42
2	A	2402	CLR	C4-C5-C10	-6.85	107.32	116.42
2	A	2403	CLR	C7-C8-C9	6.66	117.78	109.71
2	A	2403	CLR	C14-C8-C9	-6.47	100.42	109.09
2	A	2403	CLR	C19-C10-C9	-6.18	104.32	111.68
2	A	2402	CLR	C7-C8-C9	6.03	117.02	109.71
3	A	2404	8E2	C29-C28-N10	5.95	129.57	121.38
2	A	2402	CLR	C15-C14-C8	-5.81	109.51	119.08
2	A	2403	CLR	C15-C14-C8	-5.72	109.66	119.08
2	A	2401	CLR	C15-C14-C8	-5.66	109.75	119.08
2	A	2402	CLR	C19-C10-C9	-5.57	105.04	111.68
2	A	2402	CLR	C14-C8-C9	-5.35	101.93	109.09
2	A	2401	CLR	C19-C10-C9	-5.26	105.42	111.68
2	A	2401	CLR	C14-C8-C9	-5.08	102.29	109.09
2	A	2401	CLR	C7-C8-C9	4.82	115.55	109.71
2	A	2402	CLR	C10-C5-C6	-4.74	115.64	122.90
2	A	2403	CLR	C10-C5-C6	-4.67	115.76	122.90
2	A	2401	CLR	C10-C5-C6	-4.65	115.79	122.90
2	A	2402	CLR	C19-C10-C5	4.15	115.05	108.34
2	A	2403	CLR	C19-C10-C5	4.11	115.00	108.34
3	A	2404	8E2	C19-N6-N5	4.03	108.43	104.23
3	A	2404	8E2	N8-C20-N7	-3.91	111.97	114.56
2	A	2403	CLR	C12-C13-C14	3.91	113.33	107.27
2	A	2401	CLR	C19-C10-C5	3.79	114.47	108.34
2	A	2402	CLR	C11-C9-C10	-3.74	108.15	113.08
2	A	2401	CLR	C12-C13-C14	3.73	113.06	107.27
2	A	2401	CLR	C11-C9-C10	-3.59	108.35	113.08
3	A	2404	8E2	C32-C31-C30	-3.59	114.64	120.18
3	A	2404	8E2	C26-N10-C25	-3.46	103.88	111.52
2	A	2401	CLR	C21-C20-C22	-3.40	105.03	110.36
2	A	2402	CLR	C21-C20-C22	-3.40	105.03	110.36
2	A	2403	CLR	C21-C20-C22	-3.34	105.12	110.36
2	A	2402	CLR	C12-C13-C14	3.33	112.44	107.27
2	A	2401	CLR	C10-C9-C8	-3.24	107.87	112.73
2	A	2401	CLR	C16-C17-C13	-3.20	99.99	103.84
3	A	2404	8E2	C30-C29-C28	3.17	124.49	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2402	CLR	C16-C17-C13	-3.16	100.04	103.84
3	A	2404	8E2	C33-C28-C29	-3.15	112.74	119.16
2	A	2403	CLR	C18-C13-C12	-3.15	105.62	110.59
2	A	2403	CLR	C16-C17-C13	-3.04	100.17	103.84
2	A	2403	CLR	C11-C9-C10	-3.03	109.09	113.08
2	A	2402	CLR	C10-C9-C8	-3.01	108.22	112.73
2	A	2403	CLR	C16-C15-C14	-2.90	99.39	105.13
2	A	2401	CLR	C18-C13-C12	-2.87	106.06	110.59
2	A	2402	CLR	C18-C13-C12	-2.75	106.24	110.59
3	A	2404	8E2	C16-C17-N3	-2.73	117.03	121.32
2	A	2402	CLR	C16-C15-C14	-2.72	99.75	105.13
3	A	2404	8E2	C33-C32-C31	2.71	123.05	119.73
3	A	2404	8E2	C33-C28-N10	-2.68	117.68	121.38
2	A	2402	CLR	C15-C16-C17	2.66	110.40	105.13
2	A	2401	CLR	C16-C15-C14	-2.65	99.88	105.13
2	A	2403	CLR	C15-C16-C17	2.64	110.36	105.13
2	A	2402	CLR	C8-C7-C6	-2.64	108.94	112.73
2	A	2403	CLR	C10-C9-C8	-2.54	108.92	112.73
2	A	2402	CLR	O1-C3-C2	-2.48	103.86	110.16
2	A	2403	CLR	C11-C12-C13	-2.46	108.56	112.78
2	A	2401	CLR	C15-C16-C17	2.44	109.96	105.13
2	A	2402	CLR	C13-C14-C8	-2.41	110.81	114.38
2	A	2402	CLR	C22-C20-C17	2.37	115.18	110.28
2	A	2401	CLR	O1-C3-C2	-2.30	104.30	110.16
2	A	2403	CLR	C13-C14-C8	-2.30	110.97	114.38
3	A	2404	8E2	C18-N2-C15	2.28	117.97	115.36
3	A	2404	8E2	C32-C33-C28	2.28	123.32	120.32
2	A	2401	CLR	C19-C10-C1	2.25	112.98	109.43
2	A	2401	CLR	C8-C7-C6	-2.24	109.51	112.73
2	A	2402	CLR	C11-C12-C13	-2.22	108.98	112.78
2	A	2401	CLR	C7-C8-C14	-2.19	107.73	110.91
2	A	2401	CLR	C13-C14-C8	-2.16	111.18	114.38
2	A	2403	CLR	C8-C7-C6	-2.15	109.65	112.73
2	A	2403	CLR	C18-C13-C14	-2.15	107.71	111.71
2	A	2401	CLR	C3-C4-C5	-2.14	108.40	112.03
2	A	2401	CLR	C11-C12-C13	-2.09	109.20	112.78
3	A	2404	8E2	C36-C37-C38	-2.07	105.54	112.92
2	A	2403	CLR	C19-C10-C1	2.05	112.67	109.43
2	A	2403	CLR	O1-C3-C2	-2.02	105.03	110.16

There are no chirality outliers.

All (217) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2404	8E2	C34-C35-N1-C8
3	A	2404	8E2	N5-C22-C23-N9
4	A	2406	OLA	C1-C2-C3-C4
4	A	2407	OLA	C1-C2-C3-C4
4	A	2408	OLA	C1-C2-C3-C4
4	A	2409	OLA	C1-C2-C3-C4
4	A	2410	OLA	C1-C2-C3-C4
4	A	2411	OLA	C1-C2-C3-C4
4	A	2412	OLA	C1-C2-C3-C4
4	A	2413	OLA	C1-C2-C3-C4
4	A	2414	OLA	C1-C2-C3-C4
4	A	2415	OLA	C1-C2-C3-C4
4	A	2416	OLA	C1-C2-C3-C4
4	A	2417	OLA	C1-C2-C3-C4
4	A	2418	OLA	C1-C2-C3-C4
4	A	2419	OLA	C1-C2-C3-C4
4	A	2421	OLA	C1-C2-C3-C4
4	A	2422	OLA	C1-C2-C3-C4
4	A	2423	OLA	C1-C2-C3-C4
4	A	2423	OLA	C11-C10-C9-C8
4	A	2424	OLA	C1-C2-C3-C4
4	A	2425	OLA	C1-C2-C3-C4
4	A	2426	OLA	C1-C2-C3-C4
4	A	2426	OLA	C9-C10-C11-C12
4	A	2427	OLA	C1-C2-C3-C4
5	A	2432	OLC	C10-C11-C12-C13
5	A	2432	OLC	O20-C21-C22-C24
5	A	2433	OLC	C21-C22-C24-O25
5	A	2433	OLC	O20-C21-C22-C24
2	A	2402	CLR	C21-C20-C22-C23
2	A	2403	CLR	C21-C20-C22-C23
5	A	2432	OLC	O20-C21-C22-O23
2	A	2402	CLR	C17-C20-C22-C23
3	A	2404	8E2	O2-C3-C4-O3
3	A	2404	8E2	O8-C35-N1-C8
3	A	2404	8E2	C32-C31-O7-C34
3	A	2404	8E2	C30-C31-O7-C34
2	A	2401	CLR	C21-C20-C22-C23
4	A	2427	OLA	C4-C5-C6-C7
5	A	2431	OLC	O20-C21-C22-C24
4	A	2428	OLA	C4-C5-C6-C7
5	A	2433	OLC	O20-C21-C22-O23
2	A	2401	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	A	2429	OLA	C11-C10-C9-C8
2	A	2401	CLR	C13-C17-C20-C21
6	A	2434	PEG	O1-C1-C2-O2
4	A	2415	OLA	C3-C4-C5-C6
4	A	2430	OLA	C11-C10-C9-C8
2	A	2401	CLR	C22-C23-C24-C25
6	A	2434	PEG	O2-C3-C4-O4
4	A	2415	OLA	C11-C12-C13-C14
4	A	2417	OLA	C2-C3-C4-C5
4	A	2425	OLA	C4-C5-C6-C7
5	A	2432	OLC	C2-C1-O20-C21
4	A	2419	OLA	C3-C4-C5-C6
4	A	2427	OLA	C3-C4-C5-C6
4	A	2430	OLA	C4-C5-C6-C7
4	A	2421	OLA	C4-C5-C6-C7
5	A	2431	OLC	C3-C4-C5-C6
4	A	2416	OLA	C3-C4-C5-C6
4	A	2425	OLA	C5-C6-C7-C8
4	A	2423	OLA	C5-C6-C7-C8
5	A	2432	OLC	C21-C22-C24-O25
5	A	2431	OLC	O20-C21-C22-O23
4	A	2418	OLA	C6-C7-C8-C9
5	A	2431	OLC	C10-C11-C12-C13
4	A	2412	OLA	C4-C5-C6-C7
3	A	2404	8E2	O1-C1-C2-O2
4	A	2426	OLA	C3-C4-C5-C6
4	A	2411	OLA	C11-C12-C13-C14
5	A	2431	OLC	C13-C14-C15-C16
4	A	2419	OLA	C11-C10-C9-C8
4	A	2418	OLA	C5-C6-C7-C8
4	A	2420	OLA	C4-C5-C6-C7
5	A	2433	OLC	O23-C22-C24-O25
4	A	2407	OLA	C10-C11-C12-C13
4	A	2424	OLA	C6-C7-C8-C9
4	A	2417	OLA	C4-C5-C6-C7
5	A	2432	OLC	O19-C1-O20-C21
4	A	2407	OLA	C4-C5-C6-C7
4	A	2423	OLA	C12-C13-C14-C15
2	A	2401	CLR	C13-C17-C20-C22
4	A	2405	OLA	C3-C4-C5-C6
4	A	2419	OLA	C4-C5-C6-C7
6	A	2435	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	A	2424	OLA	C2-C3-C4-C5
5	A	2431	OLC	C4-C5-C6-C7
5	A	2433	OLC	C1-C2-C3-C4
4	A	2430	OLA	C2-C3-C4-C5
4	A	2413	OLA	C11-C10-C9-C8
4	A	2426	OLA	C11-C10-C9-C8
5	A	2431	OLC	C9-C10-C11-C12
5	A	2433	OLC	C6-C7-C8-C9
5	A	2431	OLC	C1-C2-C3-C4
4	A	2415	OLA	C12-C13-C14-C15
4	A	2424	OLA	C4-C5-C6-C7
5	A	2432	OLC	C6-C7-C8-C9
3	A	2404	8E2	C3-C4-O3-C5
4	A	2413	OLA	C3-C4-C5-C6
4	A	2418	OLA	C11-C10-C9-C8
4	A	2412	OLA	C3-C4-C5-C6
4	A	2414	OLA	C5-C6-C7-C8
2	A	2401	CLR	C16-C17-C20-C21
4	A	2411	OLA	C5-C6-C7-C8
4	A	2416	OLA	C2-C3-C4-C5
4	A	2414	OLA	C3-C4-C5-C6
4	A	2423	OLA	C4-C5-C6-C7
6	A	2435	PEG	O1-C1-C2-O2
4	A	2407	OLA	C14-C15-C16-C17
2	A	2403	CLR	C22-C23-C24-C25
5	A	2432	OLC	O23-C22-C24-O25
4	A	2423	OLA	C6-C7-C8-C9
5	A	2432	OLC	C11-C12-C13-C14
5	A	2433	OLC	C4-C5-C6-C7
4	A	2414	OLA	C4-C5-C6-C7
5	A	2432	OLC	C7-C8-C9-C10
5	A	2431	OLC	C21-C22-C24-O25
4	A	2426	OLA	C6-C7-C8-C9
4	A	2420	OLA	C11-C10-C9-C8
4	A	2424	OLA	C11-C10-C9-C8
4	A	2428	OLA	C3-C4-C5-C6
4	A	2415	OLA	C11-C10-C9-C8
4	A	2422	OLA	C11-C10-C9-C8
4	A	2409	OLA	C4-C5-C6-C7
4	A	2411	OLA	C2-C3-C4-C5
4	A	2407	OLA	C12-C13-C14-C15
4	A	2408	OLA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	A	2413	OLA	C4-C5-C6-C7
4	A	2429	OLA	C11-C12-C13-C14
2	A	2401	CLR	C16-C17-C20-C22
4	A	2411	OLA	C6-C7-C8-C9
4	A	2419	OLA	C5-C6-C7-C8
4	A	2430	OLA	C3-C4-C5-C6
4	A	2406	OLA	C2-C3-C4-C5
4	A	2429	OLA	C4-C5-C6-C7
3	A	2404	8E2	O3-C5-C6-O4
5	A	2431	OLC	C15-C16-C17-C18
4	A	2420	OLA	C9-C10-C11-C12
4	A	2422	OLA	C9-C10-C11-C12
4	A	2424	OLA	C9-C10-C11-C12
4	A	2428	OLA	C5-C6-C7-C8
4	A	2409	OLA	C11-C10-C9-C8
2	A	2402	CLR	C13-C17-C20-C21
5	A	2432	OLC	C4-C5-C6-C7
4	A	2408	OLA	C4-C5-C6-C7
4	A	2418	OLA	C4-C5-C6-C7
4	A	2407	OLA	C3-C4-C5-C6
4	A	2429	OLA	C3-C4-C5-C6
4	A	2418	OLA	C11-C12-C13-C14
4	A	2415	OLA	C14-C15-C16-C17
4	A	2413	OLA	C5-C6-C7-C8
4	A	2421	OLA	C3-C4-C5-C6
4	A	2407	OLA	C11-C10-C9-C8
3	A	2404	8E2	C1-C2-O2-C3
6	A	2434	PEG	C1-C2-O2-C3
4	A	2407	OLA	C5-C6-C7-C8
3	A	2404	8E2	O7-C34-C35-N1
4	A	2411	OLA	C3-C4-C5-C6
2	A	2403	CLR	C13-C17-C20-C21
5	A	2431	OLC	O23-C22-C24-O25
4	A	2419	OLA	C11-C12-C13-C14
4	A	2410	OLA	C2-C3-C4-C5
4	A	2420	OLA	C7-C8-C9-C10
4	A	2422	OLA	C4-C5-C6-C7
3	A	2404	8E2	O7-C34-C35-O8
2	A	2402	CLR	C13-C17-C20-C22
4	A	2412	OLA	C7-C8-C9-C10
4	A	2423	OLA	C9-C10-C11-C12
5	A	2433	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	2433	OLC	C9-C10-C11-C12
4	A	2406	OLA	C4-C5-C6-C7
4	A	2408	OLA	C7-C8-C9-C10
4	A	2418	OLA	C7-C8-C9-C10
3	A	2404	8E2	C35-C34-O7-C31
4	A	2414	OLA	C6-C7-C8-C9
4	A	2420	OLA	C3-C4-C5-C6
4	A	2416	OLA	C4-C5-C6-C7
4	A	2421	OLA	C10-C11-C12-C13
4	A	2426	OLA	C4-C5-C6-C7
4	A	2428	OLA	C6-C7-C8-C9
4	A	2425	OLA	C7-C8-C9-C10
4	A	2408	OLA	C11-C10-C9-C8
4	A	2418	OLA	C9-C10-C11-C12
4	A	2419	OLA	C2-C3-C4-C5
4	A	2407	OLA	C7-C8-C9-C10
4	A	2415	OLA	C9-C10-C11-C12
4	A	2421	OLA	C11-C12-C13-C14
4	A	2429	OLA	C6-C7-C8-C9
4	A	2421	OLA	C9-C10-C11-C12
4	A	2422	OLA	C7-C8-C9-C10
4	A	2429	OLA	C9-C10-C11-C12
4	A	2430	OLA	C9-C10-C11-C12
4	A	2414	OLA	C7-C8-C9-C10
5	A	2431	OLC	C14-C15-C16-C17
4	A	2430	OLA	C7-C8-C9-C10
6	A	2435	PEG	C1-C2-O2-C3
4	A	2413	OLA	C2-C3-C4-C5
4	A	2409	OLA	C7-C8-C9-C10
4	A	2419	OLA	C7-C8-C9-C10
2	A	2403	CLR	C17-C20-C22-C23
4	A	2423	OLA	C7-C8-C9-C10
4	A	2429	OLA	C7-C8-C9-C10
5	A	2431	OLC	O20-C1-C2-C3
4	A	2419	OLA	C9-C10-C11-C12
4	A	2411	OLA	C9-C10-C11-C12
4	A	2430	OLA	C6-C7-C8-C9
4	A	2415	OLA	C5-C6-C7-C8
4	A	2408	OLA	C12-C13-C14-C15
4	A	2415	OLA	C10-C11-C12-C13
5	A	2431	OLC	O19-C1-C2-C3
4	A	2408	OLA	C5-C6-C7-C8

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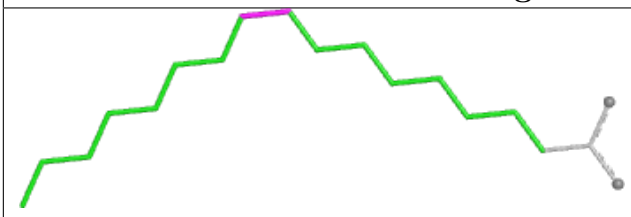
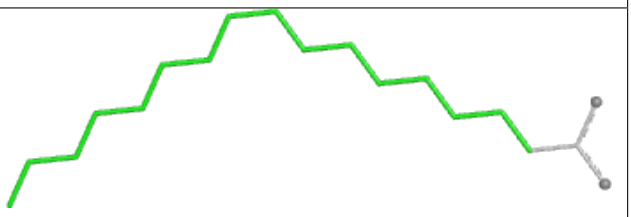
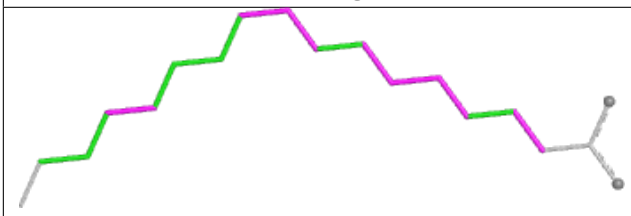
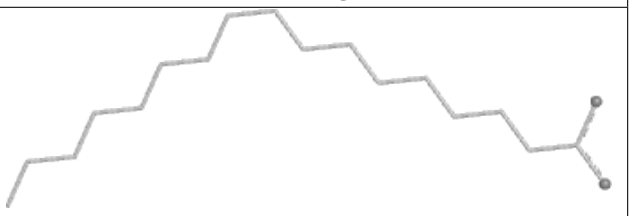
Mol	Chain	Res	Type	Atoms
4	A	2409	OLA	C3-C4-C5-C6
2	A	2402	CLR	C16-C17-C20-C21
4	A	2418	OLA	C2-C3-C4-C5
4	A	2409	OLA	C5-C6-C7-C8
4	A	2406	OLA	C3-C4-C5-C6
4	A	2405	OLA	C4-C5-C6-C7

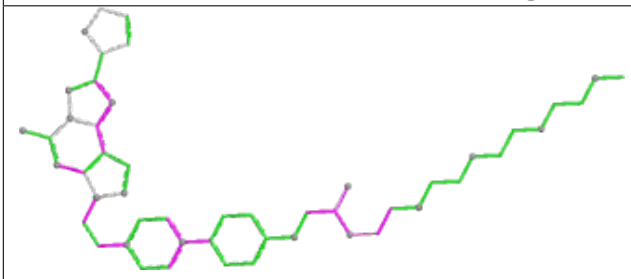
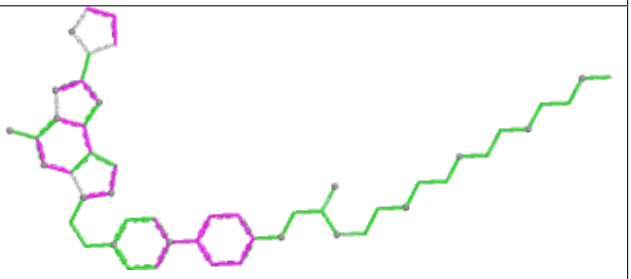
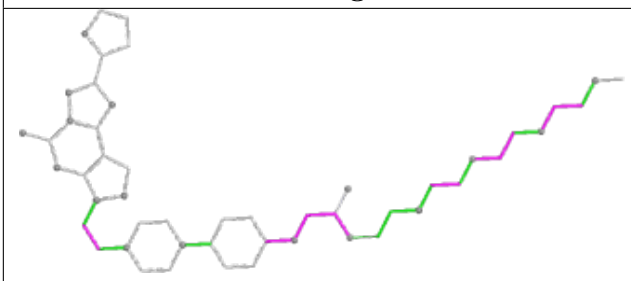
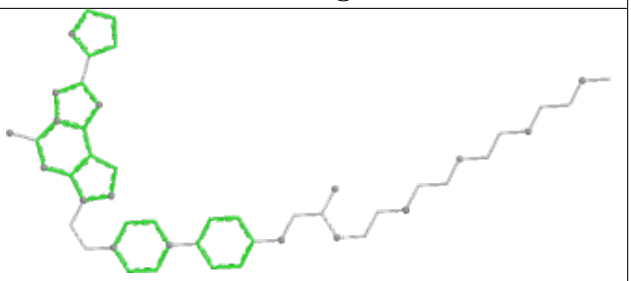
There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2403	CLR	1	0
5	A	2432	OLC	1	0
6	A	2435	PEG	1	0
4	A	2419	OLA	1	0
4	A	2410	OLA	1	0
2	A	2402	CLR	1	0
4	A	2427	OLA	1	0
2	A	2401	CLR	2	0
4	A	2428	OLA	1	0
6	A	2434	PEG	1	0

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

Ligand OLA A 2408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8E2 A 2404	
 Bond lengths	 Bond angles
 Torsions	 Rings

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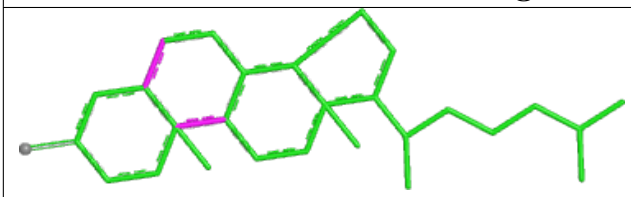
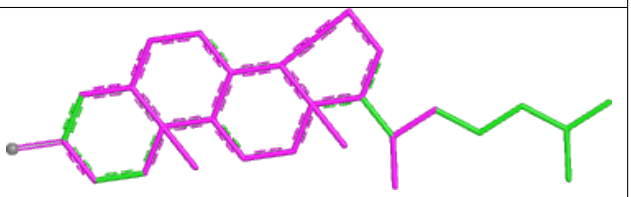
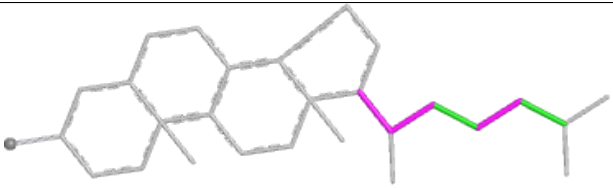
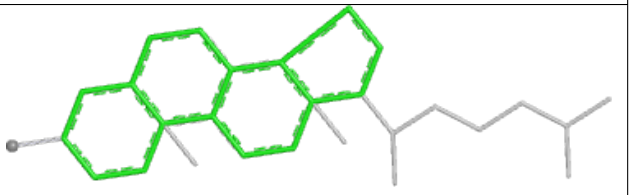
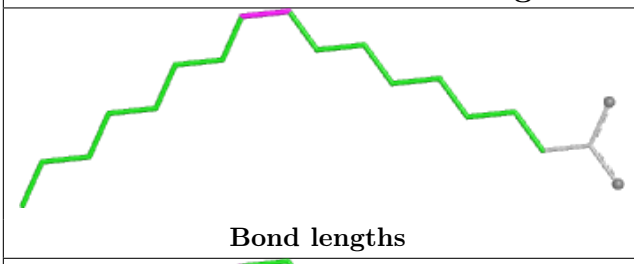
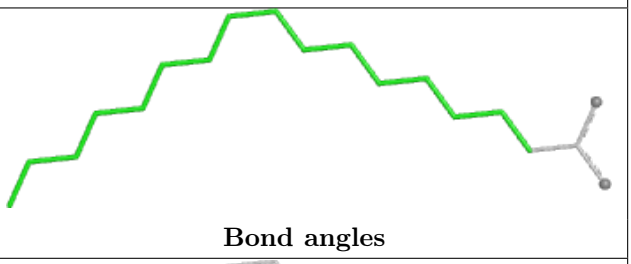
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLA A 2411


Bond lengths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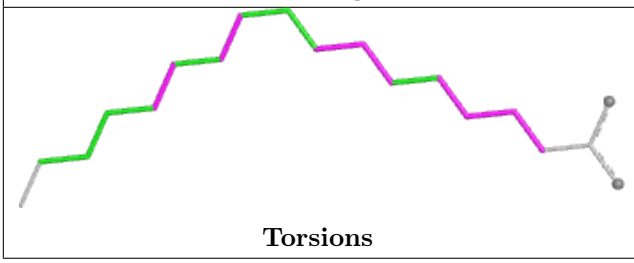
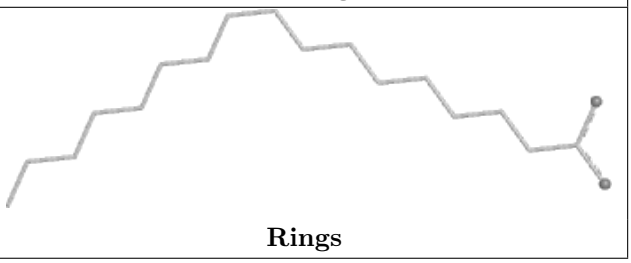
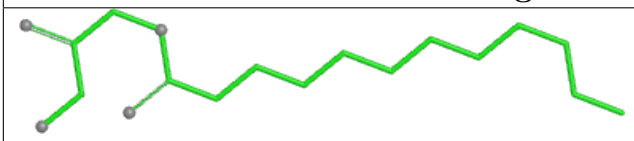
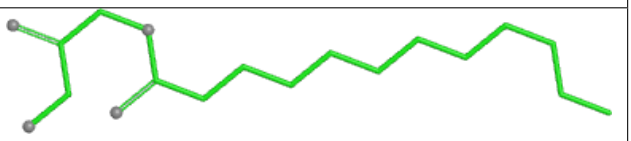
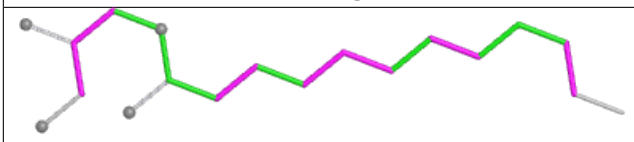

Torsions


Rings

Ligand OLC A 2433


Bond lengths


Bond angles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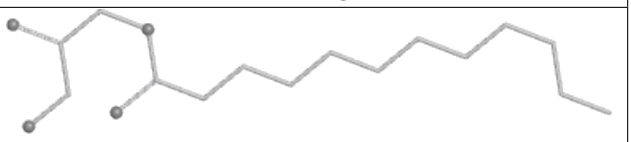
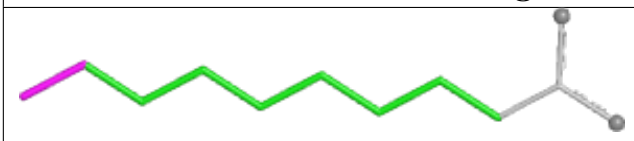

Rings

Ligand OLA A 2412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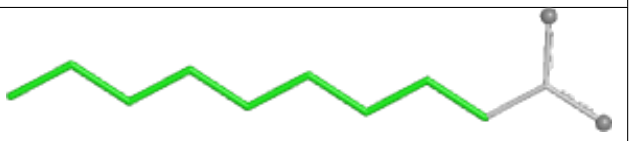
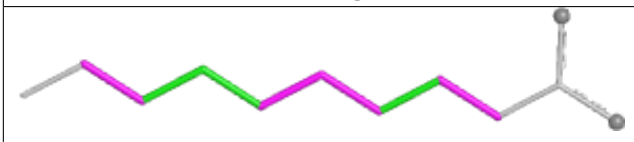

Bond angles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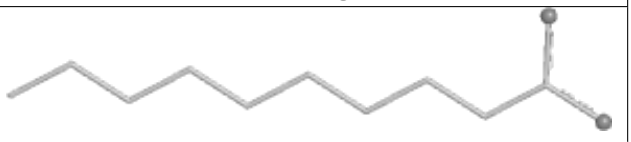
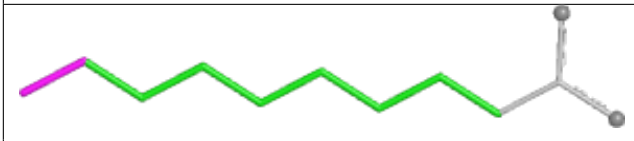

Rings

Ligand OLA A 2414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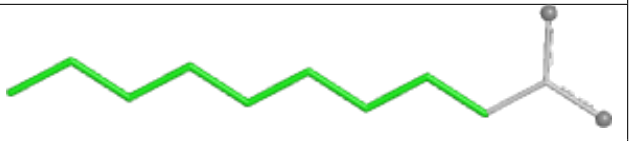
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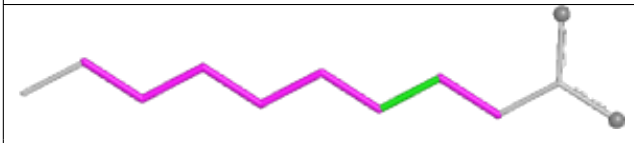
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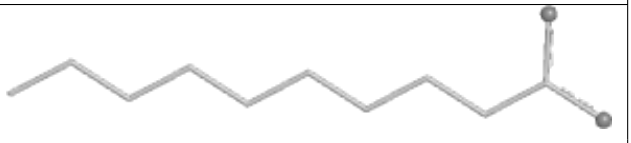
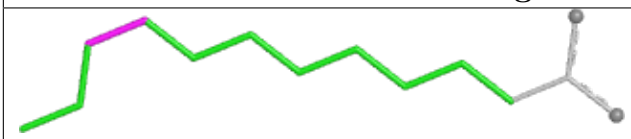
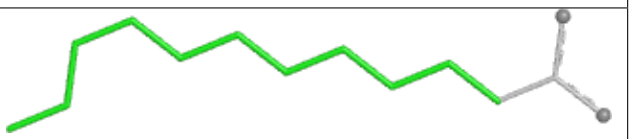
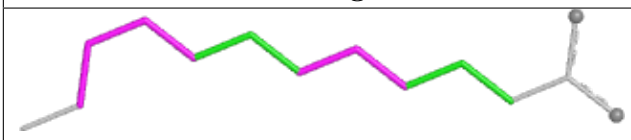
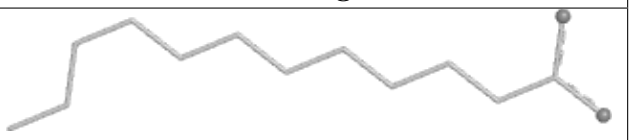
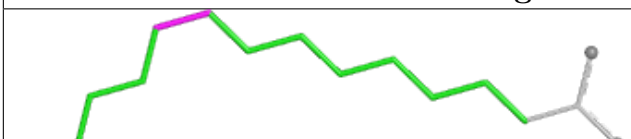
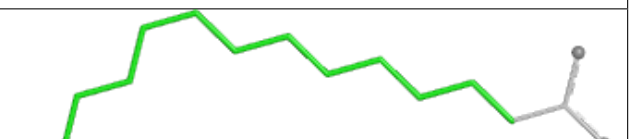
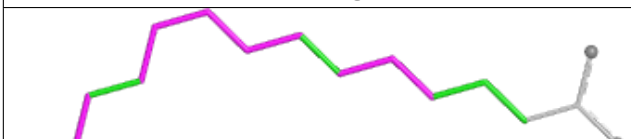

Rings

Ligand OLA A 2420	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLA A 2429	
 Bond lengths	 Bond angles
 Torsions	 Rings

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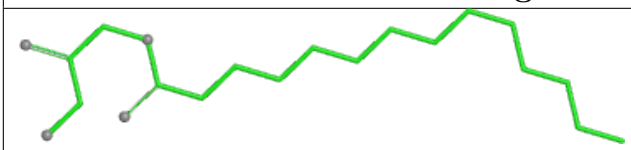
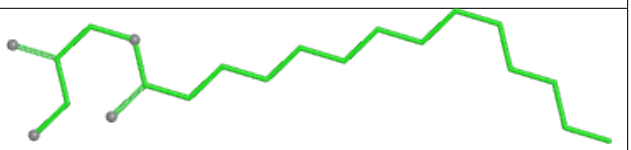
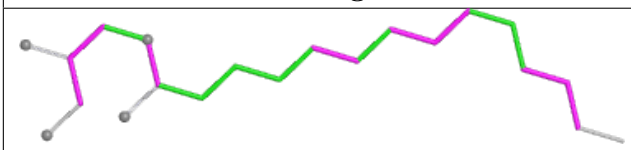
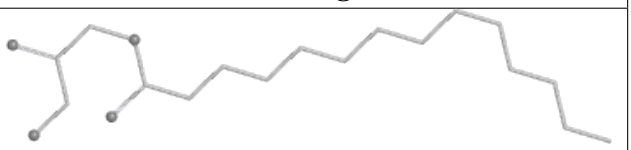
 Bond lengths	 Bond angles
 Torsions	 Rings

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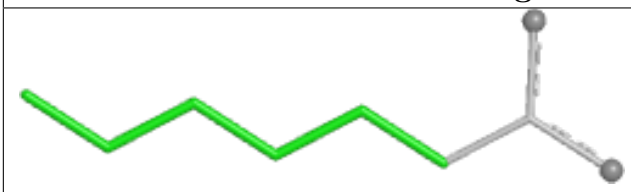
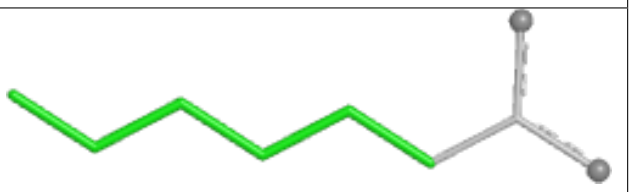
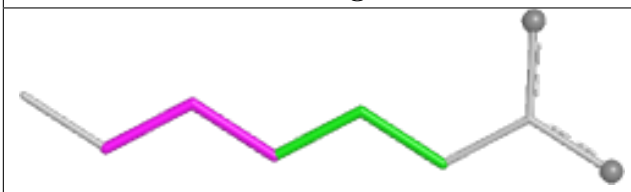
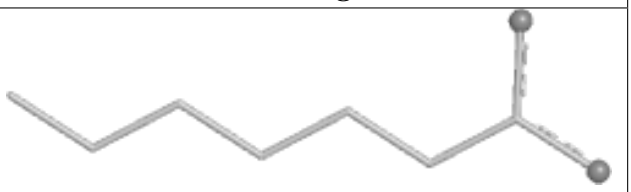
 Bond lengths	 Bond angles
 Torsions	 Rings

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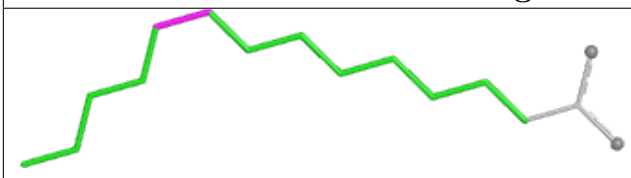
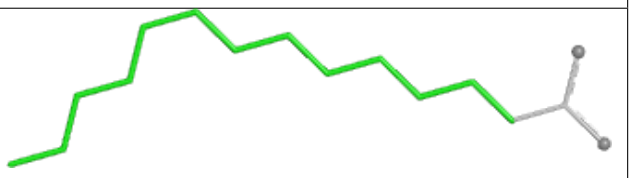
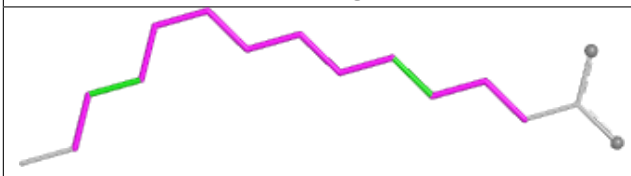
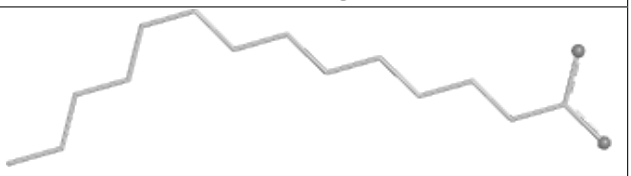
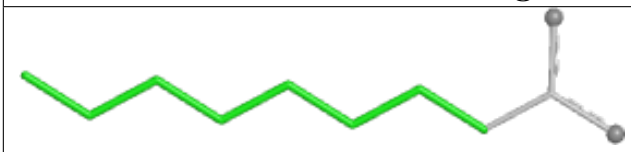
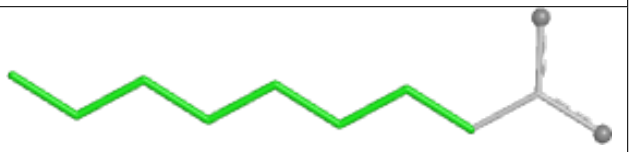
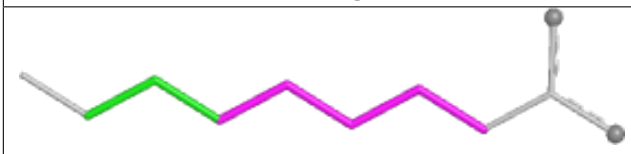
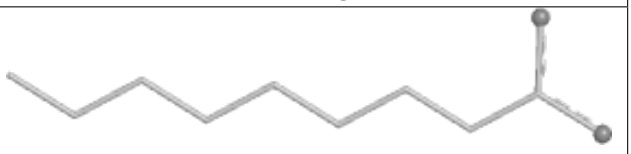
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLA A 2406	
 Bond lengths	 Bond angles
 Torsions	 Rings

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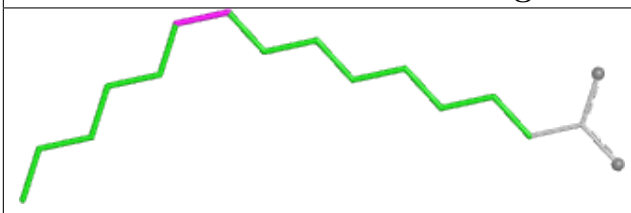
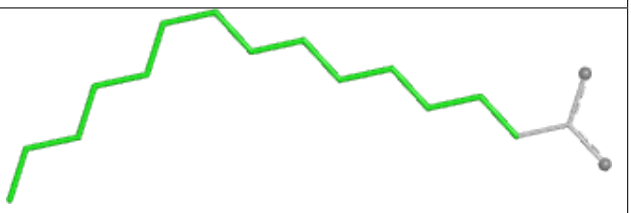
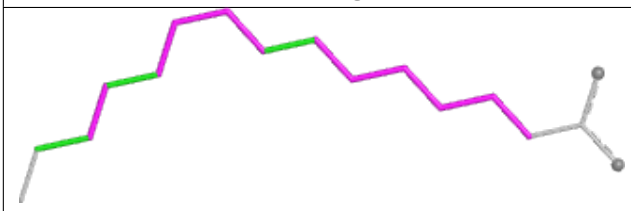
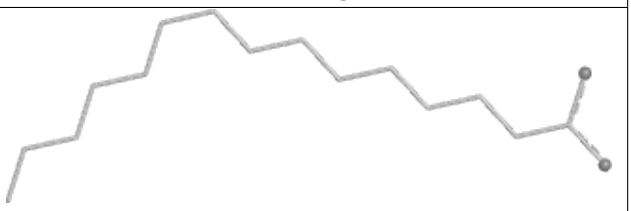
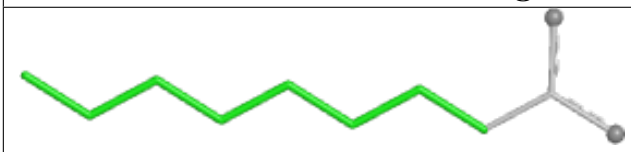
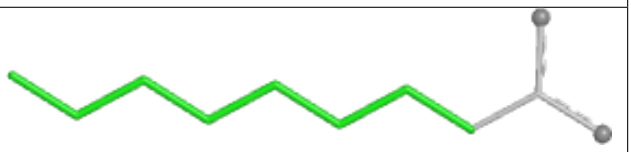
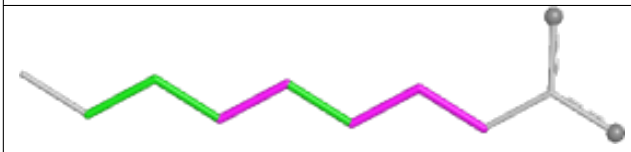
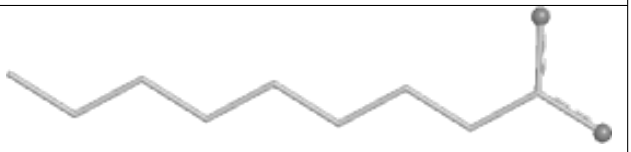
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLA A 2417	
 Bond lengths	 Bond angles
 Torsions	 Rings

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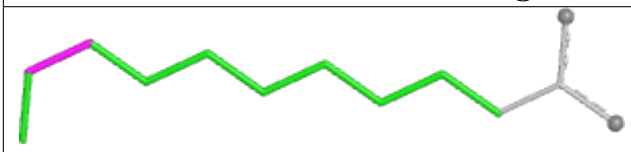
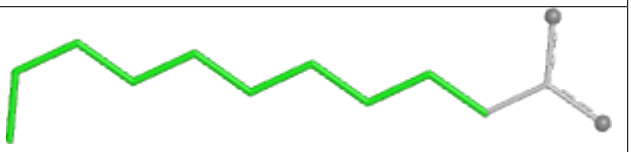
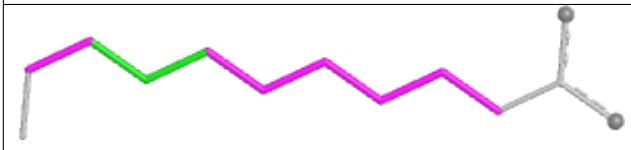
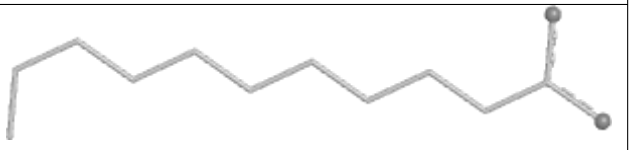
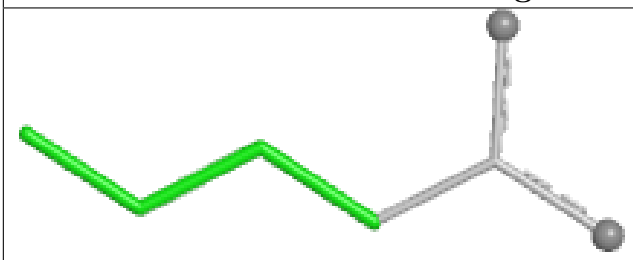
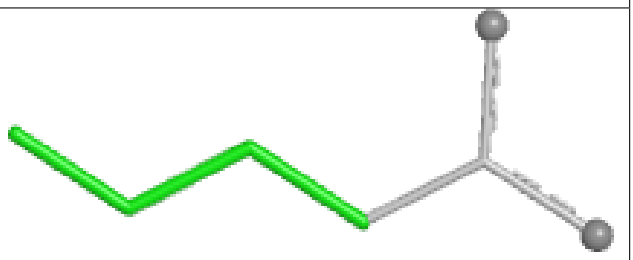
 Bond lengths	 Bond angles
 Torsions	 Rings

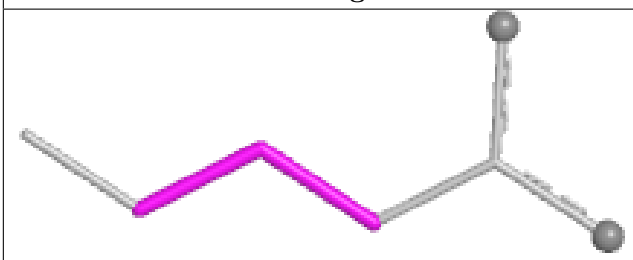
Ligand OLA A 2410



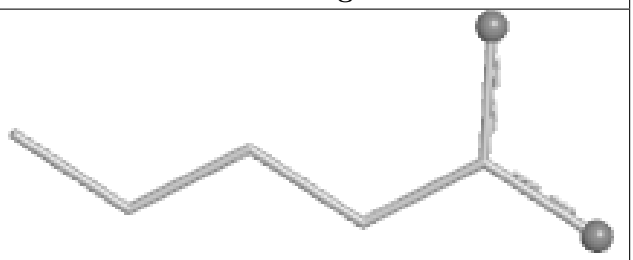
Bond lengths



Bond angles

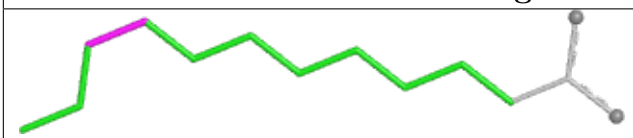


Torsions



Rings

Ligand OLA A 2426



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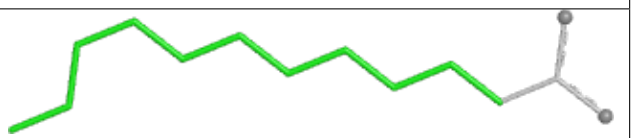
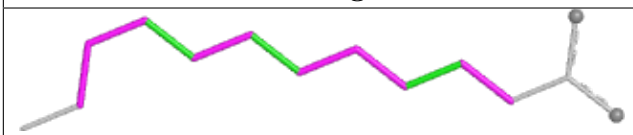
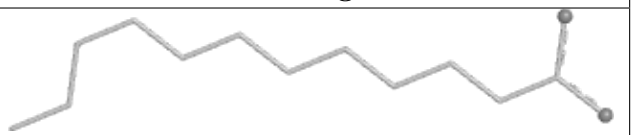


Bond angles

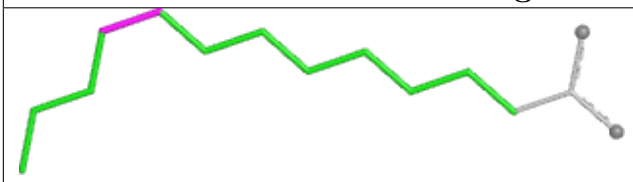


Torsions



Rings

Ligand OLA A 2430



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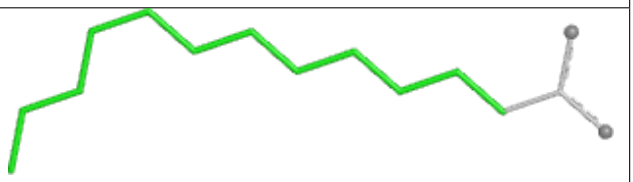
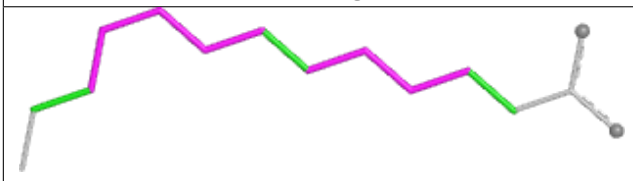
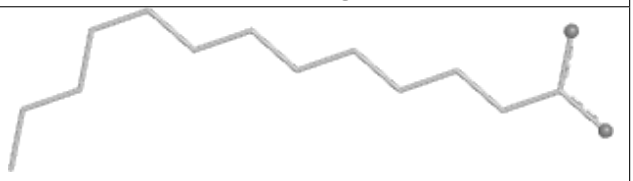


Bond angles

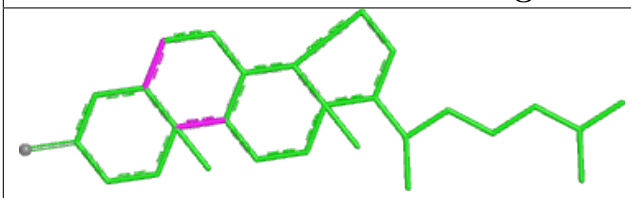


Torsions



Rings

Ligand CLR A 2402



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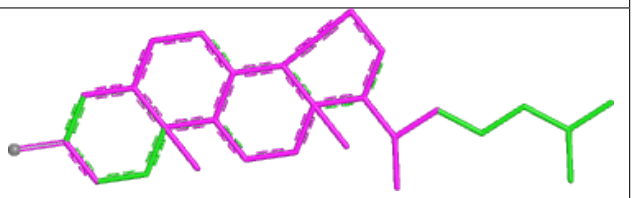
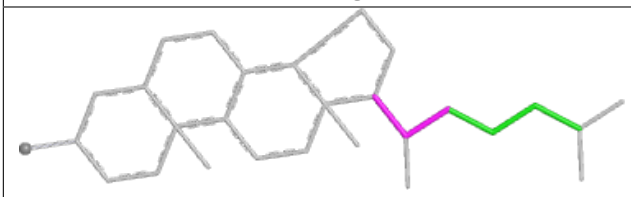
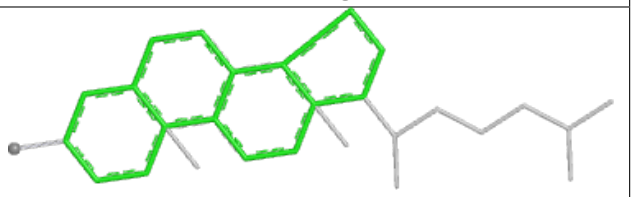


Bond angles

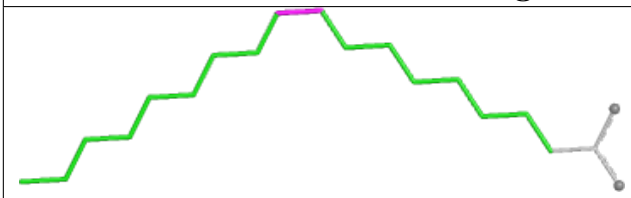


Torsions



Rings

Ligand OLA A 2407



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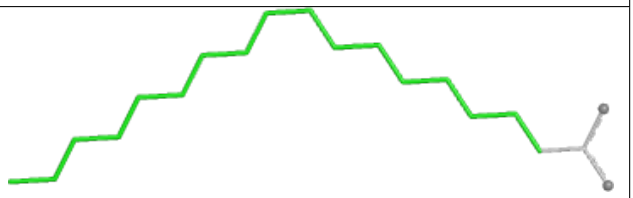
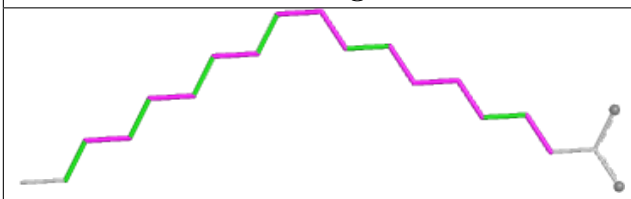
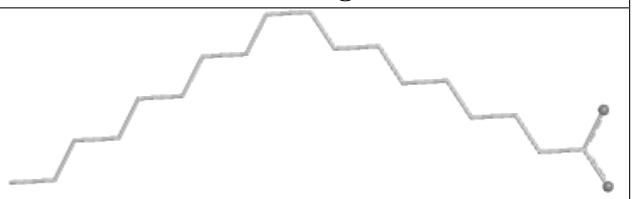


Bond angles

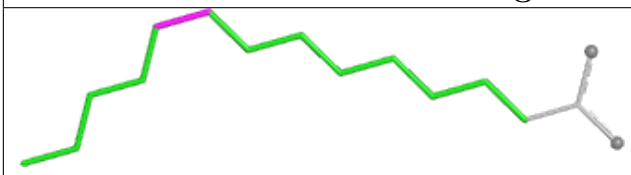


Torsions



Rings

Ligand OLA A 2421



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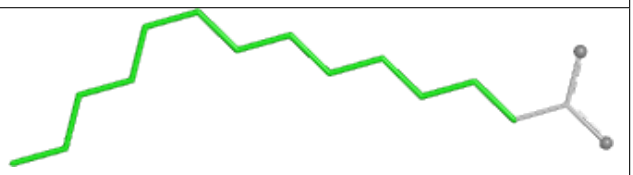
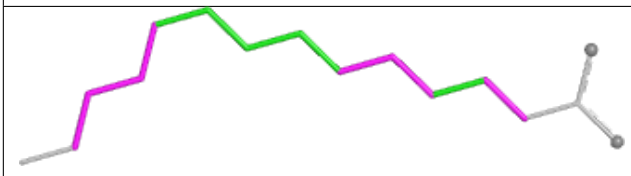
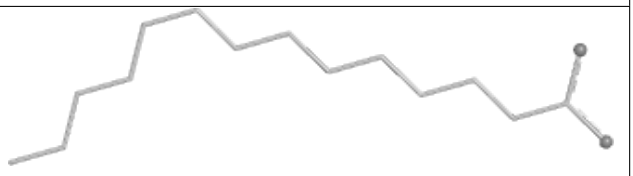


Bond angles

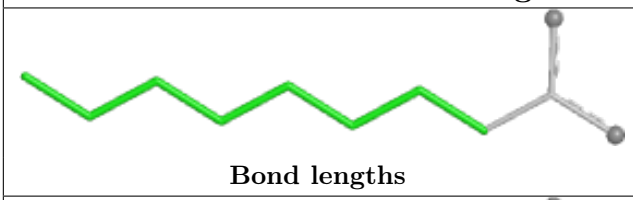


Torsions



Rings

Ligand OLA A 2427



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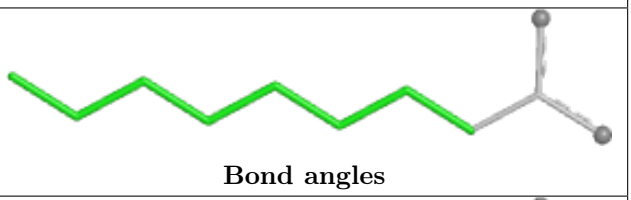
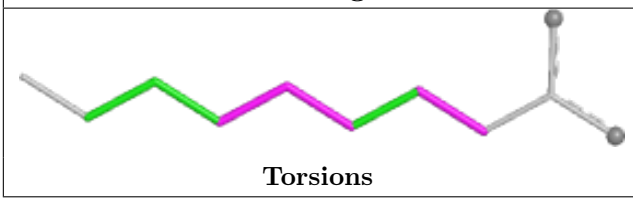
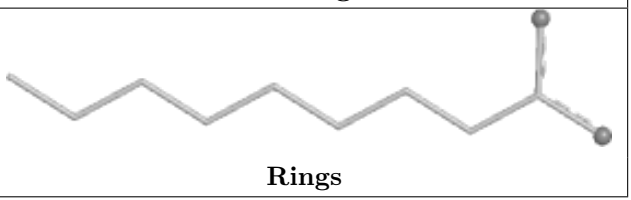


Bond angles

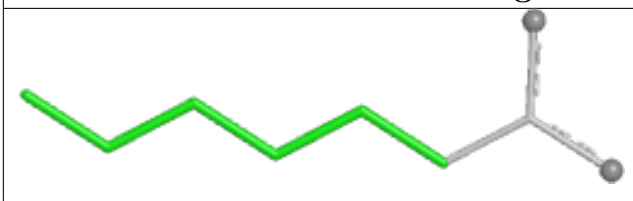


Torsions

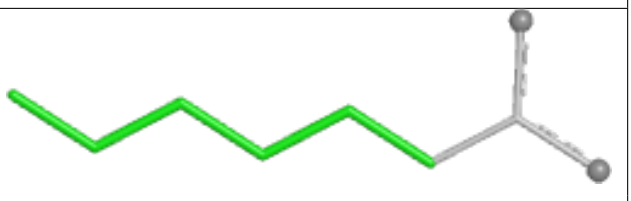


Rings

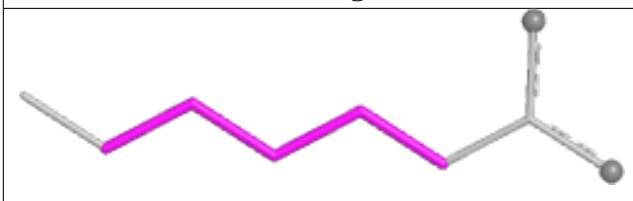
Ligand OLA A 2416



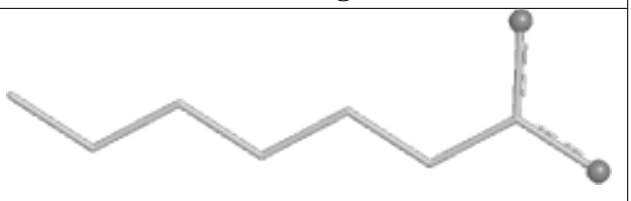
Bond lengths



Bond angles

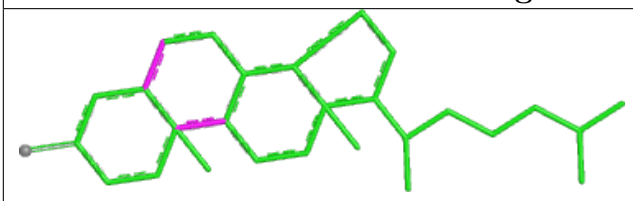


Torsions



Rings

Ligand CLR A 2401



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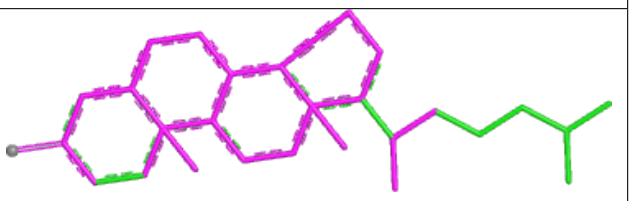
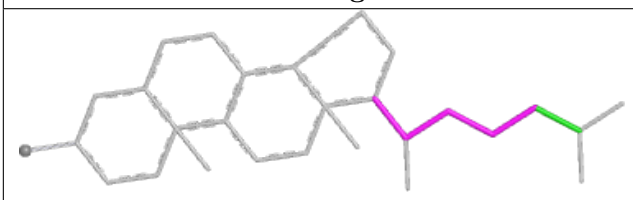
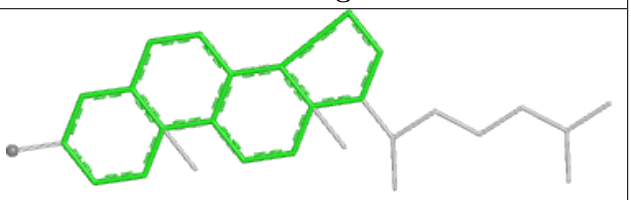


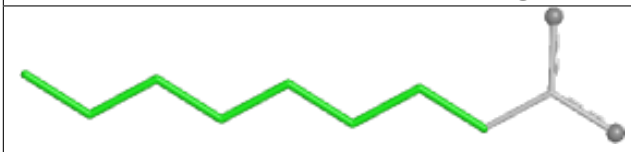
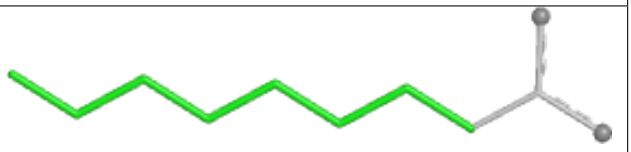
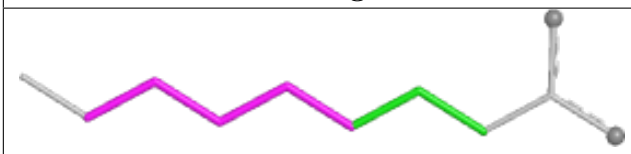
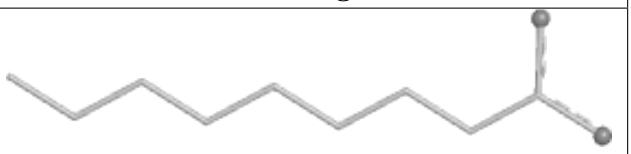
Bond angles

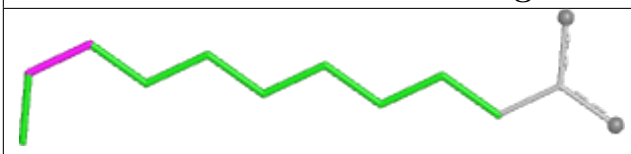
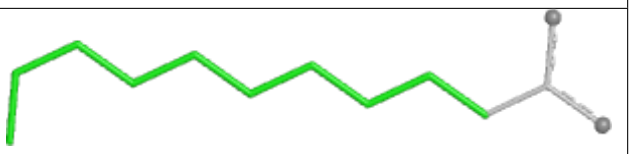
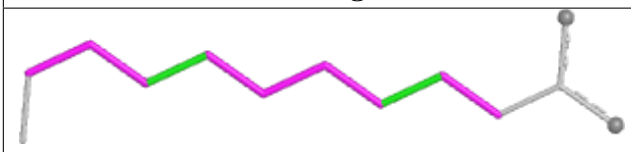
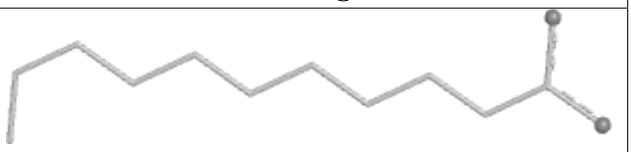


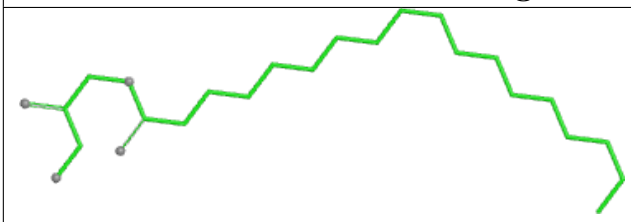
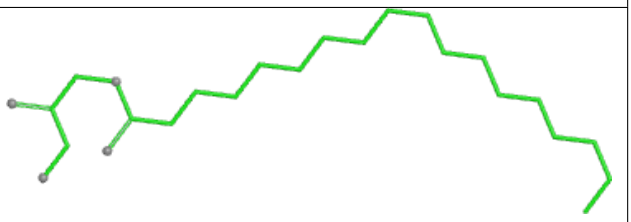
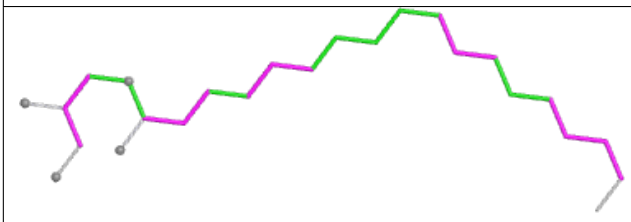
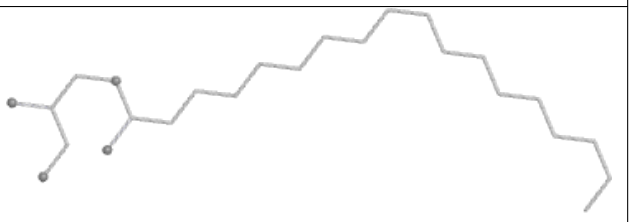
Torsions



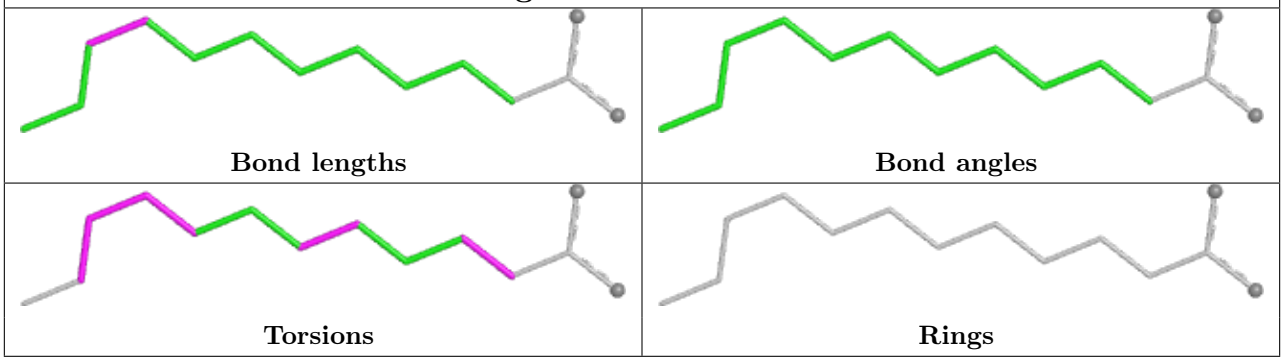
Rings

Ligand OLA A 2428	
 Bond lengths	 Bond angles
 Torsions	 Rings

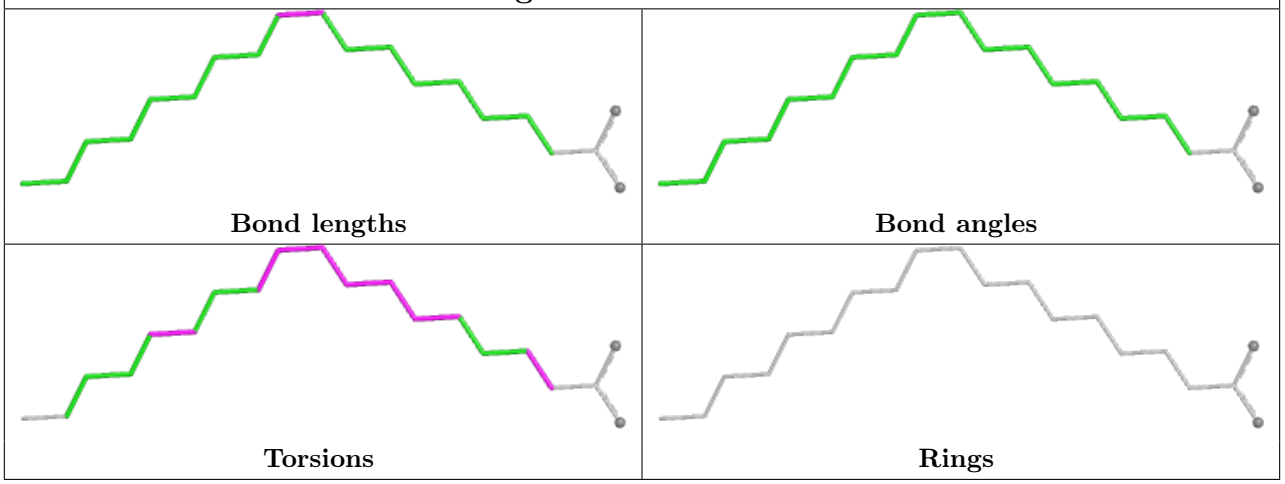
Ligand OLA A 2409	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLC A 2431	
 Bond lengths	 Bond angles
 Torsions	 Rings

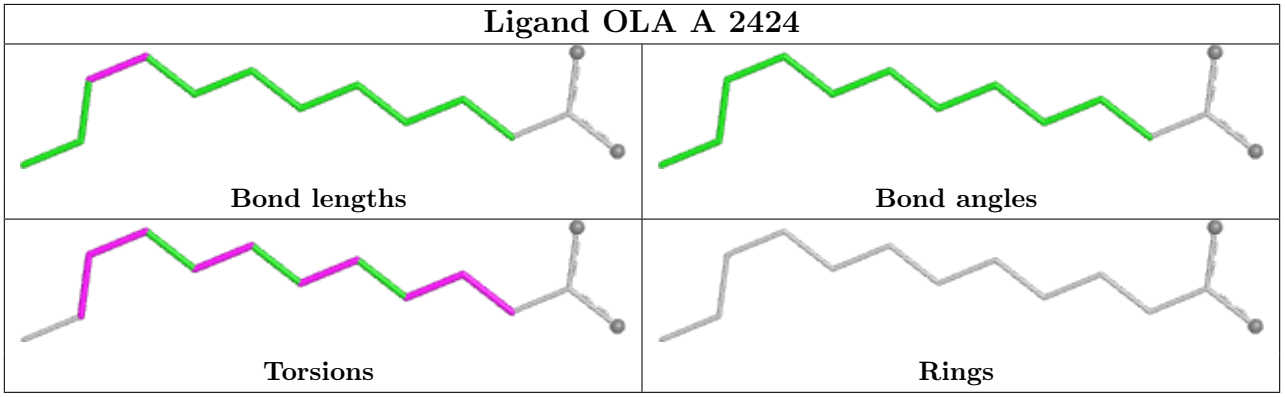
Ligand OLA A 2422

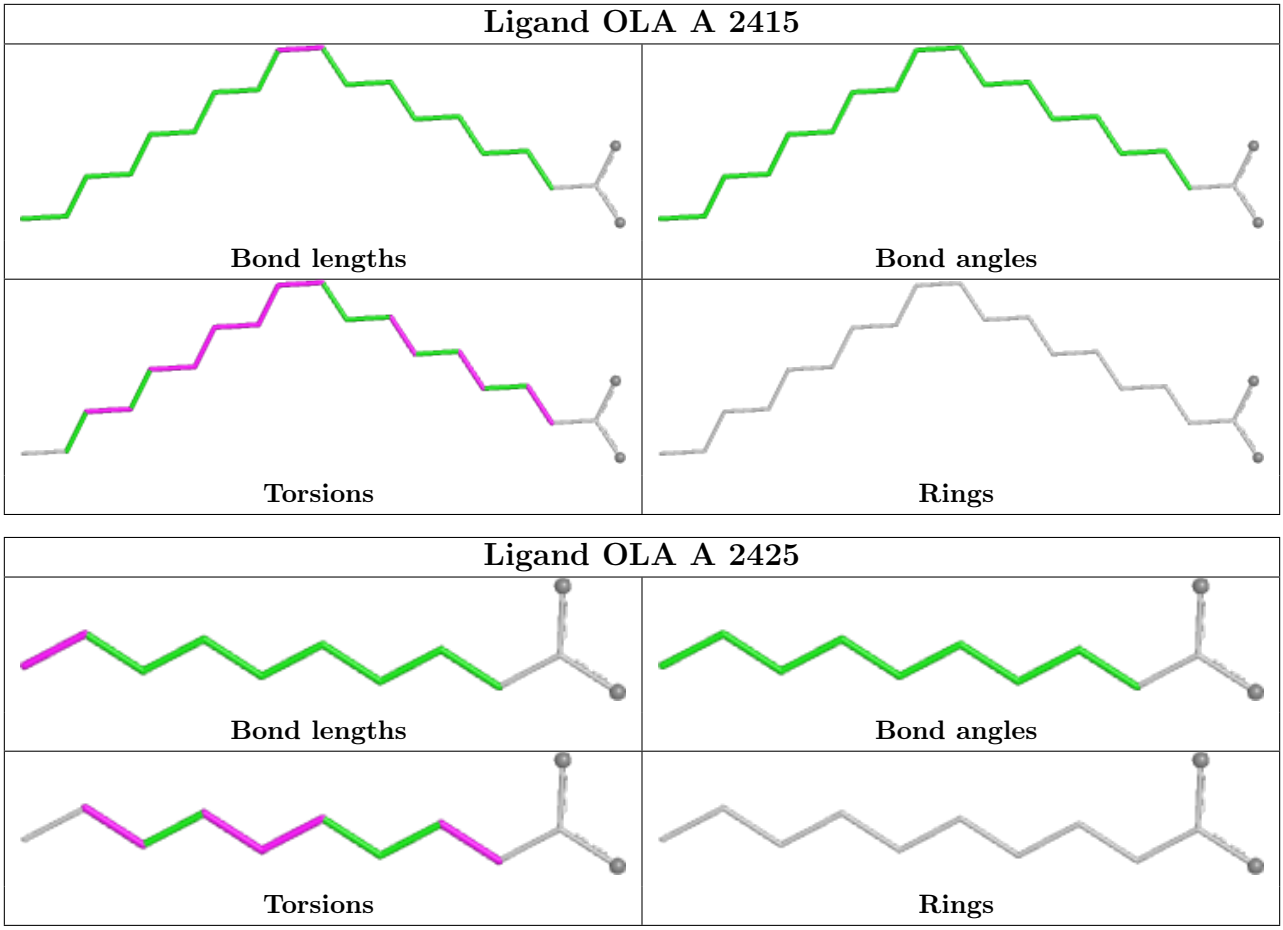


Ligand OLA A 2423



Ligand OLA 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

6.1 Protein, DNA and RNA chains

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	390/447 (87%)	0.70	57 (14%) 2 2	22, 36, 78, 99	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	7.1
1	A	1059	LYS	7.0
1	A	1058	MET	6.0
1	A	1060	ASP	5.4
1	A	1021	ASP	5.2
1	A	1063	HIS	5.1
1	A	1057	GLU	4.7
1	A	1094	LEU	4.5
1	A	1092	GLU	4.3
1	A	1091	ALA	4.0
1	A	1090	ALA	3.9
1	A	1100	ALA	3.8
1	A	1101	TYR	3.8
1	A	1066	ASP	3.7
1	A	305	SER	3.7
1	A	1033	MET	3.6
1	A	1031	THR	3.6
1	A	-2	ASP	3.5
1	A	1024	ALA	3.5
1	A	1006	ASN	3.4
1	A	156	SER	3.4
1	A	1105	TYR	3.3
1	A	1026	VAL	3.3
1	A	304	ARG	3.2
1	A	1038	LEU	3.2
1	A	111	ARG	3.2
1	A	1041	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	208	LEU	3.0
1	A	1019	LYS	3.0
1	A	1013	ASN	3.0
1	A	1028	ASP	2.9
1	A	1102	ILE	2.9
1	A	1007	TRP	2.9
1	A	1025	GLN	2.9
1	A	1016	VAL	2.8
1	A	1011	ASN	2.8
1	A	148	GLN	2.8
1	A	1076	LEU	2.7
1	A	1037	ALA	2.6
1	A	1036	ALA	2.6
1	A	152	GLY	2.5
1	A	1079	ALA	2.4
1	A	1040	ALA	2.4
1	A	29	TRP	2.4
1	A	-1	GLY	2.4
1	A	222	ARG	2.4
1	A	1084	VAL	2.3
1	A	0	ALA	2.3
1	A	1064	GLY	2.2
1	A	1020	ALA	2.2
1	A	1069	VAL	2.2
1	A	1077	LYS	2.2
1	A	1017	ILE	2.1
1	A	32	TRP	2.1
1	A	1095	LYS	2.1
1	A	1080	ASN	2.0
1	A	1023	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

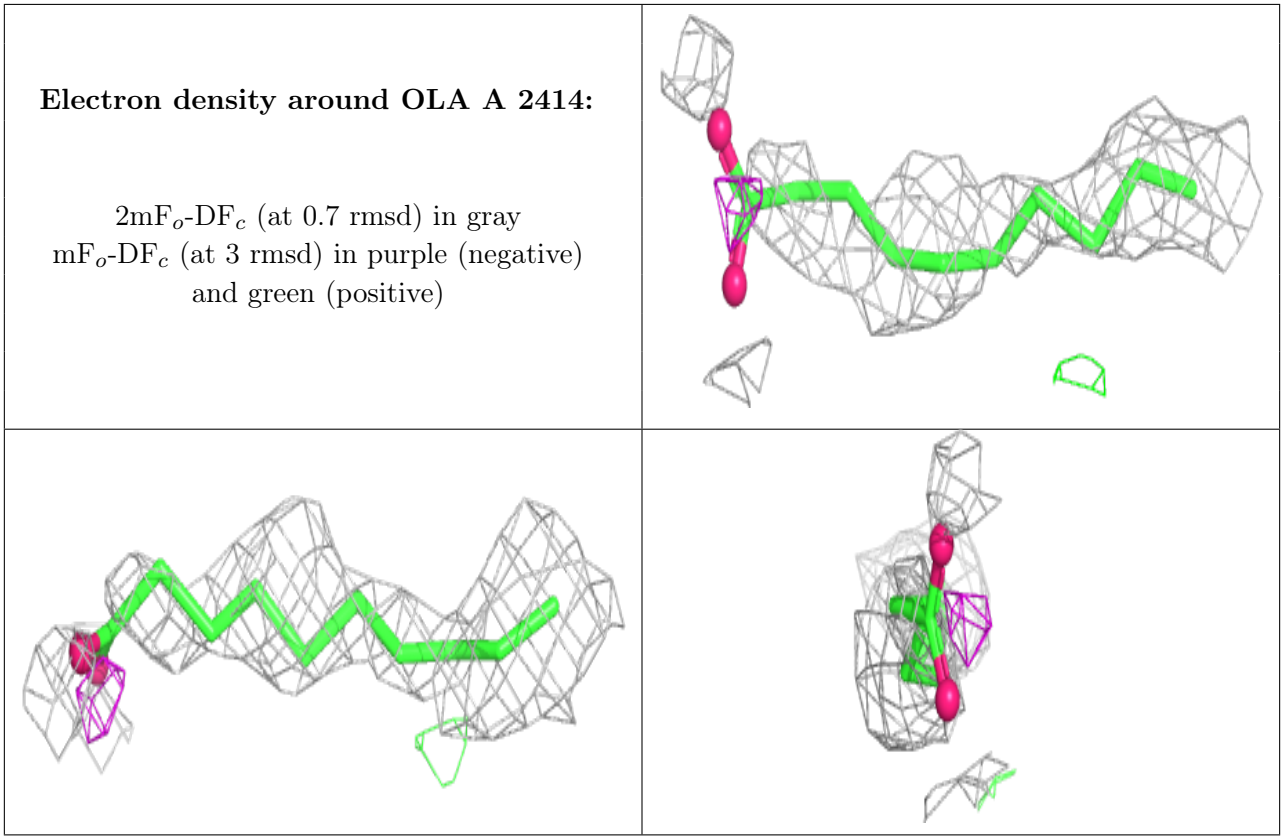
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLA	A	2414	12/20	0.37	0.38	54,62,91,94	0
4	OLA	A	2424	14/20	0.47	0.54	60,65,73,76	0
4	OLA	A	2416	9/20	0.48	0.34	48,54,60,66	0
4	OLA	A	2427	11/20	0.50	0.39	49,58,74,82	0
4	OLA	A	2426	14/20	0.55	0.32	37,57,75,78	0
4	OLA	A	2413	13/20	0.64	0.28	65,77,88,95	0
4	OLA	A	2425	12/20	0.65	0.35	59,70,84,87	0
4	OLA	A	2411	19/20	0.67	0.22	47,54,67,68	0
4	OLA	A	2415	20/20	0.70	0.30	50,60,84,91	0
4	OLA	A	2423	20/20	0.71	0.30	47,55,65,70	0
4	OLA	A	2430	15/20	0.71	0.30	49,54,69,74	0
4	OLA	A	2419	17/20	0.73	0.25	50,69,89,90	0
4	OLA	A	2408	19/20	0.74	0.25	41,49,75,80	0
4	OLA	A	2422	14/20	0.74	0.18	48,56,65,73	0
4	OLA	A	2428	11/20	0.75	0.23	50,60,75,79	0
4	OLA	A	2420	14/20	0.75	0.23	53,62,72,76	0
6	PEG	A	2435	7/7	0.75	0.20	57,67,74,75	0
4	OLA	A	2406	11/20	0.76	0.20	38,49,63,75	0
4	OLA	A	2405	9/20	0.76	0.26	42,44,52,69	0
4	OLA	A	2417	11/20	0.77	0.20	49,56,62,70	0
5	OLC	A	2431	25/25	0.77	0.26	39,52,80,85	0
4	OLA	A	2429	16/20	0.77	0.30	36,50,56,65	0
4	OLA	A	2407	20/20	0.79	0.22	39,50,62,65	0
2	CLR	A	2403	28/28	0.80	0.21	30,38,49,62	0
6	PEG	A	2434	7/7	0.80	0.24	67,72,78,82	0
4	OLA	A	2412	12/20	0.80	0.39	34,52,68,69	0
5	OLC	A	2433	19/25	0.81	0.20	32,47,75,75	0
4	OLA	A	2409	13/20	0.82	0.22	53,61,66,67	0
4	OLA	A	2421	16/20	0.82	0.21	35,56,70,73	0
5	OLC	A	2432	21/25	0.82	0.21	49,58,72,86	0
4	OLA	A	2418	16/20	0.84	0.25	32,47,63,65	0
4	OLA	A	2410	7/20	0.87	0.16	44,52,57,58	0
2	CLR	A	2401	28/28	0.87	0.15	25,33,56,60	0
2	CLR	A	2402	28/28	0.88	0.14	31,41,49,50	0
3	8E2	A	2404	50/57	0.92	0.18	21,30,85,101	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.

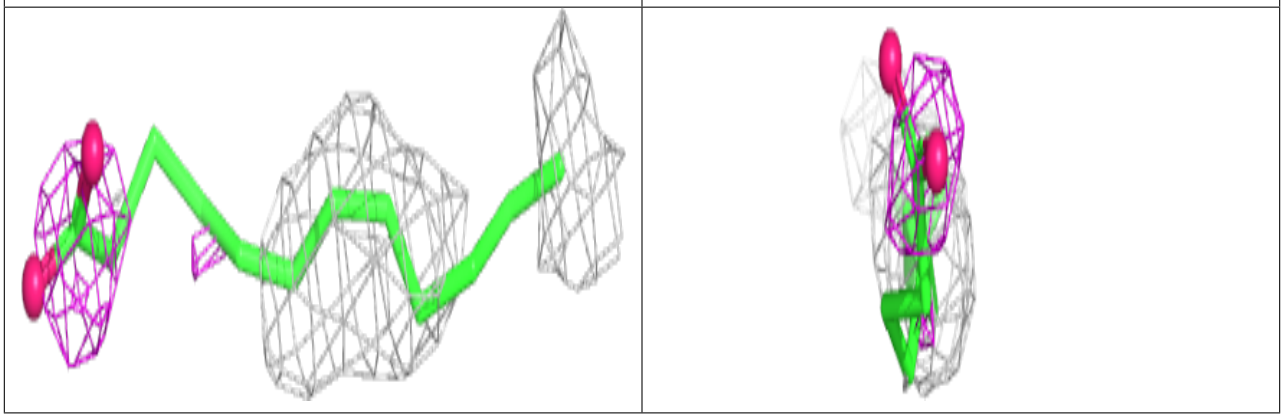
Electron density around OLA A 2414:

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



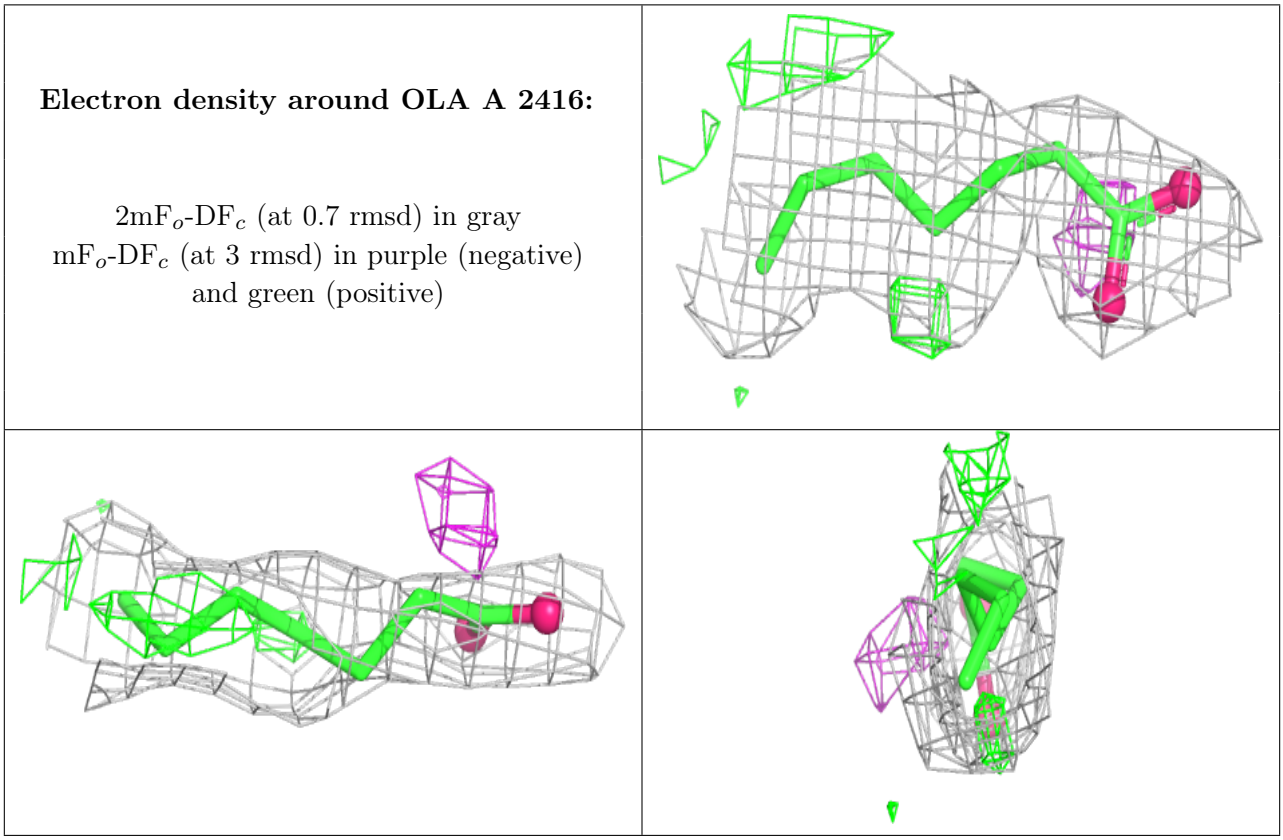
Electron density around OLA A 2424:

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



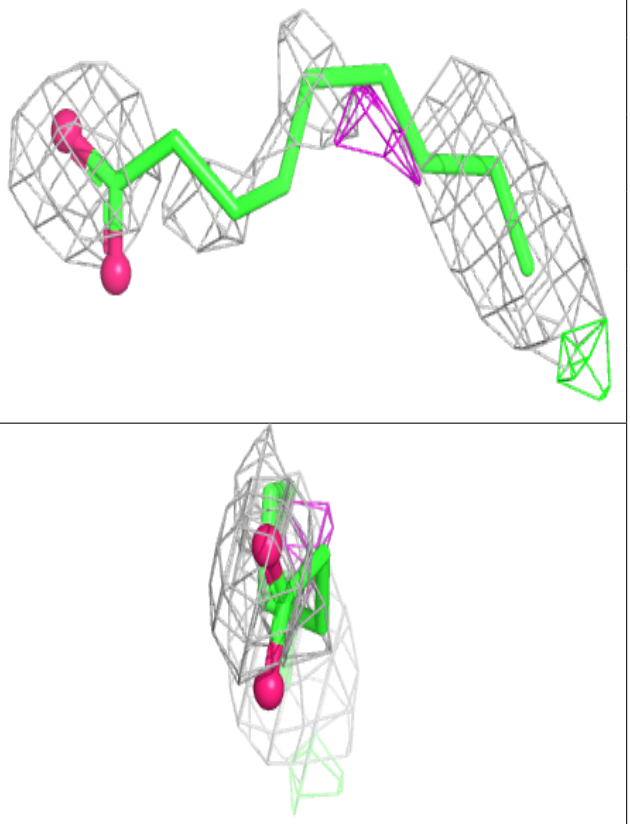
Electron density around OLA A 2416:

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



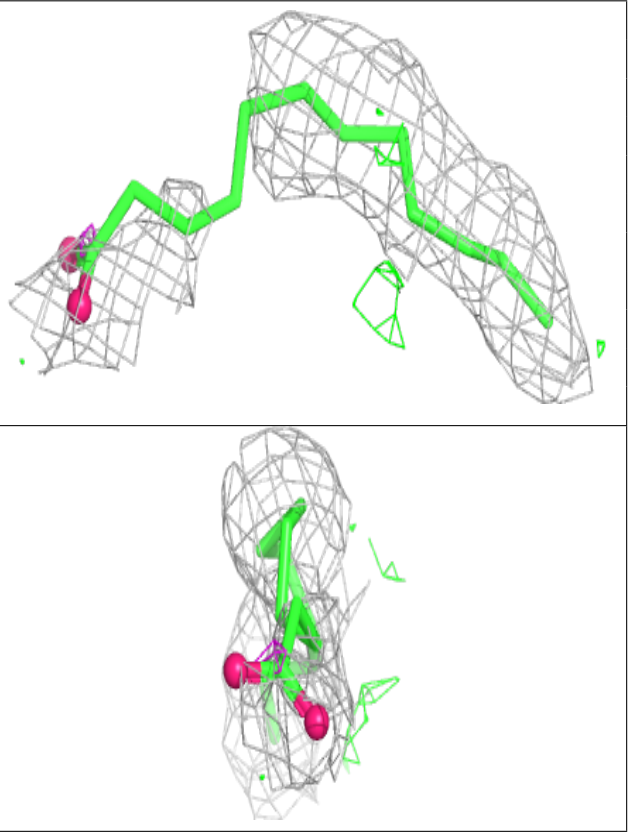
Electron density around OLA A 2427:

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



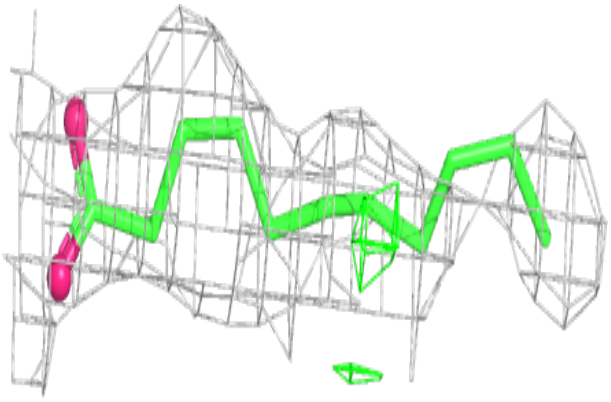
Electron density around OLA A 2426:

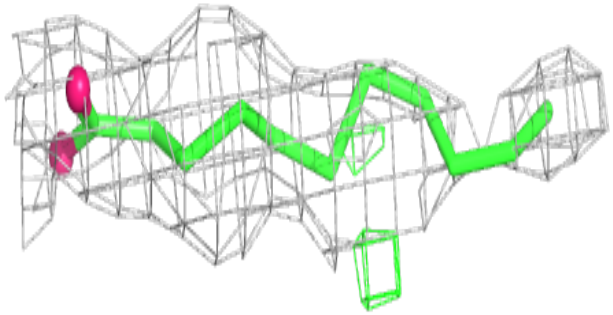
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

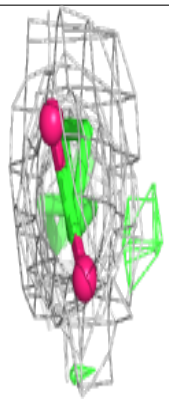


Electron density around OLA A 2413:

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

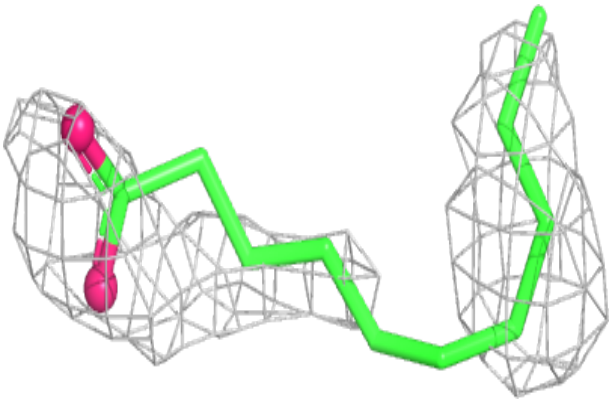


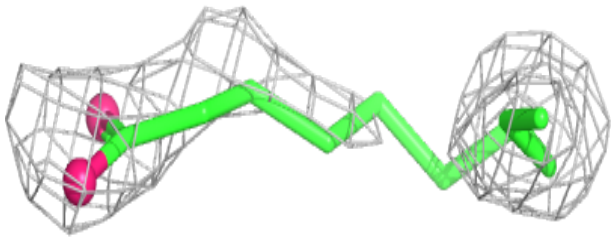


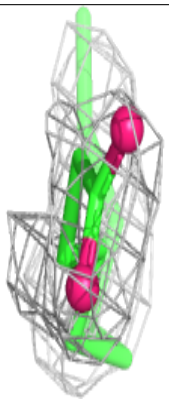


Electron density around OLA A 2425:

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

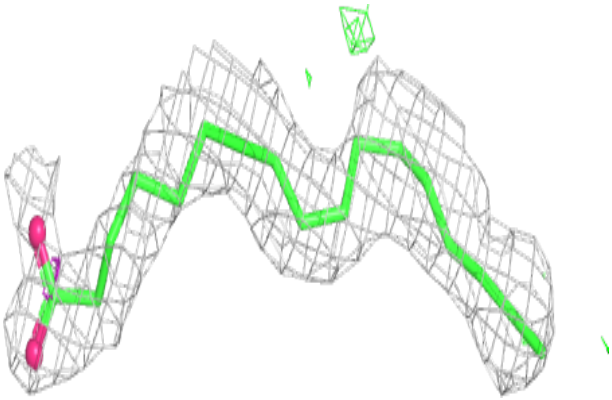


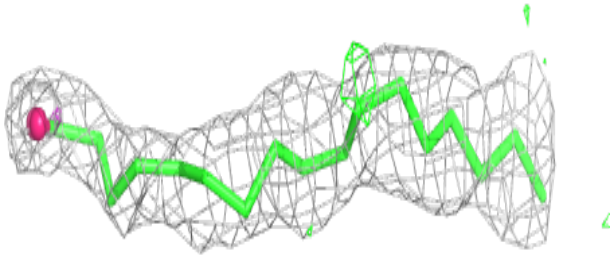




Electron density around OLA A 2411:

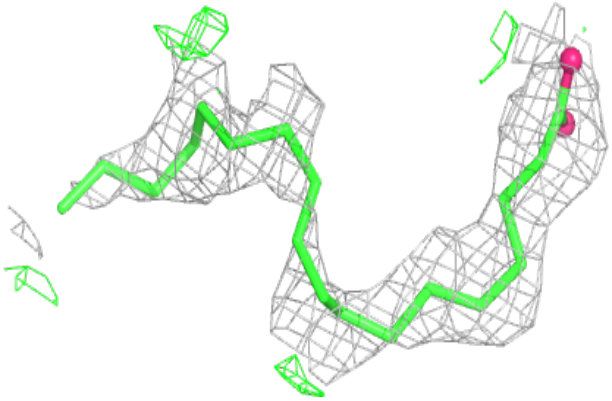
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

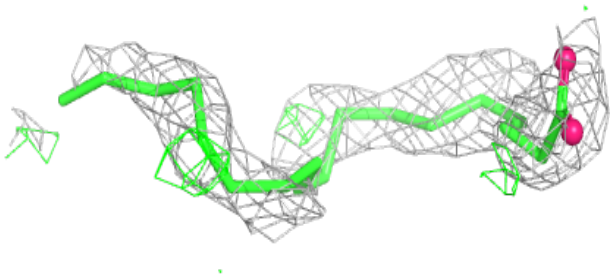


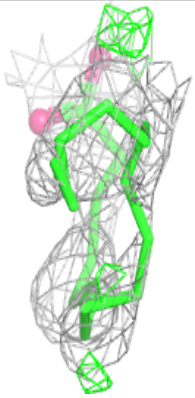


Electron density around OLA A 2415:

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

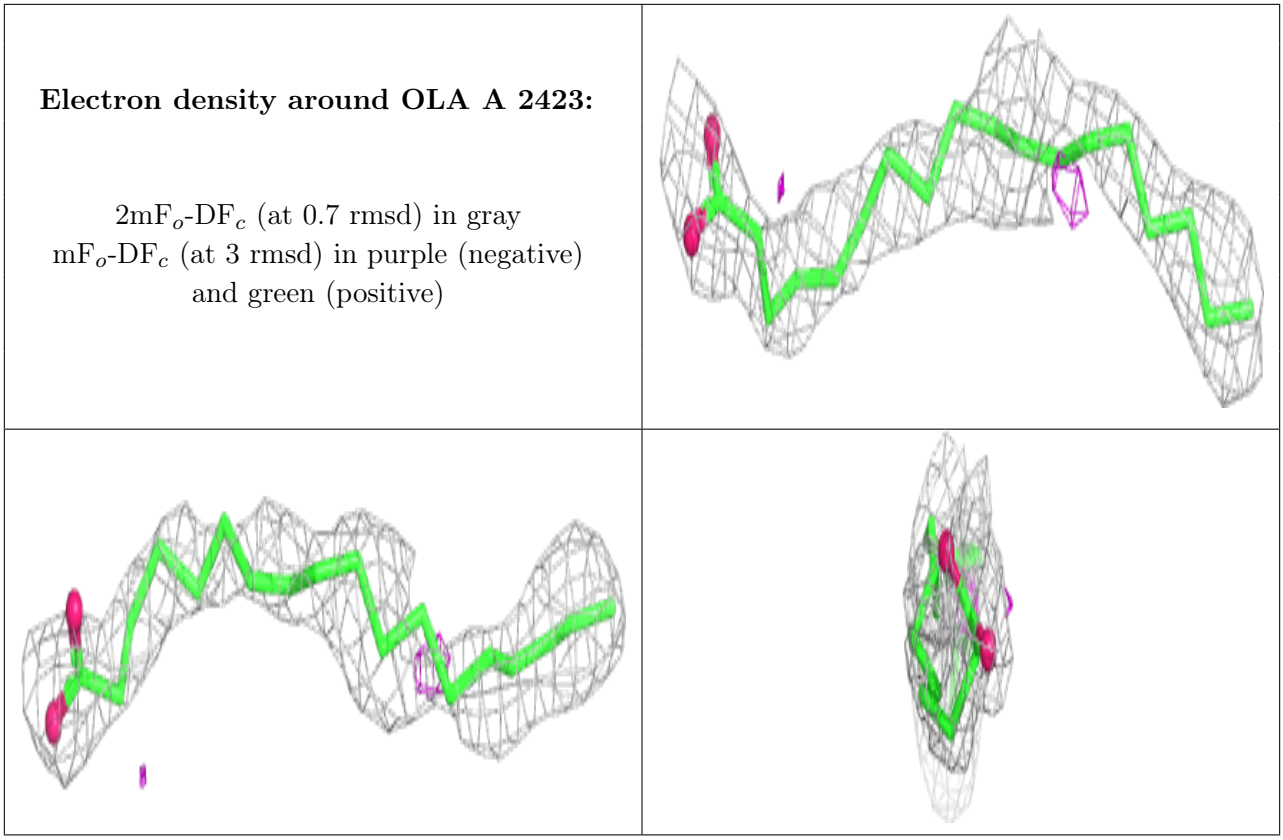






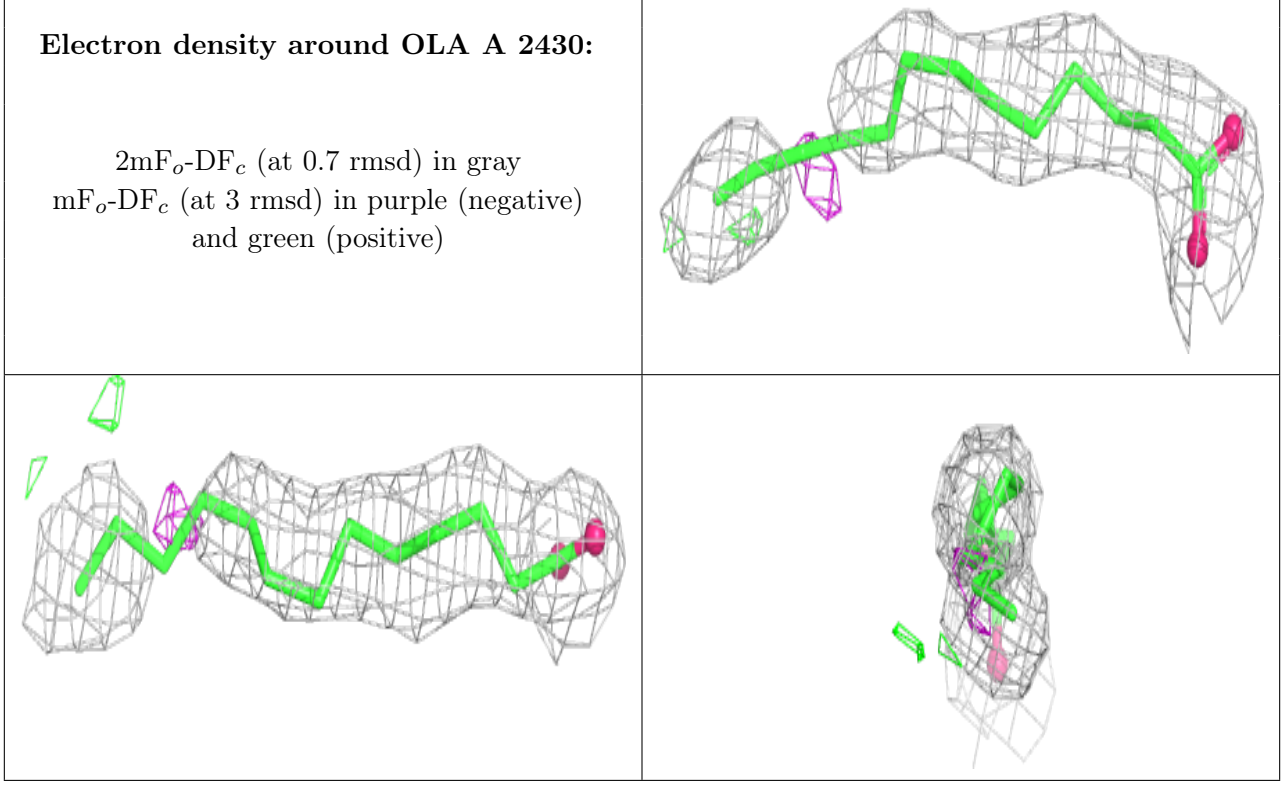
Electron density around OLA A 2423:

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



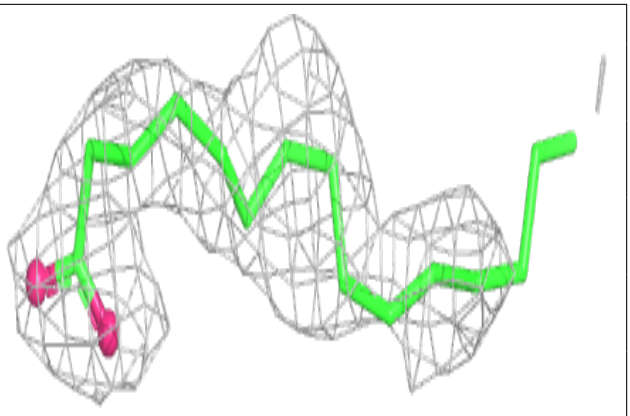
Electron density around OLA A 2430:

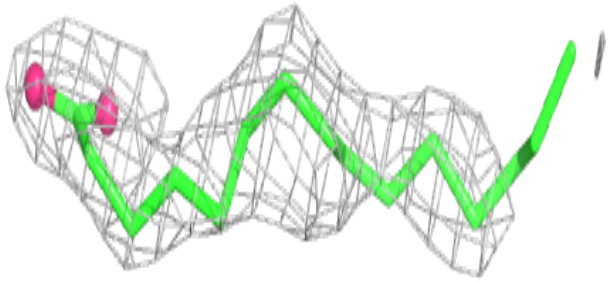
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

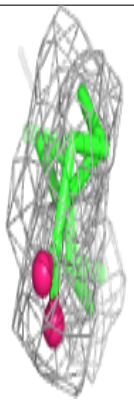


Electron density around OLA A 2419:

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

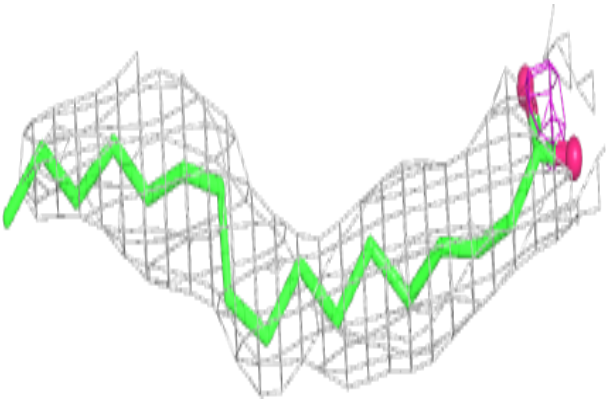


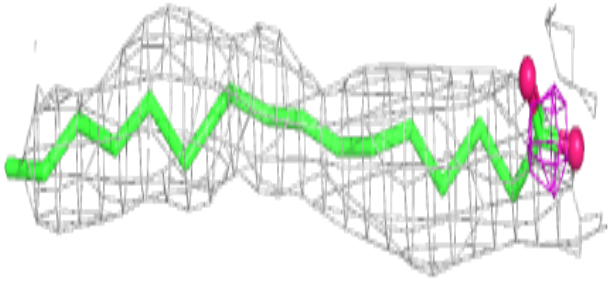


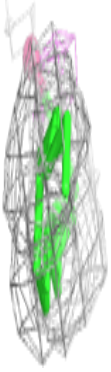


Electron density around OLA A 2408:

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

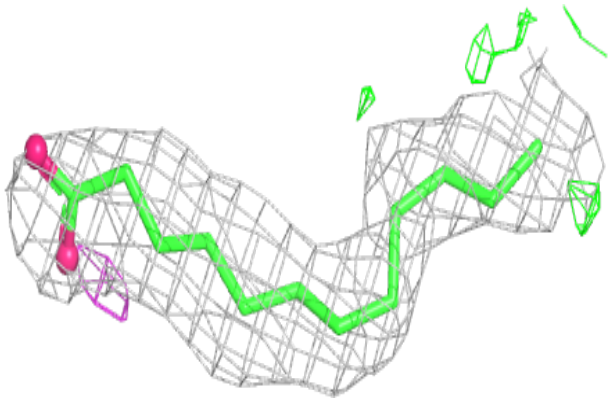


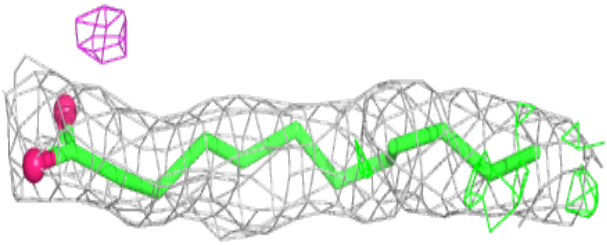


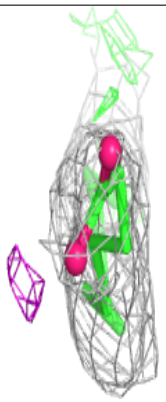


Electron density around OLA A 2422:

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

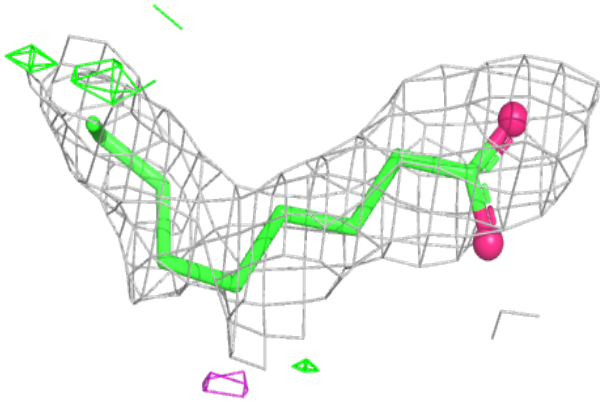


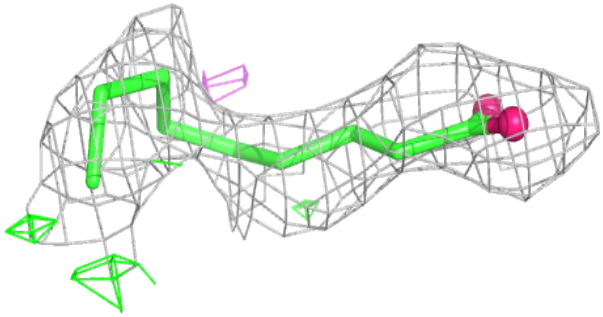


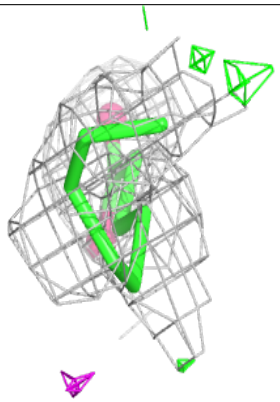


Electron density around OLA A 2428:

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

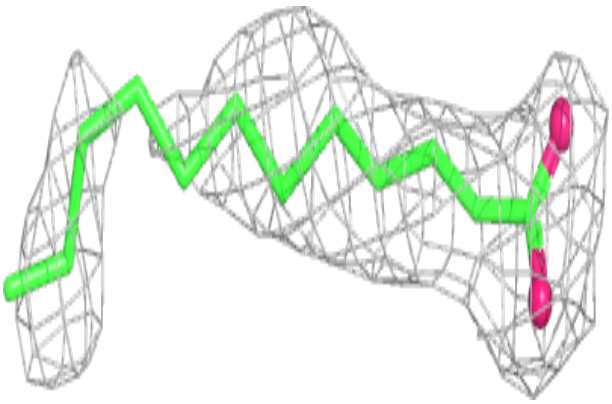


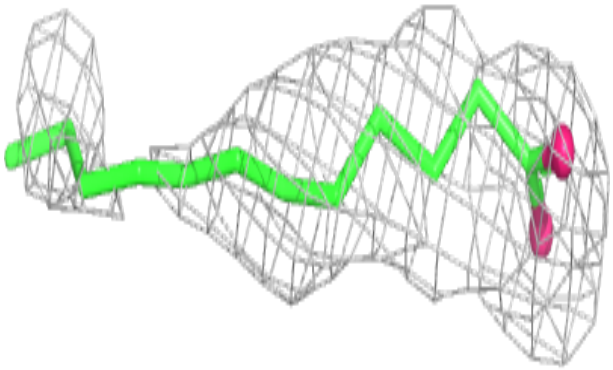


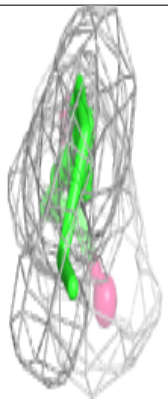


Electron density around OLA A 2420:

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

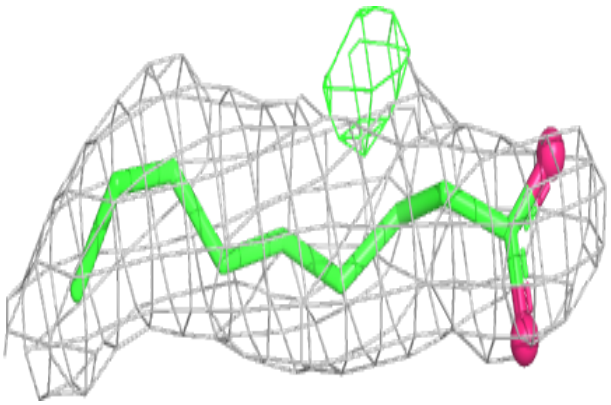


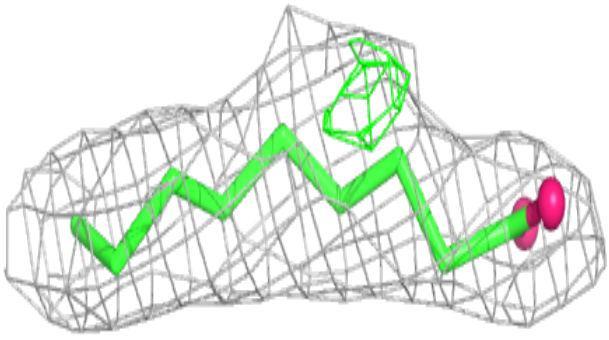


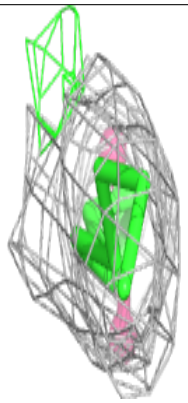


Electron density around OLA A 2406:

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

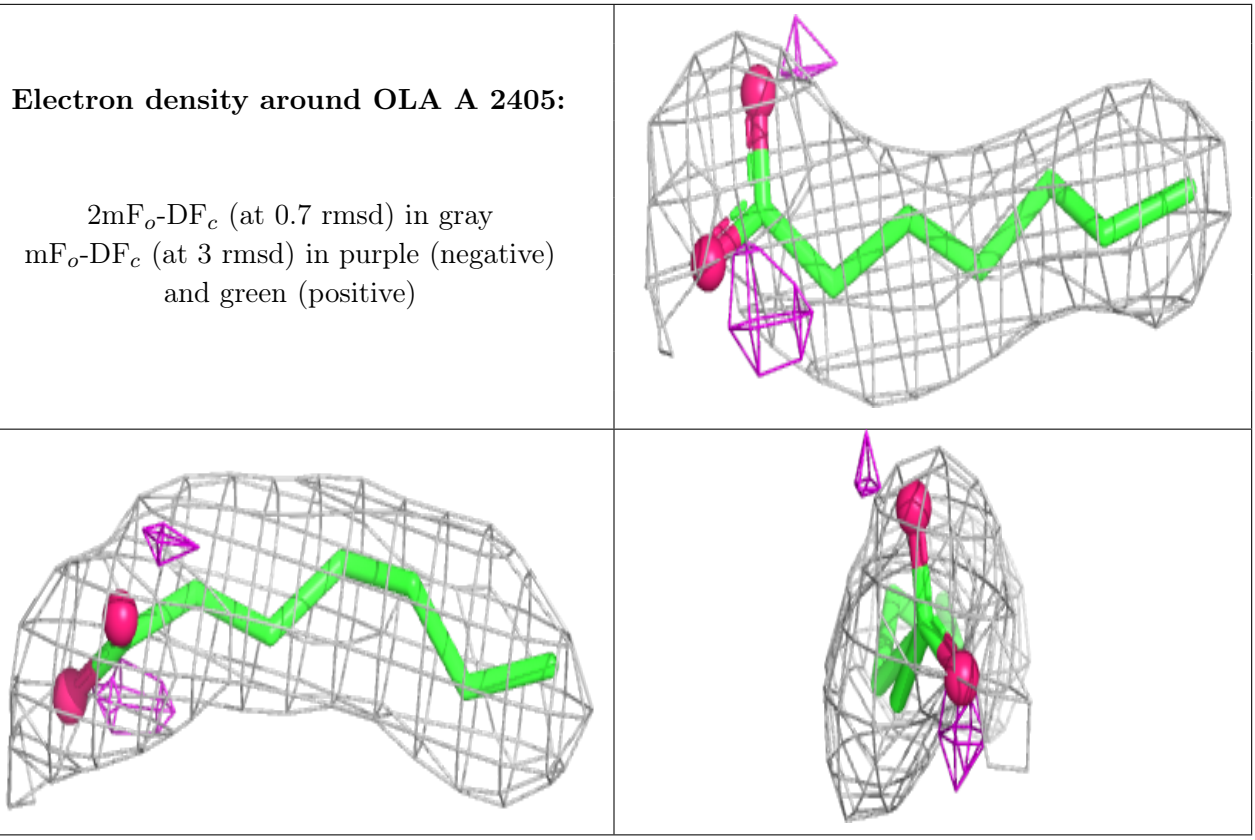






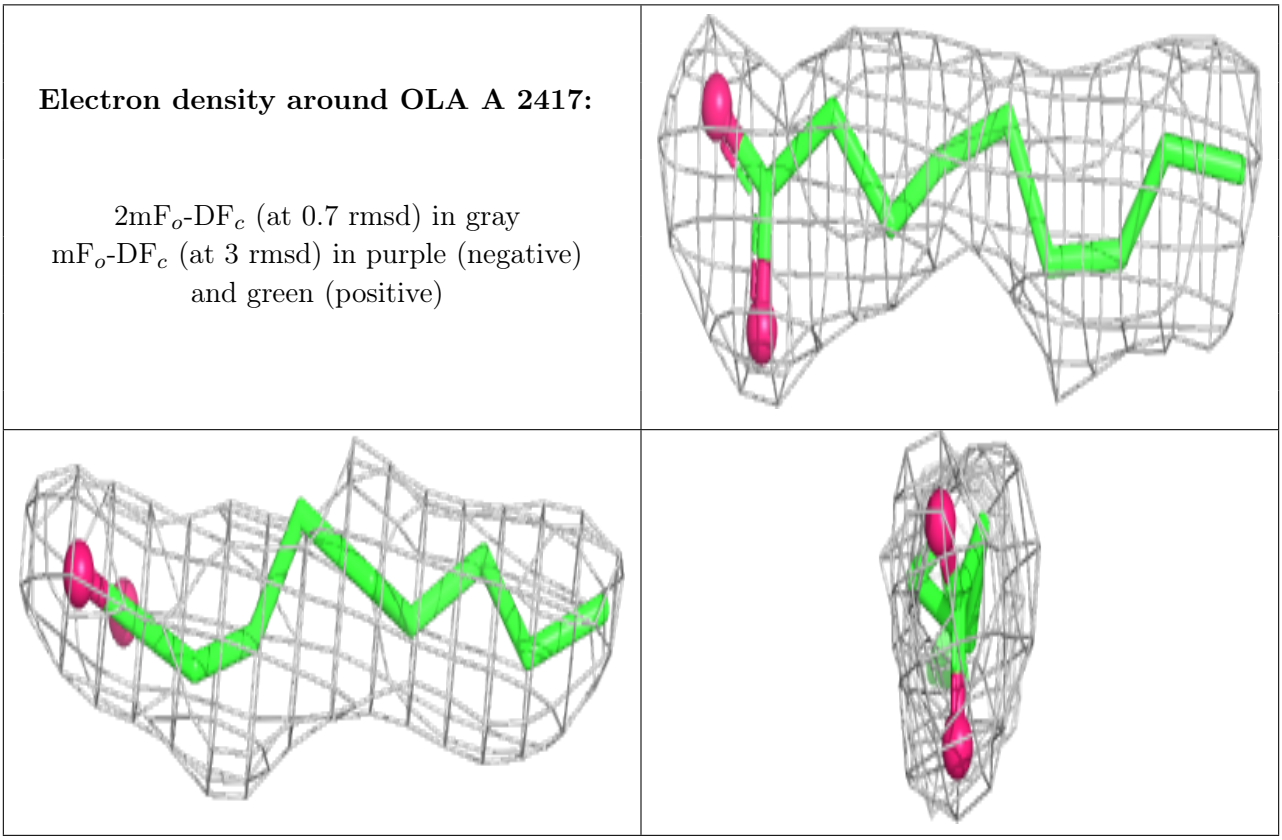
Electron density around OLA A 2405:

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



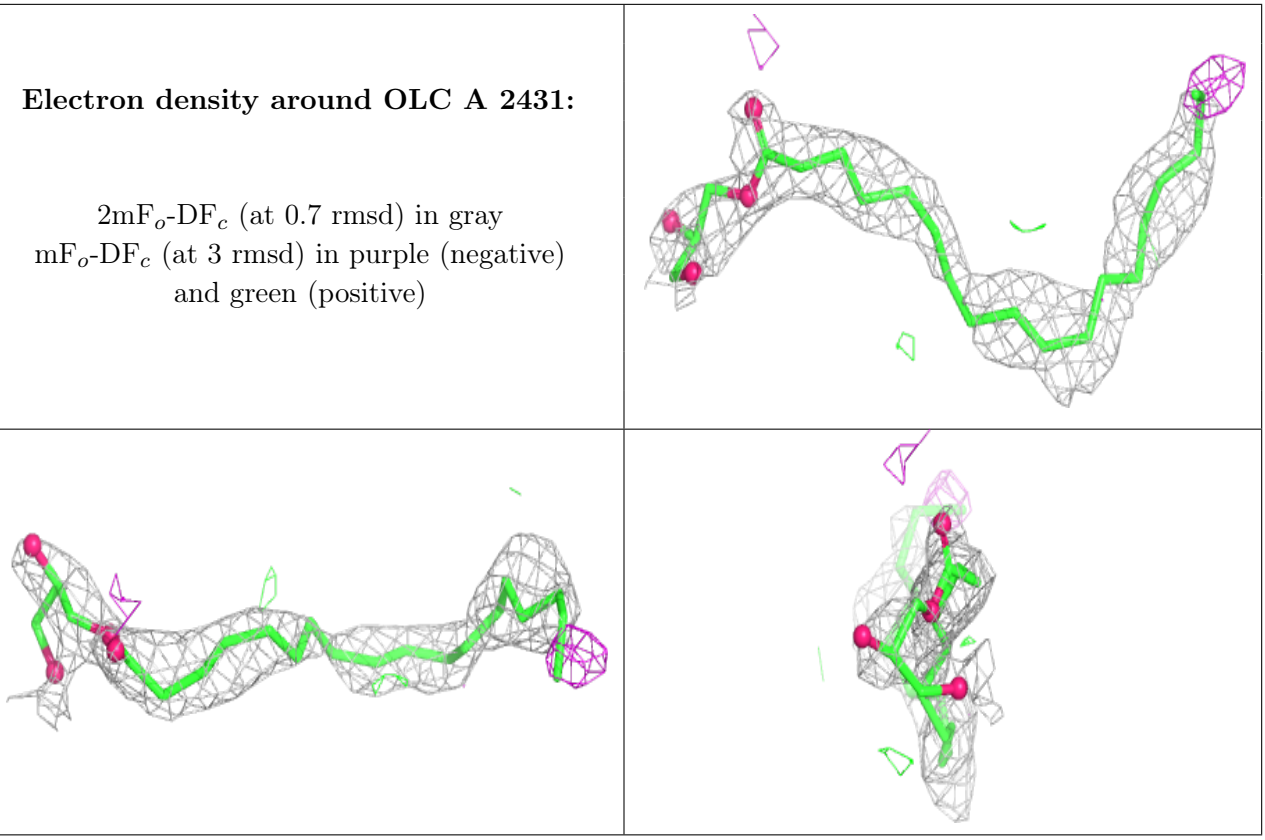
Electron density around OLA A 2417:

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



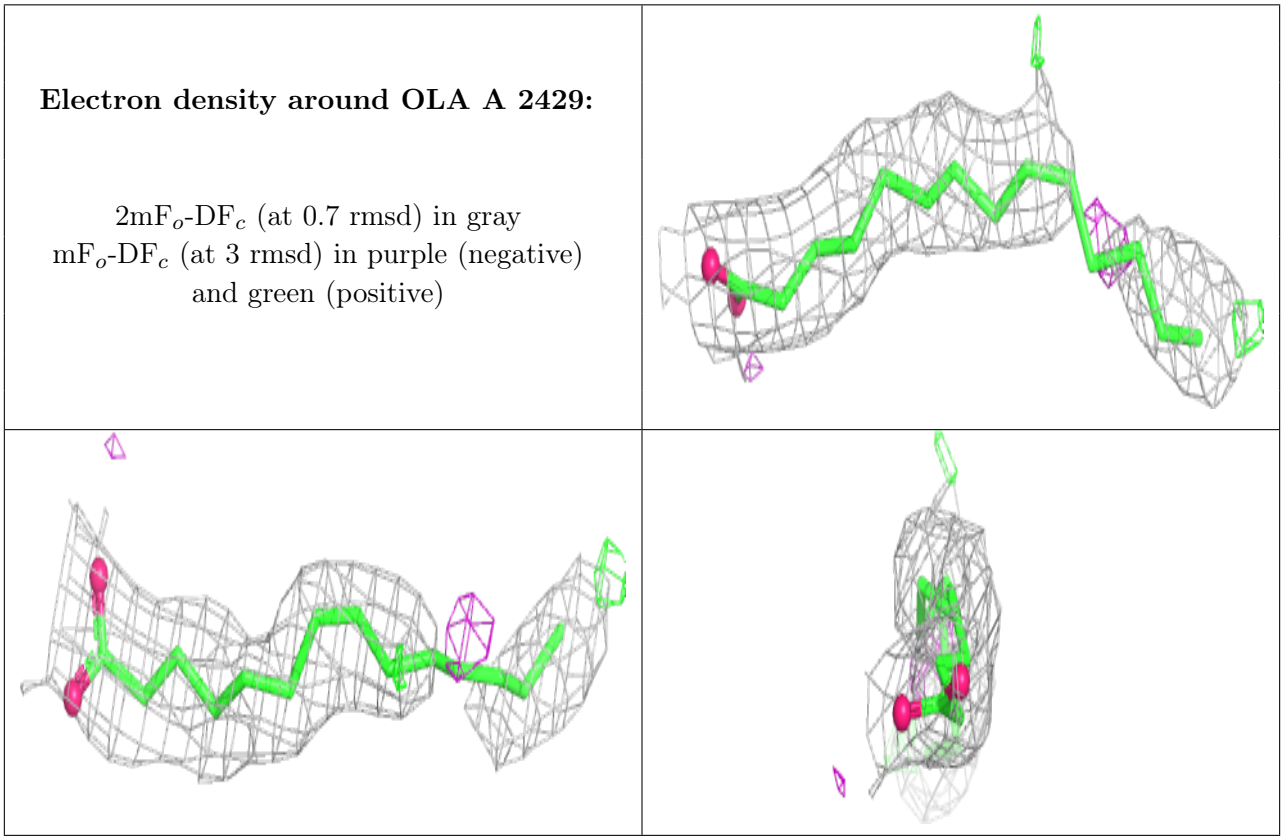
Electron density around OLC A 2431:

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



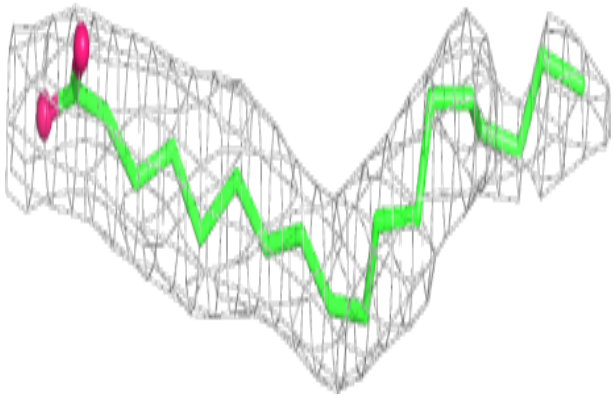
Electron density around OLA A 2429:

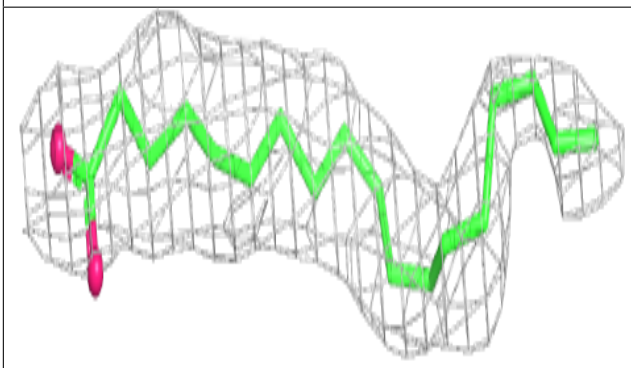
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

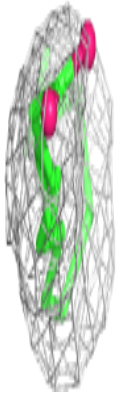


Electron density around OLA A 2407:

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

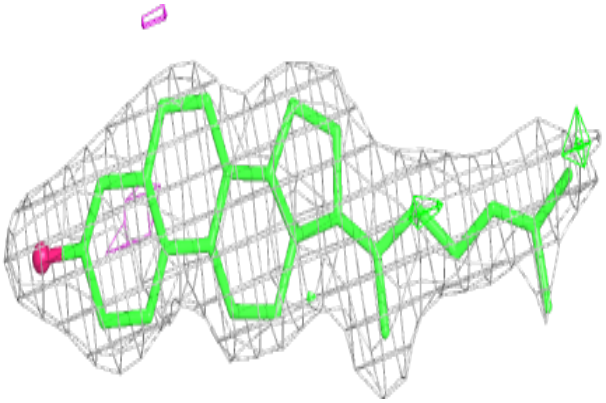


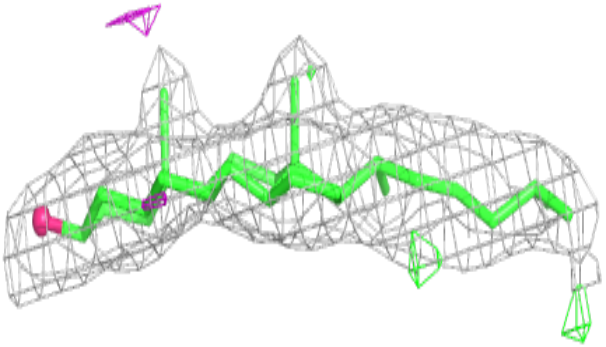


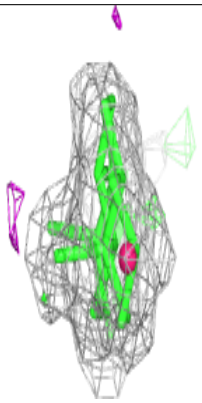


Electron density around CLR A 2403:

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

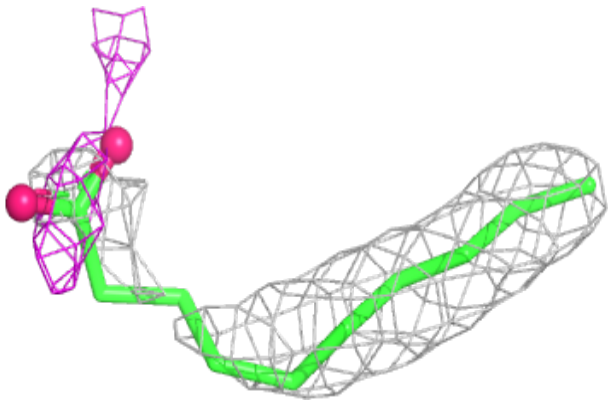


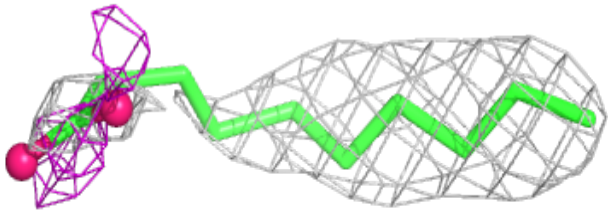


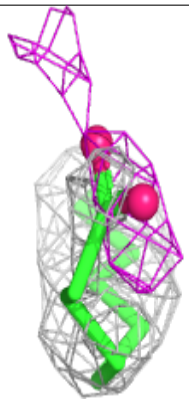


Electron density around OLA A 2412:

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

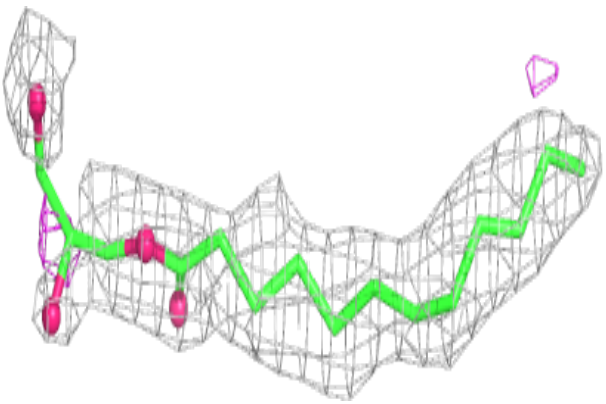


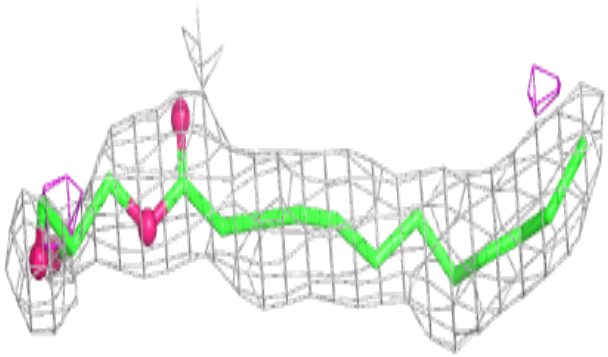


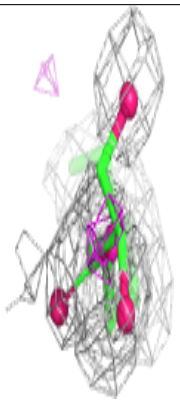


Electron density around OLC A 2433:

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

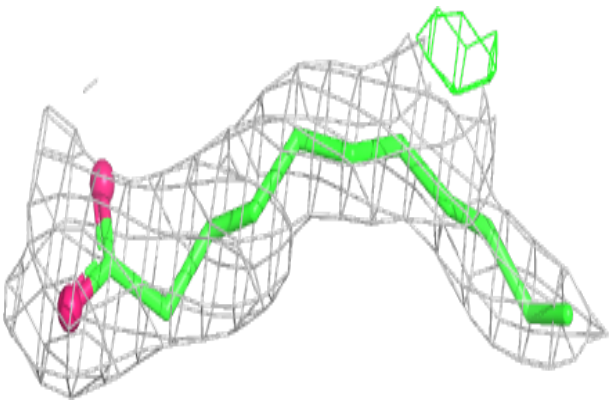


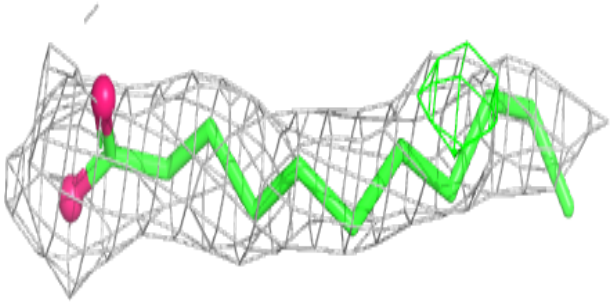


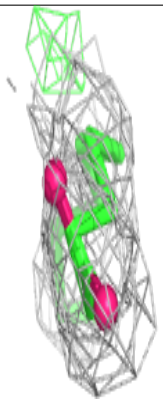


Electron density around OLA A 2409:

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

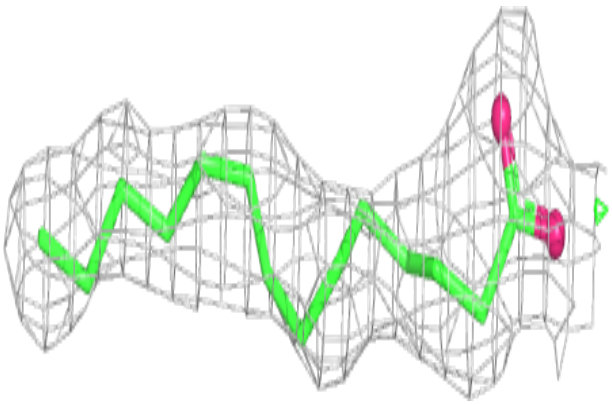


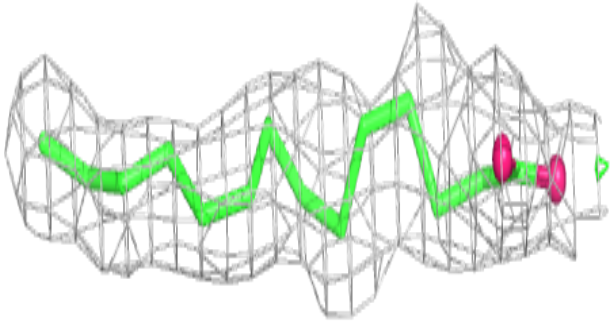


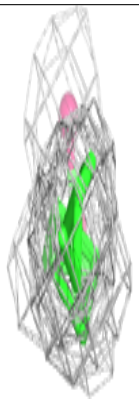


Electron density around OLA A 2421:

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

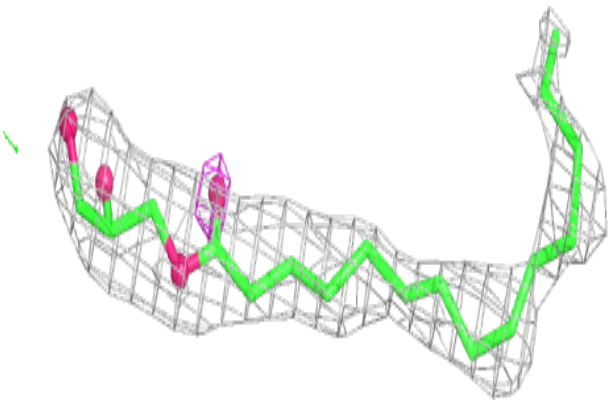


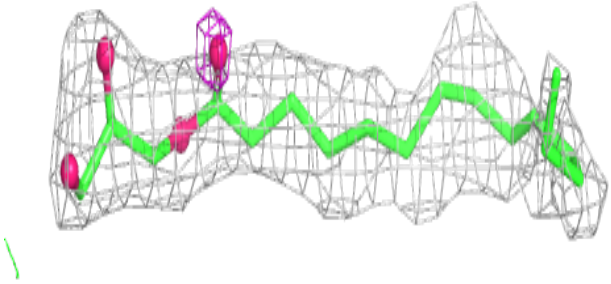


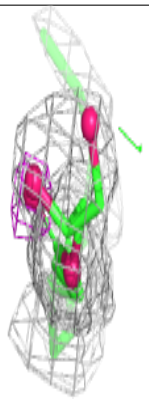


Electron density around OLC A 2432:

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

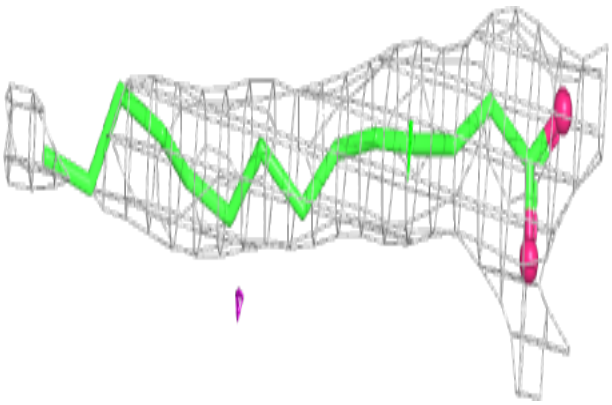


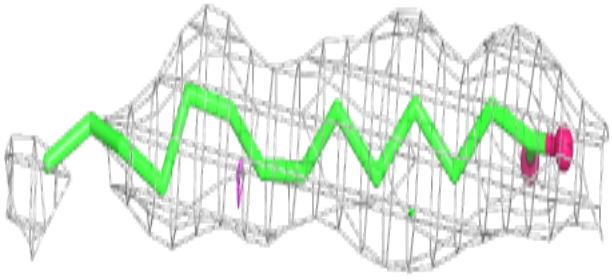


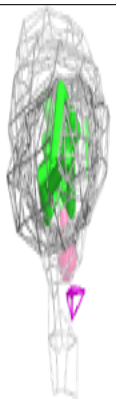


Electron density around OLA A 2418:

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

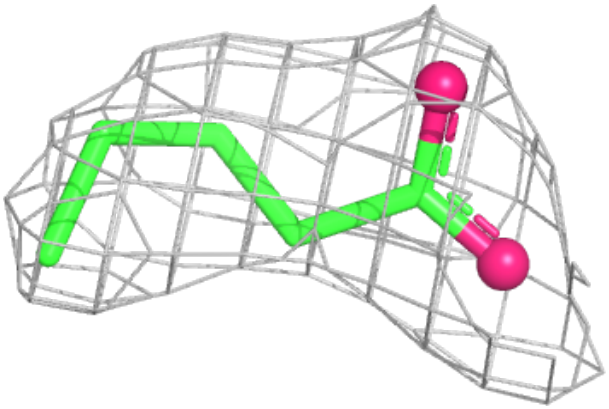


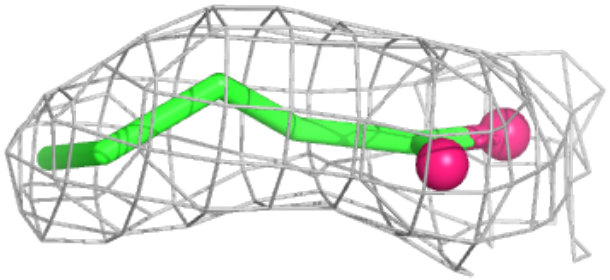


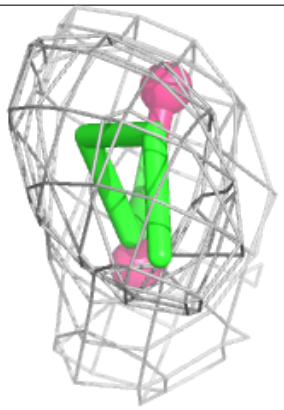


Electron density around OLA A 2410:

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

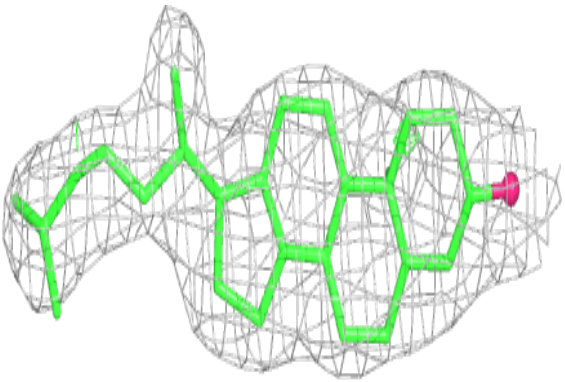


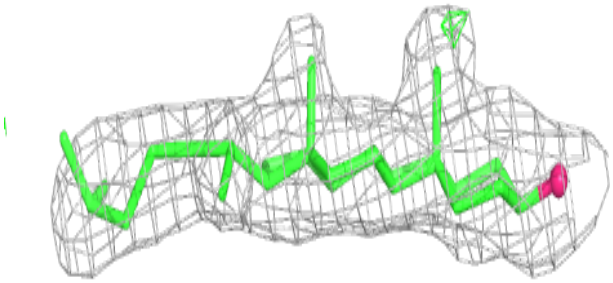


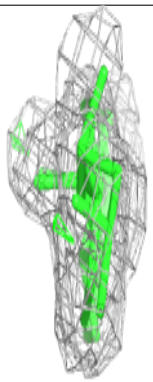


Electron density around CLR A 2401:

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

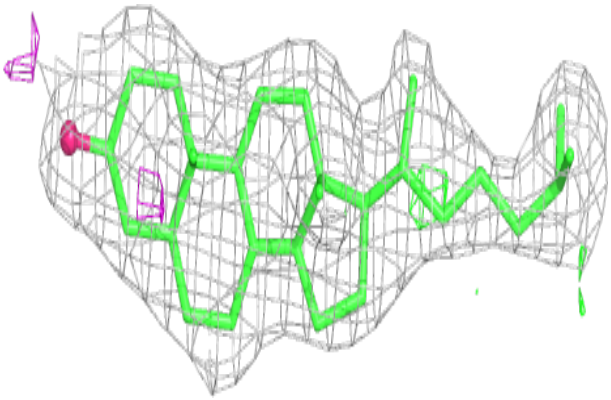


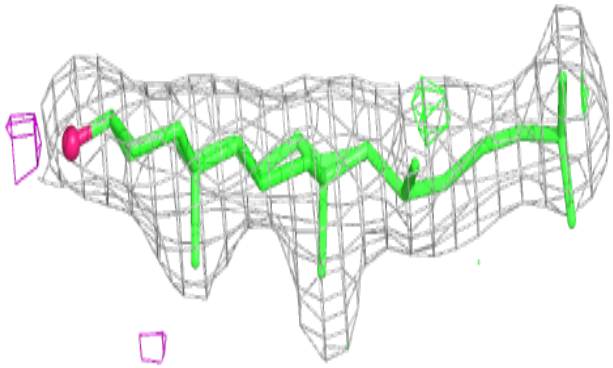


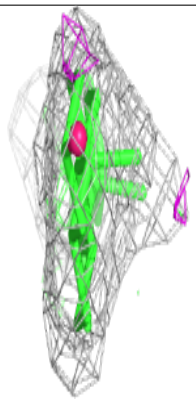


Electron density around CLR A 2402:

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

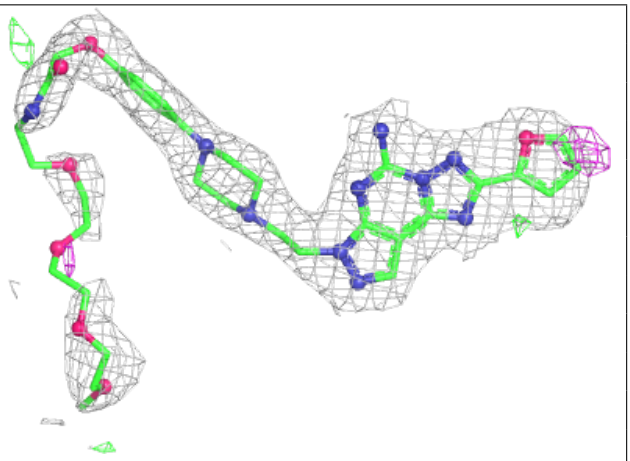


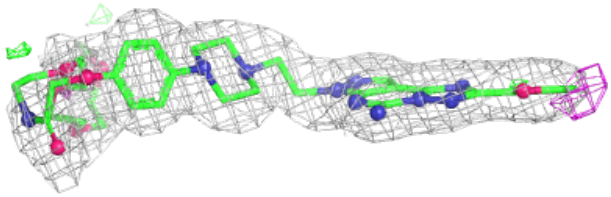


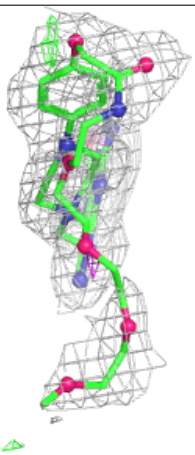


Electron density around 8E2 A 2404:

$2mF_o$-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.