



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 05:31 AM EDT

PDB ID : 5MZJ  
Title : Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with theophylline at 2.0Å resolution  
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Deposited on : 2017-01-31  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

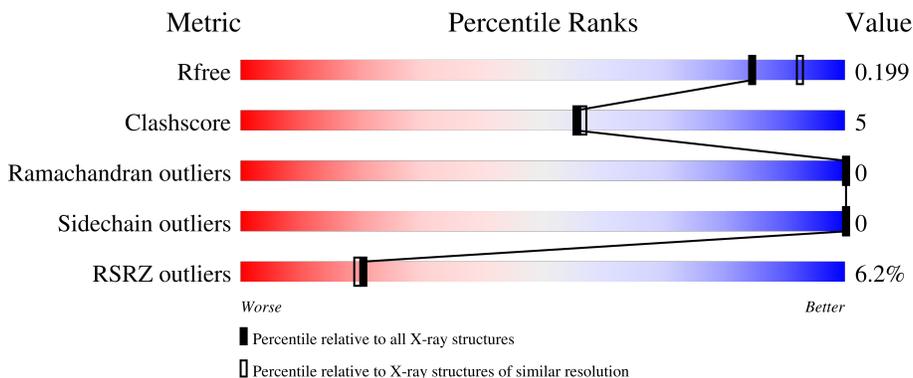
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	434	

## 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	386	3111	2029	526	533	23	0	15	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
A	54	LEU	ALA	engineered mutation	UNP P29274
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	conflict	UNP P0ABE7
A	1106	LEU	ARG	conflict	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	277	ALA	SER	engineered mutation	UNP P29274
A	318	ALA	GLY	engineered mutation	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274

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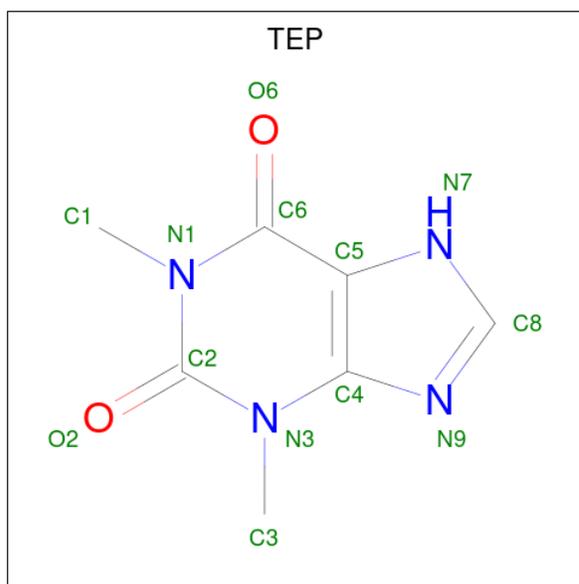
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Chain	Residue	Modelled	Actual	Comment	Reference
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

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

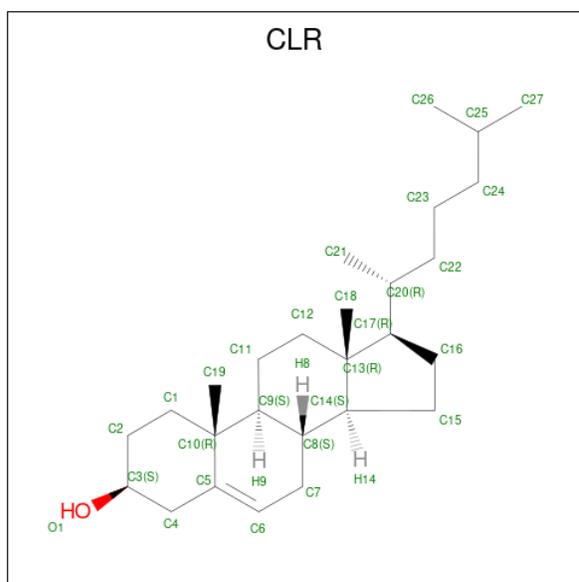
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is THEOPHYLLINE (three-letter code: TEP) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>).



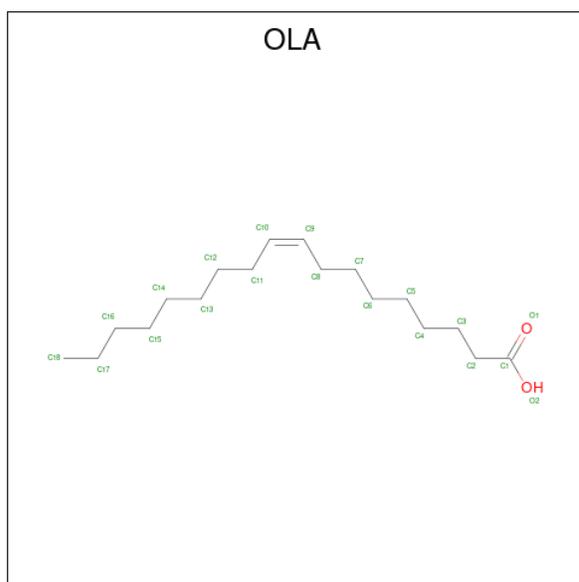
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 13 7 4 2	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



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

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



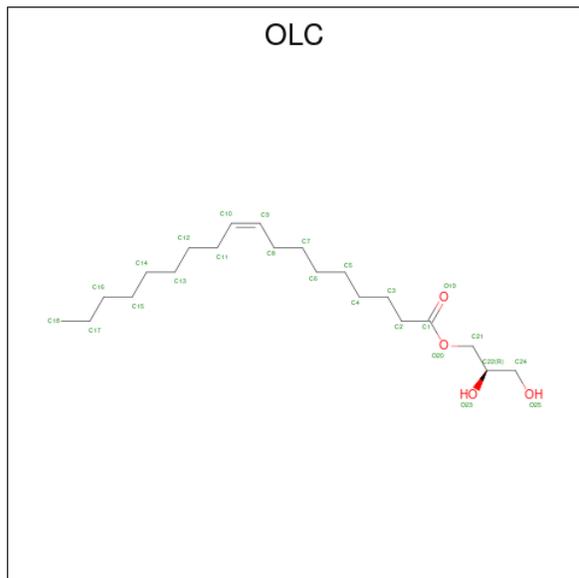
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			20	18 2		

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

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			16	12 4		
6	A	1	Total	C O	0	0
			17	13 4		
6	A	1	Total	C O	0	0
			23	19 4		
6	A	1	Total	C O	0	0
			23	19 4		
6	A	1	Total	C O	0	0
			23	19 4		
6	A	1	Total	C O	0	0
			18	14 4		
6	A	1	Total	C O	0	0
			16	12 4		

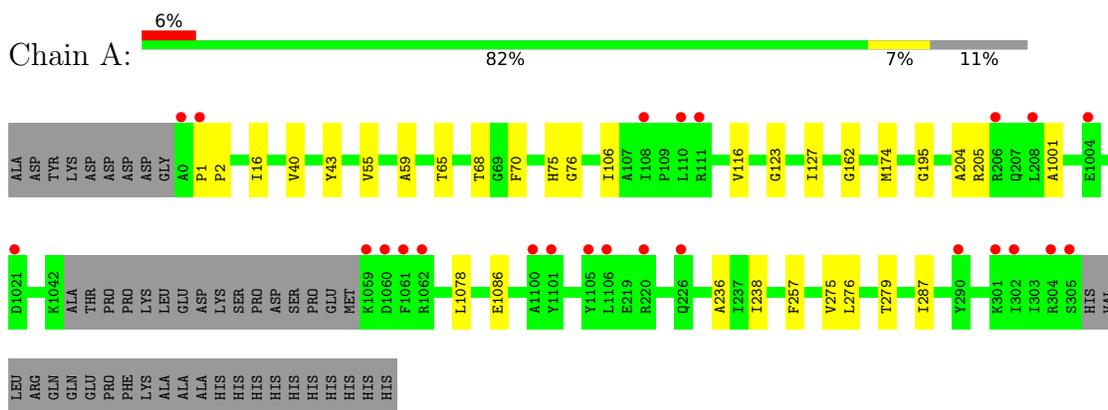
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	161	Total	O	0	0
			161	161		

### 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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.25Å 179.87Å 139.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.60 – 2.00 33.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.60-2.00) 99.9 (33.60-2.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.00Å)	Xtrriage
Refinement program	PHENIX v1.10.1_2155	Depositor
R, $R_{free}$	0.182 , 0.204 0.178 , 0.199	Depositor DCC
$R_{free}$ test set	1729 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtrriage
Anisotropy	0.344	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OLC, OLA, CLR, TEP

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	0.32	0/3174	0.42	0/4312

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3111	0	3184	25	0
2	A	1	0	0	0	0
3	A	13	0	8	0	0
4	A	84	0	138	0	0
5	A	307	0	459	22	0
6	A	136	0	186	7	0
7	A	161	0	0	2	1
All	All	3813	0	3975	39	1

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

The worst 5 of 39 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:174[B]:MET:SD	7:A:2563:HOH:O	2.43	0.76
5:A:2405:OLA:H152	6:A:2430:OLC:H12A	1.74	0.69
5:A:2424:OLA:H183	5:A:2425:OLA:C11	2.24	0.68
1:A:162:GLY:O	7:A:2501:HOH:O	2.17	0.59
5:A:2409:OLA:H151	5:A:2416:OLA:H151	1.85	0.58

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2636:HOH:O	7:A:2649:HOH:O[4_555]	2.18	0.02

### 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	392/434 (90%)	391 (100%)	1 (0%)	0	<b>100</b> <b>100</b>

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	326/353 (92%)	326 (100%)	0	<b>100</b> <b>100</b>

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	230	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	TEP	A	2401	-	6,14,14	1.45	1 (16%)	8,21,21	2.84	4 (50%)
6	OLC	A	2429	-	22,22,24	0.61	0	23,23,25	0.70	0
6	OLC	A	2431	-	22,22,24	0.64	0	23,23,25	0.75	0
5	OLA	A	2416	-	19,19,19	0.68	0	19,19,19	0.72	1 (5%)
5	OLA	A	2414	-	10,10,19	0.52	0	10,10,19	1.23	2 (20%)
6	OLC	A	2432	-	17,17,24	0.75	0	18,18,25	0.81	0
5	OLA	A	2405	-	19,19,19	0.65	0	19,19,19	0.75	1 (5%)
4	CLR	A	2404	-	31,31,31	0.77	0	48,48,48	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	OLA	A	2417	-	11,11,19	0.47	0	10,10,19	0.29	0
6	OLC	A	2427	-	15,15,24	0.68	0	16,16,25	0.94	1 (6%)
6	OLC	A	2428	-	16,16,24	0.79	0	17,17,25	0.81	0
6	OLC	A	2430	-	22,22,24	0.68	0	23,23,25	0.79	0
5	OLA	A	2422	-	7,7,19	0.27	0	6,6,19	0.31	0
5	OLA	A	2409	-	19,19,19	0.69	0	19,19,19	0.75	1 (5%)
5	OLA	A	2426	-	19,19,19	0.70	0	19,19,19	0.75	2 (10%)
5	OLA	A	2410	-	19,19,19	0.64	0	19,19,19	0.78	2 (10%)
5	OLA	A	2415	-	18,18,19	0.67	0	18,18,19	0.82	2 (11%)
4	CLR	A	2403	-	31,31,31	0.66	0	48,48,48	0.85	1 (2%)
5	OLA	A	2407	-	8,8,19	0.84	0	8,8,19	1.20	2 (25%)
5	OLA	A	2420	-	11,11,19	0.39	0	9,10,19	0.35	0
5	OLA	A	2421	-	8,8,19	0.46	0	7,7,19	0.18	0
4	CLR	A	2402	-	31,31,31	0.70	0	48,48,48	1.06	2 (4%)
5	OLA	A	2418	-	9,9,19	0.43	0	7,8,19	0.39	0
5	OLA	A	2419	-	10,10,19	0.57	0	9,9,19	0.31	0
5	OLA	A	2423	-	14,14,19	0.55	0	14,14,19	1.05	2 (14%)
5	OLA	A	2408	-	17,17,19	0.55	0	17,17,19	0.93	2 (11%)
5	OLA	A	2413	-	14,14,19	0.71	0	14,14,19	0.90	1 (7%)
5	OLA	A	2406	-	9,9,19	0.84	0	9,9,19	1.07	1 (11%)
5	OLA	A	2412	-	7,7,19	0.91	0	7,7,19	1.22	1 (14%)
5	OLA	A	2424	-	14,14,19	0.40	0	13,13,19	0.31	0
5	OLA	A	2425	-	12,12,19	0.59	0	12,12,19	1.11	2 (16%)
5	OLA	A	2411	-	11,11,19	0.80	0	11,11,19	0.96	1 (9%)
6	OLC	A	2433	-	15,15,24	0.80	0	16,16,25	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TEP	A	2401	-	-	-	0/2/2/2
6	OLC	A	2429	-	-	10/22/22/24	-
6	OLC	A	2431	-	-	9/22/22/24	-
5	OLA	A	2416	-	-	7/17/17/17	-
5	OLA	A	2414	-	-	5/8/8/17	-
6	OLC	A	2432	-	-	8/17/17/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLA	A	2405	-	-	10/17/17/17	-
4	CLR	A	2404	-	-	3/10/68/68	0/4/4/4
5	OLA	A	2417	-	-	4/9/9/17	-
6	OLC	A	2427	-	-	8/15/15/24	-
6	OLC	A	2428	-	-	11/16/16/24	-
6	OLC	A	2430	-	-	9/22/22/24	-
5	OLA	A	2422	-	-	3/5/5/17	-
5	OLA	A	2409	-	-	10/17/17/17	-
5	OLA	A	2426	-	-	11/17/17/17	-
5	OLA	A	2410	-	-	8/17/17/17	-
5	OLA	A	2415	-	-	7/16/16/17	-
4	CLR	A	2403	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2407	-	-	3/6/6/17	-
5	OLA	A	2420	-	-	7/9/9/17	-
5	OLA	A	2421	-	-	3/6/6/17	-
4	CLR	A	2402	-	-	0/10/68/68	0/4/4/4
5	OLA	A	2418	-	-	4/7/7/17	-
5	OLA	A	2419	-	-	3/8/8/17	-
5	OLA	A	2423	-	-	9/12/12/17	-
5	OLA	A	2408	-	-	6/15/15/17	-
5	OLA	A	2413	-	-	2/12/12/17	-
5	OLA	A	2406	-	-	2/7/7/17	-
5	OLA	A	2412	-	-	1/5/5/17	-
5	OLA	A	2424	-	-	6/12/12/17	-
5	OLA	A	2425	-	-	5/10/10/17	-
5	OLA	A	2411	-	-	6/9/9/17	-
6	OLC	A	2433	-	-	6/15/15/24	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2401	TEP	C6-N1	3.26	1.43	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2401	TEP	C4-C5-C6	6.29	124.00	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2401	TEP	C3-N3-C4	3.05	122.57	118.25
3	A	2401	TEP	C5-C6-N1	-2.92	115.08	118.20
5	A	2414	OLA	O2-C1-C2	2.62	122.45	114.03
5	A	2423	OLA	O2-C1-C2	2.59	122.35	114.03

There are no chirality outliers.

5 of 186 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2417	OLA	C6-C7-C8-C9
6	A	2427	OLC	O20-C21-C22-C24
6	A	2428	OLC	O20-C21-C22-O23
6	A	2429	OLC	C21-C22-C24-O25
6	A	2430	OLC	O20-C21-C22-O23

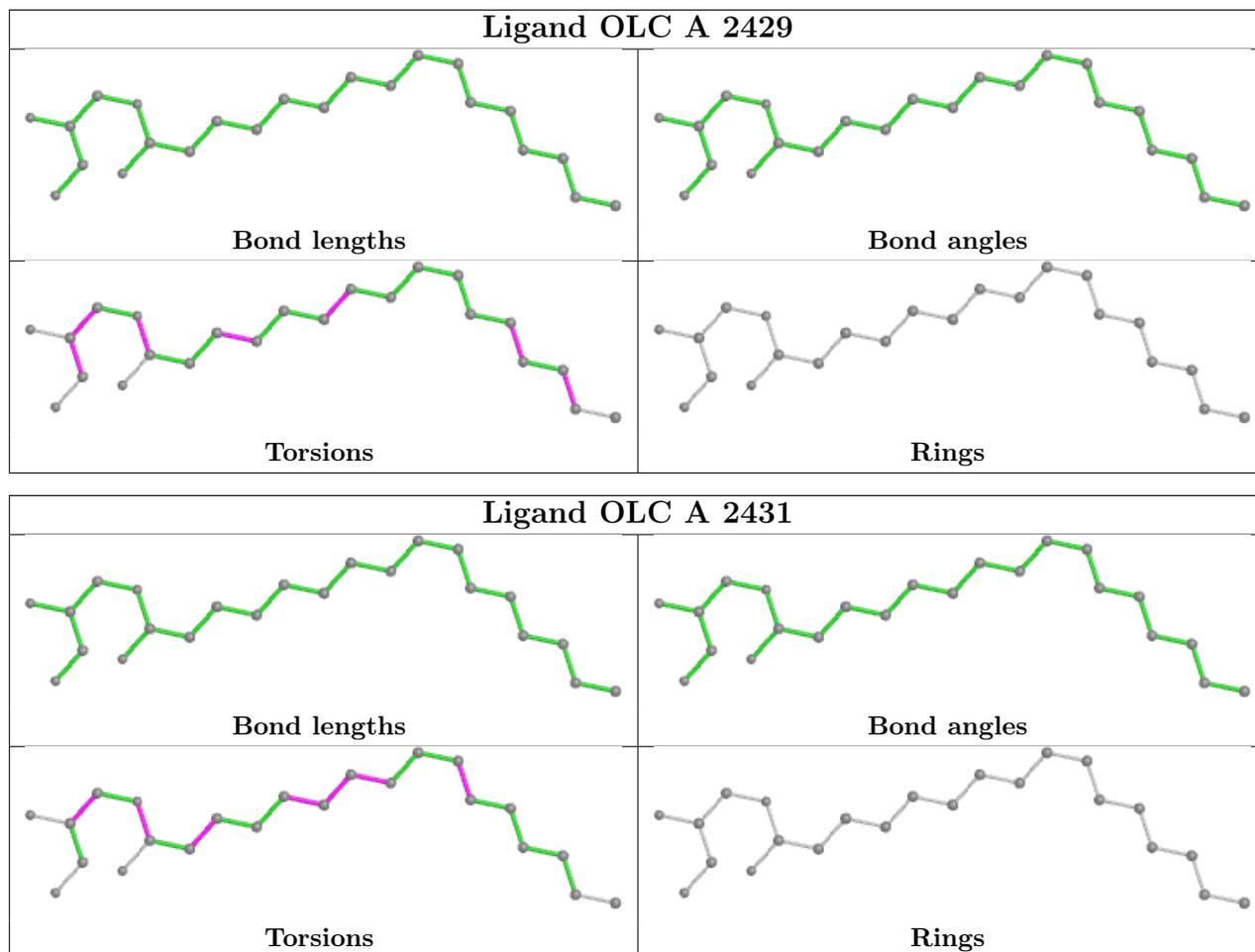
There are no ring outliers.

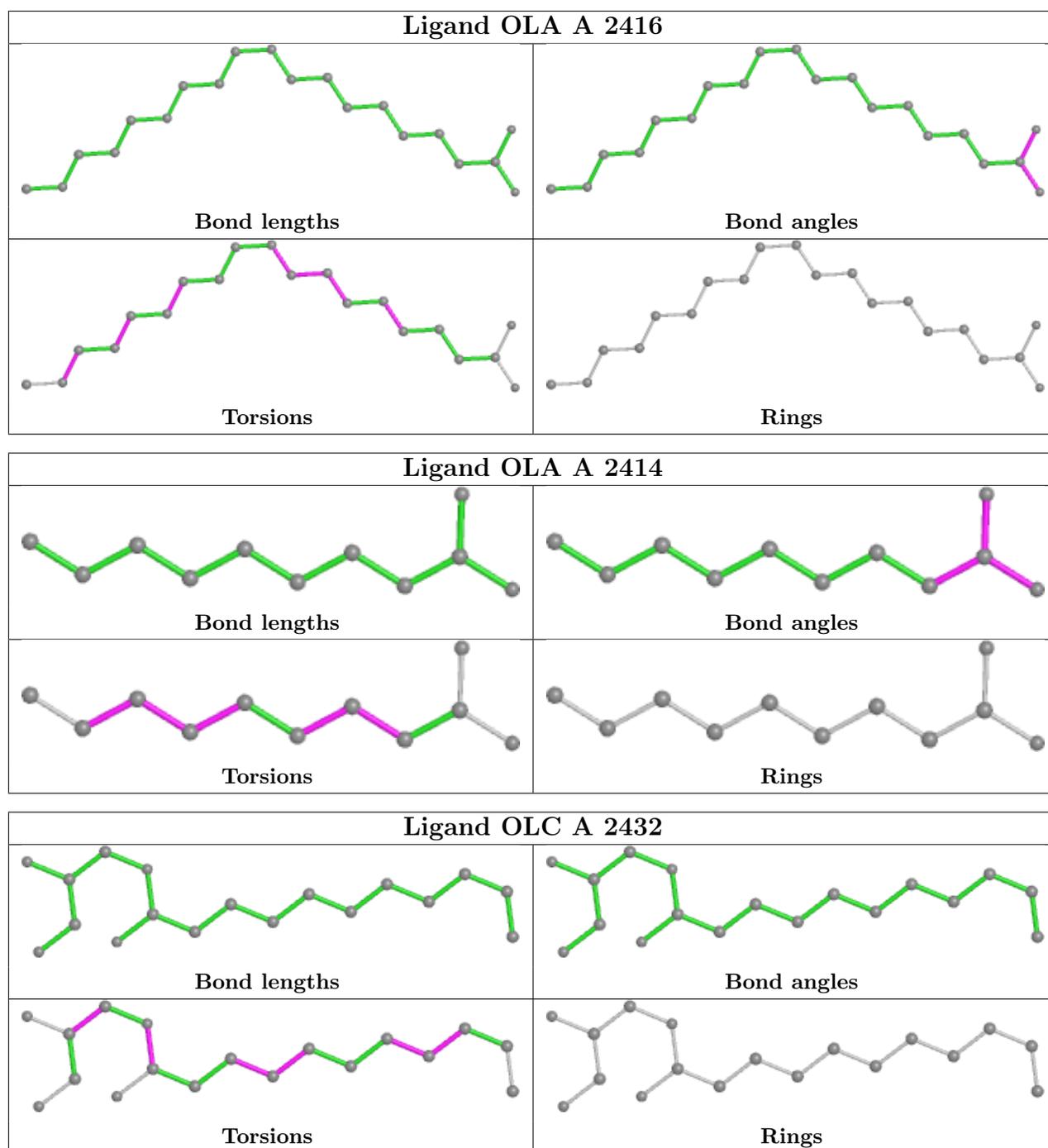
21 monomers are involved in 25 short contacts:

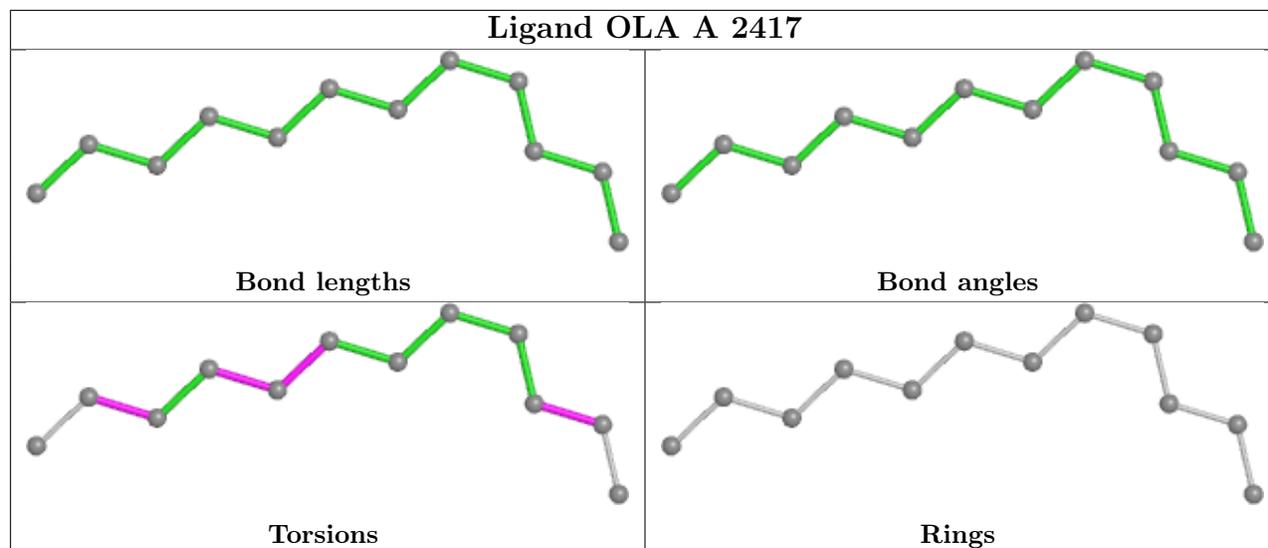
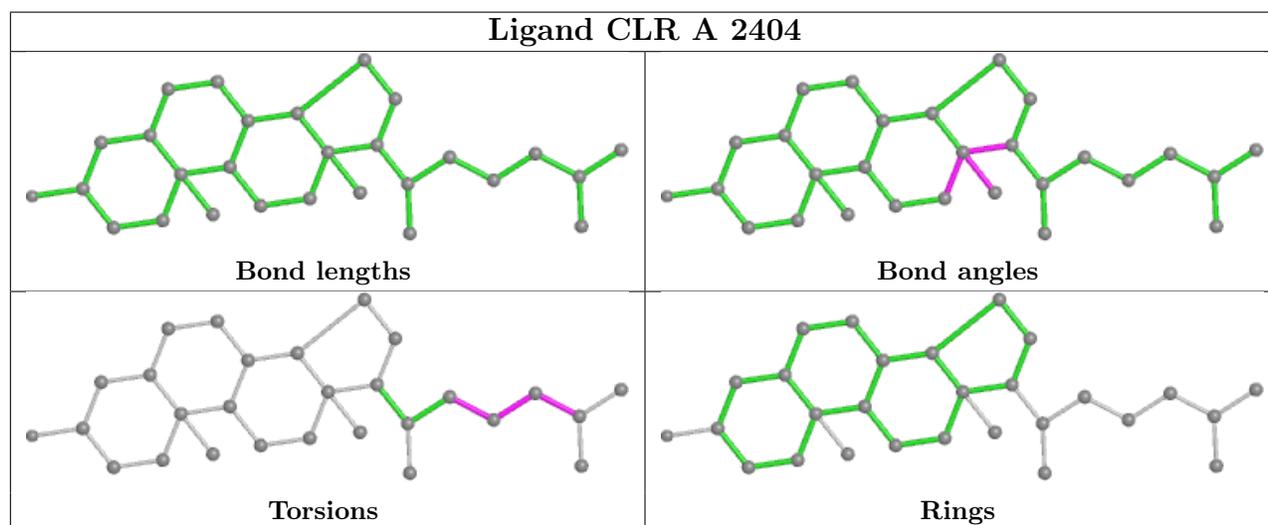
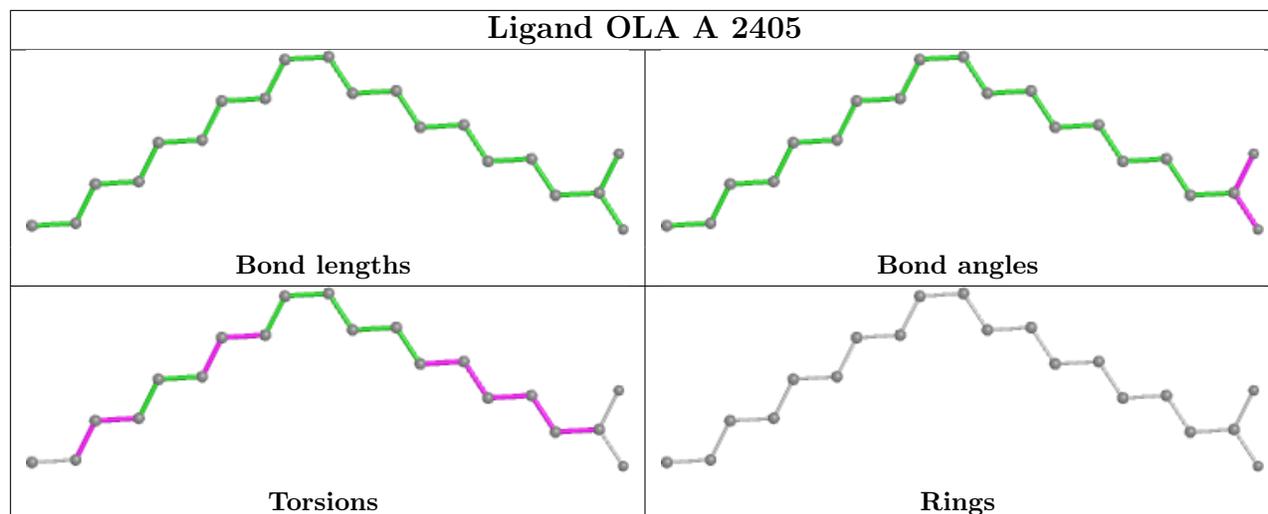
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2429	OLC	1	0
6	A	2431	OLC	1	0
5	A	2416	OLA	4	0
5	A	2405	OLA	3	0
5	A	2417	OLA	2	0
6	A	2427	OLC	1	0
6	A	2428	OLC	1	0
6	A	2430	OLC	3	0
5	A	2422	OLA	2	0
5	A	2409	OLA	2	0
5	A	2426	OLA	3	0
5	A	2410	OLA	1	0
5	A	2420	OLA	1	0
5	A	2421	OLA	2	0
5	A	2418	OLA	1	0
5	A	2419	OLA	1	0
5	A	2423	OLA	1	0
5	A	2406	OLA	1	0
5	A	2424	OLA	2	0
5	A	2425	OLA	2	0
6	A	2433	OLC	1	0

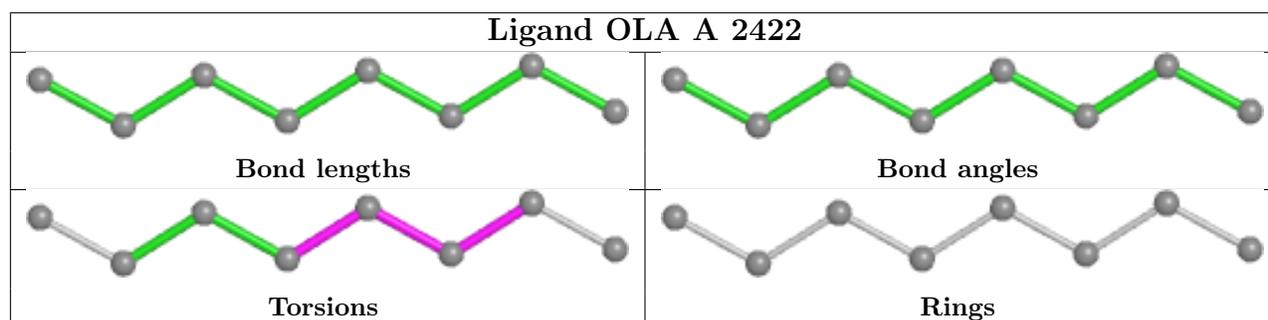
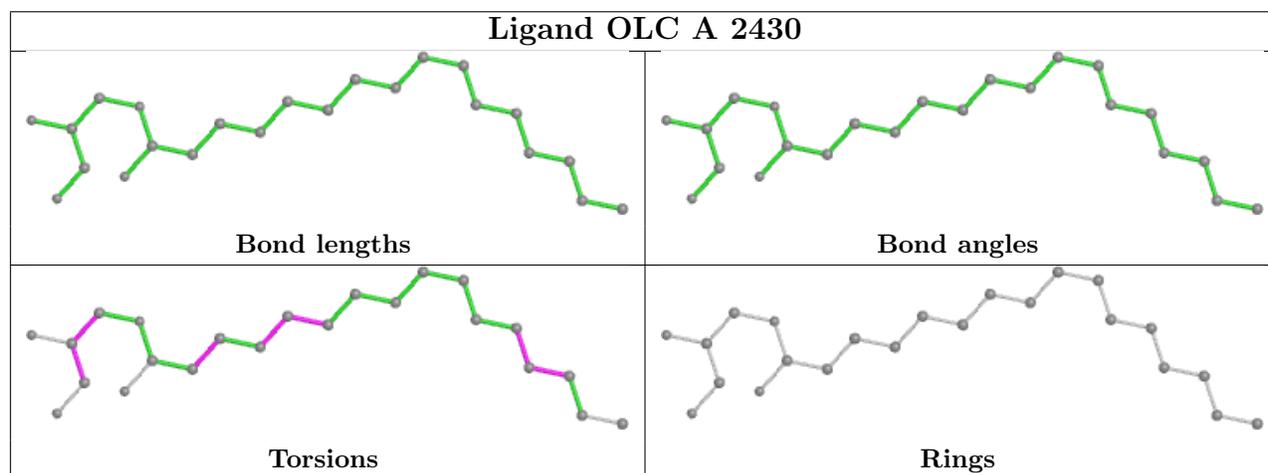
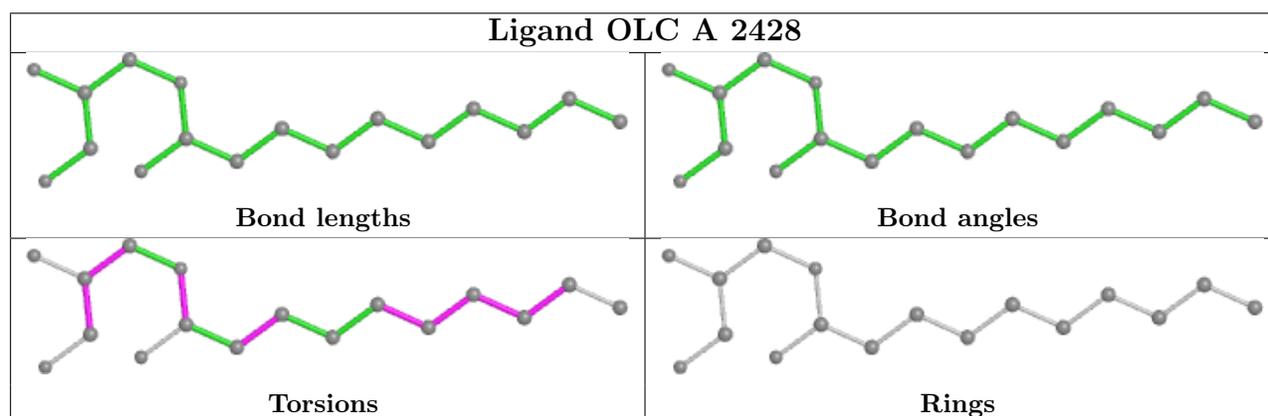
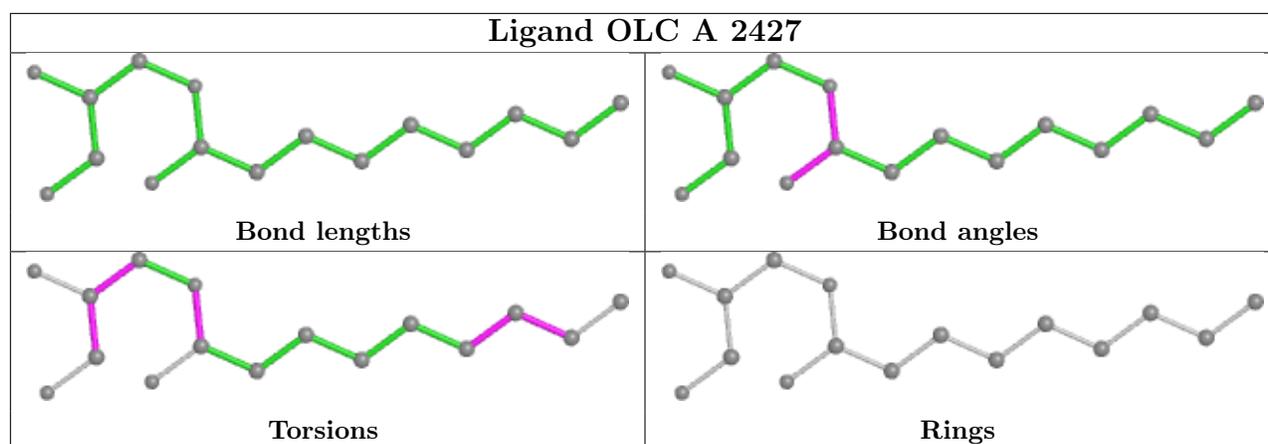
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

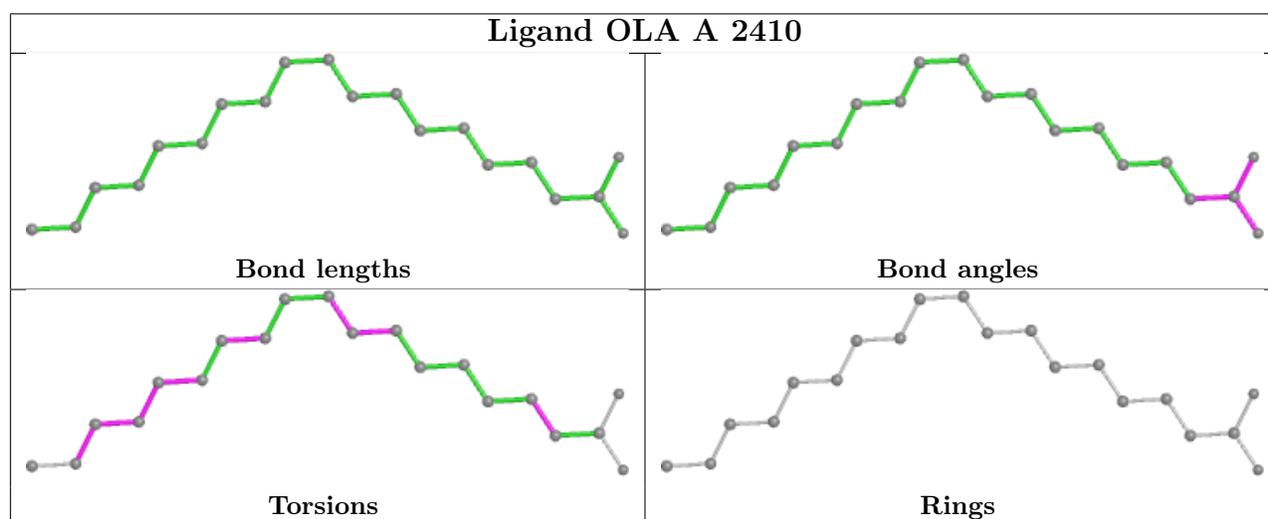
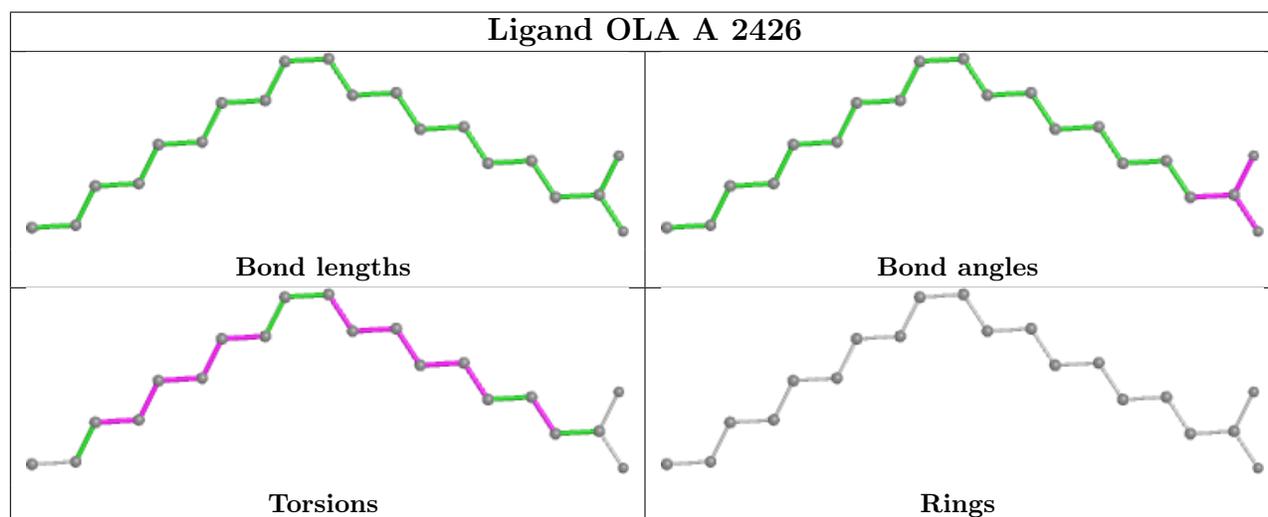
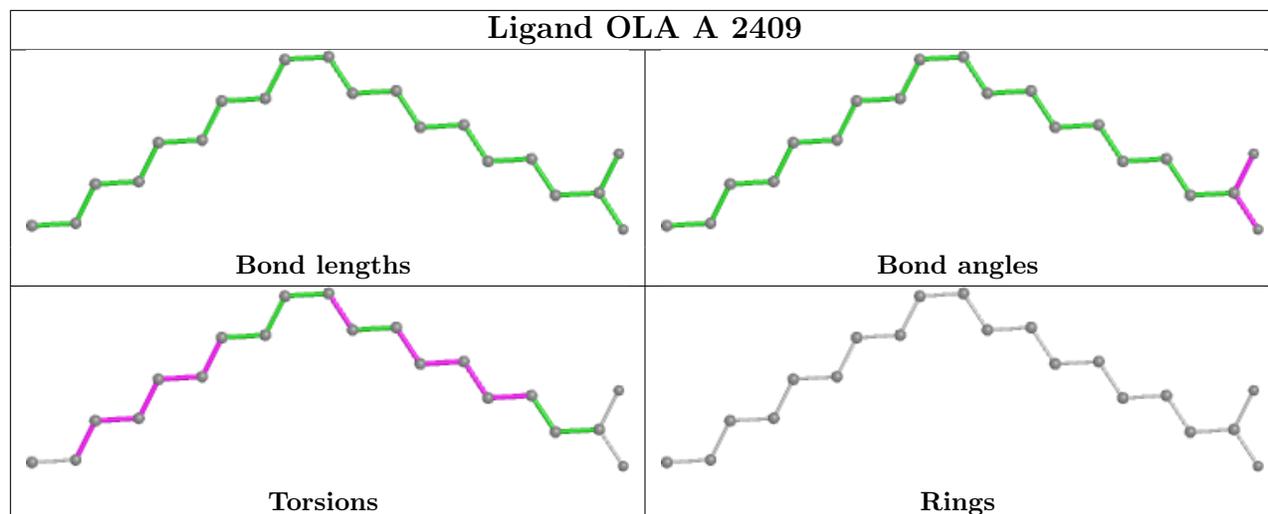
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

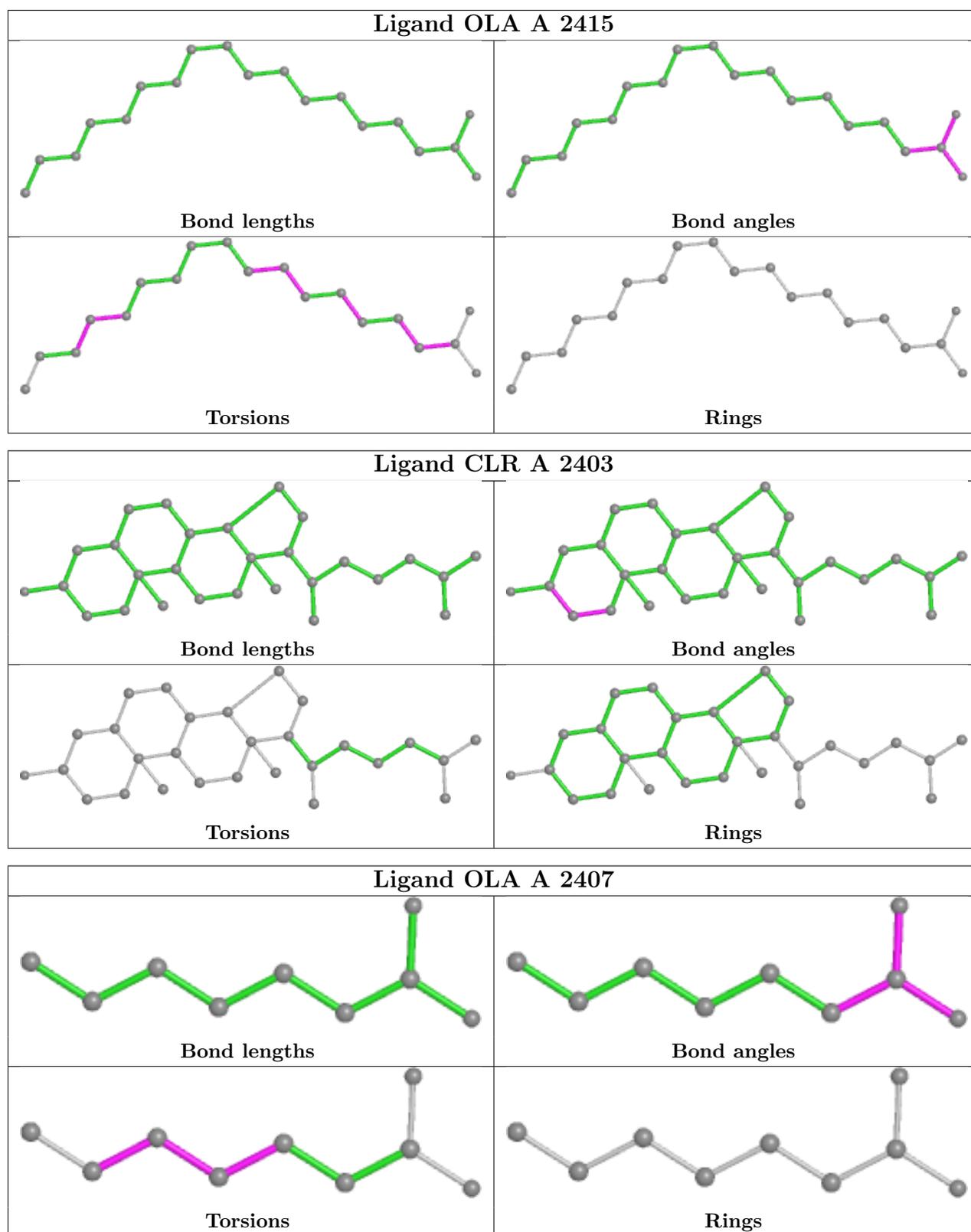


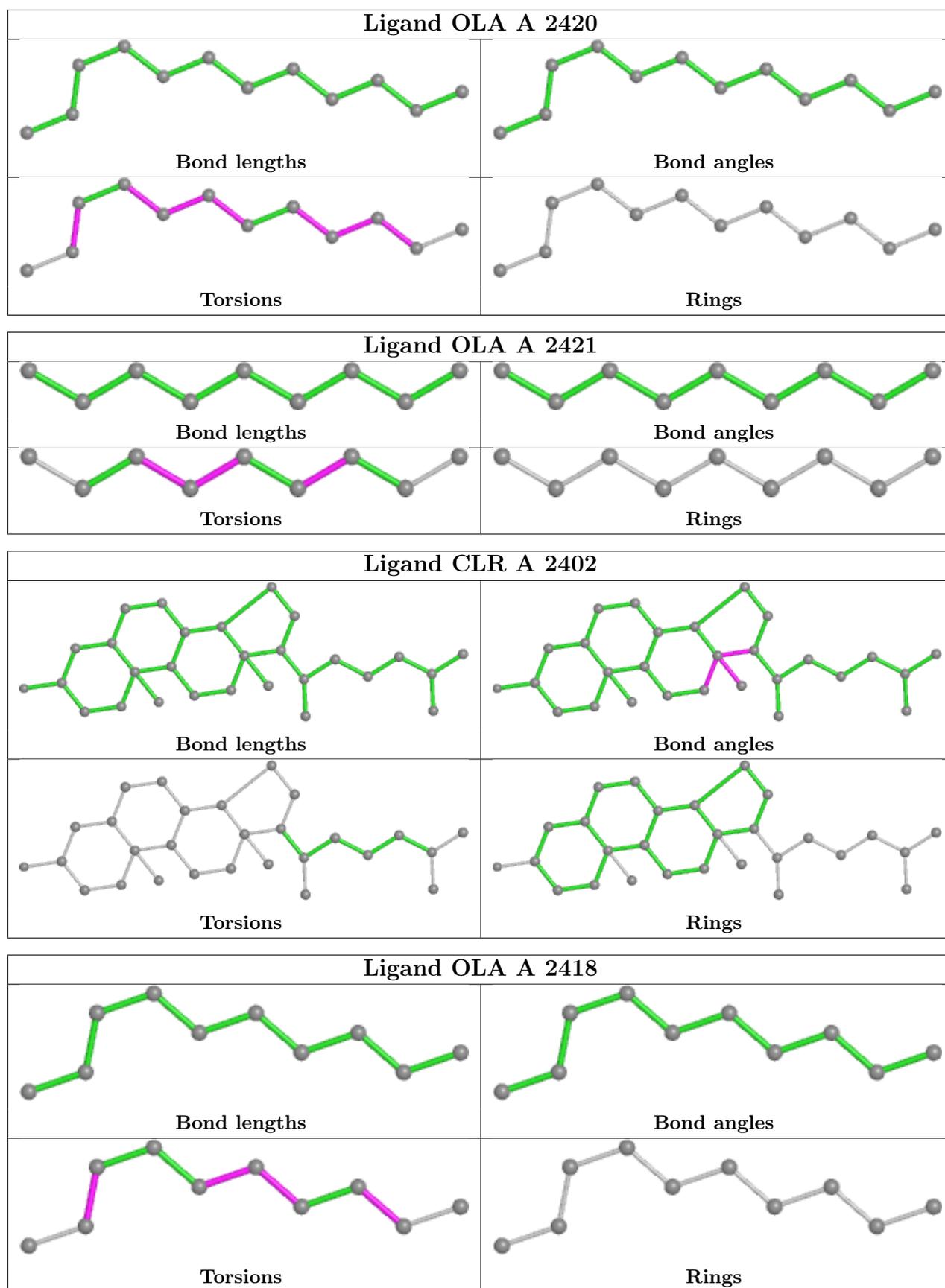


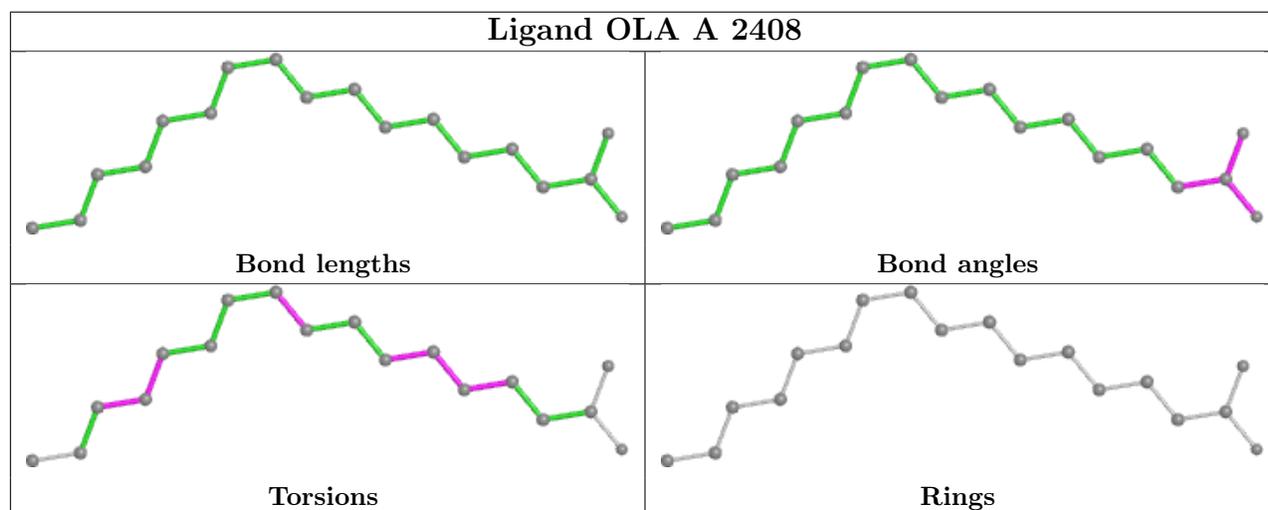
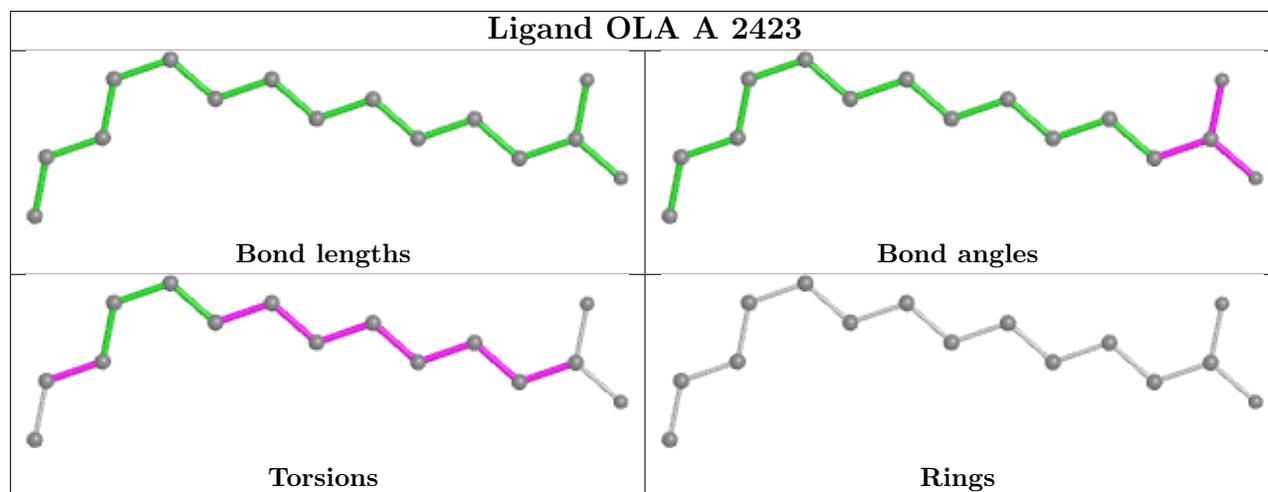
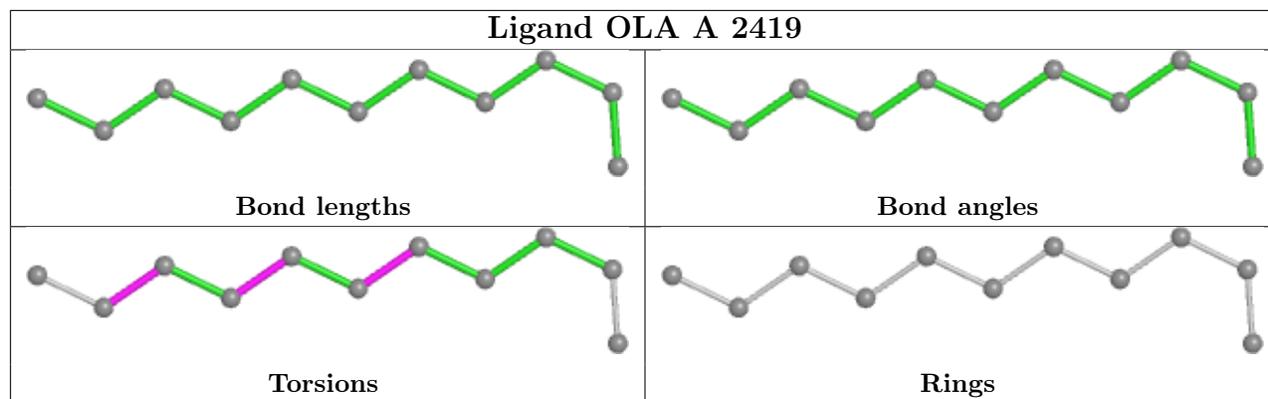


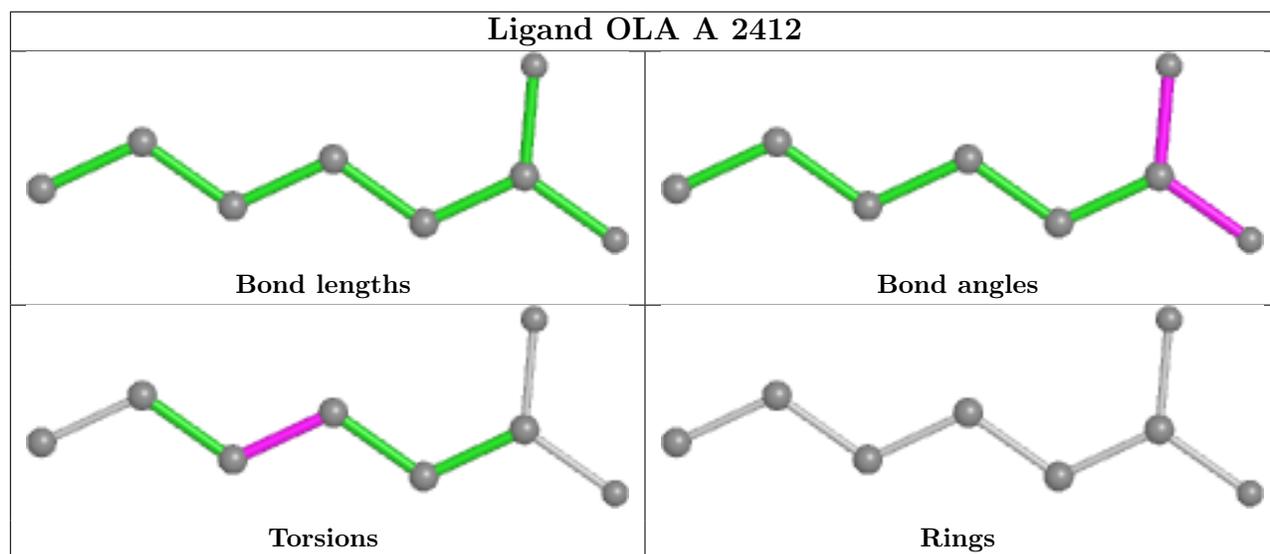
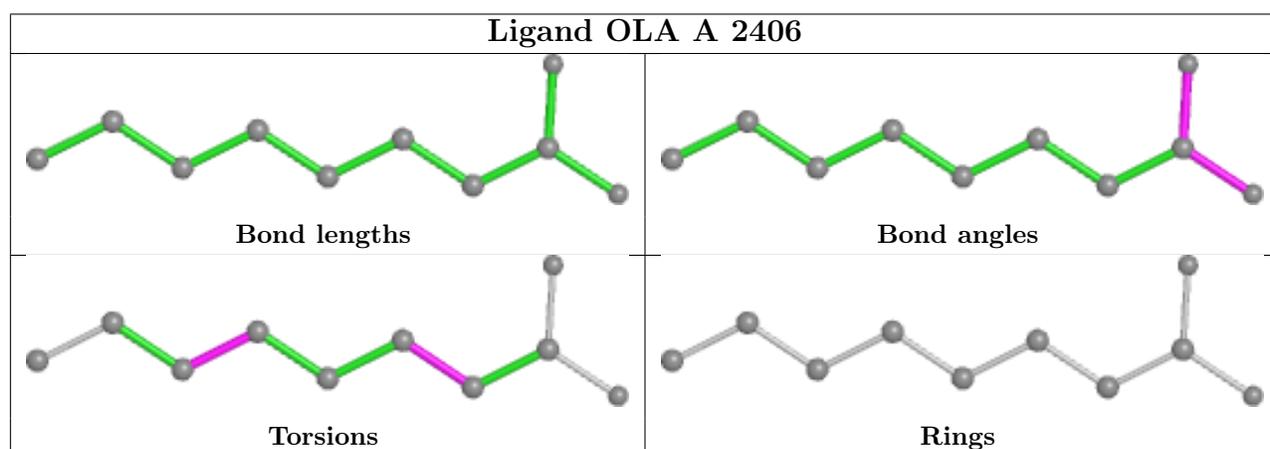
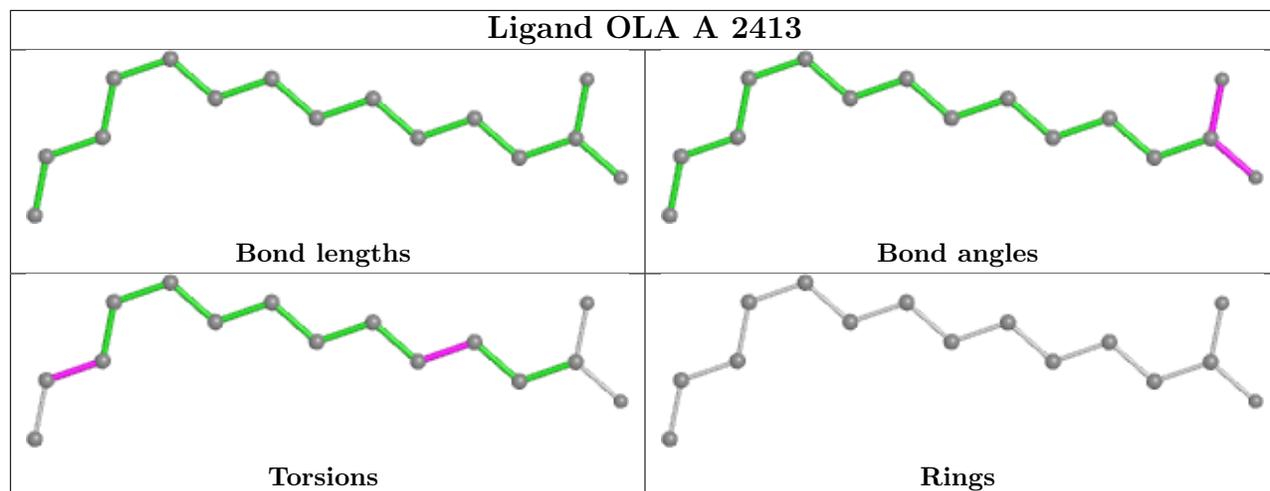


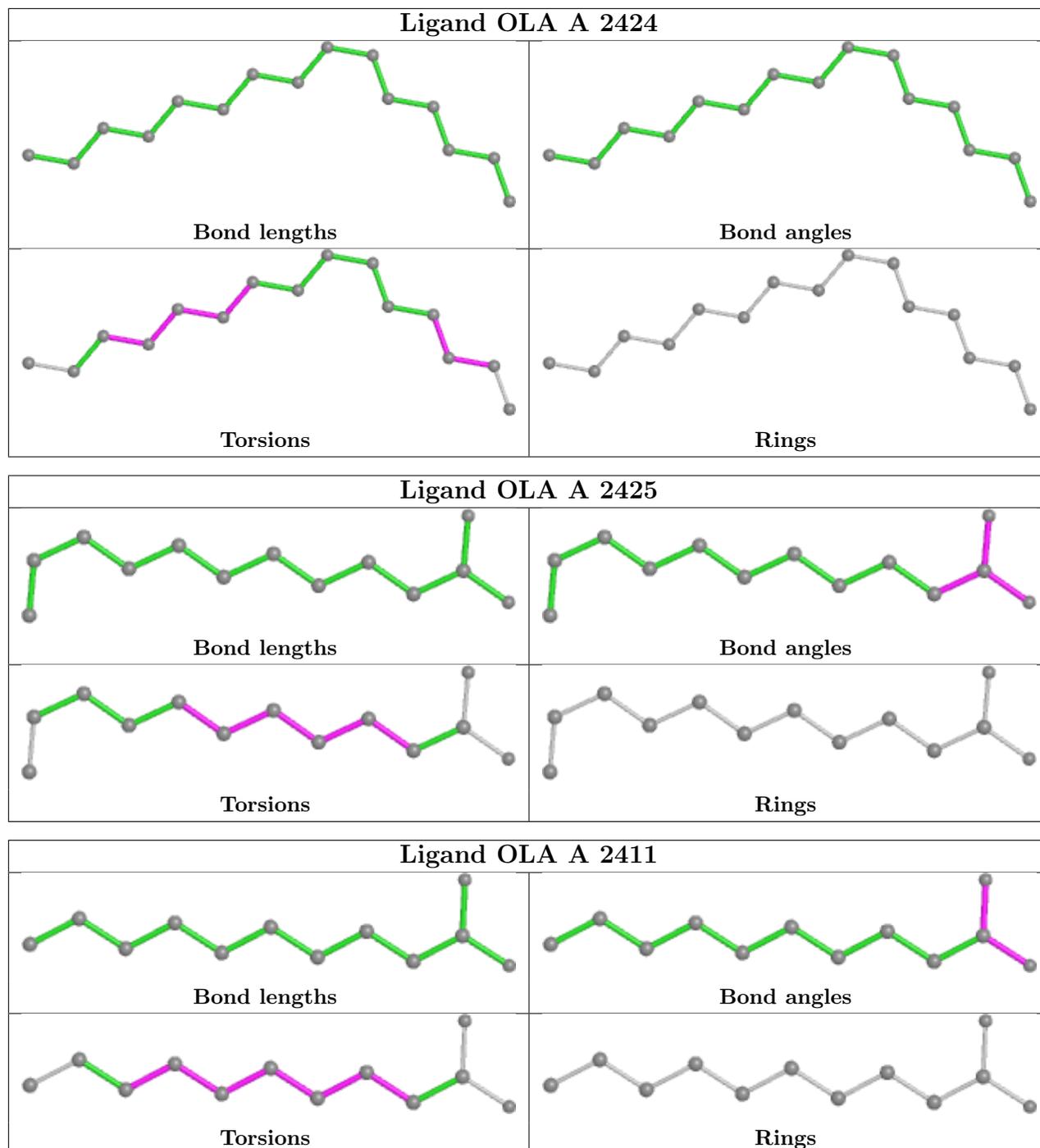


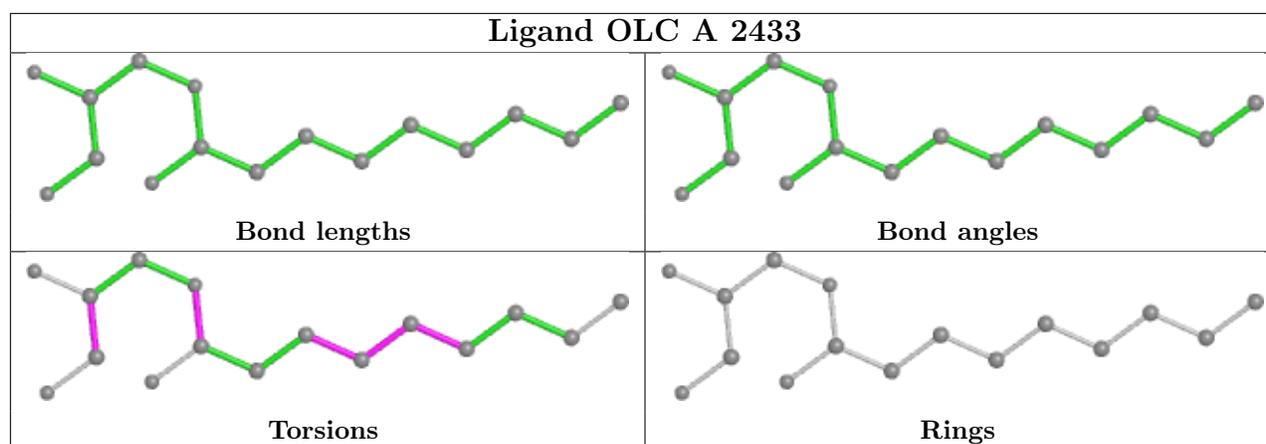












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	208[B]:LEU	C	1001:ALA	N	3.03
1	A	208[A]:LEU	C	1001:ALA	N	3.02
1	A	1106:LEU	C	219:GLU	N	2.85

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	386/434 (88%)	0.15	24 (6%) <b>20</b> <b>19</b>	15, 33, 73, 121	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1061	PHE	6.4
1	A	1059	LYS	5.7
1	A	110	LEU	3.9
1	A	1062	ARG	3.9
1	A	1105	TYR	3.6

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	OLA	A	2406	10/20	0.52	0.22	60,76,84,85	0
5	OLA	A	2426	20/20	0.58	0.26	58,66,74,76	0

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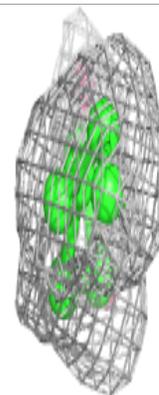
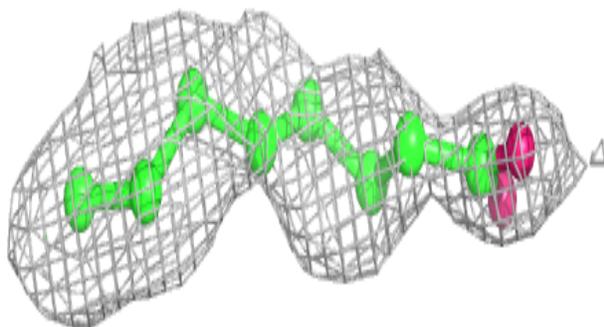
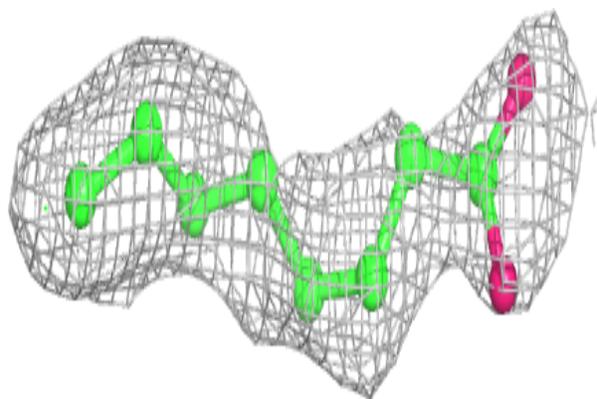
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	OLA	A	2409	20/20	0.64	0.24	46,59,75,75	0
5	OLA	A	2416	20/20	0.68	0.32	45,67,72,72	0
5	OLA	A	2423	15/20	0.70	0.19	54,58,70,71	0
6	OLC	A	2431	23/25	0.70	0.28	46,52,72,78	0
5	OLA	A	2415	19/20	0.72	0.23	54,61,69,70	0
5	OLA	A	2425	13/20	0.74	0.27	44,60,76,77	0
6	OLC	A	2432	18/25	0.74	0.27	48,59,78,83	0
5	OLA	A	2413	15/20	0.75	0.23	60,68,78,81	0
5	OLA	A	2421	9/20	0.76	0.22	53,63,66,66	0
5	OLA	A	2411	12/20	0.76	0.32	45,60,80,83	0
5	OLA	A	2410	20/20	0.76	0.25	53,63,74,74	0
5	OLA	A	2420	12/20	0.79	0.20	61,62,64,64	0
6	OLC	A	2428	17/25	0.81	0.15	51,65,83,84	0
5	OLA	A	2417	12/20	0.81	0.20	42,54,69,69	0
5	OLA	A	2412	8/20	0.81	0.14	59,62,64,64	0
5	OLA	A	2418	10/20	0.82	0.19	58,60,64,65	0
5	OLA	A	2414	11/20	0.83	0.17	49,52,70,74	0
6	OLC	A	2429	23/25	0.85	0.17	40,54,82,83	0
6	OLC	A	2427	16/25	0.85	0.18	38,47,55,60	0
5	OLA	A	2422	8/20	0.85	0.14	53,65,68,69	0
5	OLA	A	2408	18/20	0.86	0.15	47,61,72,76	0
5	OLA	A	2407	9/20	0.87	0.20	42,46,64,66	0
5	OLA	A	2405	20/20	0.88	0.14	34,54,65,66	0
6	OLC	A	2430	23/25	0.88	0.16	39,52,63,70	0
5	OLA	A	2419	11/20	0.89	0.20	38,46,58,58	0
6	OLC	A	2433	16/25	0.89	0.17	35,42,61,61	0
5	OLA	A	2424	15/20	0.90	0.15	49,54,56,56	0
4	CLR	A	2403	28/28	0.94	0.10	25,30,48,49	0
4	CLR	A	2402	28/28	0.95	0.09	21,26,51,56	0
4	CLR	A	2404	28/28	0.96	0.08	18,25,49,53	0
2	NA	A	2400	1/1	0.97	0.11	35,35,35,35	0
3	TEP	A	2401	13/13	0.98	0.19	18,20,23,25	0

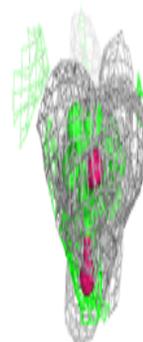
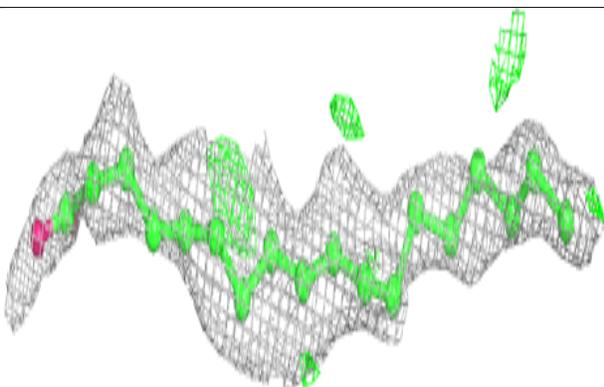
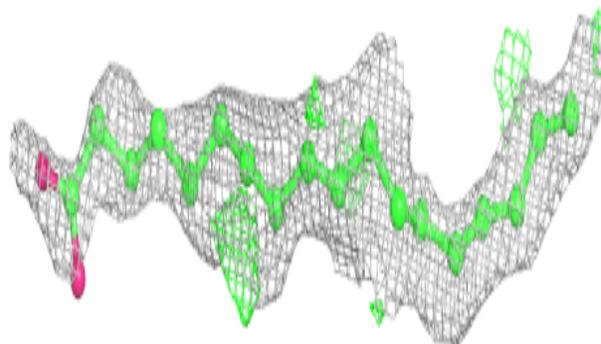
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLA A 2406:**

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

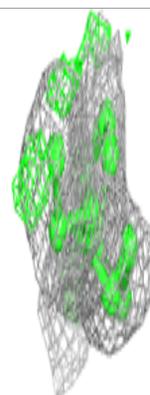
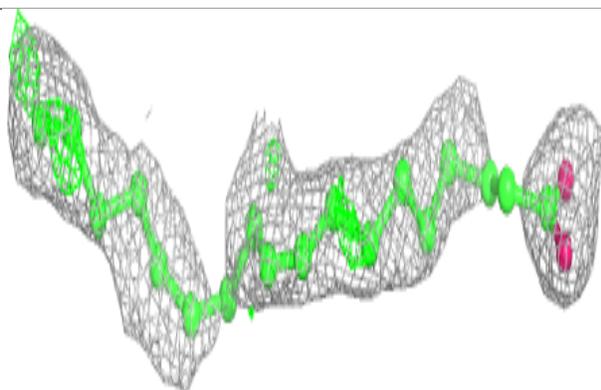
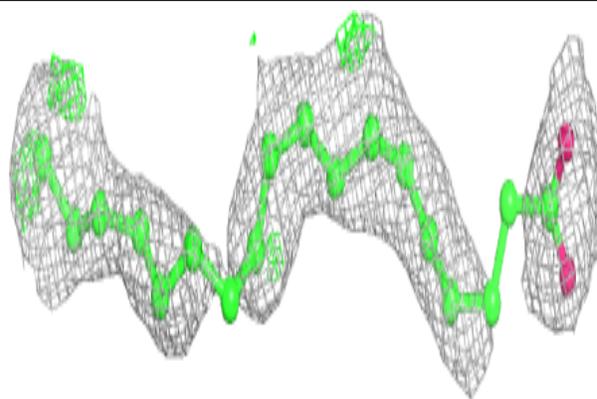
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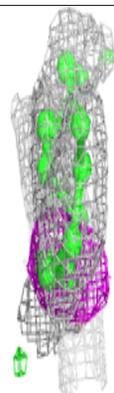
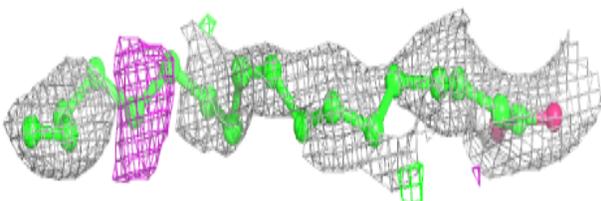
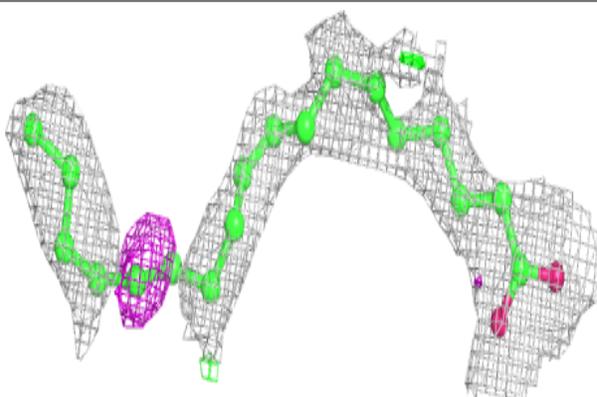


**Electron density around OLA A 2409:**

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and green (positive)

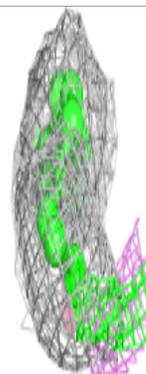
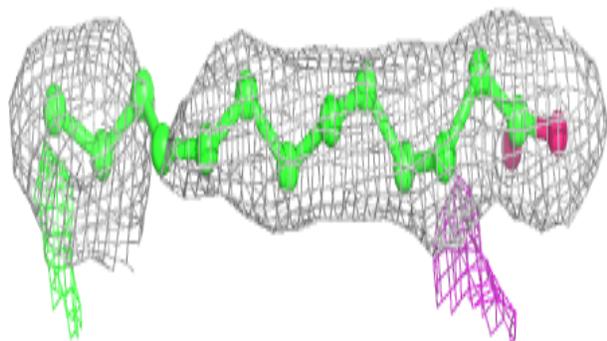
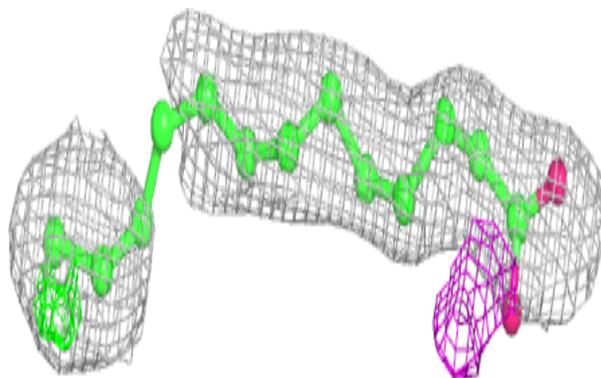
**Electron density around OLA A 2416:**

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and green (positive)

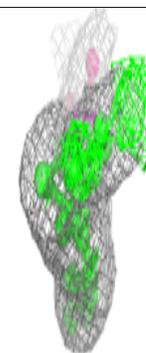
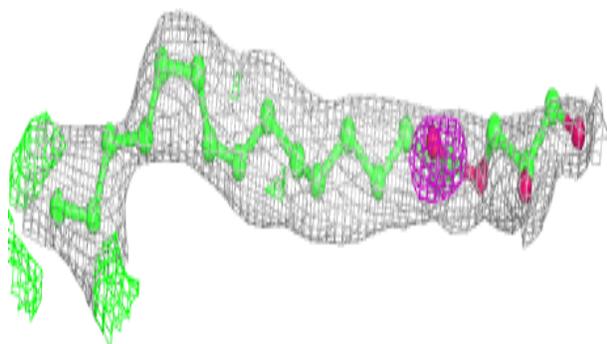
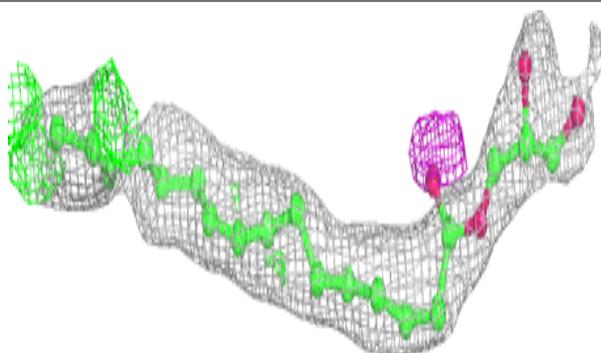


**Electron density around OLA A 2423:**

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and green (positive)

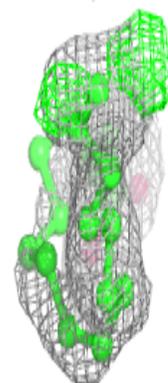
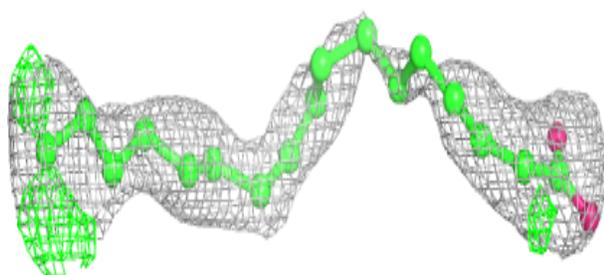
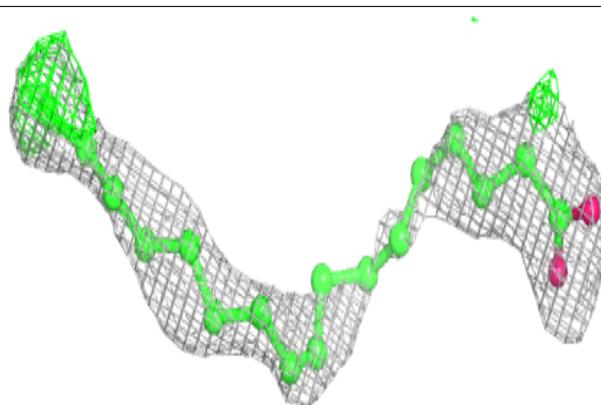
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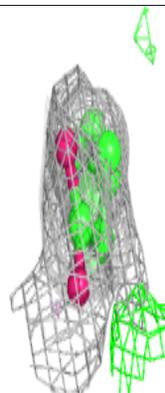
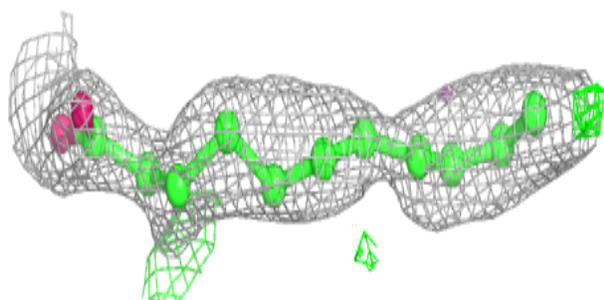
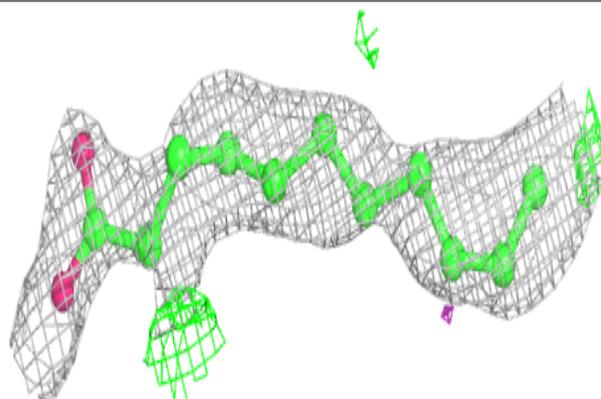


**Electron density around OLA A 2415:**

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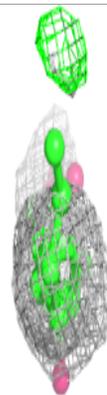
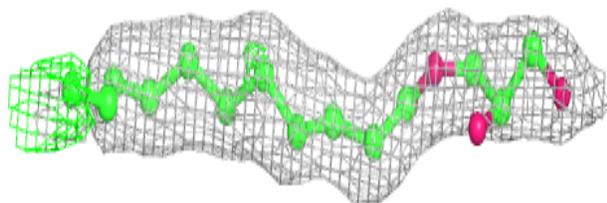
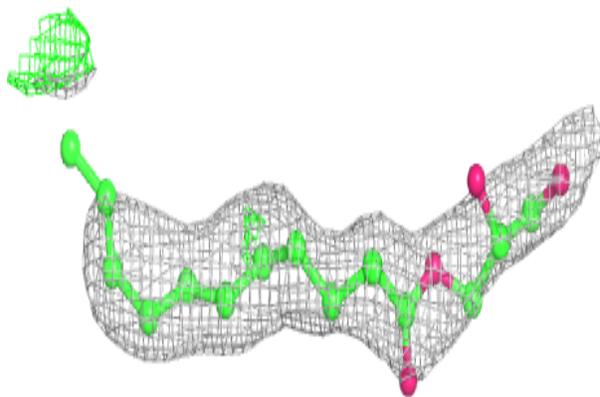
**Electron density around OLA A 2425:**

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and green (positive)

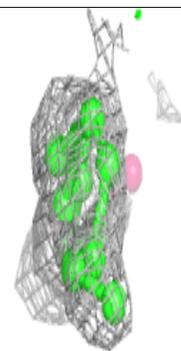
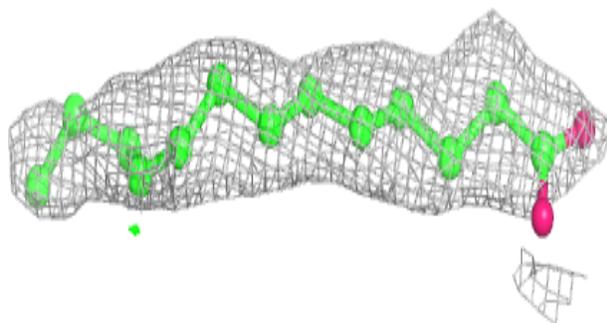
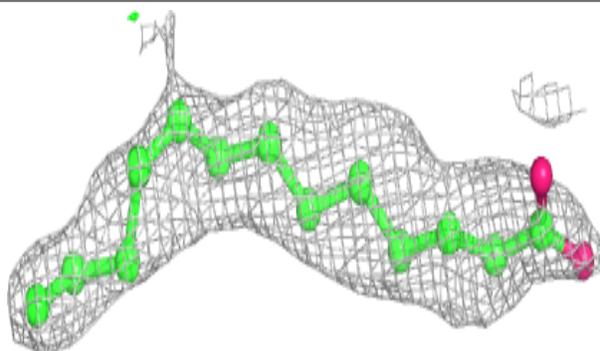


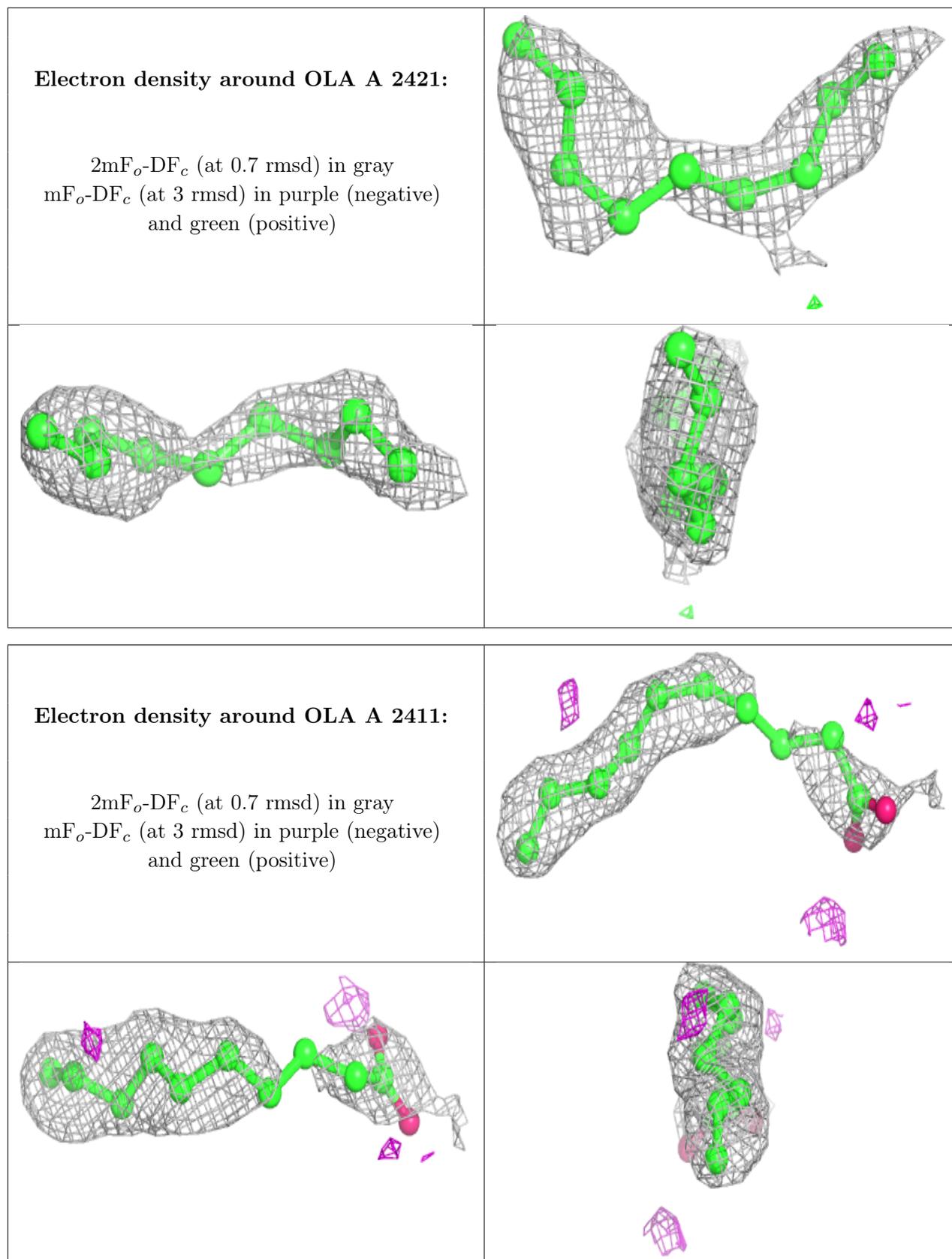
**Electron density around OLC A 2432:**

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and green (positive)

**Electron density around OLA A 2413:**

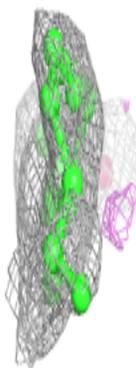
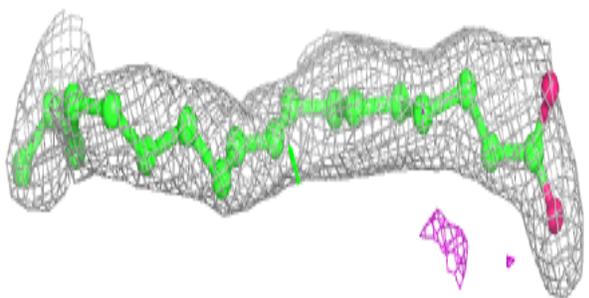
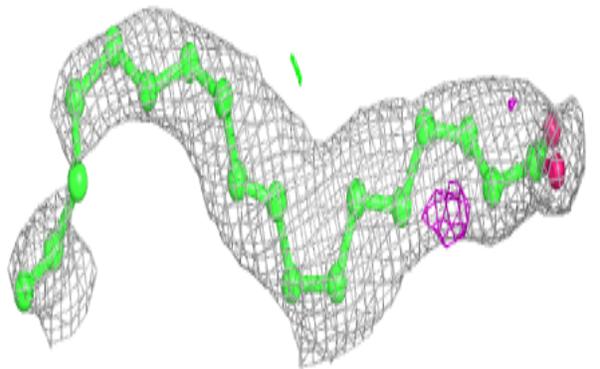
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



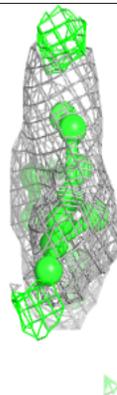
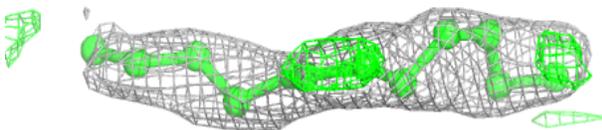
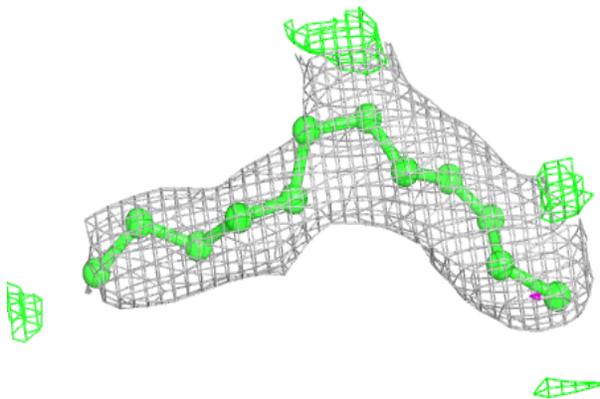


**Electron density around OLA A 2410:**

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

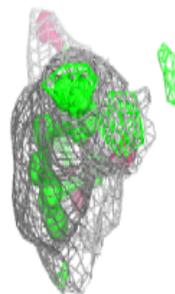
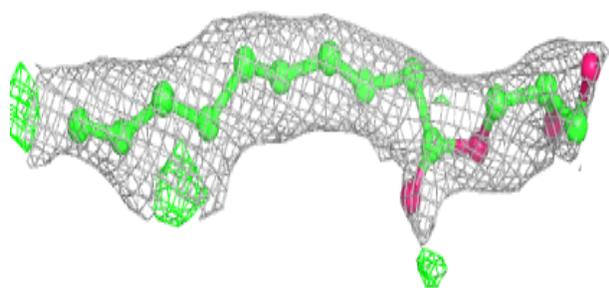
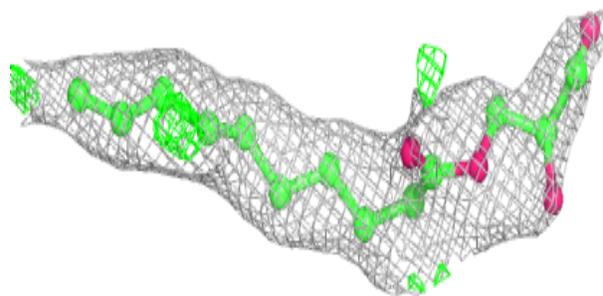
**Electron density around OLA A 2420:**

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

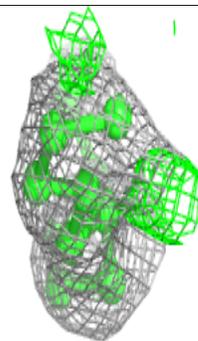
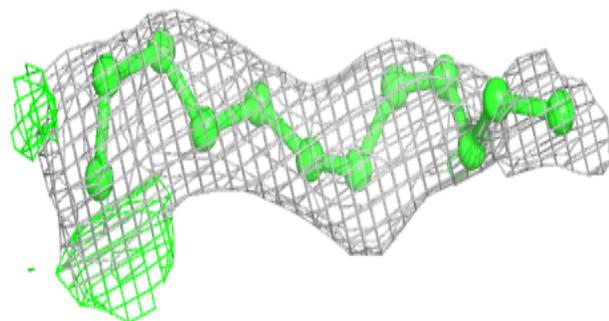
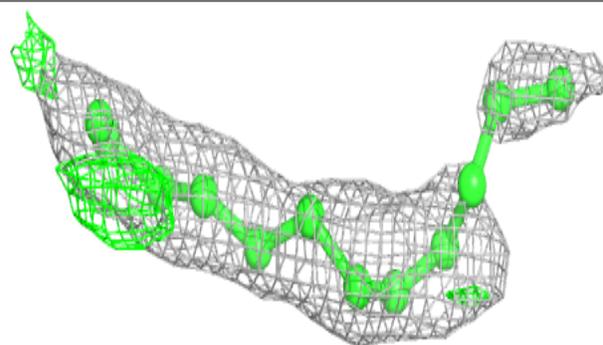


**Electron density around OLC A 2428:**

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

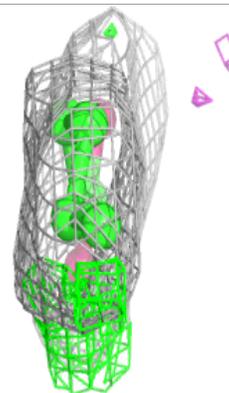
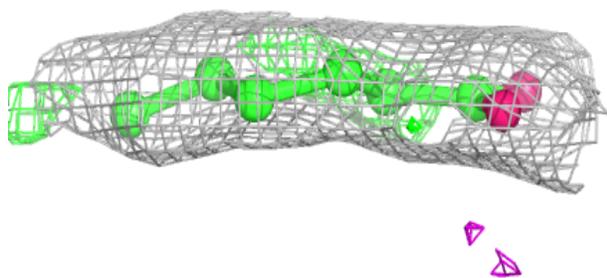
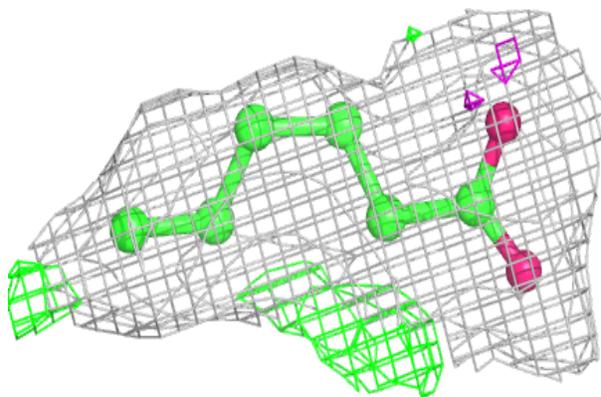
**Electron density around OLA A 2417:**

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

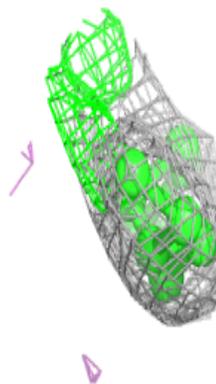
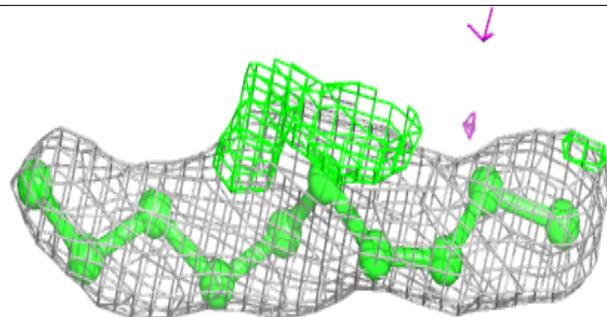
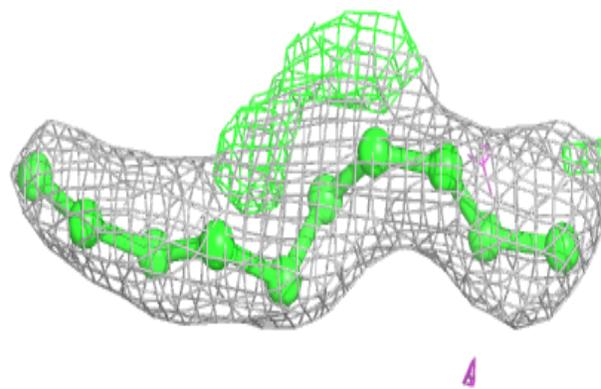


**Electron density around OLA A 2412:**

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

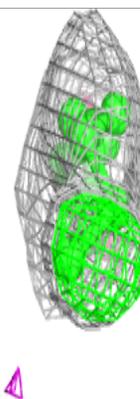
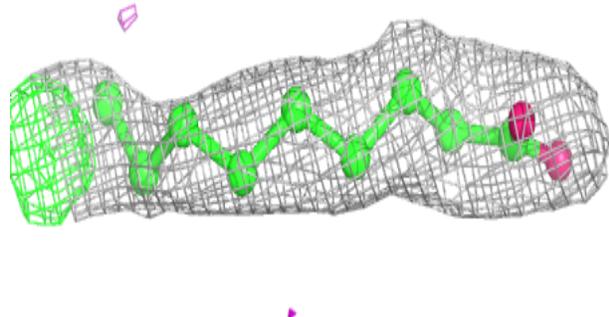
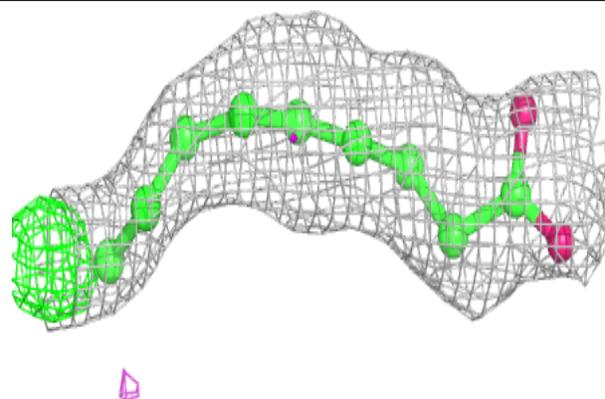
**Electron density around OLA A 2418:**

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

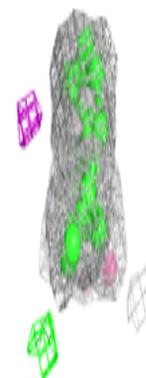
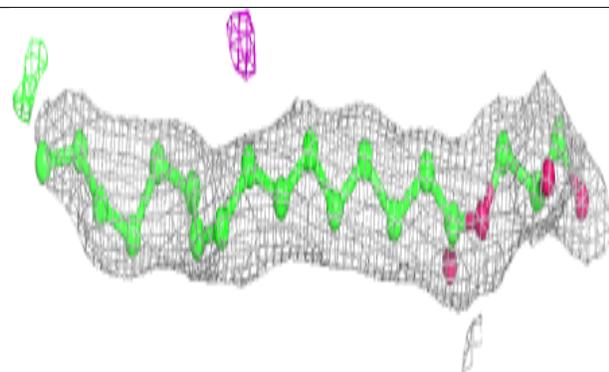
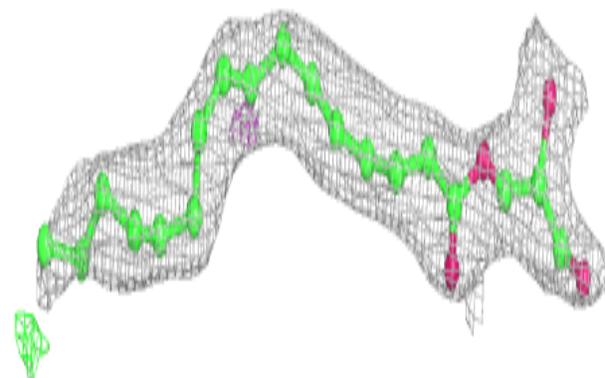


**Electron density around OLA A 2414:**

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

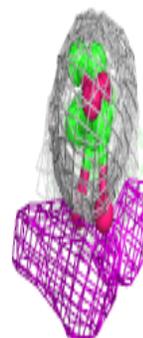
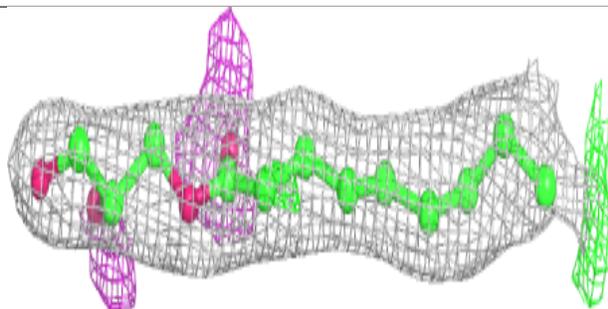
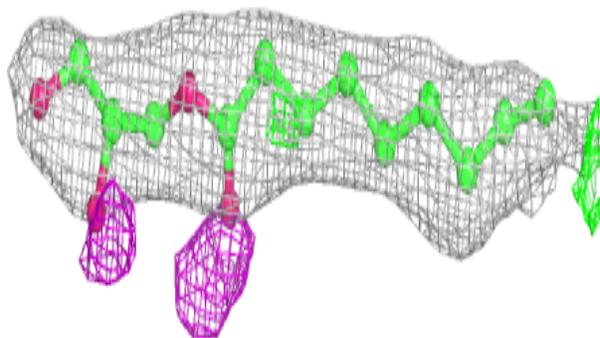
**Electron density around OLC A 2429:**

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

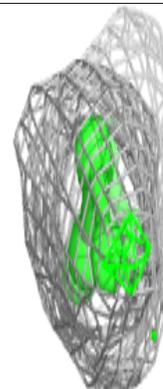
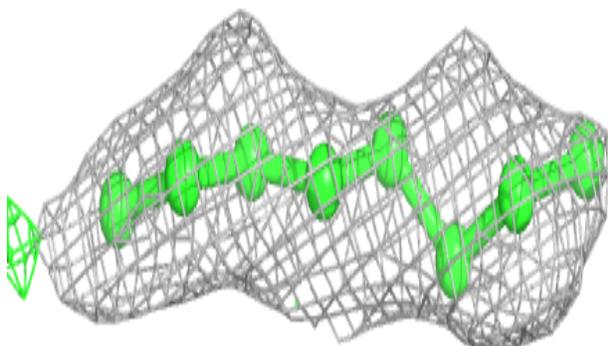
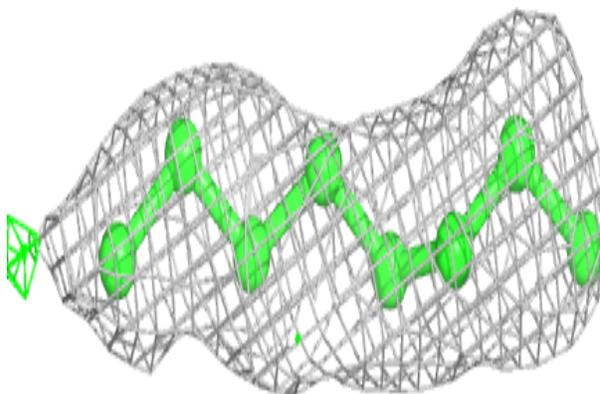


**Electron density around OLC A 2427:**

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

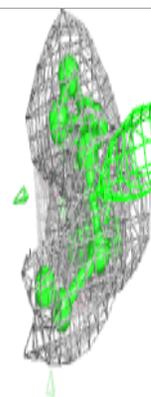
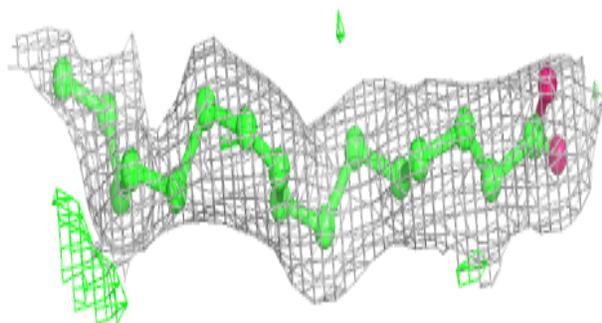
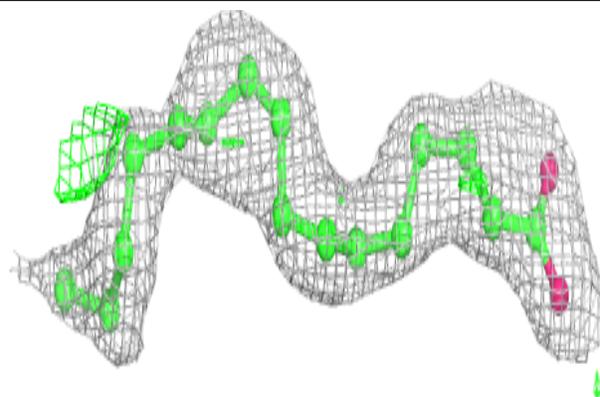
**Electron density around OLA A 2422:**

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

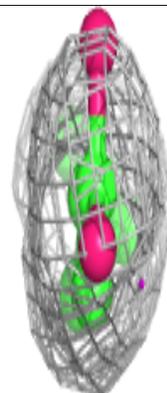
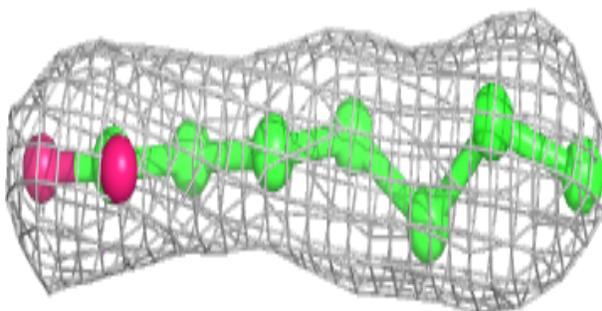
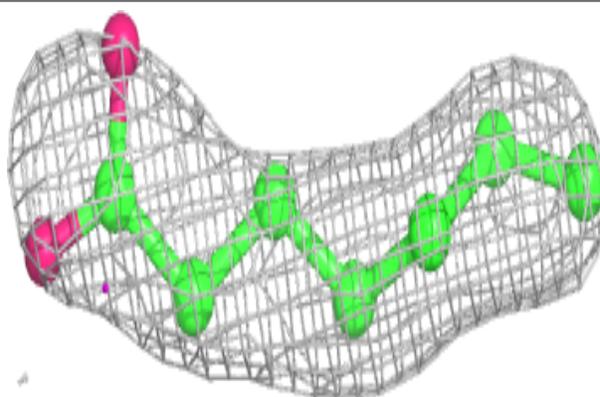


**Electron density around OLA A 2408:**

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

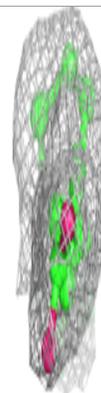
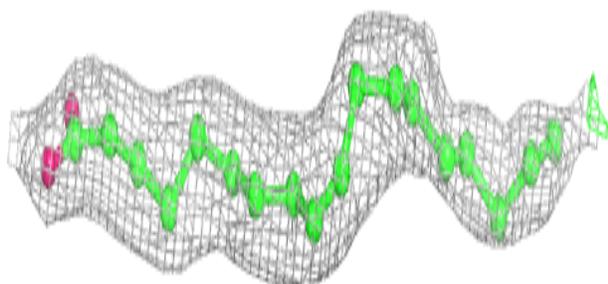
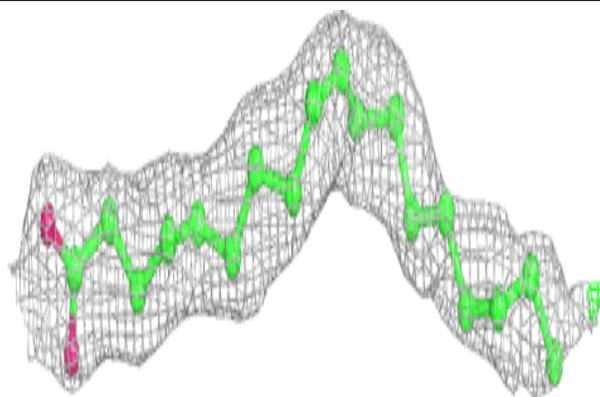
**Electron density around OLA A 2407:**

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

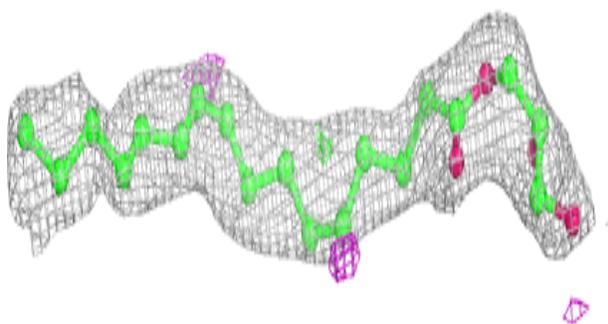
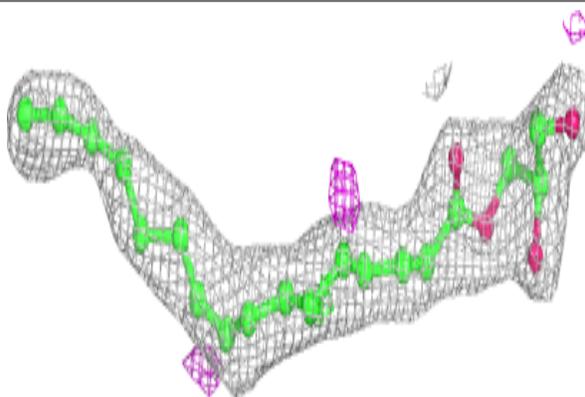


**Electron density around OLA A 2405:**

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

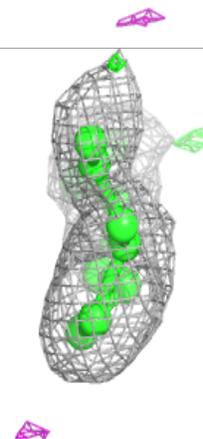
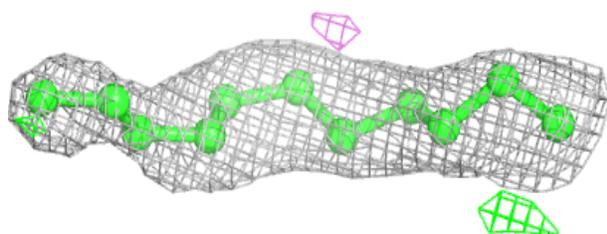
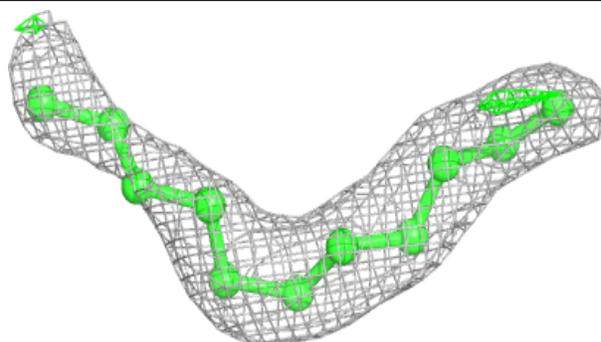
**Electron density around OLC A 2430:**

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

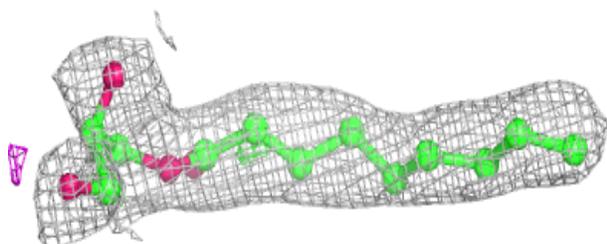
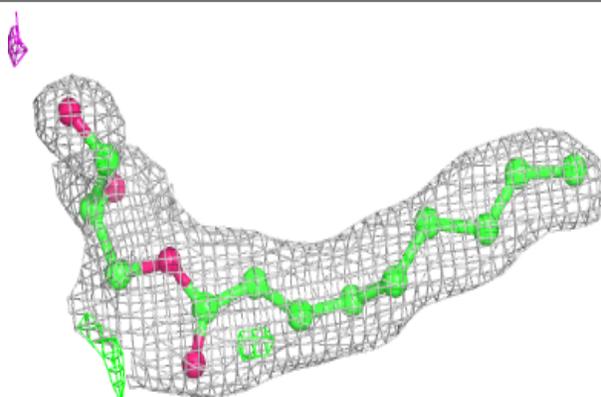


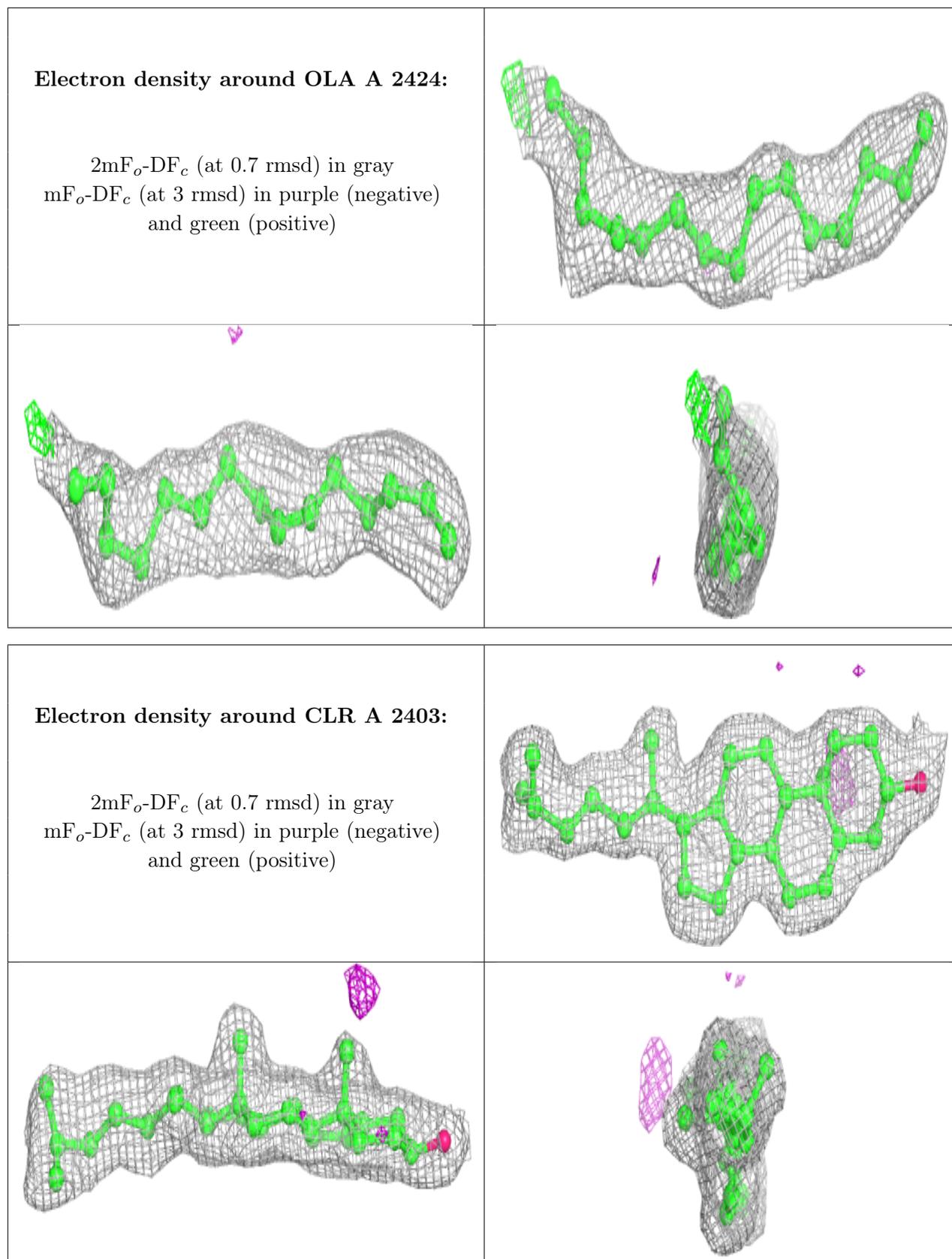
**Electron density around OLA A 2419:**

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

**Electron density around OLC A 2433:**

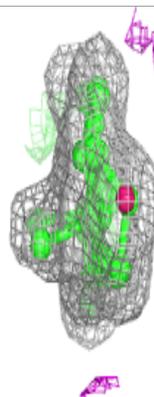
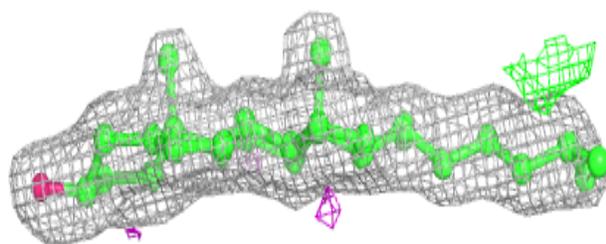
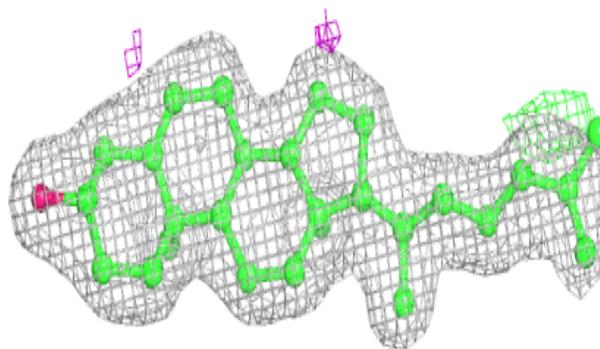
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



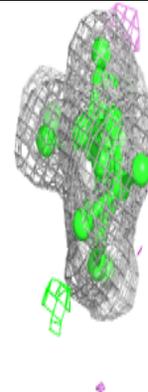
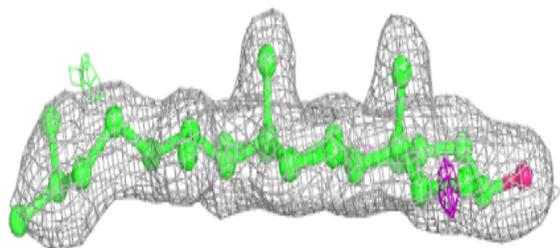
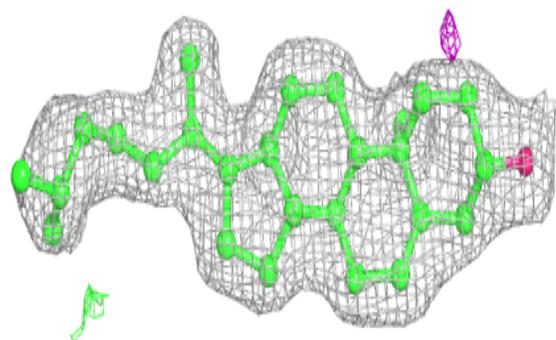


**Electron density around CLR A 2402:**

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

**Electron density around CLR A 2404:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.