



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 10:07 pm BST

PDB ID : 5T77  
Title : Crystal structure of the MOP flippase MurJ  
Authors : Kuk, A.C.Y.; Lee, S.-Y.  
Deposited on : 2016-09-02  
Resolution : 2.00 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](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.

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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 : 2.11  
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) : 2.11

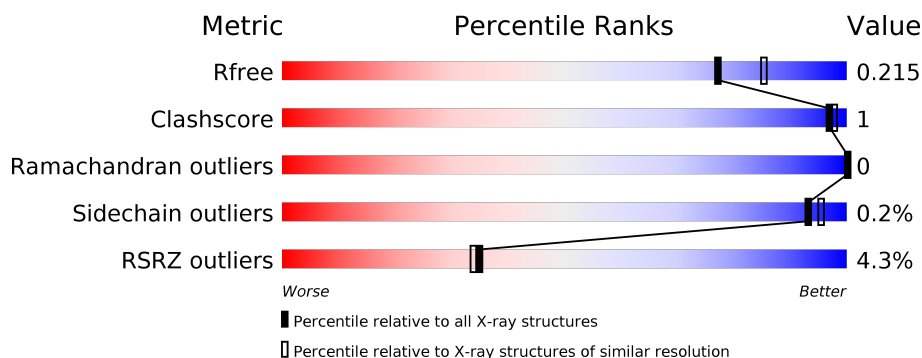
# 1 Overall quality at a glance

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 on 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	475	<div> <div>4%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8909 atoms, of which 4505 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 Putative lipid II flippase MurJ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	467	Total	C	H	N	O	S	0	2	0
			7569	2548	3826	548	639	8			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Cl	0	0
			5	5		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

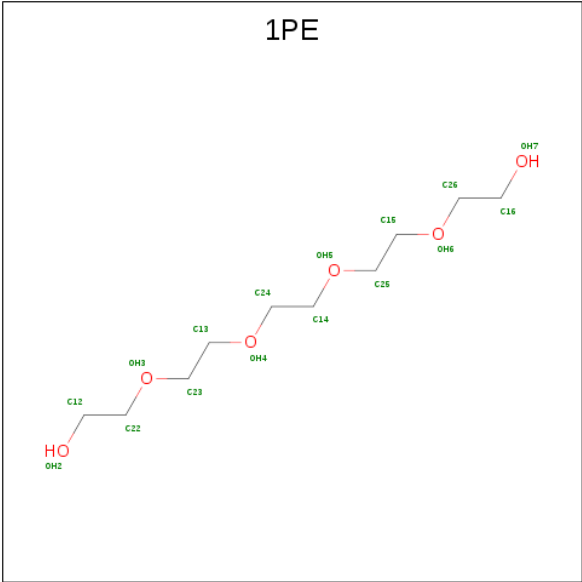
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

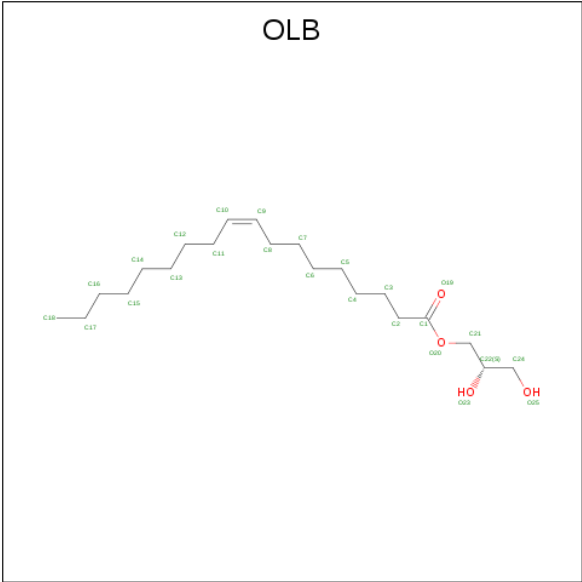
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



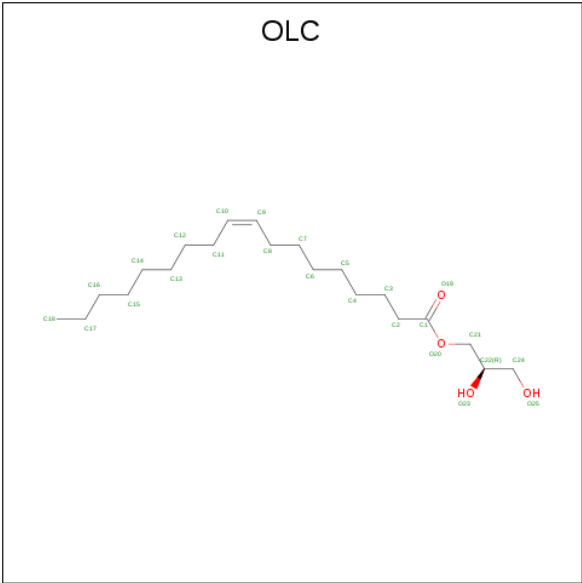
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			38	10	22	6		
6	A	1	Total	C	H	O	0	0
			38	10	22	6		
6	A	1	Total	C	H	O	0	0
			37	10	21	6		

- Molecule 7 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			28	9	15	4		
7	A	1	Total	C	H	O	0	0
			65	21	40	4		
7	A	1	Total	C	H	O	0	0
			53	18	31	4		
7	A	1	Total	C	H	O	0	0
			28	9	15	4		
7	A	1	Total	C	H	O	0	0
			29	11	16	2		
7	A	1	Total	C	H	O	0	0
			37	12	21	4		
7	A	1	Total	C	H		0	0
			30	11	19			

- Molecule 8 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
8	A	1	Total	C	H	O	0	0
			65	21	40	4		
8	A	1	Total	C	H	O	0	0
			31	10	17	4		
8	A	1	Total	C	H	O	0	0
			16	5	7	4		
8	A	1	Total	C	H	O	0	0
			37	14	20	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H 11 5 6	0	0
8	A	1	Total C H O 34 11 19 4	0	0
8	A	1	Total C H O 65 21 40 4	0	0
8	A	1	Total C H O 53 18 33 2	0	0
8	A	1	Total C H O 38 14 21 3	0	0
8	A	1	Total C H 17 7 10	0	0
8	A	1	Total C H O 27 10 14 3	0	0
8	A	1	Total C H O 55 19 32 4	0	0
8	A	1	Total C H 11 5 6	0	0
8	A	1	Total C H 17 7 10	0	0
8	A	1	Total C H 22 8 14	0	0
8	A	1	Total C H 10 4 6	0	0
8	A	1	Total C H 13 5 8	0	0
8	A	1	Total C H 13 5 8	0	0
8	A	1	Total C H 13 5 8	0	0
8	A	1	Total C H 13 5 8	0	0
8	A	1	Total C H 8 4 4	0	0
8	A	1	Total C H 8 4 4	0	0
8	A	1	Total C H O 41 14 23 4	0	0
8	A	1	Total C H 11 5 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H 11 5 6	0	0
8	A	1	Total C H 22 8 14	0	0
8	A	1	Total C H O 37 12 21 4	0	0
8	A	1	Total C H O 31 10 17 4	0	0
8	A	1	Total C H 14 6 8	0	0
8	A	1	Total C H O 15 6 6 3	0	0
8	A	1	Total C H O 25 8 13 4	0	0

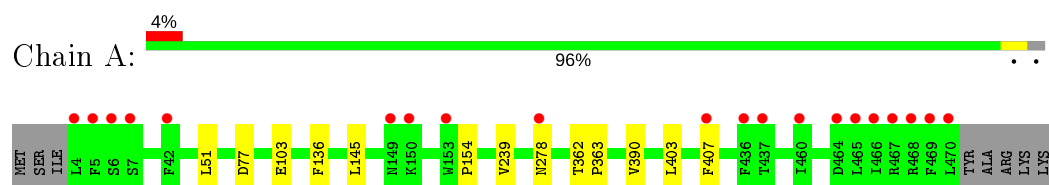
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	149	Total O 149 149	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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: Putative lipid II flippase MurJ



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.16Å 99.57Å 74.66Å 90.00° 112.91° 90.00°	Depositor
Resolution (Å)	34.19 – 2.00 34.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (34.19-2.00) 98.0 (34.19-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.189 , 0.214 0.189 , 0.215	Depositor DCC
$R_{free}$ test set	2094 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: ZN, OLC, CL, NA, CA, OLB, 1PE

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	0.27	0/3861	0.40	0/5246

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	3743	3826	3819	7	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
4	A	3	0	0	0	0
5	A	2	0	0	0	0
6	A	48	65	65	0	0
7	A	113	157	157	0	0
8	A	340	457	441	2	0
9	A	149	0	0	1	1
All	All	4404	4505	4482	8	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 1.

All (8) 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:103:GLU:OE2	8:A:524:OLC:O25	2.26	0.52
1:A:403:LEU:O	1:A:407:PHE:HD2	1.98	0.47
1:A:239:VAL:CG1	1:A:390:VAL:HG21	2.46	0.46
8:A:530:OLC:O25	8:A:530:OLC:O20	2.29	0.44
1:A:145:LEU:HD13	1:A:154:PRO:HG3	2.01	0.42
1:A:278:ASN:N	9:A:603:HOH:O	2.45	0.41
1:A:362:THR:HB	1:A:363:PRO:HD3	2.02	0.41
1:A:51:LEU:HD21	1:A:136:PHE:CE1	2.56	0.40

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)
9:A:703:HOH:O	9:A:737:HOH:O[4_9410]	2.10	0.10

## 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	467/475 (98%)	457 (98%)	10 (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	412/428 (96%)	411 (100%)	1 (0%)	93	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 53 ligands modelled in this entry, 11 are monoatomic - leaving 42 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	$\# Z  > 2$
8	OLC	A	533	4	22,22,24	0.84	1 (4%)	23,23,25	0.86	1 (4%)
7	OLB	A	518	-	12,12,24	1.10	2 (16%)	13,13,25	0.96	1 (7%)
8	OLC	A	543	-	3,3,24	0.41	0	2,2,25	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	OLC	A	524	-	8,8,24	1.08	1 (12%)	9,9,25	0.84	0
8	OLC	A	547	-	4,4,24	0.32	0	3,3,25	0.55	0
6	1PE	A	514	5	15,15,15	0.51	0	14,14,14	0.41	0
6	1PE	A	513	-	15,15,15	0.52	0	14,14,14	0.34	0
8	OLC	A	535	-	6,6,24	0.31	0	5,5,25	0.68	0
8	OLC	A	552	-	7,8,24	1.35	2 (28%)	7,9,25	1.44	1 (14%)
8	OLC	A	545	-	17,17,24	0.95	2 (11%)	18,18,25	1.04	1 (5%)
8	OLC	A	542	-	4,4,24	0.32	0	3,3,25	0.55	0
8	OLC	A	548	-	7,7,24	0.30	0	6,6,25	0.65	0
8	OLC	A	523	-	13,13,24	1.05	2 (15%)	14,14,25	1.03	1 (7%)
7	OLB	A	521	-	10,10,24	0.44	0	9,9,25	0.78	0
8	OLC	A	522	-	24,24,24	0.81	2 (8%)	25,25,25	0.95	1 (4%)
8	OLC	A	534	-	4,4,24	0.32	0	3,3,25	0.55	0
8	OLC	A	528	-	24,24,24	0.81	2 (8%)	25,25,25	0.95	1 (4%)
7	OLB	A	520	-	15,15,24	0.99	2 (13%)	16,16,25	1.03	1 (6%)
8	OLC	A	525	-	16,16,24	0.89	1 (6%)	15,16,25	0.99	1 (6%)
7	OLB	A	519	-	12,12,24	1.04	1 (8%)	12,12,25	1.16	1 (8%)
8	OLC	A	544	-	3,3,24	0.41	0	2,2,25	0.73	0
8	OLC	A	529	-	16,19,24	0.32	0	15,19,25	0.83	0
7	OLB	A	515	-	12,12,24	1.10	2 (16%)	13,13,25	1.01	1 (7%)
7	OLB	A	517	-	21,21,24	0.86	2 (9%)	22,22,25	0.92	1 (4%)
8	OLC	A	546	-	4,4,24	0.32	0	3,3,25	0.55	0
8	OLC	A	537	-	3,3,24	0.40	0	2,2,25	0.73	0
8	OLC	A	538	-	4,4,24	0.32	0	3,3,25	0.55	0
8	OLC	A	532	-	12,12,24	1.02	1 (8%)	12,12,25	1.11	1 (8%)
8	OLC	A	549	-	15,15,24	0.99	2 (13%)	16,16,25	1.03	1 (6%)
8	OLC	A	540	-	4,4,24	0.32	0	3,3,25	0.55	0
6	1PE	A	512	-	15,15,15	0.52	0	14,14,14	0.28	0
8	OLC	A	539	-	4,4,24	0.32	0	3,3,25	0.53	0
7	OLB	A	516	-	24,24,24	0.82	1 (4%)	25,25,25	0.96	1 (4%)
8	OLC	A	530	-	16,16,24	0.91	1 (6%)	16,16,25	1.03	1 (6%)
8	OLC	A	527	-	14,14,24	1.01	2 (14%)	15,15,25	1.11	1 (6%)
8	OLC	A	553	-	11,11,24	1.14	2 (18%)	12,12,25	1.01	1 (8%)
8	OLC	A	536	-	7,7,24	0.33	0	6,6,25	0.62	0
8	OLC	A	526	-	4,4,24	0.32	0	3,3,25	0.54	0
8	OLC	A	531	-	6,6,24	0.31	0	5,5,25	0.67	0
8	OLC	A	541	-	4,4,24	0.31	0	3,3,25	0.53	0
8	OLC	A	551	-	5,5,24	0.31	0	4,4,25	0.58	0
8	OLC	A	550	-	13,13,24	1.05	1 (7%)	14,14,25	0.98	1 (7%)

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
8	OLC	A	533	4	-	5/22/22/24	-
7	OLB	A	518	-	-	2/12/12/24	-
8	OLC	A	543	-	-	0/1/1/24	-
8	OLC	A	524	-	-	3/7/7/24	-
8	OLC	A	547	-	-	0/2/2/24	-
6	1PE	A	514	5	-	6/13/13/13	-
6	1PE	A	513	-	-	5/13/13/13	-
8	OLC	A	535	-	-	2/4/4/24	-
8	OLC	A	552	-	-	0/7/7/24	-
8	OLC	A	545	-	-	4/17/17/24	-
8	OLC	A	542	-	-	0/2/2/24	-
8	OLC	A	548	-	-	3/5/5/24	-
8	OLC	A	523	-	-	4/13/13/24	-
7	OLB	A	521	-	-	4/8/8/24	-
8	OLC	A	522	-	-	8/24/24/24	-
8	OLC	A	534	-	-	0/2/2/24	-
8	OLC	A	528	-	-	10/24/24/24	-
7	OLB	A	520	-	-	3/15/15/24	-
8	OLC	A	525	-	-	4/15/15/24	-
7	OLB	A	519	-	-	1/11/11/24	-
8	OLC	A	544	-	-	0/1/1/24	-
8	OLC	A	529	-	-	6/15/17/24	-
7	OLB	A	515	-	-	5/12/12/24	-
7	OLB	A	517	-	-	7/21/21/24	-
8	OLC	A	546	-	-	0/2/2/24	-
8	OLC	A	537	-	-	0/1/1/24	-
8	OLC	A	538	-	-	0/2/2/24	-
8	OLC	A	532	-	-	1/11/11/24	-
8	OLC	A	549	-	-	4/15/15/24	-
8	OLC	A	540	-	-	0/2/2/24	-
6	1PE	A	512	-	-	3/13/13/13	-
8	OLC	A	539	-	-	1/2/2/24	-
7	OLB	A	516	-	-	13/24/24/24	-
8	OLC	A	530	-	-	4/15/15/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	527	-	-	4/14/14/24	-
8	OLC	A	553	-	-	4/11/11/24	-
8	OLC	A	536	-	-	3/5/5/24	-
8	OLC	A	526	-	-	0/2/2/24	-
8	OLC	A	531	-	-	1/4/4/24	-
8	OLC	A	541	-	-	1/2/2/24	-
8	OLC	A	551	-	-	0/3/3/24	-
8	OLC	A	550	-	-	4/13/13/24	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	533	OLC	O20-C1	2.54	1.40	1.33
8	A	550	OLC	O20-C1	2.54	1.40	1.33
7	A	516	OLB	O20-C1	2.52	1.40	1.33
8	A	530	OLC	O20-C1	2.51	1.40	1.33
8	A	553	OLC	O20-C1	2.48	1.40	1.33
7	A	520	OLB	O20-C1	2.45	1.40	1.33
8	A	532	OLC	O20-C1	2.44	1.40	1.33
8	A	549	OLC	O20-C1	2.44	1.40	1.33
8	A	552	OLC	O20-C1	2.43	1.40	1.33
8	A	528	OLC	O20-C1	2.42	1.40	1.33
7	A	517	OLB	O20-C1	2.42	1.40	1.33
7	A	518	OLB	O20-C1	2.42	1.40	1.33
7	A	519	OLB	O20-C1	2.41	1.40	1.33
8	A	545	OLC	O20-C1	2.41	1.40	1.33
8	A	527	OLC	O20-C1	2.40	1.40	1.33
8	A	522	OLC	O20-C1	2.39	1.40	1.33
8	A	523	OLC	O20-C1	2.39	1.40	1.33
7	A	515	OLB	O20-C1	2.39	1.40	1.33
8	A	525	OLC	O20-C1	2.36	1.40	1.33
7	A	515	OLB	O20-C21	-2.16	1.40	1.45
8	A	545	OLC	O20-C21	-2.11	1.40	1.45
8	A	523	OLC	O20-C21	-2.10	1.40	1.45
8	A	552	OLC	O20-C21	-2.10	1.40	1.45
7	A	517	OLB	O20-C21	-2.10	1.40	1.45
8	A	522	OLC	O20-C21	-2.09	1.40	1.45
8	A	524	OLC	O20-C21	-2.09	1.40	1.45
7	A	518	OLB	O20-C21	-2.08	1.40	1.45
8	A	549	OLC	O20-C21	-2.07	1.40	1.45
8	A	528	OLC	O20-C21	-2.06	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	520	OLB	O20-C21	-2.06	1.40	1.45
8	A	527	OLC	O20-C21	-2.06	1.40	1.45
8	A	553	OLC	O20-C21	-2.03	1.40	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	552	OLC	O20-C1-C2	3.24	119.87	111.38
7	A	516	OLB	O20-C1-C2	2.85	120.85	111.91
8	A	527	OLC	O20-C1-C2	2.71	120.41	111.91
7	A	520	OLB	O20-C1-C2	2.66	120.27	111.91
8	A	550	OLC	O20-C1-C2	2.61	120.09	111.91
7	A	519	OLB	O20-C1-C2	2.60	120.07	111.91
8	A	522	OLC	O20-C1-C2	2.59	120.02	111.91
8	A	528	OLC	O20-C1-C2	2.59	120.02	111.91
8	A	523	OLC	O20-C1-C2	2.58	120.00	111.91
7	A	517	OLB	O20-C1-C2	2.57	119.97	111.91
8	A	532	OLC	O20-C1-C2	2.57	119.97	111.91
8	A	553	OLC	O20-C1-C2	2.52	119.81	111.91
8	A	549	OLC	O20-C1-C2	2.48	119.69	111.91
8	A	545	OLC	O20-C1-C2	2.47	119.65	111.91
7	A	518	OLB	O20-C1-C2	2.43	119.53	111.91
7	A	515	OLB	O20-C1-C2	2.40	119.42	111.91
8	A	533	OLC	O20-C1-C2	2.28	119.06	111.91
8	A	530	OLC	O20-C1-C2	2.22	118.86	111.91
8	A	525	OLC	O20-C1-C2	2.18	118.75	111.91

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	533	OLC	C21-C22-C24-O25
8	A	528	OLC	C21-C22-C24-O25
7	A	520	OLB	O20-C21-C22-O23
7	A	517	OLB	C21-C22-C24-O25
8	A	530	OLC	O20-C21-C22-C24
6	A	514	1PE	OH4-C13-C23-OH3
6	A	514	1PE	OH6-C15-C25-OH5
7	A	520	OLB	O20-C21-C22-C24
8	A	522	OLC	O20-C21-C22-C24
8	A	527	OLC	O20-C21-C22-C24
8	A	522	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
6	A	512	1PE	OH5-C14-C24-OH4
8	A	530	OLC	C1-C2-C3-C4
8	A	527	OLC	O23-C22-C24-O25
7	A	516	OLB	C1-C2-C3-C4
8	A	523	OLC	O20-C21-C22-O23
8	A	527	OLC	O20-C21-C22-O23
6	A	513	1PE	OH4-C13-C23-OH3
7	A	521	OLB	C12-C13-C14-C15
7	A	516	OLB	C5-C6-C7-C8
8	A	523	OLC	O20-C21-C22-C24
8	A	528	OLC	C2-C3-C4-C5
8	A	529	OLC	C14-C15-C16-C17
8	A	524	OLC	C21-C22-C24-O25
7	A	515	OLB	C21-C22-C24-O25
8	A	549	OLC	C21-C22-C24-O25
7	A	516	OLB	C21-C22-C24-O25
8	A	527	OLC	C21-C22-C24-O25
8	A	525	OLC	C5-C6-C7-C8
7	A	516	OLB	C11-C12-C13-C14
7	A	516	OLB	C12-C13-C14-C15
6	A	513	1PE	OH2-C12-C22-OH3
8	A	549	OLC	C5-C6-C7-C8
7	A	520	OLB	C2-C3-C4-C5
8	A	533	OLC	O23-C22-C24-O25
7	A	517	OLB	O23-C22-C24-O25
8	A	528	OLC	C14-C15-C16-C17
8	A	533	OLC	C2-C3-C4-C5
8	A	529	OLC	C6-C7-C8-C9
7	A	518	OLB	C1-C2-C3-C4
8	A	536	OLC	C2-C3-C4-C5
6	A	513	1PE	OH6-C15-C25-OH5
8	A	548	OLC	C2-C3-C4-C5
8	A	536	OLC	C3-C4-C5-C6
8	A	529	OLC	C11-C12-C13-C14
6	A	513	1PE	C12-C22-OH3-C23
8	A	530	OLC	C2-C3-C4-C5
8	A	524	OLC	O23-C22-C24-O25
8	A	522	OLC	C5-C6-C7-C8
7	A	521	OLB	C13-C14-C15-C16
8	A	550	OLC	O20-C21-C22-O23
8	A	525	OLC	C3-C4-C5-C6
8	A	533	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	A	550	OLC	O20-C21-C22-C24
8	A	533	OLC	C11-C12-C13-C14
8	A	528	OLC	O23-C22-C24-O25
8	A	528	OLC	C11-C12-C13-C14
8	A	545	OLC	C3-C4-C5-C6
8	A	525	OLC	C9-C10-C11-C12
7	A	516	OLB	C14-C15-C16-C17
7	A	518	OLB	C2-C3-C4-C5
6	A	514	1PE	C13-C23-OH3-C22
8	A	531	OLC	C2-C3-C4-C5
8	A	548	OLC	C3-C4-C5-C6
6	A	512	1PE	C23-C13-OH4-C24
7	A	515	OLB	O20-C21-C22-O23
8	A	524	OLC	O20-C21-C22-C24
8	A	522	OLC	C11-C12-C13-C14
8	A	535	OLC	C3-C4-C5-C6
6	A	512	1PE	C24-C14-OH5-C25
7	A	515	OLB	O20-C21-C22-C24
8	A	525	OLC	C7-C8-C9-C10
6	A	514	1PE	C25-C15-OH6-C26
8	A	541	OLC	C2-C3-C4-C5
7	A	515	OLB	O23-C22-C24-O25
6	A	514	1PE	OH5-C14-C24-OH4
7	A	516	OLB	C2-C3-C4-C5
7	A	516	OLB	C6-C7-C8-C9
7	A	517	OLB	O20-C1-C2-C3
8	A	545	OLC	C7-C8-C9-C10
8	A	530	OLC	C7-C8-C9-C10
7	A	519	OLB	C5-C6-C7-C8
8	A	553	OLC	O20-C21-C22-C24
8	A	528	OLC	C9-C10-C11-C12
8	A	539	OLC	C1-C2-C3-C4
7	A	521	OLB	C10-C11-C12-C13
8	A	522	OLC	C1-C2-C3-C4
8	A	523	OLC	C3-C4-C5-C6
8	A	528	OLC	C7-C8-C9-C10
8	A	545	OLC	C21-C22-C24-O25
7	A	517	OLB	C9-C10-C11-C12
8	A	532	OLC	O20-C21-C22-O23
8	A	529	OLC	C2-C3-C4-C5
8	A	549	OLC	O23-C22-C24-O25
7	A	515	OLB	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
8	A	529	OLC	C9-C10-C11-C12
7	A	516	OLB	O20-C1-C2-C3
7	A	521	OLB	C9-C10-C11-C12
8	A	522	OLC	C9-C10-C11-C12
8	A	522	OLC	C6-C7-C8-C9
8	A	553	OLC	O20-C1-C2-C3
8	A	550	OLC	O20-C1-C2-C3
8	A	523	OLC	C4-C5-C6-C7
8	A	549	OLC	C4-C5-C6-C7
7	A	516	OLB	C9-C10-C11-C12
7	A	516	OLB	O23-C22-C24-O25
8	A	553	OLC	O20-C21-C22-O23
8	A	536	OLC	C4-C5-C6-C7
7	A	516	OLB	C7-C8-C9-C10
8	A	528	OLC	O20-C21-C22-C24
7	A	517	OLB	C11-C12-C13-C14
6	A	513	1PE	OH5-C14-C24-OH4
7	A	516	OLB	O19-C1-C2-C3
7	A	517	OLB	C7-C8-C9-C10
8	A	528	OLC	C15-C16-C17-C18
8	A	522	OLC	C21-C22-C24-O25
6	A	514	1PE	OH2-C12-C22-OH3
7	A	517	OLB	C10-C11-C12-C13
8	A	529	OLC	C5-C6-C7-C8
8	A	553	OLC	O19-C1-C2-C3
8	A	550	OLC	O19-C1-C2-C3
8	A	545	OLC	O23-C22-C24-O25
8	A	528	OLC	O20-C1-C2-C3
8	A	548	OLC	C4-C5-C6-C7
8	A	535	OLC	C1-C2-C3-C4

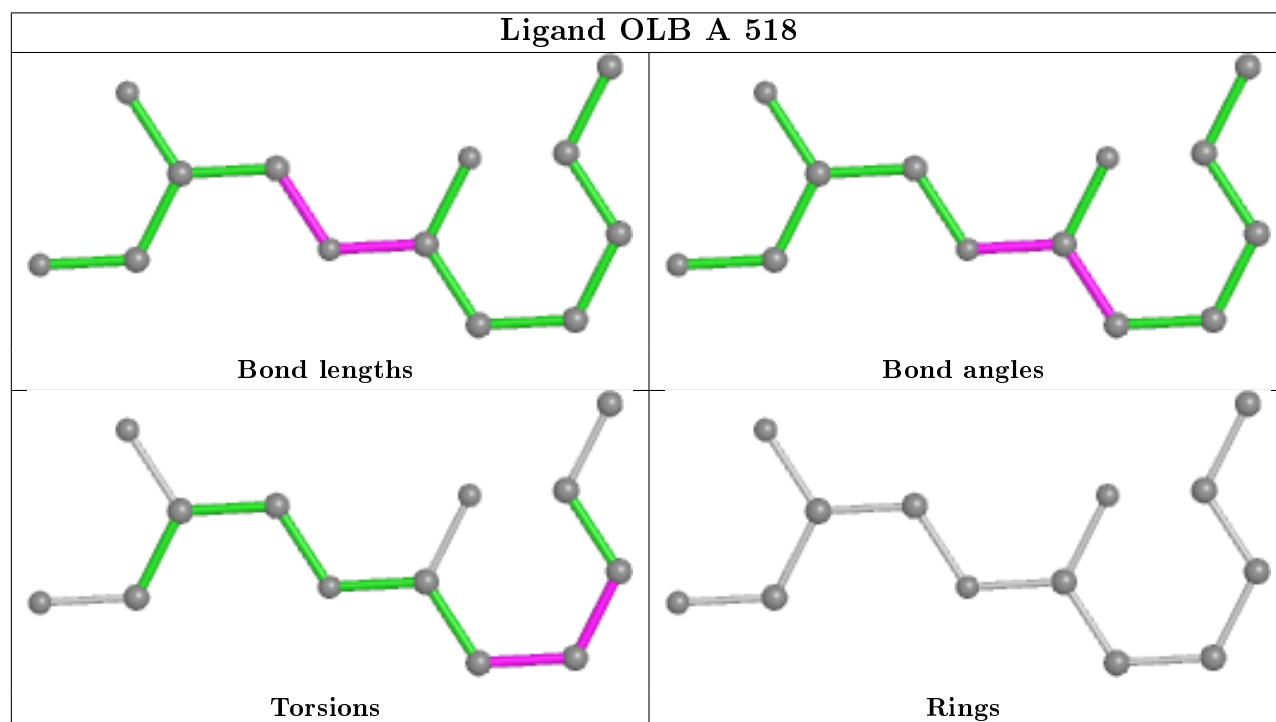
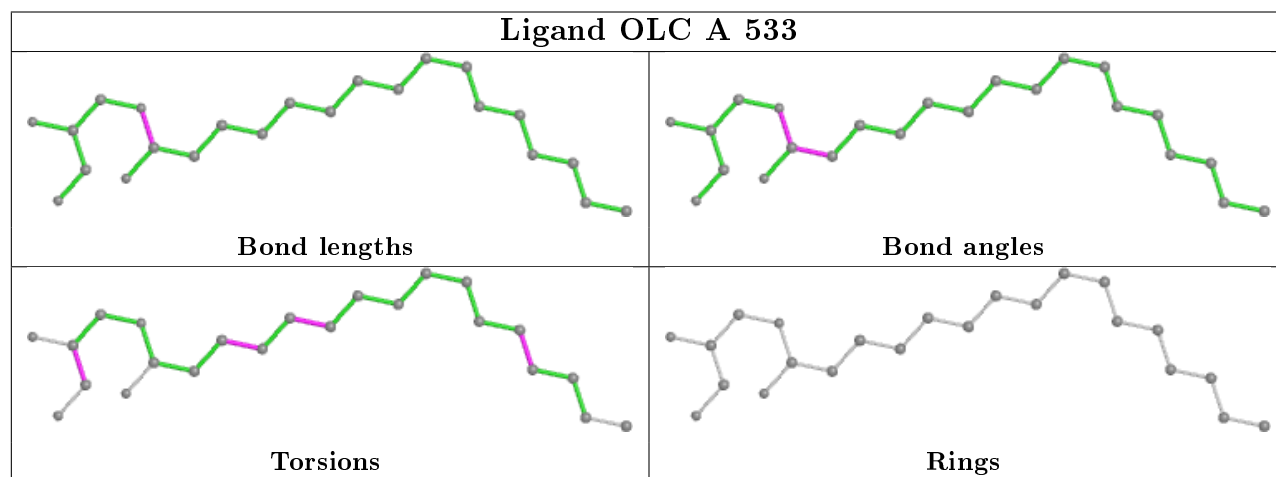
There are no ring outliers.

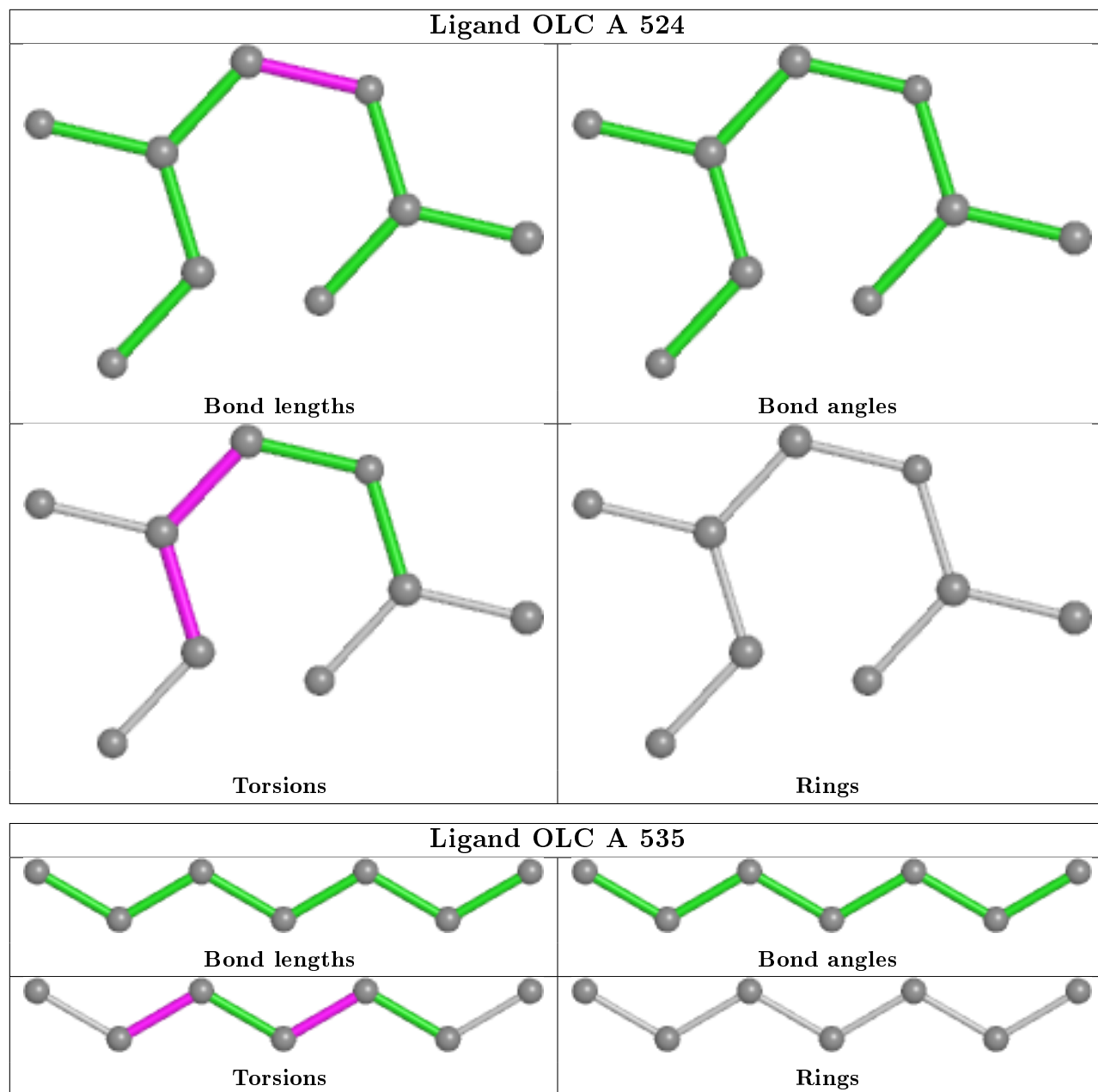
2 monomers are involved in 2 short contacts:

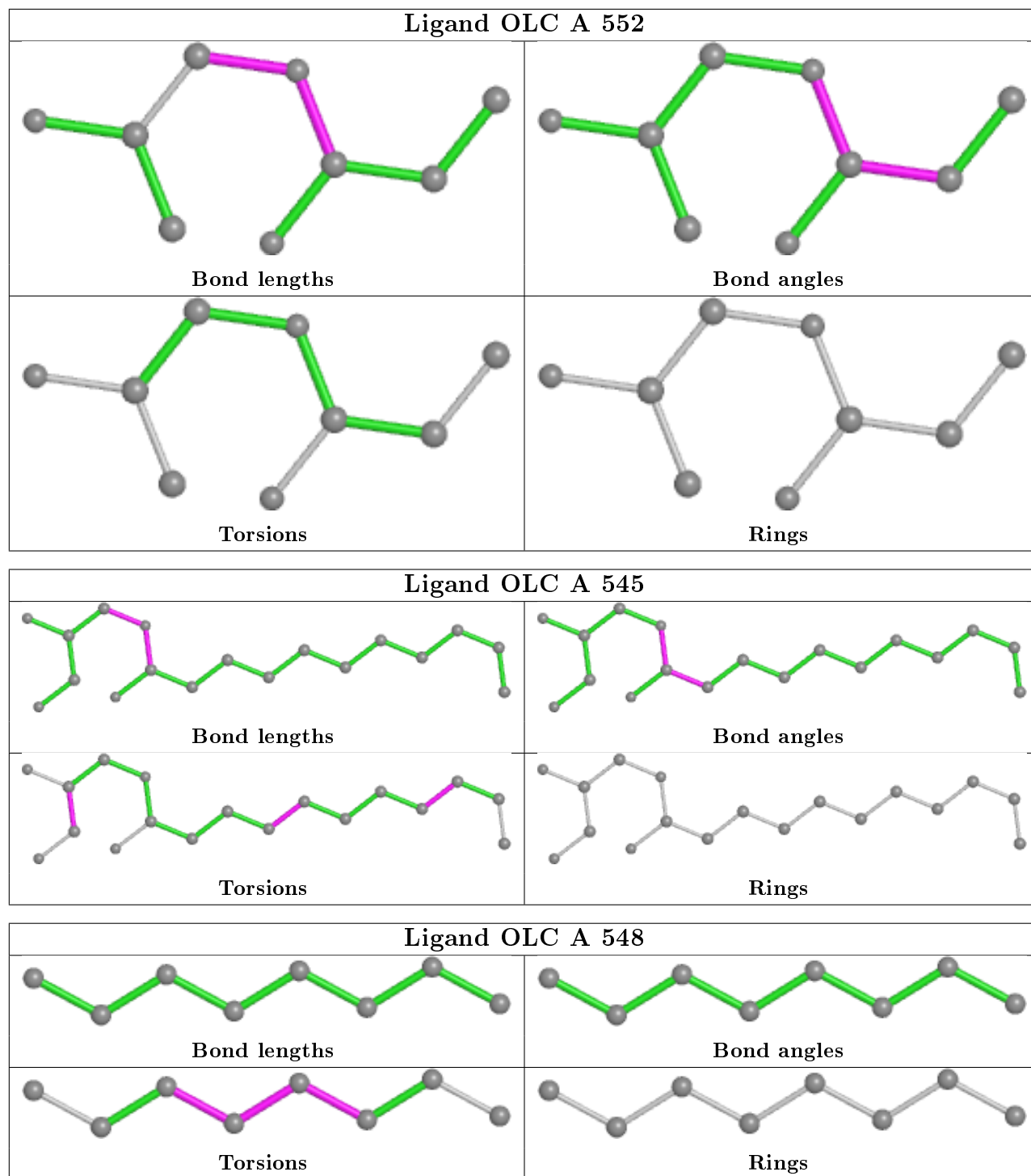
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	524	OLC	1	0
8	A	530	OLC	1	0

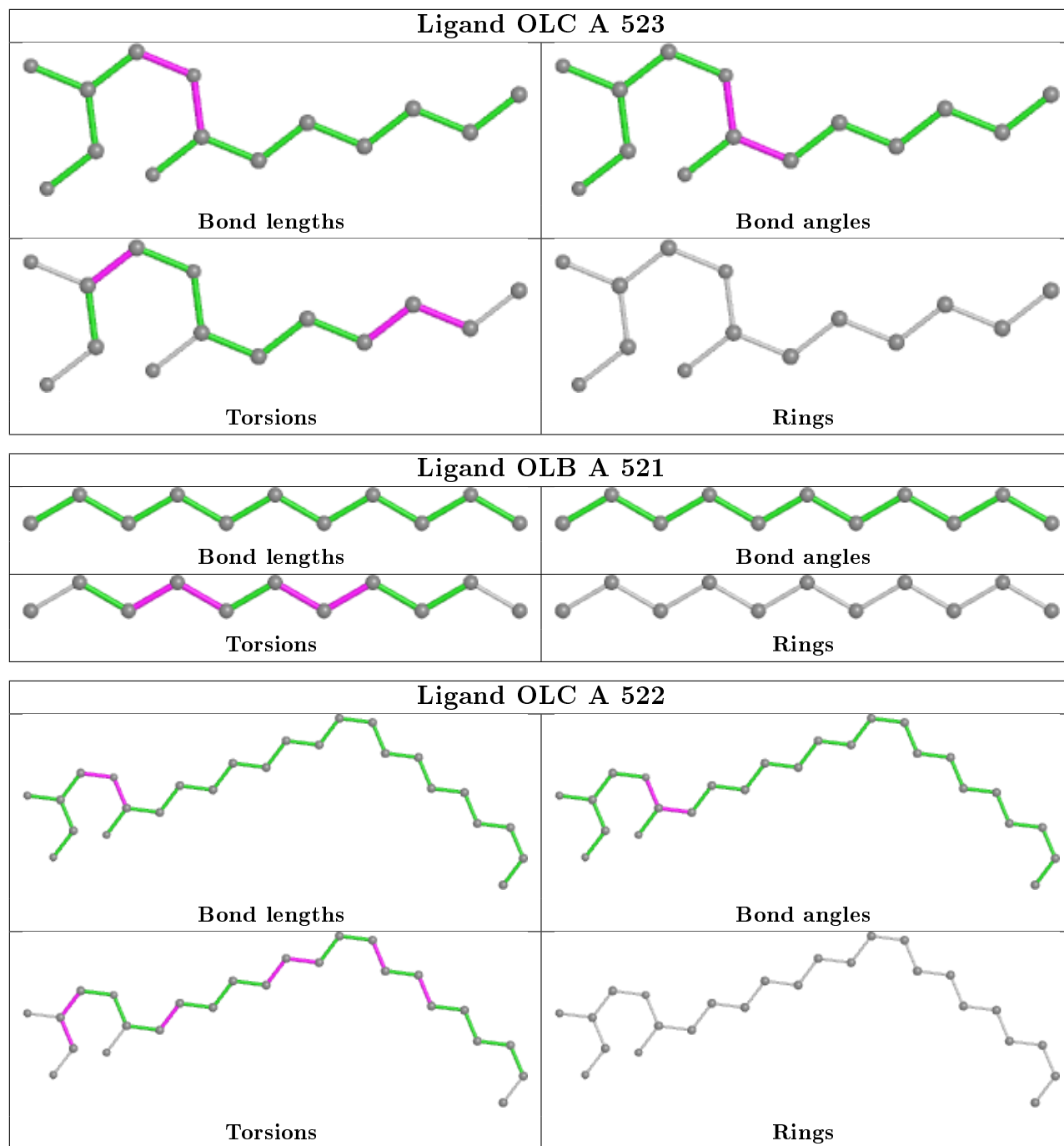
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

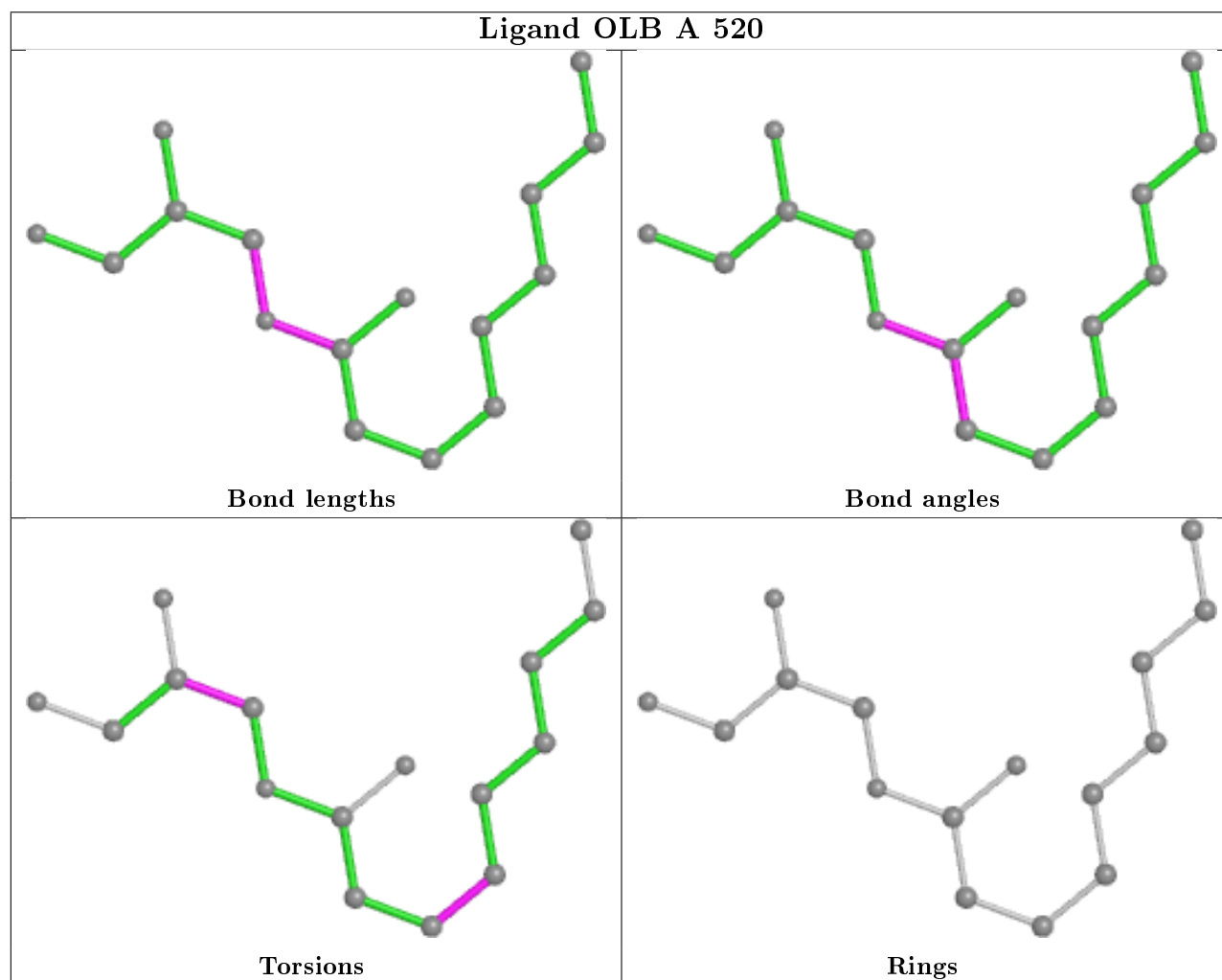
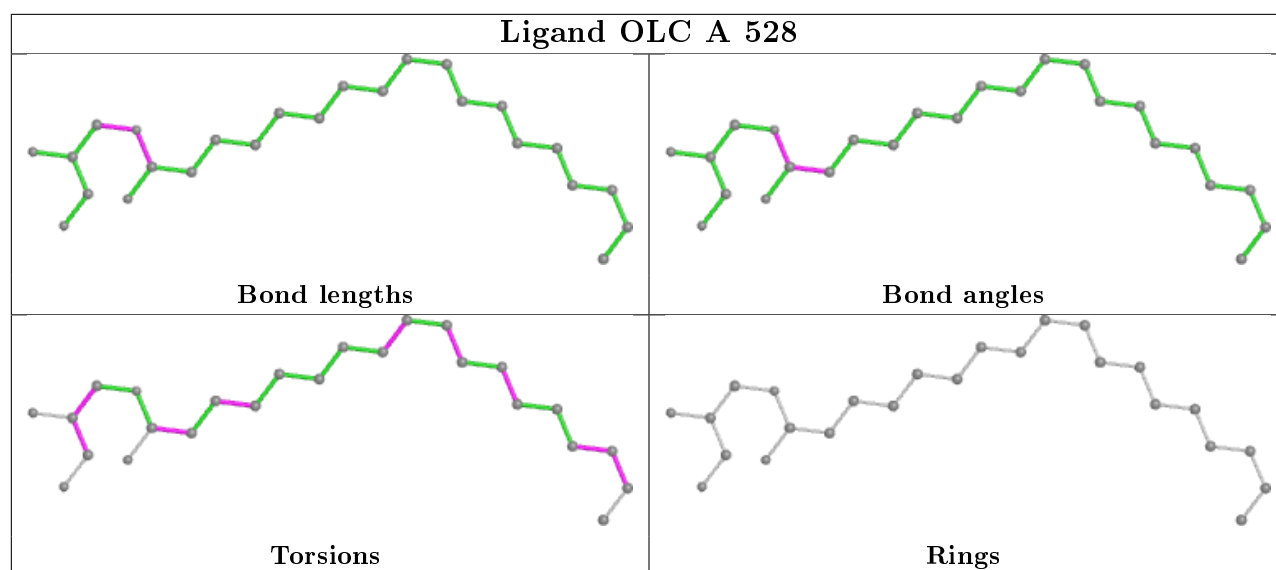
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

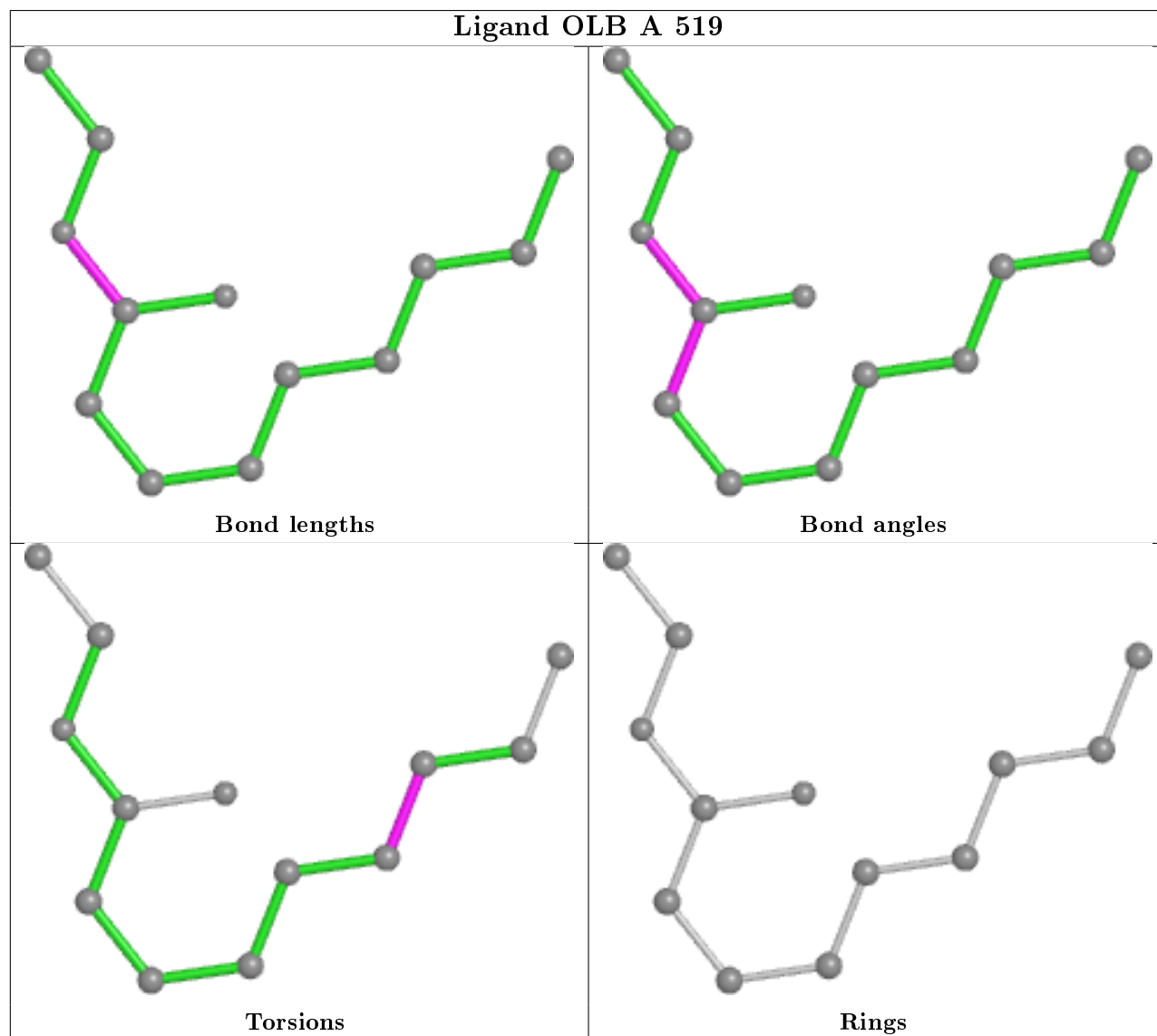
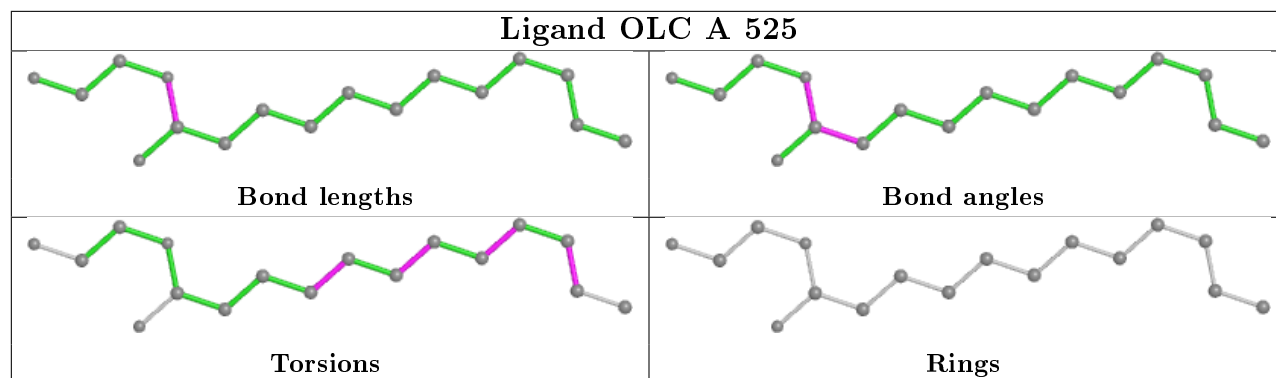


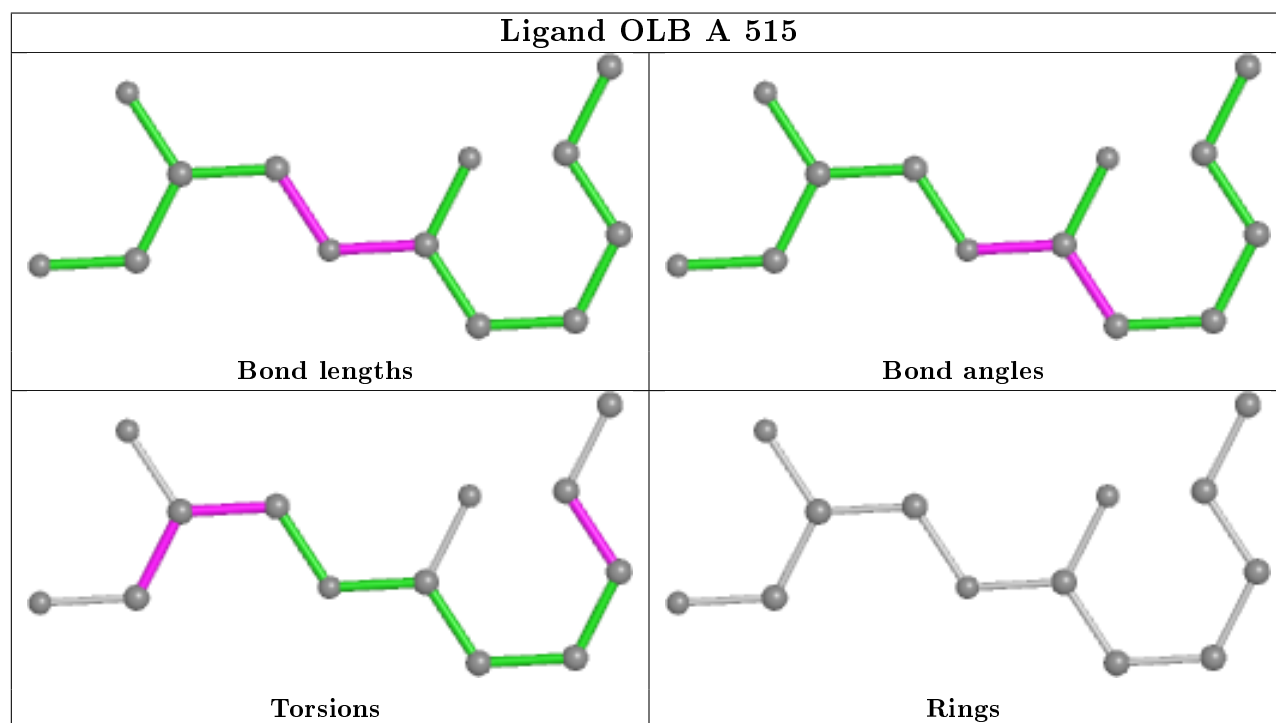
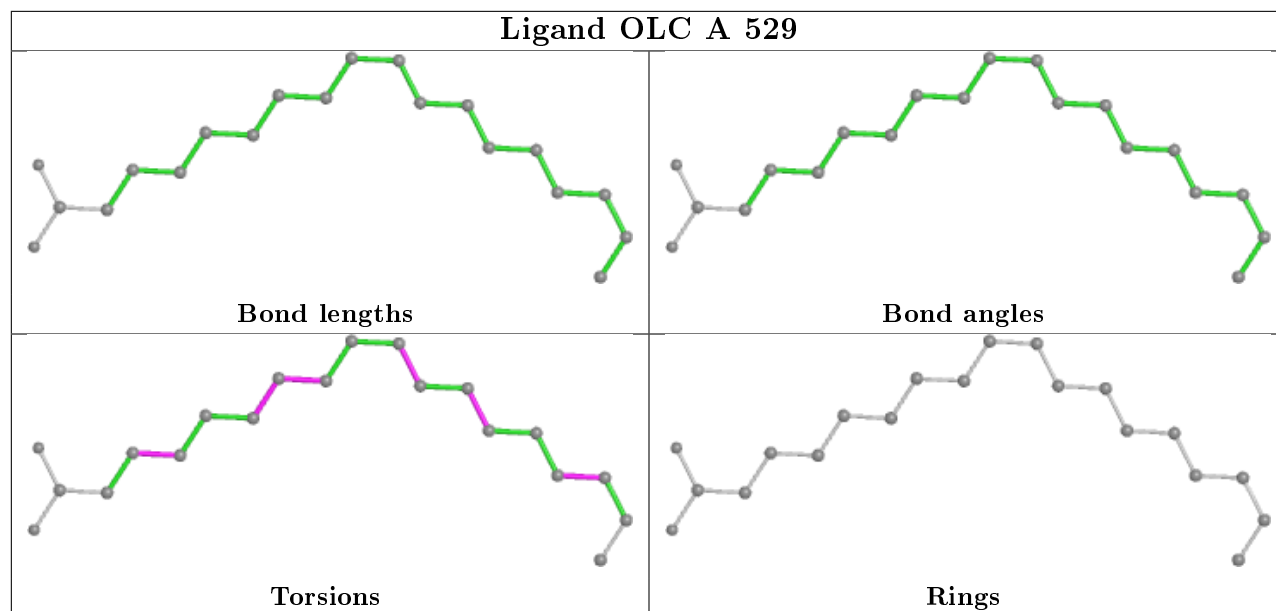


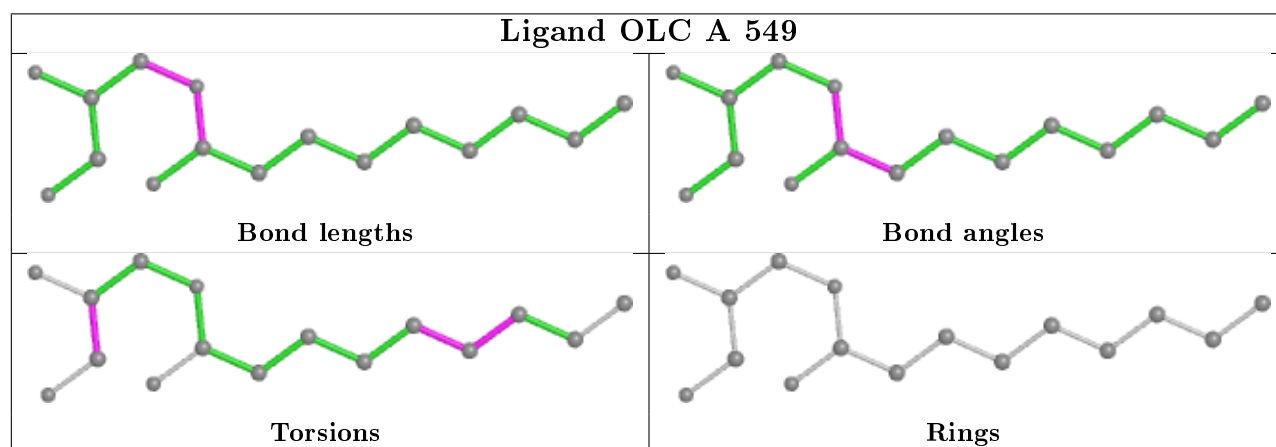
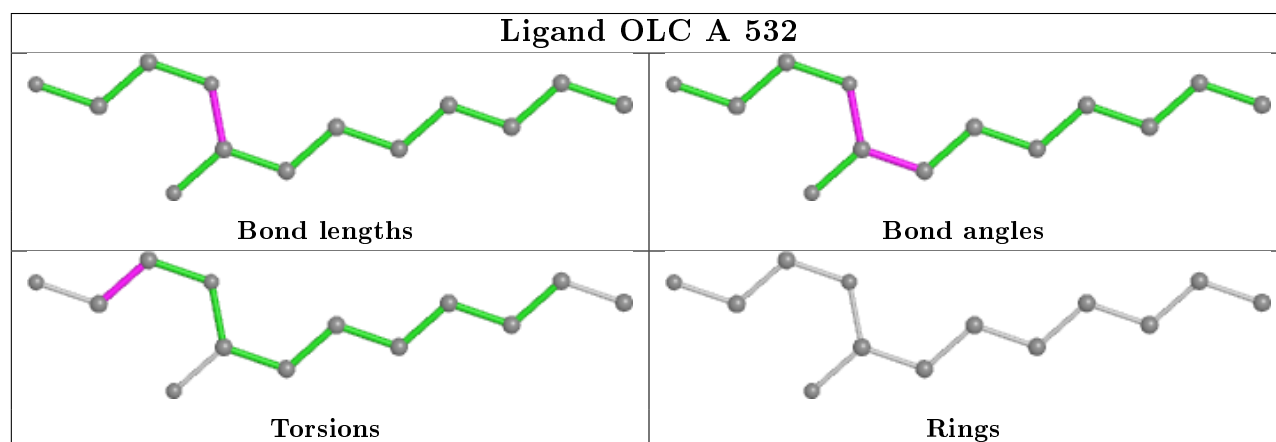
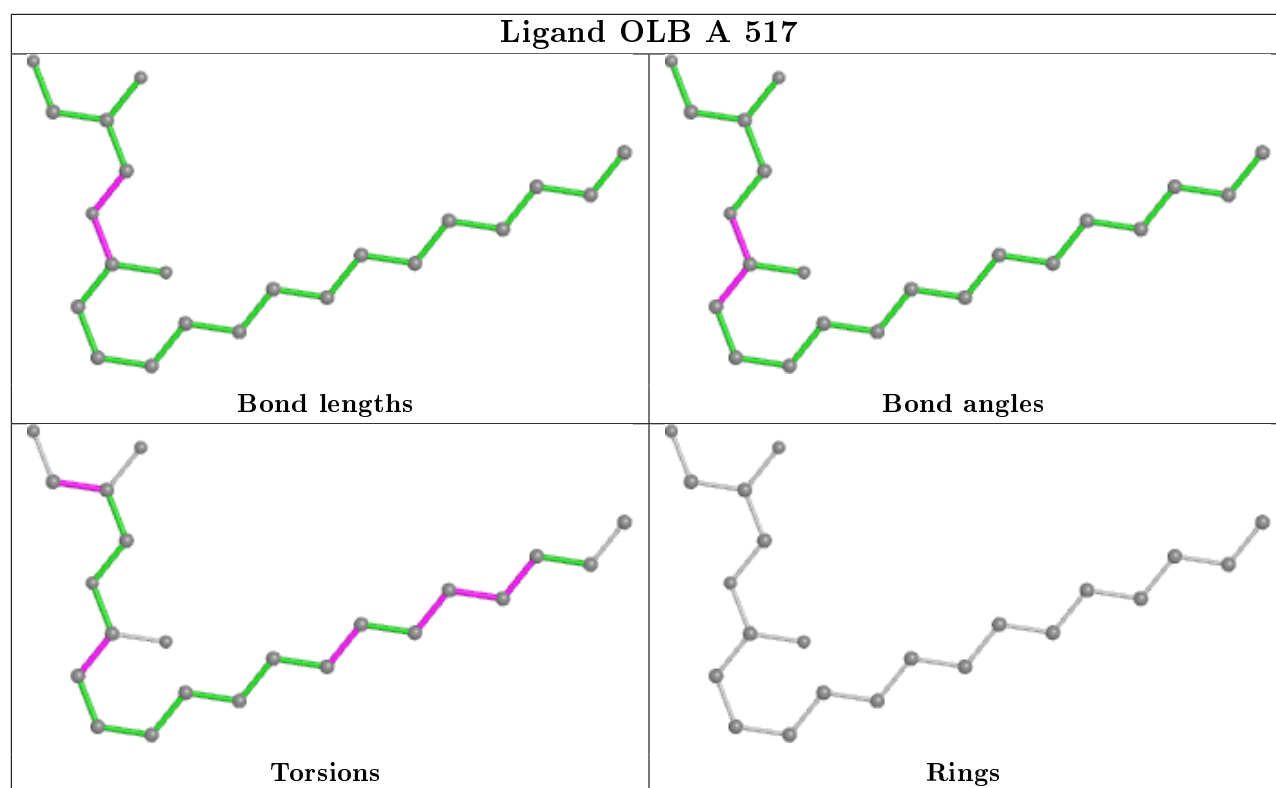


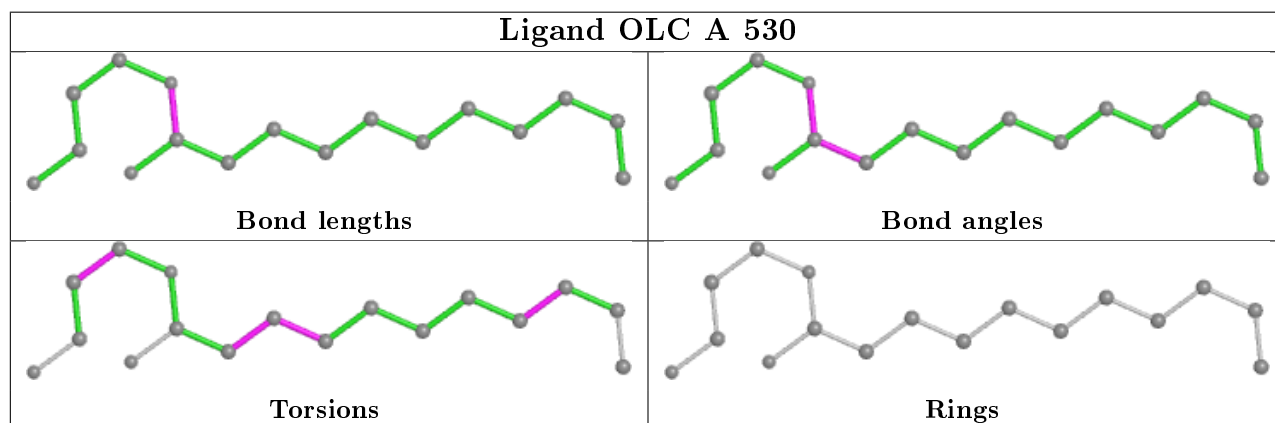
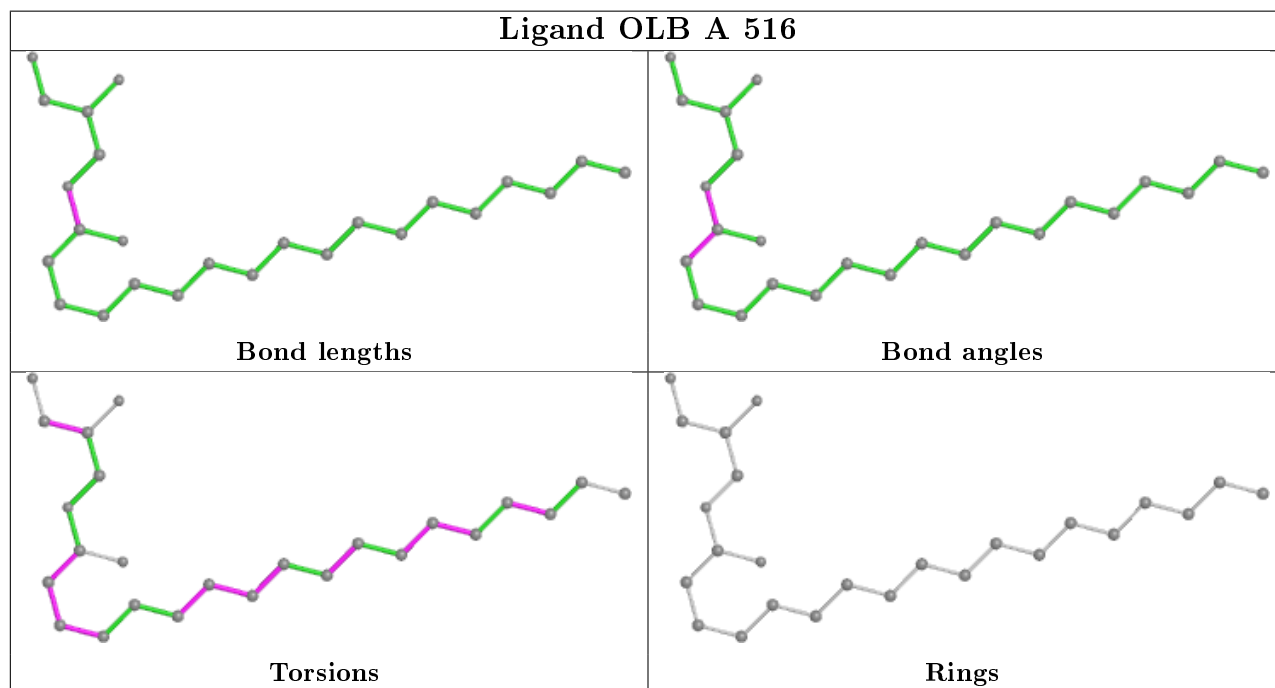
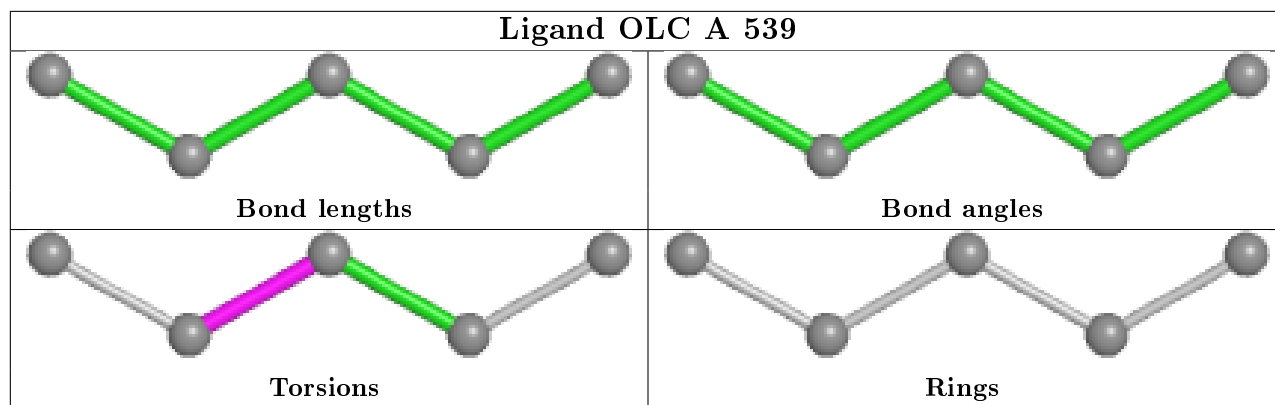


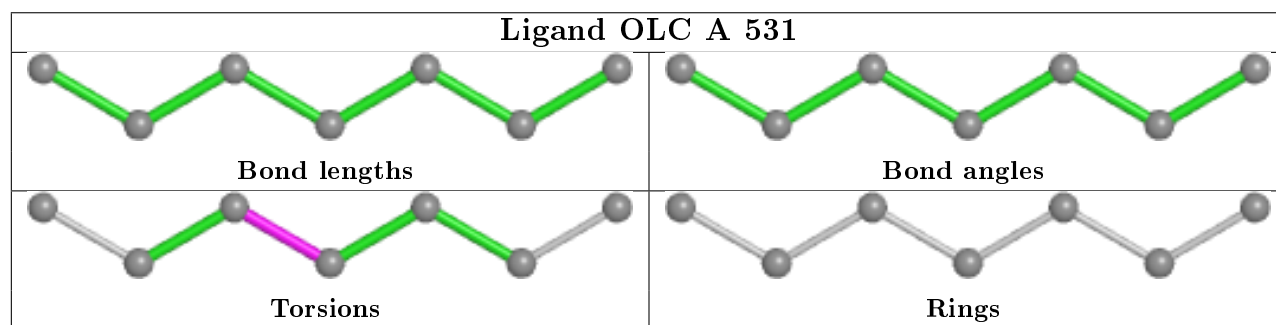
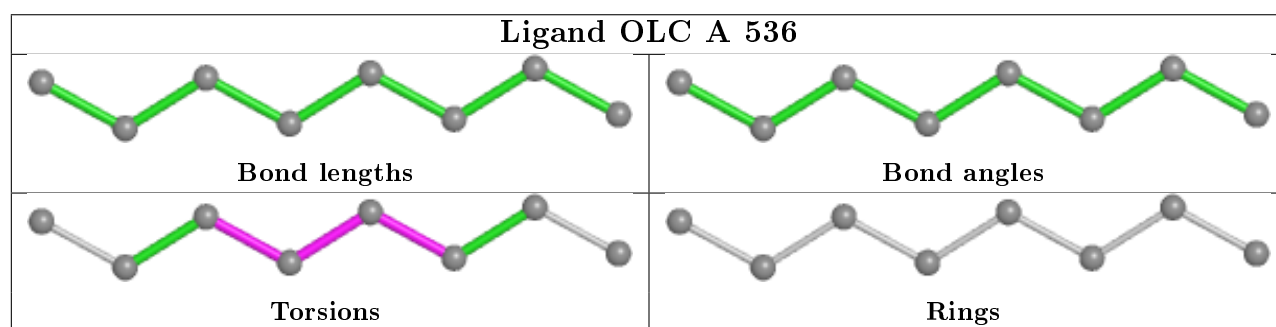
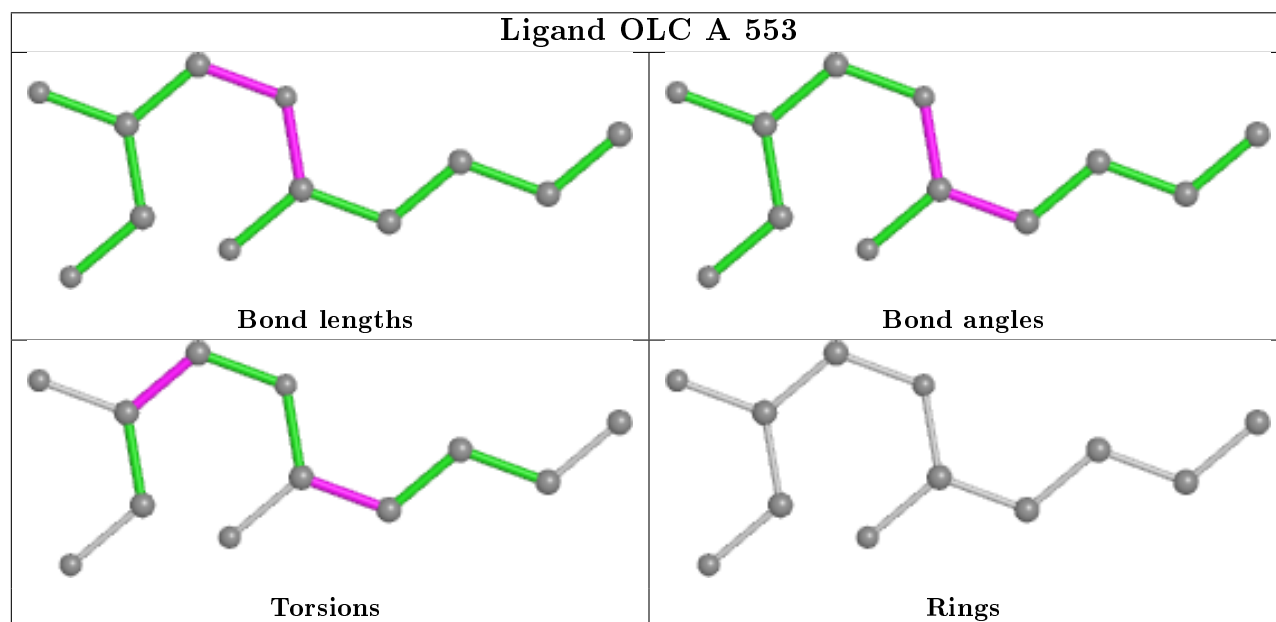
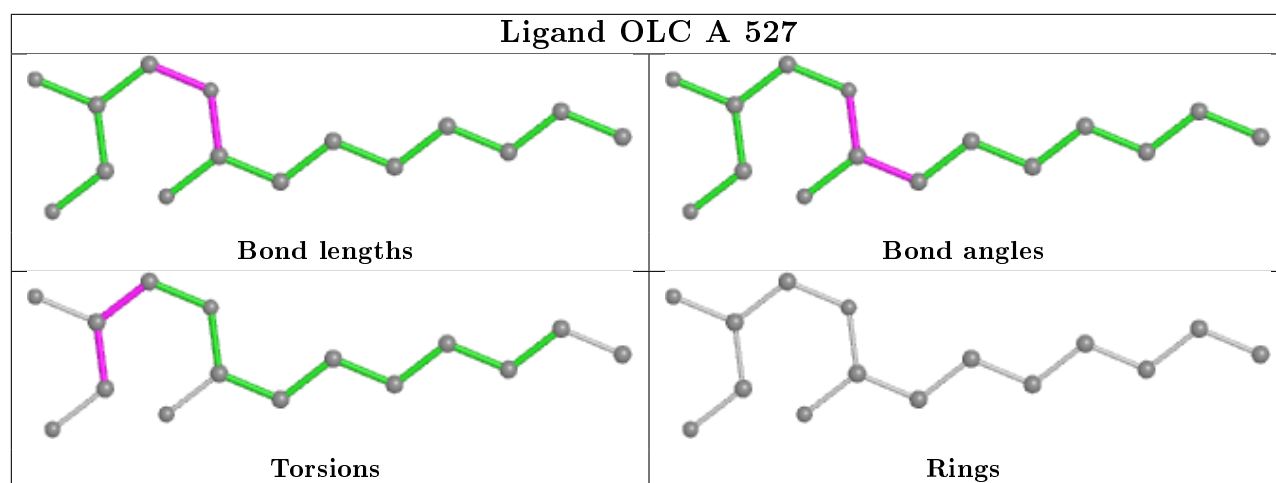


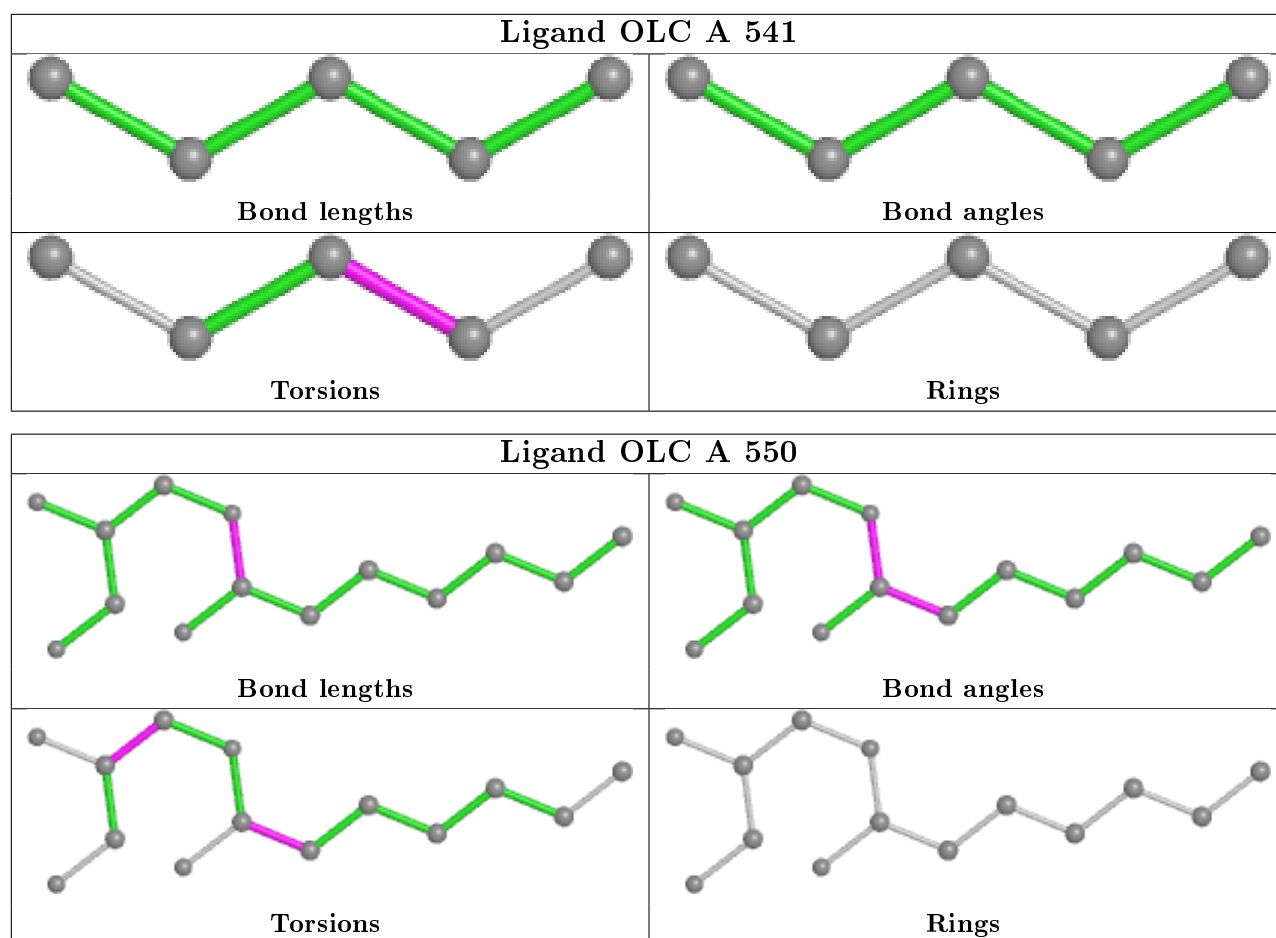












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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<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	467/475 (98%)	0.02	20 (4%) 35 34	21, 34, 65, 115	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	LEU	9.4
1	A	6	SER	9.0
1	A	470	LEU	6.2
1	A	466	ILE	5.9
1	A	469	PHE	5.6
1	A	5	PHE	5.4
1	A	436	PHE	5.2
1	A	7	SER	4.6
1	A	464	ASP	4.3
1	A	465	LEU	4.2
1	A	437	THR	4.1
1	A	468	ARG	3.6
1	A	149	ASN	3.6
1	A	467	ARG	3.5
1	A	153	TRP	3.4
1	A	407	PHE	2.7
1	A	278	ASN	2.5
1	A	460	ILE	2.3
1	A	42	PHE	2.2
1	A	150	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
8	OLC	A	543	4/25	0.57	0.32	64,68,82,82	0
8	OLC	A	550	14/25	0.59	0.27	80,96,108,111	0
8	OLC	A	528	25/25	0.61	0.21	67,86,114,116	0
7	OLB	A	516	25/25	0.67	0.21	57,74,86,89	0
8	OLC	A	551	6/25	0.68	0.19	61,73,79,79	0
8	OLC	A	553	12/25	0.68	0.26	80,96,111,116	0
8	OLC	A	549	16/25	0.69	0.17	73,89,105,107	0
7	OLB	A	515	13/25	0.70	0.20	65,79,88,94	0
8	OLC	A	536	8/25	0.71	0.19	49,64,75,76	0
6	1PE	A	514	16/16	0.71	0.22	50,97,119,120	0
8	OLC	A	533	23/25	0.71	0.21	62,80,102,105	0
8	OLC	A	546	5/25	0.72	0.17	55,59,70,70	0
7	OLB	A	518	13/25	0.73	0.19	59,70,78,87	0
8	OLC	A	527	15/25	0.74	0.22	63,77,95,98	0
8	OLC	A	542	5/25	0.76	0.14	67,81,83,83	0
8	OLC	A	548	8/25	0.76	0.18	68,85,93,93	0
8	OLC	A	523	14/25	0.77	0.15	58,71,97,103	0
8	OLC	A	529	20/25	0.77	0.27	65,81,92,92	0
7	OLB	A	517	22/25	0.78	0.21	61,76,99,105	0
7	OLB	A	519	13/25	0.78	0.25	59,73,88,96	0
7	OLB	A	520	16/25	0.78	0.21	60,75,94,106	0
7	OLB	A	521	11/25	0.79	0.17	45,69,84,84	0
8	OLC	A	530	17/25	0.80	0.21	52,66,80,85	0
8	OLC	A	541	5/25	0.80	0.13	55,70,79,79	0
8	OLC	A	552	9/25	0.81	0.33	85,91,108,108	0
8	OLC	A	535	7/25	0.81	0.20	41,59,72,72	0
8	OLC	A	545	18/25	0.82	0.18	66,80,89,101	0
8	OLC	A	531	7/25	0.82	0.18	58,72,83,83	0
6	1PE	A	513	16/16	0.82	0.14	67,81,89,90	0
8	OLC	A	524	9/25	0.82	0.31	52,66,85,85	0
8	OLC	A	544	4/25	0.82	0.22	62,63,76,76	0
8	OLC	A	522	25/25	0.83	0.18	51,67,98,102	0

*Continued on next page...*

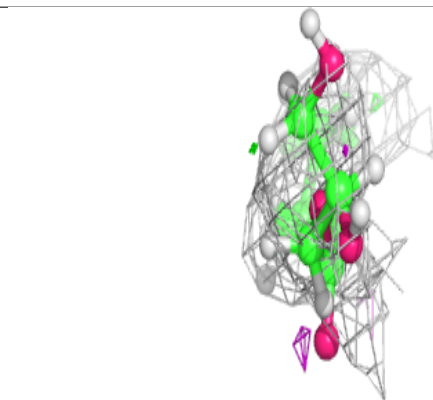
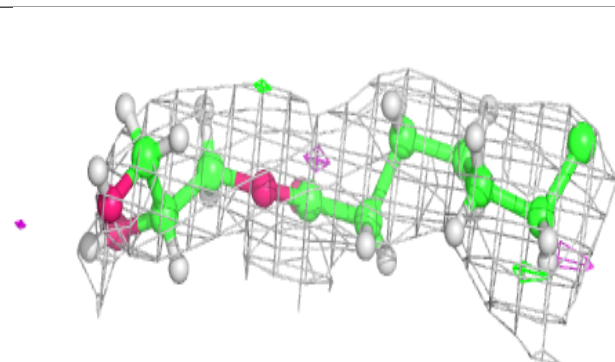
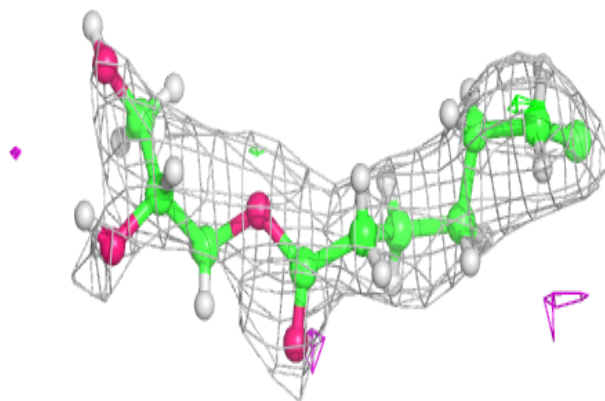
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	OLC	A	532	13/25	0.83	0.16	51,64,77,89	0
8	OLC	A	537	4/25	0.84	0.14	58,69,71,71	0
8	OLC	A	540	5/25	0.84	0.14	61,75,82,82	0
8	OLC	A	539	5/25	0.84	0.12	59,71,76,76	0
8	OLC	A	538	5/25	0.86	0.17	61,73,78,78	0
8	OLC	A	526	5/25	0.86	0.20	53,55,66,66	0
8	OLC	A	525	17/25	0.89	0.15	36,50,70,79	0
5	NA	A	510	1/1	0.89	0.18	57,57,57,57	0
8	OLC	A	547	5/25	0.91	0.14	58,63,76,76	0
6	1PE	A	512	16/16	0.94	0.12	36,48,73,83	0
8	OLC	A	534	5/25	0.94	0.10	49,54,65,65	0
5	NA	A	511	1/1	0.94	0.17	35,35,35,35	0
2	CL	A	503	1/1	0.95	0.04	38,38,38,38	0
4	CA	A	509	1/1	0.96	0.08	52,52,52,52	0
4	CA	A	507	1/1	0.96	0.06	60,60,60,60	0
2	CL	A	505	1/1	0.98	0.08	33,33,33,33	0
3	ZN	A	506	1/1	0.99	0.06	33,33,33,33	0
2	CL	A	504	1/1	0.99	0.07	35,35,35,35	0
4	CA	A	508	1/1	0.99	0.05	42,42,42,42	0
2	CL	A	501	1/1	1.00	0.19	30,30,30,30	0
2	CL	A	502	1/1	1.00	0.11	35,35,35,35	0

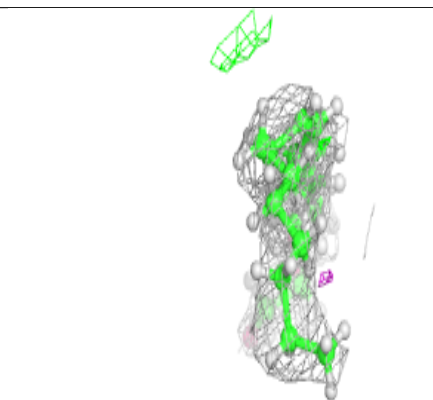
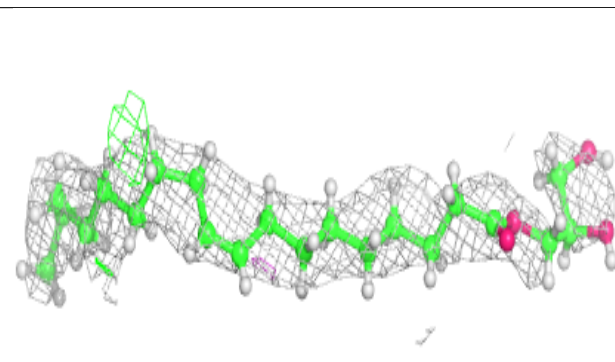
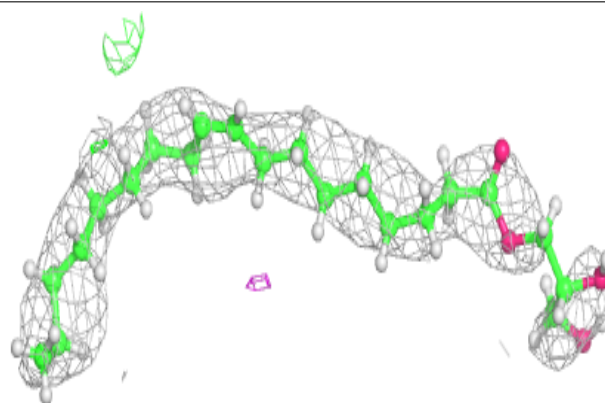
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC A 550:**

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

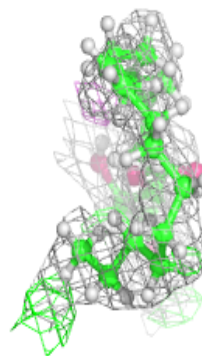
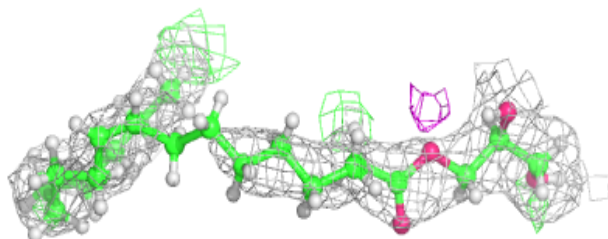
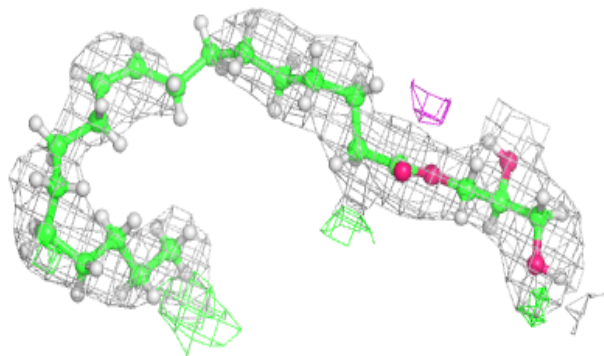
**Electron density around OLC A 528:**

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

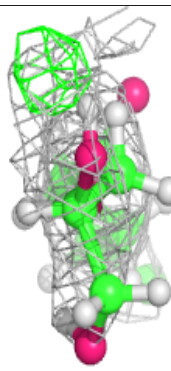
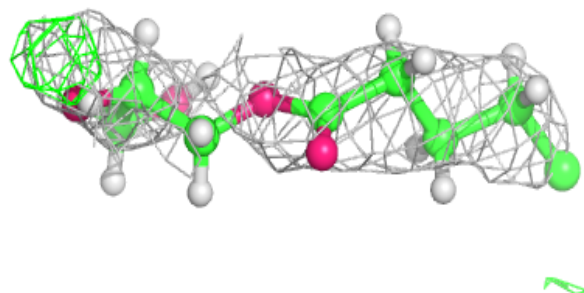
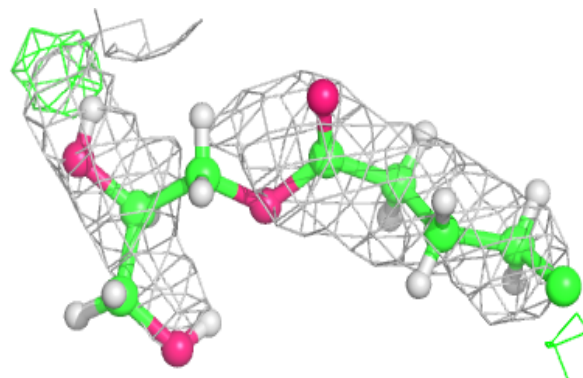


**Electron density around OLB A 516:**

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

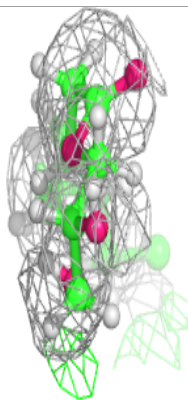
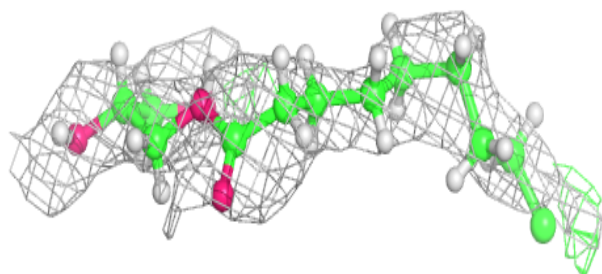
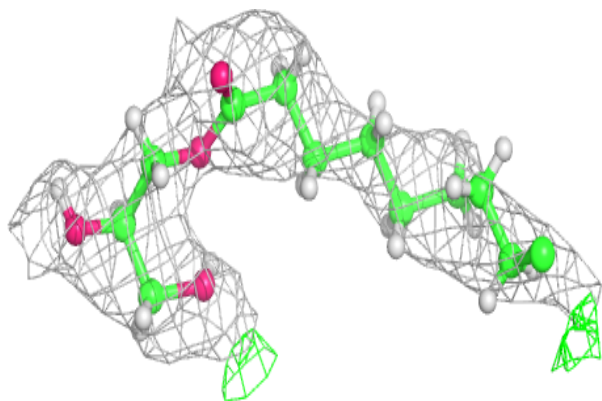
**Electron density around OLC A 553:**

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

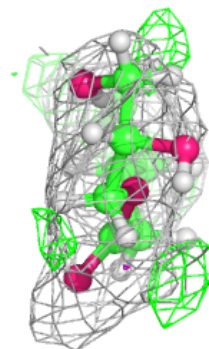
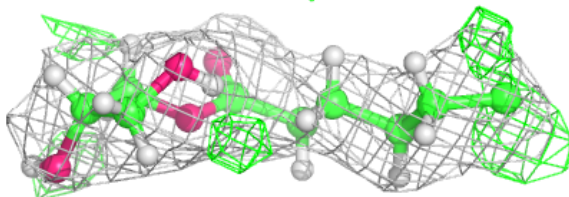
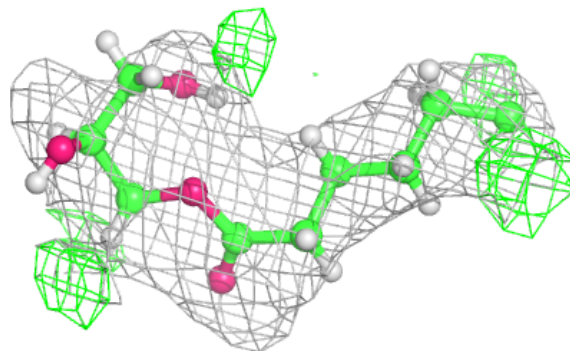


**Electron density around OLC A 549:**

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

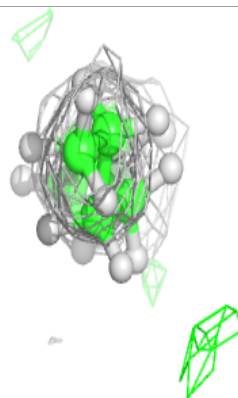
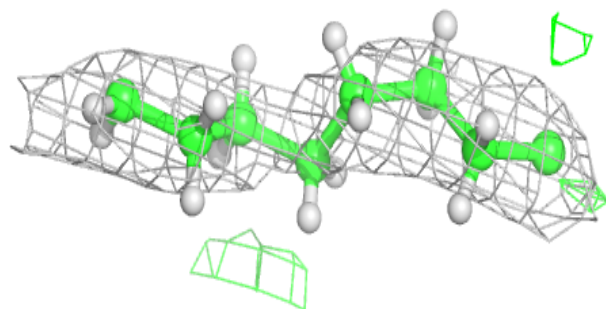
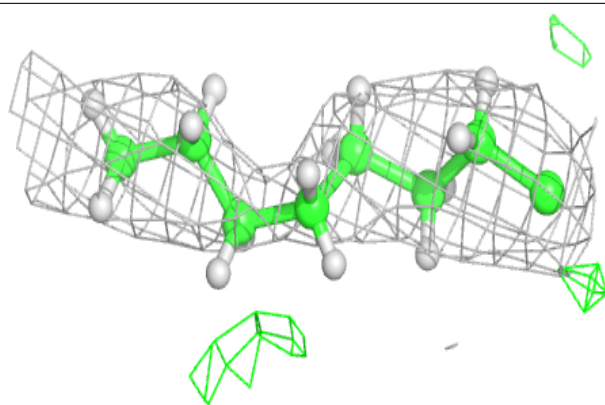
**Electron density around OLB A 515:**

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

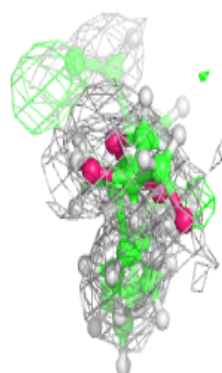
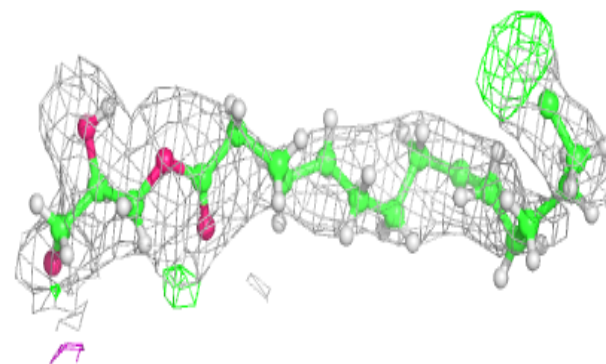
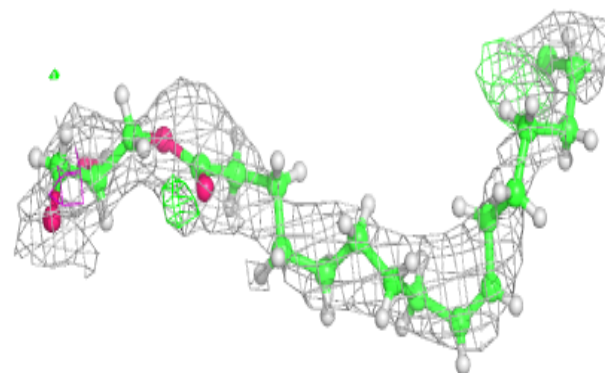


**Electron density around OLC A 536:**

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

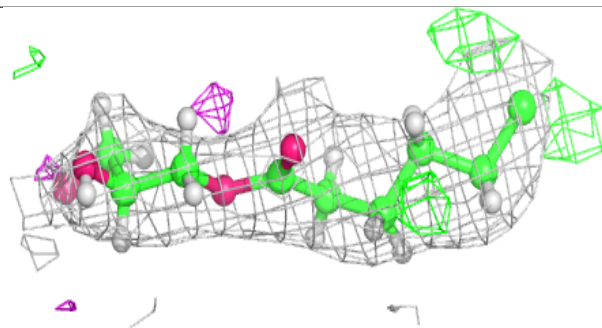
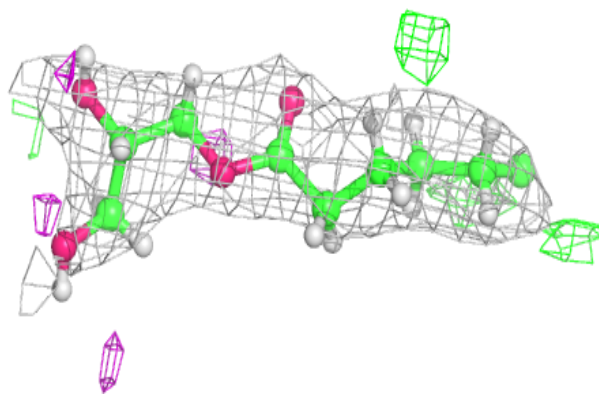
**Electron density around OLC A 533:**

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

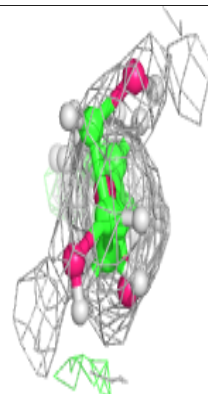
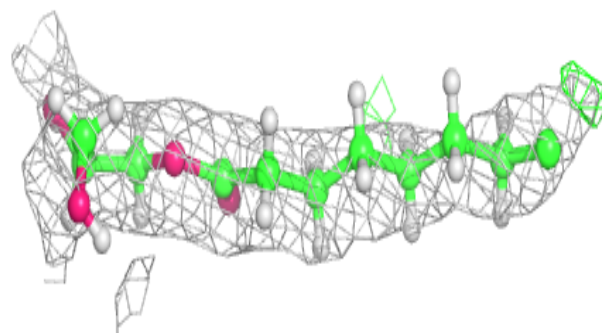
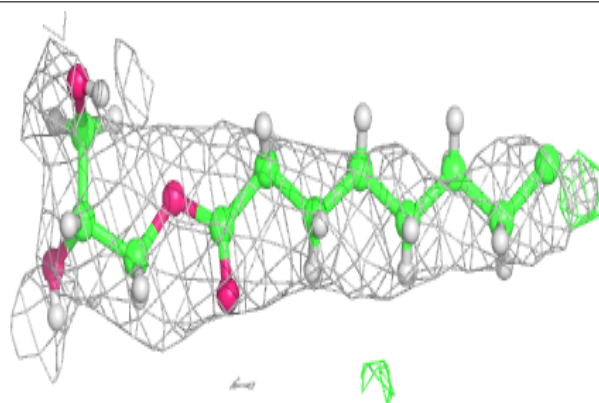


**Electron density around OLB A 518:**

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

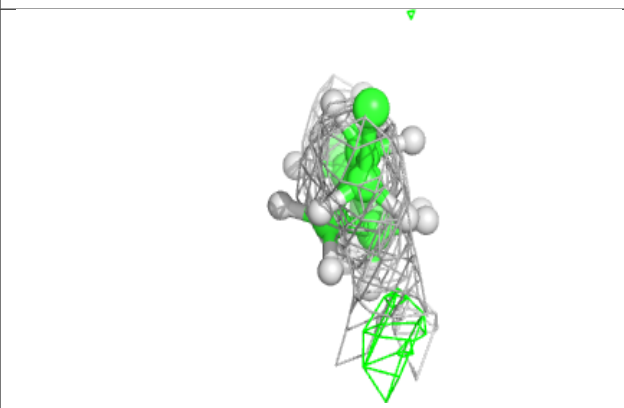
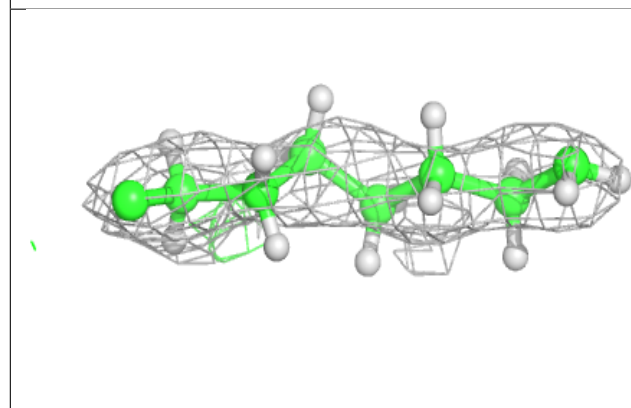
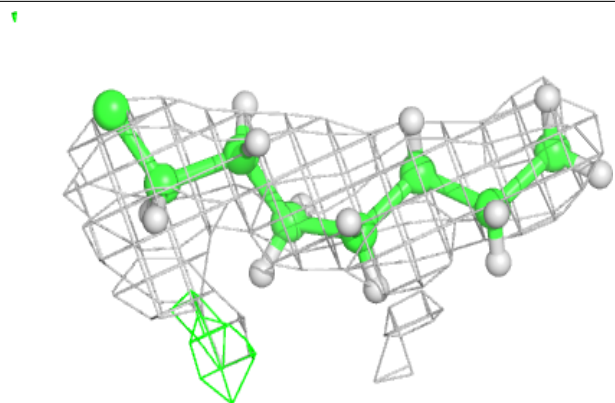
**Electron density around OLC A 527:**

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

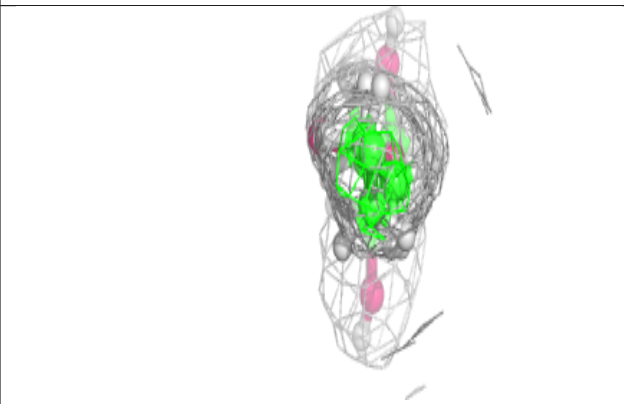
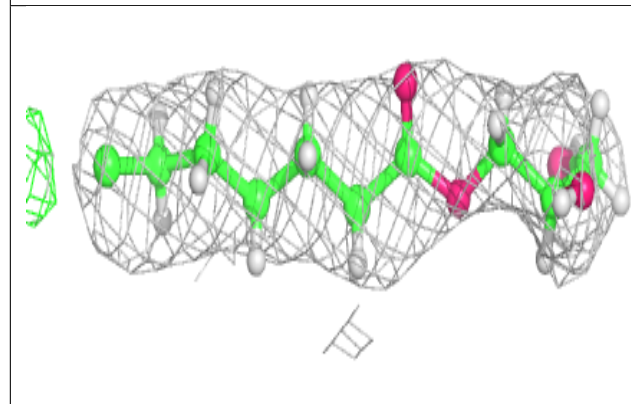
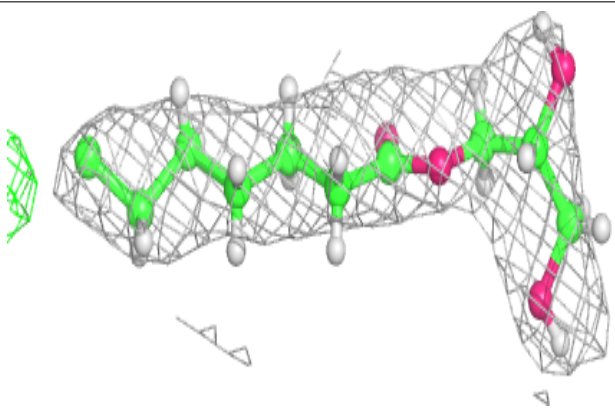


**Electron density around OLC A 548:**

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

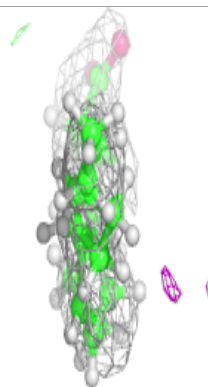
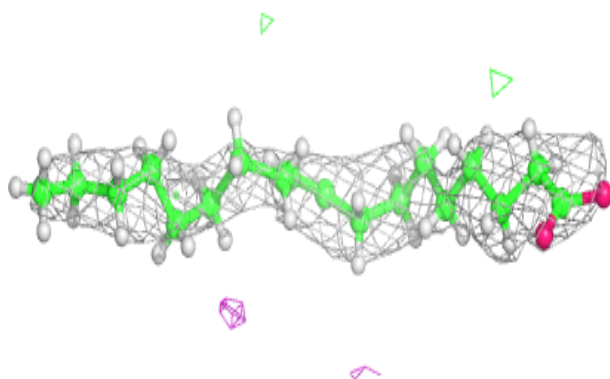
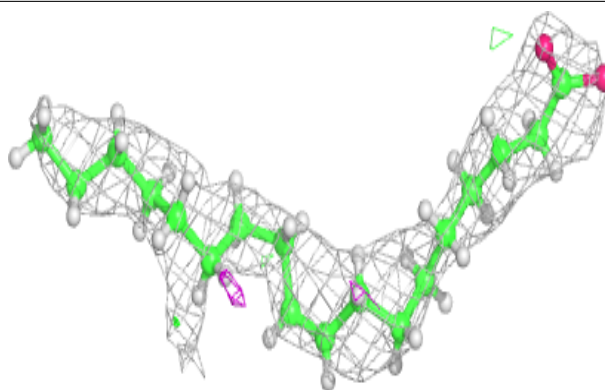
**Electron density around OLC A 523:**

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

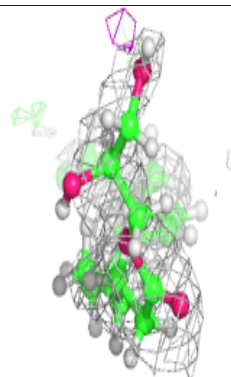
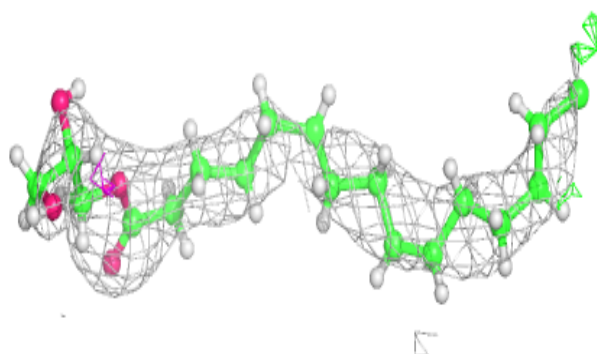
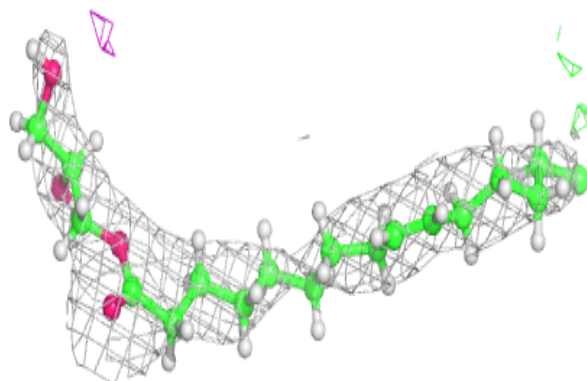


**Electron density around OLC A 529:**

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

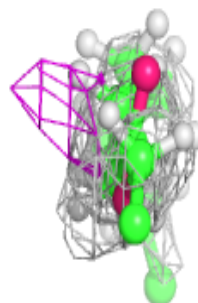
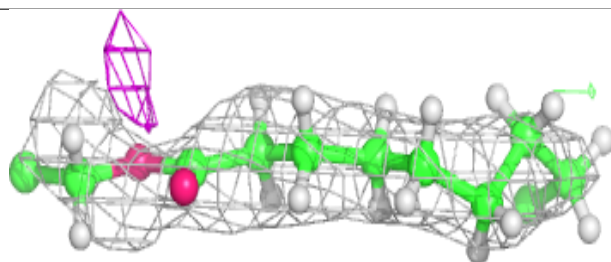
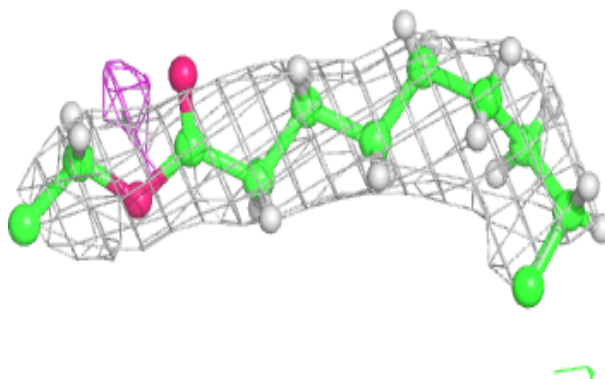
**Electron density around OLB A 517:**

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

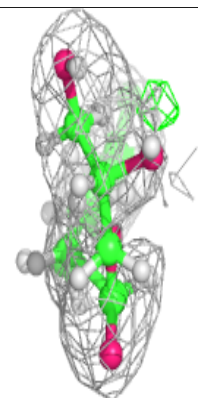
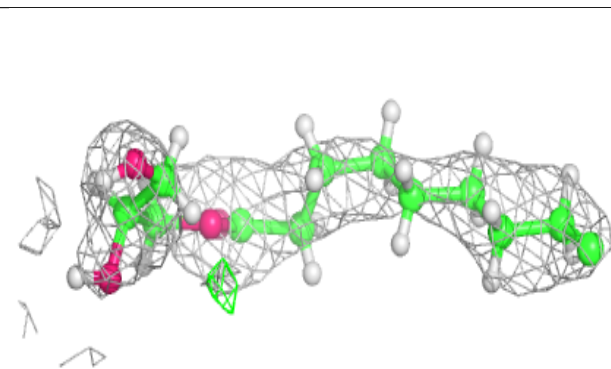
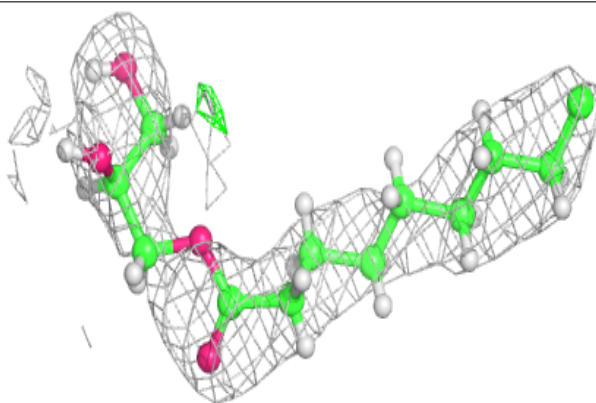


**Electron density around OLB A 519:**

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

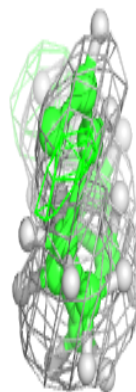
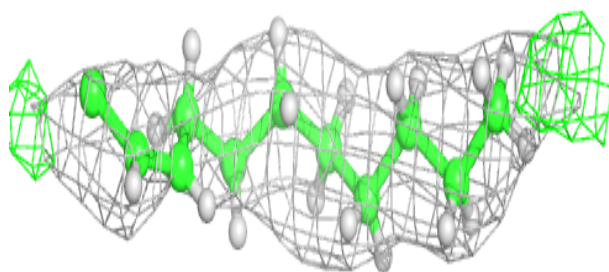
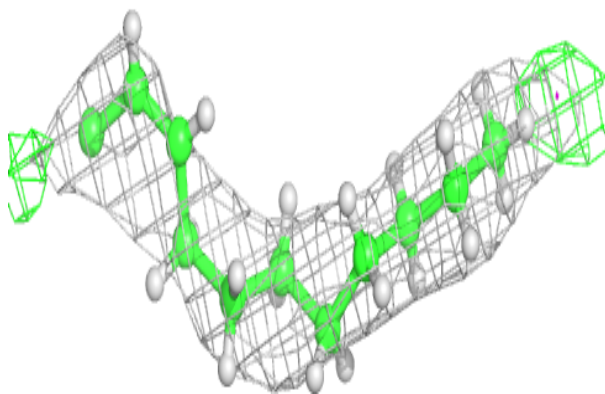
**Electron density around OLB A 520:**

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

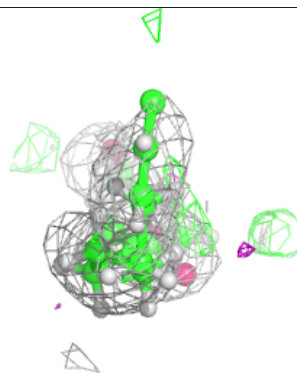
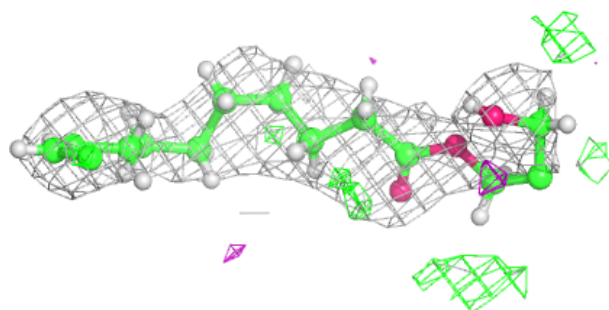
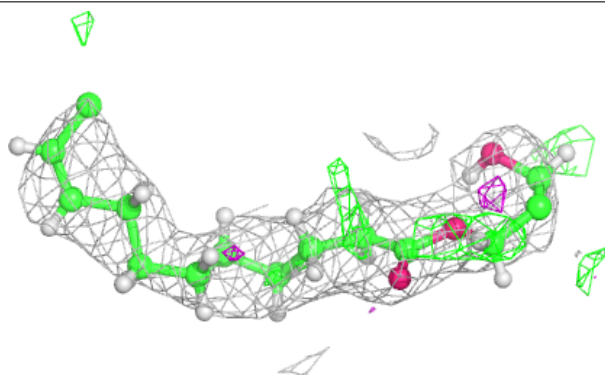


**Electron density around OLB A 521:**

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

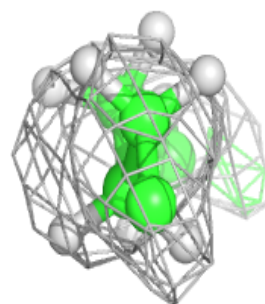
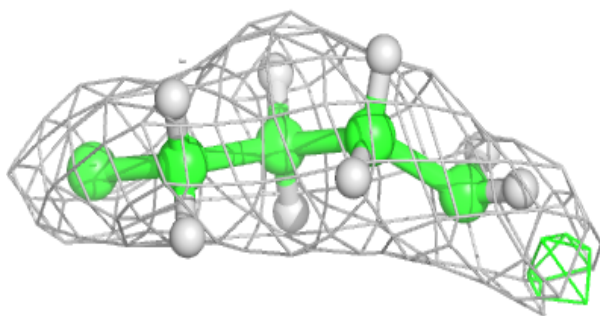
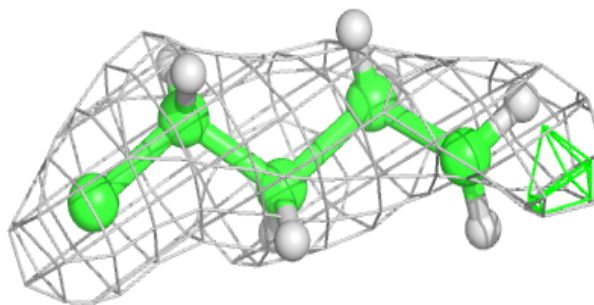
**Electron density around OLC A 530:**

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

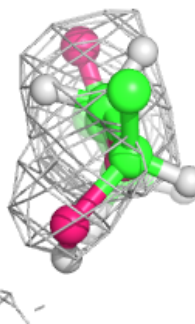
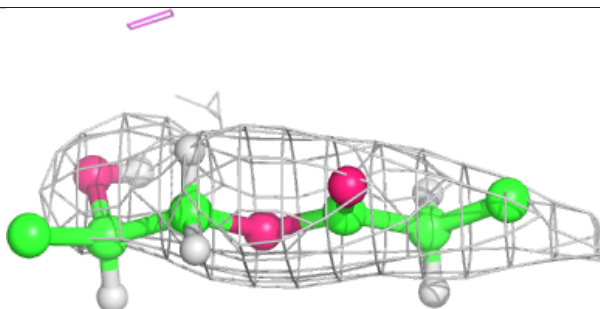
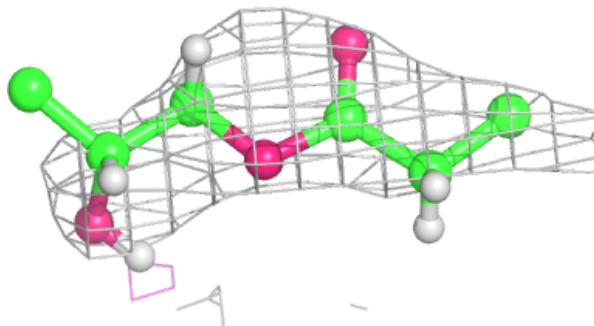


**Electron density around OLC A 541:**

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

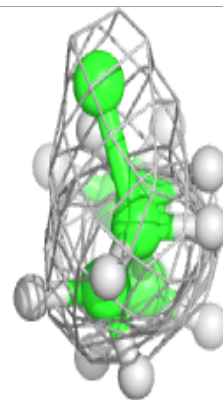
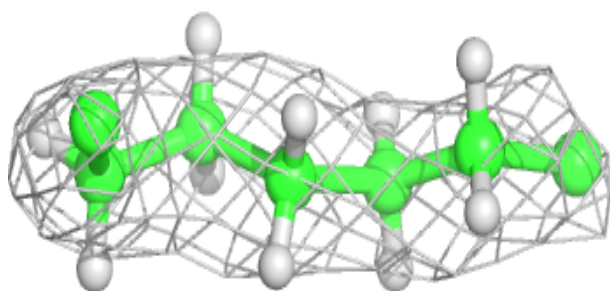
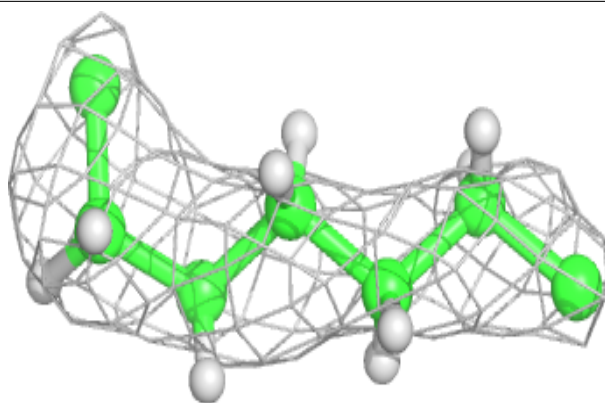
**Electron density around OLC A 552:**

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

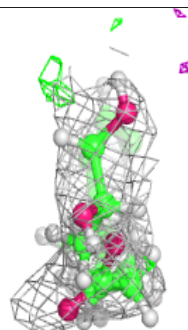
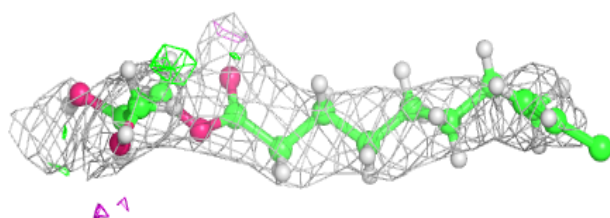
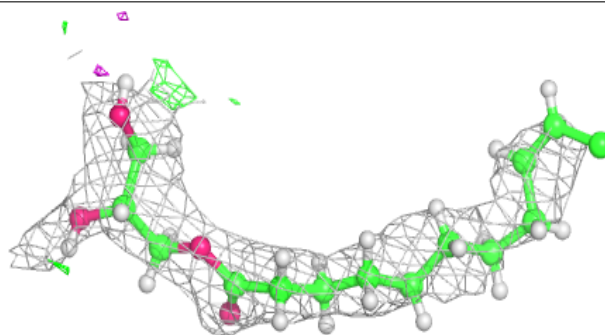


**Electron density around OLC A 535:**

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

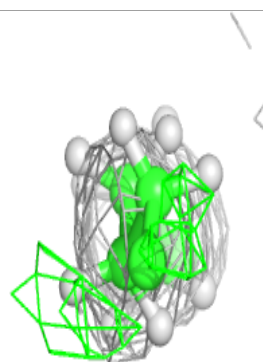
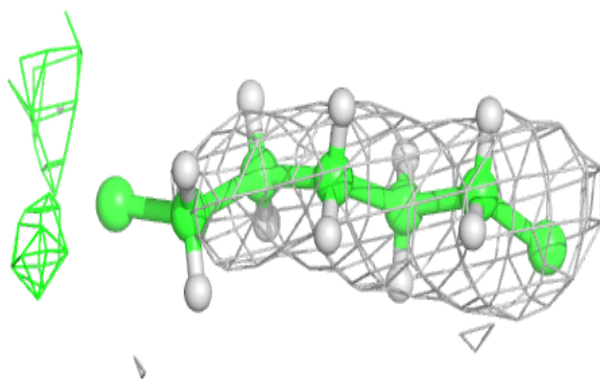
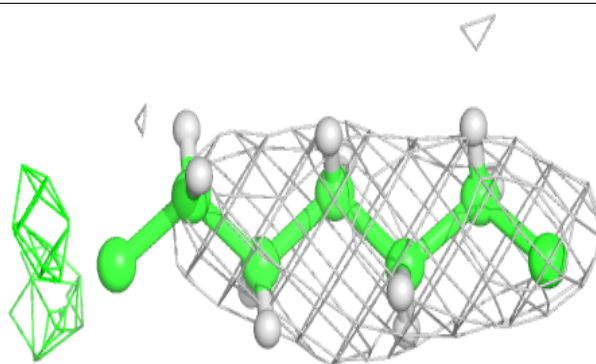
**Electron density around OLC A 545:**

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

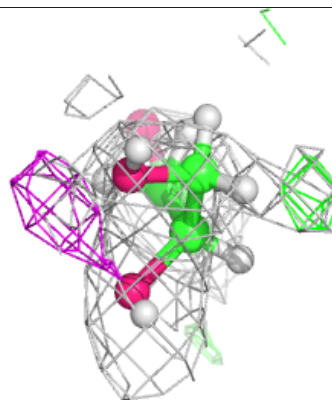
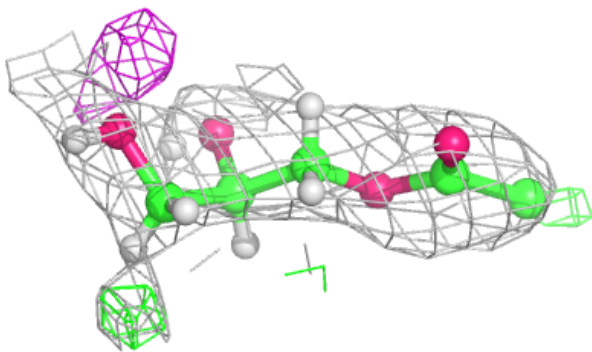
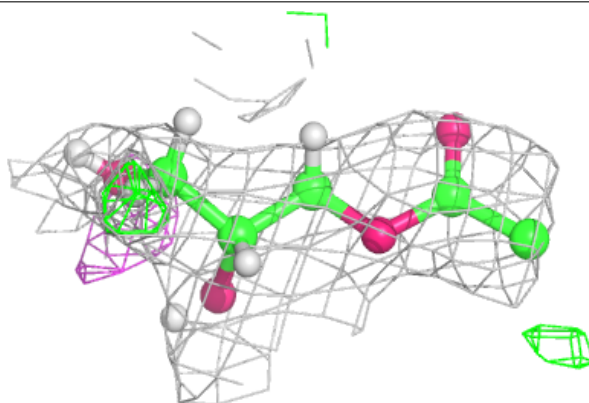


**Electron density around OLC A 531:**

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

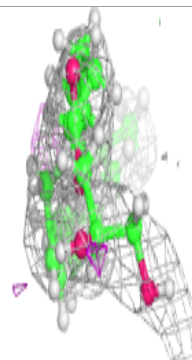
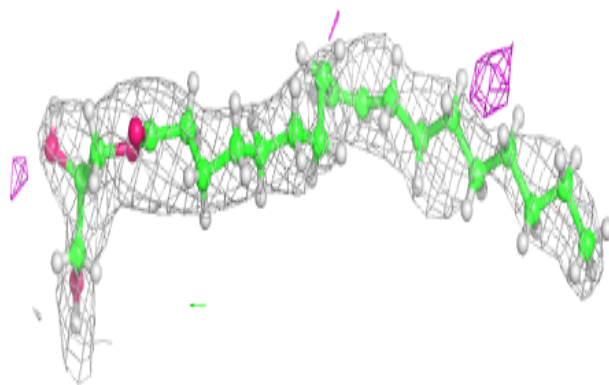
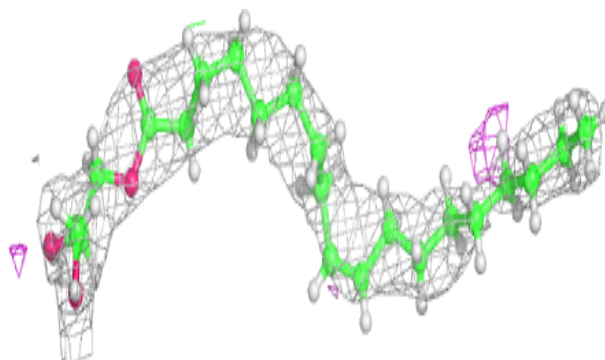
**Electron density around OLC A 524:**

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

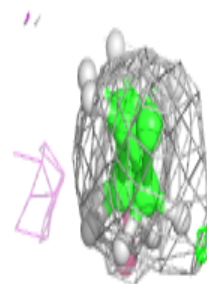
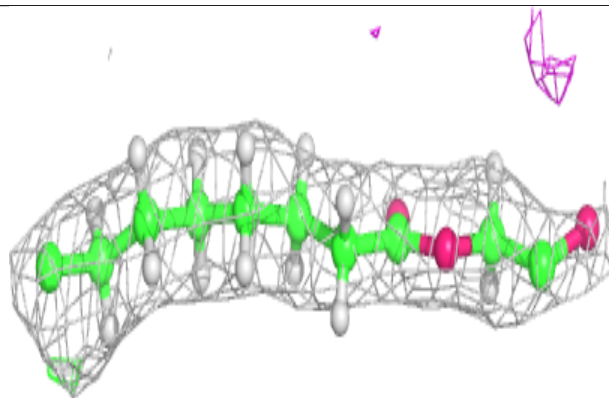
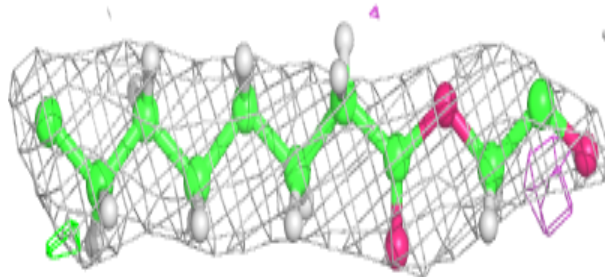


**Electron density around OLC A 522:**

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

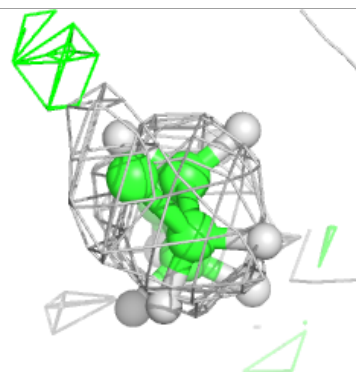
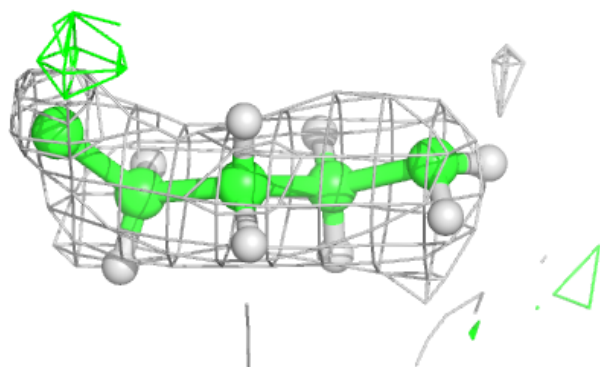
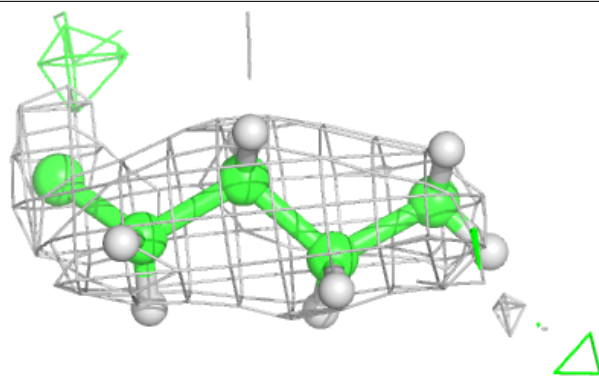
**Electron density around OLC A 532:**

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

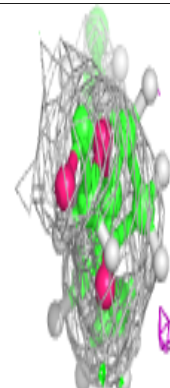
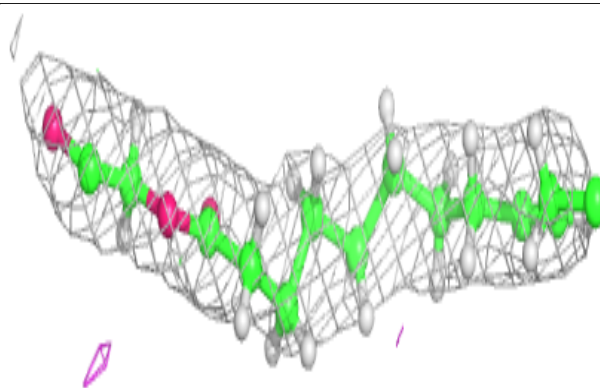
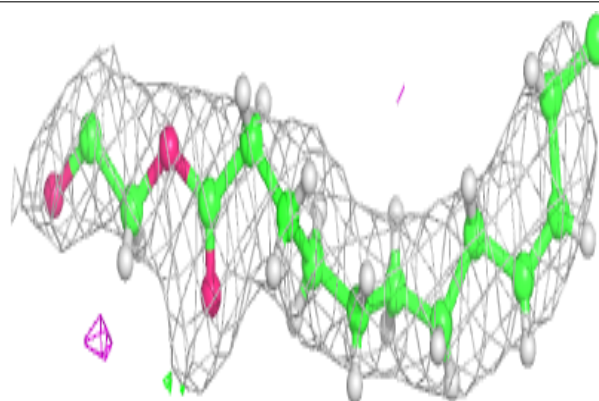


**Electron density around OLC A 539:**

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

**Electron density around OLC A 525:**

$2mF_o-DF_c$  (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.