



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:16 PM BST

PDB ID : 6RF3
Title : Crystal structure of the potassium-pumping G263F mutant of the light-driven sodium pump KR2 in the pentameric form, pH 8.0
Authors : Kovalev, K.; Polovinkin, V.; Gushchin, I.; Borshchevskiy, V.; Gordeliy, V.
Deposited on : 2019-04-12
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

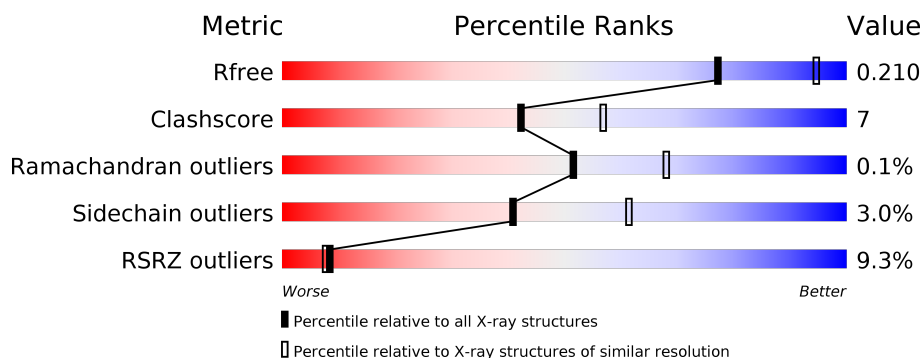
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 ≥ 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	288	<div> <div>9%</div> <div>81% 14% • 5%</div> </div>
1	B	288	<div> <div>8%</div> <div>80% 14% • 5%</div> </div>
1	C	288	<div> <div>8%</div> <div>80% 14% • 5%</div> </div>
1	D	288	<div> <div>11%</div> <div>82% 12% 5%</div> </div>
1	E	288	<div> <div>8%</div> <div>82% 11% • 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OLC	A	301	-	-	-	X
2	OLC	A	304	-	-	-	X
2	OLC	A	306	-	-	-	X
2	OLC	A	307	-	-	-	X
2	OLC	A	308	-	-	-	X
2	OLC	A	310	-	-	-	X
2	OLC	B	303	-	-	-	X
2	OLC	B	307	-	-	-	X
2	OLC	B	309	-	-	-	X
2	OLC	B	311	-	-	-	X
2	OLC	C	303	-	-	-	X
2	OLC	C	308	-	-	-	X
2	OLC	C	309	-	-	-	X
2	OLC	C	310	-	-	-	X
2	OLC	D	302	-	-	-	X
2	OLC	D	305	-	-	-	X
2	OLC	D	306	-	-	-	X
2	OLC	E	303	-	-	-	X
2	OLC	E	306	-	-	-	X
2	OLC	E	308	-	-	-	X
2	OLC	E	312	-	-	-	X
2	OLC	E	313	-	-	-	X
2	OLC	E	314	-	-	-	X
3	LFA	B	302	-	-	-	X
3	LFA	C	302	-	-	-	X
3	LFA	C	319	-	-	-	X
3	LFA	E	302	-	-	-	X
3	LFA	E	319	-	-	-	X
3	LFA	E	323	-	-	-	X
5	BOG	A	320	-	-	-	X
5	BOG	B	321	-	-	-	X
5	BOG	C	321	-	-	-	X
5	BOG	D	317	-	-	-	X
5	BOG	E	321	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13092 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 Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2200	1475	329	387	9			
1	B	273	Total	C	N	O	S	0	0	0
			2194	1470	330	385	9			
1	C	273	Total	C	N	O	S	0	0	0
			2199	1474	329	387	9			
1	D	273	Total	C	N	O	S	0	0	0
			2191	1469	329	384	9			
1	E	273	Total	C	N	O	S	0	0	0
			2193	1471	329	384	9			

There are 45 discrepancies between the modelled and reference sequences:

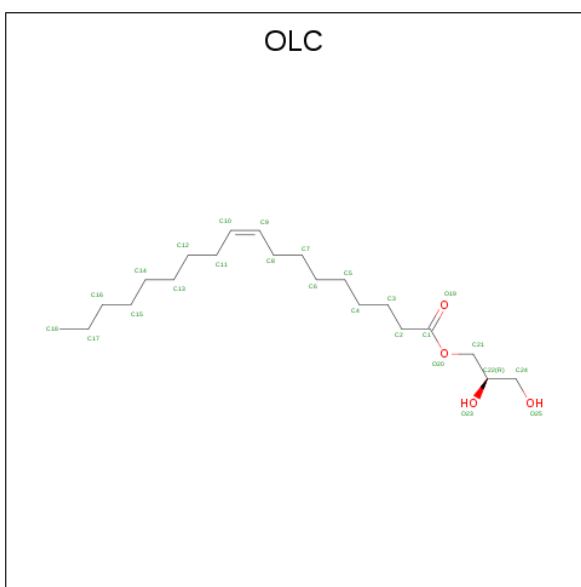
Chain	Residue	Modelled	Actual	Comment	Reference
A	263	PHE	GLY	engineered mutation	UNP N0DKS8
A	281	LEU	-	expression tag	UNP N0DKS8
A	282	GLU	-	expression tag	UNP N0DKS8
A	283	HIS	-	expression tag	UNP N0DKS8
A	284	HIS	-	expression tag	UNP N0DKS8
A	285	HIS	-	expression tag	UNP N0DKS8
A	286	HIS	-	expression tag	UNP N0DKS8
A	287	HIS	-	expression tag	UNP N0DKS8
A	288	HIS	-	expression tag	UNP N0DKS8
B	263	PHE	GLY	engineered mutation	UNP N0DKS8
B	281	LEU	-	expression tag	UNP N0DKS8
B	282	GLU	-	expression tag	UNP N0DKS8
B	283	HIS	-	expression tag	UNP N0DKS8
B	284	HIS	-	expression tag	UNP N0DKS8
B	285	HIS	-	expression tag	UNP N0DKS8
B	286	HIS	-	expression tag	UNP N0DKS8
B	287	HIS	-	expression tag	UNP N0DKS8
B	288	HIS	-	expression tag	UNP N0DKS8
C	263	PHE	GLY	engineered mutation	UNP N0DKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	281	LEU	-	expression tag	UNP N0DKS8
C	282	GLU	-	expression tag	UNP N0DKS8
C	283	HIS	-	expression tag	UNP N0DKS8
C	284	HIS	-	expression tag	UNP N0DKS8
C	285	HIS	-	expression tag	UNP N0DKS8
C	286	HIS	-	expression tag	UNP N0DKS8
C	287	HIS	-	expression tag	UNP N0DKS8
C	288	HIS	-	expression tag	UNP N0DKS8
D	263	PHE	GLY	engineered mutation	UNP N0DKS8
D	281	LEU	-	expression tag	UNP N0DKS8
D	282	GLU	-	expression tag	UNP N0DKS8
D	283	HIS	-	expression tag	UNP N0DKS8
D	284	HIS	-	expression tag	UNP N0DKS8
D	285	HIS	-	expression tag	UNP N0DKS8
D	286	HIS	-	expression tag	UNP N0DKS8
D	287	HIS	-	expression tag	UNP N0DKS8
D	288	HIS	-	expression tag	UNP N0DKS8
E	263	PHE	GLY	engineered mutation	UNP N0DKS8
E	281	LEU	-	expression tag	UNP N0DKS8
E	282	GLU	-	expression tag	UNP N0DKS8
E	283	HIS	-	expression tag	UNP N0DKS8
E	284	HIS	-	expression tag	UNP N0DKS8
E	285	HIS	-	expression tag	UNP N0DKS8
E	286	HIS	-	expression tag	UNP N0DKS8
E	287	HIS	-	expression tag	UNP N0DKS8
E	288	HIS	-	expression tag	UNP N0DKS8

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 15	C 11	O 4	0	0
2	A	1	Total 25	C 21	O 4	0	0
2	A	1	Total 22	C 18	O 4	0	0
2	A	1	Total 25	C 21	O 4	0	0
2	A	1	Total 13	C 9	O 4	0	0
2	A	1	Total 15	C 11	O 4	0	0
2	A	1	Total 16	C 12	O 4	0	0
2	A	1	Total 25	C 21	O 4	0	0
2	A	1	Total 15	C 11	O 4	0	0
2	A	1	Total 16	C 12	O 4	0	0
2	A	1	Total 16	C 12	O 4	0	0
2	A	1	Total 25	C 21	O 4	0	0
2	B	1	Total 25	C 21	O 4	0	0
2	B	1	Total 14	C 10	O 4	0	0

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

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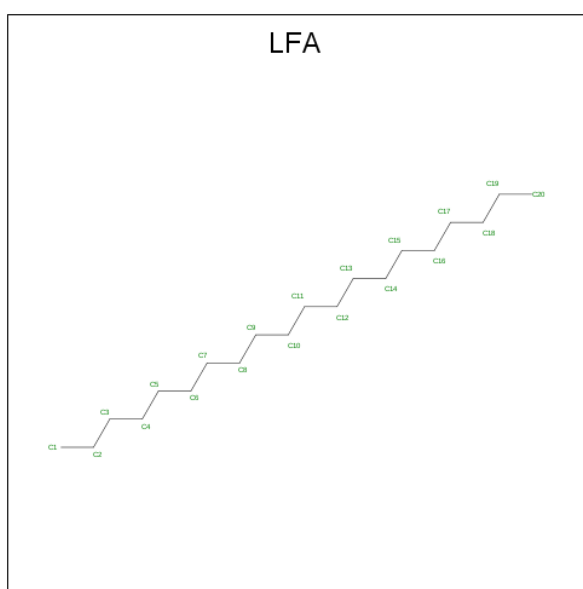
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	D	1	Total	C	O	0	0
			18	14	4		
2	D	1	Total	C	O	0	0
			13	9	4		
2	D	1	Total	C	O	0	0
			25	21	4		
2	D	1	Total	C	O	0	0
			18	14	4		
2	D	1	Total	C	O	0	0
			23	19	4		
2	D	1	Total	C	O	0	0
			25	21	4		
2	D	1	Total	C	O	0	0
			14	10	4		
2	D	1	Total	C	O	0	0
			15	11	4		
2	D	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			14	10	4		
2	E	1	Total	C	O	0	0
			16	12	4		
2	E	1	Total	C	O	0	0
			24	20	4		
2	E	1	Total	C	O	0	0
			24	20	4		
2	E	1	Total	C	O	0	0
			20	16	4		
2	E	1	Total	C	O	0	0
			15	11	4		
2	E	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			15	11	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			11	7	4		
2	E	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			20	16	4		
2	E	1	Total	C	O	0	0
			25	21	4		

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			7	7		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			12	12		
3	A	1	Total	C	0	0
			4	4		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			20	20		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 20 20	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 11 11	0	0
3	C	1	Total C 4 4	0	0
3	C	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	E	1	Total C 20 20	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0

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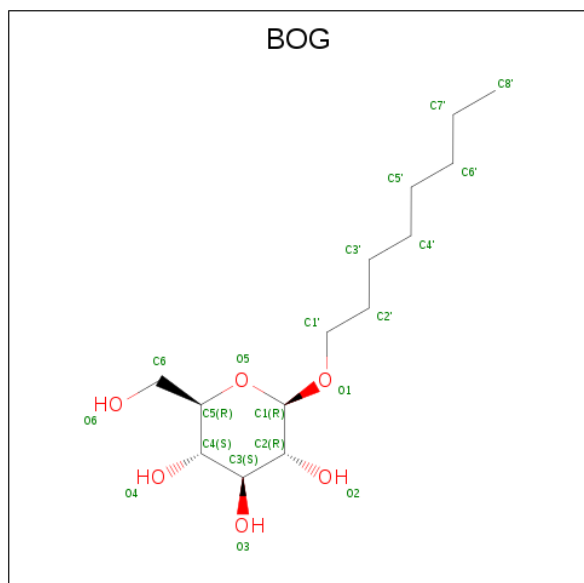
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0
3	E	1	Total C 20 20	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 14 14	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			20	14	6		
5	B	1	Total	C	O	0	0
			20	14	6		
5	C	1	Total	C	O	0	0
			20	14	6		
5	D	1	Total	C	O	0	0
			20	14	6		
5	E	1	Total	C	O	0	0
			20	14	6		

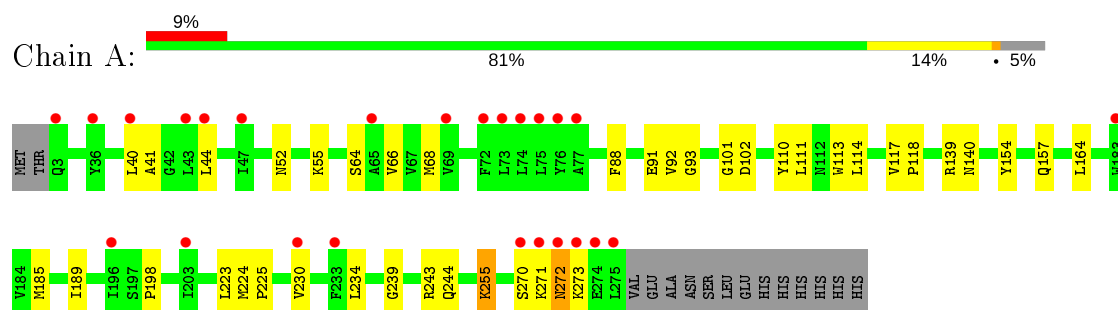
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total	O	0	0
			97	97		
6	B	86	Total	O	0	0
			86	86		
6	C	94	Total	O	0	0
			94	94		
6	D	89	Total	O	0	0
			89	89		
6	E	96	Total	O	0	0
			96	96		

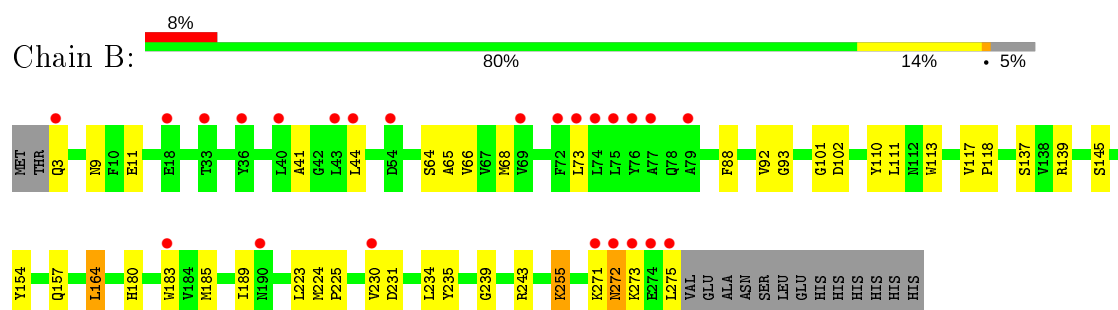
3 Residue-property plots [i](#)

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.

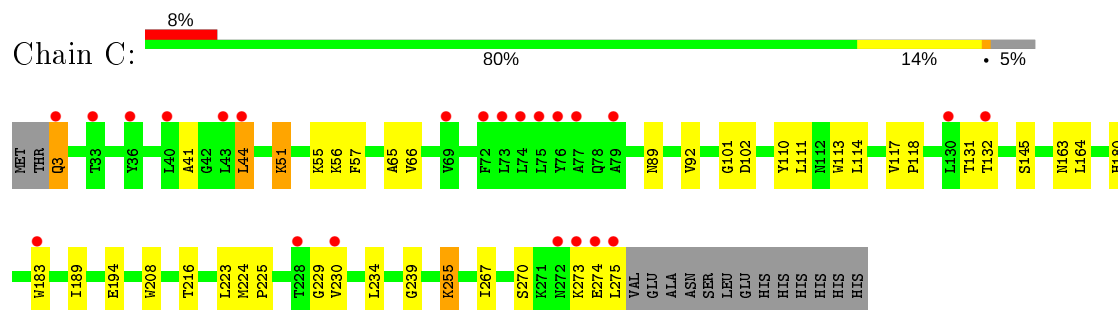
• Molecule 1: Sodium pumping rhodopsin



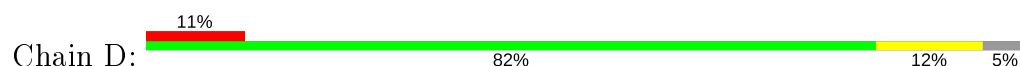
• Molecule 1: Sodium pumping rhodopsin

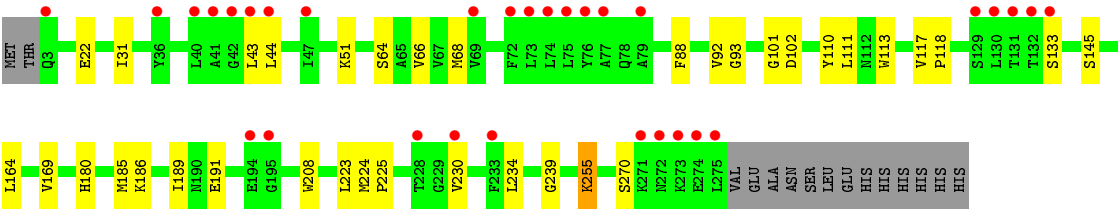


• Molecule 1: Sodium pumping rhodopsin

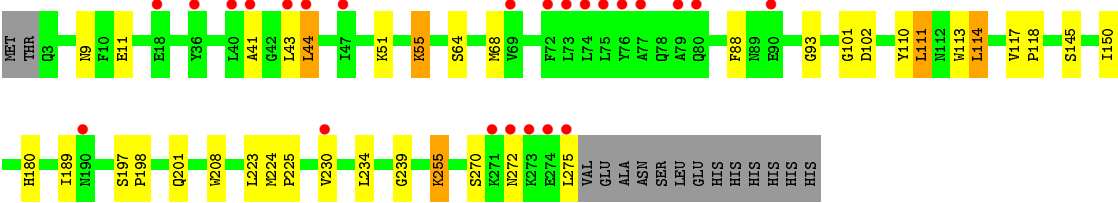
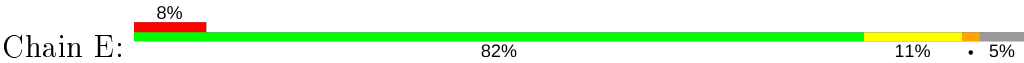


• Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.68Å 239.69Å 134.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.97 – 2.40 47.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.97-2.40) 99.9 (47.94-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.172 , 0.205 0.184 , 0.210	Depositor DCC
R_{free} test set	4195 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13092	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OLC, LFA, LYR, BOG

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	0.29	0/2229	0.42	0/3030
1	B	0.29	0/2223	0.42	0/3023
1	C	0.28	0/2228	0.42	0/3029
1	D	0.28	0/2220	0.43	0/3018
1	E	0.29	0/2222	0.42	0/3021
All	All	0.28	0/11122	0.42	0/15121

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	B	243	ARG	Sidechain
1	B	273	LYS	Peptide
1	C	270	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2200	0	2184	33	0
1	B	2194	0	2179	36	0
1	C	2199	0	2182	39	0
1	D	2191	0	2172	28	0
1	E	2193	0	2179	27	0
2	A	228	0	326	7	0
2	B	269	0	378	7	0
2	C	240	0	343	5	0
2	D	176	0	250	2	0
2	E	259	0	371	13	0
3	A	65	0	126	1	0
3	B	54	0	106	1	0
3	C	90	0	182	6	0
3	D	78	0	153	3	0
3	E	89	0	176	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	20	0	28	3	0
5	B	20	0	28	4	0
5	C	20	0	28	1	0
5	D	20	0	28	1	0
5	E	20	0	28	0	0
6	A	97	0	0	4	0
6	B	86	0	0	1	0
6	C	94	0	0	3	0
6	D	89	0	0	2	0
6	E	96	0	0	4	0
All	All	13092	0	13447	179	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (179) 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)
3:E:316:LFA:H141	3:E:317:LFA:H201	1.51	0.89
1:C:267:ILE:HG21	1:C:275:LEU:HB3	1.57	0.85
3:E:316:LFA:C14	3:E:317:LFA:H201	2.05	0.84
1:B:255:LYR:H9	1:B:255:LYR:H183	1.60	0.82
1:A:164:LEU:HD21	5:A:320:BOG:H2'1	1.61	0.80
1:A:255:LYR:H9	1:A:255:LYR:H183	1.62	0.80
1:D:255:LYR:H9	1:D:255:LYR:H183	1.62	0.80
1:C:255:LYR:H9	1:C:255:LYR:H183	1.62	0.79
1:E:255:LYR:H183	1:E:255:LYR:H9	1.64	0.79
1:A:272:ASN:HD22	1:A:272:ASN:N	1.84	0.76
1:B:272:ASN:N	1:B:272:ASN:HD22	1.84	0.76
1:B:231:ASP:H	5:B:321:BOG:HO6	1.34	0.75
1:C:51:LYS:HD3	6:C:447:HOH:O	1.86	0.75
2:A:307:OLC:O19	2:A:308:OLC:H21A	1.88	0.72
2:A:301:OLC:C8	2:B:304:OLC:H10	2.21	0.70
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.74	0.70
1:E:145:SER:OG	1:E:180:HIS:HD2	1.75	0.69
1:C:145:SER:OG	1:C:180:HIS:HD2	1.76	0.68
2:E:303:OLC:C24	3:E:315:LFA:C13	2.72	0.68
1:B:145:SER:OG	1:B:180:HIS:HD2	1.75	0.68
1:C:183:TRP:CZ3	3:C:314:LFA:H61	2.29	0.68
1:D:145:SER:OG	1:D:180:HIS:HD2	1.76	0.68
2:E:303:OLC:H24	3:E:315:LFA:C13	2.26	0.66
3:D:313:LFA:C17	2:E:301:OLC:H21A	2.25	0.65
2:B:313:OLC:H2	2:B:315:OLC:H24A	1.79	0.64
1:A:139:ARG:HH22	2:A:302:OLC:H24A	1.63	0.63
1:C:224:MET:N	1:C:225:PRO:HD2	2.16	0.60
1:A:224:MET:N	1:A:225:PRO:HD2	2.16	0.60
1:D:234:LEU:O	1:D:239:GLY:HA3	2.02	0.60
1:A:52:ASN:OD1	6:A:401:HOH:O	2.17	0.59
1:E:234:LEU:O	1:E:239:GLY:HA3	2.02	0.59
1:D:224:MET:N	1:D:225:PRO:HD2	2.17	0.59
3:D:313:LFA:H172	2:E:301:OLC:H21A	1.84	0.59
6:A:418:HOH:O	1:B:3:GLN:HG3	2.02	0.59
1:B:255:LYR:C9	1:B:255:LYR:H183	2.32	0.59
1:E:224:MET:N	1:E:225:PRO:HD2	2.17	0.58
1:C:164:LEU:HD21	5:C:321:BOG:H2'1	1.86	0.58
1:E:55:LYS:HE3	6:E:480:HOH:O	2.04	0.58
1:B:224:MET:N	1:B:225:PRO:HD2	2.17	0.58
1:C:216:THR:CG2	3:C:318:LFA:H201	2.34	0.58
1:A:255:LYR:C9	1:A:255:LYR:H183	2.33	0.57
1:A:140:ASN:HB3	2:A:304:OLC:H2A	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.87	0.57
1:C:255:LYR:C9	1:C:255:LYR:H183	2.33	0.57
1:A:234:LEU:O	1:A:239:GLY:HA3	2.05	0.56
2:E:305:OLC:C17	2:E:312:OLC:H11A	2.36	0.56
1:C:234:LEU:O	1:C:239:GLY:HA3	2.05	0.56
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.88	0.56
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.88	0.56
2:E:304:OLC:O19	2:E:304:OLC:H4	2.05	0.55
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.88	0.55
1:B:234:LEU:O	1:B:239:GLY:HA3	2.05	0.55
1:C:189:ILE:HD12	1:C:208:TRP:HB2	1.89	0.55
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.88	0.54
1:E:198:PRO:HG2	6:E:485:HOH:O	2.07	0.54
1:A:272:ASN:ND2	1:A:272:ASN:N	2.55	0.54
1:E:111:LEU:O	1:E:114:LEU:HB2	2.09	0.53
2:E:310:OLC:O19	2:E:312:OLC:O25	2.25	0.52
1:C:267:ILE:CG2	1:C:275:LEU:HB3	2.34	0.52
1:C:55:LYS:NZ	6:C:404:HOH:O	2.42	0.52
1:D:255:LYR:H183	1:D:255:LYR:C9	2.33	0.52
1:B:139:ARG:HH11	2:B:301:OLC:C24	2.23	0.52
2:E:303:OLC:H24A	3:E:315:LFA:C13	2.39	0.51
1:B:139:ARG:NH1	2:B:301:OLC:C24	2.73	0.51
3:C:302:LFA:H32	3:E:323:LFA:H102	1.92	0.51
1:C:216:THR:HG22	3:C:318:LFA:H201	1.91	0.51
1:B:183:TRP:CZ3	3:B:316:LFA:H182	2.45	0.51
2:B:306:OLC:H10	1:C:114:LEU:HD22	1.93	0.51
1:D:44:LEU:HD21	1:E:43:LEU:HD11	1.92	0.51
1:B:164:LEU:HD11	5:B:321:BOG:H2'1	1.93	0.50
2:E:305:OLC:C17	2:E:312:OLC:C11	2.90	0.50
1:B:231:ASP:N	5:B:321:BOG:O6	2.22	0.50
1:C:163:ASN:HD22	2:C:311:OLC:C24	2.25	0.50
1:E:255:LYR:H183	1:E:255:LYR:C9	2.35	0.50
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.94	0.49
1:C:183:TRP:CE3	3:C:314:LFA:H41	2.46	0.49
1:D:164:LEU:HD21	5:D:317:BOG:H2'1	1.94	0.49
6:B:409:HOH:O	1:C:3:GLN:HB2	2.13	0.49
1:D:255:LYR:H9	1:D:255:LYR:H192	1.95	0.49
1:C:255:LYR:H9	1:C:255:LYR:H192	1.95	0.49
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.94	0.48
1:A:164:LEU:HD21	5:A:320:BOG:C2'	2.38	0.48
1:A:40:LEU:HD23	1:B:73:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:VAL:HG11	2:D:304:OLC:H2	1.96	0.48
1:C:101:GLY:O	1:C:102:ASP:HB2	2.13	0.48
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.94	0.48
2:E:306:OLC:H2	2:E:306:OLC:H5	1.64	0.48
1:A:164:LEU:CD2	5:A:320:BOG:H2'1	2.40	0.47
1:B:255:LYR:H192	1:B:255:LYR:H9	1.96	0.47
1:B:101:GLY:O	1:B:102:ASP:HB2	2.15	0.47
1:D:51:LYS:HG2	6:D:460:HOH:O	2.13	0.47
1:B:223:LEU:C	1:B:225:PRO:HD2	2.35	0.47
1:C:229:GLY:HA3	2:C:309:OLC:H22	1.95	0.47
1:E:255:LYR:H192	1:E:255:LYR:H9	1.96	0.47
1:E:51:LYS:HD3	6:E:407:HOH:O	2.14	0.47
1:C:44:LEU:HD11	1:D:43:LEU:HD11	1.98	0.46
1:A:223:LEU:C	1:A:225:PRO:HD2	2.34	0.46
1:A:244:GLN:HG2	6:A:425:HOH:O	2.16	0.46
1:C:223:LEU:C	1:C:225:PRO:HD2	2.35	0.46
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.51	0.46
1:A:101:GLY:O	1:A:102:ASP:HB2	2.15	0.46
1:A:255:LYR:H9	1:A:255:LYR:H192	1.98	0.46
1:B:185:MET:O	1:B:189:ILE:HG12	2.15	0.46
2:E:304:OLC:O19	2:E:304:OLC:C4	2.64	0.46
3:A:315:LFA:H102	3:A:315:LFA:H72	1.80	0.45
1:E:101:GLY:O	1:E:102:ASP:HB2	2.16	0.45
1:E:223:LEU:C	1:E:225:PRO:HD2	2.37	0.45
2:A:311:OLC:H5A	2:B:301:OLC:H17	1.97	0.45
1:D:51:LYS:HE2	6:D:460:HOH:O	2.16	0.45
1:D:255:LYR:H192	1:D:255:LYR:C9	2.47	0.45
1:B:272:ASN:N	1:B:272:ASN:ND2	2.56	0.45
1:D:223:LEU:C	1:D:225:PRO:HD2	2.38	0.45
2:C:304:OLC:H11A	2:C:304:OLC:H8	1.79	0.44
1:D:186:LYS:HD3	1:D:208:TRP:CZ2	2.52	0.44
1:A:164:LEU:HD23	2:A:306:OLC:H24	1.98	0.44
1:A:185:MET:O	1:A:189:ILE:HG12	2.18	0.44
1:A:224:MET:N	1:A:225:PRO:CD	2.81	0.44
1:C:110:TYR:O	1:C:113:TRP:HB2	2.17	0.44
1:A:88:PHE:CZ	1:A:93:GLY:HA2	2.53	0.44
1:C:56:LYS:HG2	6:C:484:HOH:O	2.18	0.44
1:A:44:LEU:HD21	1:B:65:ALA:HB1	2.00	0.44
1:B:271:LYS:C	1:B:272:ASN:HD22	2.22	0.44
1:C:216:THR:HG21	3:C:318:LFA:H201	2.00	0.44
2:C:305:OLC:H7	2:C:305:OLC:H11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LYR:C9	1:B:255:LYR:H192	2.48	0.43
1:D:185:MET:O	1:D:189:ILE:HG12	2.18	0.43
1:B:224:MET:N	1:B:225:PRO:CD	2.81	0.43
1:C:131:THR:HG21	1:C:194:GLU:OE1	2.19	0.43
1:C:255:LYR:H192	1:C:255:LYR:C9	2.48	0.43
1:E:197:SER:O	1:E:201:GLN:HG3	2.19	0.43
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.99	0.43
1:E:224:MET:N	1:E:225:PRO:CD	2.82	0.43
1:C:224:MET:N	1:C:225:PRO:CD	2.81	0.43
1:D:64:SER:O	1:D:68:MET:HG2	2.19	0.43
1:A:110:TYR:HA	1:A:113:TRP:CE3	2.54	0.43
1:D:133:SER:OG	1:D:191:GLU:OE2	2.36	0.43
2:C:304:OLC:H3	3:D:311:LFA:H202	2.01	0.43
1:B:110:TYR:O	1:B:113:TRP:HB2	2.19	0.42
1:A:114:LEU:O	1:A:118:PRO:HG2	2.18	0.42
2:E:305:OLC:C17	2:E:312:OLC:C10	2.97	0.42
1:A:255:LYR:H192	1:A:255:LYR:C9	2.49	0.42
1:B:88:PHE:CZ	1:B:93:GLY:HA2	2.53	0.42
1:C:89:ASN:OD1	1:C:92:VAL:HG13	2.19	0.42
1:E:189:ILE:CD1	1:E:208:TRP:HB2	2.49	0.42
1:E:255:LYR:H192	1:E:255:LYR:C9	2.48	0.42
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.20	0.42
1:A:271:LYS:C	1:A:272:ASN:HD22	2.23	0.42
1:E:64:SER:O	1:E:68:MET:HG2	2.20	0.42
1:A:110:TYR:O	1:A:113:TRP:HB2	2.19	0.42
1:D:224:MET:N	1:D:225:PRO:CD	2.83	0.42
1:E:114:LEU:HA	1:E:114:LEU:HD12	1.87	0.41
1:D:110:TYR:HA	1:D:113:TRP:CE3	2.55	0.41
2:D:302:OLC:C6	2:E:309:OLC:C18	2.98	0.41
1:E:110:TYR:O	1:E:113:TRP:HB2	2.20	0.41
1:A:198:PRO:HD2	6:A:426:HOH:O	2.19	0.41
1:D:22:GLU:HB2	6:E:412:HOH:O	2.21	0.41
1:D:88:PHE:CZ	1:D:93:GLY:HA2	2.55	0.41
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.20	0.41
1:C:110:TYR:HA	1:C:113:TRP:CE3	2.56	0.41
1:D:110:TYR:O	1:D:113:TRP:HB2	2.20	0.41
1:D:255:LYR:H10	1:D:255:LYR:H81	1.88	0.41
1:E:44:LEU:HA	1:E:44:LEU:HD23	1.82	0.41
1:B:110:TYR:HA	1:B:113:TRP:CE3	2.55	0.41
1:B:154:TYR:O	1:B:157:GLN:HG3	2.21	0.41
1:B:44:LEU:HD21	1:C:65:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:LEU:O	1:C:118:PRO:HG2	2.21	0.41
1:D:101:GLY:O	1:D:102:ASP:HB2	2.21	0.41
1:E:114:LEU:O	1:E:118:PRO:HG2	2.21	0.41
1:B:235:TYR:CD1	5:B:321:BOG:H62	2.56	0.41
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.81	0.41
1:C:56:LYS:HD3	1:C:57:PHE:CE1	2.56	0.41
1:C:255:LYR:H81	1:C:255:LYR:H10	1.90	0.40
2:A:310:OLC:C9	2:A:311:OLC:H21	2.52	0.40
1:B:64:SER:O	1:B:68:MET:HG2	2.21	0.40
1:A:154:TYR:O	1:A:157:GLN:HG3	2.20	0.40
1:A:64:SER:O	1:A:68:MET:HG2	2.21	0.40
1:B:255:LYR:H81	1:B:255:LYR:H10	1.89	0.40
1:B:139:ARG:HH11	2:B:301:OLC:H24A	1.86	0.40
1:D:31:ILE:HA	1:D:31:ILE:HD12	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	270/288 (94%)	265 (98%)	5 (2%)	0	100	100
1	B	270/288 (94%)	264 (98%)	6 (2%)	0	100	100
1	C	270/288 (94%)	265 (98%)	5 (2%)	0	100	100
1	D	270/288 (94%)	265 (98%)	5 (2%)	0	100	100
1	E	270/288 (94%)	265 (98%)	4 (2%)	1 (0%)	34	48
All	All	1350/1440 (94%)	1324 (98%)	25 (2%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	272	ASN

5.3.2 Protein sidechains ⓘ

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	230/248 (93%)	222 (96%)	8 (4%)	36	55
1	B	230/248 (93%)	223 (97%)	7 (3%)	41	61
1	C	230/248 (93%)	222 (96%)	8 (4%)	36	55
1	D	228/248 (92%)	224 (98%)	4 (2%)	59	76
1	E	229/248 (92%)	222 (97%)	7 (3%)	40	60
All	All	1147/1240 (92%)	1113 (97%)	34 (3%)	41	61

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	91	GLU
1	A	92	VAL
1	A	111	LEU
1	A	230	VAL
1	A	270	SER
1	A	272	ASN
1	A	273	LYS
1	B	92	VAL
1	B	111	LEU
1	B	137	SER
1	B	164	LEU
1	B	230	VAL
1	B	272	ASN
1	B	275	LEU
1	C	3	GLN
1	C	44	LEU
1	C	51	LYS
1	C	111	LEU

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Mol	Chain	Res	Type
1	C	132	THR
1	C	230	VAL
1	C	273	LYS
1	C	274	GLU
1	D	92	VAL
1	D	111	LEU
1	D	230	VAL
1	D	270	SER
1	E	44	LEU
1	E	55	LYS
1	E	111	LEU
1	E	114	LEU
1	E	230	VAL
1	E	270	SER
1	E	275	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	ASN
1	B	180	HIS
1	B	272	ASN
1	C	3	GLN
1	C	180	HIS
1	D	3	GLN
1	D	180	HIS
1	E	180	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LYR	E	255	1	27,29,30	0.66	0	30,37,39	1.87	8 (26%)
1	LYR	B	255	1	27,29,30	0.62	0	30,37,39	1.85	8 (26%)
1	LYR	D	255	1	27,29,30	0.62	0	30,37,39	1.86	8 (26%)
1	LYR	A	255	1	27,29,30	0.63	0	30,37,39	1.82	8 (26%)
1	LYR	C	255	1	27,29,30	0.61	0	30,37,39	1.84	8 (26%)

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
1	LYR	E	255	1	-	3/22/40/42	0/1/1/1
1	LYR	B	255	1	-	4/22/40/42	0/1/1/1
1	LYR	D	255	1	-	4/22/40/42	0/1/1/1
1	LYR	A	255	1	-	4/22/40/42	0/1/1/1
1	LYR	C	255	1	-	3/22/40/42	0/1/1/1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	255	LYR	C1-NZ-CE	5.37	121.84	113.33
1	D	255	LYR	C1-NZ-CE	5.33	121.78	113.33
1	C	255	LYR	C1-NZ-CE	5.31	121.75	113.33
1	B	255	LYR	C1-NZ-CE	5.02	121.28	113.33
1	A	255	LYR	C1-NZ-CE	4.54	120.52	113.33
1	E	255	LYR	C13-C12-C11	-4.34	119.66	124.53
1	A	255	LYR	C13-C12-C11	-4.29	119.70	124.53
1	C	255	LYR	C13-C12-C11	-4.27	119.73	124.53
1	B	255	LYR	C13-C12-C11	-4.14	119.88	124.53
1	D	255	LYR	C13-C12-C11	-4.09	119.94	124.53
1	A	255	LYR	C10-C9-C80	-3.05	121.63	126.23
1	D	255	LYR	C10-C9-C80	-3.00	121.70	126.23
1	B	255	LYR	C10-C9-C80	-2.91	121.83	126.23
1	C	255	LYR	C10-C9-C80	-2.76	122.06	126.23
1	B	255	LYR	C1-C2-C3	-2.57	122.04	126.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	255	LYR	C10-C9-C80	-2.52	122.42	126.23
1	E	255	LYR	C1-C2-C3	-2.48	122.21	126.97
1	A	255	LYR	C1-C2-C3	-2.46	122.26	126.97
1	B	255	LYR	C7-C6-C5	-2.43	115.63	123.22
1	C	255	LYR	C1-C2-C3	-2.38	122.41	126.97
1	A	255	LYR	C7-C6-C5	-2.35	115.87	123.22
1	D	255	LYR	C6-C7-C80	-2.31	124.01	127.31
1	E	255	LYR	C8-C80-C9	2.31	121.72	118.08
1	D	255	LYR	C1-C2-C3	-2.30	122.55	126.97
1	D	255	LYR	C4-C3-C5	2.30	121.70	118.08
1	B	255	LYR	C8-C80-C9	2.29	121.68	118.08
1	C	255	LYR	C6-C7-C80	-2.26	124.09	127.31
1	D	255	LYR	C7-C6-C5	-2.25	116.18	123.22
1	A	255	LYR	C6-C7-C80	-2.22	124.14	127.31
1	E	255	LYR	C7-C6-C5	-2.22	116.28	123.22
1	B	255	LYR	C4-C3-C5	2.21	121.55	118.08
1	C	255	LYR	C4-C3-C5	2.20	121.55	118.08
1	A	255	LYR	C8-C80-C9	2.19	121.53	118.08
1	B	255	LYR	C6-C7-C80	-2.19	124.19	127.31
1	D	255	LYR	C8-C80-C9	2.18	121.50	118.08
1	C	255	LYR	C8-C80-C9	2.15	121.46	118.08
1	E	255	LYR	C6-C7-C80	-2.13	124.27	127.31
1	C	255	LYR	C7-C6-C5	-2.09	116.70	123.22
1	A	255	LYR	C4-C3-C5	2.07	121.35	118.08
1	E	255	LYR	C4-C3-C5	2.05	121.30	118.08

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	255	LYR	C2-C1-NZ-CE
1	A	255	LYR	C2-C1-NZ-CE
1	C	255	LYR	C2-C1-NZ-CE
1	B	255	LYR	C2-C1-NZ-CE
1	D	255	LYR	C2-C1-NZ-CE
1	D	255	LYR	CE-CD-CG-CB
1	A	255	LYR	CE-CD-CG-CB
1	C	255	LYR	CE-CD-CG-CB
1	B	255	LYR	CE-CD-CG-CB
1	E	255	LYR	CE-CD-CG-CB
1	E	255	LYR	CD-CE-NZ-C1
1	A	255	LYR	CD-CE-NZ-C1

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Mol	Chain	Res	Type	Atoms
1	B	255	LYR	CG-CD-CE-NZ
1	A	255	LYR	CG-CD-CE-NZ
1	B	255	LYR	CD-CE-NZ-C1
1	D	255	LYR	CD-CE-NZ-C1
1	D	255	LYR	CG-CD-CE-NZ
1	C	255	LYR	CD-CE-NZ-C1

There are no ring outliers.

5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	255	LYR	4	0
1	B	255	LYR	5	0
1	D	255	LYR	5	0
1	A	255	LYR	4	0
1	C	255	LYR	5	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 103 ligands modelled in this entry, 5 are monoatomic - leaving 98 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	$\# Z > 2$
2	OLC	B	312	-	15,15,24	1.13	1 (6%)	16,16,25	0.92	1 (6%)
2	OLC	C	312	-	15,15,24	1.21	1 (6%)	16,16,25	1.01	1 (6%)
3	LFA	D	310	-	19,19,19	0.29	0	18,18,18	0.53	0
2	OLC	A	306	-	14,14,24	1.22	1 (7%)	15,15,25	0.99	1 (6%)
5	BOG	B	321	-	20,20,20	0.60	1 (5%)	25,25,25	0.61	0
3	LFA	D	312	-	7,7,19	0.29	0	6,6,18	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	B	315	-	15,15,24	1.26	1 (6%)	16,16,25	0.96	1 (6%)
3	LFA	B	318	-	9,9,19	0.31	0	8,8,18	0.49	0
3	LFA	E	322	-	3,3,19	0.37	0	2,2,18	0.60	0
2	OLC	E	311	-	10,10,24	1.47	1 (10%)	11,11,25	1.19	2 (18%)
5	BOG	D	317	-	20,20,20	0.54	0	25,25,25	0.70	0
2	OLC	B	301	-	24,24,24	0.95	1 (4%)	25,25,25	0.89	1 (4%)
2	OLC	D	308	-	14,14,24	1.24	1 (7%)	15,15,25	0.91	1 (6%)
3	LFA	B	302	-	19,19,19	0.36	0	18,18,18	0.39	0
2	OLC	E	306	-	23,23,24	0.99	1 (4%)	24,24,25	0.84	1 (4%)
2	OLC	D	304	-	17,17,24	1.13	1 (5%)	18,18,25	1.05	1 (5%)
2	OLC	B	314	-	14,14,24	1.26	1 (7%)	15,15,25	0.99	1 (6%)
2	OLC	E	313	-	19,19,24	1.09	1 (5%)	20,20,25	0.98	1 (5%)
3	LFA	D	315	-	5,5,19	0.33	0	4,4,18	0.28	0
2	OLC	A	308	-	24,24,24	0.97	1 (4%)	25,25,25	0.87	1 (4%)
3	LFA	D	311	-	19,19,19	0.26	0	18,18,18	0.55	0
2	OLC	C	309	-	15,15,24	1.23	1 (6%)	16,16,25	1.08	1 (6%)
3	LFA	C	316	-	19,19,19	0.28	0	18,18,18	0.50	0
2	OLC	E	314	-	24,24,24	0.95	1 (4%)	25,25,25	0.85	1 (4%)
3	LFA	A	318	-	19,19,19	0.28	0	18,18,18	0.51	0
3	LFA	E	302	-	19,19,19	0.38	0	18,18,18	0.36	0
2	OLC	E	312	-	24,24,24	0.98	1 (4%)	25,25,25	0.84	1 (4%)
3	LFA	C	318	-	3,3,19	0.34	0	2,2,18	0.66	0
5	BOG	A	320	-	20,20,20	0.55	0	25,25,25	0.64	0
5	BOG	E	321	-	20,20,20	0.54	0	25,25,25	0.53	0
2	OLC	A	310	-	15,15,24	1.17	1 (6%)	16,16,25	0.92	1 (6%)
2	OLC	B	309	-	20,20,24	1.05	1 (5%)	21,21,25	0.99	1 (4%)
2	OLC	B	311	-	24,24,24	0.97	1 (4%)	25,25,25	0.84	2 (8%)
2	OLC	A	307	-	15,15,24	1.20	1 (6%)	16,16,25	1.27	2 (12%)
2	OLC	D	306	-	24,24,24	1.00	1 (4%)	25,25,25	0.91	1 (4%)
2	OLC	B	313	-	16,16,24	1.17	1 (6%)	17,17,25	0.97	1 (5%)
2	OLC	D	303	-	24,24,24	0.97	1 (4%)	25,25,25	0.91	1 (4%)
2	OLC	E	310	-	14,14,24	1.22	1 (7%)	15,15,25	0.93	1 (6%)
3	LFA	A	314	-	7,7,19	0.27	0	6,6,18	0.44	0
2	OLC	B	303	-	13,13,24	1.26	1 (7%)	14,14,25	1.08	1 (7%)
2	OLC	C	313	-	15,15,24	1.25	1 (6%)	16,16,25	1.07	1 (6%)
3	LFA	C	302	-	19,19,19	0.39	0	18,18,18	0.29	0
3	LFA	A	316	-	3,3,19	0.38	0	2,2,18	0.60	0
2	OLC	E	303	-	13,13,24	1.29	1 (7%)	14,14,25	1.05	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	C	315	-	7,7,19	0.28	0	6,6,18	0.36	0
2	OLC	B	305	-	14,14,24	1.24	1 (7%)	15,15,25	0.97	1 (6%)
3	LFA	E	315	-	7,7,19	0.27	0	6,6,18	0.48	0
2	OLC	E	309	-	24,24,24	0.92	1 (4%)	25,25,25	0.87	2 (8%)
2	OLC	A	321	-	24,24,24	0.95	1 (4%)	25,25,25	0.86	1 (4%)
3	LFA	C	317	-	10,10,19	0.31	0	9,9,18	0.48	0
2	OLC	C	307	-	24,24,24	0.97	1 (4%)	25,25,25	0.89	1 (4%)
3	LFA	C	314	-	6,6,19	0.33	0	5,5,18	0.34	0
2	OLC	D	309	-	24,24,24	0.96	1 (4%)	25,25,25	0.77	1 (4%)
2	OLC	E	305	-	23,23,24	0.95	1 (4%)	24,24,25	0.95	2 (8%)
2	OLC	A	311	-	15,15,24	1.24	1 (6%)	16,16,25	1.00	1 (6%)
2	OLC	D	307	-	13,13,24	1.24	1 (7%)	14,14,25	1.05	2 (14%)
2	OLC	B	304	-	24,24,24	0.98	1 (4%)	25,25,25	0.86	1 (4%)
2	OLC	C	304	-	20,20,24	1.06	1 (5%)	21,21,25	0.89	1 (4%)
2	OLC	A	304	-	24,24,24	0.97	1 (4%)	25,25,25	0.83	1 (4%)
2	OLC	E	308	-	14,14,24	1.24	1 (7%)	15,15,25	1.05	1 (6%)
2	OLC	C	301	-	20,20,24	0.97	1 (5%)	21,21,25	0.95	1 (4%)
2	OLC	C	305	-	22,22,24	0.98	1 (4%)	23,23,25	0.89	2 (8%)
3	LFA	E	316	-	13,13,19	0.28	0	12,12,18	0.50	0
3	LFA	A	317	-	5,5,19	0.27	0	4,4,18	0.35	0
3	LFA	E	317	-	3,3,19	0.34	0	2,2,18	0.65	0
3	LFA	B	316	-	8,8,19	0.30	0	7,7,18	0.44	0
3	LFA	B	317	-	7,7,19	0.27	0	6,6,18	0.46	0
2	OLC	B	306	-	19,19,24	1.07	1 (5%)	20,20,25	0.88	1 (5%)
3	LFA	B	319	-	6,6,19	0.31	0	5,5,18	0.35	0
3	LFA	A	315	-	11,11,19	0.30	0	10,10,18	0.46	0
2	OLC	A	302	-	24,24,24	0.97	1 (4%)	25,25,25	0.82	1 (4%)
2	OLC	A	305	-	12,12,24	1.31	1 (8%)	13,13,25	1.17	2 (15%)
3	LFA	E	323	-	13,13,19	0.30	0	12,12,18	0.48	0
3	LFA	E	319	-	19,19,19	0.40	0	18,18,18	0.31	0
3	LFA	E	318	-	4,4,19	0.29	0	3,3,18	0.37	0
2	OLC	B	310	-	15,15,24	1.21	1 (6%)	16,16,25	1.01	1 (6%)
2	OLC	B	307	-	23,23,24	0.98	1 (4%)	24,24,25	0.85	1 (4%)
2	OLC	C	306	-	24,24,24	0.97	1 (4%)	25,25,25	0.89	1 (4%)
3	LFA	D	314	-	6,6,19	0.31	0	5,5,18	0.37	0
2	OLC	C	310	-	24,24,24	0.96	1 (4%)	25,25,25	0.82	1 (4%)
5	BOG	C	321	-	20,20,20	0.56	0	25,25,25	0.60	0
2	OLC	E	307	-	19,19,24	1.05	1 (5%)	20,20,25	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	C	308	-	21,21,24	1.01	1 (4%)	22,22,25	0.94	2 (9%)
2	OLC	A	301	-	14,14,24	1.22	1 (7%)	15,15,25	1.00	1 (6%)
2	OLC	D	305	-	22,22,24	0.99	1 (4%)	23,23,25	0.82	1 (4%)
2	OLC	E	301	-	24,24,24	0.95	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	D	301	-	17,17,24	1.13	1 (5%)	18,18,25	1.00	1 (5%)
2	OLC	B	308	-	19,19,24	1.07	1 (5%)	20,20,25	0.95	2 (10%)
2	OLC	A	303	-	21,21,24	0.99	1 (4%)	22,22,25	0.86	2 (9%)
2	OLC	E	304	-	15,15,24	1.18	1 (6%)	16,16,25	1.03	2 (12%)
2	OLC	D	302	-	12,12,24	1.34	1 (8%)	13,13,25	1.10	1 (7%)
2	OLC	A	309	-	14,14,24	1.23	1 (7%)	15,15,25	1.12	2 (13%)
2	OLC	C	311	-	15,15,24	1.18	1 (6%)	16,16,25	0.97	2 (12%)
3	LFA	C	319	-	19,19,19	0.36	0	18,18,18	0.41	0
3	LFA	A	312	-	6,6,19	0.29	0	5,5,18	0.38	0
2	OLC	C	303	-	13,13,24	1.27	1 (7%)	14,14,25	1.03	1 (7%)
3	LFA	D	313	-	16,16,19	0.31	0	15,15,18	0.48	0
3	LFA	A	313	-	7,7,19	0.29	0	6,6,18	0.44	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
2	OLC	B	312	-	-	5/15/15/24	-
2	OLC	C	312	-	-	11/15/15/24	-
3	LFA	D	310	-	-	11/17/17/17	-
2	OLC	A	306	-	-	5/14/14/24	-
5	BOG	B	321	-	-	5/11/31/31	0/1/1/1
3	LFA	D	312	-	-	4/5/5/17	-
2	OLC	B	315	-	-	7/15/15/24	-
3	LFA	B	318	-	-	5/7/7/17	-
3	LFA	E	322	-	-	0/1/1/17	-
2	OLC	E	311	-	-	6/10/10/24	-
5	BOG	D	317	-	-	2/11/31/31	0/1/1/1
2	OLC	B	301	-	-	10/24/24/24	-
2	OLC	D	308	-	-	11/14/14/24	-
3	LFA	B	302	-	-	6/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	E	306	-	-	14/23/23/24	-
2	OLC	D	304	-	-	5/17/17/24	-
2	OLC	B	314	-	-	8/14/14/24	-
2	OLC	E	313	-	-	12/19/19/24	-
3	LFA	D	315	-	-	0/3/3/17	-
2	OLC	A	308	-	-	15/24/24/24	-
3	LFA	D	311	-	-	8/17/17/17	-
2	OLC	C	309	-	-	8/15/15/24	-
3	LFA	C	316	-	-	11/17/17/17	-
2	OLC	E	314	-	-	10/24/24/24	-
3	LFA	A	318	-	-	8/17/17/17	-
3	LFA	E	302	-	-	8/17/17/17	-
2	OLC	E	312	-	-	10/24/24/24	-
3	LFA	C	318	-	-	1/1/1/17	-
5	BOG	A	320	-	-	5/11/31/31	0/1/1/1
5	BOG	E	321	-	-	9/11/31/31	0/1/1/1
2	OLC	A	310	-	-	8/15/15/24	-
2	OLC	B	309	-	-	9/20/20/24	-
2	OLC	B	311	-	-	15/24/24/24	-
2	OLC	A	307	-	-	4/15/15/24	-
2	OLC	D	306	-	-	12/24/24/24	-
2	OLC	B	313	-	-	10/16/16/24	-
2	OLC	D	303	-	-	10/24/24/24	-
2	OLC	E	310	-	-	8/14/14/24	-
3	LFA	A	314	-	-	3/5/5/17	-
2	OLC	B	303	-	-	8/13/13/24	-
2	OLC	C	313	-	-	9/15/15/24	-
3	LFA	C	302	-	-	12/17/17/17	-
3	LFA	A	316	-	-	0/1/1/17	-
2	OLC	E	303	-	-	5/13/13/24	-
3	LFA	C	315	-	-	4/5/5/17	-
2	OLC	B	305	-	-	4/14/14/24	-
3	LFA	E	315	-	-	1/5/5/17	-
2	OLC	E	309	-	-	17/24/24/24	-
2	OLC	A	321	-	-	10/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	C	317	-	-	3/8/8/17	-
2	OLC	C	307	-	-	6/24/24/24	-
3	LFA	C	314	-	-	3/4/4/17	-
2	OLC	D	309	-	-	13/24/24/24	-
2	OLC	E	305	-	-	12/23/23/24	-
2	OLC	A	311	-	-	7/15/15/24	-
2	OLC	D	307	-	-	7/13/13/24	-
2	OLC	B	304	-	-	9/24/24/24	-
2	OLC	C	304	-	-	9/20/20/24	-
2	OLC	A	304	-	-	14/24/24/24	-
2	OLC	E	308	-	-	9/14/14/24	-
2	OLC	C	301	-	-	12/20/20/24	-
2	OLC	C	305	-	-	11/22/22/24	-
3	LFA	E	316	-	-	5/11/11/17	-
3	LFA	A	317	-	-	1/3/3/17	-
3	LFA	E	317	-	-	1/1/1/17	-
3	LFA	B	316	-	-	3/6/6/17	-
3	LFA	B	317	-	-	4/5/5/17	-
2	OLC	B	306	-	-	10/19/19/24	-
3	LFA	B	319	-	-	2/4/4/17	-
3	LFA	A	315	-	-	5/9/9/17	-
2	OLC	A	302	-	-	15/24/24/24	-
2	OLC	A	305	-	-	1/12/12/24	-
3	LFA	E	323	-	-	4/11/11/17	-
3	LFA	E	319	-	-	10/17/17/17	-
3	LFA	E	318	-	-	1/2/2/17	-
2	OLC	B	310	-	-	9/15/15/24	-
2	OLC	B	307	-	-	8/23/23/24	-
2	OLC	C	306	-	-	10/24/24/24	-
3	LFA	D	314	-	-	3/4/4/17	-
2	OLC	C	310	-	-	13/24/24/24	-
5	BOG	C	321	-	-	3/11/31/31	0/1/1/1
2	OLC	E	307	-	-	7/19/19/24	-
2	OLC	C	308	-	-	8/21/21/24	-
2	OLC	A	301	-	-	6/14/14/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	D	305	-	-	7/22/22/24	-
2	OLC	E	301	-	-	13/24/24/24	-
2	OLC	D	301	-	-	9/17/17/24	-
2	OLC	B	308	-	-	6/19/19/24	-
2	OLC	A	303	-	-	7/21/21/24	-
2	OLC	E	304	-	-	6/15/15/24	-
2	OLC	D	302	-	-	7/12/12/24	-
2	OLC	A	309	-	-	8/14/14/24	-
2	OLC	C	311	-	-	7/15/15/24	-
3	LFA	C	319	-	-	9/17/17/17	-
3	LFA	A	312	-	-	3/4/4/17	-
2	OLC	C	303	-	-	9/13/13/24	-
3	LFA	D	313	-	-	9/14/14/17	-
3	LFA	A	313	-	-	1/5/5/17	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	OLC	O20-C1	4.66	1.47	1.33
2	A	311	OLC	O20-C1	4.62	1.46	1.33
2	D	306	OLC	O20-C1	4.62	1.46	1.33
2	C	313	OLC	O20-C1	4.60	1.46	1.33
2	C	309	OLC	O20-C1	4.57	1.46	1.33
2	E	312	OLC	O20-C1	4.56	1.46	1.33
2	E	313	OLC	O20-C1	4.50	1.46	1.33
2	C	304	OLC	O20-C1	4.50	1.46	1.33
2	B	310	OLC	O20-C1	4.48	1.46	1.33
2	A	307	OLC	O20-C1	4.48	1.46	1.33
2	D	303	OLC	O20-C1	4.48	1.46	1.33
2	C	306	OLC	O20-C1	4.47	1.46	1.33
2	E	303	OLC	O20-C1	4.47	1.46	1.33
2	A	304	OLC	O20-C1	4.47	1.46	1.33
2	D	302	OLC	O20-C1	4.47	1.46	1.33
2	B	309	OLC	O20-C1	4.47	1.46	1.33
2	B	314	OLC	O20-C1	4.46	1.46	1.33
2	A	302	OLC	O20-C1	4.46	1.46	1.33
2	E	308	OLC	O20-C1	4.46	1.46	1.33
2	C	312	OLC	O20-C1	4.46	1.46	1.33
2	A	308	OLC	O20-C1	4.46	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	306	OLC	O20-C1	4.45	1.46	1.33
2	B	311	OLC	O20-C1	4.45	1.46	1.33
2	B	305	OLC	O20-C1	4.44	1.46	1.33
2	E	311	OLC	O20-C1	4.43	1.46	1.33
2	A	321	OLC	O20-C1	4.43	1.46	1.33
2	C	307	OLC	O20-C1	4.43	1.46	1.33
2	E	301	OLC	O20-C1	4.42	1.46	1.33
2	B	307	OLC	O20-C1	4.42	1.46	1.33
2	B	304	OLC	O20-C1	4.42	1.46	1.33
2	E	314	OLC	O20-C1	4.41	1.46	1.33
2	D	304	OLC	O20-C1	4.40	1.46	1.33
2	B	301	OLC	O20-C1	4.40	1.46	1.33
2	D	309	OLC	O20-C1	4.39	1.46	1.33
2	A	309	OLC	O20-C1	4.39	1.46	1.33
2	A	301	OLC	O20-C1	4.39	1.46	1.33
2	D	305	OLC	O20-C1	4.39	1.46	1.33
2	C	310	OLC	O20-C1	4.38	1.46	1.33
2	B	308	OLC	O20-C1	4.38	1.46	1.33
2	E	307	OLC	O20-C1	4.38	1.46	1.33
2	C	308	OLC	O20-C1	4.38	1.46	1.33
2	C	303	OLC	O20-C1	4.37	1.46	1.33
2	D	308	OLC	O20-C1	4.37	1.46	1.33
2	A	305	OLC	O20-C1	4.36	1.46	1.33
2	B	313	OLC	O20-C1	4.36	1.46	1.33
2	E	304	OLC	O20-C1	4.36	1.46	1.33
2	D	301	OLC	O20-C1	4.35	1.46	1.33
2	B	306	OLC	O20-C1	4.34	1.46	1.33
2	B	303	OLC	O20-C1	4.32	1.46	1.33
2	C	311	OLC	O20-C1	4.32	1.46	1.33
2	A	306	OLC	O20-C1	4.32	1.46	1.33
2	A	310	OLC	O20-C1	4.32	1.46	1.33
2	E	310	OLC	O20-C1	4.30	1.45	1.33
2	C	305	OLC	O20-C1	4.30	1.45	1.33
2	E	305	OLC	O20-C1	4.26	1.45	1.33
2	D	307	OLC	O20-C1	4.24	1.45	1.33
2	A	303	OLC	O20-C1	4.21	1.45	1.33
2	E	309	OLC	O20-C1	4.19	1.45	1.33
2	C	301	OLC	O20-C1	4.13	1.45	1.33
2	B	312	OLC	O20-C1	4.11	1.45	1.33
5	B	321	BOG	O1-C1	2.22	1.44	1.40

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	307	OLC	O20-C1-C2	3.46	122.77	111.91
2	A	305	OLC	O20-C1-C2	3.08	121.58	111.91
2	E	313	OLC	O20-C1-C2	3.07	121.54	111.91
2	A	309	OLC	O20-C1-C2	3.06	121.51	111.91
2	C	307	OLC	O20-C1-C2	3.04	121.45	111.91
2	C	313	OLC	O20-C1-C2	3.02	121.38	111.91
2	B	309	OLC	O20-C1-C2	3.02	121.37	111.91
2	C	309	OLC	O20-C1-C2	3.00	121.33	111.91
2	C	308	OLC	O20-C1-C2	2.96	121.19	111.91
2	D	304	OLC	O20-C1-C2	2.95	121.16	111.91
2	E	304	OLC	O20-C1-C2	2.91	121.05	111.91
2	C	306	OLC	O20-C1-C2	2.90	121.02	111.91
2	D	303	OLC	O20-C1-C2	2.88	120.96	111.91
2	D	306	OLC	O20-C1-C2	2.87	120.93	111.91
2	C	301	OLC	O20-C1-C2	2.87	120.93	111.91
2	B	304	OLC	O20-C1-C2	2.87	120.90	111.91
2	E	305	OLC	O20-C1-C2	2.86	120.90	111.91
2	D	302	OLC	O20-C1-C2	2.86	120.88	111.91
2	B	303	OLC	O20-C1-C2	2.85	120.84	111.91
2	E	307	OLC	O20-C1-C2	2.85	120.84	111.91
2	D	307	OLC	O20-C1-C2	2.84	120.81	111.91
2	E	311	OLC	O20-C1-C2	2.83	120.80	111.91
2	E	308	OLC	O20-C1-C2	2.83	120.78	111.91
2	B	311	OLC	O20-C1-C2	2.81	120.73	111.91
2	C	305	OLC	O20-C1-C2	2.81	120.73	111.91
2	B	301	OLC	O20-C1-C2	2.80	120.68	111.91
2	E	303	OLC	O20-C1-C2	2.79	120.67	111.91
2	B	308	OLC	O20-C1-C2	2.79	120.67	111.91
2	E	309	OLC	O20-C1-C2	2.77	120.61	111.91
2	A	311	OLC	O20-C1-C2	2.76	120.56	111.91
2	B	310	OLC	O20-C1-C2	2.75	120.55	111.91
2	C	312	OLC	O20-C1-C2	2.74	120.52	111.91
2	A	308	OLC	O20-C1-C2	2.74	120.50	111.91
2	E	306	OLC	O20-C1-C2	2.72	120.45	111.91
2	A	304	OLC	O20-C1-C2	2.72	120.45	111.91
2	A	301	OLC	O20-C1-C2	2.72	120.44	111.91
2	A	302	OLC	O20-C1-C2	2.71	120.41	111.91
2	B	307	OLC	O20-C1-C2	2.71	120.41	111.91
2	C	303	OLC	O20-C1-C2	2.71	120.41	111.91
2	A	303	OLC	O20-C1-C2	2.70	120.39	111.91
2	E	312	OLC	O20-C1-C2	2.69	120.36	111.91
2	E	314	OLC	O20-C1-C2	2.69	120.35	111.91
2	D	301	OLC	O20-C1-C2	2.68	120.33	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	306	OLC	O20-C1-C2	2.67	120.28	111.91
2	C	304	OLC	O20-C1-C2	2.66	120.27	111.91
2	C	311	OLC	O20-C1-C2	2.63	120.16	111.91
2	B	306	OLC	O20-C1-C2	2.62	120.13	111.91
2	A	321	OLC	O20-C1-C2	2.61	120.11	111.91
2	B	305	OLC	O20-C1-C2	2.61	120.10	111.91
2	E	301	OLC	O20-C1-C2	2.61	120.09	111.91
2	B	314	OLC	O20-C1-C2	2.59	120.03	111.91
2	C	310	OLC	O20-C1-C2	2.58	120.00	111.91
2	B	315	OLC	O20-C1-C2	2.57	119.98	111.91
2	B	313	OLC	O20-C1-C2	2.57	119.98	111.91
2	E	310	OLC	O20-C1-C2	2.50	119.74	111.91
2	D	309	OLC	O20-C1-C2	2.45	119.60	111.91
2	A	310	OLC	O20-C1-C2	2.42	119.51	111.91
2	D	308	OLC	O20-C1-C2	2.42	119.49	111.91
2	D	305	OLC	O20-C1-C2	2.41	119.48	111.91
2	B	312	OLC	O20-C1-C2	2.38	119.38	111.91
2	A	309	OLC	O20-C1-O19	-2.30	117.79	123.59
2	E	309	OLC	O20-C1-O19	-2.29	117.81	123.59
2	A	305	OLC	O20-C1-O19	-2.25	117.90	123.59
2	E	304	OLC	O20-C1-O19	-2.22	118.00	123.59
2	A	307	OLC	O20-C1-O19	-2.14	118.19	123.59
2	B	311	OLC	O20-C1-O19	-2.13	118.21	123.59
2	C	311	OLC	O20-C1-O19	-2.11	118.27	123.59
2	E	311	OLC	O20-C1-O19	-2.11	118.28	123.59
2	C	305	OLC	O20-C1-O19	-2.10	118.29	123.59
2	B	308	OLC	O20-C1-O19	-2.08	118.35	123.59
2	D	307	OLC	O20-C1-O19	-2.08	118.35	123.59
2	A	303	OLC	O20-C1-O19	-2.04	118.44	123.59
2	E	305	OLC	O20-C1-O19	-2.04	118.45	123.59
2	C	308	OLC	O20-C1-O19	-2.02	118.50	123.59

There are no chirality outliers.

All (714) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	312	OLC	C21-C22-C24-O25
2	C	312	OLC	O23-C22-C24-O25
2	C	312	OLC	O20-C21-C22-C24
2	C	312	OLC	C2-C1-O20-C21
2	C	312	OLC	O19-C1-O20-C21
2	B	315	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
2	B	315	OLC	O20-C21-C22-O23
2	E	311	OLC	C21-C22-C24-O25
2	D	308	OLC	O20-C21-C22-C24
2	D	308	OLC	O20-C21-C22-O23
2	E	306	OLC	C21-C22-C24-O25
2	B	314	OLC	O20-C21-C22-C24
2	B	314	OLC	O20-C21-C22-O23
2	E	313	OLC	C21-C22-C24-O25
2	A	308	OLC	C21-C22-C24-O25
2	A	308	OLC	O20-C21-C22-O23
2	C	309	OLC	C21-C22-C24-O25
5	A	320	BOG	C2'-C1'-O1-C1
5	E	321	BOG	C2'-C1'-O1-C1
2	A	310	OLC	C21-C22-C24-O25
2	A	310	OLC	O20-C21-C22-C24
2	A	310	OLC	O20-C21-C22-O23
2	B	311	OLC	O20-C21-C22-C24
2	A	307	OLC	O20-C21-C22-C24
2	A	307	OLC	O20-C21-C22-O23
2	B	313	OLC	O20-C21-C22-C24
2	B	313	OLC	O20-C21-C22-O23
2	D	303	OLC	O20-C21-C22-O23
2	E	310	OLC	C21-C22-C24-O25
2	E	310	OLC	O20-C21-C22-O23
2	B	303	OLC	C21-C22-C24-O25
2	C	313	OLC	O20-C21-C22-O23
2	E	309	OLC	O20-C21-C22-C24
2	E	309	OLC	O20-C21-C22-O23
2	C	307	OLC	C21-C22-C24-O25
2	D	309	OLC	C21-C22-C24-O25
2	E	305	OLC	C21-C22-C24-O25
2	E	305	OLC	O20-C21-C22-C24
2	A	311	OLC	C21-C22-C24-O25
2	D	307	OLC	C21-C22-C24-O25
2	E	308	OLC	O20-C21-C22-O23
2	C	301	OLC	C21-C22-C24-O25
2	C	310	OLC	C21-C22-C24-O25
2	E	307	OLC	C10-C11-C12-C13
2	C	308	OLC	C21-C22-C24-O25
2	A	301	OLC	O20-C21-C22-O23
2	B	308	OLC	C10-C11-C12-C13
2	E	304	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
2	D	302	OLC	C21-C22-C24-O25
2	D	302	OLC	O20-C21-C22-C24
2	A	309	OLC	C21-C22-C24-O25
2	C	303	OLC	C21-C22-C24-O25
2	C	303	OLC	O20-C21-C22-O23
2	C	305	OLC	O19-C1-O20-C21
2	A	302	OLC	O19-C1-O20-C21
2	A	309	OLC	O19-C1-O20-C21
2	C	305	OLC	C2-C1-O20-C21
2	B	314	OLC	C2-C1-O20-C21
2	C	304	OLC	C2-C1-O20-C21
2	A	302	OLC	C2-C1-O20-C21
2	A	309	OLC	C2-C1-O20-C21
2	D	309	OLC	O19-C1-O20-C21
2	A	306	OLC	C2-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
2	A	321	OLC	C2-C1-O20-C21
2	D	309	OLC	C2-C1-O20-C21
2	B	308	OLC	C2-C1-O20-C21
2	A	306	OLC	O19-C1-O20-C21
2	B	314	OLC	O19-C1-O20-C21
2	E	309	OLC	O19-C1-O20-C21
2	A	321	OLC	O19-C1-O20-C21
2	C	304	OLC	O19-C1-O20-C21
2	B	312	OLC	C2-C1-O20-C21
2	A	304	OLC	C2-C1-O20-C21
2	C	311	OLC	C2-C1-O20-C21
2	C	312	OLC	O20-C21-C22-O23
2	B	311	OLC	O20-C21-C22-O23
2	C	311	OLC	O20-C21-C22-O23
2	B	301	OLC	O19-C1-O20-C21
2	E	306	OLC	C2-C3-C4-C5
2	E	309	OLC	C2-C1-O20-C21
2	B	308	OLC	O19-C1-O20-C21
2	C	311	OLC	O19-C1-O20-C21
2	B	312	OLC	O19-C1-O20-C21
2	A	304	OLC	O19-C1-O20-C21
2	D	301	OLC	C2-C1-O20-C21
2	D	301	OLC	O19-C1-O20-C21
2	E	311	OLC	C2-C1-O20-C21
2	D	304	OLC	C2-C1-O20-C21
2	A	308	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	C	309	OLC	C2-C1-O20-C21
2	D	303	OLC	C2-C1-O20-C21
2	C	303	OLC	C2-C1-O20-C21
2	E	311	OLC	O20-C21-C22-C24
2	E	310	OLC	O20-C21-C22-C24
2	A	301	OLC	O20-C21-C22-C24
2	C	311	OLC	O20-C21-C22-C24
5	E	321	BOG	C2-C1-O1-C1'
2	E	311	OLC	O19-C1-O20-C21
2	E	311	OLC	O20-C21-C22-O23
2	E	305	OLC	O20-C21-C22-O23
2	D	302	OLC	O20-C21-C22-O23
2	C	310	OLC	C1-C2-C3-C4
2	C	309	OLC	O19-C1-O20-C21
2	D	303	OLC	O19-C1-O20-C21
2	B	311	OLC	C2-C1-O20-C21
2	A	306	OLC	C1-C2-C3-C4
2	B	313	OLC	C1-C2-C3-C4
2	D	307	OLC	C1-C2-C3-C4
2	E	301	OLC	C1-C2-C3-C4
2	D	308	OLC	O23-C22-C24-O25
2	B	305	OLC	O23-C22-C24-O25
2	D	309	OLC	O23-C22-C24-O25
2	C	301	OLC	O23-C22-C24-O25
2	E	304	OLC	O23-C22-C24-O25
2	D	304	OLC	C1-C2-C3-C4
2	E	313	OLC	C1-C2-C3-C4
2	A	304	OLC	C1-C2-C3-C4
2	A	302	OLC	C1-C2-C3-C4
2	A	321	OLC	C2-C3-C4-C5
2	B	306	OLC	C1-C2-C3-C4
2	C	303	OLC	O19-C1-O20-C21
2	D	304	OLC	O19-C1-O20-C21
5	E	321	BOG	O5-C1-O1-C1'
2	B	314	OLC	C1-C2-C3-C4
5	B	321	BOG	O5-C5-C6-O6
5	E	321	BOG	O5-C5-C6-O6
2	E	303	OLC	C2-C1-O20-C21
2	C	301	OLC	C2-C1-O20-C21
2	A	308	OLC	O19-C1-O20-C21
2	B	311	OLC	O19-C1-O20-C21
2	C	310	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	B	304	OLC	C1-C2-C3-C4
5	E	321	BOG	C4-C5-C6-O6
2	E	313	OLC	O20-C21-C22-O23
2	E	303	OLC	O20-C21-C22-O23
2	C	301	OLC	O20-C21-C22-O23
2	B	306	OLC	O20-C21-C22-O23
2	C	306	OLC	O20-C21-C22-O23
2	D	301	OLC	O20-C21-C22-O23
5	B	321	BOG	C4-C5-C6-O6
2	E	305	OLC	C2-C1-O20-C21
5	E	321	BOG	O1-C1'-C2'-C3'
2	D	303	OLC	C5-C6-C7-C8
2	B	313	OLC	C5-C6-C7-C8
2	A	302	OLC	C4-C5-C6-C7
2	B	307	OLC	C3-C4-C5-C6
2	C	310	OLC	C2-C1-O20-C21
2	E	313	OLC	O20-C21-C22-C24
2	C	313	OLC	O20-C21-C22-C24
2	E	303	OLC	O20-C21-C22-C24
2	E	308	OLC	O20-C21-C22-C24
2	B	306	OLC	O20-C21-C22-C24
2	D	301	OLC	O20-C21-C22-C24
2	C	303	OLC	O20-C21-C22-C24
3	B	302	LFA	C16-C17-C18-C19
2	A	308	OLC	C4-C5-C6-C7
2	B	305	OLC	C4-C5-C6-C7
2	C	301	OLC	C5-C6-C7-C8
3	B	316	LFA	C16-C17-C18-C19
3	C	319	LFA	C12-C13-C14-C15
3	D	313	LFA	C7-C8-C9-C10
2	B	314	OLC	C4-C5-C6-C7
2	C	305	OLC	C4-C5-C6-C7
2	B	313	OLC	C4-C5-C6-C7
2	B	304	OLC	C14-C15-C16-C17
2	C	305	OLC	C3-C4-C5-C6
3	A	315	LFA	C11-C10-C9-C8
3	D	312	LFA	C2-C3-C4-C5
2	B	304	OLC	C4-C5-C6-C7
3	B	317	LFA	C2-C3-C4-C5
2	C	310	OLC	C5-C6-C7-C8
3	B	318	LFA	C5-C6-C7-C8
2	A	308	OLC	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	C	316	LFA	C12-C13-C14-C15
2	B	309	OLC	C2-C3-C4-C5
2	D	309	OLC	C2-C3-C4-C5
3	B	317	LFA	C3-C4-C5-C6
2	B	306	OLC	C5-C6-C7-C8
3	D	314	LFA	C16-C17-C18-C19
2	D	305	OLC	C5-C6-C7-C8
2	A	303	OLC	C3-C4-C5-C6
3	C	319	LFA	C9-C10-C11-C12
2	E	305	OLC	O19-C1-O20-C21
5	E	321	BOG	C2'-C3'-C4'-C5'
2	D	309	OLC	C11-C12-C13-C14
2	C	310	OLC	C2-C3-C4-C5
3	D	310	LFA	C6-C7-C8-C9
2	A	302	OLC	C11-C12-C13-C14
3	E	319	LFA	C6-C7-C8-C9
2	D	305	OLC	C3-C4-C5-C6
2	C	311	OLC	C3-C4-C5-C6
2	C	301	OLC	O19-C1-O20-C21
2	E	306	OLC	C5-C6-C7-C8
3	A	318	LFA	C11-C12-C13-C14
2	A	302	OLC	C5-C6-C7-C8
3	D	314	LFA	C15-C16-C17-C18
3	C	319	LFA	C10-C11-C12-C13
2	D	308	OLC	C21-C22-C24-O25
2	B	314	OLC	C21-C22-C24-O25
2	D	306	OLC	C21-C22-C24-O25
2	B	305	OLC	C21-C22-C24-O25
2	E	309	OLC	C21-C22-C24-O25
2	A	304	OLC	C21-C22-C24-O25
2	E	308	OLC	C21-C22-C24-O25
2	C	305	OLC	C21-C22-C24-O25
2	A	302	OLC	C21-C22-C24-O25
2	B	310	OLC	C21-C22-C24-O25
2	E	301	OLC	C21-C22-C24-O25
2	B	310	OLC	O20-C21-C22-O23
2	E	309	OLC	C2-C3-C4-C5
3	D	313	LFA	C15-C16-C17-C18
2	A	308	OLC	C10-C11-C12-C13
2	A	321	OLC	C10-C11-C12-C13
2	C	304	OLC	C10-C11-C12-C13
2	A	304	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	C	305	OLC	C10-C11-C12-C13
2	C	310	OLC	C6-C7-C8-C9
2	D	305	OLC	C6-C7-C8-C9
2	E	301	OLC	C10-C11-C12-C13
2	A	303	OLC	C6-C7-C8-C9
2	D	302	OLC	C1-C2-C3-C4
2	A	308	OLC	C11-C12-C13-C14
3	A	314	LFA	C16-C17-C18-C19
2	D	309	OLC	C13-C14-C15-C16
2	D	309	OLC	C12-C13-C14-C15
2	E	312	OLC	C11-C12-C13-C14
2	B	311	OLC	C4-C5-C6-C7
3	C	315	LFA	C16-C17-C18-C19
2	A	321	OLC	C12-C13-C14-C15
2	E	305	OLC	C3-C4-C5-C6
2	B	306	OLC	C3-C4-C5-C6
3	E	323	LFA	C3-C4-C5-C6
3	A	318	LFA	C5-C6-C7-C8
2	B	311	OLC	C5-C6-C7-C8
2	E	310	OLC	C3-C4-C5-C6
2	D	305	OLC	C4-C5-C6-C7
2	C	303	OLC	C2-C3-C4-C5
2	A	301	OLC	C1-C2-C3-C4
3	D	310	LFA	C3-C4-C5-C6
3	A	318	LFA	C6-C7-C8-C9
3	A	318	LFA	C15-C16-C17-C18
3	C	302	LFA	C3-C4-C5-C6
3	C	319	LFA	C11-C10-C9-C8
3	E	323	LFA	C4-C5-C6-C7
5	B	321	BOG	C1'-C2'-C3'-C4'
3	D	310	LFA	C9-C10-C11-C12
2	A	321	OLC	C5-C6-C7-C8
2	D	307	OLC	C2-C3-C4-C5
3	E	319	LFA	C16-C17-C18-C19
2	E	303	OLC	O19-C1-O20-C21
3	E	319	LFA	C13-C14-C15-C16
3	D	312	LFA	C4-C5-C6-C7
2	B	304	OLC	C3-C4-C5-C6
2	B	310	OLC	C2-C3-C4-C5
3	B	302	LFA	C7-C8-C9-C10
2	C	308	OLC	C11-C12-C13-C14
2	E	306	OLC	O23-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
2	E	313	OLC	O23-C22-C24-O25
2	A	308	OLC	O23-C22-C24-O25
2	C	309	OLC	O23-C22-C24-O25
2	E	310	OLC	O23-C22-C24-O25
2	B	303	OLC	O23-C22-C24-O25
2	E	309	OLC	O23-C22-C24-O25
2	C	307	OLC	O23-C22-C24-O25
2	A	311	OLC	O23-C22-C24-O25
2	D	307	OLC	O23-C22-C24-O25
2	A	302	OLC	O23-C22-C24-O25
2	B	310	OLC	O23-C22-C24-O25
2	C	310	OLC	O23-C22-C24-O25
2	C	308	OLC	O23-C22-C24-O25
2	D	302	OLC	O23-C22-C24-O25
2	A	309	OLC	O23-C22-C24-O25
2	C	303	OLC	O23-C22-C24-O25
2	D	304	OLC	C5-C6-C7-C8
3	E	302	LFA	C7-C8-C9-C10
2	E	308	OLC	C4-C5-C6-C7
2	E	307	OLC	C3-C4-C5-C6
2	B	301	OLC	C10-C11-C12-C13
2	E	306	OLC	C6-C7-C8-C9
2	E	313	OLC	C6-C7-C8-C9
2	C	304	OLC	C6-C7-C8-C9
2	D	301	OLC	C6-C7-C8-C9
2	B	311	OLC	C1-C2-C3-C4
2	B	303	OLC	C1-C2-C3-C4
2	E	307	OLC	C5-C6-C7-C8
2	C	305	OLC	C12-C13-C14-C15
3	B	316	LFA	C14-C15-C16-C17
2	C	310	OLC	O19-C1-O20-C21
2	E	305	OLC	C11-C12-C13-C14
2	C	311	OLC	C4-C5-C6-C7
2	E	314	OLC	C12-C13-C14-C15
2	A	310	OLC	C4-C5-C6-C7
2	B	307	OLC	C4-C5-C6-C7
2	D	309	OLC	C1-C2-C3-C4
3	A	318	LFA	C9-C10-C11-C12
2	C	306	OLC	C3-C4-C5-C6
2	B	305	OLC	C2-C3-C4-C5
3	B	319	LFA	C15-C16-C17-C18
5	D	317	BOG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
2	E	309	OLC	C3-C4-C5-C6
2	C	301	OLC	C4-C5-C6-C7
2	B	310	OLC	C4-C5-C6-C7
5	D	317	BOG	C1'-C2'-C3'-C4'
2	B	311	OLC	C11-C12-C13-C14
3	C	302	LFA	C15-C16-C17-C18
2	E	307	OLC	C4-C5-C6-C7
2	D	306	OLC	C6-C7-C8-C9
2	E	309	OLC	C6-C7-C8-C9
2	C	307	OLC	C6-C7-C8-C9
2	B	307	OLC	C6-C7-C8-C9
2	A	303	OLC	C10-C11-C12-C13
2	D	306	OLC	C1-C2-C3-C4
2	D	301	OLC	C1-C2-C3-C4
2	E	304	OLC	C2-C1-O20-C21
2	A	302	OLC	C12-C13-C14-C15
2	C	306	OLC	C14-C15-C16-C17
2	A	303	OLC	C4-C5-C6-C7
3	C	302	LFA	C7-C8-C9-C10
3	E	316	LFA	C14-C15-C16-C17
3	E	323	LFA	C2-C3-C4-C5
2	B	310	OLC	C1-C2-C3-C4
2	E	312	OLC	O20-C21-C22-C24
2	A	309	OLC	O20-C21-C22-C24
2	C	312	OLC	C2-C3-C4-C5
3	B	302	LFA	C6-C7-C8-C9
3	B	316	LFA	C15-C16-C17-C18
2	E	314	OLC	C2-C1-O20-C21
3	C	316	LFA	C15-C16-C17-C18
3	C	317	LFA	C4-C5-C6-C7
3	D	313	LFA	C9-C10-C11-C12
3	C	302	LFA	C16-C17-C18-C19
3	C	317	LFA	C3-C4-C5-C6
3	E	319	LFA	C14-C15-C16-C17
3	C	302	LFA	C9-C10-C11-C12
2	E	314	OLC	C5-C6-C7-C8
2	B	310	OLC	C5-C6-C7-C8
2	A	308	OLC	C6-C7-C8-C9
2	B	309	OLC	C10-C11-C12-C13
2	E	309	OLC	C10-C11-C12-C13
2	C	308	OLC	C6-C7-C8-C9
2	C	306	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	E	309	OLC	C1-C2-C3-C4
2	C	309	OLC	C2-C3-C4-C5
2	E	312	OLC	C4-C5-C6-C7
2	A	302	OLC	C3-C4-C5-C6
2	E	301	OLC	C14-C15-C16-C17
5	C	321	BOG	C1'-C2'-C3'-C4'
2	A	304	OLC	C13-C14-C15-C16
3	E	319	LFA	C12-C13-C14-C15
2	E	301	OLC	C4-C5-C6-C7
2	D	305	OLC	C2-C1-O20-C21
2	E	313	OLC	C3-C4-C5-C6
3	D	313	LFA	C13-C14-C15-C16
2	B	307	OLC	C11-C12-C13-C14
2	E	313	OLC	C5-C6-C7-C8
2	A	302	OLC	C2-C3-C4-C5
2	E	314	OLC	C6-C7-C8-C9
2	E	305	OLC	C6-C7-C8-C9
2	E	309	OLC	C11-C12-C13-C14
3	E	302	LFA	C11-C10-C9-C8
2	C	306	OLC	C5-C6-C7-C8
2	E	314	OLC	C13-C14-C15-C16
2	B	306	OLC	C4-C5-C6-C7
5	B	321	BOG	C5'-C6'-C7'-C8'
3	C	316	LFA	C16-C17-C18-C19
2	A	310	OLC	C6-C7-C8-C9
3	E	318	LFA	C17-C18-C19-C20
2	C	312	OLC	C6-C7-C8-C9
3	D	310	LFA	C11-C10-C9-C8
2	B	301	OLC	C15-C16-C17-C18
5	C	321	BOG	C5'-C6'-C7'-C8'
2	B	315	OLC	O23-C22-C24-O25
2	E	311	OLC	O23-C22-C24-O25
2	E	305	OLC	O23-C22-C24-O25
3	B	318	LFA	C7-C8-C9-C10
3	D	311	LFA	C11-C12-C13-C14
2	B	311	OLC	C10-C11-C12-C13
2	C	301	OLC	C10-C11-C12-C13
2	E	314	OLC	O19-C1-O20-C21
2	E	304	OLC	O19-C1-O20-C21
2	E	306	OLC	C13-C14-C15-C16
3	D	312	LFA	C5-C6-C7-C8
2	B	315	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	E	306	OLC	C11-C12-C13-C14
2	E	301	OLC	C5-C6-C7-C8
2	D	303	OLC	O20-C21-C22-C24
3	D	311	LFA	C1-C2-C3-C4
5	E	321	BOG	C5'-C6'-C7'-C8'
2	B	303	OLC	C4-C5-C6-C7
3	A	312	LFA	C15-C16-C17-C18
3	D	313	LFA	C16-C17-C18-C19
3	A	313	LFA	C1-C2-C3-C4
2	D	306	OLC	C4-C5-C6-C7
3	C	315	LFA	C13-C14-C15-C16
2	E	309	OLC	C12-C13-C14-C15
3	C	317	LFA	C1-C2-C3-C4
2	C	310	OLC	C4-C5-C6-C7
2	A	308	OLC	C3-C4-C5-C6
3	C	316	LFA	C9-C10-C11-C12
2	B	304	OLC	C13-C14-C15-C16
3	D	313	LFA	C5-C6-C7-C8
2	D	306	OLC	C2-C1-O20-C21
2	D	309	OLC	C4-C5-C6-C7
2	C	304	OLC	C4-C5-C6-C7
2	C	313	OLC	C4-C5-C6-C7
2	D	305	OLC	O19-C1-O20-C21
2	D	309	OLC	C10-C11-C12-C13
3	A	318	LFA	C1-C2-C3-C4
2	E	312	OLC	C22-C21-O20-C1
2	D	306	OLC	O19-C1-O20-C21
3	C	316	LFA	C13-C14-C15-C16
2	B	311	OLC	C12-C13-C14-C15
2	C	303	OLC	C4-C5-C6-C7
3	C	302	LFA	C13-C14-C15-C16
3	D	314	LFA	C14-C15-C16-C17
2	E	312	OLC	O20-C21-C22-O23
2	C	304	OLC	O20-C21-C22-O23
2	D	308	OLC	C2-C1-O20-C21
2	C	313	OLC	C2-C1-O20-C21
3	D	311	LFA	C10-C11-C12-C13
3	C	315	LFA	C17-C18-C19-C20
2	A	302	OLC	C6-C7-C8-C9
3	D	310	LFA	C16-C17-C18-C19
3	D	311	LFA	C3-C4-C5-C6
2	C	310	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	D	311	LFA	C14-C15-C16-C17
3	C	302	LFA	C2-C3-C4-C5
2	E	309	OLC	C14-C15-C16-C17
2	B	303	OLC	C2-C1-O20-C21
2	A	311	OLC	C2-C1-O20-C21
2	C	301	OLC	C11-C12-C13-C14
3	E	316	LFA	C9-C10-C11-C12
5	E	321	BOG	C1'-C2'-C3'-C4'
2	C	312	OLC	C5-C6-C7-C8
3	B	318	LFA	C1-C2-C3-C4
3	E	316	LFA	C7-C8-C9-C10
2	E	301	OLC	C3-C4-C5-C6
2	C	303	OLC	C3-C4-C5-C6
5	A	320	BOG	C5'-C6'-C7'-C8'
2	C	313	OLC	C2-C3-C4-C5
2	C	308	OLC	C2-C3-C4-C5
2	A	308	OLC	O20-C21-C22-C24
2	C	309	OLC	O20-C21-C22-C24
2	B	310	OLC	O20-C21-C22-C24
2	B	303	OLC	O20-C21-C22-O23
5	A	320	BOG	O1-C1'-C2'-C3'
2	C	305	OLC	C5-C6-C7-C8
2	D	301	OLC	C2-C3-C4-C5
2	D	303	OLC	C1-C2-C3-C4
2	A	311	OLC	C1-C2-C3-C4
2	B	301	OLC	O23-C22-C24-O25
2	D	306	OLC	O23-C22-C24-O25
2	B	313	OLC	C2-C1-O20-C21
2	C	313	OLC	C3-C4-C5-C6
3	C	314	LFA	C4-C5-C6-C7
2	B	311	OLC	C6-C7-C8-C9
3	C	319	LFA	C4-C5-C6-C7
2	E	306	OLC	C3-C4-C5-C6
2	C	310	OLC	C15-C16-C17-C18
2	E	314	OLC	C14-C15-C16-C17
5	C	321	BOG	C3'-C4'-C5'-C6'
2	E	304	OLC	C1-C2-C3-C4
2	C	305	OLC	O20-C21-C22-O23
2	D	308	OLC	C2-C3-C4-C5
2	B	308	OLC	C4-C5-C6-C7
3	C	316	LFA	C4-C5-C6-C7
3	C	316	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	D	310	LFA	C17-C18-C19-C20
3	C	314	LFA	C2-C3-C4-C5
2	C	313	OLC	O19-C1-O20-C21
2	E	304	OLC	C4-C5-C6-C7
2	C	308	OLC	C4-C5-C6-C7
2	B	309	OLC	C5-C6-C7-C8
3	D	310	LFA	C4-C5-C6-C7
2	A	307	OLC	C6-C7-C8-C9
2	B	315	OLC	O20-C21-C22-C24
2	B	309	OLC	O20-C21-C22-C24
3	A	318	LFA	C17-C18-C19-C20
2	B	310	OLC	C3-C4-C5-C6
2	E	313	OLC	C4-C5-C6-C7
3	E	316	LFA	C13-C14-C15-C16
2	E	305	OLC	C10-C11-C12-C13
2	B	304	OLC	C10-C11-C12-C13
2	A	309	OLC	O20-C21-C22-O23
2	D	308	OLC	O19-C1-O20-C21
2	B	303	OLC	O19-C1-O20-C21
2	B	313	OLC	O20-C1-C2-C3
3	D	310	LFA	C7-C8-C9-C10
2	E	312	OLC	C13-C14-C15-C16
2	B	311	OLC	C2-C3-C4-C5
2	A	311	OLC	O19-C1-O20-C21
2	A	306	OLC	C4-C5-C6-C7
2	B	309	OLC	C4-C5-C6-C7
2	B	313	OLC	O19-C1-O20-C21
2	E	312	OLC	O23-C22-C24-O25
2	A	310	OLC	O23-C22-C24-O25
2	C	313	OLC	O23-C22-C24-O25
2	E	308	OLC	O23-C22-C24-O25
2	D	301	OLC	O23-C22-C24-O25
2	D	306	OLC	C10-C11-C12-C13
2	B	303	OLC	C2-C3-C4-C5
3	C	302	LFA	C17-C18-C19-C20
2	E	312	OLC	C14-C15-C16-C17
3	A	317	LFA	C2-C3-C4-C5
2	C	304	OLC	C21-C22-C24-O25
2	A	305	OLC	O20-C21-C22-O23
5	A	320	BOG	C1'-C2'-C3'-C4'
3	A	312	LFA	C16-C17-C18-C19
3	A	315	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	312	LFA	C17-C18-C19-C20
2	C	307	OLC	C12-C13-C14-C15
2	E	306	OLC	C2-C1-O20-C21
2	B	312	OLC	C6-C7-C8-C9
2	A	304	OLC	C5-C6-C7-C8
2	D	306	OLC	C5-C6-C7-C8
2	E	303	OLC	C2-C3-C4-C5
3	B	302	LFA	C5-C6-C7-C8
2	A	307	OLC	C5-C6-C7-C8
3	D	313	LFA	C4-C5-C6-C7
3	E	319	LFA	C9-C10-C11-C12
2	E	305	OLC	C22-C21-O20-C1
2	C	309	OLC	O20-C21-C22-O23
2	A	302	OLC	C14-C15-C16-C17
2	C	306	OLC	C15-C16-C17-C18
2	C	306	OLC	C1-C2-C3-C4
3	C	318	LFA	C17-C18-C19-C20
3	E	317	LFA	C17-C18-C19-C20
3	A	315	LFA	C7-C8-C9-C10
2	D	309	OLC	C5-C6-C7-C8
2	E	301	OLC	C13-C14-C15-C16
2	A	309	OLC	C5-C6-C7-C8
2	A	309	OLC	C2-C3-C4-C5
2	D	308	OLC	C3-C4-C5-C6
3	C	314	LFA	C1-C2-C3-C4
5	B	321	BOG	C3'-C4'-C5'-C6'
2	A	308	OLC	C12-C13-C14-C15
2	C	306	OLC	C13-C14-C15-C16
2	B	315	OLC	C6-C7-C8-C9
2	E	306	OLC	O19-C1-O20-C21
3	C	319	LFA	C15-C16-C17-C18
2	B	314	OLC	O23-C22-C24-O25
3	B	318	LFA	C6-C7-C8-C9
2	E	309	OLC	C15-C16-C17-C18
3	C	302	LFA	C4-C5-C6-C7
2	E	306	OLC	O20-C21-C22-O23
2	C	307	OLC	O20-C21-C22-O23
2	A	308	OLC	C9-C10-C11-C12
2	E	301	OLC	C7-C8-C9-C10
3	E	319	LFA	C7-C8-C9-C10
2	D	307	OLC	C4-C5-C6-C7
2	C	304	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	A	310	OLC	C3-C4-C5-C6
2	D	306	OLC	C3-C4-C5-C6
3	C	302	LFA	C1-C2-C3-C4
2	A	321	OLC	C13-C14-C15-C16
3	D	311	LFA	C16-C17-C18-C19
3	A	314	LFA	C15-C16-C17-C18
2	C	309	OLC	C1-C2-C3-C4
2	C	305	OLC	C9-C10-C11-C12
3	E	315	LFA	C17-C18-C19-C20
3	C	319	LFA	C16-C17-C18-C19
3	C	316	LFA	C2-C3-C4-C5
2	B	301	OLC	C11-C12-C13-C14
3	A	318	LFA	C4-C5-C6-C7
2	D	302	OLC	C3-C4-C5-C6
2	B	301	OLC	C5-C6-C7-C8
2	D	306	OLC	C7-C8-C9-C10
2	D	305	OLC	C9-C10-C11-C12
3	D	311	LFA	C4-C5-C6-C7
3	C	315	LFA	C15-C16-C17-C18
2	E	313	OLC	C2-C1-O20-C21
2	B	301	OLC	C6-C7-C8-C9
2	E	310	OLC	O19-C1-O20-C21
2	E	310	OLC	C2-C1-O20-C21
3	E	316	LFA	C11-C12-C13-C14
5	A	320	BOG	C2'-C3'-C4'-C5'
2	E	301	OLC	C6-C7-C8-C9
2	C	305	OLC	C7-C8-C9-C10
3	E	302	LFA	C5-C6-C7-C8
2	E	313	OLC	O19-C1-O20-C21
2	B	309	OLC	C2-C1-O20-C21
2	E	310	OLC	C5-C6-C7-C8
2	E	314	OLC	C7-C8-C9-C10
2	A	304	OLC	C9-C10-C11-C12
2	C	306	OLC	C7-C8-C9-C10
3	C	316	LFA	C3-C4-C5-C6
2	B	307	OLC	O20-C1-C2-C3
2	B	304	OLC	C5-C6-C7-C8
3	B	318	LFA	C4-C5-C6-C7
3	B	317	LFA	C1-C2-C3-C4
3	E	302	LFA	C4-C5-C6-C7
3	B	317	LFA	C5-C6-C7-C8
2	D	301	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	E	319	LFA	C11-C10-C9-C8
3	E	319	LFA	C11-C12-C13-C14
2	E	301	OLC	C15-C16-C17-C18
2	A	304	OLC	O20-C21-C22-C24
2	A	302	OLC	C10-C11-C12-C13
2	B	309	OLC	C7-C8-C9-C10
2	D	309	OLC	C7-C8-C9-C10
2	A	304	OLC	C7-C8-C9-C10
3	D	312	LFA	C1-C2-C3-C4
2	B	311	OLC	C14-C15-C16-C17
2	B	309	OLC	O19-C1-O20-C21
2	E	305	OLC	C5-C6-C7-C8
2	C	310	OLC	C11-C12-C13-C14
2	E	312	OLC	C15-C16-C17-C18
2	E	313	OLC	C9-C10-C11-C12
2	B	315	OLC	C5-C6-C7-C8
3	D	313	LFA	C10-C11-C12-C13
2	C	307	OLC	C5-C6-C7-C8
3	D	311	LFA	C2-C3-C4-C5
2	A	301	OLC	O19-C1-O20-C21
2	A	301	OLC	C2-C1-O20-C21
2	B	311	OLC	C15-C16-C17-C18
3	C	302	LFA	C12-C13-C14-C15
2	B	307	OLC	O20-C21-C22-C24
3	C	316	LFA	C11-C10-C9-C8
2	C	313	OLC	C21-C22-C24-O25
2	B	306	OLC	C21-C22-C24-O25
3	B	319	LFA	C16-C17-C18-C19
3	D	313	LFA	C11-C10-C9-C8
2	D	303	OLC	C4-C5-C6-C7
2	B	307	OLC	C12-C13-C14-C15
2	A	303	OLC	C2-C3-C4-C5
2	B	301	OLC	C7-C8-C9-C10
2	E	306	OLC	C7-C8-C9-C10
2	B	311	OLC	C9-C10-C11-C12
2	B	304	OLC	C7-C8-C9-C10
2	C	308	OLC	C7-C8-C9-C10
3	E	302	LFA	C14-C15-C16-C17
2	C	304	OLC	O23-C22-C24-O25
2	E	301	OLC	O23-C22-C24-O25
2	D	308	OLC	C4-C5-C6-C7
2	E	308	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
3	D	310	LFA	C14-C15-C16-C17
2	A	301	OLC	C3-C4-C5-C6
2	D	303	OLC	C9-C10-C11-C12
2	E	309	OLC	C9-C10-C11-C12
2	B	307	OLC	C9-C10-C11-C12
2	B	308	OLC	C7-C8-C9-C10
2	B	306	OLC	C10-C11-C12-C13
2	E	308	OLC	O20-C1-C2-C3
3	E	302	LFA	C11-C12-C13-C14
2	A	310	OLC	C2-C3-C4-C5
2	A	304	OLC	C15-C16-C17-C18
2	D	308	OLC	O20-C1-C2-C3
2	E	312	OLC	C7-C8-C9-C10
2	A	321	OLC	C7-C8-C9-C10
2	E	307	OLC	C9-C10-C11-C12
2	E	309	OLC	C13-C14-C15-C16
3	C	319	LFA	C17-C18-C19-C20
2	C	306	OLC	C4-C5-C6-C7
2	E	308	OLC	C2-C1-O20-C21
2	A	304	OLC	O20-C1-C2-C3
2	D	302	OLC	C2-C3-C4-C5
2	B	304	OLC	C9-C10-C11-C12
3	A	314	LFA	C14-C15-C16-C17
3	C	302	LFA	C14-C15-C16-C17
3	E	302	LFA	C17-C18-C19-C20
2	D	303	OLC	C13-C14-C15-C16
2	D	307	OLC	O20-C1-C2-C3
2	D	306	OLC	C9-C10-C11-C12
2	C	301	OLC	C7-C8-C9-C10
2	B	306	OLC	C9-C10-C11-C12
2	A	303	OLC	C9-C10-C11-C12
2	C	312	OLC	O20-C1-C2-C3
2	C	308	OLC	C12-C13-C14-C15
3	D	310	LFA	C13-C14-C15-C16
2	A	304	OLC	C3-C4-C5-C6
2	C	301	OLC	C3-C4-C5-C6
2	E	314	OLC	C9-C10-C11-C12
2	C	311	OLC	C2-C3-C4-C5
3	B	302	LFA	C11-C12-C13-C14
2	E	307	OLC	O20-C21-C22-O23
2	E	314	OLC	C10-C11-C12-C13
2	E	306	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	302	OLC	C9-C10-C11-C12
2	B	308	OLC	C9-C10-C11-C12
2	A	308	OLC	C2-C3-C4-C5
3	D	310	LFA	C15-C16-C17-C18
2	E	307	OLC	C1-C2-C3-C4
2	B	312	OLC	C3-C4-C5-C6
3	C	316	LFA	C14-C15-C16-C17
2	A	321	OLC	C14-C15-C16-C17
2	A	306	OLC	C21-C22-C24-O25
2	B	301	OLC	C21-C22-C24-O25
2	B	309	OLC	O20-C21-C22-O23
3	E	323	LFA	C6-C7-C8-C9
3	E	319	LFA	C15-C16-C17-C18
2	C	312	OLC	O19-C1-C2-C3
2	D	307	OLC	O19-C1-C2-C3
2	A	304	OLC	O19-C1-C2-C3
2	E	308	OLC	O19-C1-C2-C3
3	C	319	LFA	C3-C4-C5-C6
2	D	303	OLC	O20-C1-C2-C3
2	E	301	OLC	C2-C3-C4-C5
2	A	311	OLC	C5-C6-C7-C8
2	E	306	OLC	O20-C1-C2-C3
2	D	308	OLC	O19-C1-C2-C3
2	C	301	OLC	O20-C21-C22-C24
3	B	302	LFA	C17-C18-C19-C20
2	B	313	OLC	O19-C1-C2-C3
2	B	312	OLC	C5-C6-C7-C8
3	E	302	LFA	C15-C16-C17-C18
2	B	306	OLC	C7-C8-C9-C10
2	A	311	OLC	C6-C7-C8-C9
2	D	304	OLC	C3-C4-C5-C6
2	A	321	OLC	C15-C16-C17-C18
3	A	315	LFA	C1-C2-C3-C4
3	A	315	LFA	C9-C10-C11-C12
2	A	303	OLC	O20-C21-C22-O23
2	B	313	OLC	C3-C4-C5-C6

There are no ring outliers.

42 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	306	OLC	1	0

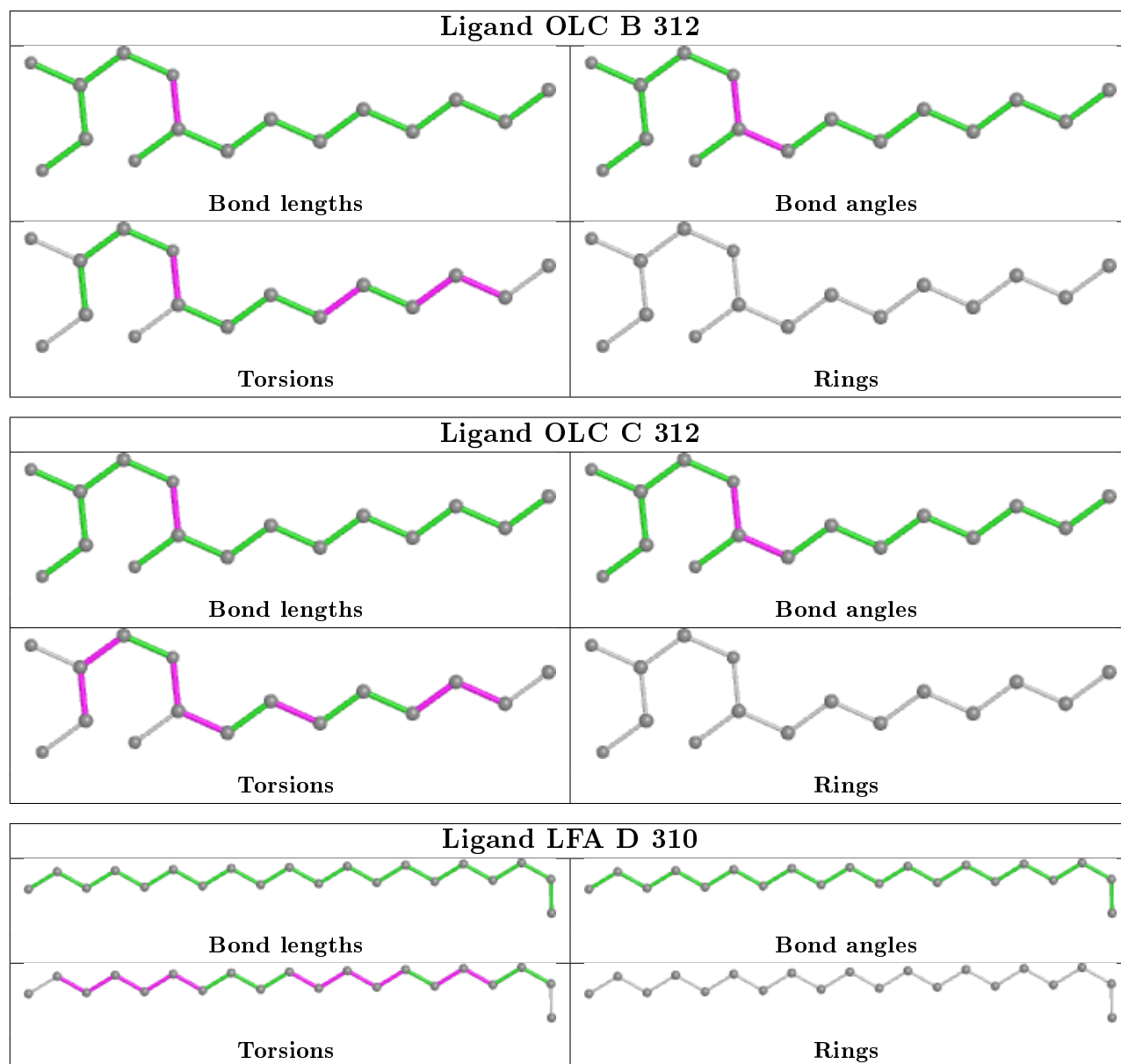
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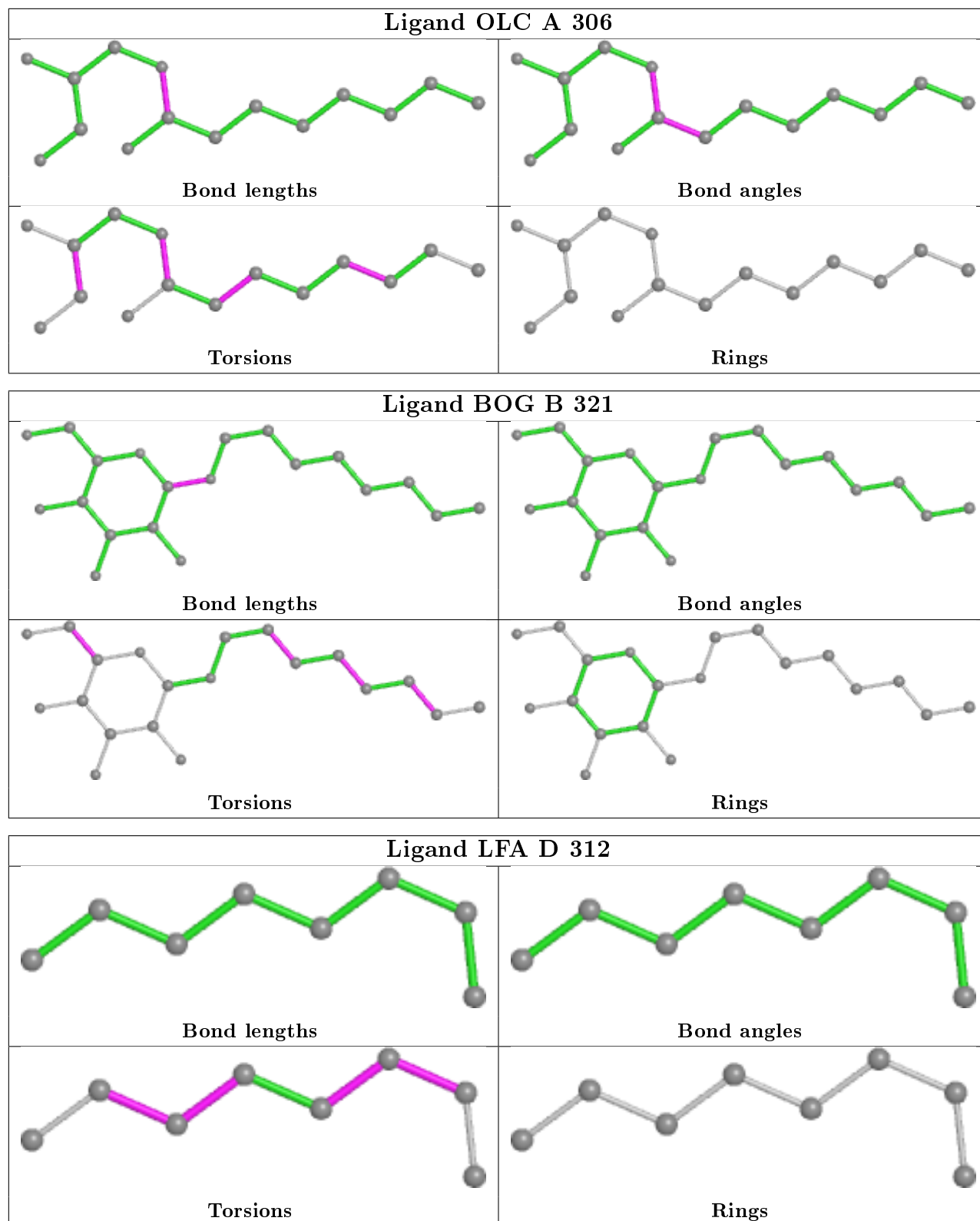
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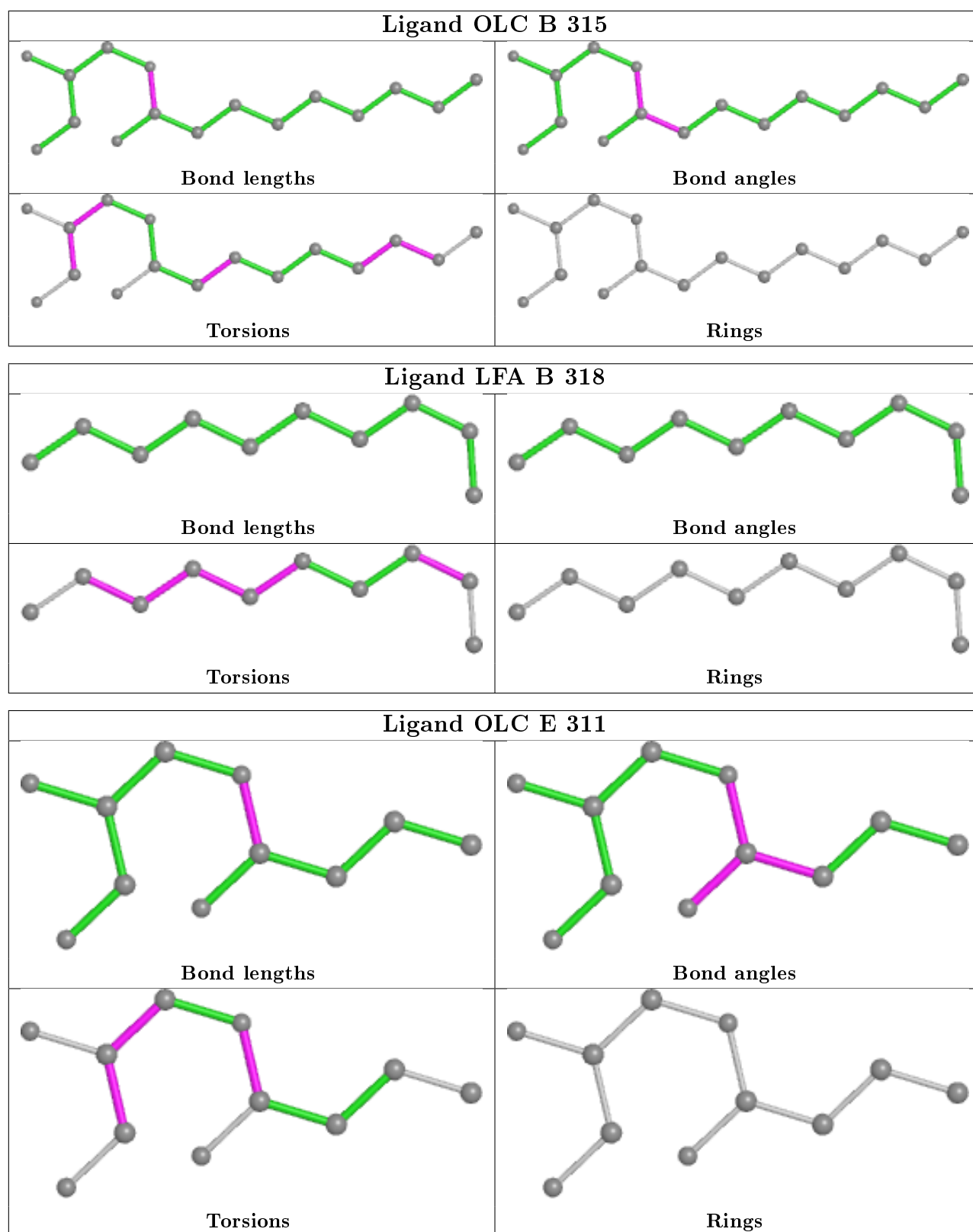
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	321	BOG	4	0
2	B	315	OLC	1	0
5	D	317	BOG	1	0
2	B	301	OLC	4	0
2	E	306	OLC	1	0
2	D	304	OLC	1	0
2	A	308	OLC	1	0
3	D	311	LFA	1	0
2	C	309	OLC	1	0
2	E	312	OLC	4	0
3	C	318	LFA	3	0
5	A	320	BOG	3	0
2	A	310	OLC	1	0
2	A	307	OLC	1	0
2	B	313	OLC	1	0
2	E	310	OLC	1	0
3	C	302	LFA	1	0
2	E	303	OLC	3	0
3	E	315	LFA	3	0
2	E	309	OLC	1	0
3	C	314	LFA	2	0
2	E	305	OLC	3	0
2	A	311	OLC	2	0
2	B	304	OLC	1	0
2	C	304	OLC	2	0
2	A	304	OLC	1	0
2	C	305	OLC	1	0
3	E	316	LFA	2	0
3	E	317	LFA	2	0
3	B	316	LFA	1	0
2	B	306	OLC	1	0
3	A	315	LFA	1	0
2	A	302	OLC	1	0
3	E	323	LFA	1	0
5	C	321	BOG	1	0
2	A	301	OLC	1	0
2	E	301	OLC	2	0
2	E	304	OLC	2	0
2	D	302	OLC	1	0
2	C	311	OLC	1	0
3	D	313	LFA	2	0

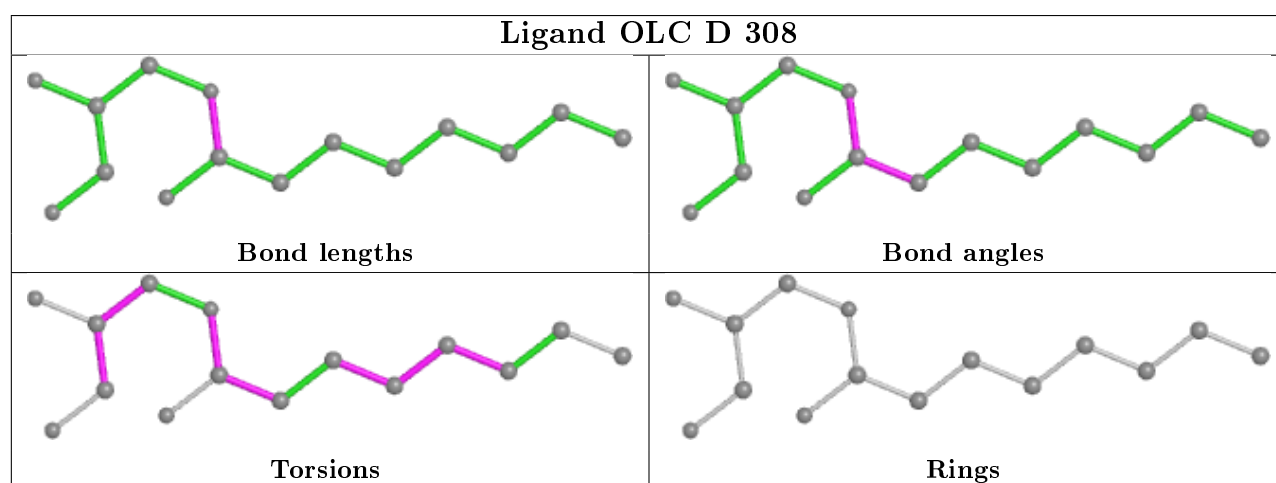
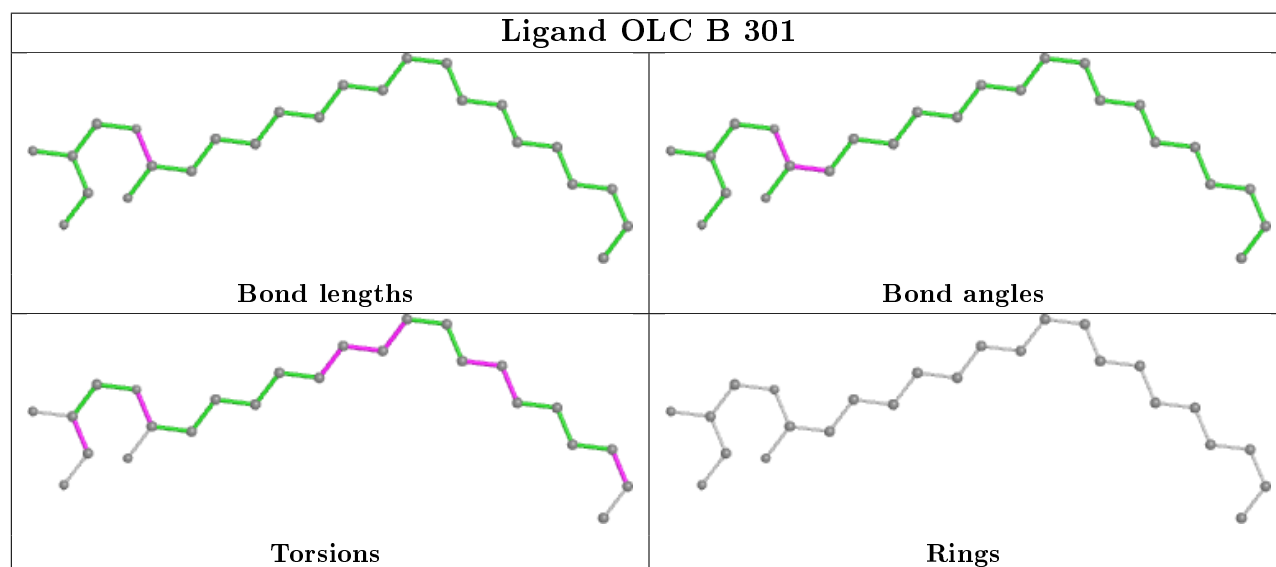
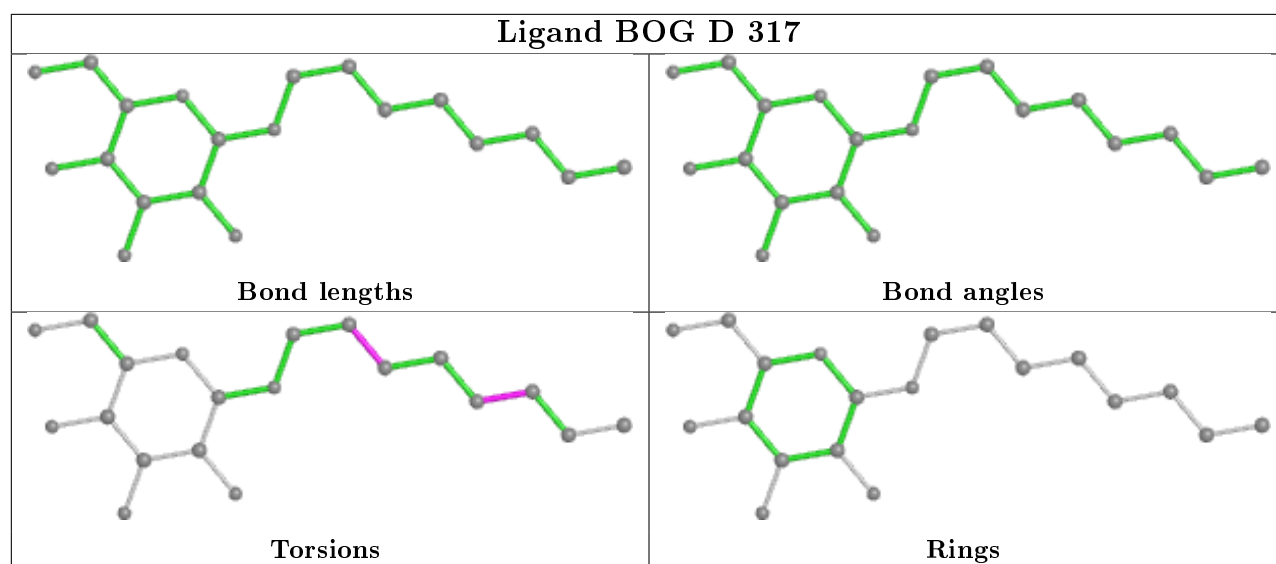
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

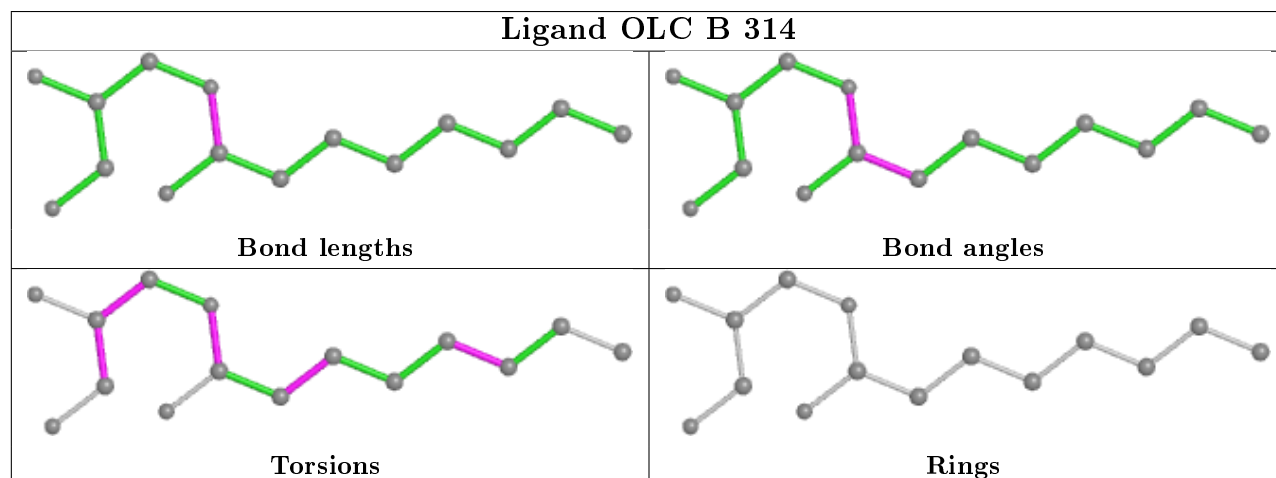
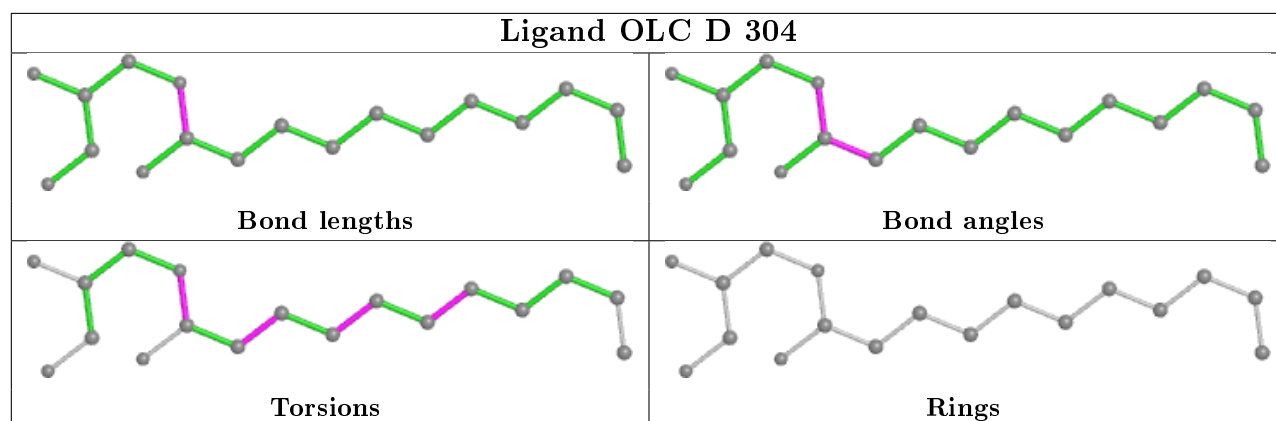
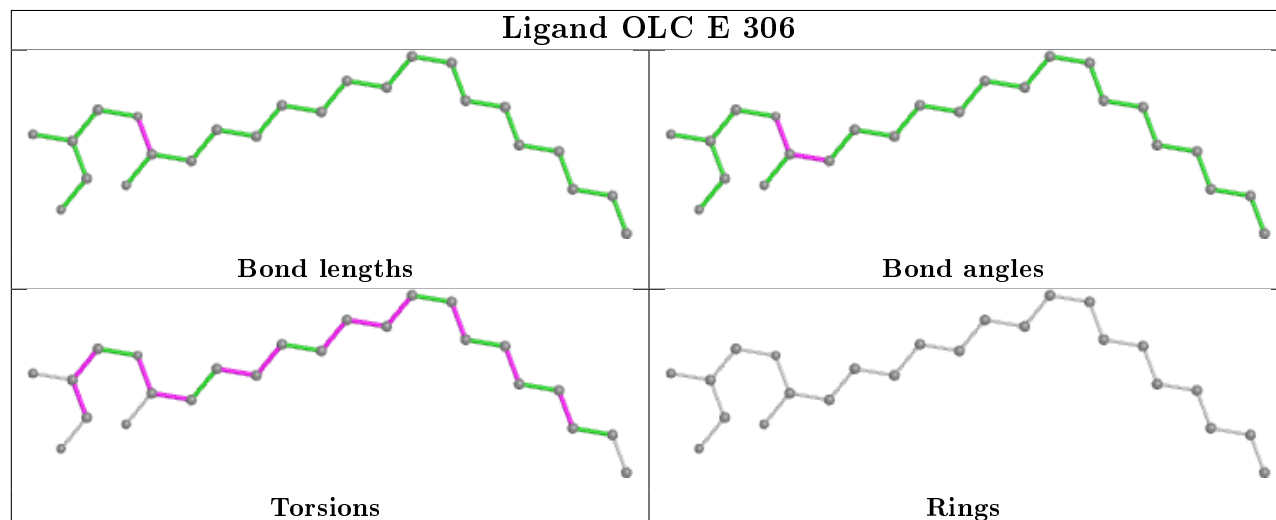
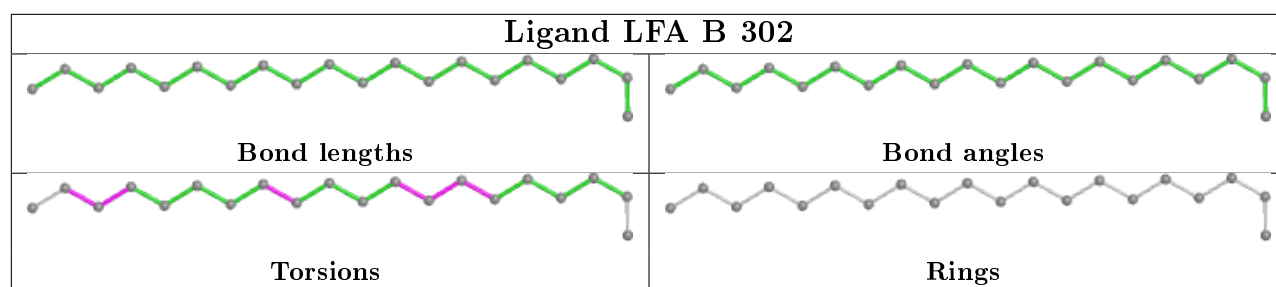
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

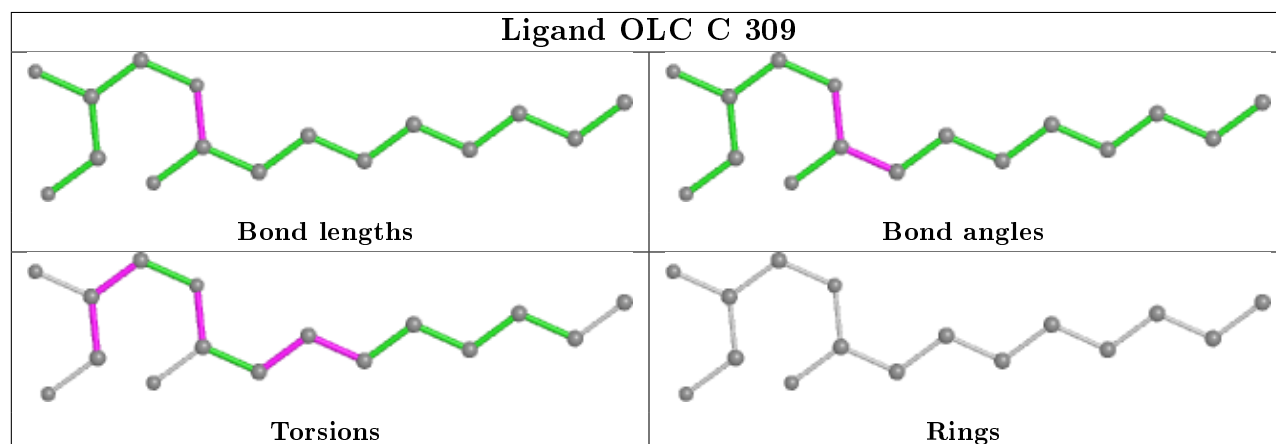
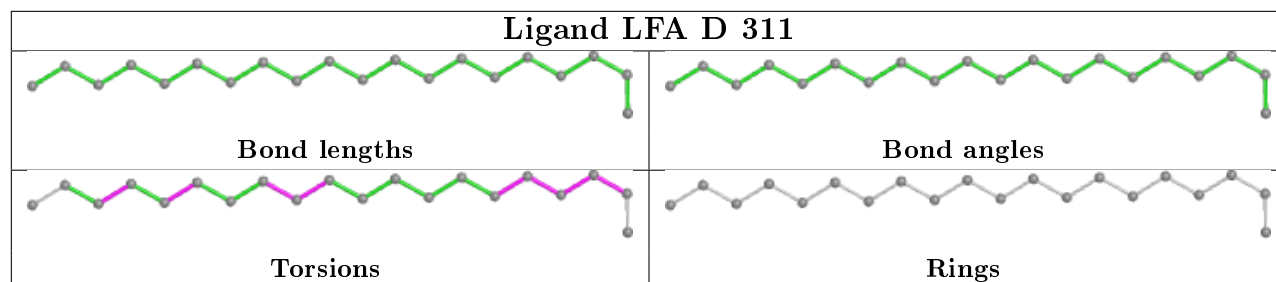
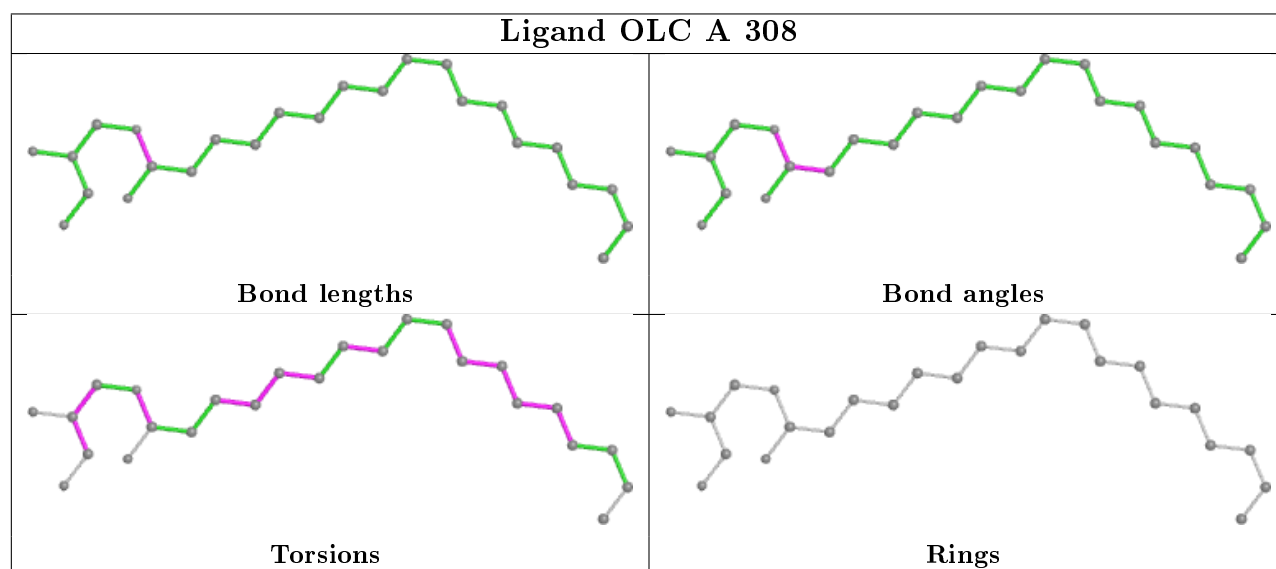
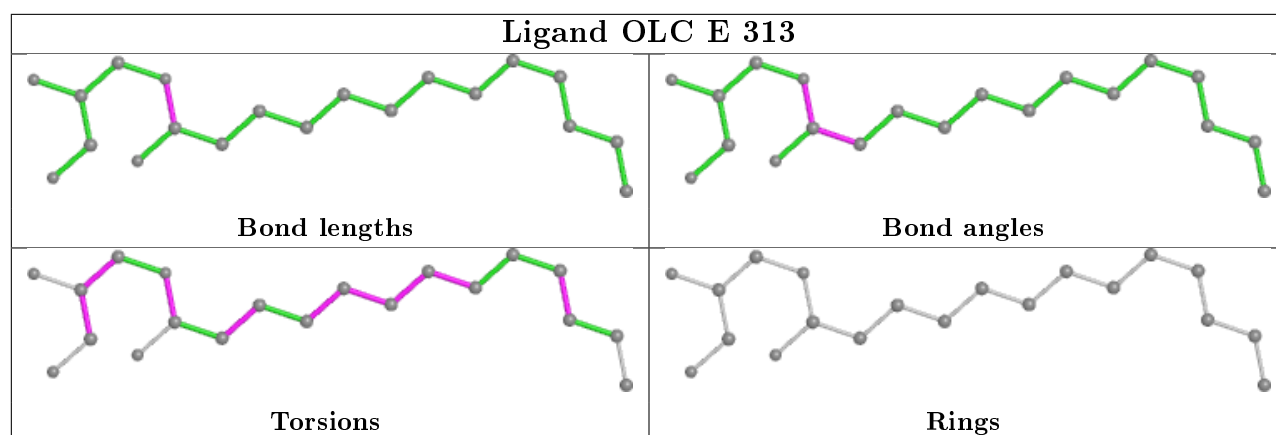


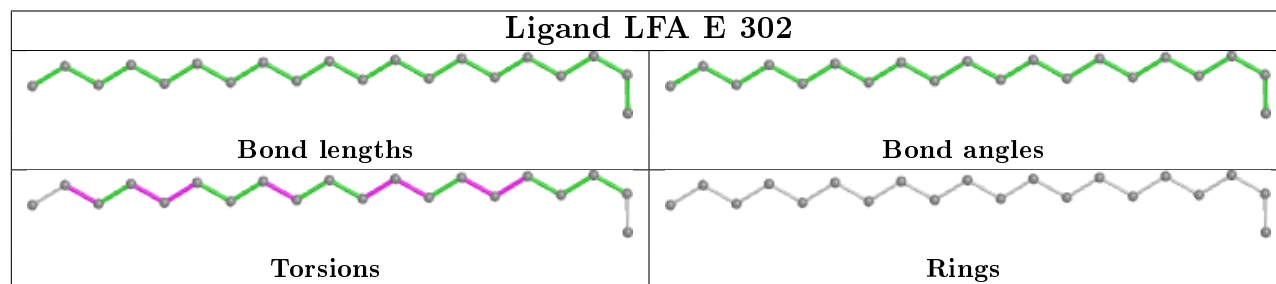
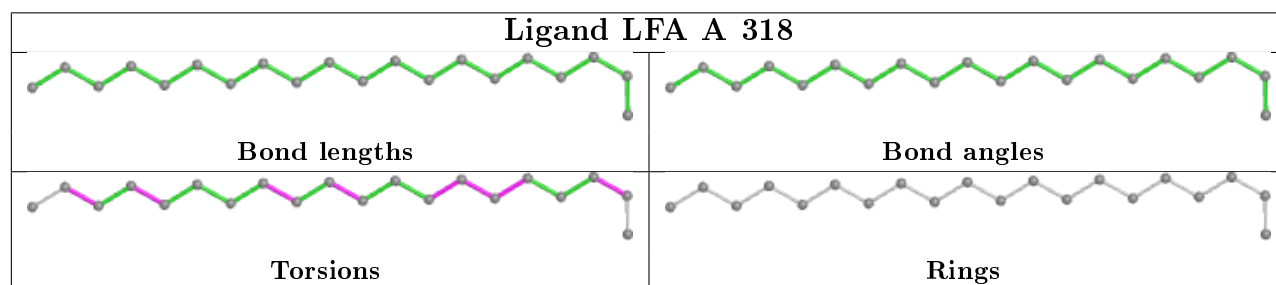
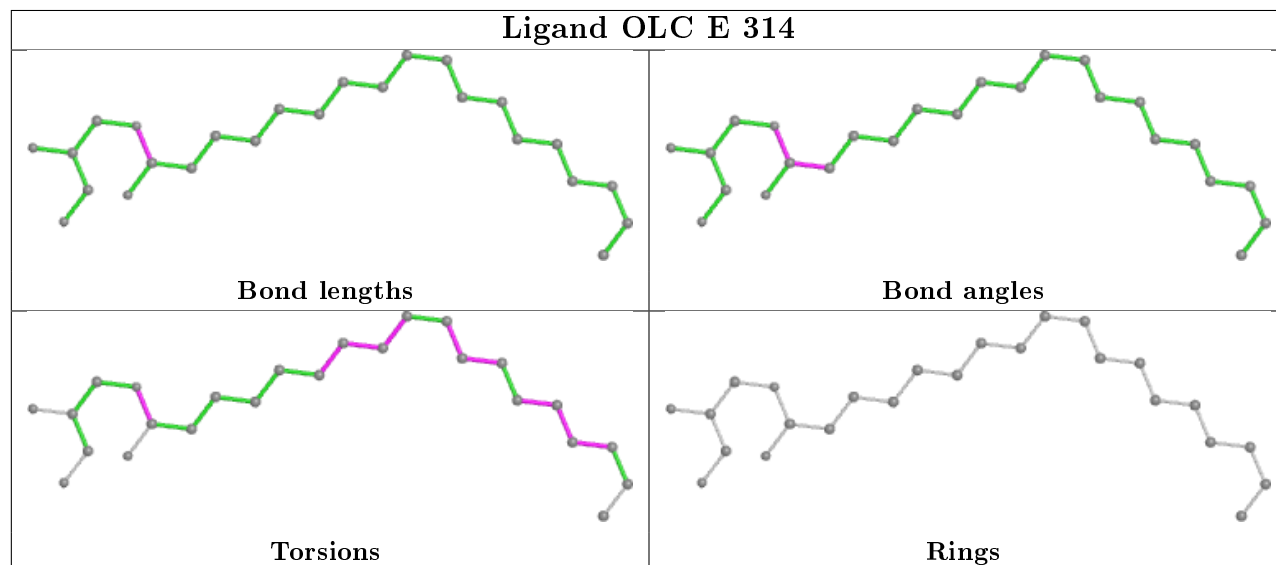
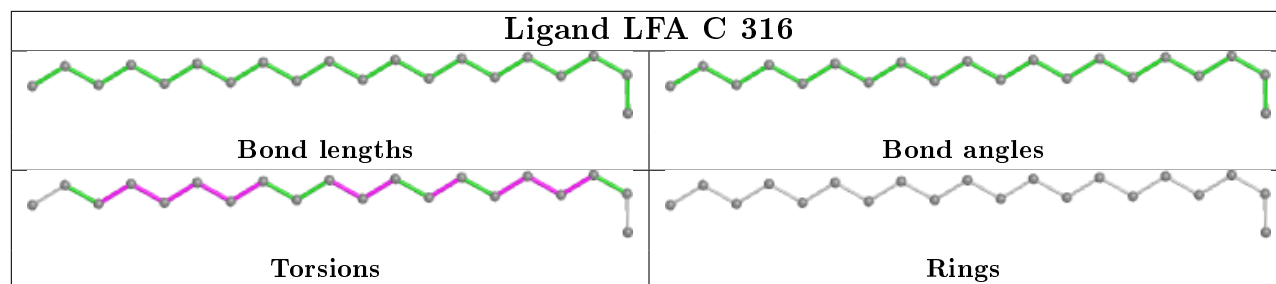




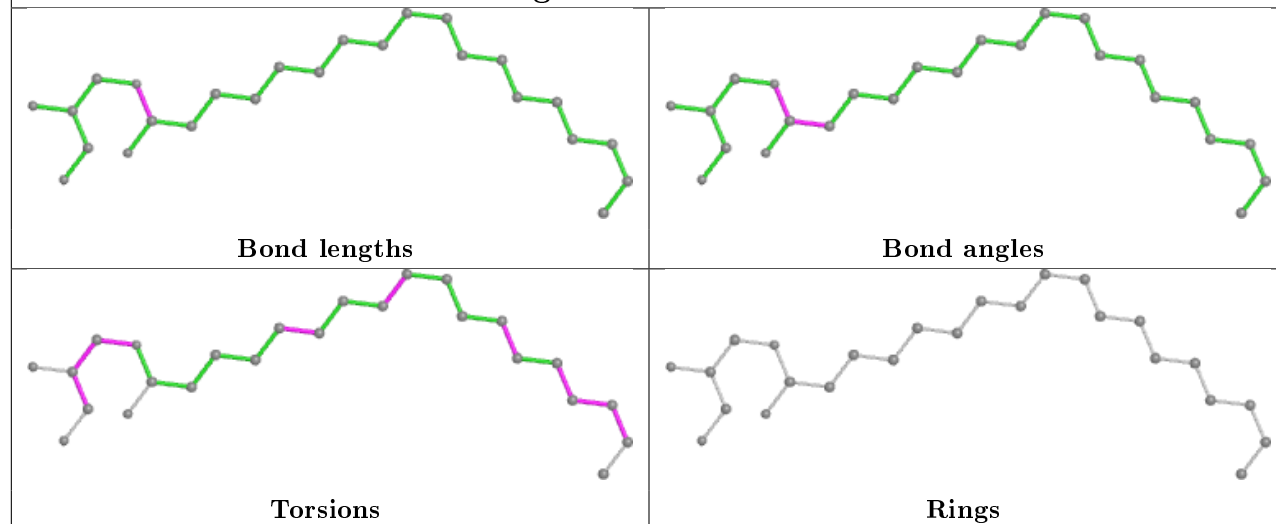




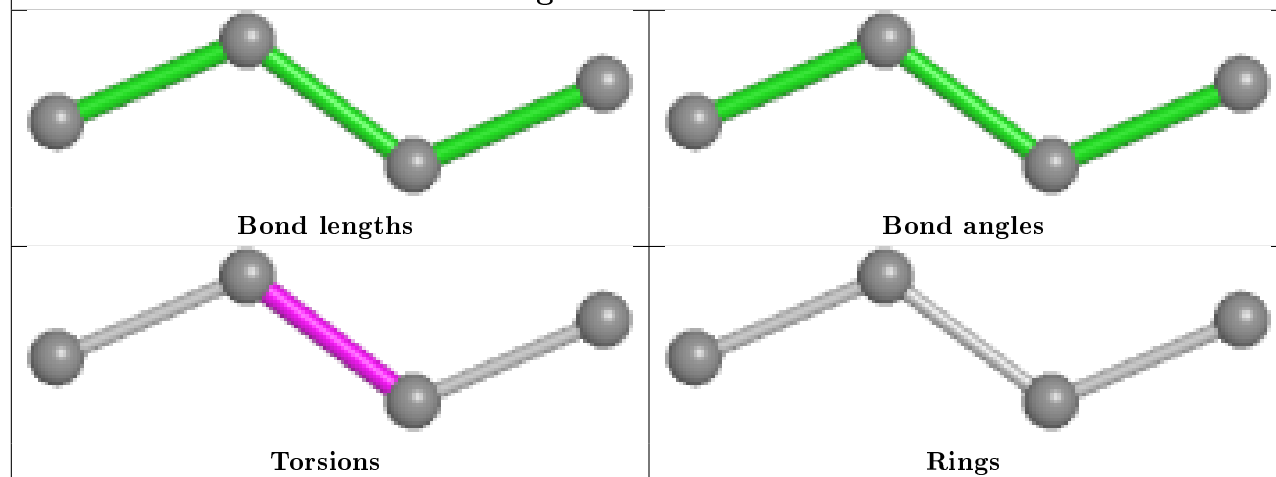




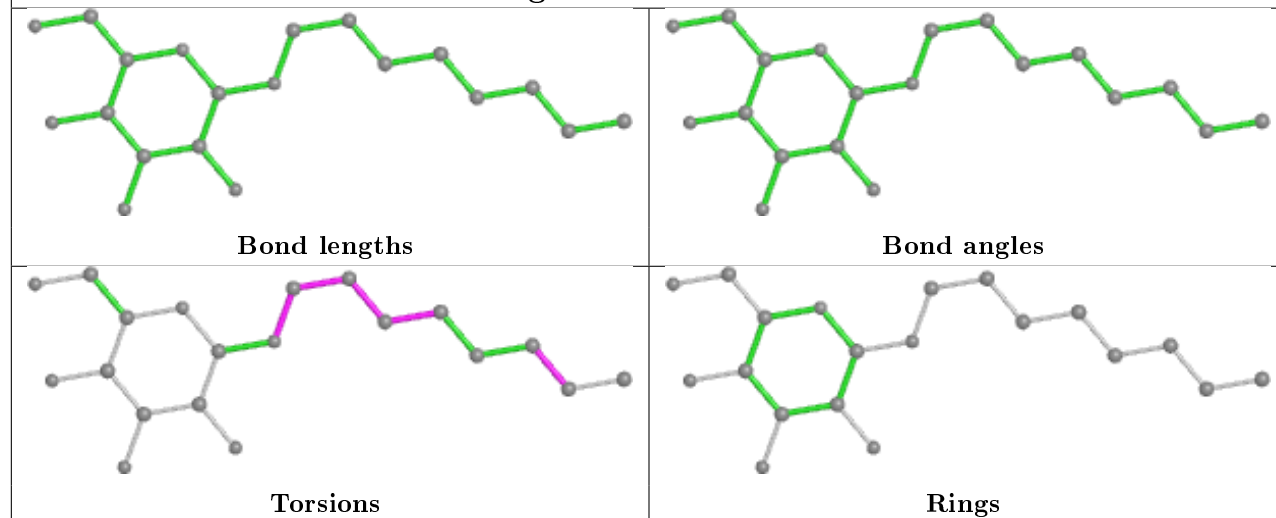
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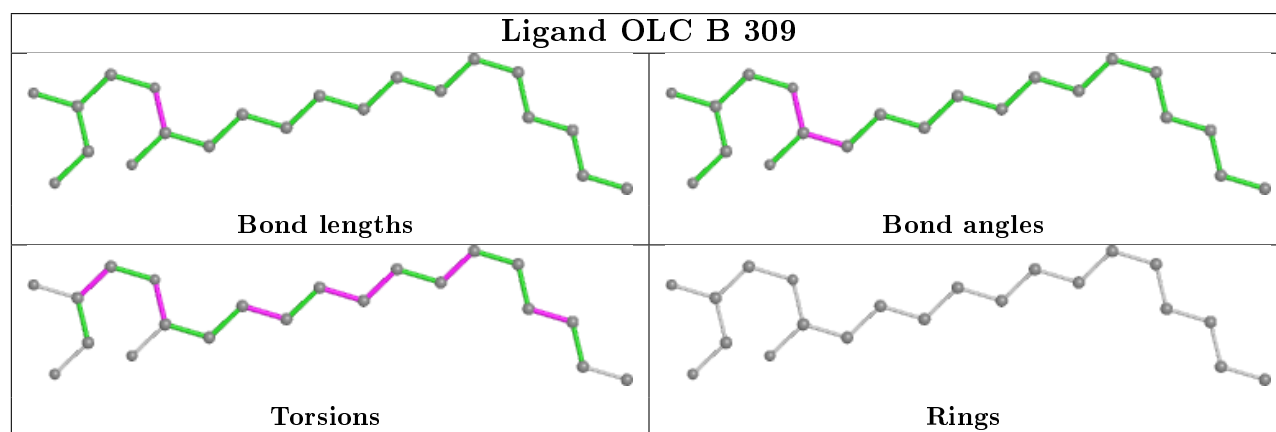
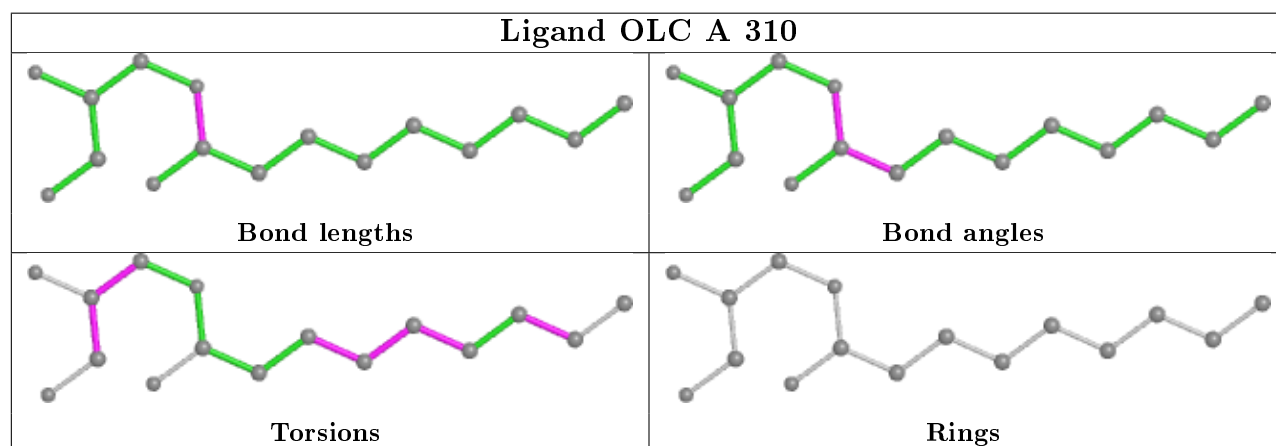
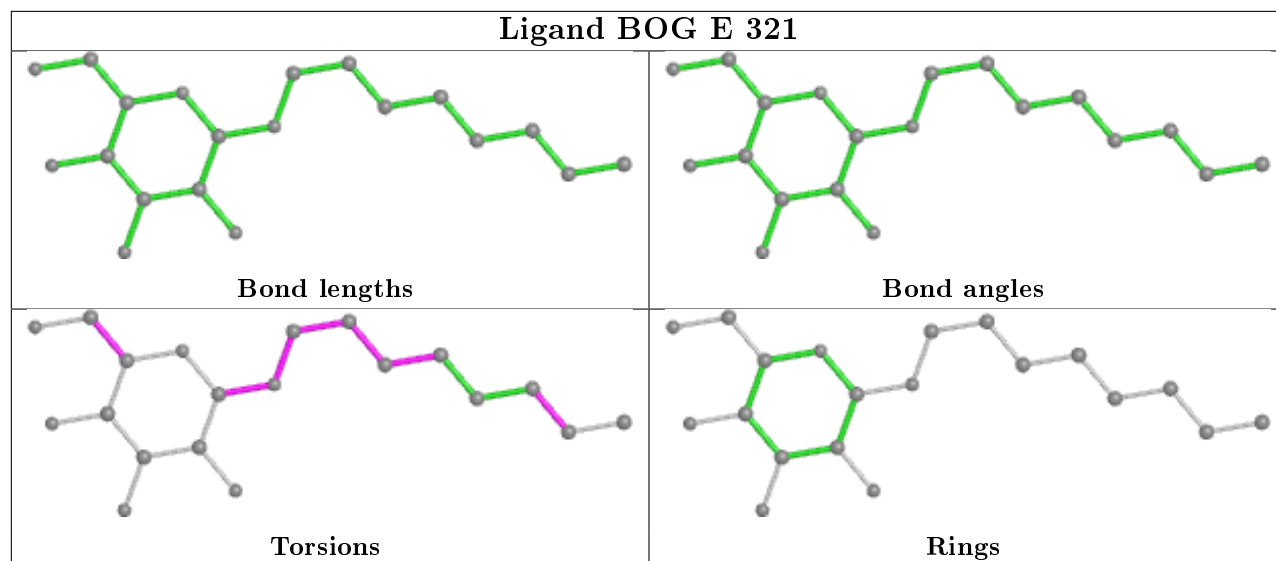


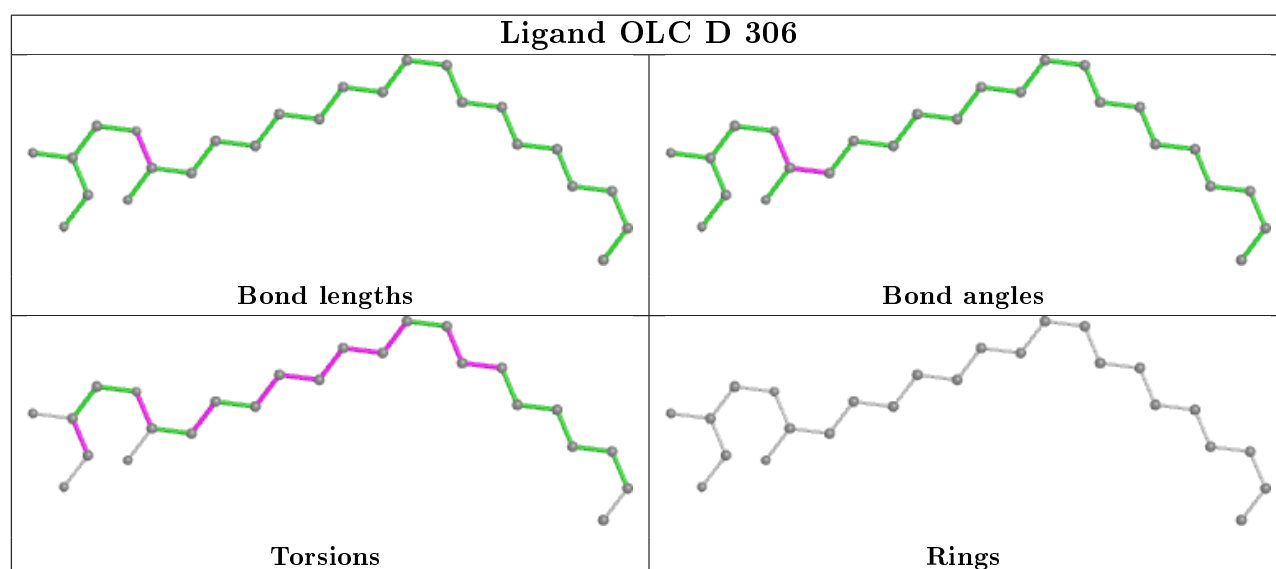
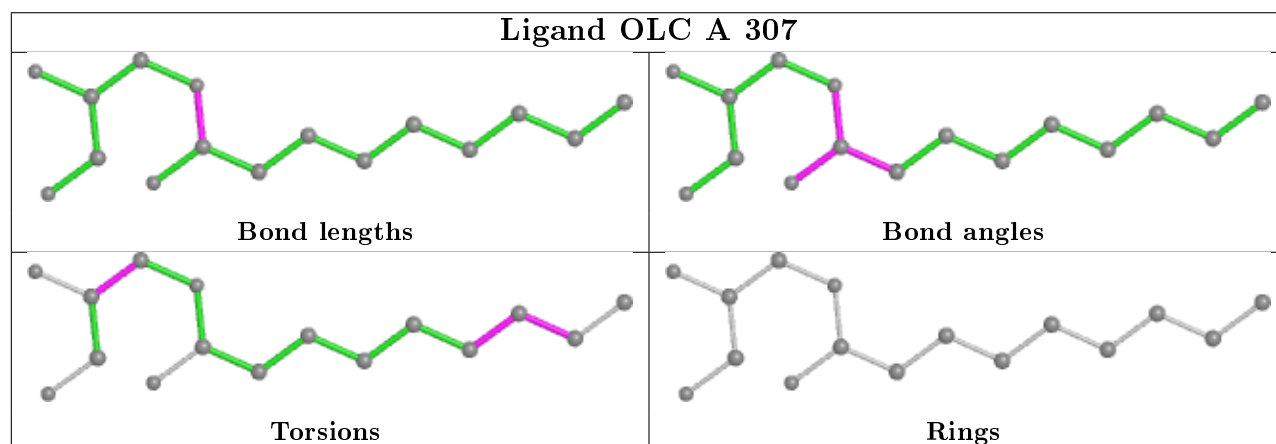
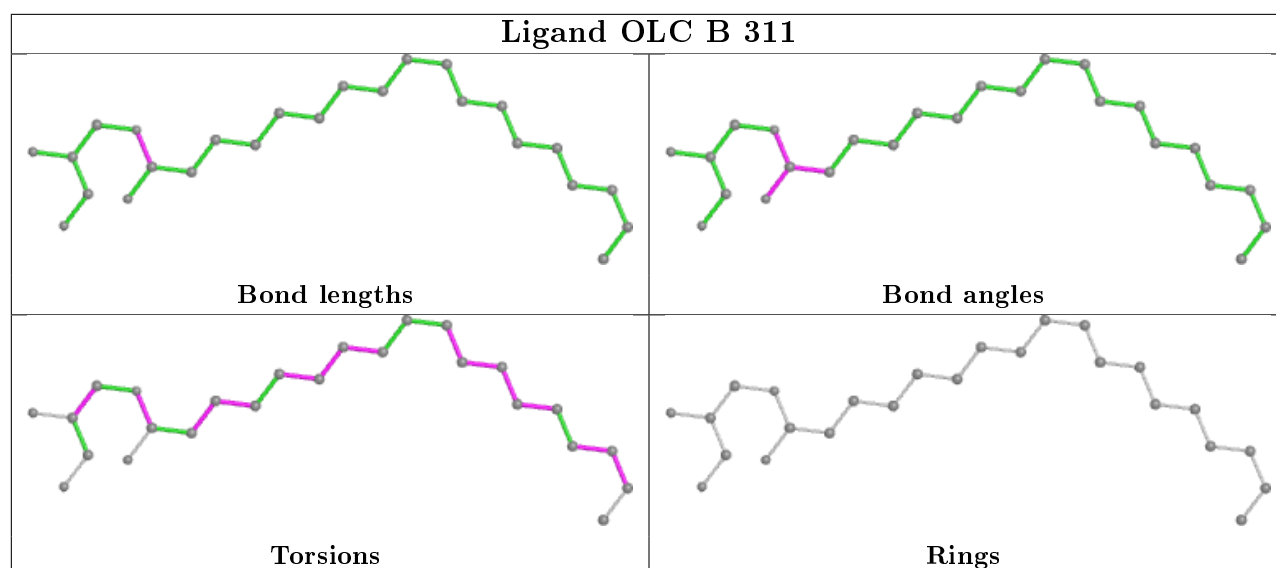
Ligand LFA C 318

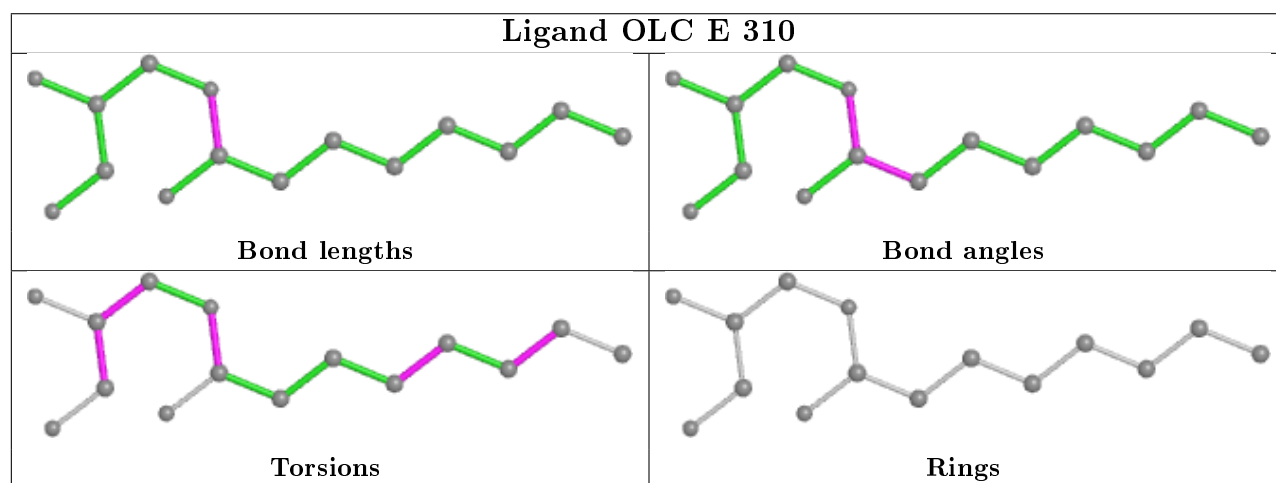
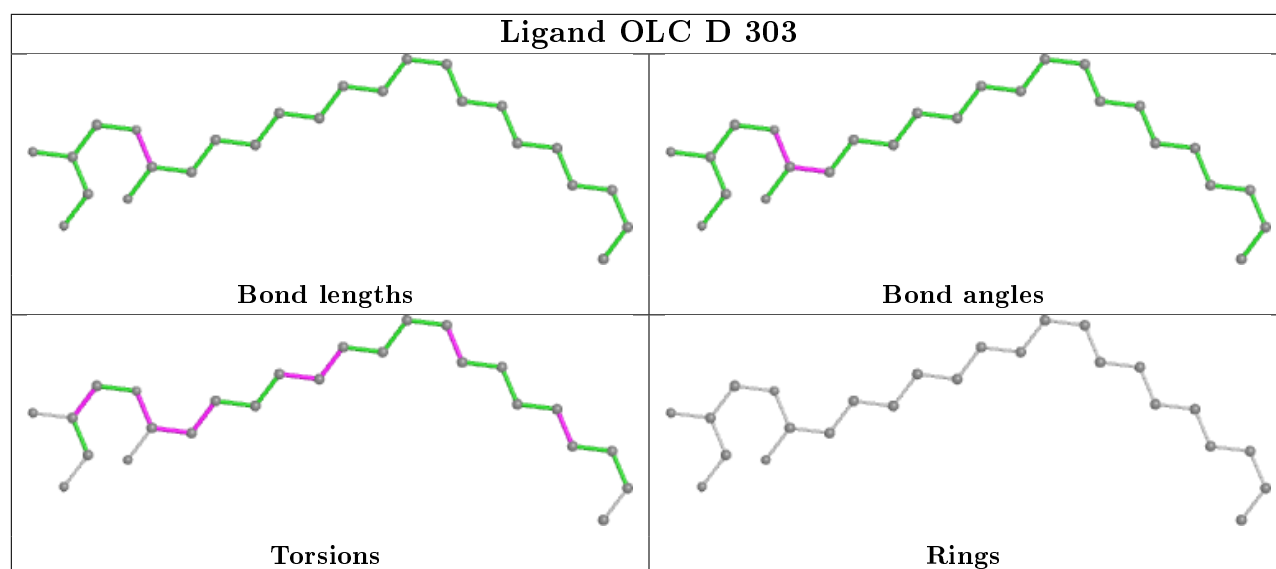
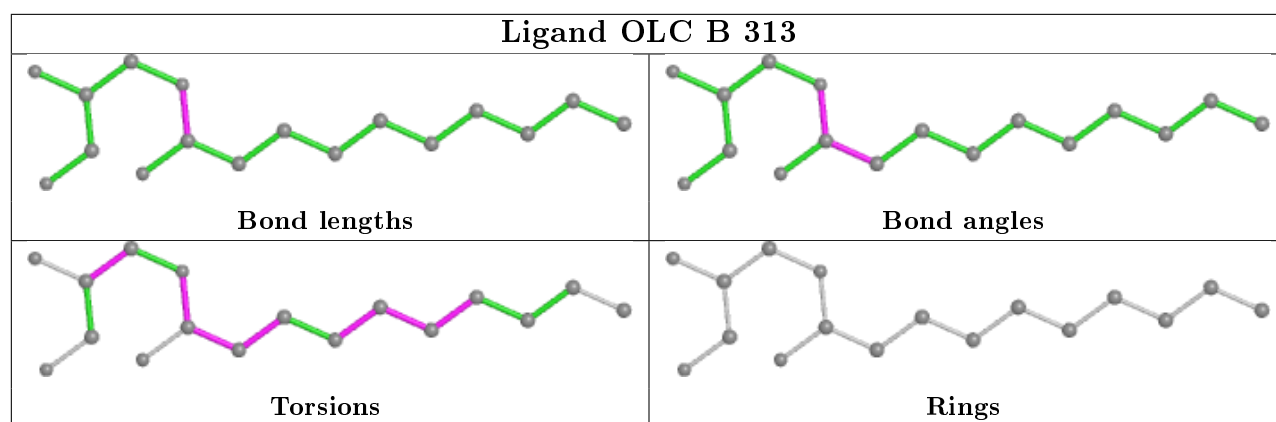


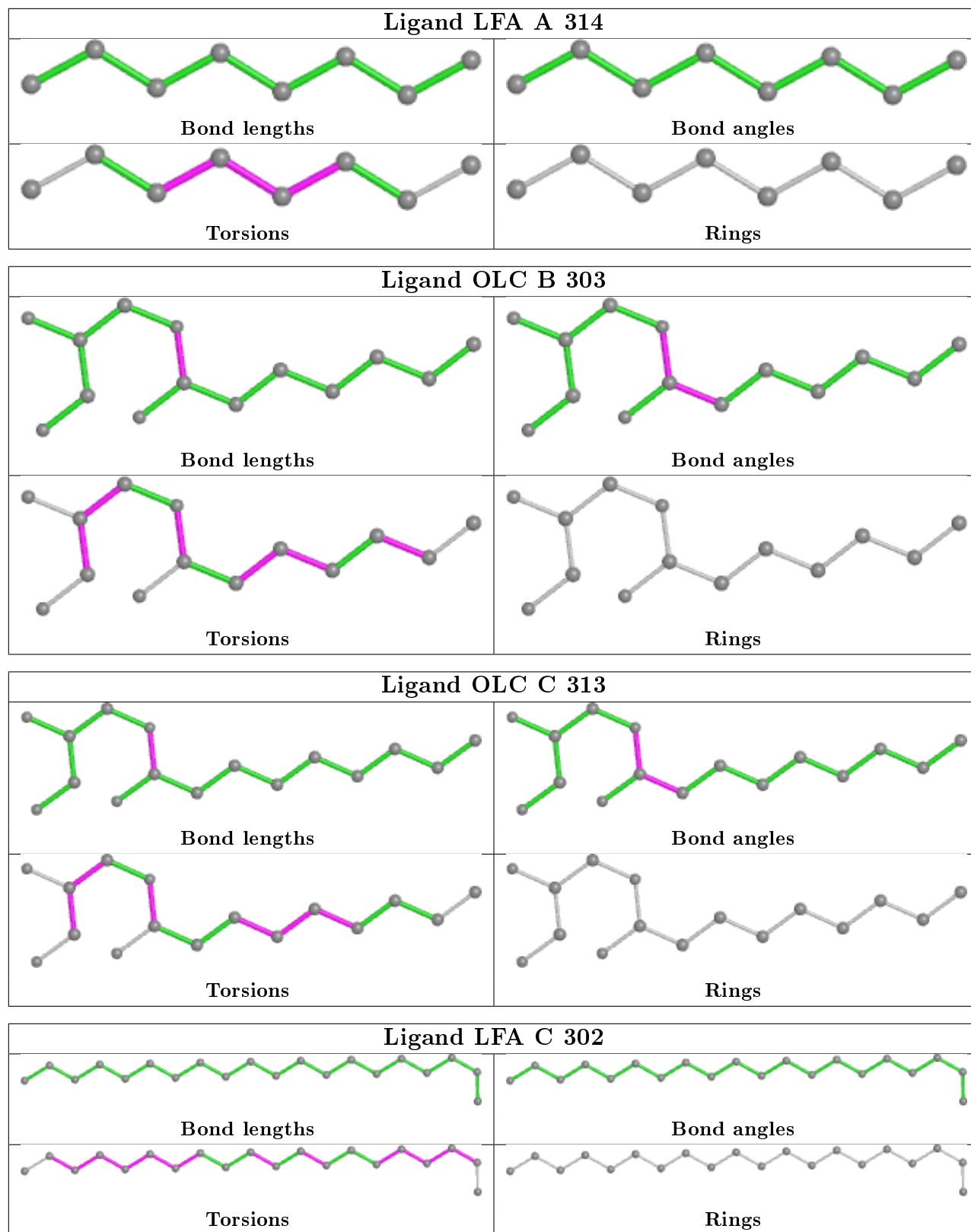
Ligand BOG A 320

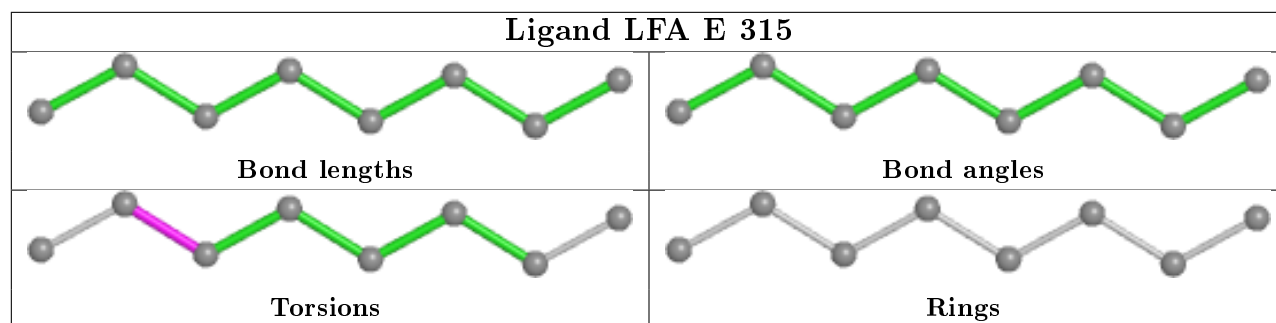
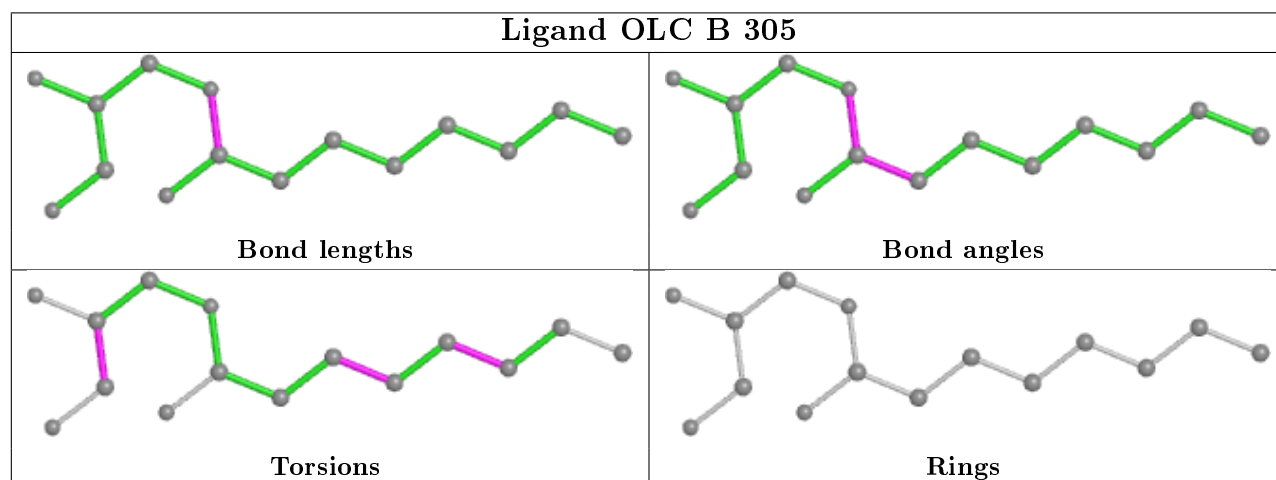
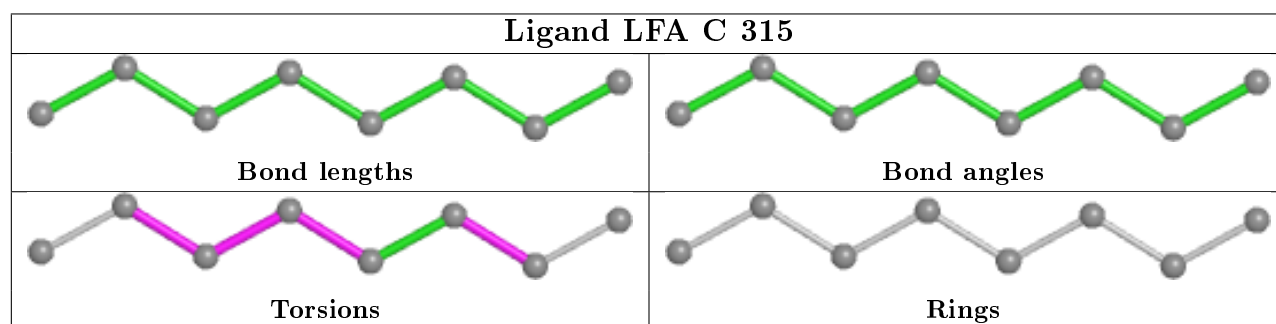
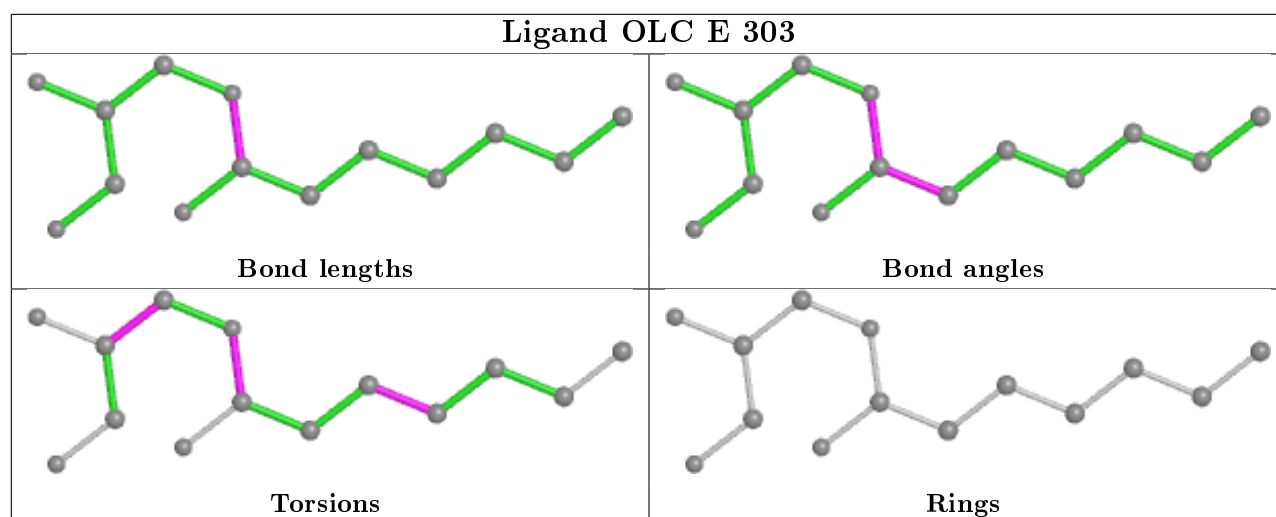


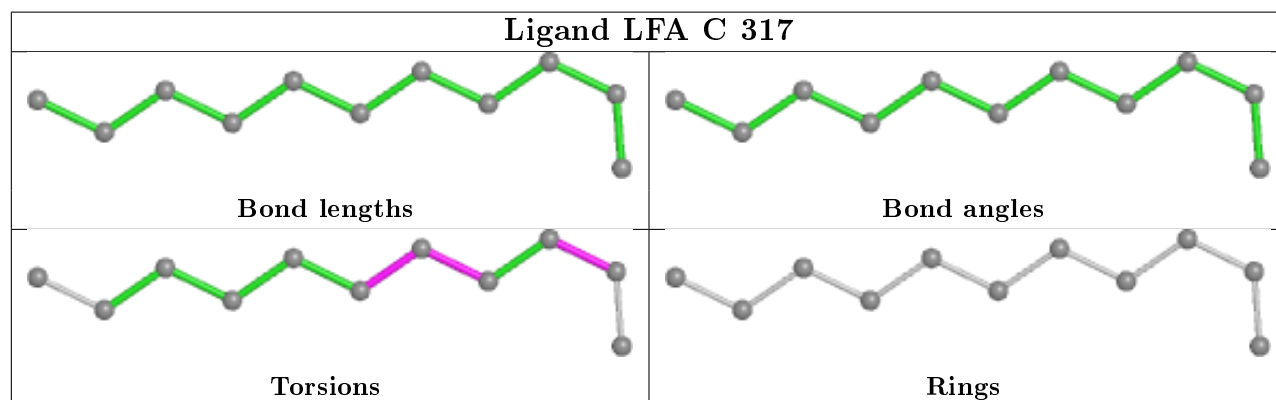
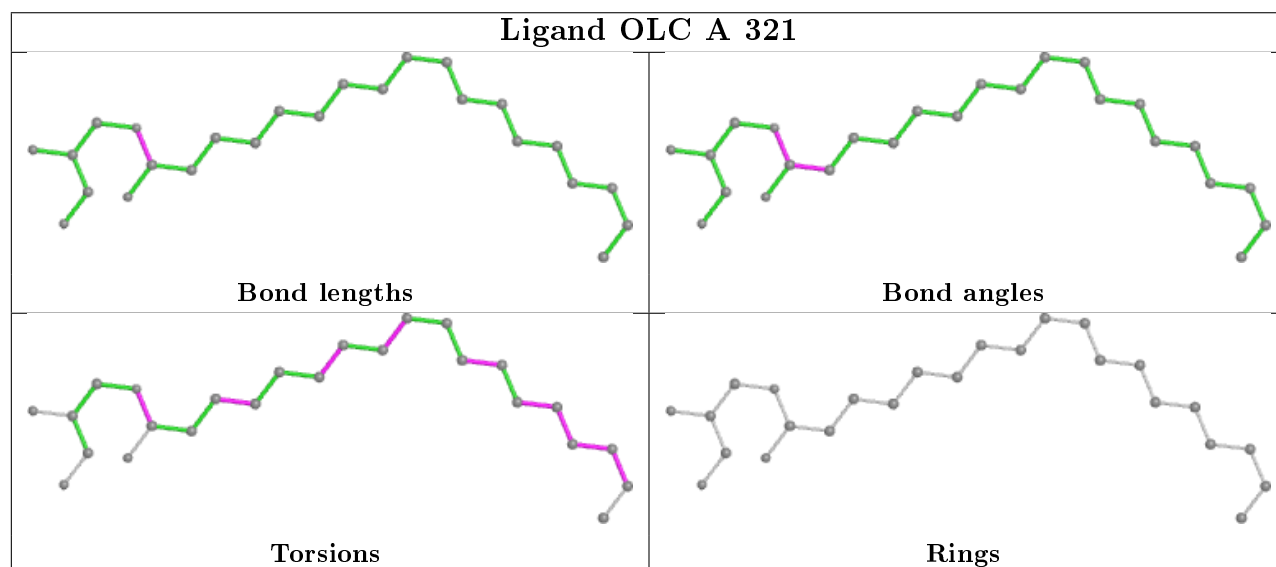
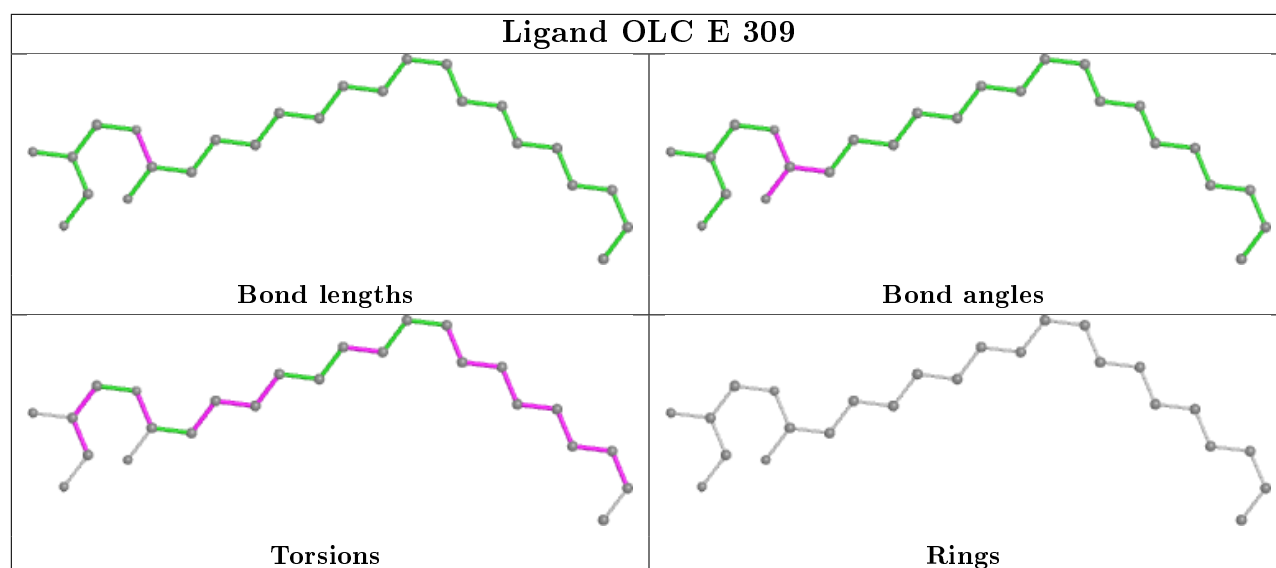


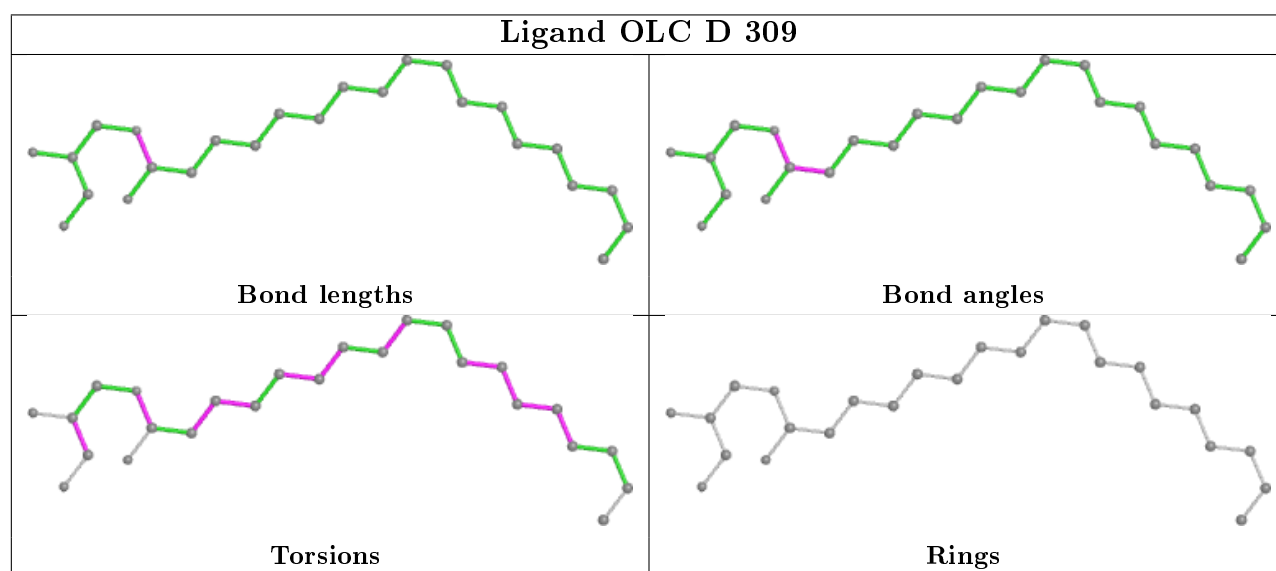
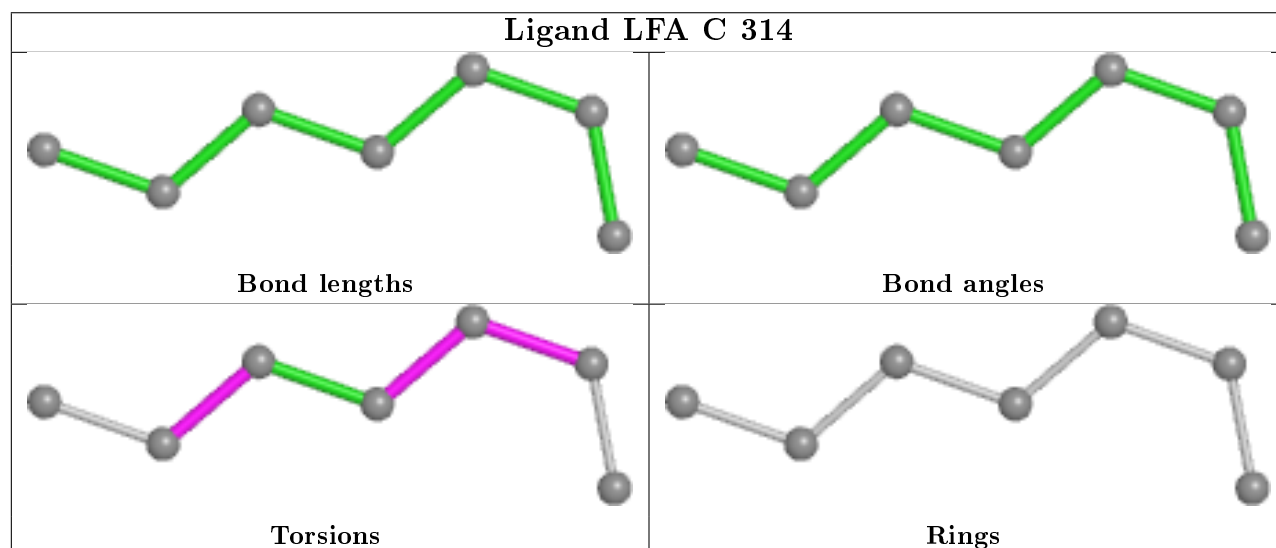
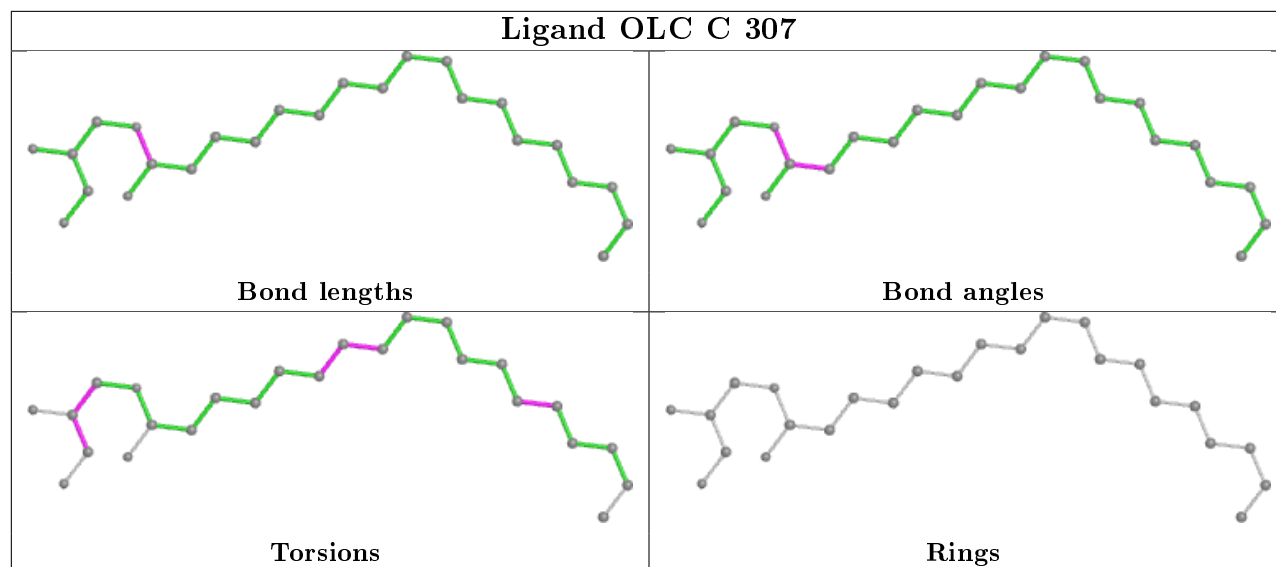


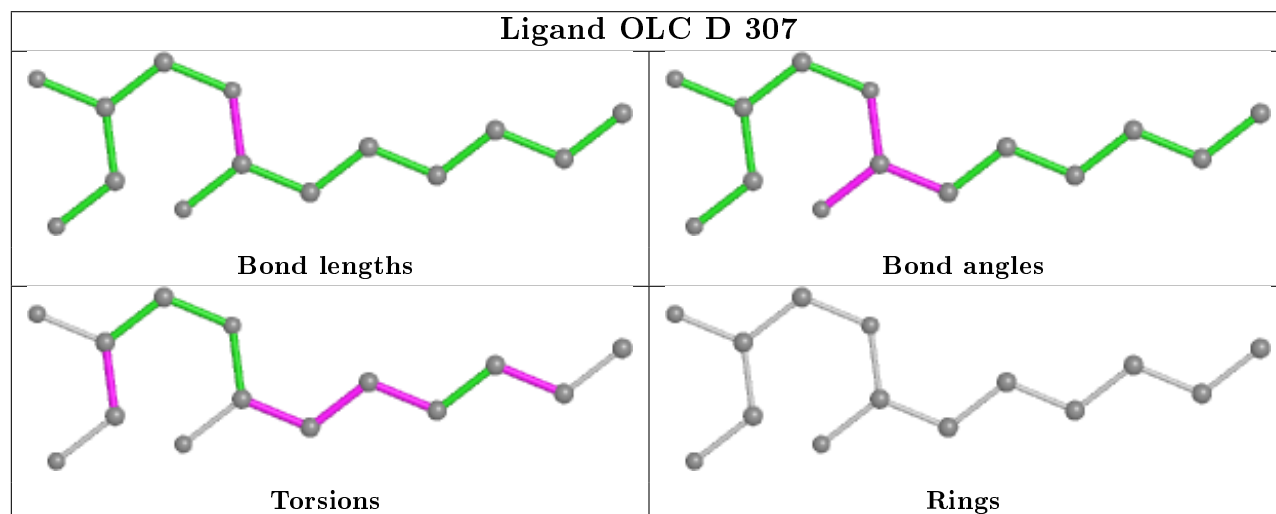
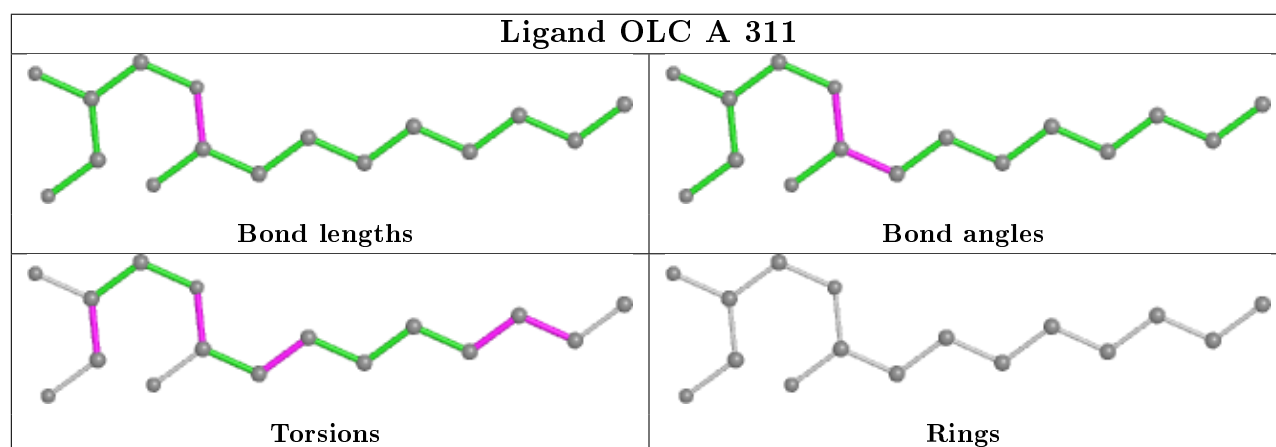
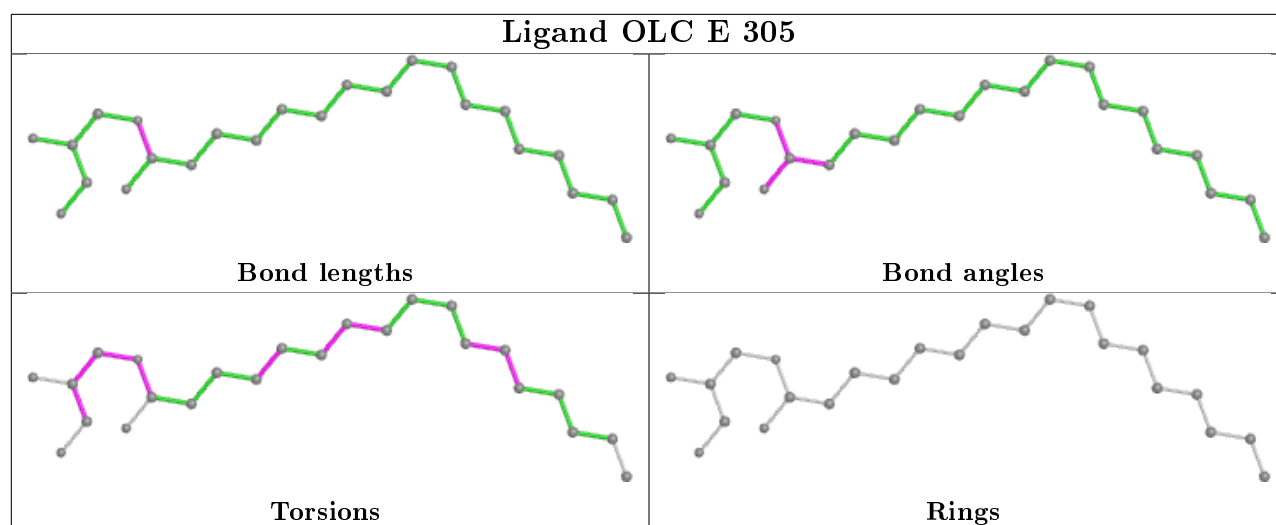


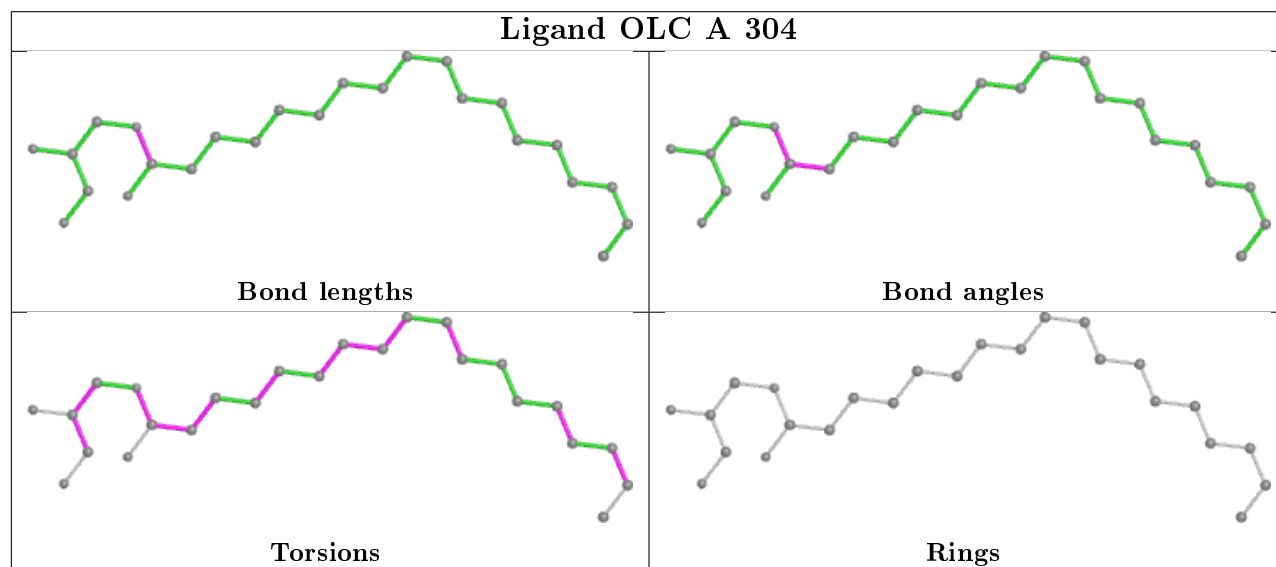
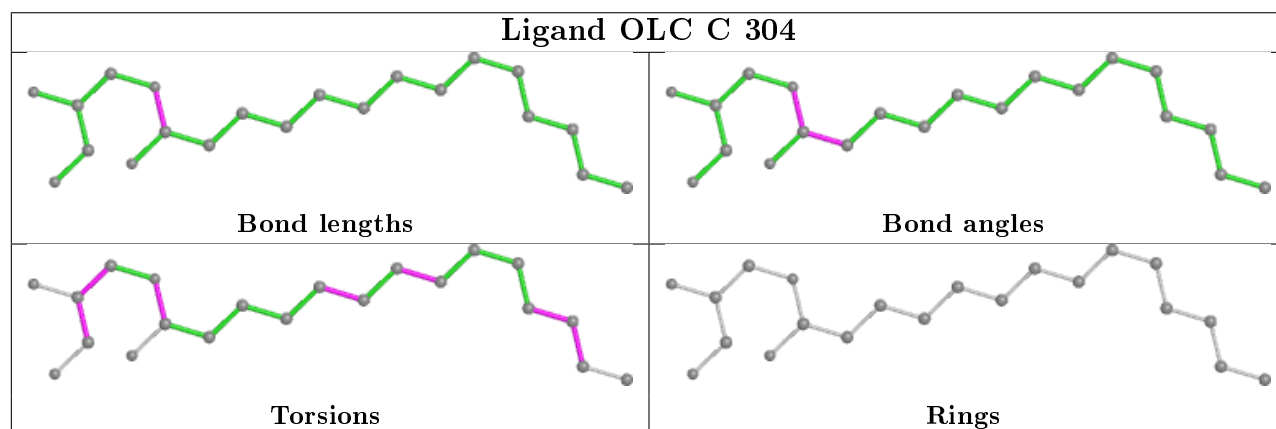
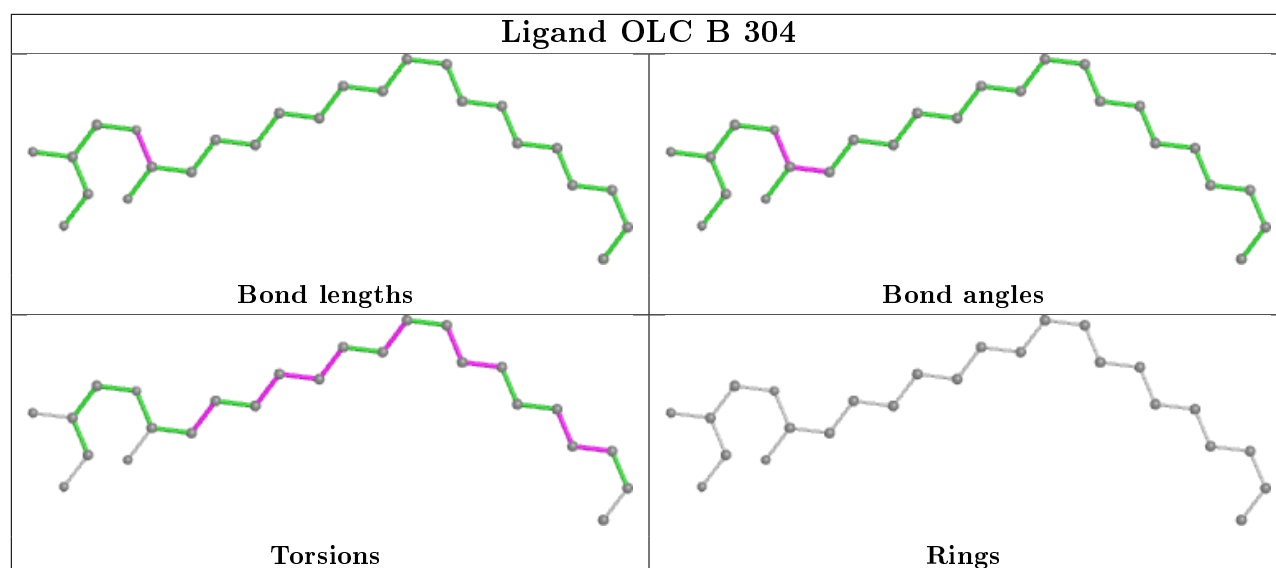


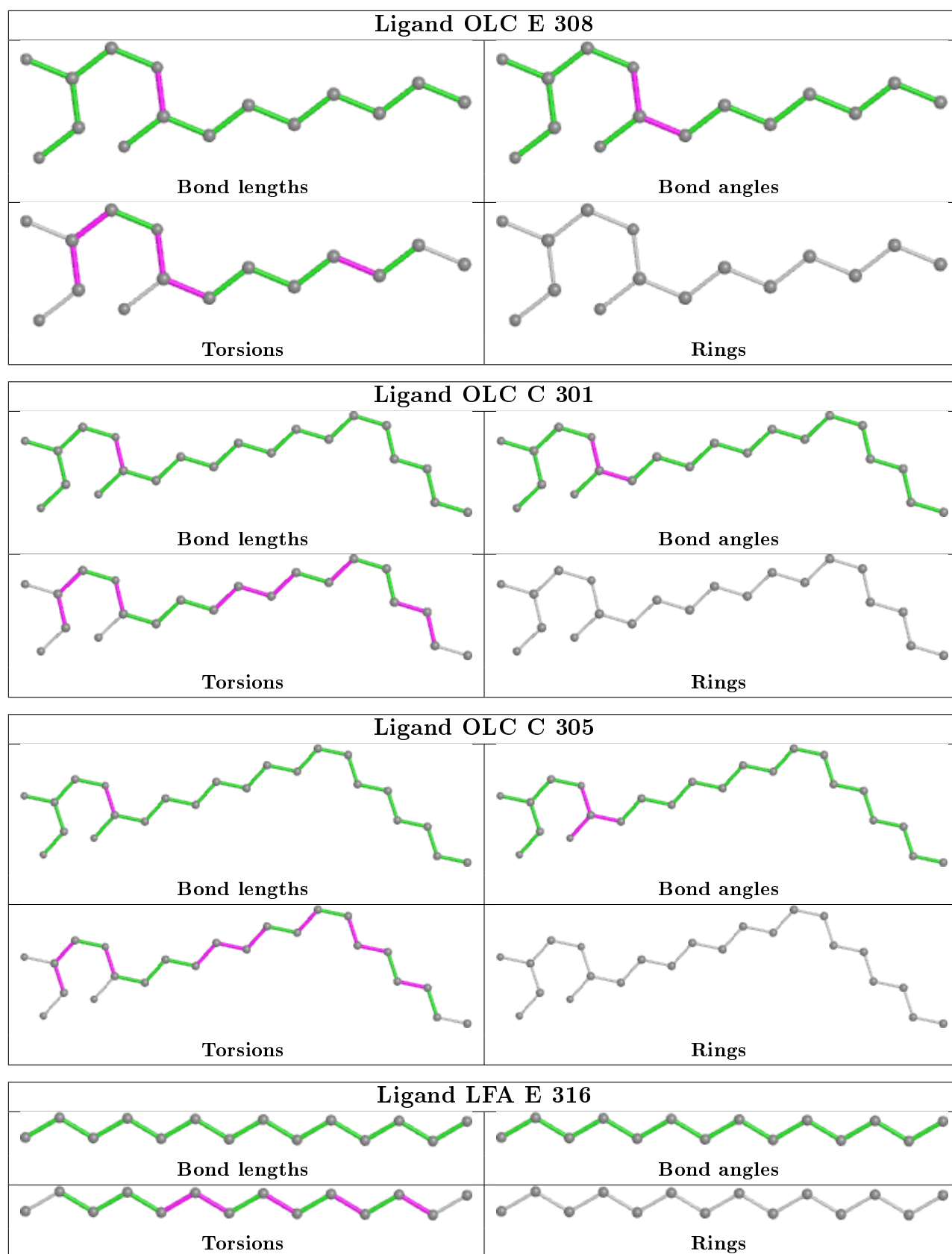


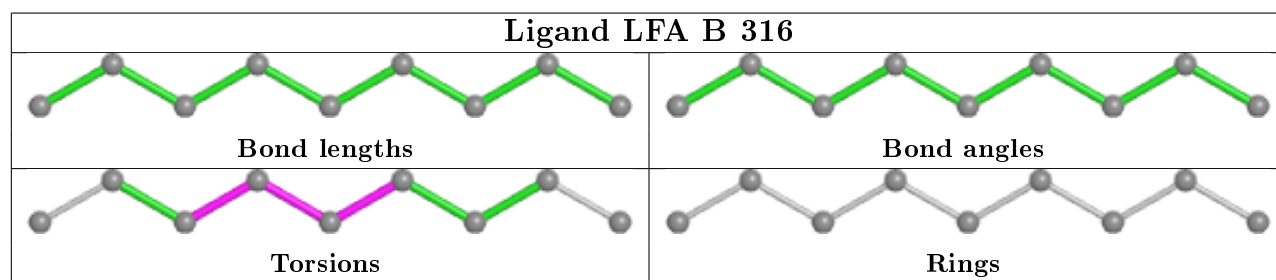
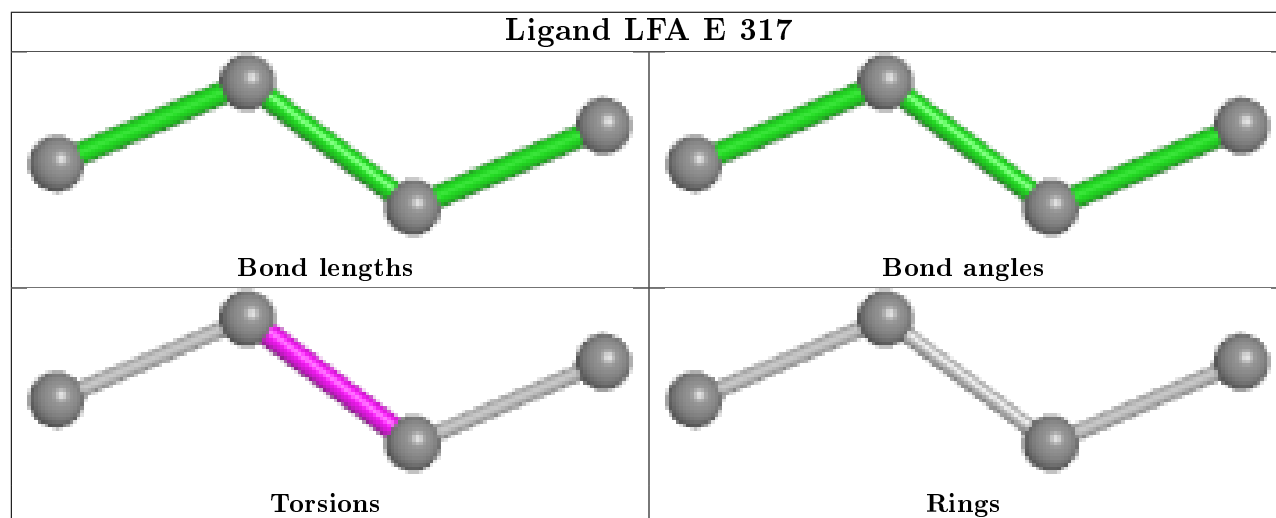
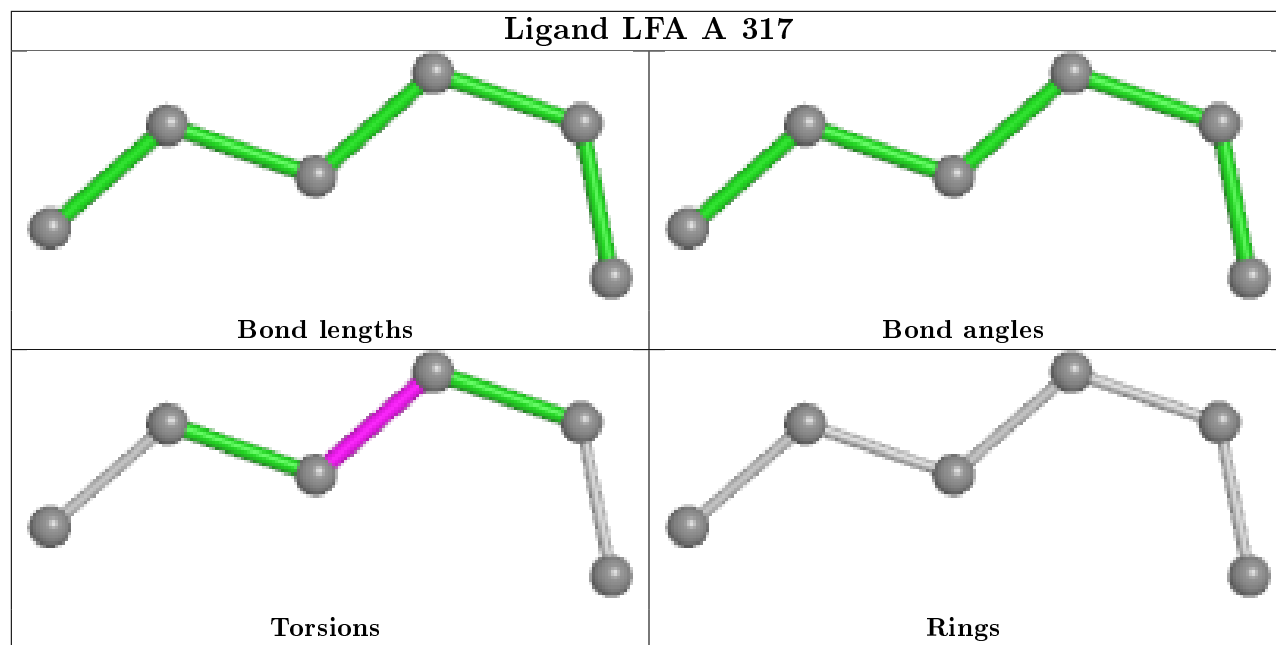


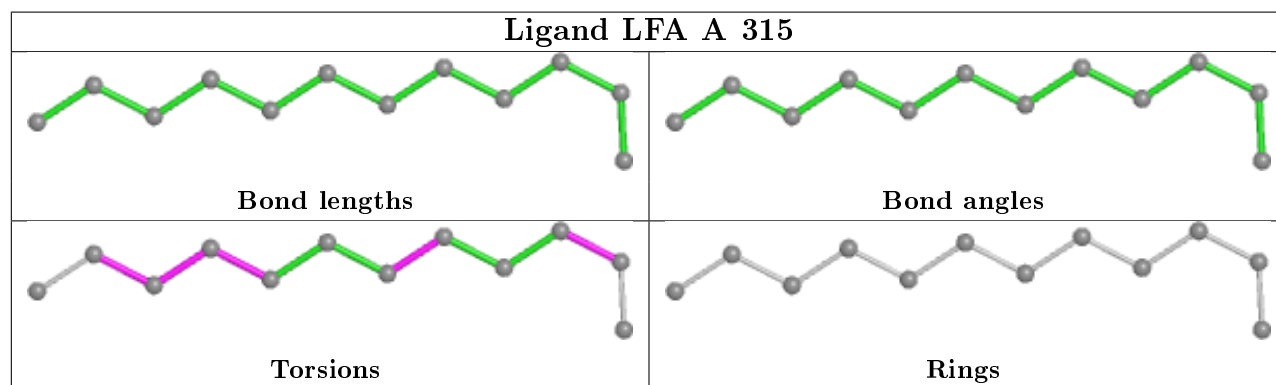
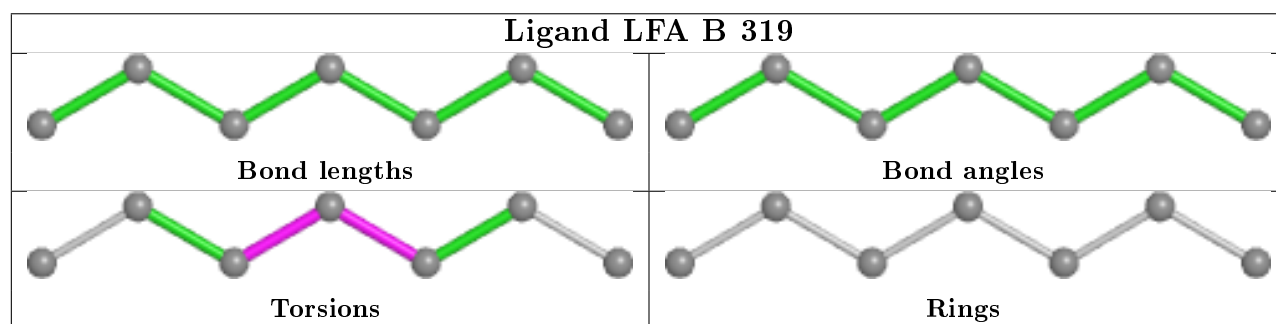
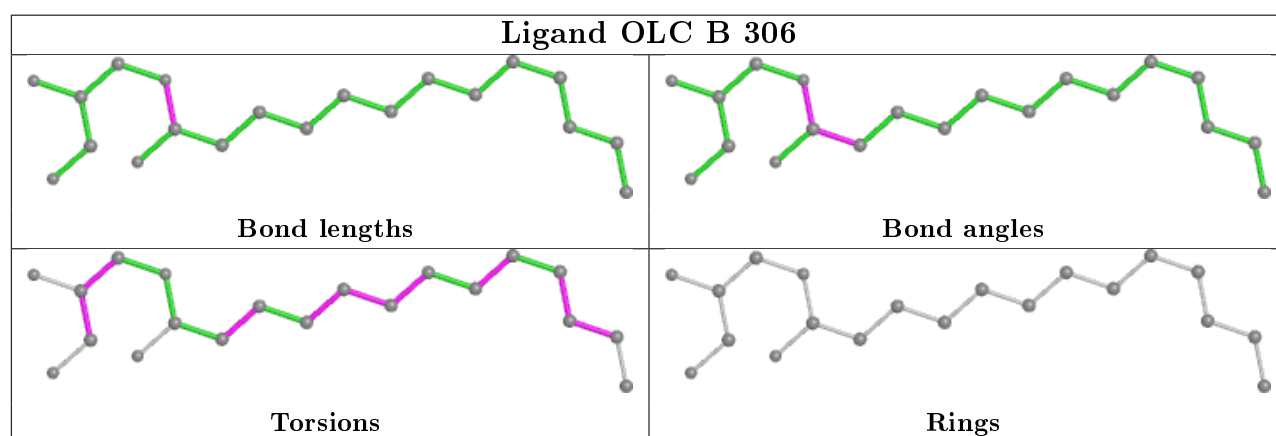
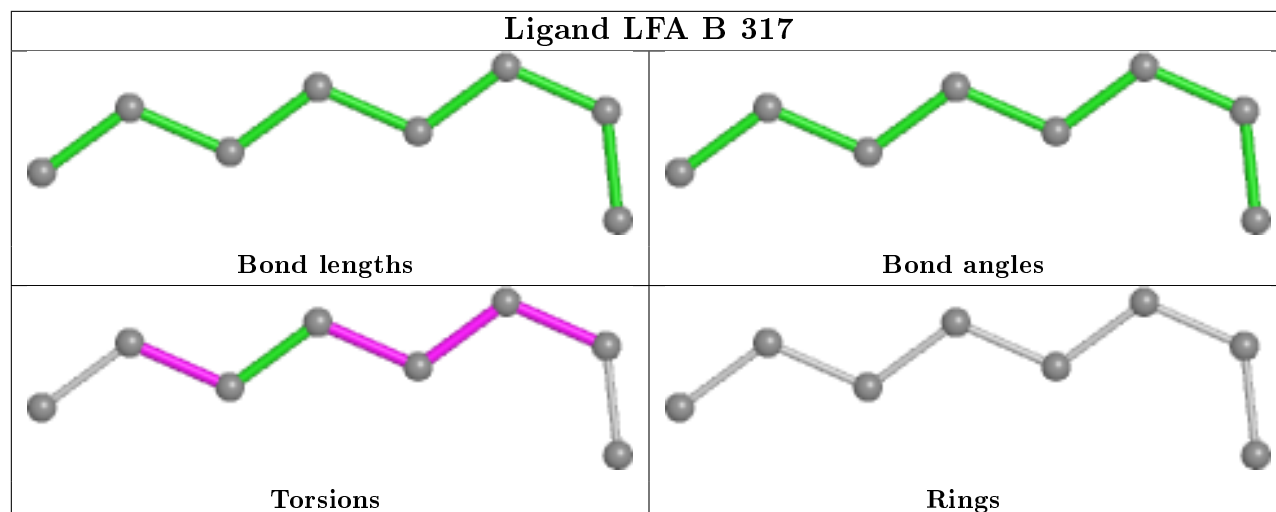


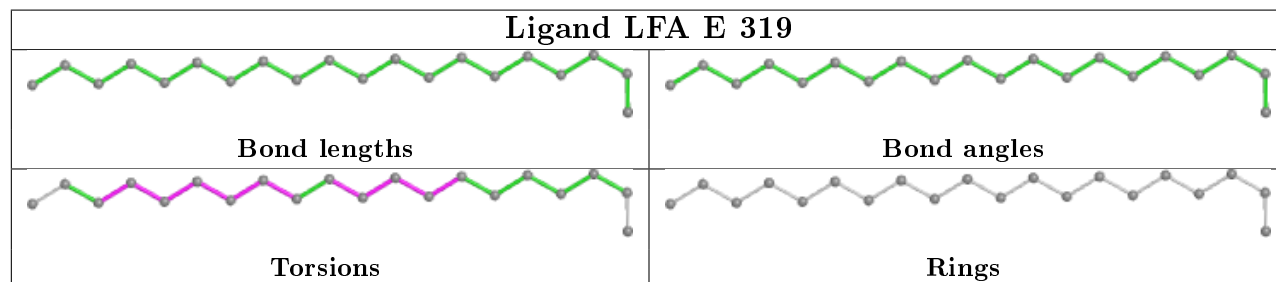
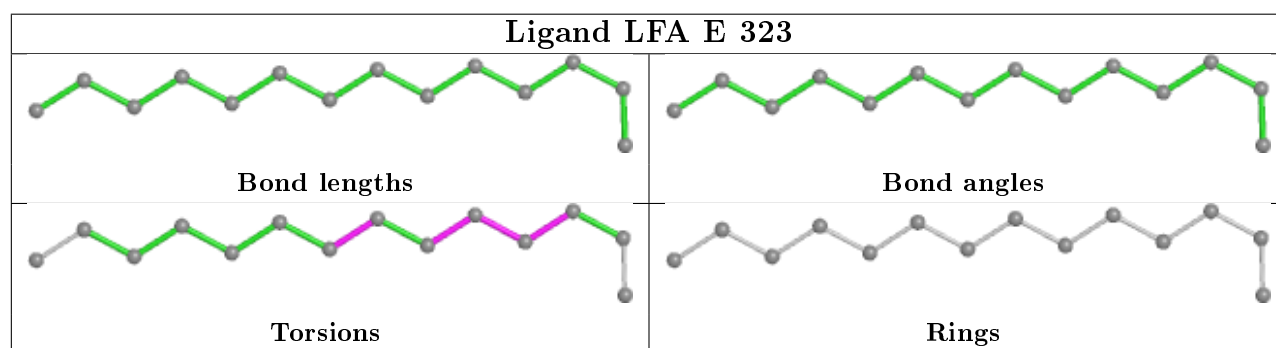
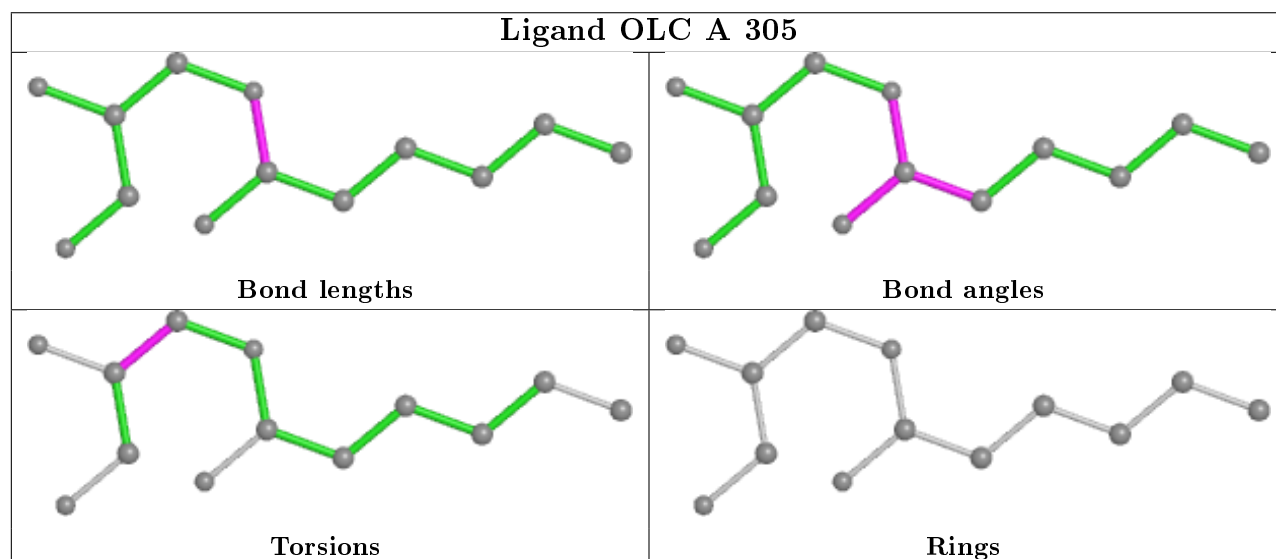
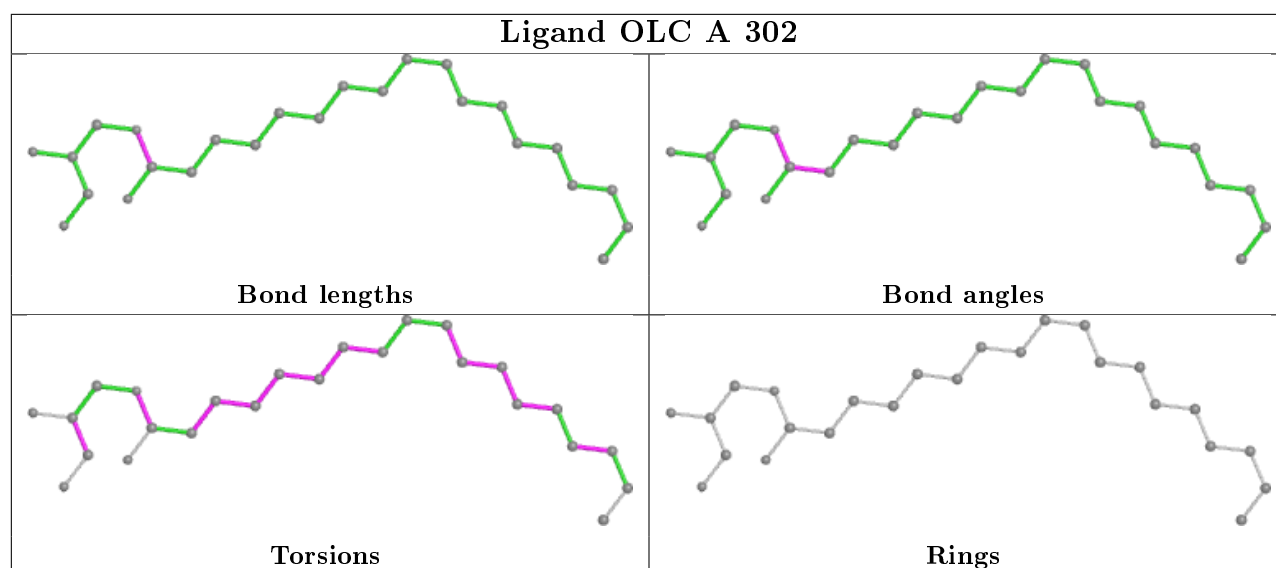


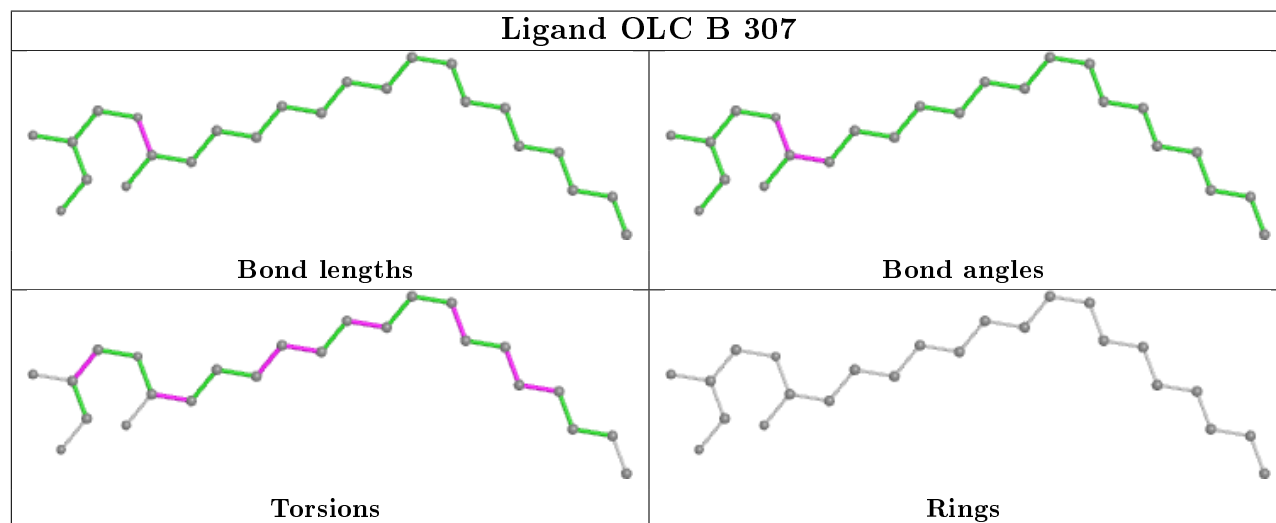
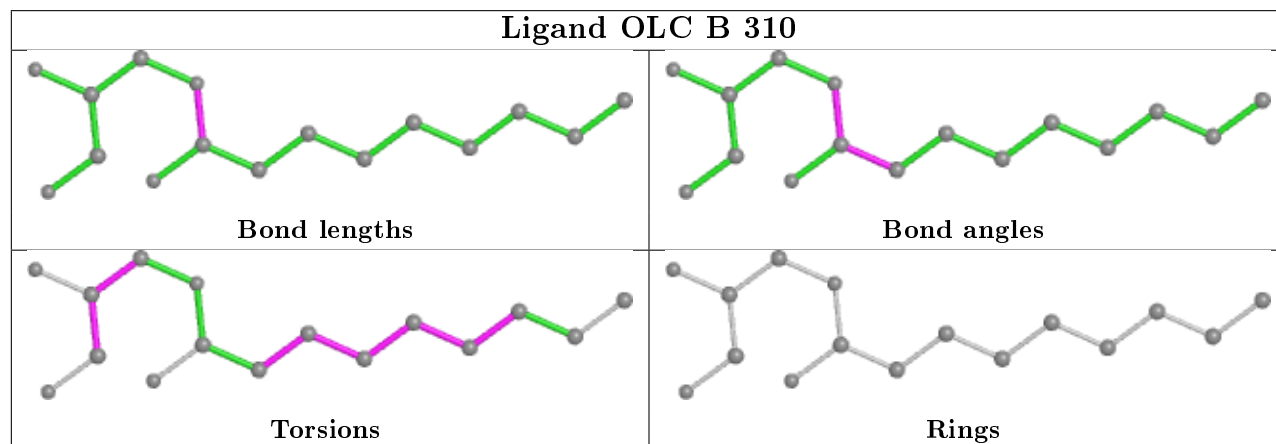
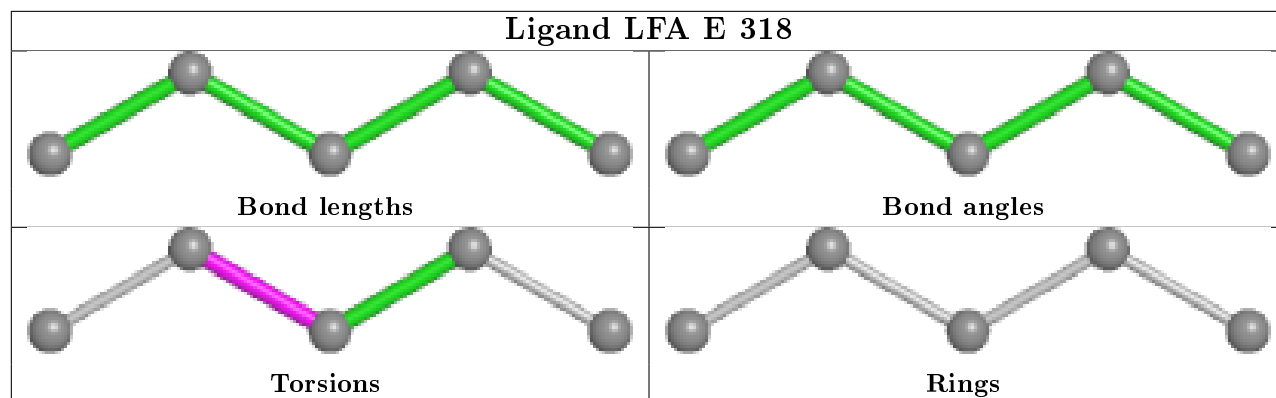


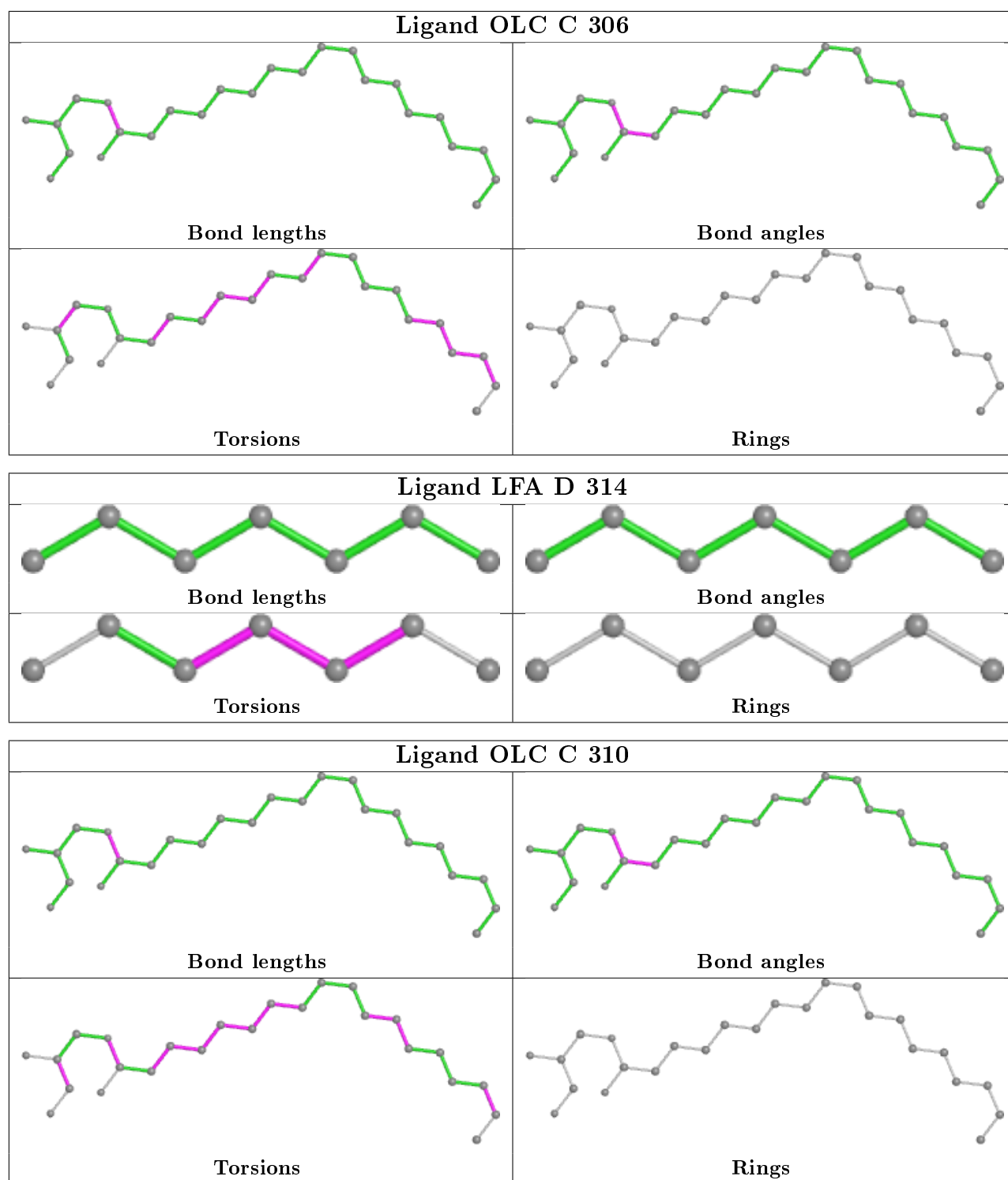


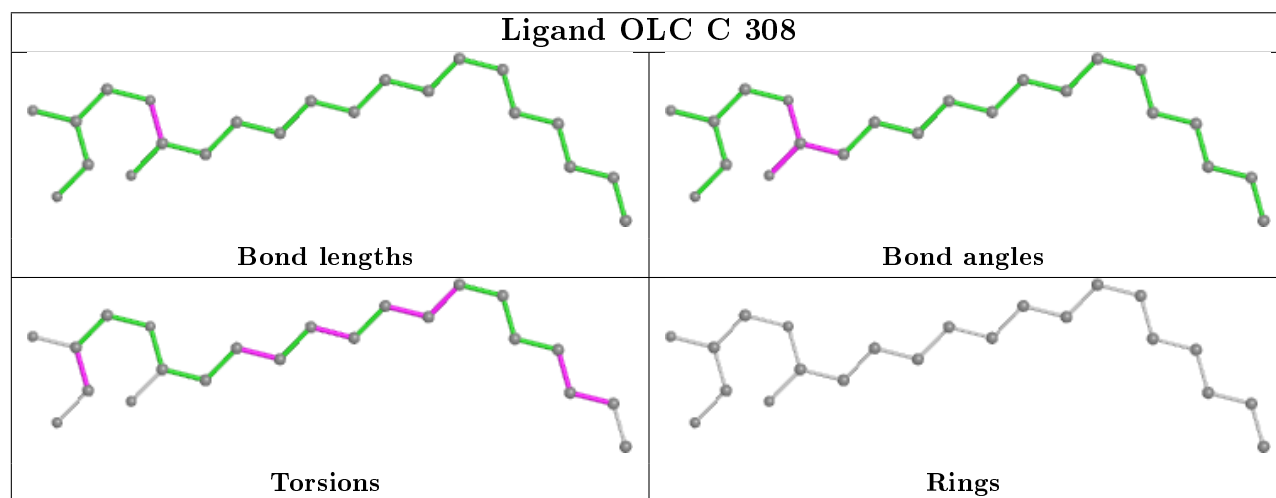
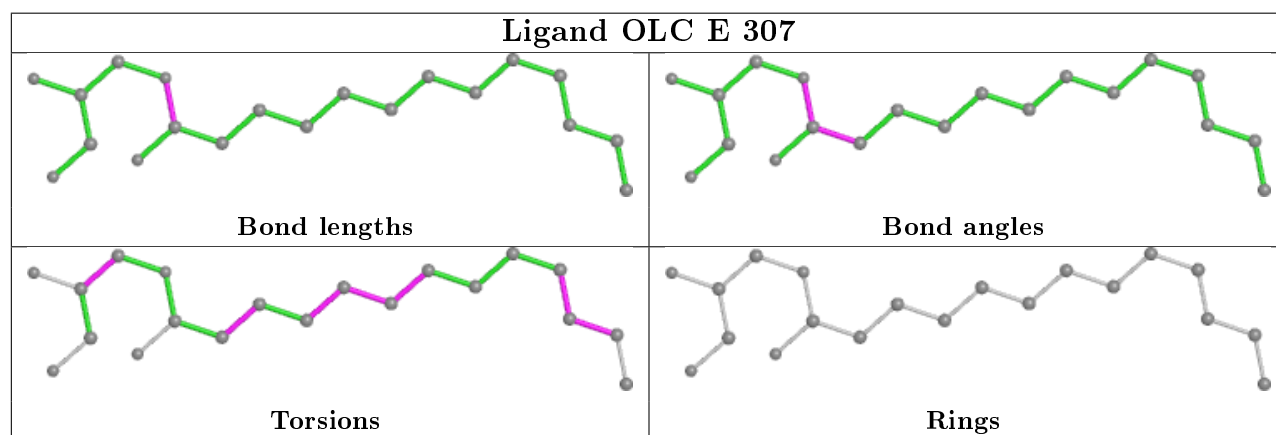
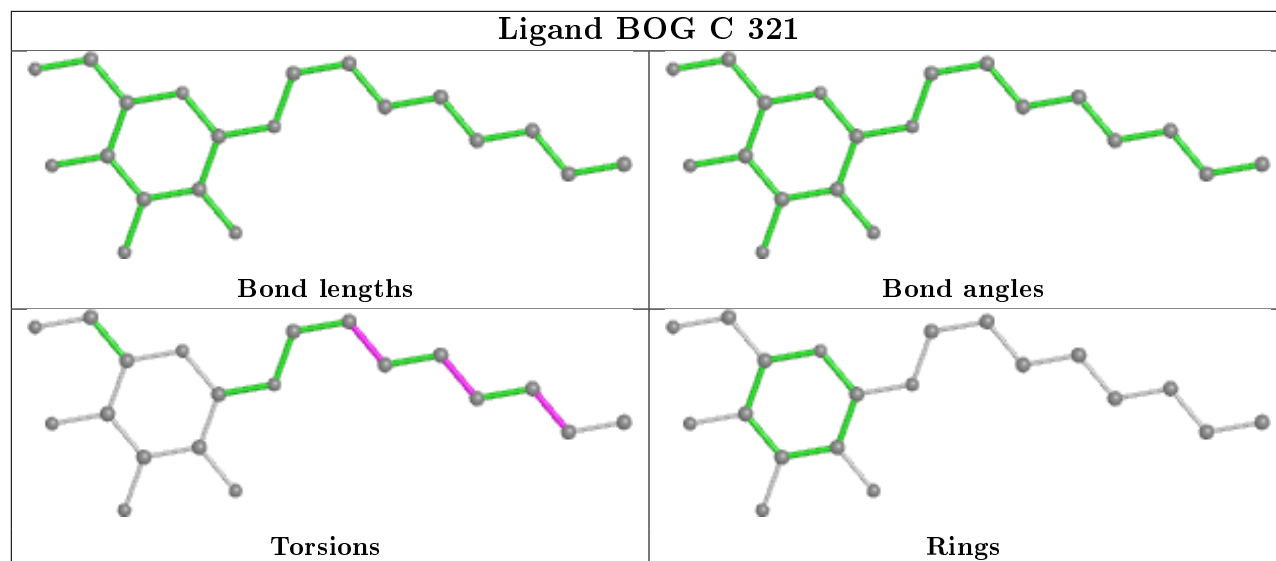


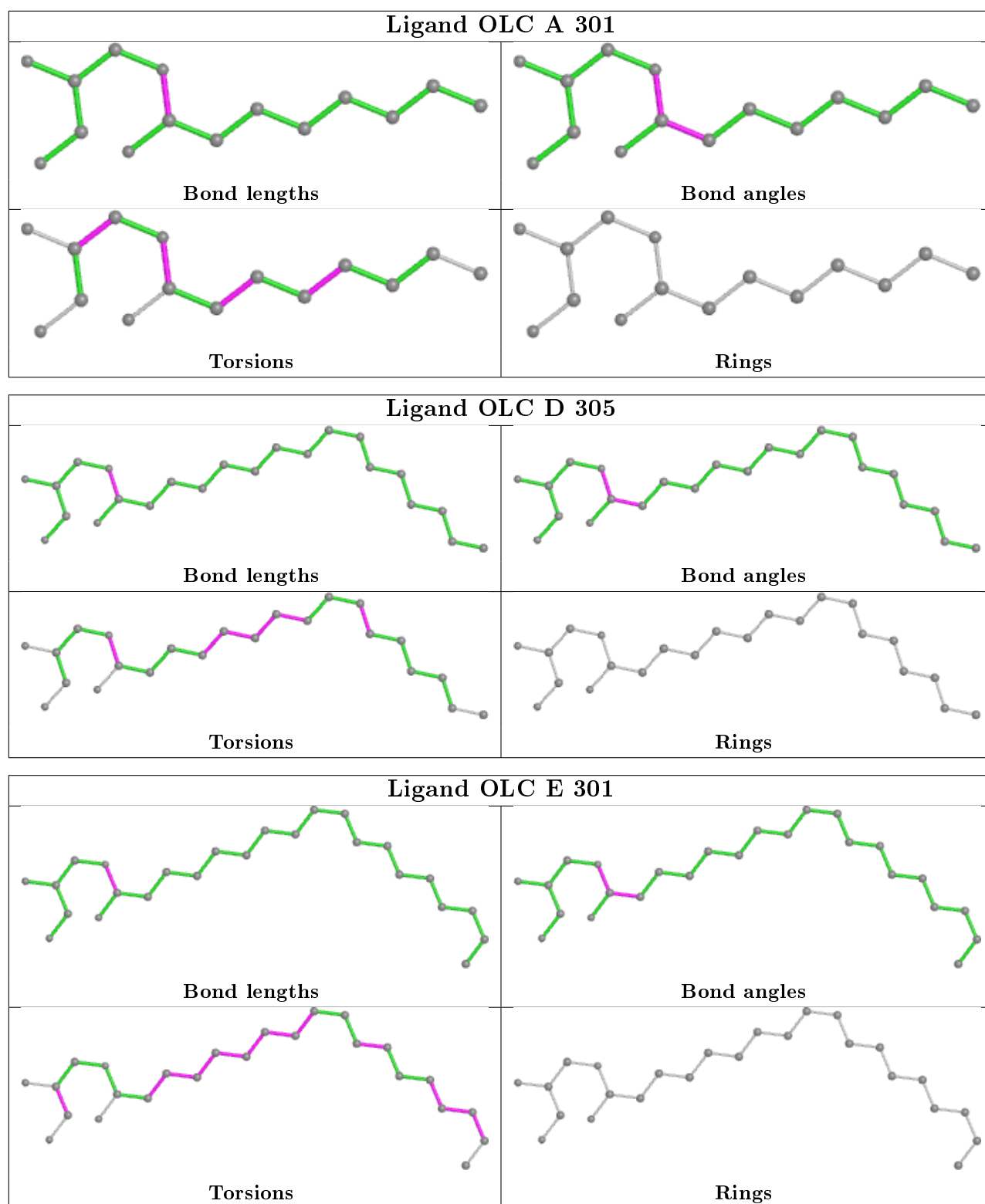


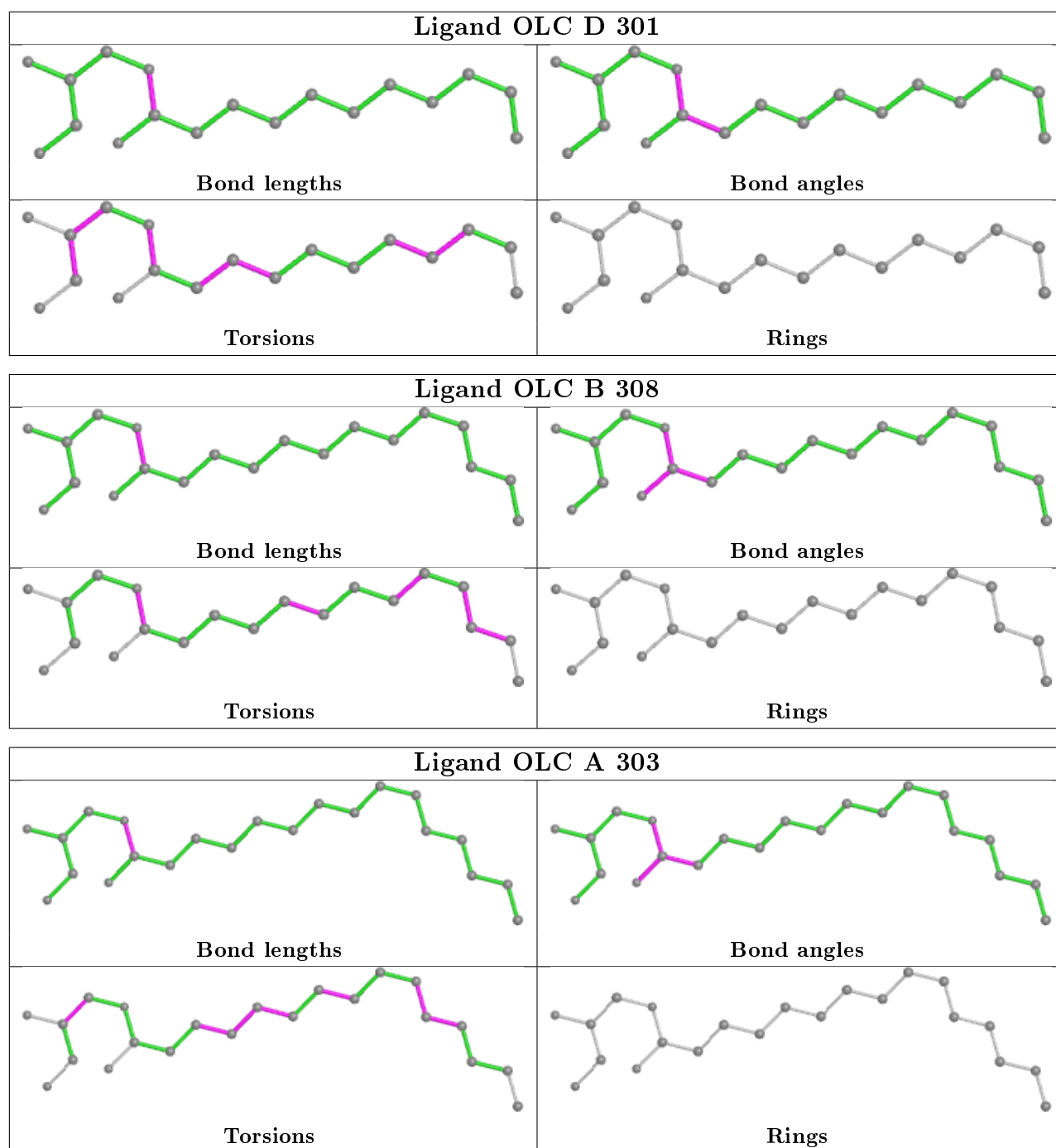


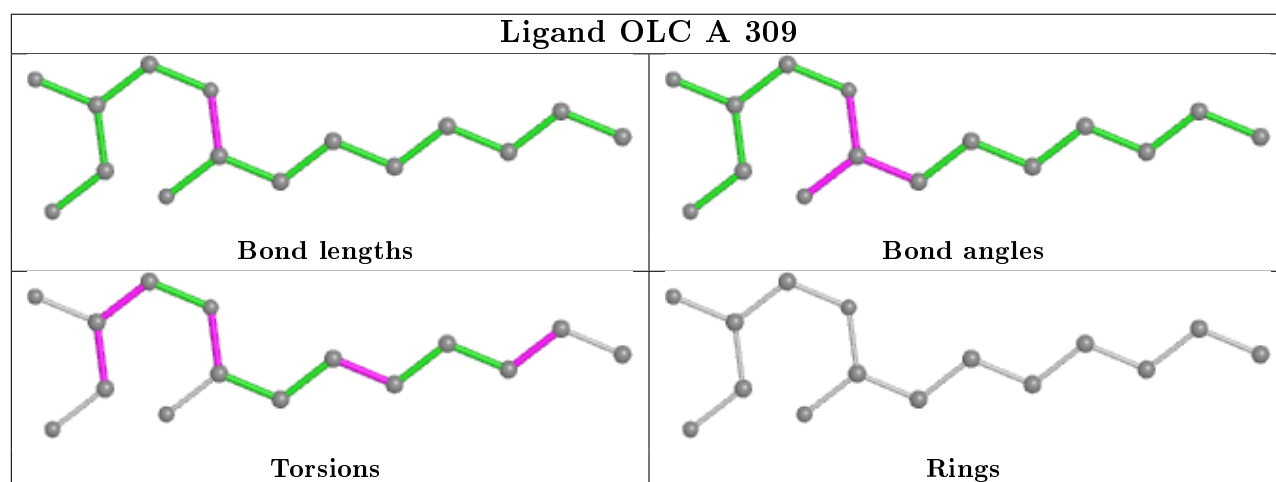
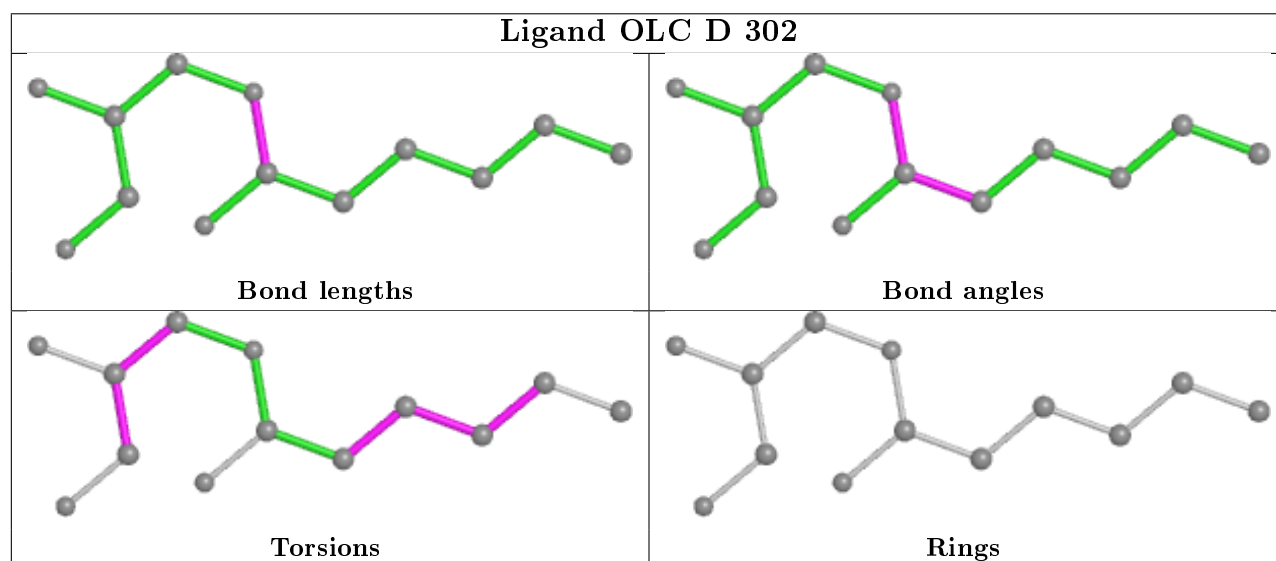
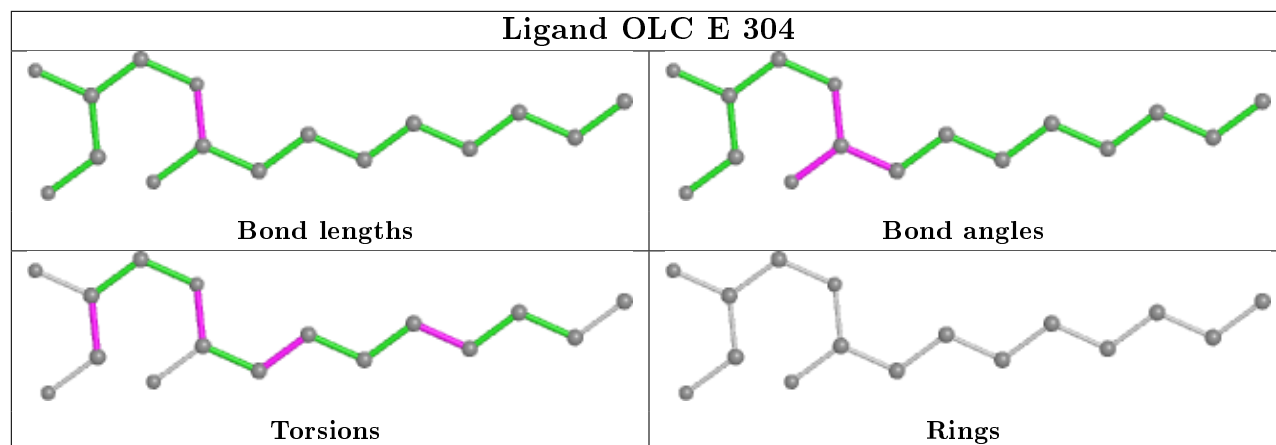


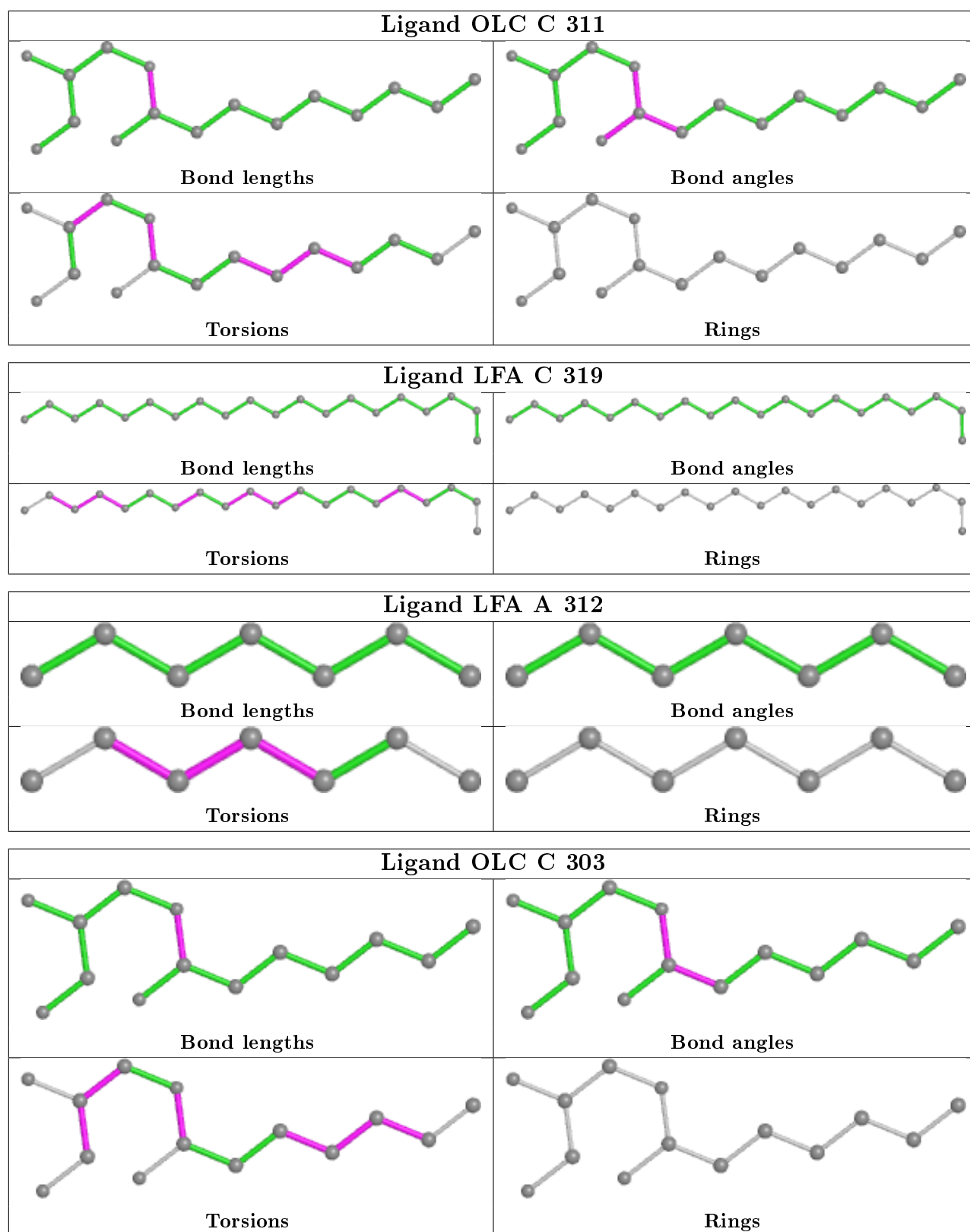


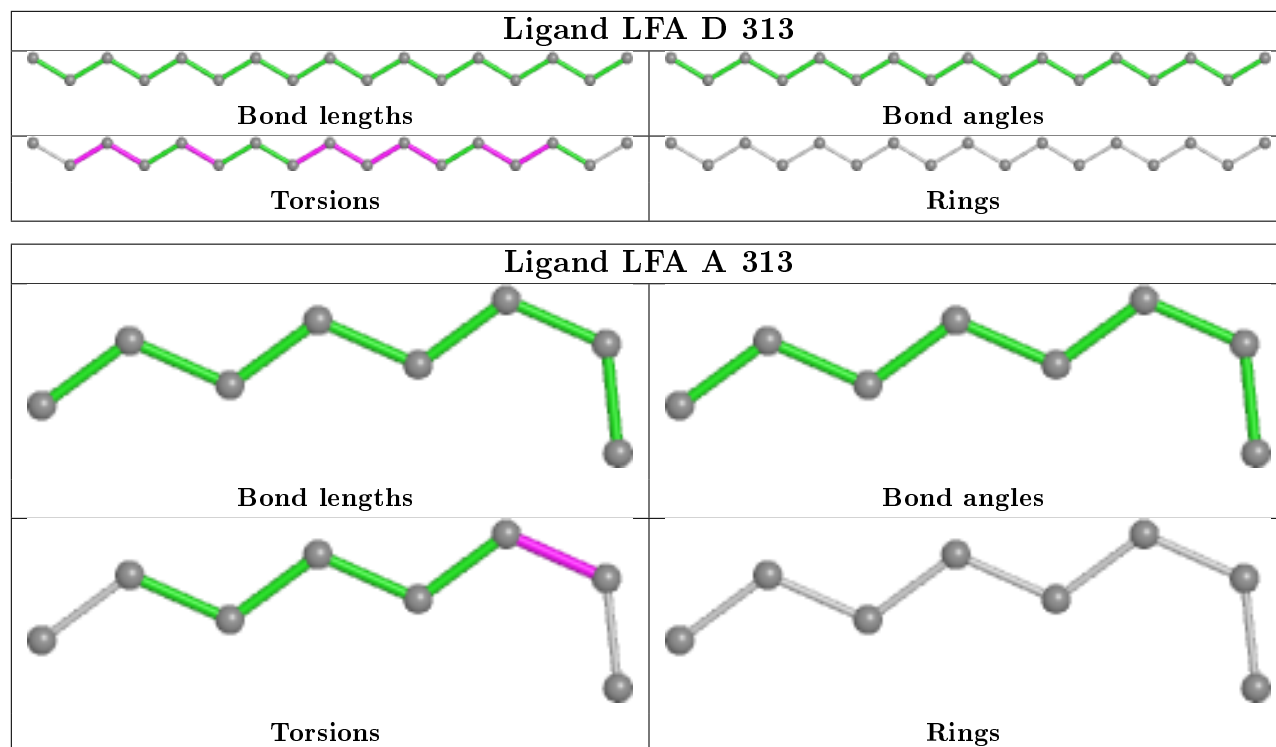












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/288 (94%)	0.33	25 (9%) 9 8	34, 45, 68, 152	0
1	B	272/288 (94%)	0.27	24 (8%) 10 9	36, 45, 69, 148	0
1	C	272/288 (94%)	0.28	23 (8%) 10 10	35, 45, 68, 179	0
1	D	272/288 (94%)	0.48	31 (11%) 5 4	35, 47, 74, 176	0
1	E	272/288 (94%)	0.34	24 (8%) 10 9	33, 45, 69, 179	0
All	All	1360/1440 (94%)	0.34	127 (9%) 8 8	33, 45, 70, 179	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	274	GLU	11.3
1	A	275	LEU	10.7
1	E	274	GLU	9.5
1	A	272	ASN	9.1
1	C	275	LEU	8.1
1	B	275	LEU	8.1
1	D	275	LEU	7.8
1	E	275	LEU	7.8
1	B	272	ASN	7.7
1	A	274	GLU	6.7
1	B	273	LYS	6.0
1	B	274	GLU	6.0
1	E	272	ASN	6.0
1	B	230	VAL	5.9
1	E	273	LYS	5.9
1	D	272	ASN	5.6
1	C	272	ASN	5.6
1	C	230	VAL	5.4
1	A	73	LEU	5.0
1	A	273	LYS	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	40	LEU	4.9
1	C	40	LEU	4.8
1	D	131	THR	4.8
1	E	73	LEU	4.6
1	D	273	LYS	4.5
1	C	76	TYR	4.4
1	D	230	VAL	4.4
1	B	76	TYR	4.3
1	D	43	LEU	4.3
1	D	76	TYR	4.3
1	E	40	LEU	4.2
1	E	76	TYR	4.2
1	B	40	LEU	4.2
1	A	40	LEU	4.2
1	A	76	TYR	4.2
1	E	72	PHE	4.1
1	D	69	VAL	4.1
1	D	36	TYR	4.0
1	A	3	GLN	4.0
1	A	69	VAL	4.0
1	C	273	LYS	3.8
1	E	36	TYR	3.7
1	B	72	PHE	3.6
1	B	3	GLN	3.6
1	A	271	LYS	3.6
1	A	72	PHE	3.6
1	D	73	LEU	3.6
1	D	72	PHE	3.5
1	C	72	PHE	3.5
1	E	43	LEU	3.5
1	D	79	ALA	3.4
1	D	233	PHE	3.3
1	D	74	LEU	3.3
1	D	75	LEU	3.3
1	A	183	TRP	3.3
1	C	36	TYR	3.3
1	C	44	LEU	3.2
1	E	74	LEU	3.2
1	E	69	VAL	3.2
1	D	132	THR	3.2
1	E	44	LEU	3.2
1	B	271	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	77	ALA	3.2
1	A	233	PHE	3.1
1	D	130	LEU	3.1
1	E	47	ILE	3.1
1	A	74	LEU	3.1
1	A	230	VAL	3.1
1	C	73	LEU	3.1
1	C	132	THR	3.1
1	C	43	LEU	3.0
1	A	36	TYR	2.9
1	B	73	LEU	2.9
1	E	79	ALA	2.9
1	D	271	LYS	2.9
1	D	77	ALA	2.8
1	B	36	TYR	2.8
1	B	79	ALA	2.8
1	A	43	LEU	2.8
1	C	74	LEU	2.8
1	C	69	VAL	2.7
1	C	77	ALA	2.7
1	D	3	GLN	2.7
1	B	74	LEU	2.7
1	D	129	SER	2.6
1	B	77	ALA	2.6
1	D	44	LEU	2.6
1	E	230	VAL	2.6
1	D	42	GLY	2.6
1	C	274	GLU	2.6
1	C	130	LEU	2.5
1	B	75	LEU	2.5
1	B	190	ASN	2.5
1	A	75	LEU	2.5
1	E	271	LYS	2.4
1	C	79	ALA	2.4
1	A	44	LEU	2.4
1	B	183	TRP	2.4
1	C	3	GLN	2.4
1	E	90	GLU	2.4
1	D	41	ALA	2.4
1	E	190	ASN	2.3
1	D	133	SER	2.3
1	B	44	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	47	ILE	2.3
1	E	75	LEU	2.3
1	A	270	SER	2.3
1	E	77	ALA	2.3
1	C	33	THR	2.2
1	B	33	THR	2.2
1	C	75	LEU	2.2
1	E	18	GLU	2.2
1	C	228	THR	2.2
1	B	69	VAL	2.2
1	D	194	GLU	2.2
1	A	196	ILE	2.2
1	A	203	ILE	2.1
1	A	65	ALA	2.1
1	E	41	ALA	2.1
1	E	80	GLN	2.1
1	B	43	LEU	2.1
1	D	228	THR	2.1
1	D	47	ILE	2.1
1	B	18	GLU	2.0
1	C	183	TRP	2.0
1	D	195	GLY	2.0
1	B	54	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LYR	A	255	29/30	0.91	0.16	34,40,48,51	0
1	LYR	B	255	29/30	0.93	0.17	33,39,53,57	0
1	LYR	D	255	29/30	0.94	0.17	35,42,49,49	0
1	LYR	E	255	29/30	0.94	0.16	34,39,44,47	0
1	LYR	C	255	29/30	0.95	0.15	34,42,48,52	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	D	306	25/25	0.29	0.45	80,101,115,122	0
2	OLC	C	309	16/25	0.34	0.52	82,110,137,140	0
2	OLC	E	303	14/25	0.44	0.41	104,126,146,183	0
2	OLC	A	301	15/25	0.45	0.51	95,124,172,178	0
2	OLC	A	308	25/25	0.46	0.42	78,103,127,132	0
2	OLC	B	303	14/25	0.47	0.42	101,136,164,188	0
2	OLC	A	310	16/25	0.51	0.43	76,105,138,148	0
2	OLC	A	307	16/25	0.54	0.48	90,107,122,128	0
5	BOG	C	321	20/20	0.57	0.54	76,93,115,115	0
2	OLC	E	312	25/25	0.58	0.43	80,98,116,135	0
2	OLC	B	313	17/25	0.58	0.29	73,99,129,136	0
3	LFA	E	302	20/20	0.59	1.39	57,76,93,105	0
2	OLC	B	311	25/25	0.59	0.43	82,102,121,127	0
5	BOG	A	320	20/20	0.59	0.61	76,107,122,122	0
3	LFA	C	314	7/20	0.60	0.26	67,79,104,106	0
2	OLC	B	310	16/25	0.60	0.37	71,96,130,131	0
2	OLC	D	303	25/25	0.60	0.38	75,101,114,115	0
2	OLC	B	305	15/25	0.60	0.32	87,114,139,139	0
2	OLC	E	310	15/25	0.61	0.31	58,97,131,132	0
5	BOG	E	321	20/20	0.61	0.46	73,106,121,123	0
2	OLC	E	304	16/25	0.61	0.39	67,116,151,155	0
3	LFA	E	323	14/20	0.62	1.50	101,125,159,162	0
2	OLC	E	313	20/25	0.62	0.56	65,112,127,135	0
2	OLC	A	306	15/25	0.62	0.56	69,96,128,137	0
2	OLC	B	314	15/25	0.62	0.28	90,107,125,126	0
2	OLC	E	308	15/25	0.62	0.53	84,107,142,147	0
2	OLC	C	308	22/25	0.63	0.45	58,98,127,148	0
2	OLC	C	303	14/25	0.63	0.44	93,115,149,167	0
2	OLC	D	305	23/25	0.64	0.45	60,112,160,166	0
5	BOG	B	321	20/20	0.65	0.54	75,102,116,129	0
3	LFA	B	318	10/20	0.65	0.28	75,92,103,104	0
2	OLC	E	314	25/25	0.65	0.46	86,115,149,161	0
2	OLC	C	304	21/25	0.66	0.33	74,115,144,153	0
2	OLC	B	307	24/25	0.66	0.41	83,112,130,134	0
3	LFA	B	302	20/20	0.66	1.25	59,75,86,93	0
2	OLC	B	304	25/25	0.66	0.34	78,107,124,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	D	308	15/25	0.67	0.32	66,90,129,139	0
3	LFA	C	317	11/20	0.67	0.30	72,88,105,107	0
2	OLC	C	307	25/25	0.67	0.24	69,93,114,123	0
3	LFA	C	319	20/20	0.67	1.18	55,68,79,80	0
3	LFA	D	312	8/20	0.67	0.30	74,83,108,109	0
2	OLC	A	321	25/25	0.68	0.31	65,91,126,134	0
2	OLC	D	302	13/25	0.68	0.47	116,129,142,171	0
3	LFA	E	319	20/20	0.69	1.24	52,75,89,95	0
2	OLC	B	308	20/25	0.70	0.22	64,86,109,114	0
3	LFA	B	316	9/20	0.70	0.33	75,92,99,101	0
2	OLC	B	306	20/25	0.70	0.31	75,90,119,120	0
2	OLC	E	306	24/25	0.70	0.45	85,103,140,162	0
2	OLC	C	306	25/25	0.70	0.29	72,95,117,128	0
2	OLC	C	312	16/25	0.71	0.27	65,90,118,120	0
2	OLC	B	315	16/25	0.71	0.35	75,88,123,145	0
2	OLC	C	313	16/25	0.72	0.37	64,85,112,122	0
2	OLC	E	311	11/25	0.72	0.28	94,110,127,133	0
2	OLC	A	304	25/25	0.73	0.44	70,98,119,137	0
3	LFA	A	312	7/20	0.73	0.24	86,90,92,101	0
2	OLC	A	311	16/25	0.73	0.36	73,91,128,145	0
3	LFA	B	319	7/20	0.74	0.26	65,76,100,111	0
2	OLC	D	309	25/25	0.74	0.38	79,95,116,131	0
3	LFA	C	315	8/20	0.74	0.24	79,90,98,101	0
3	LFA	A	314	8/20	0.74	0.24	66,91,111,123	0
3	LFA	D	315	6/20	0.74	0.26	73,87,99,104	0
2	OLC	E	301	25/25	0.74	0.32	63,92,133,149	0
2	OLC	A	303	22/25	0.75	0.33	48,65,121,170	0
3	LFA	E	316	14/20	0.75	0.27	69,91,104,110	0
3	LFA	D	310	20/20	0.75	0.26	81,94,105,115	0
3	LFA	C	302	20/20	0.75	1.12	61,71,77,81	0
5	BOG	D	317	20/20	0.75	0.60	89,102,112,114	0
2	OLC	C	305	23/25	0.75	0.34	49,66,121,135	0
2	OLC	A	302	25/25	0.76	0.26	74,111,124,141	0
3	LFA	E	315	8/20	0.76	0.31	72,99,104,104	0
3	LFA	A	315	12/20	0.76	0.19	92,99,111,112	0
2	OLC	C	310	25/25	0.76	0.47	89,100,121,127	0
3	LFA	A	313	8/20	0.76	0.28	74,83,90,91	0
3	LFA	D	314	7/20	0.78	0.19	71,82,99,105	0
3	LFA	A	318	20/20	0.79	0.32	80,107,126,131	0
3	LFA	E	318	5/20	0.79	0.24	83,83,92,101	0
3	LFA	E	317	4/20	0.79	0.28	68,71,76,85	0
2	OLC	D	301	18/25	0.79	0.30	77,96,118,128	0

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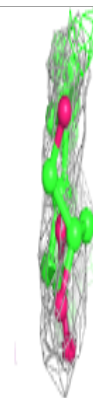
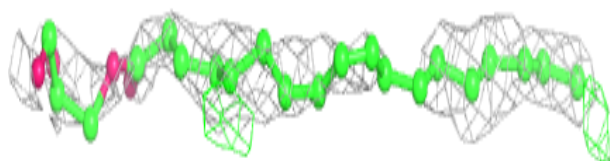
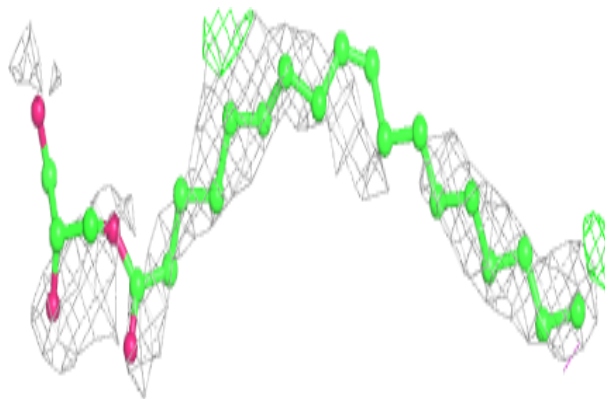
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	E	305	24/25	0.80	0.34	51,66,129,145	0
2	OLC	B	309	21/25	0.80	0.42	58,87,118,143	0
2	OLC	B	301	25/25	0.80	0.25	74,90,122,124	0
3	LFA	D	311	20/20	0.82	0.28	70,98,113,113	0
2	OLC	A	305	13/25	0.82	0.25	64,73,86,86	0
3	LFA	C	316	20/20	0.82	0.25	63,92,121,125	0
2	OLC	D	304	18/25	0.83	0.30	74,96,115,118	0
2	OLC	C	301	21/25	0.83	0.29	48,62,101,113	0
3	LFA	A	316	4/20	0.83	0.27	81,85,93,95	0
2	OLC	E	307	20/25	0.84	0.29	75,96,108,113	0
3	LFA	C	318	4/20	0.84	0.42	87,93,94,97	0
3	LFA	B	317	8/20	0.85	0.31	75,103,106,107	0
3	LFA	D	313	17/20	0.88	0.47	49,57,84,85	0
2	OLC	C	311	16/25	0.88	0.20	60,86,99,103	0
2	OLC	B	312	16/25	0.89	0.23	65,83,97,111	0
2	OLC	E	309	25/25	0.90	0.26	56,98,132,140	0
2	OLC	A	309	15/25	0.90	0.15	60,76,101,104	0
2	OLC	D	307	14/25	0.92	0.12	56,82,98,102	0
3	LFA	A	317	6/20	0.92	0.24	64,73,82,82	0
3	LFA	E	322	4/20	0.95	2.40	73,79,81,83	0
4	NA	E	320	1/1	0.95	0.07	38,38,38,38	0
4	NA	A	319	1/1	0.96	0.11	45,45,45,45	0
4	NA	B	320	1/1	0.97	0.08	39,39,39,39	0
4	NA	D	316	1/1	0.98	0.08	41,41,41,41	0
4	NA	C	320	1/1	0.99	0.10	42,42,42,42	0

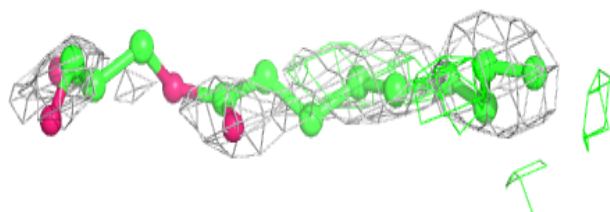
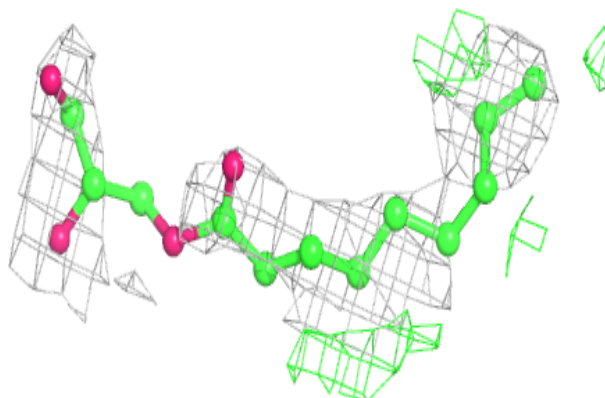
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC D 306:

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

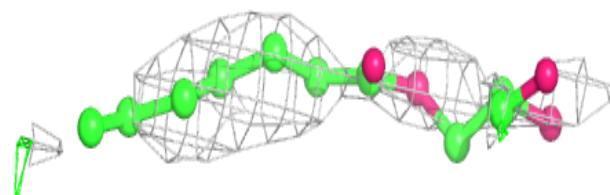
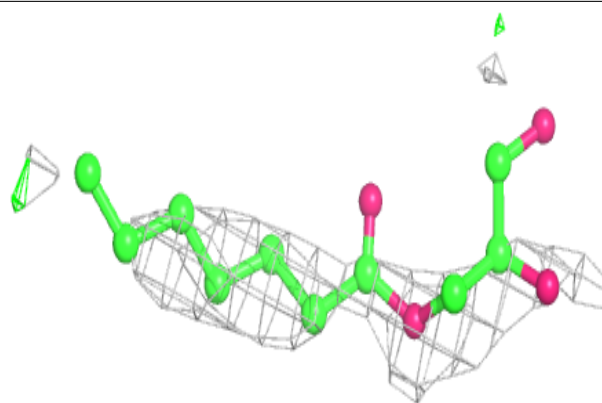
**Electron density around OLC C 309:**

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

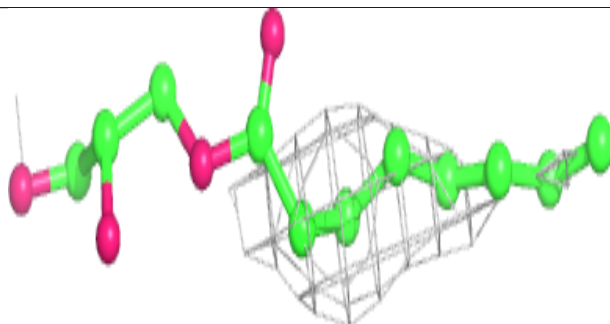
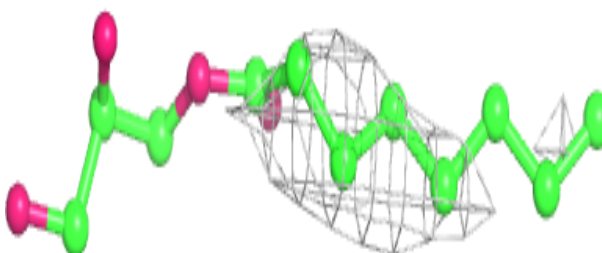


Electron density around OLC E 303:

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

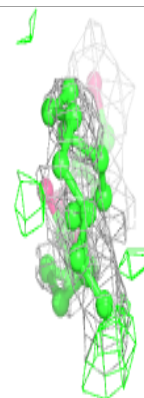
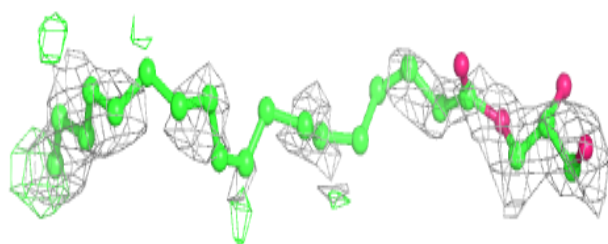
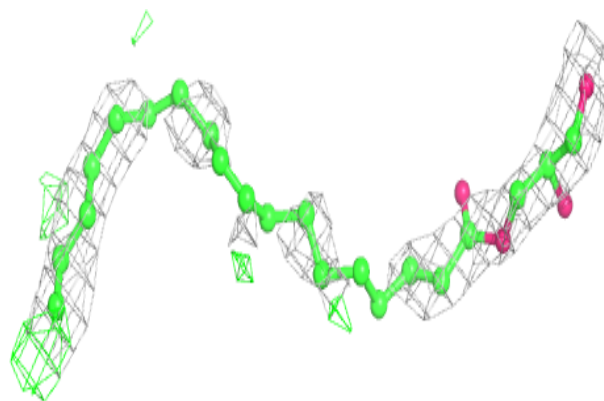
**Electron density around OLC A 301:**

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

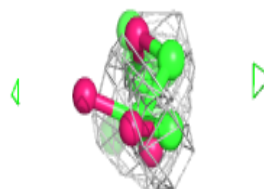
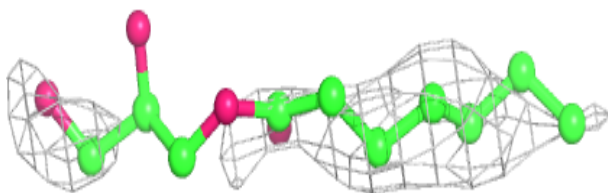
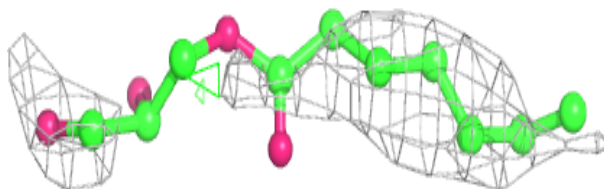


Electron density around OLC A 308:

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

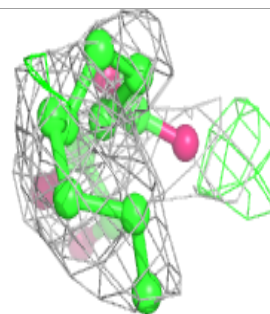
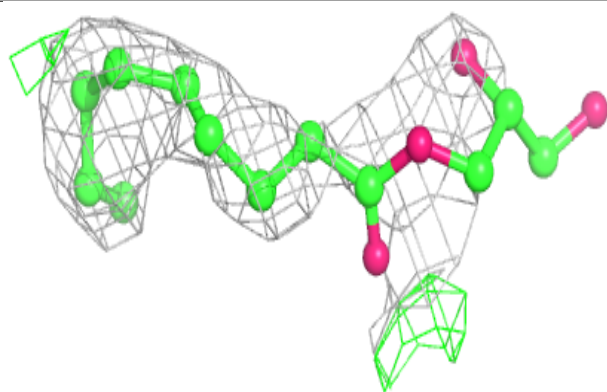
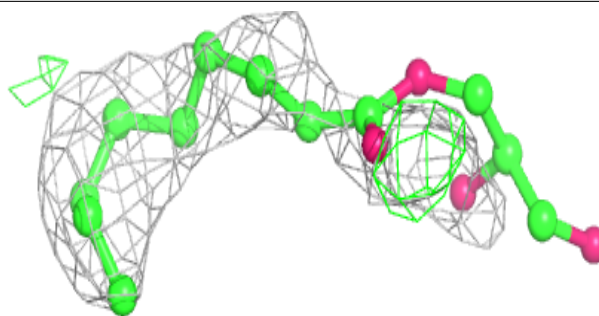
**Electron density around OLC B 303:**

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

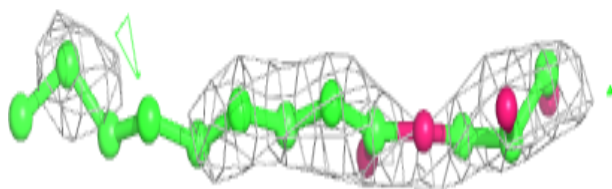
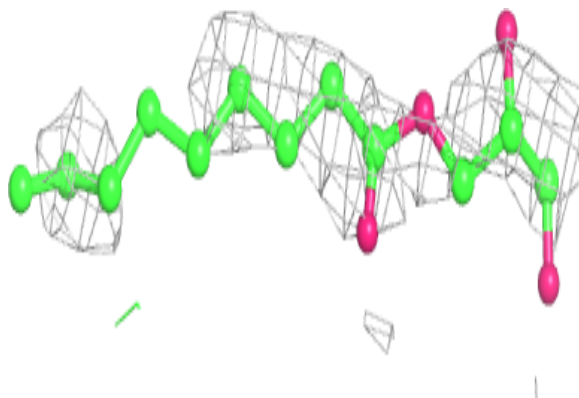


Electron density around OLC A 310:

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

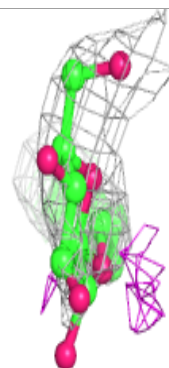
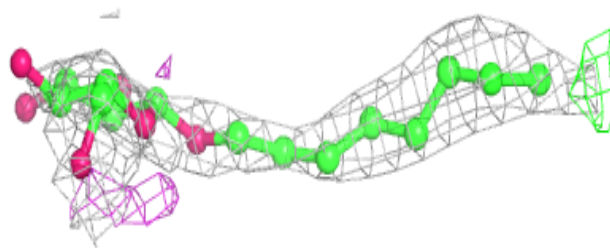
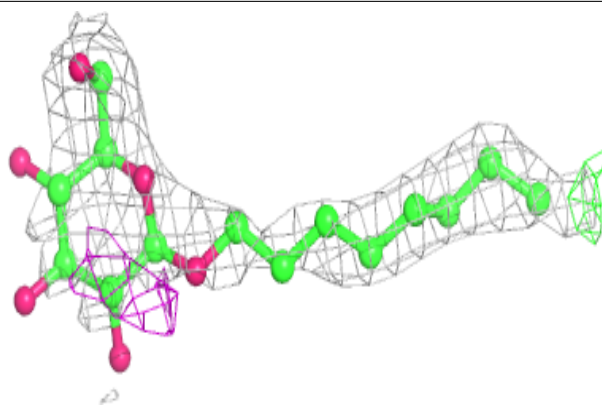
**Electron density around OLC A 307:**

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

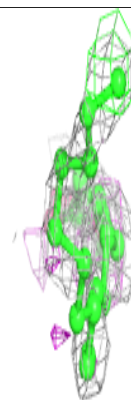
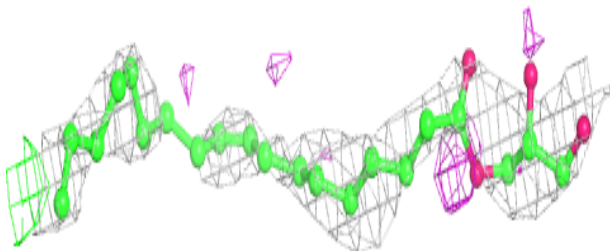
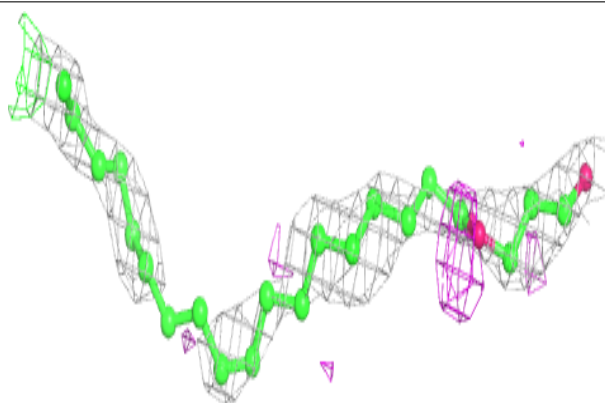


Electron density around BOG C 321:

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

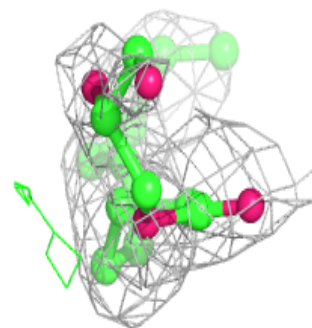
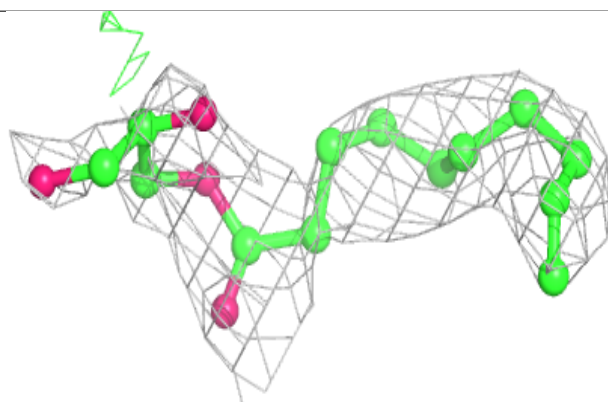
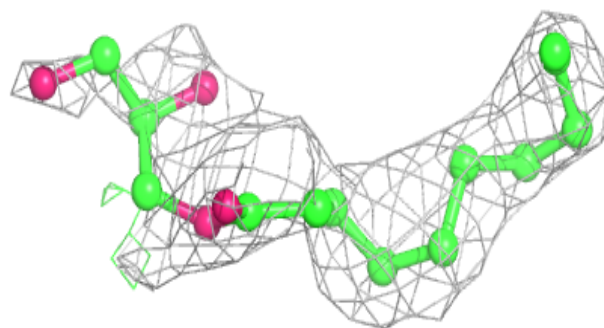
**Electron density around OLC E 312:**

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

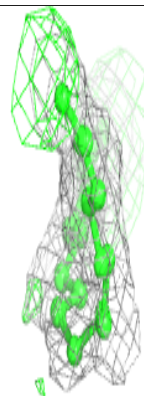
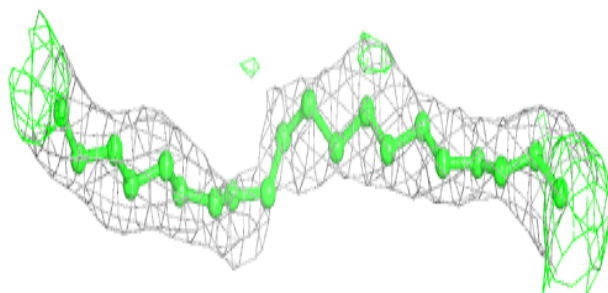
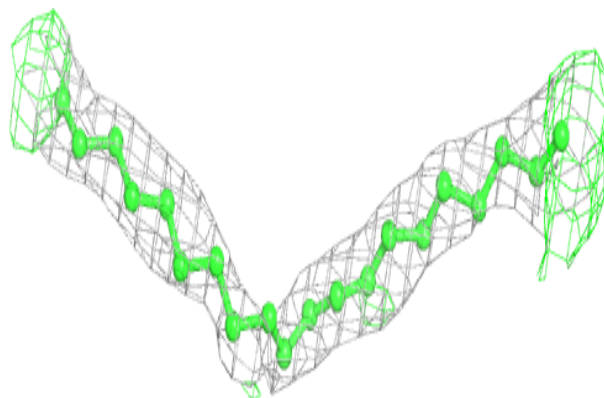


Electron density around OLC B 313:

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

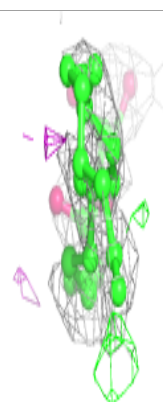
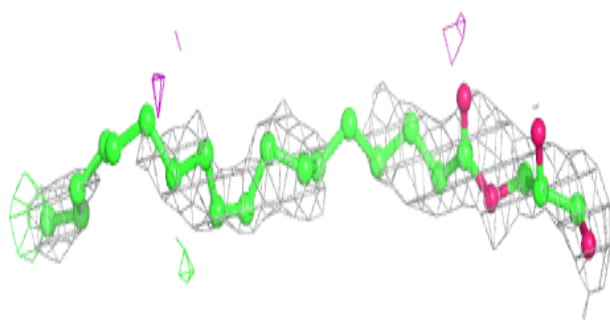
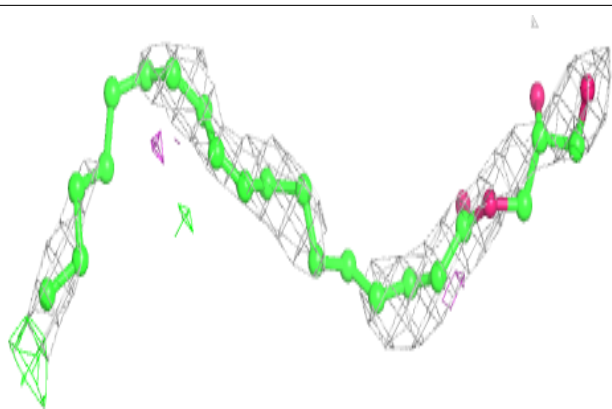
**Electron density around LFA E 302:**

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

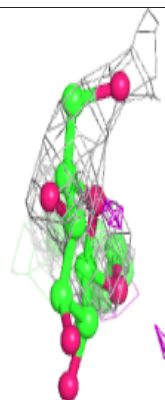
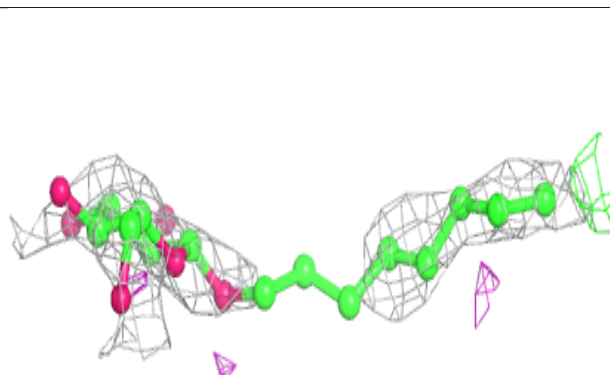
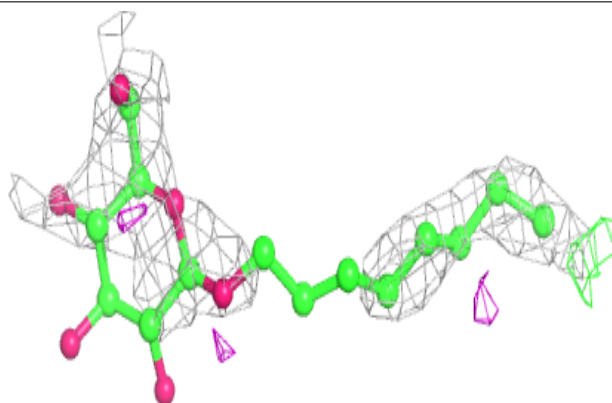


Electron density around OLC B 311:

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

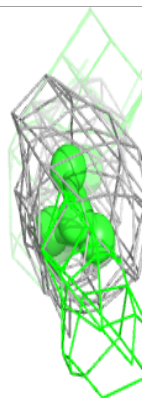
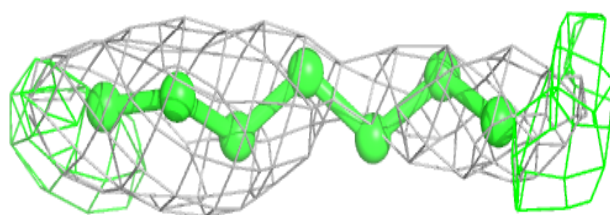
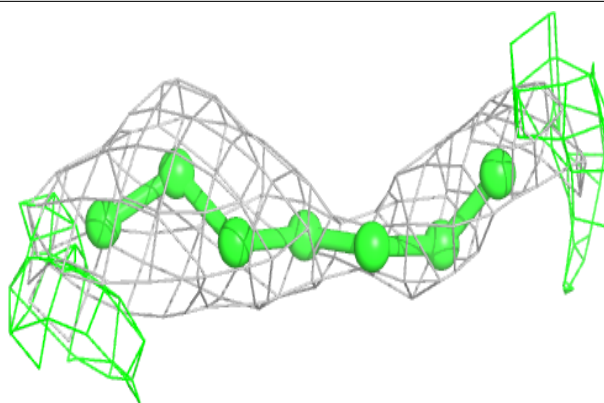
**Electron density around BOG A 320:**

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

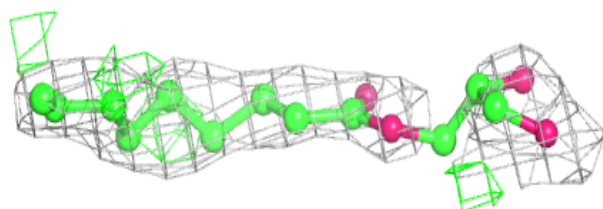
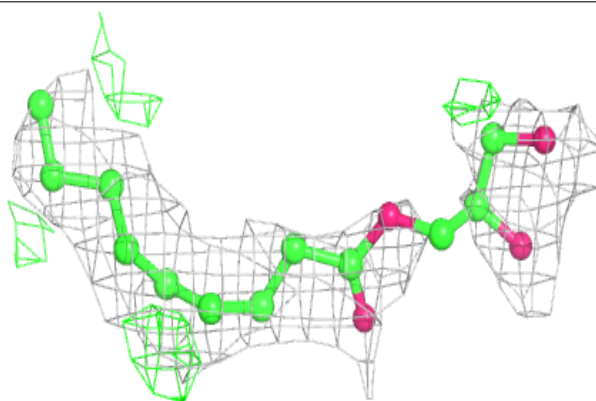


Electron density around LFA C 314:

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

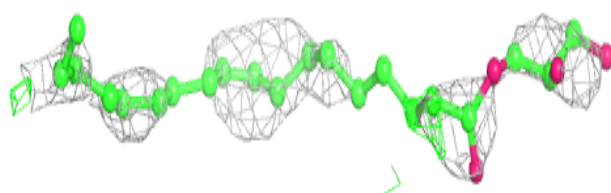
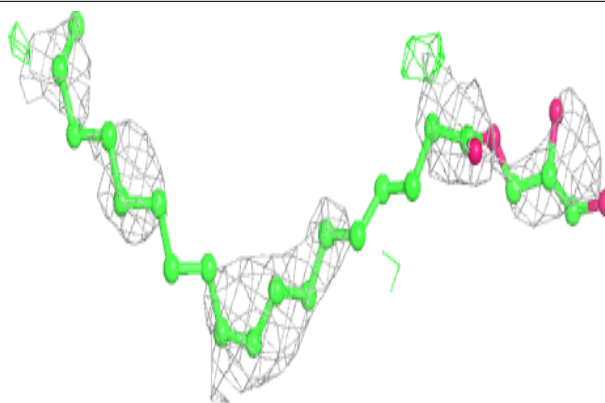
**Electron density around OLC B 310:**

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

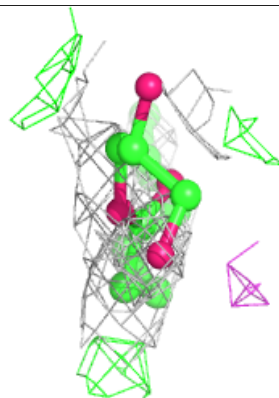
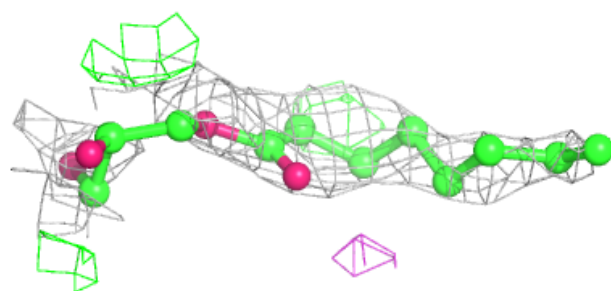
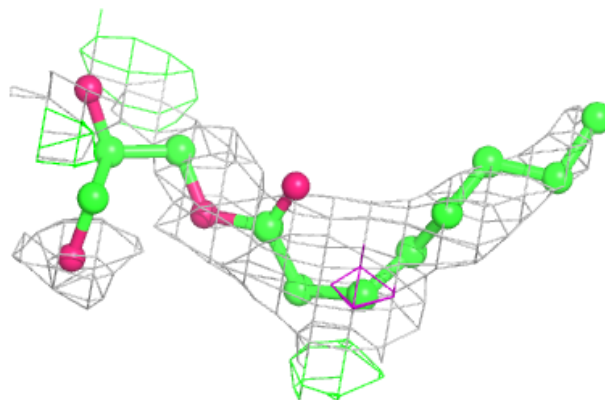


Electron density around OLC D 303:

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

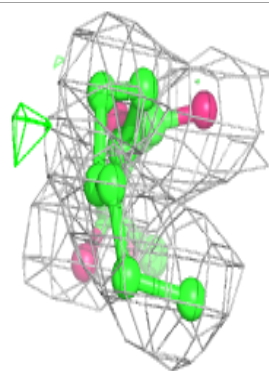
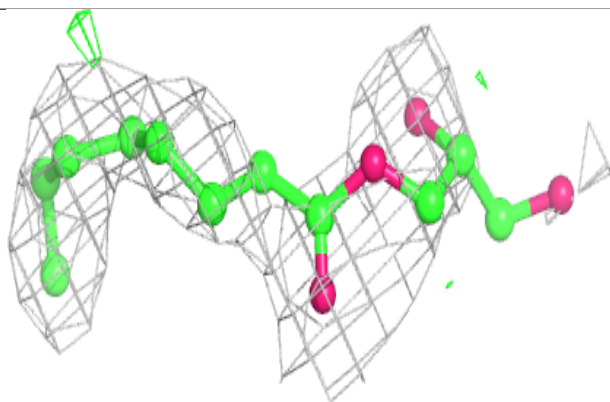
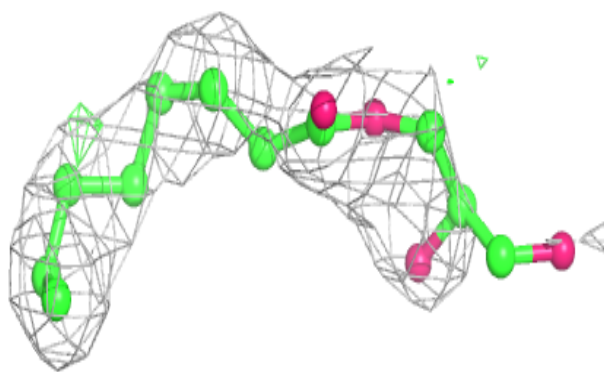
**Electron density around OLC B 305:**

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

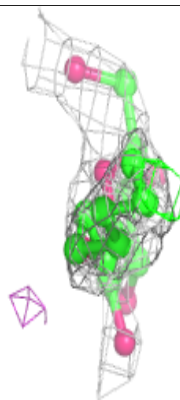
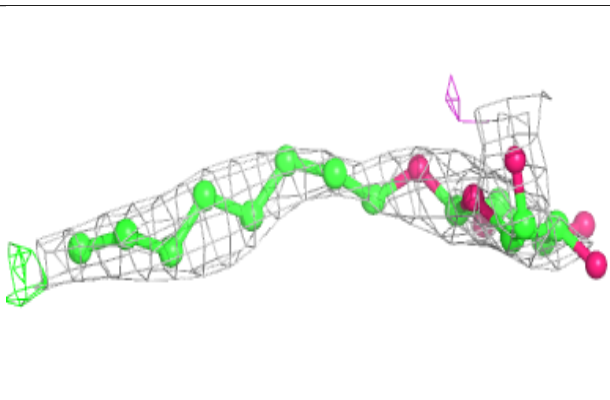
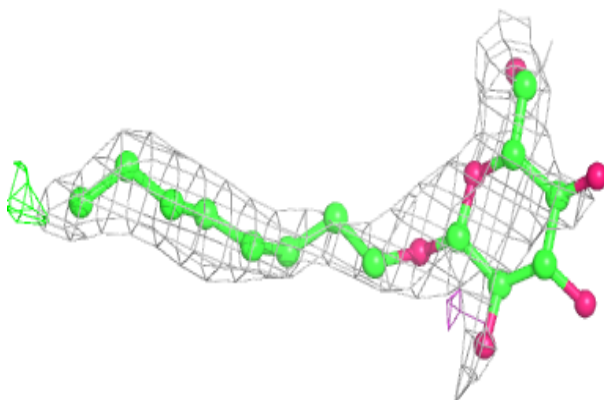


Electron density around OLC E 310:

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

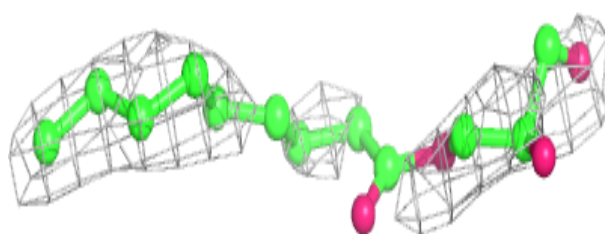
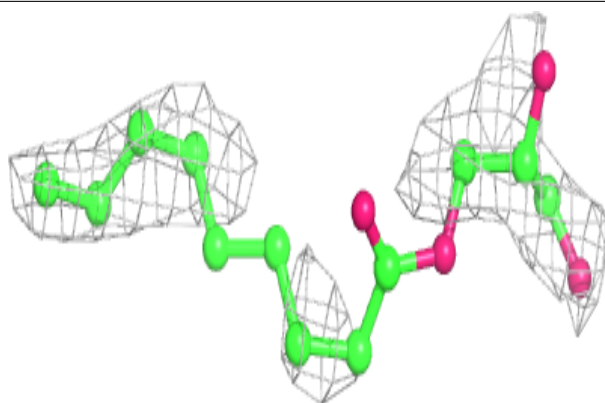
**Electron density around BOG E 321:**

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

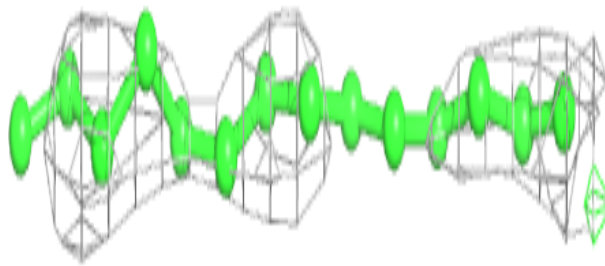
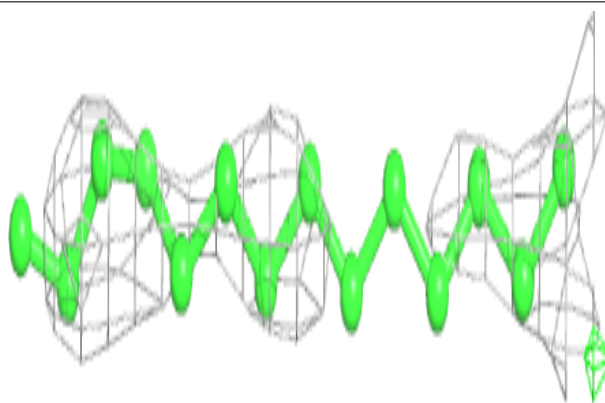


Electron density around OLC E 304:

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

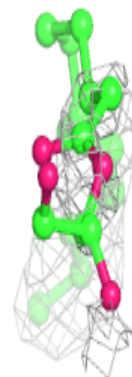
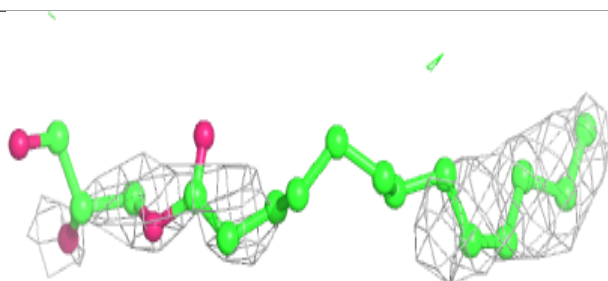
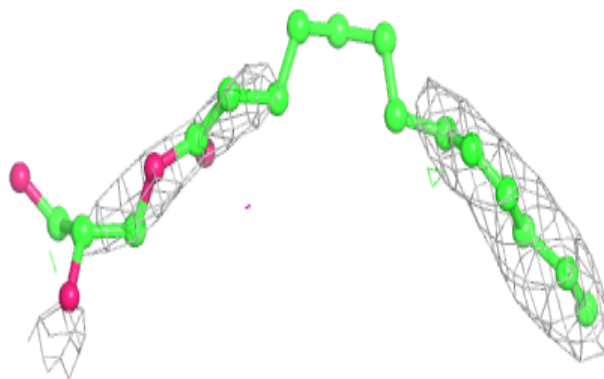
**Electron density around LFA E 323:**

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

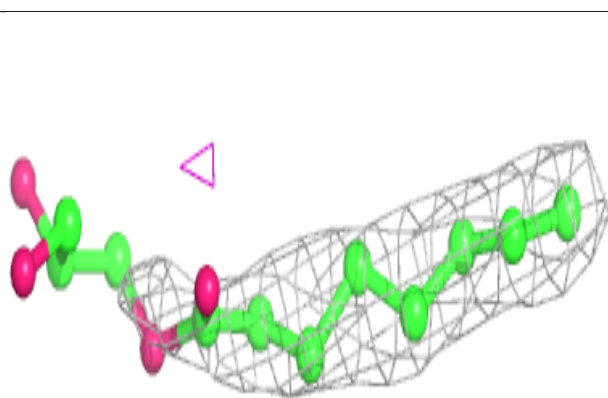
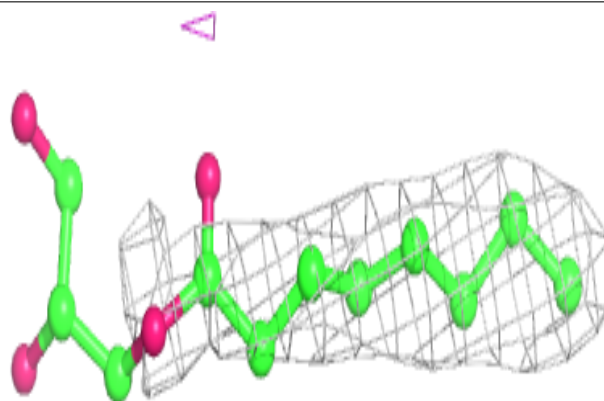


Electron density around OLC E 313:

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

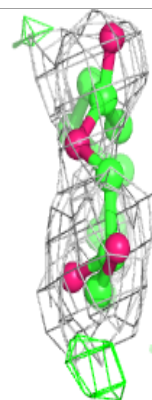
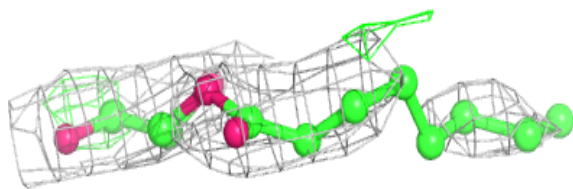
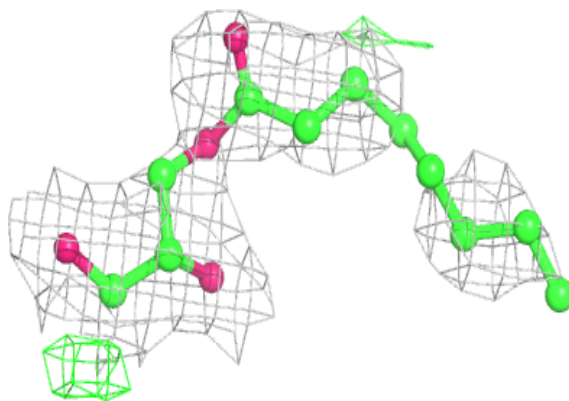
**Electron density around OLC A 306:**

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

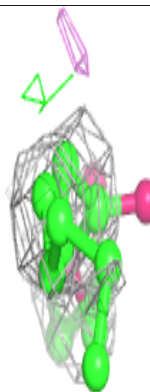
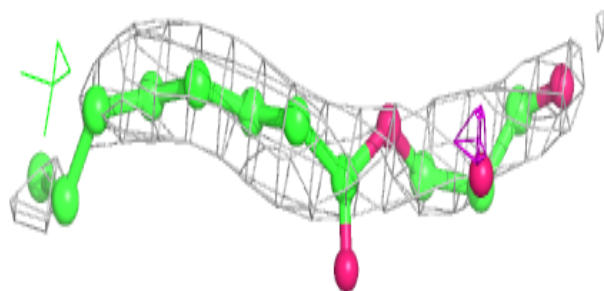
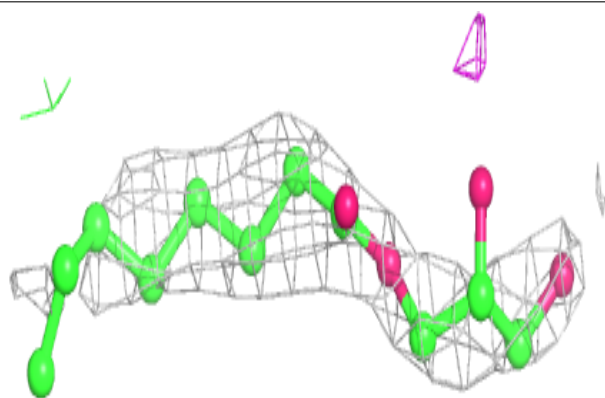


Electron density around OLC B 314:

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

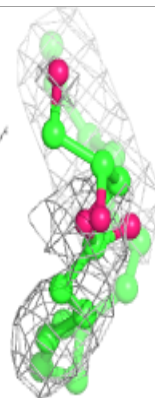
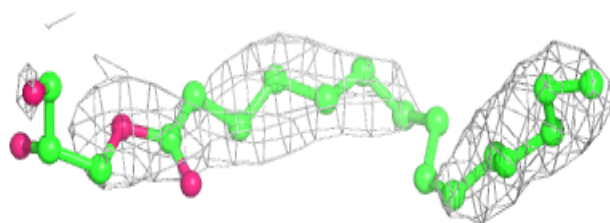
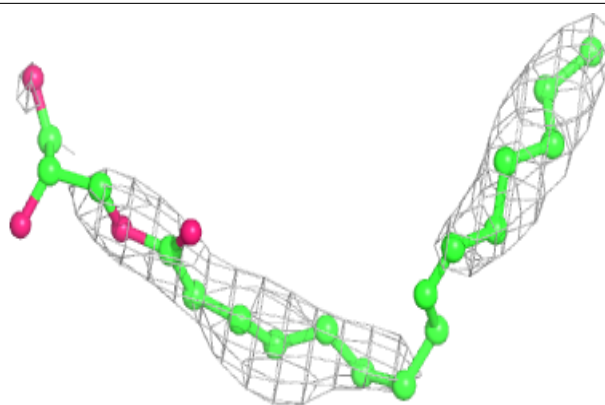
**Electron density around OLC E 308:**

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

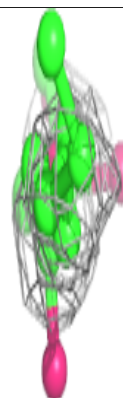
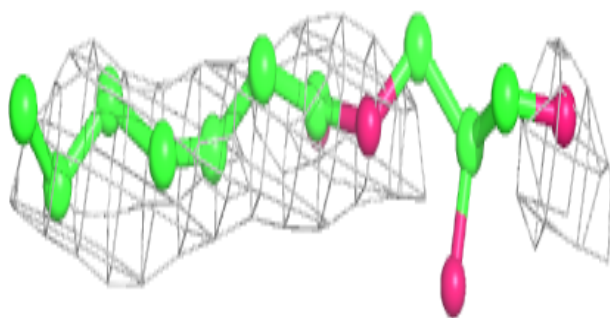
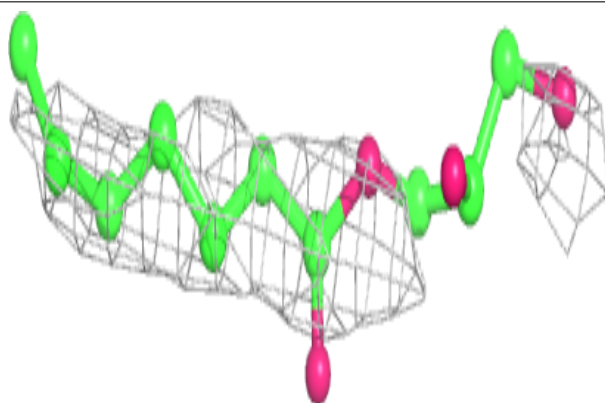


Electron density around OLC C 308:

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

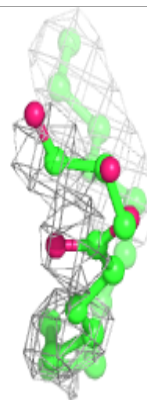
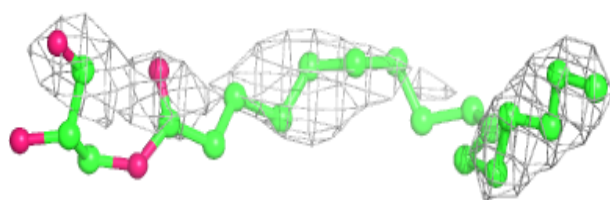
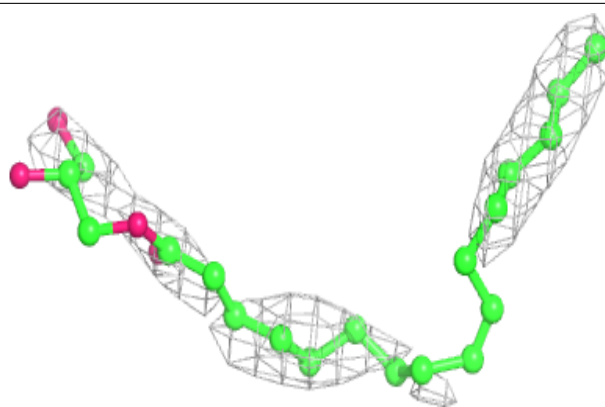
**Electron density around OLC C 303:**

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

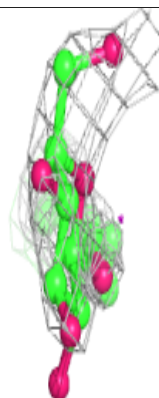
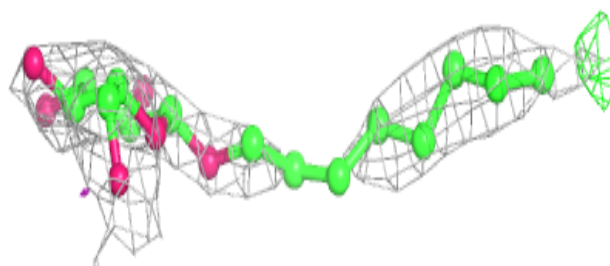
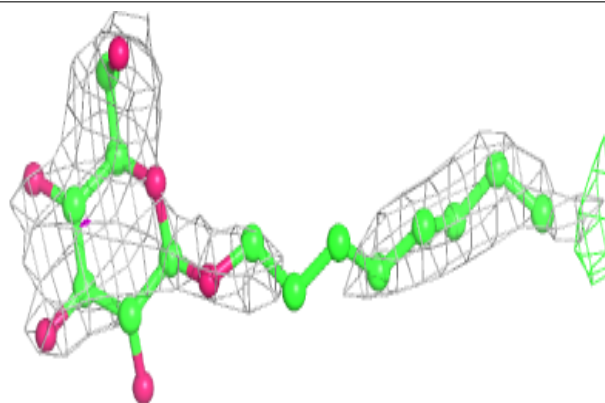


Electron density around OLC D 305:

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

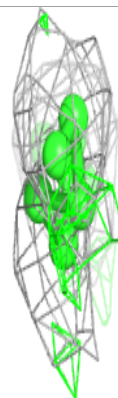
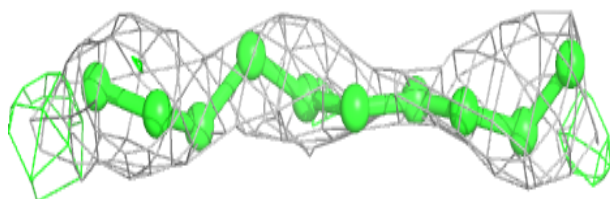
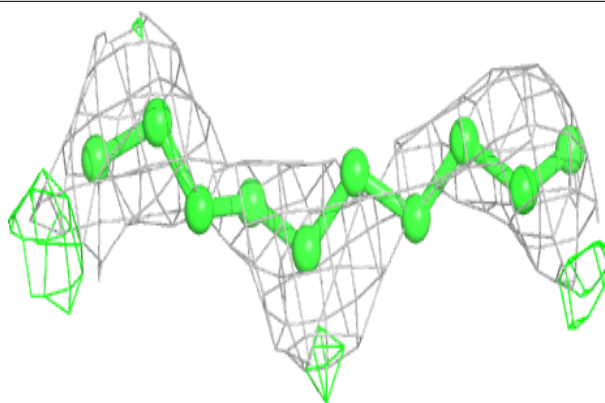
**Electron density around BOG B 321:**

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

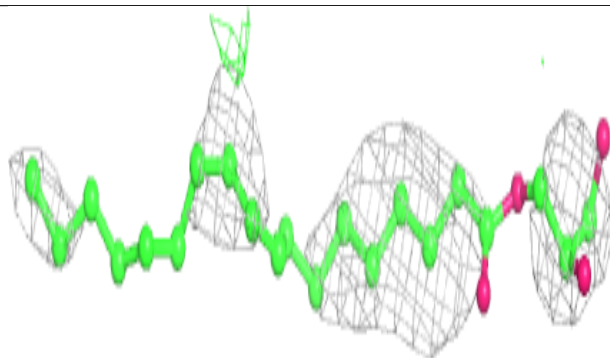
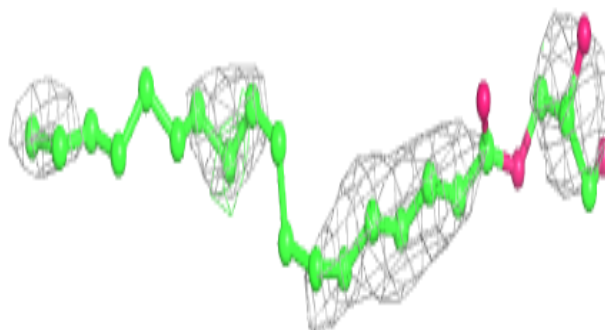


Electron density around LFA B 318:

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

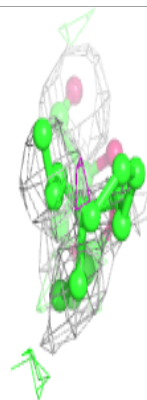
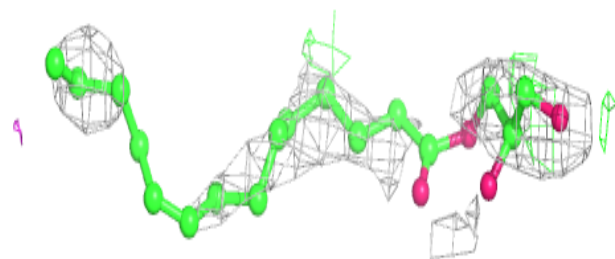
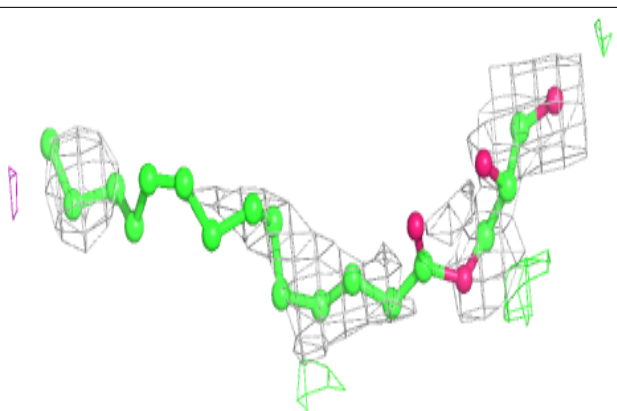
**Electron density around OLC E 314:**

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

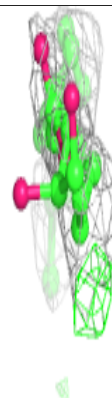
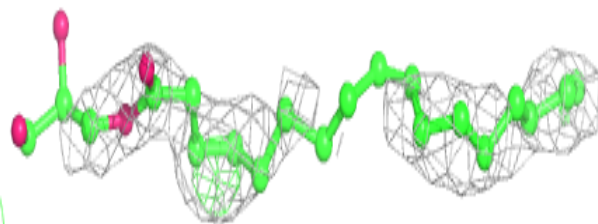
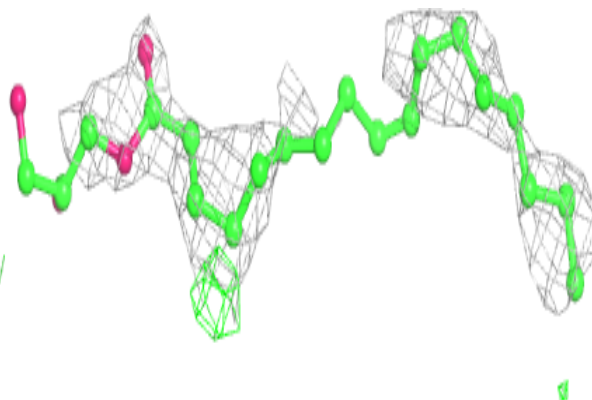


Electron density around OLC C 304:

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

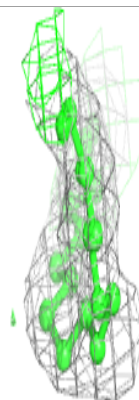
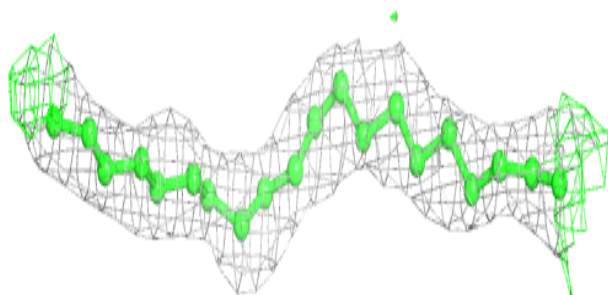
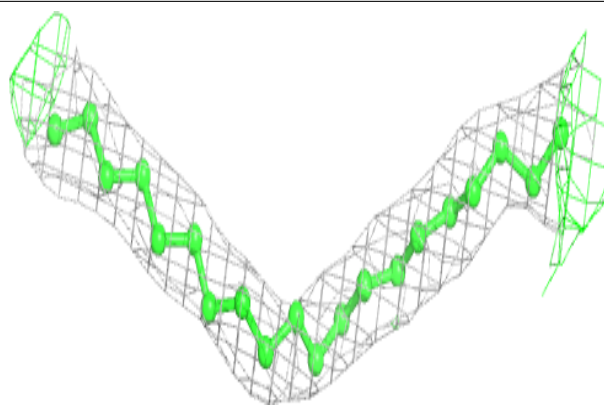
**Electron density around OLC B 307:**

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

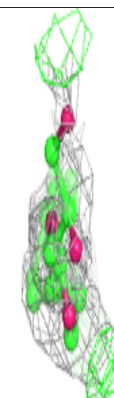
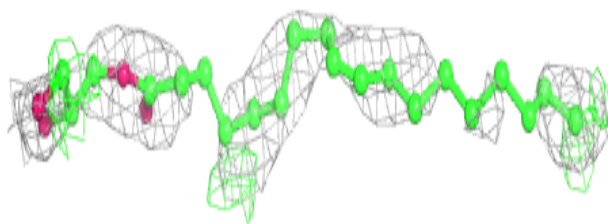
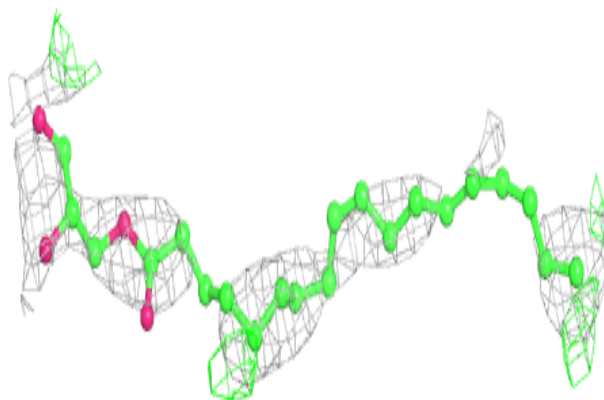


Electron density around LFA B 302:

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

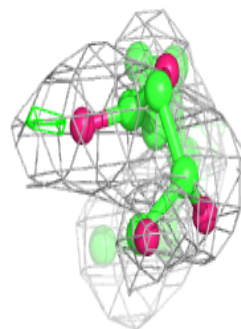
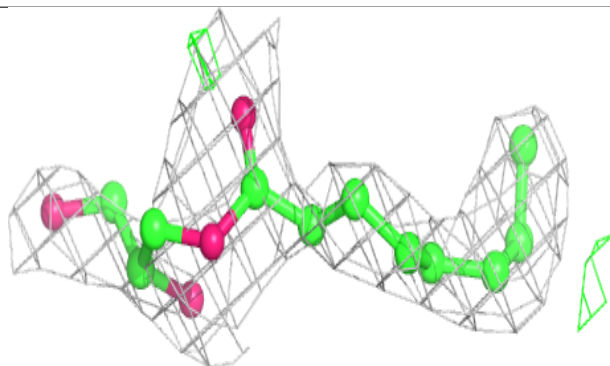
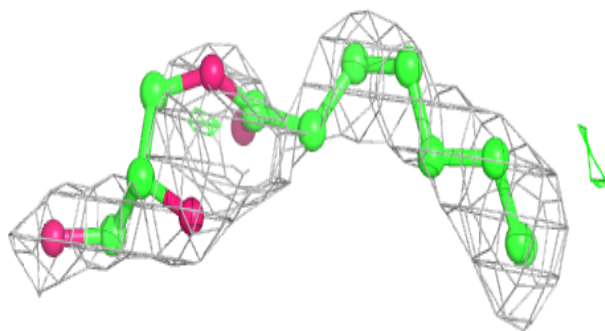
**Electron density around OLC B 304:**

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

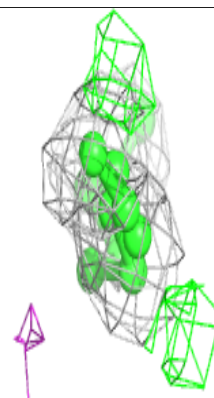
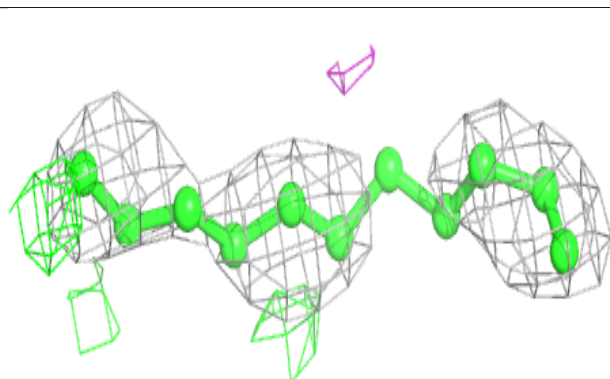
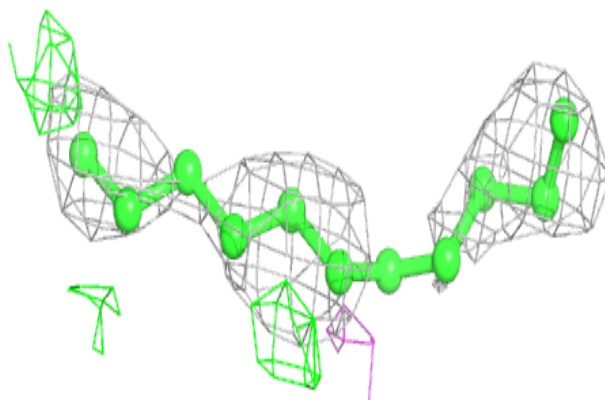


Electron density around OLC D 308:

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

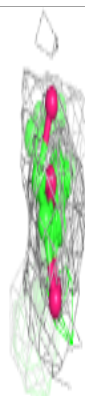
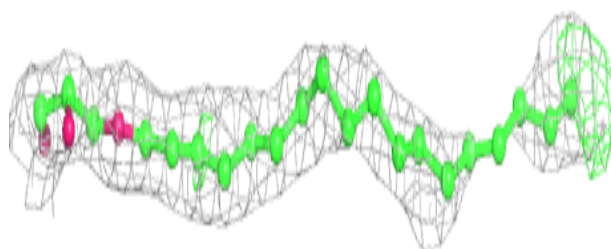
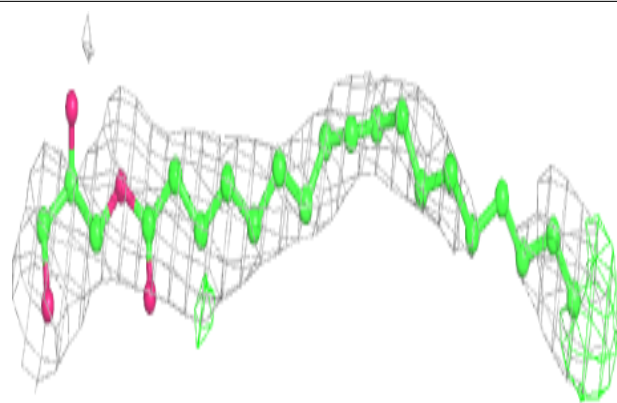
**Electron density around LFA C 317:**

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

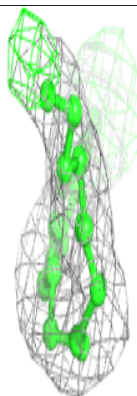
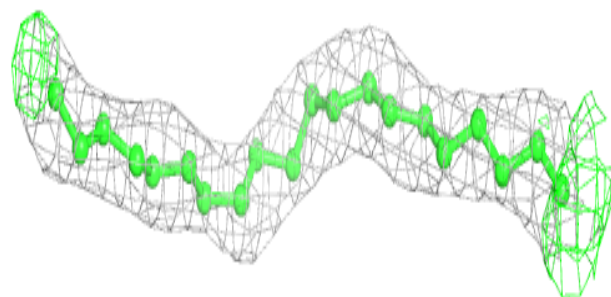
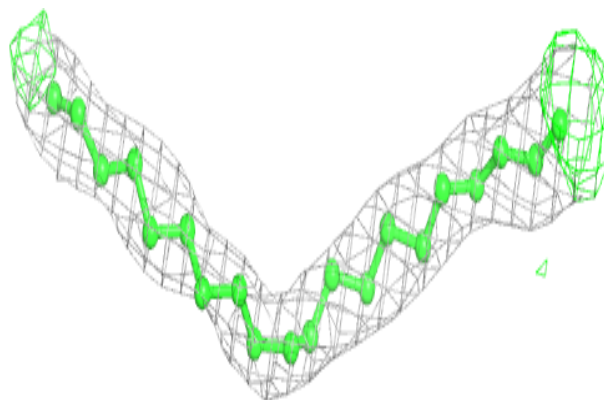


Electron density around OLC C 307:

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

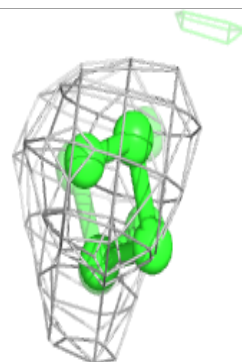
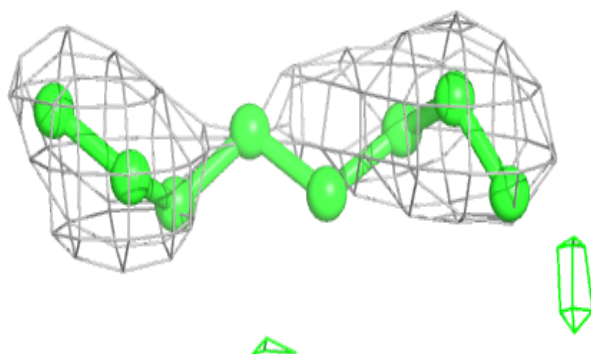
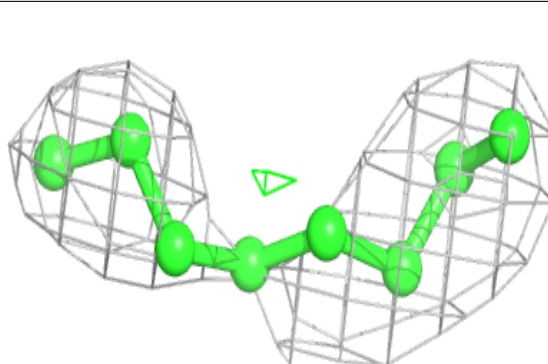
**Electron density around LFA C 319:**

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

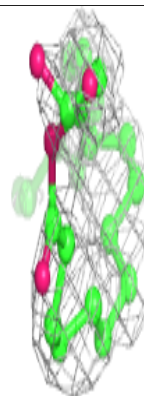
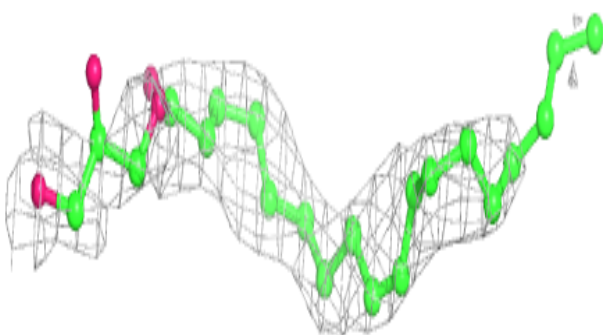
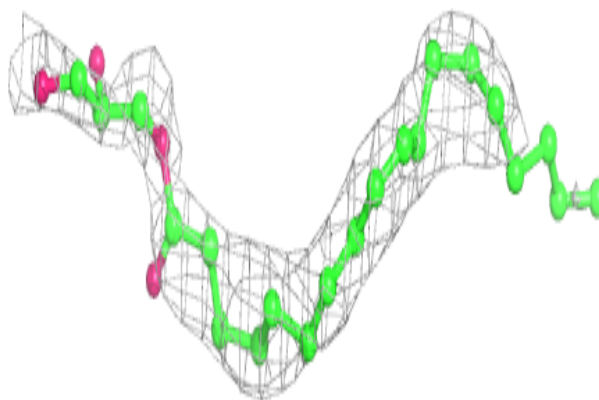


Electron density around LFA D 312:

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

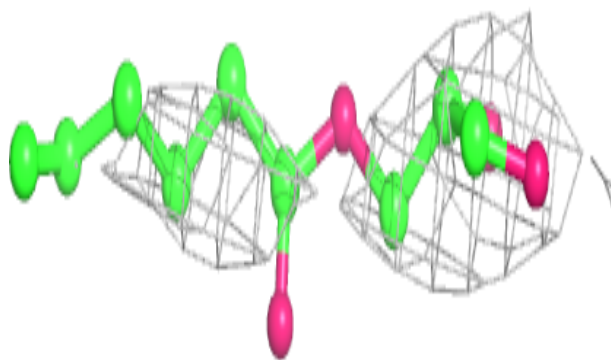
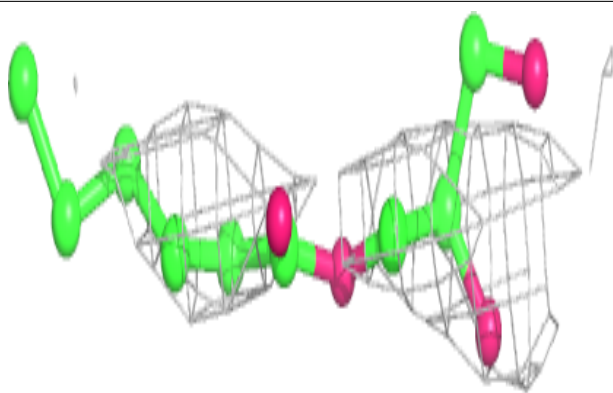
**Electron density around OLC A 321:**

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

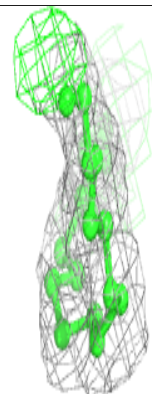
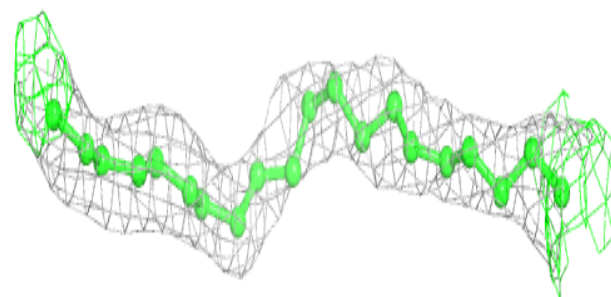
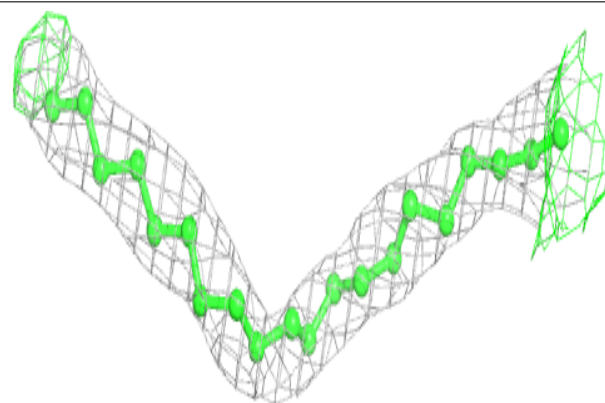


Electron density around OLC D 302:

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

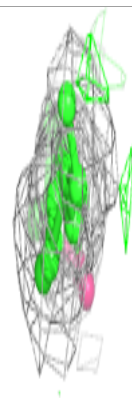
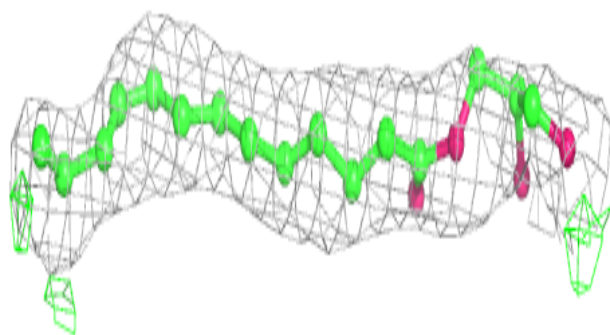
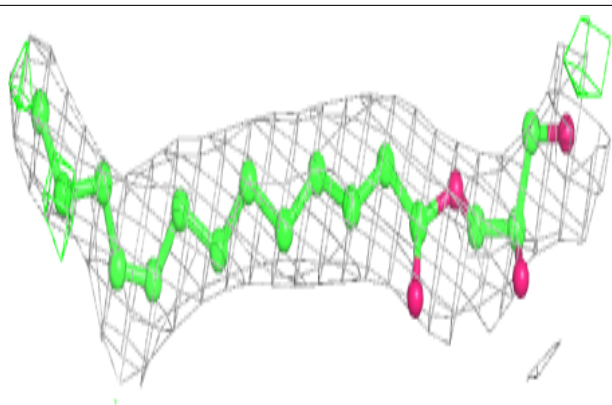
**Electron density around LFA E 319:**

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

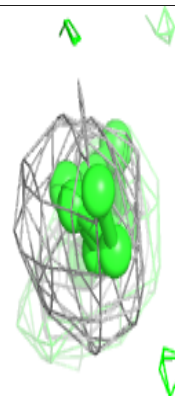
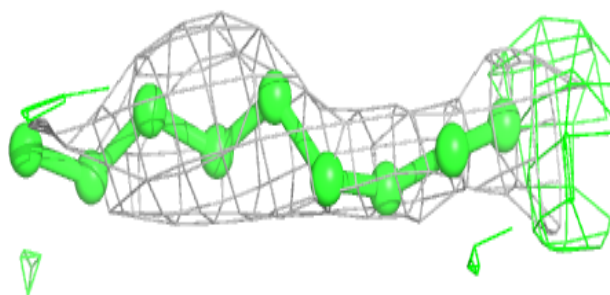
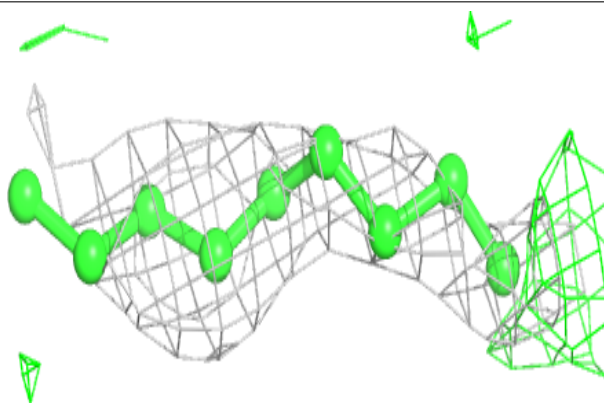


Electron density around OLC B 308:

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

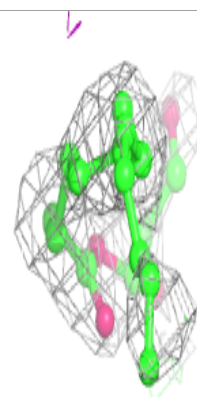
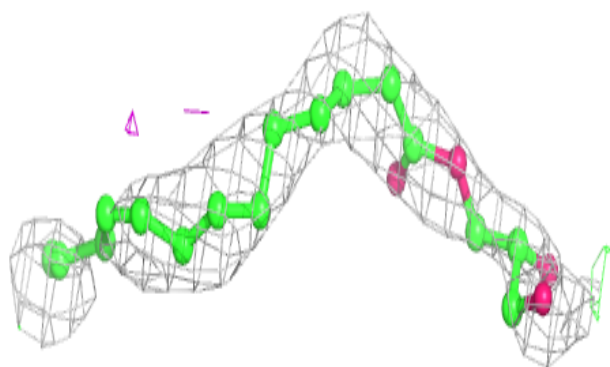
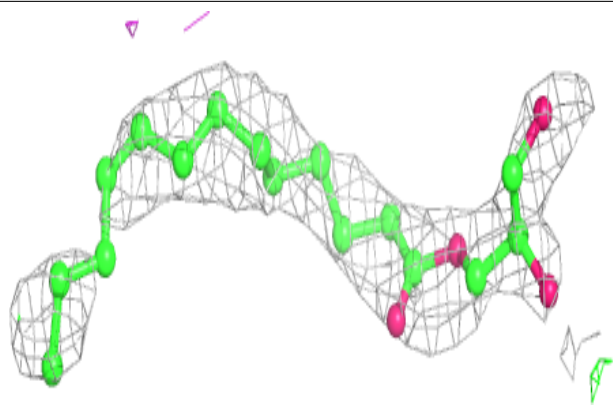
**Electron density around LFA B 316:**

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

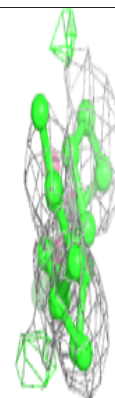
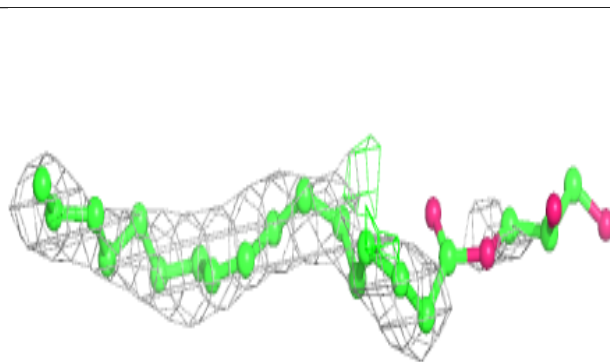
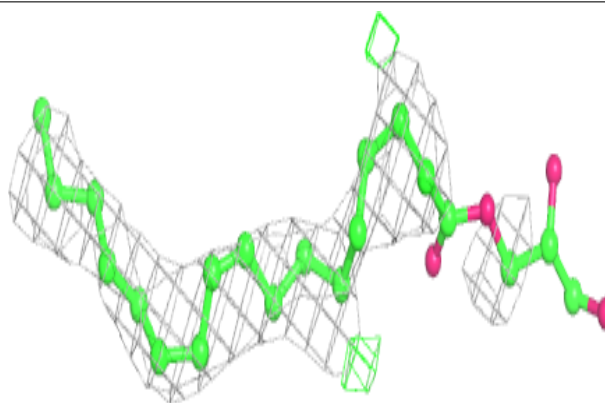


Electron density around OLC B 306:

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

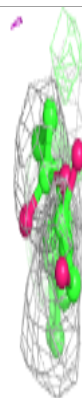
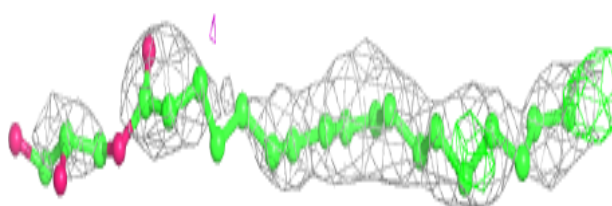
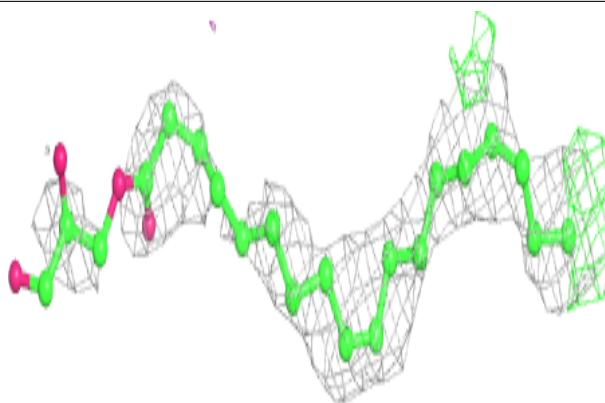
**Electron density around OLC E 306:**

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

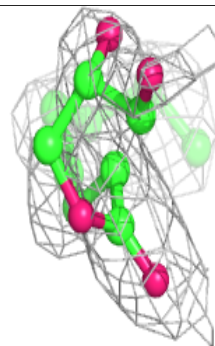
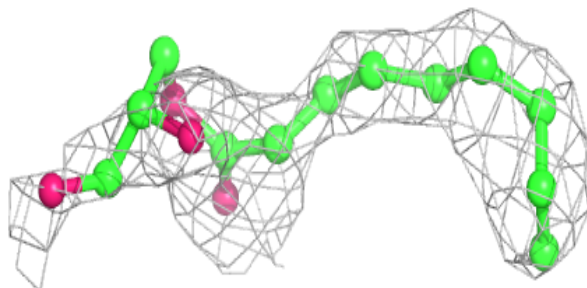
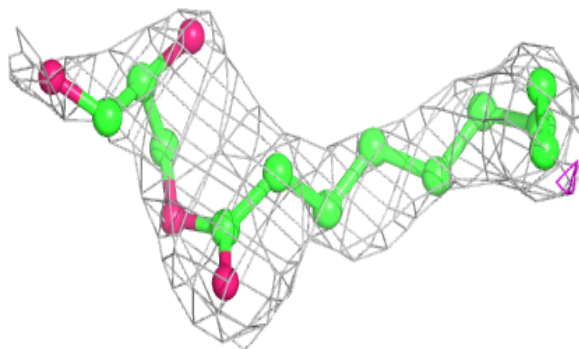


Electron density around OLC C 306:

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

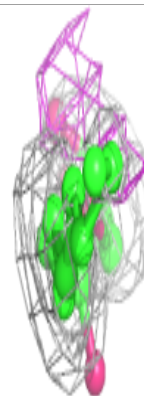
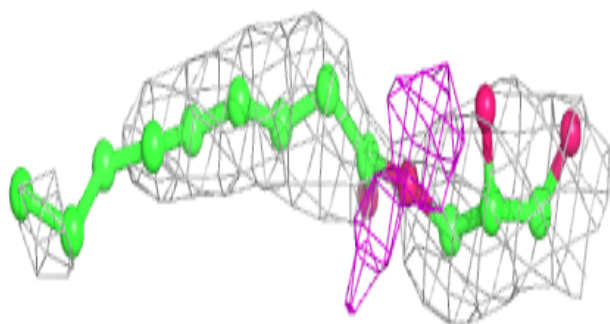
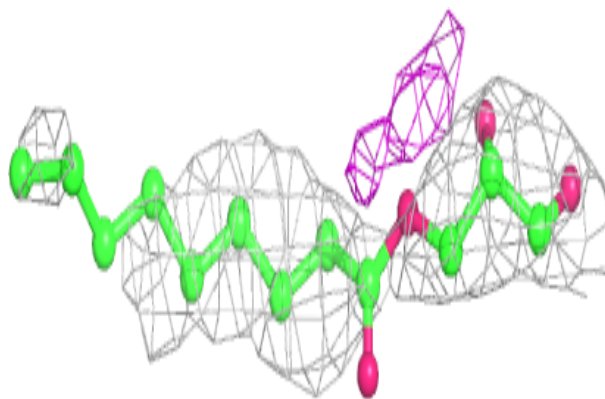
**Electron density around OLC C 312:**

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

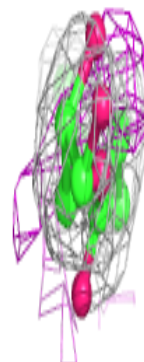
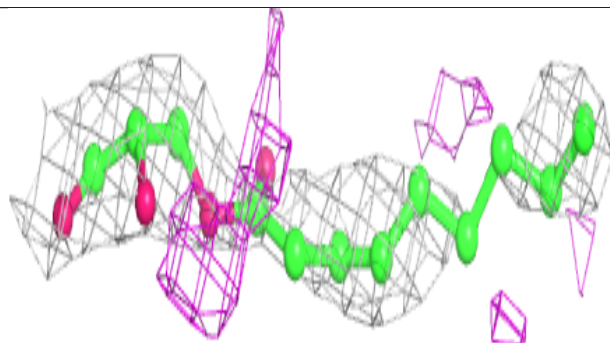
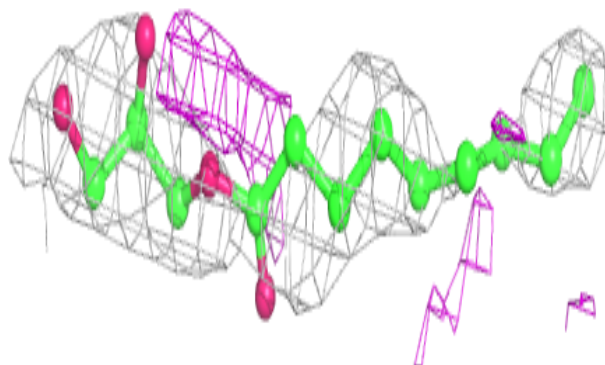


Electron density around OLC B 315:

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

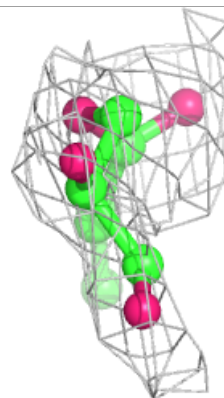
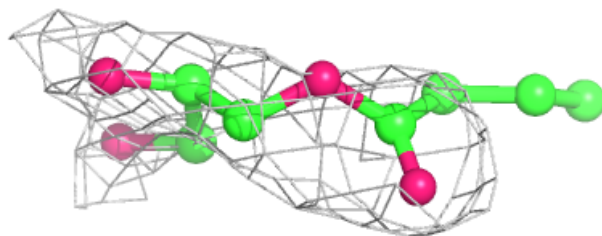
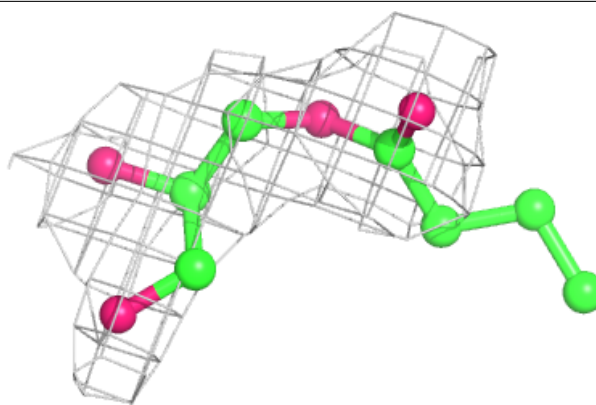
**Electron density around OLC C 313:**

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

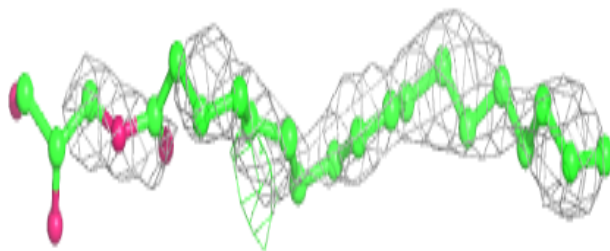
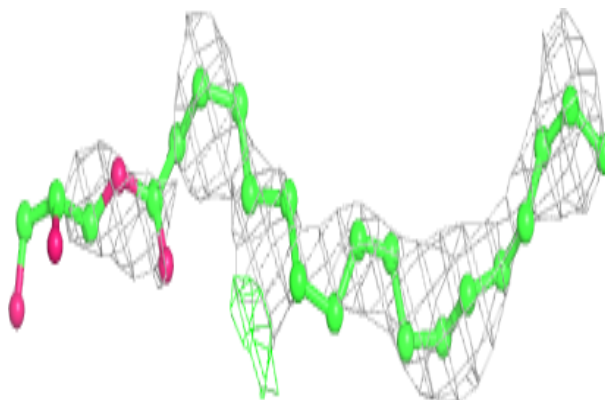


Electron density around OLC E 311:

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

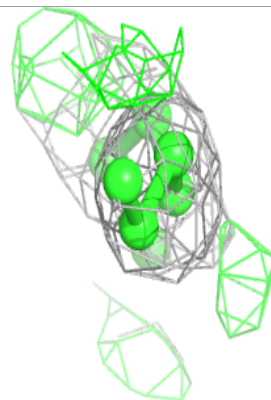
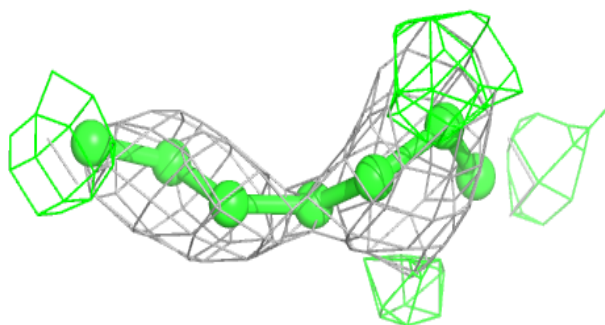
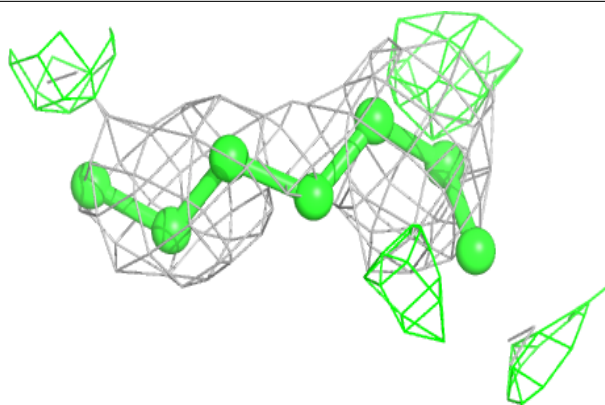
**Electron density around OLC A 304:**

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

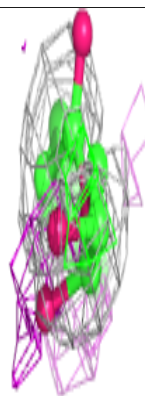
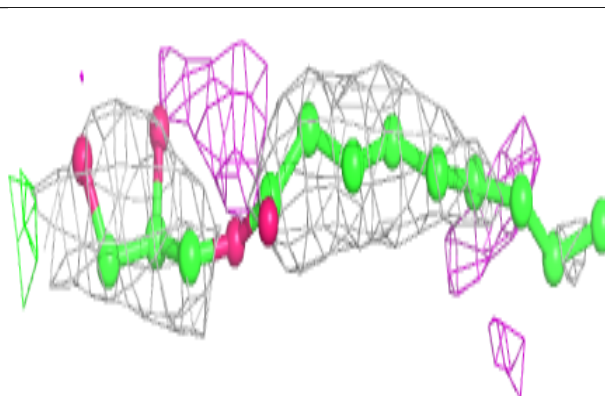
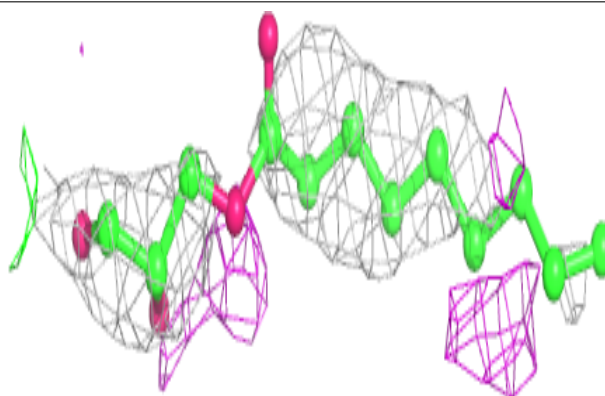


Electron density around LFA A 312:

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

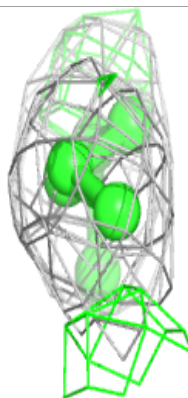
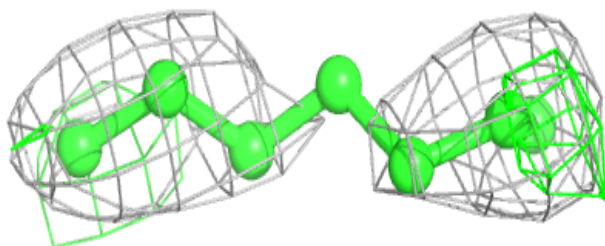
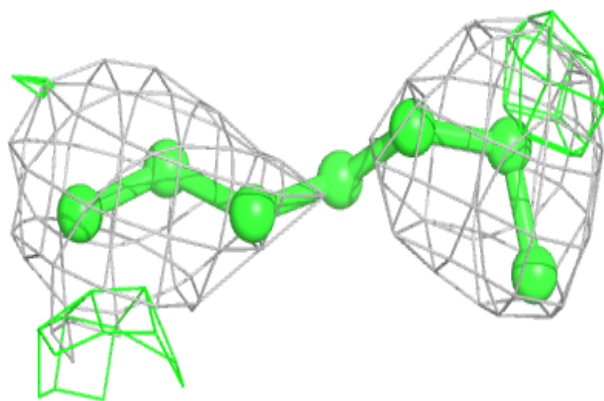
**Electron density around OLC A 311:**

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

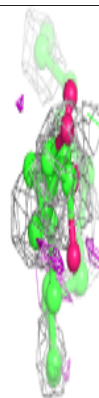
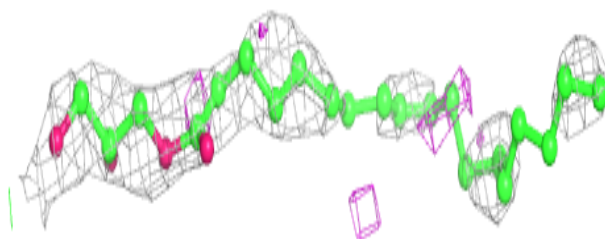
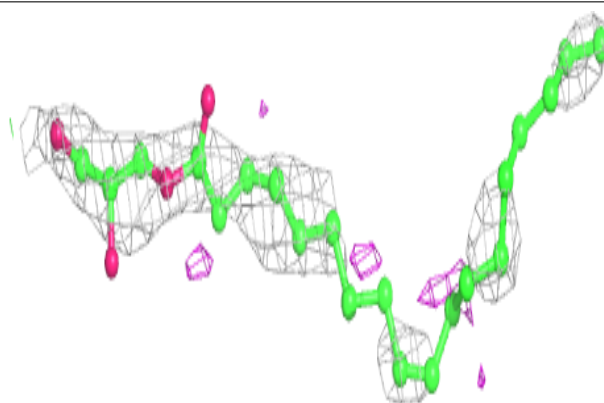


Electron density around LFA B 319:

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

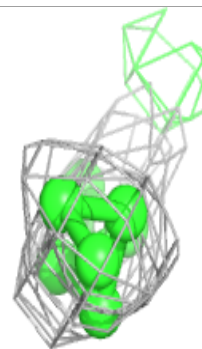
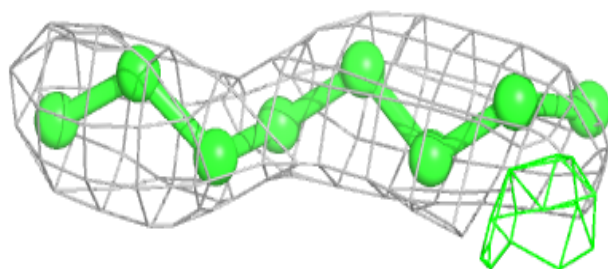
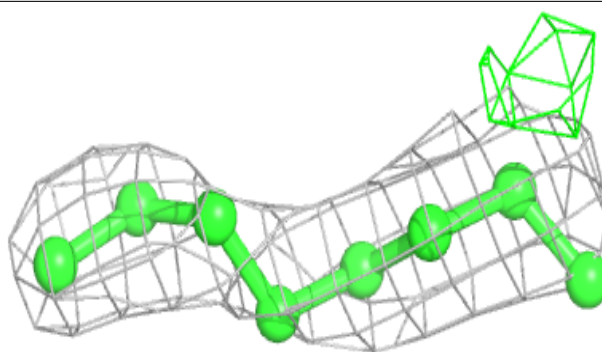
**Electron density around OLC D 309:**

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

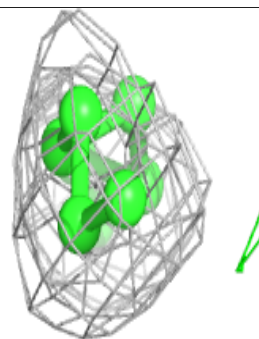
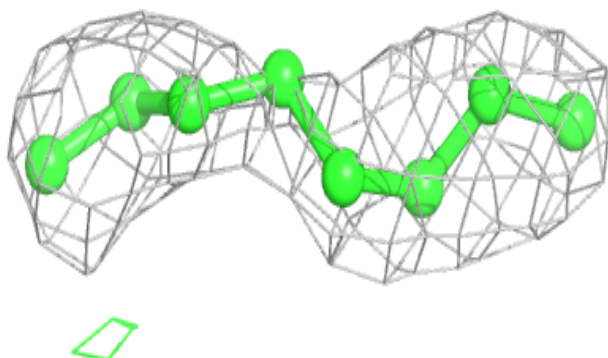
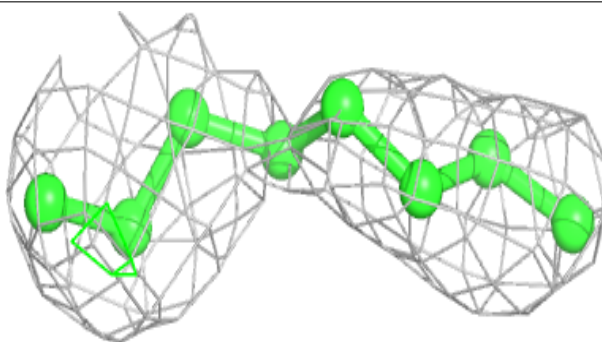


Electron density around LFA C 315:

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

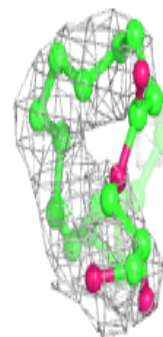
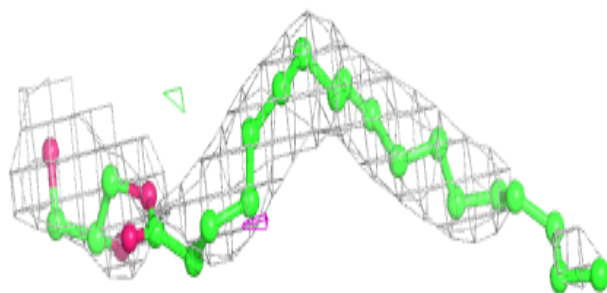
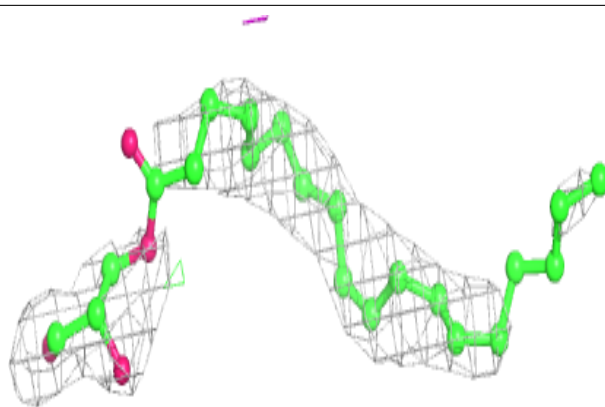
**Electron density around LFA A 314:**

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

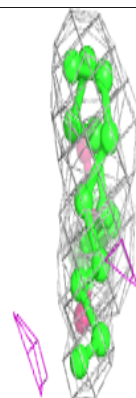
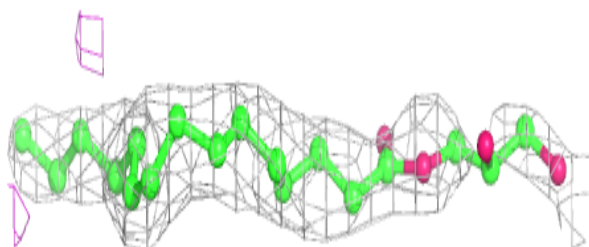
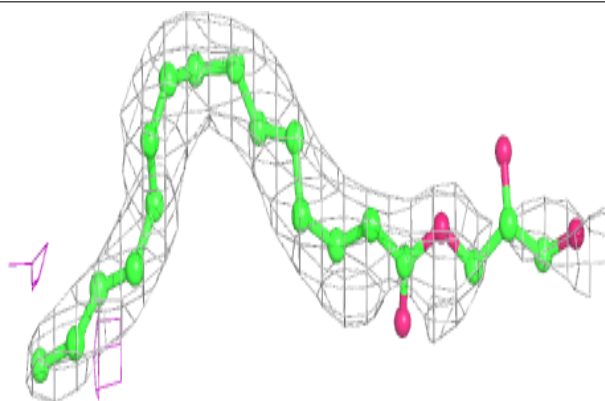


Electron density around OLC E 301:

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

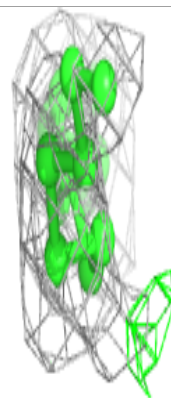
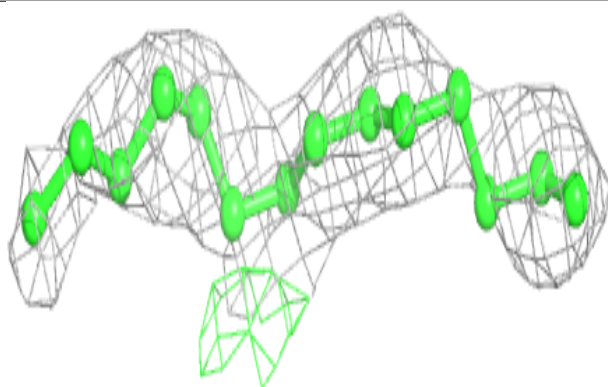
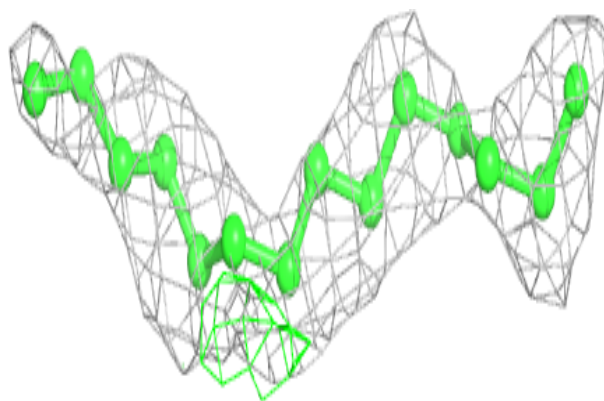
**Electron density around OLC A 303:**

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

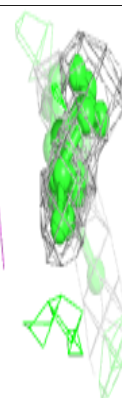
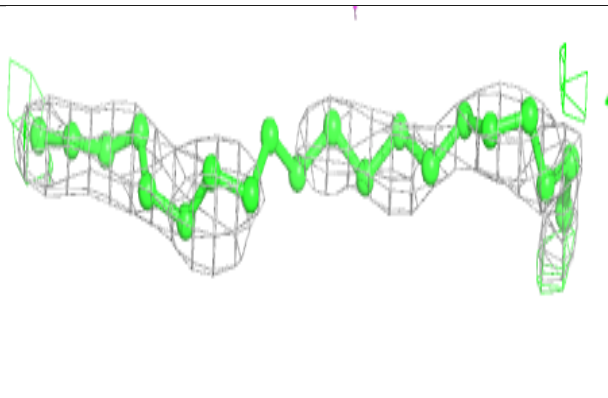
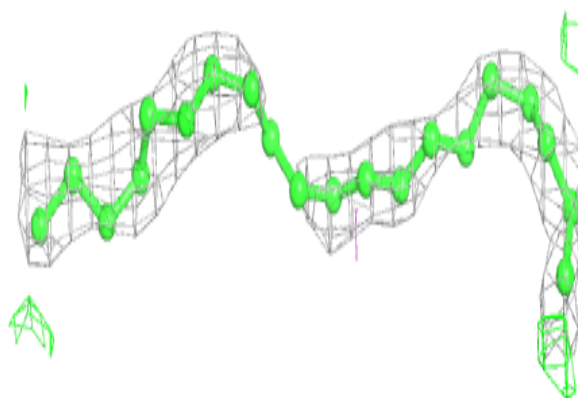


Electron density around LFA E 316:

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

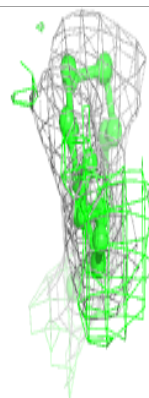
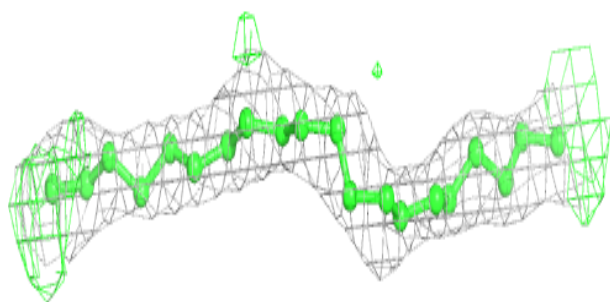
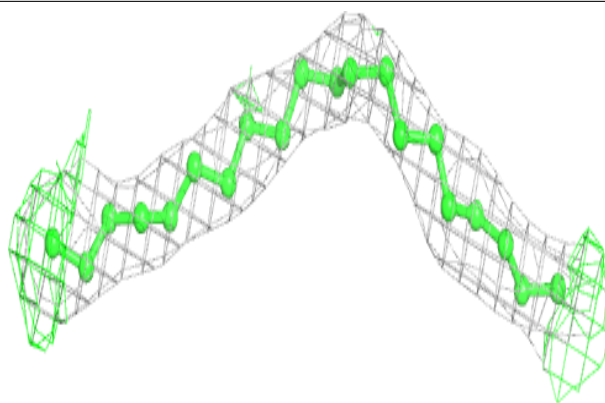
**Electron density around LFA D 310:**

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

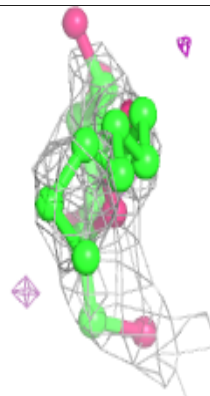
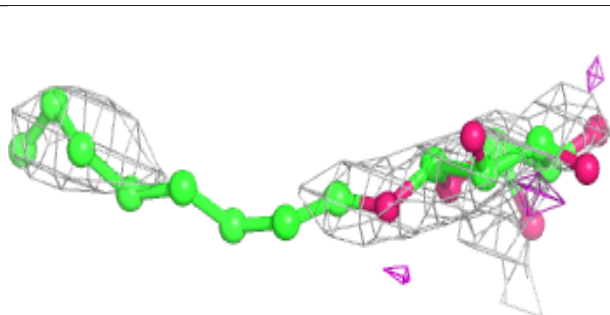
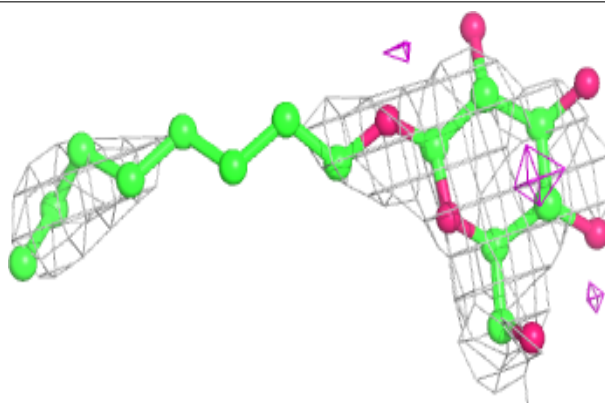


Electron density around LFA C 302:

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

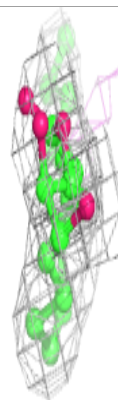
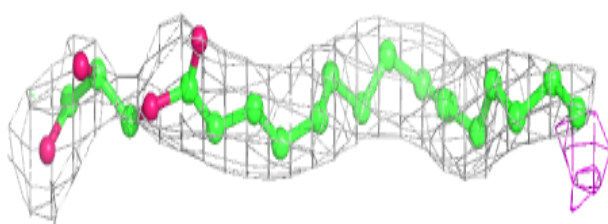
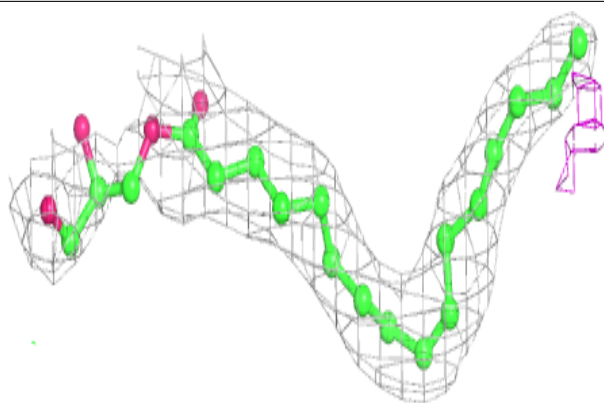
**Electron density around BOG D 317:**

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

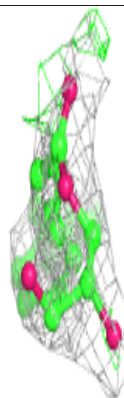
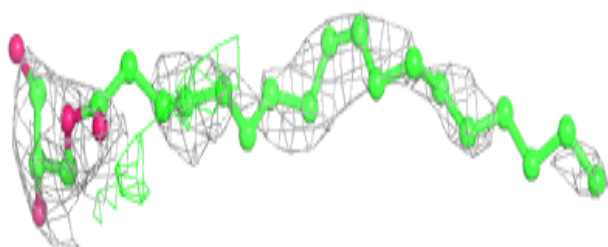
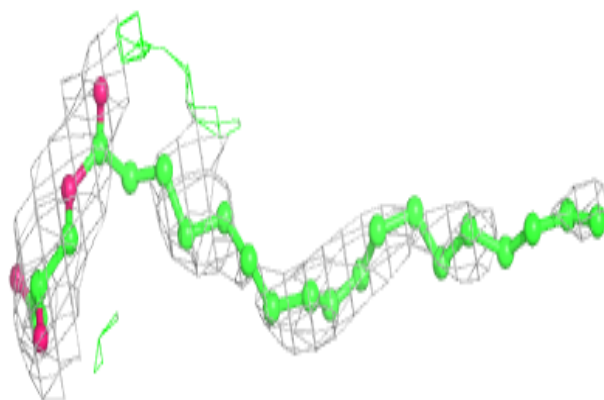


Electron density around OLC C 305:

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

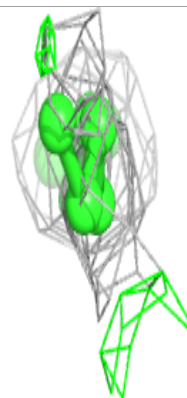
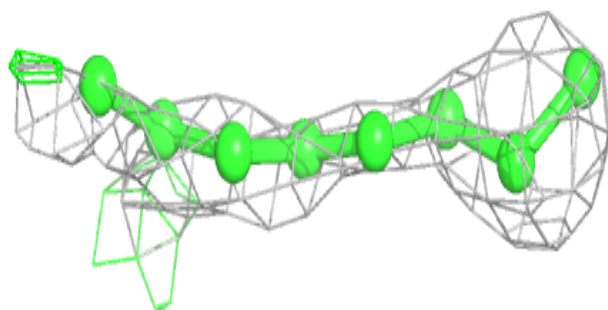
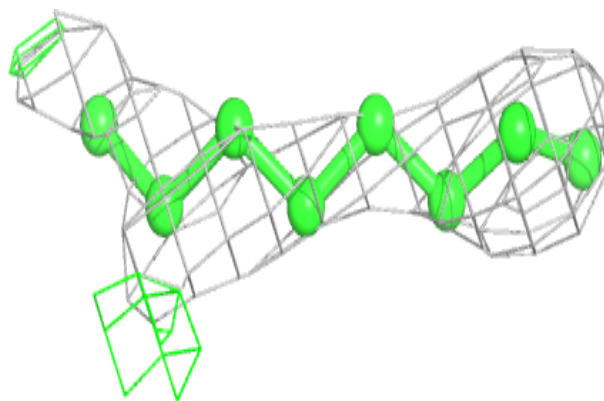
**Electron density around OLC A 302:**

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

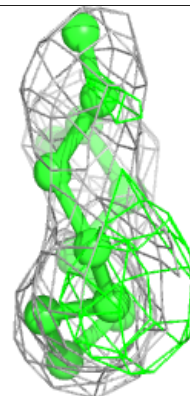
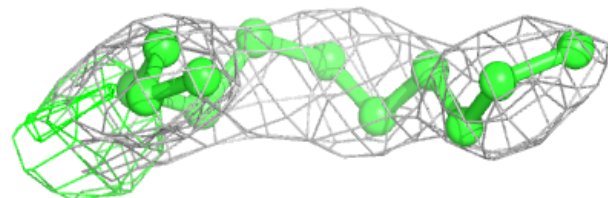
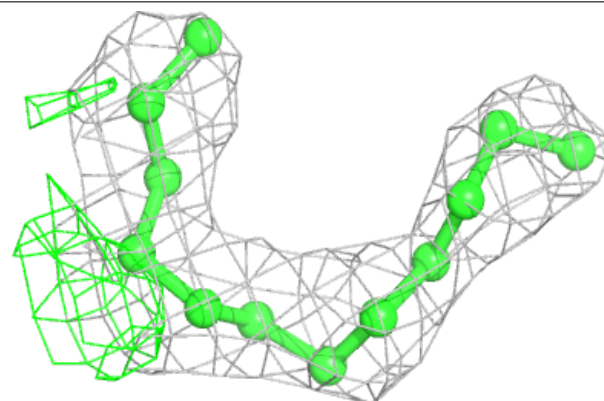


Electron density around LFA E 315:

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

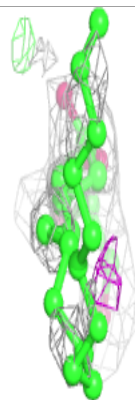
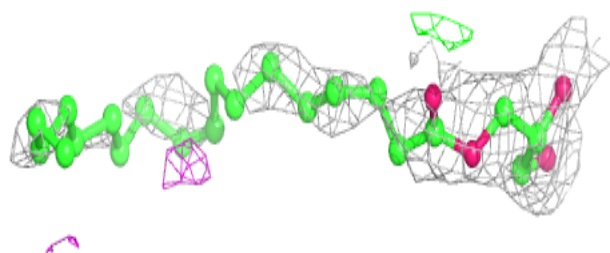
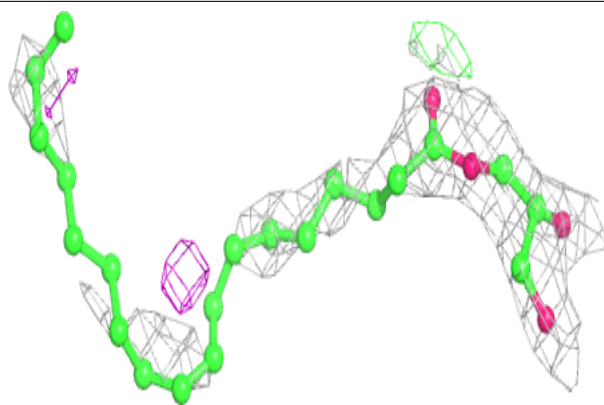
**Electron density around LFA A 315:**

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

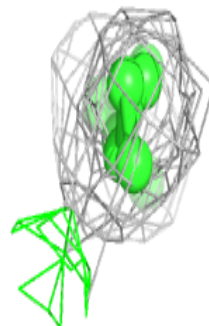
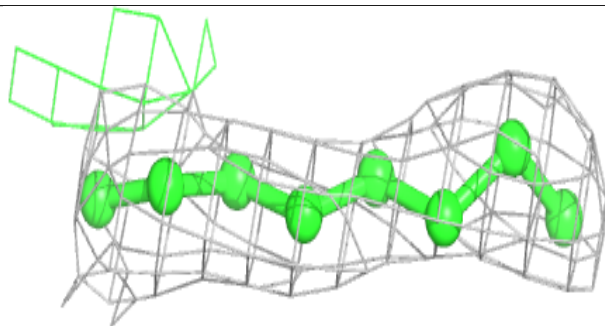
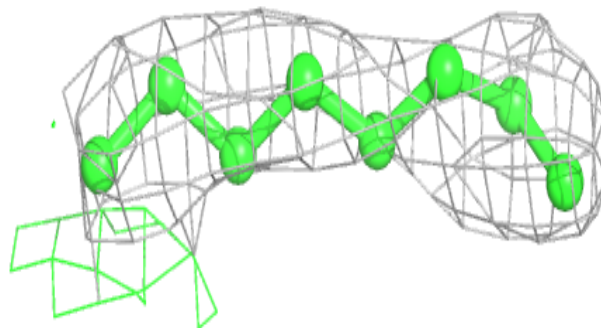


Electron density around OLC C 310:

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

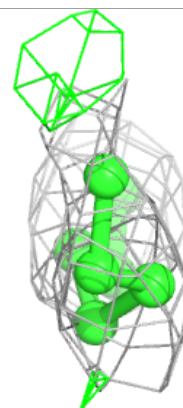
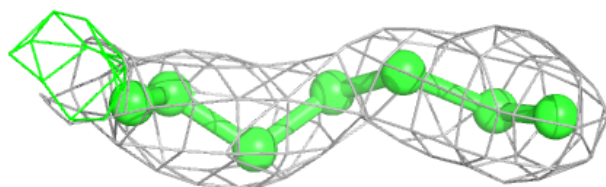
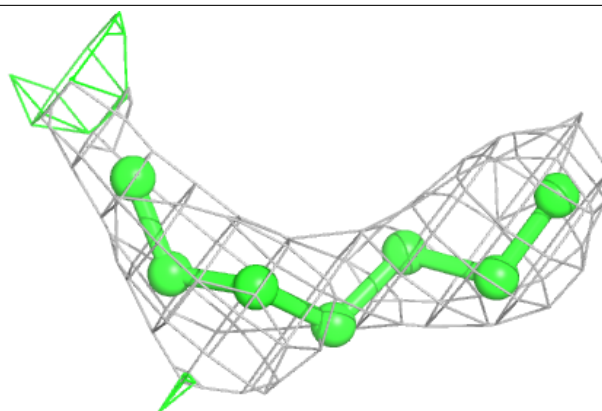
**Electron density around LFA A 313:**

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

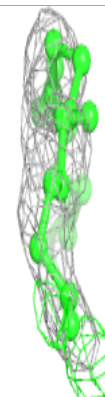
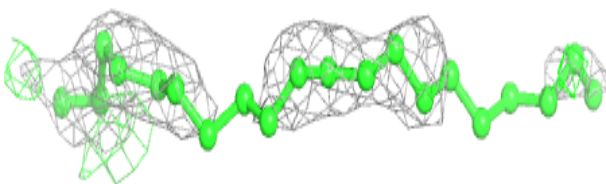
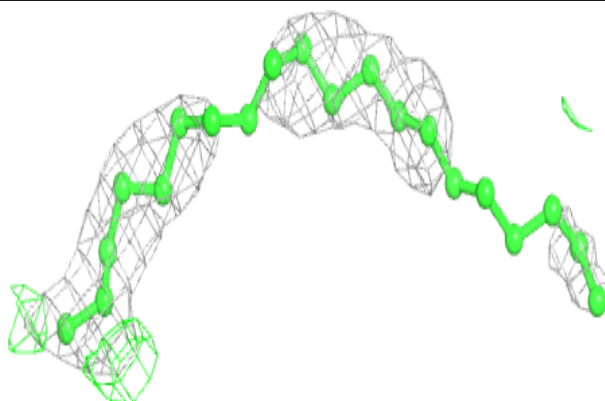


Electron density around LFA D 314:

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

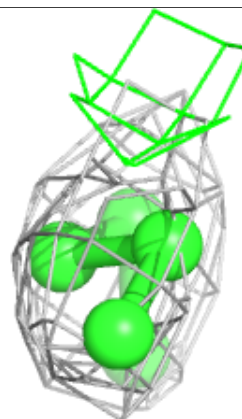
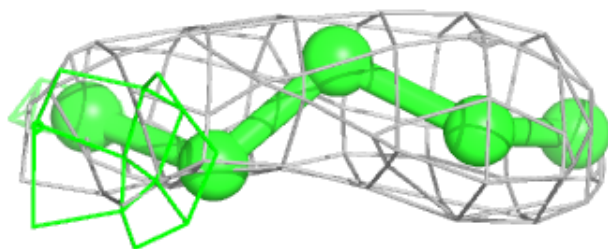
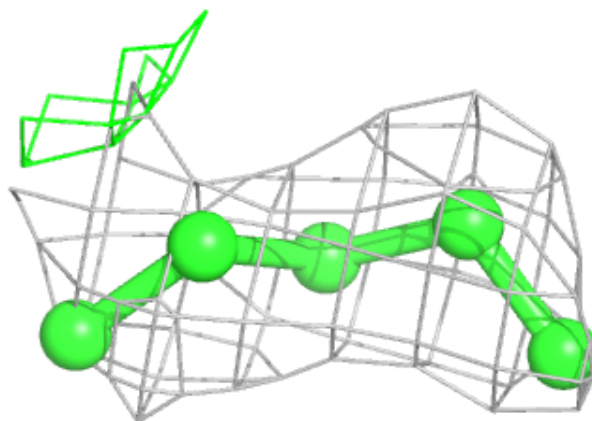
**Electron density around LFA A 318:**

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



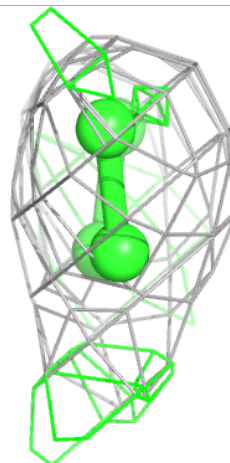
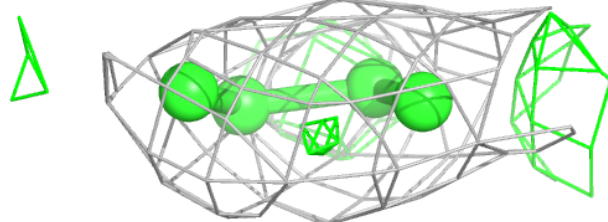
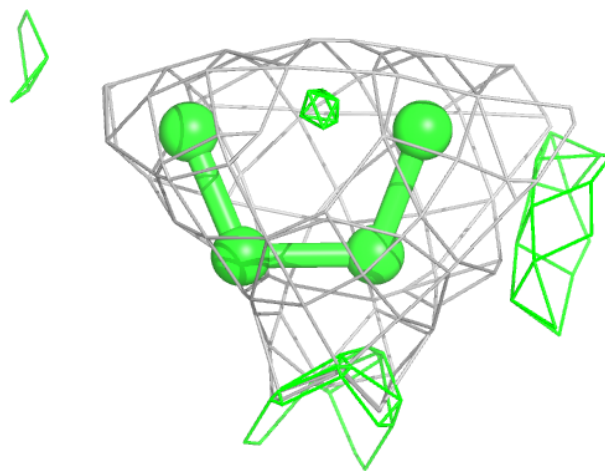
Electron density around LFA E 318:

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



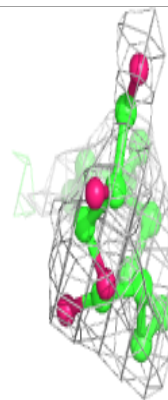
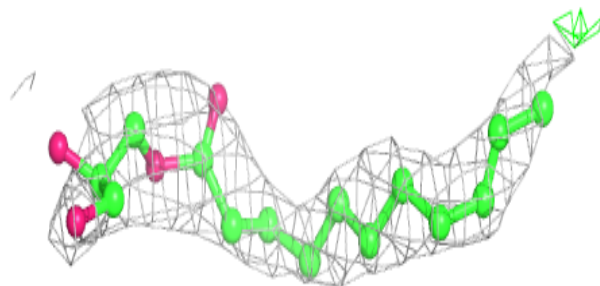
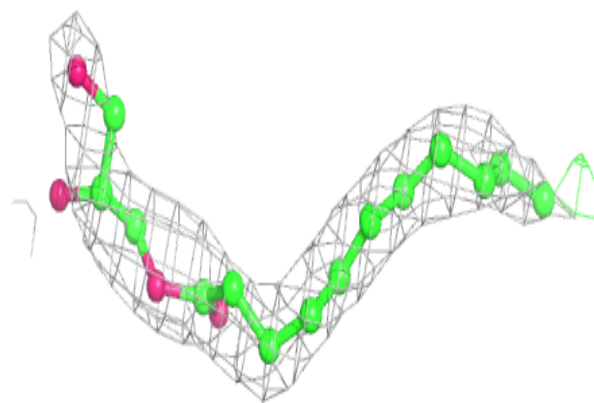
Electron density around LFA E 317:

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

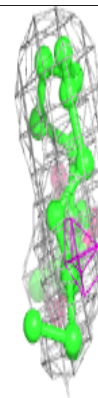
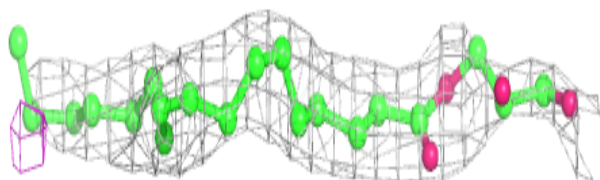
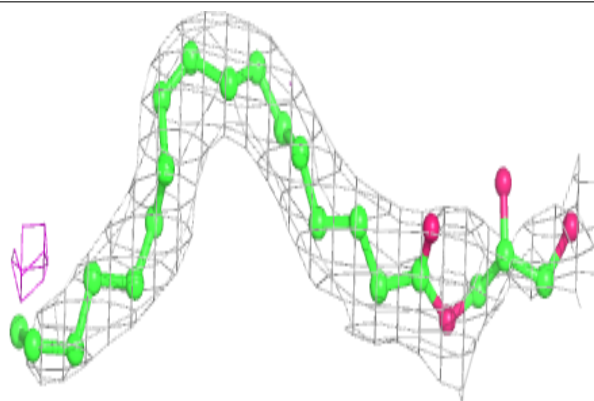


Electron density around OLC D 301:

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

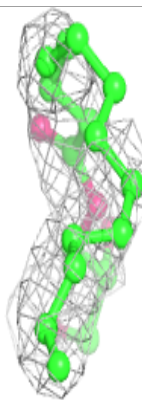
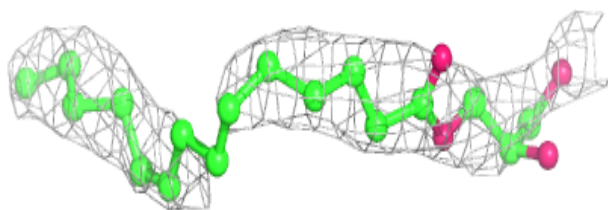
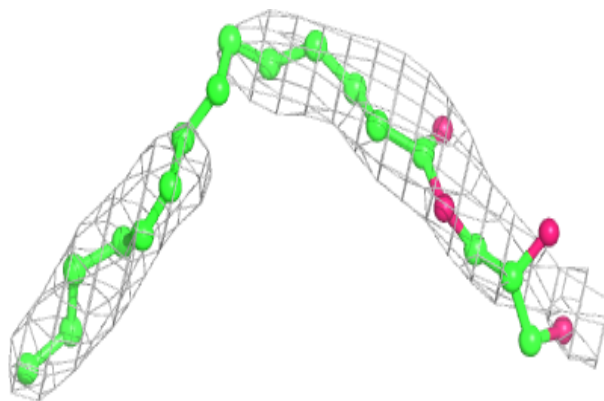
**Electron density around OLC E 305:**

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

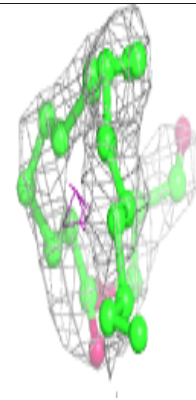
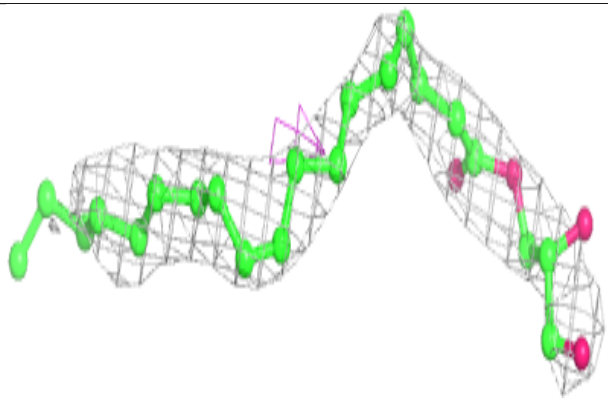
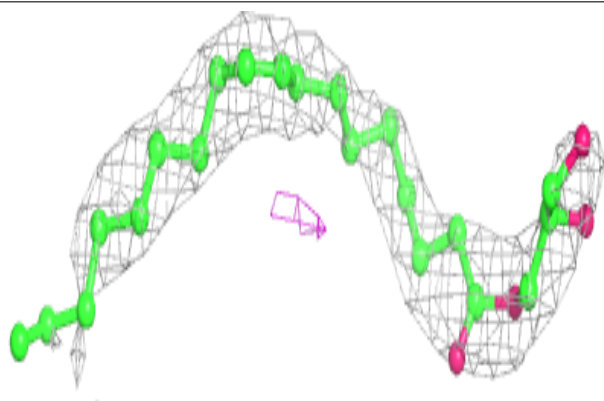


Electron density around OLC B 309:

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

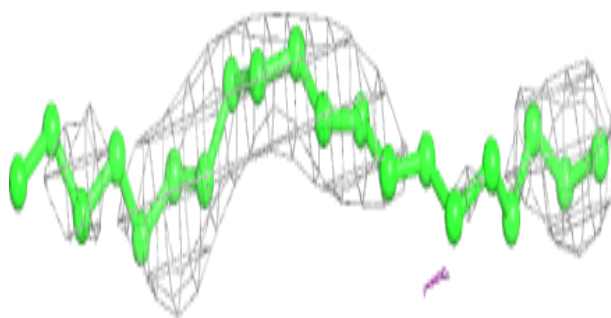
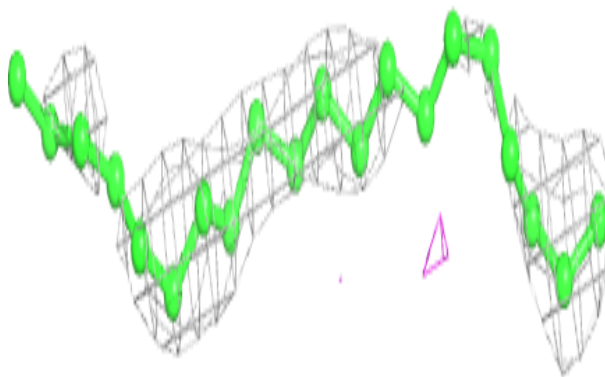
**Electron density around OLC B 301:**

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

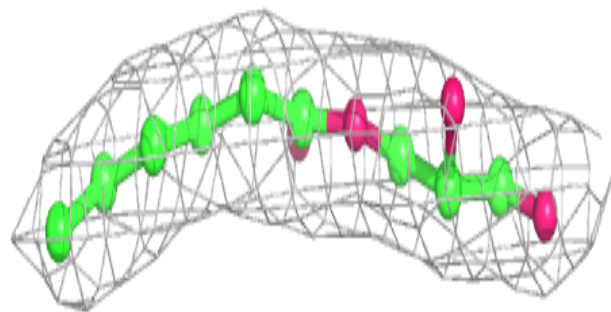
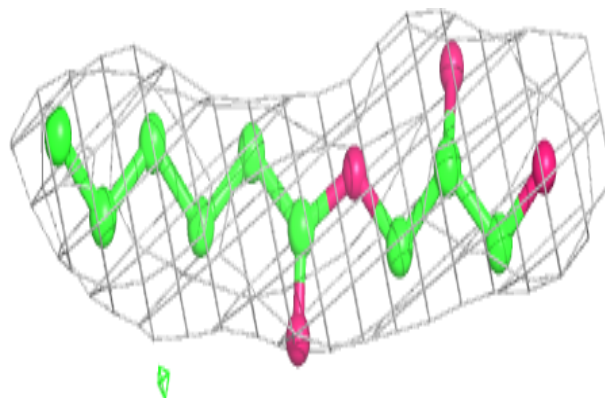


Electron density around LFA D 311:

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

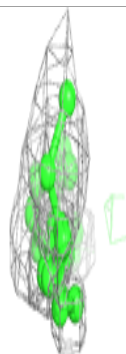
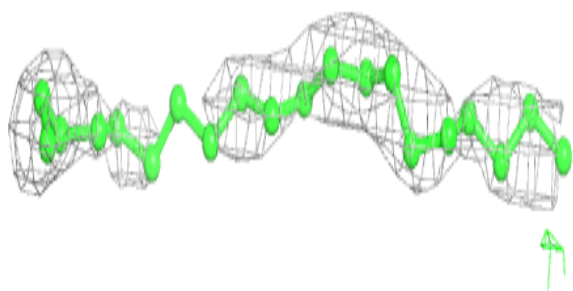
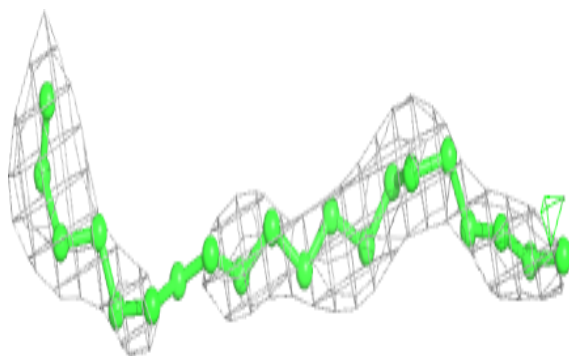
**Electron density around OLC A 305:**

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

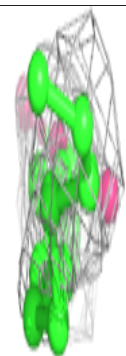
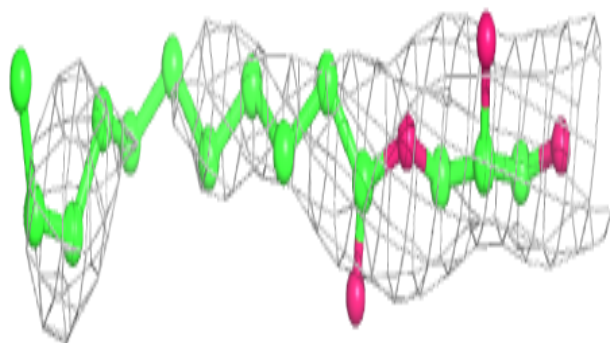
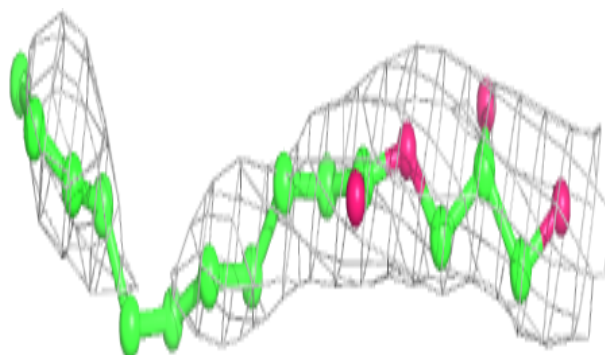


Electron density around LFA C 316:

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

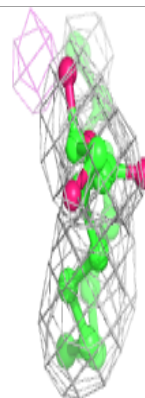
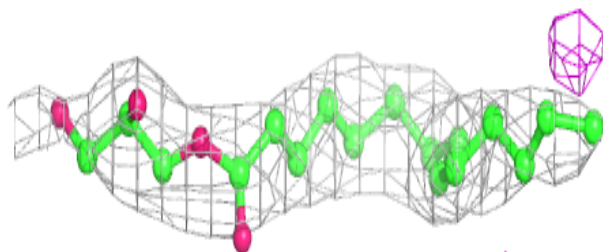
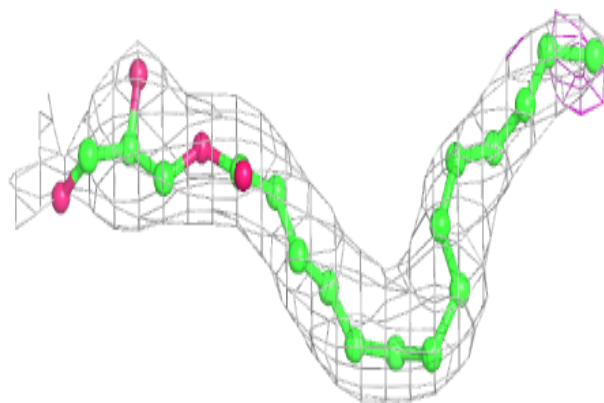
**Electron density around OLC D 304:**

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

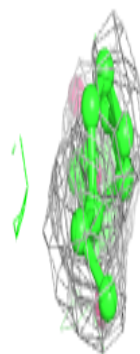
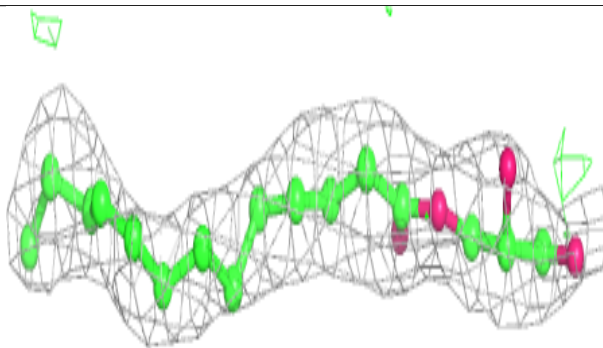
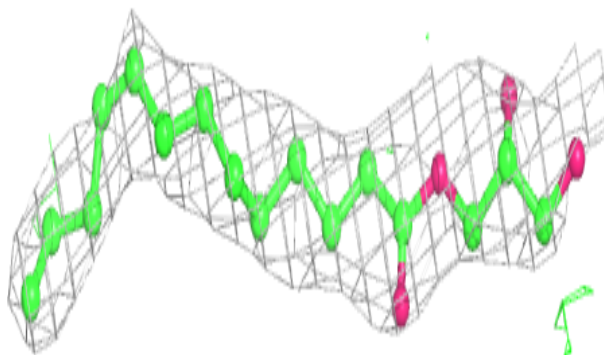


Electron density around OLC C 301:

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

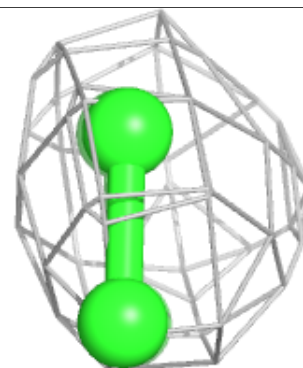
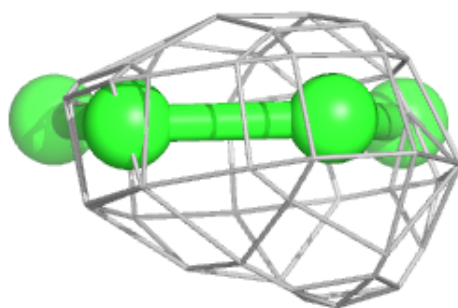
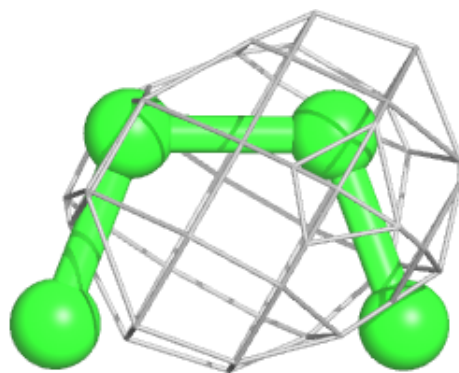
**Electron density around OLC E 307:**

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



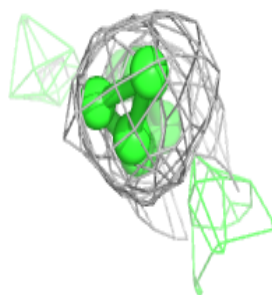
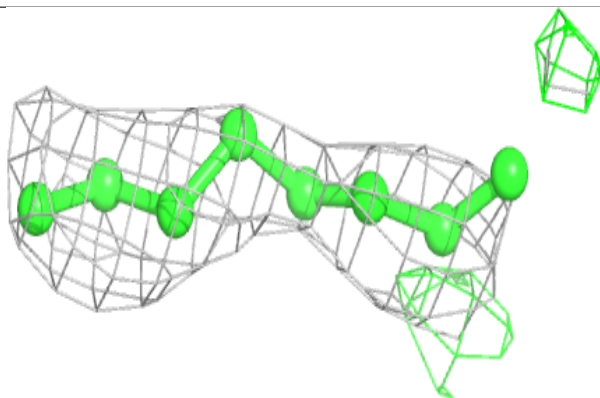
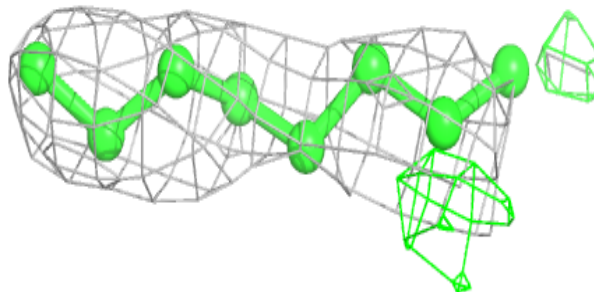
Electron density around LFA C 318:

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

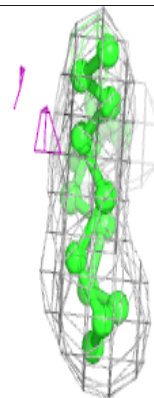
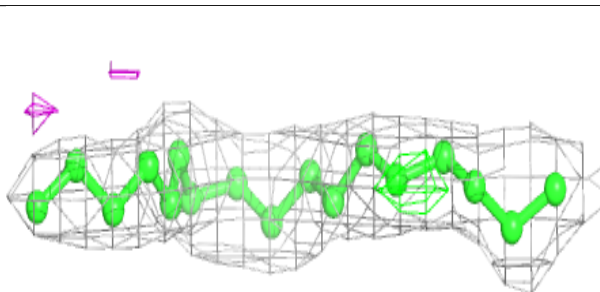
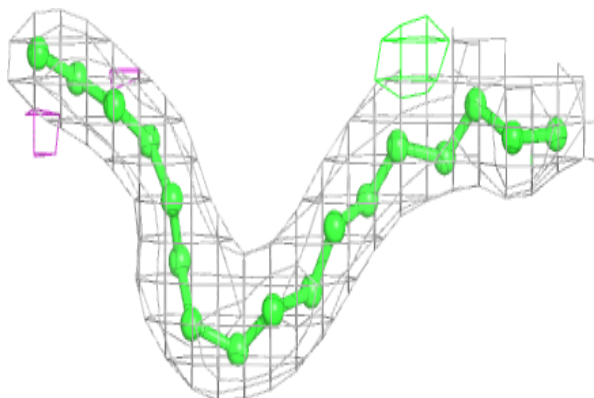


Electron density around LFA B 317:

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

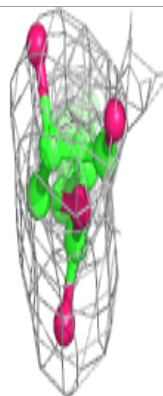
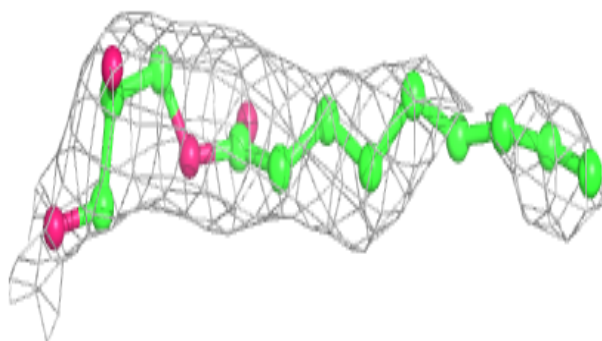
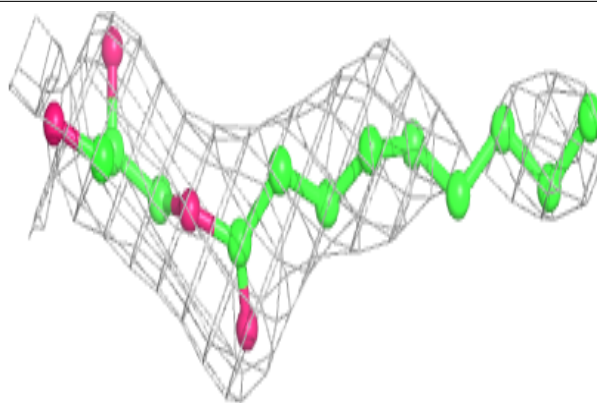
**Electron density around LFA D 313:**

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

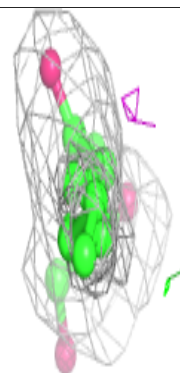
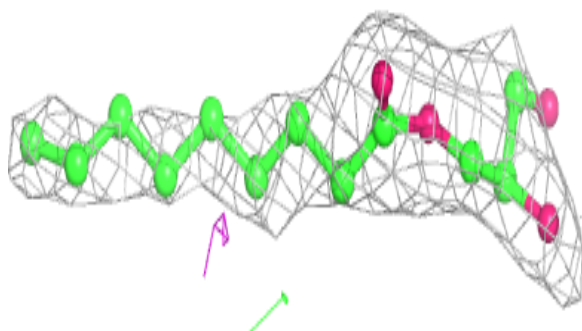
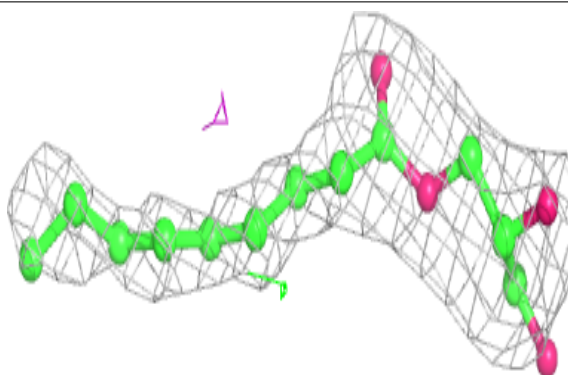


Electron density around OLC C 311:

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

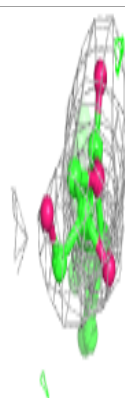
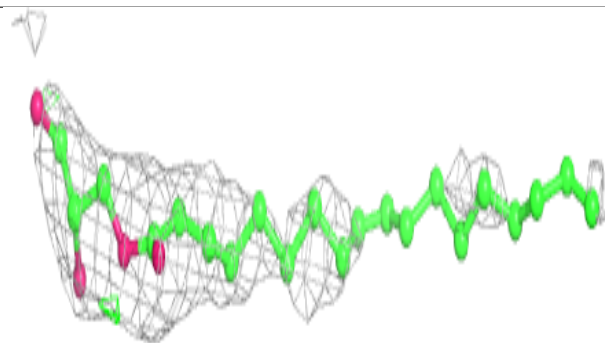
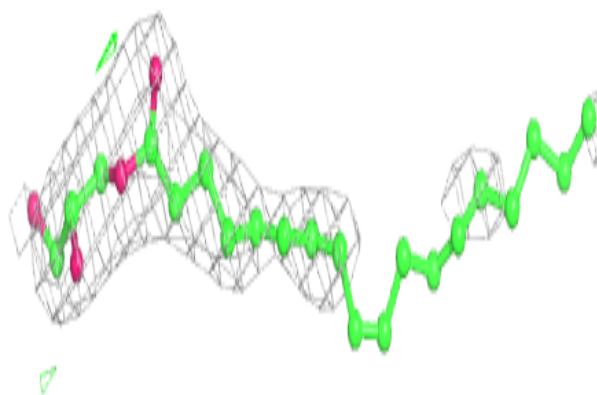
**Electron density around OLC B 312:**

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

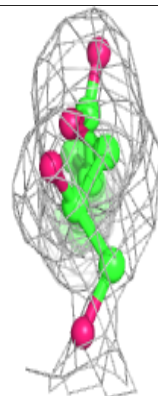
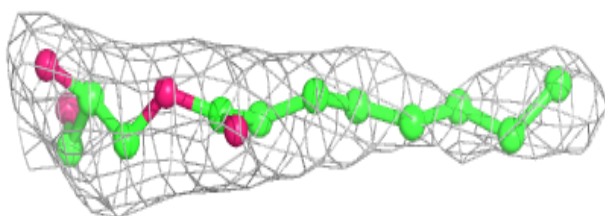
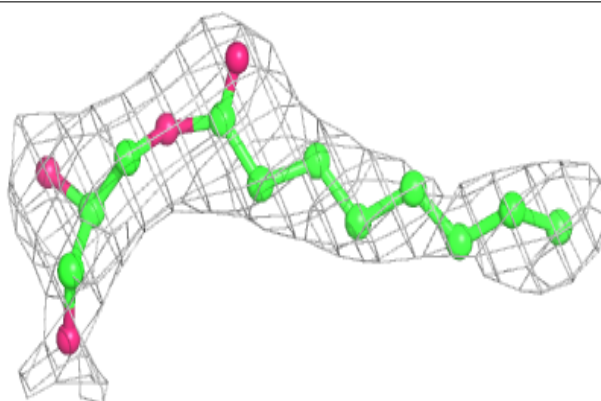


Electron density around OLC E 309:

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

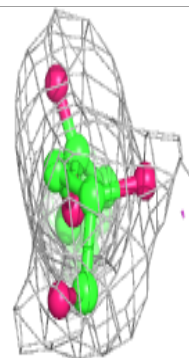
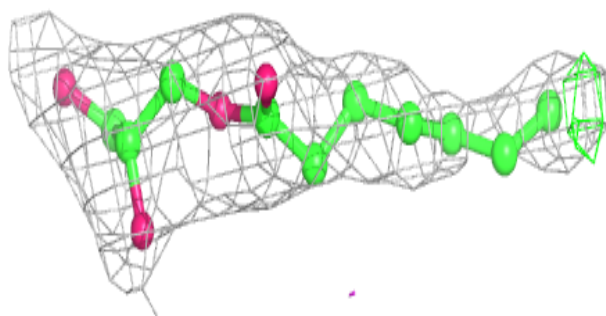
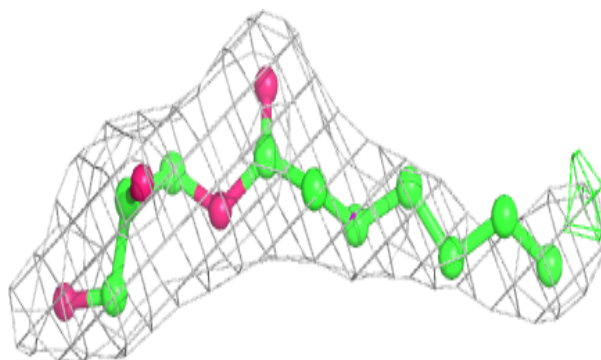
**Electron density around OLC A 309:**

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

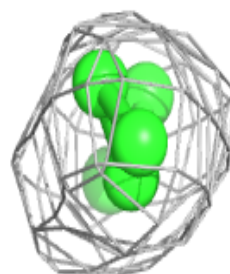
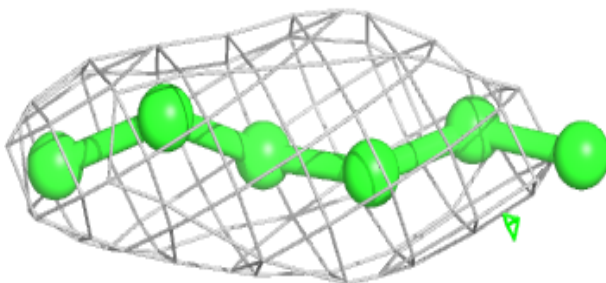
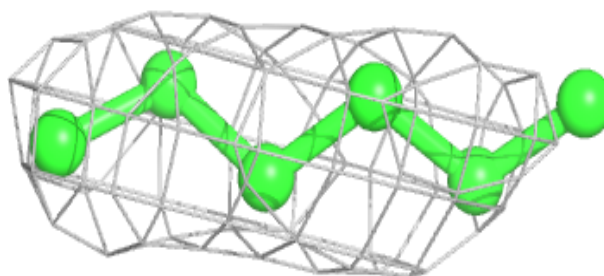


Electron density around OLC D 307:

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

**Electron density around LFA A 317:**

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



6.5 Other polymers

There are no such residues in this entry.