



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 10:54 AM BST

PDB ID : 6REW
Title : Crystal structure 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 : 2.20 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

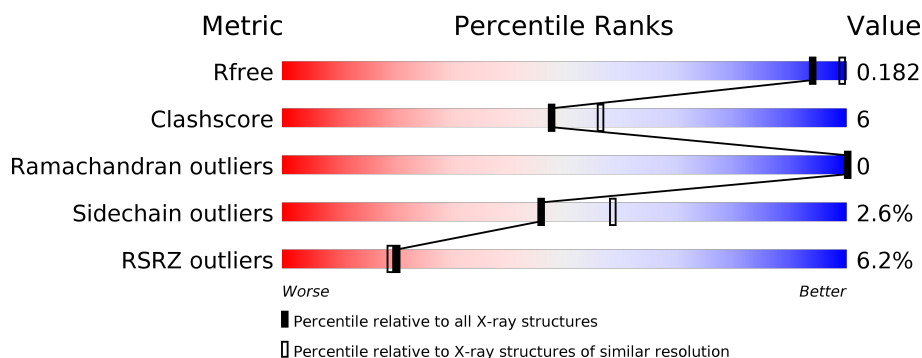
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	273	<div> <div>6%</div> <div>88% 12%</div> </div>
1	B	273	<div> <div>4%</div> <div>87% 13%</div> </div>
1	C	273	<div> <div>6%</div> <div>87% 12%</div> </div>
1	D	273	<div> <div>8%</div> <div>89% 11%</div> </div>
1	E	273	<div> <div>5%</div> <div>86% 12%</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
3	LFA	E	302	-	-	-	X
5	BOG	A	316	-	-	-	X
5	BOG	B	314	-	-	-	X

2 Entry composition i

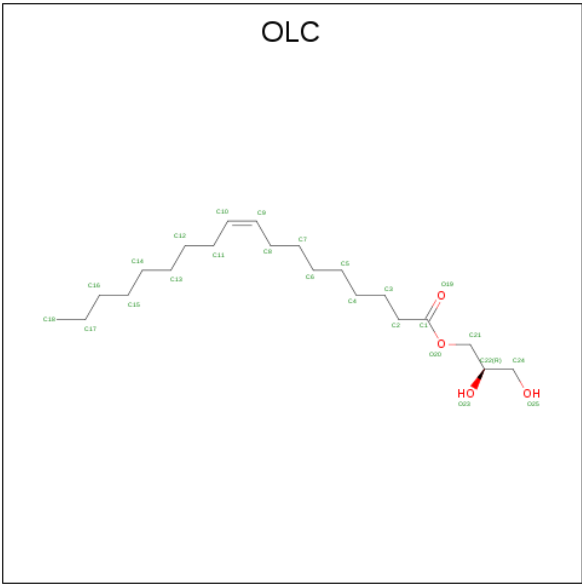
There are 7 unique types of molecules in this entry. The entry contains 12742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			2179	1451	330	389	9			
1	B	273	Total	C	N	O	S	0	1	0
			2173	1446	331	387	9			
1	C	273	Total	C	N	O	S	0	1	0
			2178	1450	330	389	9			
1	D	273	Total	C	N	O	S	0	2	0
			2177	1449	331	388	9			
1	E	273	Total	C	N	O	S	0	2	0
			2179	1451	331	388	9			

- 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	C	0	0
			9	9		

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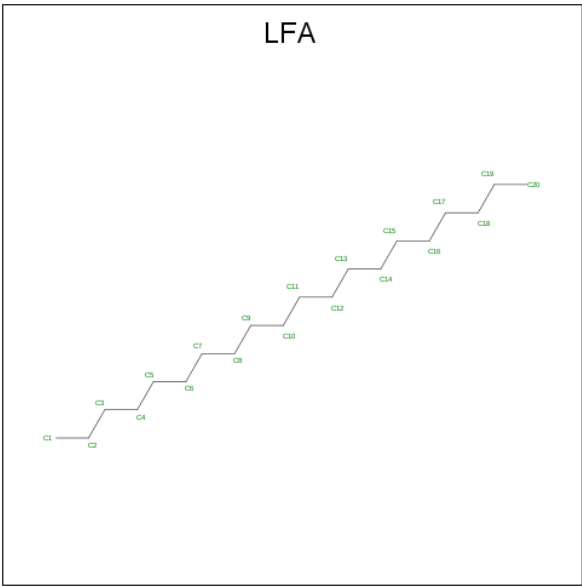
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			13	9	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	A	1	Total	C		0	0
			7	7			
2	A	1	Total	C	O	0	0
			16	12	4		
2	A	1	Total	C	O	0	0
			19	17	2		
2	A	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			22	18	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			21	17	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		0	0
			7	7			
2	C	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			12	8	4		
2	C	1	Total	C	O	0	0
			23	19	4		
2	C	1	Total	C	O	0	0
			22	18	4		
2	C	1	Total	C	O	0	0
			20	16	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C 7 7	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 16 12 4	0	0
2	D	1	Total C O 13 9 4	0	0
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 18 16 2	0	0
2	D	1	Total C O 14 10 4	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C O 25 21 4	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 8 8	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 20 16 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C 6 6	0	0
2	E	1	Total C O 22 18 4	0	0
2	E	1	Total C O 20 16 4	0	0

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 20 20	0	0
3	A	1	Total C 9 9	0	0
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

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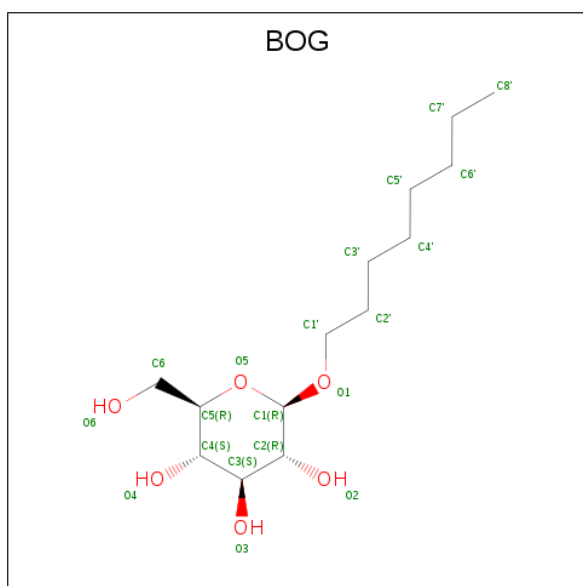
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 4 4	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 14 14	0	0
3	D	1	Total C 20 20	0	0
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
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0
3	E	1	Total C 4 4	0	0

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

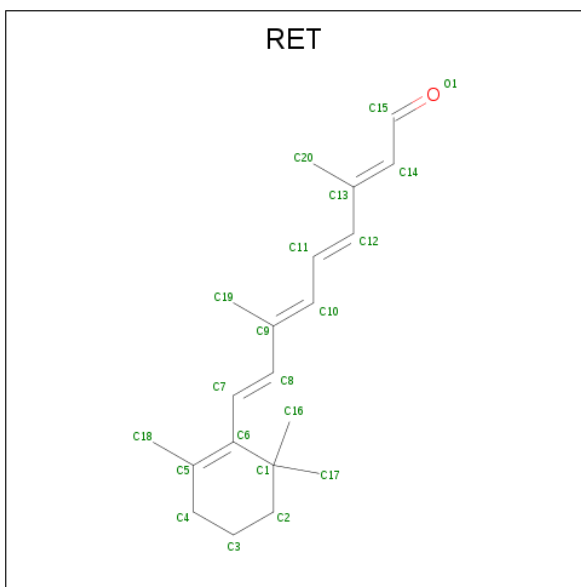
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 6 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



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

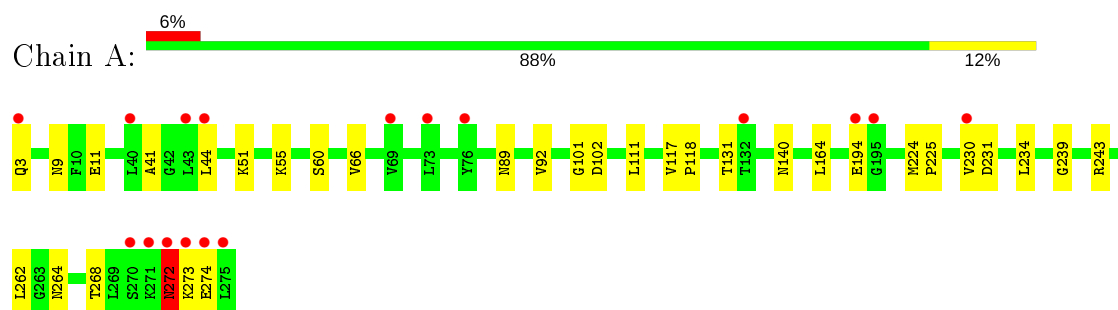
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	110	Total O 110 110	0	0
7	B	112	Total O 112 112	0	0
7	C	111	Total O 111 111	0	0
7	D	96	Total O 96 96	0	0
7	E	112	Total O 112 112	0	0

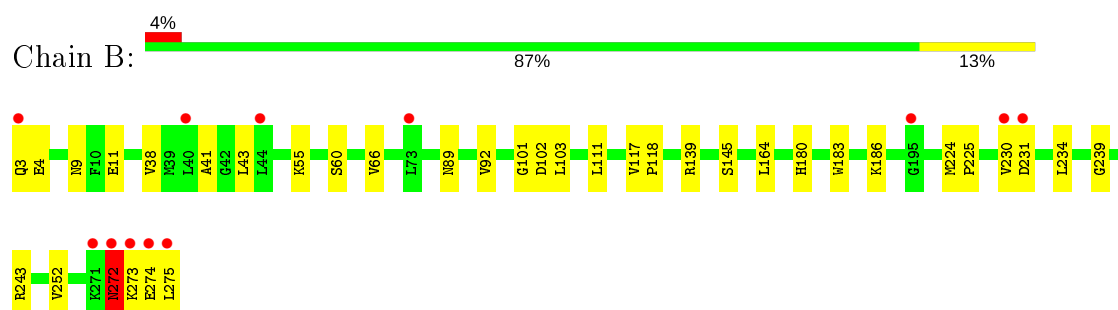
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

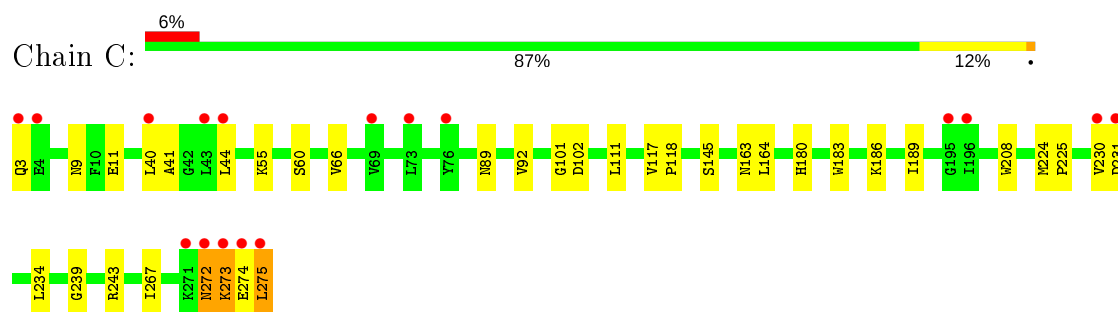
- Molecule 1: Sodium pumping rhodopsin



- Molecule 1: Sodium pumping rhodopsin

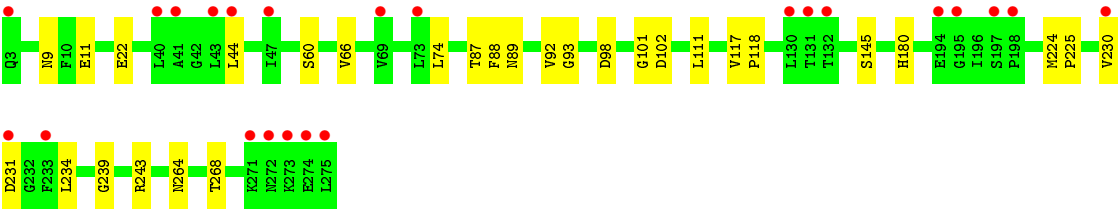


- Molecule 1: Sodium pumping rhodopsin

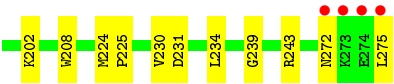
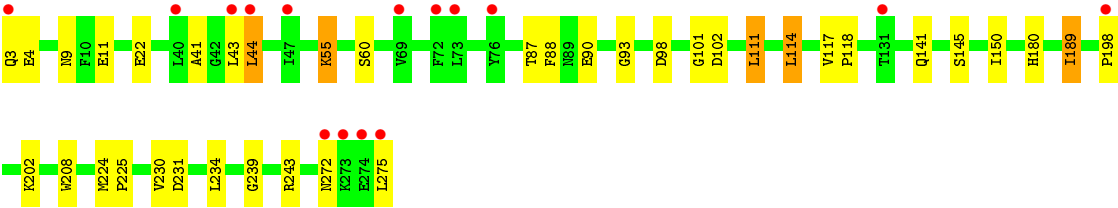
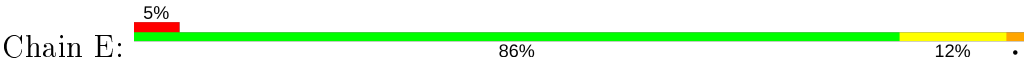


- Molecule 1: Sodium pumping rhodopsin





● 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	131.36Å 239.59Å 135.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.03 – 2.20 48.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.03-2.20) 100.0 (48.03-2.20)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.149 , 0.172 0.162 , 0.182	Depositor DCC
R_{free} test set	5464 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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	12742	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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, RET, 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	0.31	0/2237	0.44	0/3041
1	B	0.32	0/2231	0.44	0/3034
1	C	0.31	0/2236	0.44	0/3040
1	D	0.31	0/2235	0.45	0/3039
1	E	0.31	0/2237	0.44	0/3042
All	All	0.31	0/11176	0.44	0/15196

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	2
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	A	272	ASN	Peptide
1	B	243	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	272	ASN	Peptide
1	C	272	ASN	Peptide
1	D	243	ARG	Sidechain
1	E	243	ARG	Sidechain
1	E	272	ASN	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	2179	0	2154	24	0
1	B	2173	0	2149	27	0
1	C	2178	0	2152	25	0
1	D	2177	0	2148	22	0
1	E	2179	0	2155	28	0
2	A	171	0	249	2	0
2	B	132	0	186	2	0
2	C	142	0	193	6	0
2	D	154	0	215	3	0
2	E	147	0	209	2	0
3	A	78	0	151	0	0
3	B	54	0	106	2	0
3	C	99	0	196	6	0
3	D	78	0	156	1	0
3	E	55	0	107	1	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	2	0
5	B	20	0	28	3	0
5	C	20	0	28	2	0
5	D	20	0	28	1	0
5	E	20	0	28	4	0
6	A	20	0	27	4	0
6	B	20	0	27	4	0
6	C	20	0	27	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	20	0	27	5	0
6	E	20	0	27	6	0
7	A	110	0	0	6	0
7	B	112	0	0	3	0
7	C	111	0	0	5	0
7	D	96	0	0	4	0
7	E	112	0	0	10	0
All	All	12742	0	12801	152	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 6.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:315:RET:H8	6:B:315:RET:H161	1.65	0.78
6:C:319:RET:H161	6:C:319:RET:H8	1.65	0.78
6:D:318:RET:H8	6:D:318:RET:H161	1.65	0.77
1:E:87[B]:THR:HG21	1:E:98:ASP:OD2	1.85	0.77
6:A:321:RET:H8	6:A:321:RET:H161	1.67	0.75
1:D:87[B]:THR:HG21	1:D:98:ASP:OD2	1.86	0.74
1:B:272:ASN:H	1:B:272:ASN:HD22	1.36	0.73
6:E:318:RET:H161	6:E:318:RET:H8	1.70	0.73
1:D:231:ASP:N	5:D:317:BOG:O6	2.19	0.73
1:E:60:SER:OG	7:E:401:HOH:O	2.06	0.72
1:C:55:LYS:NZ	7:C:402:HOH:O	2.22	0.72
1:D:60:SER:OG	7:D:401:HOH:O	2.07	0.72
1:B:231:ASP:H	5:B:314:BOG:HO6	1.37	0.72
1:B:231:ASP:N	5:B:314:BOG:O6	2.19	0.71
1:A:164:LEU:HD21	5:A:316:BOG:H2'1	1.72	0.70
1:A:272:ASN:H	1:A:272:ASN:HD22	1.40	0.70
1:D:87[B]:THR:HG22	7:D:438:HOH:O	1.93	0.68
2:C:304:OLC:H11	2:C:304:OLC:H7	1.74	0.68
7:A:407:HOH:O	1:B:3:GLN:HG3	1.94	0.68
1:E:189:ILE:HD12	1:E:208:TRP:HB2	1.76	0.67
1:A:231:ASP:N	5:A:316:BOG:O6	2.27	0.66
1:C:60:SER:OG	7:C:401:HOH:O	2.14	0.66
1:B:145:SER:OG	1:B:180:HIS:HD2	1.79	0.65
1:E:145:SER:OG	1:E:180:HIS:HD2	1.80	0.64
1:C:189:ILE:HD12	1:C:208:TRP:HB2	1.80	0.64
1:D:145:SER:OG	1:D:180:HIS:HD2	1.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:N	1:B:272:ASN:HD22	1.95	0.63
1:C:145:SER:OG	1:C:180:HIS:HD2	1.82	0.62
2:C:304:OLC:H13	2:D:301:OLC:H4A	1.82	0.62
1:A:140:ASN:HB3	2:A:303:OLC:H2A	1.82	0.61
1:A:272:ASN:HD22	1:A:272:ASN:N	1.97	0.60
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.83	0.60
1:E:87[B]:THR:HG22	7:E:453:HOH:O	2.01	0.60
1:A:44:LEU:HD21	1:B:43:LEU:HD11	1.84	0.59
1:D:60:SER:CB	7:D:401:HOH:O	2.51	0.57
1:E:141:GLN:HG2	2:E:304:OLC:H5A	1.87	0.56
1:C:183:TRP:CE3	3:C:310:LFA:H41	2.40	0.56
1:C:60:SER:CB	7:C:401:HOH:O	2.54	0.56
1:C:231:ASP:N	5:C:317:BOG:O6	2.32	0.56
1:E:111:LEU:O	1:E:114:LEU:HB2	2.07	0.53
1:E:55:LYS:HE3	7:E:452:HOH:O	2.07	0.53
1:C:224:MET:N	1:C:225:PRO:HD2	2.23	0.53
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.89	0.53
1:D:22:GLU:HB2	7:E:411:HOH:O	2.08	0.53
1:A:60:SER:OG	7:A:401:HOH:O	2.19	0.52
1:B:231:ASP:N	5:B:314:BOG:HO6	2.03	0.52
1:A:140:ASN:HD22	2:A:303:OLC:H21	1.75	0.52
1:C:60:SER:HB3	7:C:401:HOH:O	2.09	0.52
6:B:315:RET:C8	6:B:315:RET:H161	2.39	0.52
1:B:101:GLY:O	1:B:102:ASP:HB2	2.10	0.52
1:D:224:MET:N	1:D:225:PRO:HD2	2.25	0.51
1:A:224:MET:N	1:A:225:PRO:HD2	2.26	0.51
1:E:101:GLY:O	1:E:102:ASP:HB2	2.11	0.51
6:C:319:RET:H161	6:C:319:RET:C8	2.39	0.51
2:C:309:OLC:C3	2:D:302:OLC:H24A	2.41	0.51
1:B:273:LYS:O	7:B:401:HOH:O	2.18	0.51
6:A:321:RET:C8	6:A:321:RET:H161	2.39	0.51
1:B:224:MET:N	1:B:225:PRO:HD2	2.26	0.51
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.93	0.51
1:C:186:LYS:HG2	3:C:310:LFA:C5	2.41	0.51
1:E:60:SER:CB	7:E:401:HOH:O	2.60	0.50
1:B:272:ASN:N	1:B:272:ASN:ND2	2.58	0.50
1:B:186:LYS:HG2	3:B:309:LFA:H192	1.93	0.50
1:A:101:GLY:O	1:A:102:ASP:HB2	2.12	0.50
1:E:234:LEU:O	1:E:239:GLY:HA3	2.11	0.50
1:A:234:LEU:O	1:A:239:GLY:HA3	2.12	0.50
1:C:101:GLY:O	1:C:102:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ASN:OD1	1:C:92:VAL:HG13	2.11	0.50
1:D:234:LEU:O	1:D:239:GLY:HA3	2.12	0.50
1:A:3:GLN:HG2	7:E:407:HOH:O	2.13	0.49
1:B:234:LEU:O	1:B:239:GLY:HA3	2.11	0.49
1:E:198:PRO:HG2	7:E:492:HOH:O	2.12	0.49
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.94	0.49
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.94	0.49
1:C:186:LYS:HG2	3:C:310:LFA:H51	1.94	0.49
1:D:87[B]:THR:HG23	1:D:98:ASP:CB	2.42	0.49
1:C:234:LEU:O	1:C:239:GLY:HA3	2.13	0.49
1:B:139:ARG:NH1	2:B:301:OLC:H24	2.27	0.49
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.94	0.49
2:E:310:OLC:H21	5:E:316:BOG:H3'1	1.95	0.49
1:B:274:GLU:O	1:B:275:LEU:CB	2.61	0.49
1:E:224:MET:N	1:E:225:PRO:HD2	2.27	0.48
1:E:87[B]:THR:HG23	1:E:98:ASP:CB	2.43	0.48
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.95	0.48
1:D:60:SER:HB3	7:D:401:HOH:O	2.11	0.48
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.94	0.48
1:C:163:ASN:HD22	2:C:308:OLC:C24	2.27	0.48
1:E:202:LYS:CD	7:E:498:HOH:O	2.61	0.48
1:A:272:ASN:ND2	1:A:272:ASN:N	2.60	0.47
6:D:318:RET:H161	6:D:318:RET:C8	2.38	0.47
1:E:87[B]:THR:HG23	1:E:98:ASP:HB2	1.96	0.47
1:D:101:GLY:O	1:D:102:ASP:HB2	2.15	0.47
1:C:40:LEU:HD11	3:C:303:LFA:H142	1.97	0.46
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.96	0.46
7:A:408:HOH:O	1:E:22:GLU:HB2	2.16	0.46
1:C:267:ILE:HG21	1:C:275:LEU:HB3	1.98	0.46
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.16	0.46
6:C:319:RET:H8	6:C:319:RET:H171	1.98	0.46
1:A:131:THR:HG21	1:A:194:GLU:OE1	2.16	0.45
6:B:315:RET:H8	6:B:315:RET:H171	1.98	0.45
6:E:318:RET:H8	6:E:318:RET:H171	1.97	0.45
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.16	0.45
1:A:89:ASN:OD1	1:A:92:VAL:HG13	2.16	0.45
1:B:183:TRP:CZ3	3:B:309:LFA:H182	2.51	0.45
3:E:312:LFA:H141	3:E:313:LFA:H191	1.98	0.45
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.17	0.45
1:D:87[B]:THR:HG23	1:D:98:ASP:HB2	1.98	0.45
1:A:51:LYS:CD	7:A:477:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LEU:HD21	5:C:317:BOG:H2'1	1.98	0.44
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.16	0.44
1:C:183:TRP:CZ3	3:C:310:LFA:H61	2.52	0.44
1:E:55:LYS:CE	7:E:452:HOH:O	2.64	0.44
6:A:321:RET:H171	6:A:321:RET:H8	2.00	0.44
1:B:60:SER:CB	7:B:402:HOH:O	2.65	0.44
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.18	0.44
6:C:319:RET:C8	6:C:319:RET:H171	2.48	0.44
1:B:139:ARG:HH11	2:B:301:OLC:C24	2.30	0.44
1:C:243:ARG:NH2	7:C:405:HOH:O	2.52	0.43
1:D:89:ASN:OD1	1:D:92:VAL:HG13	2.17	0.43
6:B:315:RET:C8	6:B:315:RET:H171	2.48	0.43
6:D:318:RET:H8	6:D:318:RET:H171	2.01	0.43
6:E:318:RET:H161	6:E:318:RET:C8	2.42	0.43
1:A:3:GLN:NE2	1:E:90:GLU:OE1	2.52	0.43
1:D:74:LEU:HD22	1:D:74:LEU:HA	1.87	0.43
6:E:318:RET:H171	6:E:318:RET:C8	2.47	0.43
1:E:44:LEU:HA	1:E:44:LEU:HD23	1.83	0.43
7:A:455:HOH:O	1:B:55:LYS:HE3	2.18	0.43
1:B:60:SER:HB3	7:B:402:HOH:O	2.19	0.43
6:A:321:RET:H171	6:A:321:RET:C8	2.49	0.42
6:D:318:RET:H171	6:D:318:RET:C8	2.49	0.42
1:C:272:ASN:HB2	1:C:273:LYS:HD3	2.01	0.42
2:D:309:OLC:H11A	3:D:313:LFA:H12	2.00	0.42
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.54	0.42
6:E:318:RET:H7	6:E:318:RET:H181	1.73	0.42
1:A:264:ASN:O	1:A:268:THR:HG23	2.19	0.42
1:C:41:ALA:HB1	1:D:66:VAL:HG13	2.00	0.42
1:E:231:ASP:H	5:E:316:BOG:HO6	1.61	0.42
1:D:264:ASN:O	1:D:268:THR:HG23	2.19	0.42
6:D:318:RET:H191	6:D:318:RET:H11	1.92	0.42
1:B:89:ASN:OD1	1:B:92:VAL:HG13	2.19	0.42
2:C:301:OLC:H12A	3:C:312:LFA:H111	2.01	0.42
2:C:306:OLC:H2A	2:C:308:OLC:H21A	2.02	0.42
5:E:316:BOG:H5	7:E:455:HOH:O	2.19	0.42
6:E:318:RET:H11	6:E:318:RET:H191	1.90	0.42
1:A:60:SER:CB	7:A:401:HOH:O	2.67	0.41
1:D:44:LEU:HD21	1:E:43:LEU:HD11	2.01	0.41
1:E:231:ASP:N	5:E:316:BOG:O6	2.35	0.41
1:B:38:VAL:HG11	1:B:252:VAL:HG22	2.02	0.41
1:D:88:PHE:CZ	1:D:93:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.97	0.41
1:D:87[B]:THR:CG2	1:D:98:ASP:OD2	2.65	0.41
6:C:319:RET:H7	6:C:319:RET:H181	1.75	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	272/273 (100%)	266 (98%)	6 (2%)	0	100	100
1	B	272/273 (100%)	265 (97%)	7 (3%)	0	100	100
1	C	272/273 (100%)	266 (98%)	6 (2%)	0	100	100
1	D	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
1	E	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
All	All	1362/1365 (100%)	1333 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	231/234 (99%)	225 (97%)	6 (3%)	46	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	231/234 (99%)	225 (97%)	6 (3%)	46	58
1	C	231/234 (99%)	224 (97%)	7 (3%)	41	53
1	D	230/234 (98%)	228 (99%)	2 (1%)	78	88
1	E	231/234 (99%)	222 (96%)	9 (4%)	32	41
All	All	1154/1170 (99%)	1124 (97%)	30 (3%)	46	58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	111	LEU
1	A	230	VAL
1	A	272	ASN
1	A	273	LYS
1	A	274	GLU
1	B	4	GLU
1	B	103	LEU
1	B	111	LEU
1	B	164	LEU
1	B	230	VAL
1	B	272	ASN
1	C	3	GLN
1	C	44	LEU
1	C	111	LEU
1	C	230	VAL
1	C	273	LYS
1	C	274	GLU
1	C	275	LEU
1	D	111	LEU
1	D	230	VAL
1	E	3	GLN
1	E	4	GLU
1	E	44	LEU
1	E	55	LYS
1	E	111	LEU
1	E	114	LEU
1	E	189	ILE
1	E	230	VAL
1	E	275	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 91 ligands modelled in this entry, 5 are monoatomic - leaving 86 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	E	303	-	7,7,24	0.29	0	6,6,25	0.41	0
2	OLC	D	307	-	13,13,24	1.24	1 (7%)	14,14,25	0.93	1 (7%)
6	RET	E	318	1	20,20,21	0.74	1 (5%)	27,27,28	1.63	6 (22%)
2	OLC	D	308	-	6,6,24	0.33	0	5,5,25	0.36	0
2	OLC	B	301	-	21,21,24	0.97	1 (4%)	22,22,25	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	A	318	-	16,19,24	0.27	0	15,19,25	0.54	0
2	OLC	E	304	-	15,15,24	0.27	0	14,14,25	0.51	0
3	LFA	D	312	-	7,7,19	0.30	0	6,6,18	0.39	0
3	LFA	A	313	-	5,5,19	0.28	0	4,4,18	0.37	0
3	LFA	E	312	-	13,13,19	0.28	0	12,12,18	0.48	0
3	LFA	E	311	-	7,7,19	0.28	0	6,6,18	0.43	0
2	OLC	E	308	-	5,5,24	0.32	0	4,4,25	0.30	0
2	OLC	E	310	-	19,19,24	1.08	1 (5%)	20,20,25	0.99	1 (5%)
3	LFA	B	312	-	6,6,19	0.27	0	5,5,18	0.39	0
3	LFA	E	313	-	3,3,19	0.34	0	2,2,18	0.60	0
3	LFA	D	310	-	19,19,19	0.26	0	18,18,18	0.56	0
3	LFA	A	312	-	3,3,19	0.37	0	2,2,18	0.61	0
2	OLC	C	305	-	21,21,24	1.04	1 (4%)	22,22,25	0.91	1 (4%)
3	LFA	C	318	-	13,13,19	0.28	0	12,12,18	0.49	0
2	OLC	A	302	-	21,21,24	0.98	1 (4%)	22,22,25	0.86	2 (9%)
2	OLC	B	308	-	6,6,24	0.46	0	5,5,25	0.58	0
2	OLC	E	305	-	19,19,24	1.08	1 (5%)	20,20,25	1.00	1 (5%)
6	RET	C	319	1	20,20,21	0.68	0	27,27,28	1.62	6 (22%)
2	OLC	B	303	-	24,24,24	0.95	1 (4%)	25,25,25	0.82	1 (4%)
3	LFA	B	310	-	7,7,19	0.28	0	6,6,18	0.41	0
3	LFA	B	309	-	8,8,19	0.28	0	7,7,18	0.44	0
2	OLC	D	304	-	24,24,24	0.94	1 (4%)	25,25,25	0.83	1 (4%)
2	OLC	A	304	-	12,12,24	1.30	1 (8%)	13,13,25	1.26	2 (15%)
6	RET	D	318	1	20,20,21	0.68	0	27,27,28	1.61	7 (25%)
3	LFA	A	311	-	7,7,19	0.29	0	6,6,18	0.40	0
5	BOG	D	317	-	20,20,20	0.56	0	25,25,25	0.63	0
3	LFA	A	320	-	8,8,19	0.29	0	7,7,18	0.41	0
2	OLC	E	309	-	21,21,24	1.03	1 (4%)	22,22,25	0.87	1 (4%)
2	OLC	A	303	-	24,24,24	0.97	1 (4%)	25,25,25	0.83	1 (4%)
3	LFA	C	312	-	19,19,19	0.26	0	18,18,18	0.53	0
2	OLC	D	301	-	17,17,24	1.11	1 (5%)	18,18,25	1.01	1 (5%)
3	LFA	C	310	-	6,6,19	0.31	0	5,5,18	0.37	0
2	OLC	E	307	-	14,14,24	1.14	1 (7%)	15,15,25	0.97	2 (13%)
3	LFA	B	311	-	9,9,19	0.31	0	8,8,18	0.41	0
3	LFA	A	309	-	6,6,19	0.27	0	5,5,18	0.41	0
2	OLC	B	304	-	20,20,24	0.99	1 (5%)	21,21,25	0.96	1 (4%)
2	OLC	C	306	-	19,19,24	1.07	1 (5%)	20,20,25	0.92	1 (5%)
2	OLC	A	305	-	24,24,24	0.98	1 (4%)	25,25,25	0.84	1 (4%)
3	LFA	A	310	-	7,7,19	0.32	0	6,6,18	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	D	306	-	14,17,24	0.28	0	13,17,25	0.54	0
2	OLC	D	303	-	12,12,24	1.35	1 (8%)	13,13,25	1.05	1 (7%)
2	OLC	C	309	-	6,6,24	0.30	0	5,5,25	0.36	0
3	LFA	B	302	-	19,19,19	0.36	0	18,18,18	0.36	0
3	LFA	A	319	-	19,19,19	0.35	0	18,18,18	0.36	0
2	OLC	D	309	-	24,24,24	0.93	1 (4%)	25,25,25	0.76	1 (4%)
6	RET	B	315	1	20,20,21	0.69	0	27,27,28	1.62	6 (22%)
2	OLC	A	301	-	8,8,24	0.36	0	6,7,25	0.45	0
3	LFA	C	314	-	3,3,19	0.37	0	2,2,18	0.58	0
2	OLC	C	304	-	22,22,24	0.94	1 (4%)	23,23,25	0.88	2 (8%)
2	OLC	B	307	-	15,15,24	1.13	1 (6%)	16,16,25	0.97	1 (6%)
3	LFA	E	317	-	3,3,19	0.36	0	2,2,18	0.59	0
3	LFA	D	315	-	5,5,19	0.31	0	4,4,18	0.31	0
3	LFA	C	315	-	19,19,19	0.34	0	18,18,18	0.39	0
2	OLC	B	305	-	19,19,24	1.05	1 (5%)	20,20,25	0.99	2 (10%)
5	BOG	B	314	-	20,20,20	0.55	1 (5%)	25,25,25	0.57	0
2	OLC	A	307	-	6,6,24	0.27	0	5,5,25	0.47	0
2	OLC	C	307	-	21,21,24	1.02	1 (4%)	22,22,25	0.92	1 (4%)
2	OLC	B	306	-	20,20,24	1.04	1 (5%)	21,21,25	0.95	1 (4%)
5	BOG	A	316	-	20,20,20	0.57	1 (5%)	25,25,25	0.62	0
5	BOG	C	317	-	20,20,20	0.50	0	25,25,25	0.61	0
2	OLC	E	301	-	24,24,24	0.93	1 (4%)	25,25,25	0.89	1 (4%)
2	OLC	A	306	-	14,14,24	1.21	1 (7%)	15,15,25	0.99	1 (6%)
3	LFA	C	311	-	7,7,19	0.29	0	6,6,18	0.35	0
5	BOG	E	316	-	20,20,20	0.57	1 (5%)	25,25,25	0.62	0
3	LFA	E	314	-	4,4,19	0.29	0	3,3,18	0.37	0
3	LFA	A	314	-	15,15,19	0.29	0	14,14,18	0.49	0
3	LFA	C	313	-	5,5,19	0.34	0	4,4,18	0.33	0
2	OLC	C	302	-	11,11,24	1.44	1 (9%)	12,12,25	1.08	1 (8%)
3	LFA	D	314	-	6,6,19	0.29	0	5,5,18	0.37	0
2	OLC	A	308	-	15,15,24	1.23	1 (6%)	16,16,25	0.98	1 (6%)
2	OLC	A	317	-	15,18,24	0.22	0	14,18,25	0.59	0
2	OLC	C	308	-	15,15,24	1.17	1 (6%)	16,16,25	0.90	1 (6%)
2	OLC	C	301	-	19,19,24	1.08	1 (5%)	20,20,25	0.92	2 (10%)
2	OLC	D	305	-	17,17,24	1.12	1 (5%)	18,18,25	1.10	2 (11%)
3	LFA	D	311	-	19,19,19	0.28	0	18,18,18	0.51	0
2	OLC	D	302	-	15,15,24	1.24	1 (6%)	16,16,25	1.06	2 (12%)
6	RET	A	321	1	20,20,21	0.75	1 (5%)	27,27,28	1.64	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	D	313	-	16,16,19	0.28	0	15,15,18	0.48	0
3	LFA	E	302	-	19,19,19	0.37	0	18,18,18	0.40	0
2	OLC	E	306	-	14,14,24	1.24	1 (7%)	15,15,25	1.07	1 (6%)
3	LFA	C	303	-	19,19,19	0.36	0	18,18,18	0.31	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	E	303	-	-	2/5/5/24	-
2	OLC	D	307	-	-	4/13/13/24	-
6	RET	E	318	1	-	0/13/30/31	0/1/1/1
2	OLC	D	308	-	-	1/4/4/24	-
2	OLC	B	301	-	-	7/21/21/24	-
2	OLC	A	318	-	-	9/15/17/24	-
2	OLC	E	304	-	-	8/13/13/24	-
3	LFA	D	312	-	-	4/5/5/17	-
3	LFA	A	313	-	-	2/3/3/17	-
3	LFA	E	312	-	-	5/11/11/17	-
3	LFA	E	311	-	-	2/5/5/17	-
2	OLC	E	308	-	-	0/3/3/24	-
2	OLC	E	310	-	-	12/19/19/24	-
3	LFA	B	312	-	-	1/4/4/17	-
3	LFA	E	313	-	-	1/1/1/17	-
3	LFA	D	310	-	-	11/17/17/17	-
3	LFA	A	312	-	-	0/1/1/17	-
2	OLC	C	305	-	-	7/21/21/24	-
3	LFA	C	318	-	-	4/11/11/17	-
2	OLC	A	302	-	-	10/21/21/24	-
2	OLC	B	308	-	-	2/4/4/24	-
2	OLC	E	305	-	-	6/19/19/24	-
6	RET	C	319	1	-	0/13/30/31	0/1/1/1
2	OLC	B	303	-	-	14/24/24/24	-
3	LFA	B	310	-	-	3/5/5/17	-
3	LFA	B	309	-	-	3/6/6/17	-
2	OLC	D	304	-	-	10/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	304	-	-	2/12/12/24	-
6	RET	D	318	1	-	0/13/30/31	0/1/1/1
3	LFA	A	311	-	-	3/5/5/17	-
5	BOG	D	317	-	-	4/11/31/31	0/1/1/1
3	LFA	A	320	-	-	3/6/6/17	-
2	OLC	E	309	-	-	6/21/21/24	-
2	OLC	A	303	-	-	17/24/24/24	-
3	LFA	C	312	-	-	13/17/17/17	-
2	OLC	D	301	-	-	8/17/17/24	-
3	LFA	C	310	-	-	2/4/4/17	-
2	OLC	E	307	-	-	9/14/14/24	-
3	LFA	B	311	-	-	4/7/7/17	-
3	LFA	A	309	-	-	2/4/4/17	-
2	OLC	B	304	-	-	11/20/20/24	-
2	OLC	C	306	-	-	5/19/19/24	-
2	OLC	A	305	-	-	13/24/24/24	-
3	LFA	A	310	-	-	3/5/5/17	-
2	OLC	D	306	-	-	7/13/15/24	-
2	OLC	D	303	-	-	6/12/12/24	-
2	OLC	C	309	-	-	3/4/4/24	-
3	LFA	B	302	-	-	7/17/17/17	-
3	LFA	A	319	-	-	10/17/17/17	-
2	OLC	D	309	-	-	13/24/24/24	-
6	RET	B	315	1	-	0/13/30/31	0/1/1/1
2	OLC	A	301	-	-	3/6/6/24	-
3	LFA	C	314	-	-	1/1/1/17	-
2	OLC	C	304	-	-	9/22/22/24	-
2	OLC	B	307	-	-	3/15/15/24	-
3	LFA	E	317	-	-	0/1/1/17	-
3	LFA	D	315	-	-	0/3/3/17	-
3	LFA	C	315	-	-	6/17/17/17	-
2	OLC	B	305	-	-	6/19/19/24	-
5	BOG	B	314	-	-	5/11/31/31	0/1/1/1
2	OLC	A	307	-	-	3/4/4/24	-
2	OLC	C	307	-	-	10/21/21/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	306	-	-	12/20/20/24	-
5	BOG	A	316	-	-	5/11/31/31	0/1/1/1
5	BOG	C	317	-	-	3/11/31/31	0/1/1/1
2	OLC	E	301	-	-	14/24/24/24	-
2	OLC	A	306	-	-	7/14/14/24	-
3	LFA	C	311	-	-	4/5/5/17	-
5	BOG	E	316	-	-	9/11/31/31	0/1/1/1
3	LFA	E	314	-	-	1/2/2/17	-
3	LFA	A	314	-	-	9/13/13/17	-
3	LFA	C	313	-	-	0/3/3/17	-
2	OLC	C	302	-	-	5/11/11/24	-
3	LFA	D	314	-	-	3/4/4/17	-
2	OLC	A	308	-	-	6/15/15/24	-
2	OLC	A	317	-	-	7/14/16/24	-
2	OLC	C	308	-	-	7/15/15/24	-
2	OLC	C	301	-	-	11/19/19/24	-
2	OLC	D	305	-	-	4/17/17/24	-
3	LFA	D	311	-	-	9/17/17/17	-
2	OLC	D	302	-	-	7/15/15/24	-
6	RET	A	321	1	-	0/13/30/31	0/1/1/1
3	LFA	D	313	-	-	9/14/14/17	-
3	LFA	E	302	-	-	5/17/17/17	-
2	OLC	E	306	-	-	5/14/14/24	-
3	LFA	C	303	-	-	12/17/17/17	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	OLC	O20-C1	4.61	1.46	1.33
2	A	308	OLC	O20-C1	4.55	1.46	1.33
2	D	302	OLC	O20-C1	4.55	1.46	1.33
2	C	305	OLC	O20-C1	4.51	1.46	1.33
2	A	305	OLC	O20-C1	4.50	1.46	1.33
2	A	303	OLC	O20-C1	4.49	1.46	1.33
2	D	303	OLC	O20-C1	4.49	1.46	1.33
2	E	305	OLC	O20-C1	4.48	1.46	1.33
2	C	306	OLC	O20-C1	4.44	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	310	OLC	O20-C1	4.44	1.46	1.33
2	E	309	OLC	O20-C1	4.43	1.46	1.33
2	E	306	OLC	O20-C1	4.43	1.46	1.33
2	C	301	OLC	O20-C1	4.41	1.46	1.33
2	B	306	OLC	O20-C1	4.40	1.46	1.33
2	D	305	OLC	O20-C1	4.40	1.46	1.33
2	C	307	OLC	O20-C1	4.39	1.46	1.33
2	B	303	OLC	O20-C1	4.35	1.46	1.33
2	D	304	OLC	O20-C1	4.34	1.46	1.33
2	A	304	OLC	O20-C1	4.33	1.46	1.33
2	C	308	OLC	O20-C1	4.32	1.46	1.33
2	D	301	OLC	O20-C1	4.31	1.45	1.33
2	E	301	OLC	O20-C1	4.31	1.45	1.33
2	B	305	OLC	O20-C1	4.31	1.45	1.33
2	A	306	OLC	O20-C1	4.30	1.45	1.33
2	D	309	OLC	O20-C1	4.27	1.45	1.33
2	D	307	OLC	O20-C1	4.26	1.45	1.33
2	B	304	OLC	O20-C1	4.24	1.45	1.33
2	B	301	OLC	O20-C1	4.20	1.45	1.33
2	A	302	OLC	O20-C1	4.19	1.45	1.33
2	B	307	OLC	O20-C1	4.13	1.45	1.33
2	C	304	OLC	O20-C1	4.10	1.45	1.33
2	E	307	OLC	O20-C1	3.97	1.44	1.33
6	A	321	RET	C14-C13	2.26	1.35	1.33
6	E	318	RET	C14-C13	2.18	1.35	1.33
5	A	316	BOG	O1-C1	2.02	1.43	1.40
5	B	314	BOG	O1-C1	2.01	1.43	1.40
5	E	316	BOG	O1-C1	2.01	1.43	1.40

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	321	RET	C18-C5-C6	-3.79	120.28	124.53
6	E	318	RET	C18-C5-C6	-3.77	120.29	124.53
6	C	319	RET	C18-C5-C6	-3.66	120.42	124.53
6	D	318	RET	C18-C5-C6	-3.48	120.62	124.53
6	B	315	RET	C18-C5-C6	-3.47	120.64	124.53
2	A	304	OLC	O20-C1-C2	3.26	122.15	111.91
2	D	305	OLC	O20-C1-C2	3.11	121.65	111.91
2	E	305	OLC	O20-C1-C2	3.09	121.61	111.91
2	E	310	OLC	O20-C1-C2	3.04	121.46	111.91
2	B	304	OLC	O20-C1-C2	2.98	121.27	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	305	OLC	O20-C1-C2	2.94	121.15	111.91
2	B	306	OLC	O20-C1-C2	2.94	121.14	111.91
2	D	302	OLC	O20-C1-C2	2.93	121.10	111.91
6	B	315	RET	C7-C8-C9	-2.91	121.84	126.23
2	E	306	OLC	O20-C1-C2	2.90	120.99	111.91
2	C	307	OLC	O20-C1-C2	2.86	120.88	111.91
6	D	318	RET	C7-C8-C9	-2.84	121.94	126.23
6	B	315	RET	C11-C10-C9	-2.82	123.29	127.31
2	C	306	OLC	O20-C1-C2	2.80	120.69	111.91
2	C	301	OLC	O20-C1-C2	2.79	120.66	111.91
6	A	321	RET	C11-C10-C9	-2.78	123.34	127.31
2	A	303	OLC	O20-C1-C2	2.77	120.59	111.91
2	C	305	OLC	O20-C1-C2	2.77	120.59	111.91
2	A	302	OLC	O20-C1-C2	2.72	120.46	111.91
2	E	309	OLC	O20-C1-C2	2.72	120.45	111.91
2	D	301	OLC	O20-C1-C2	2.72	120.43	111.91
2	B	301	OLC	O20-C1-C2	2.71	120.42	111.91
2	E	301	OLC	O20-C1-C2	2.71	120.41	111.91
2	A	305	OLC	O20-C1-C2	2.70	120.39	111.91
6	C	319	RET	C11-C10-C9	-2.70	123.46	127.31
2	A	308	OLC	O20-C1-C2	2.69	120.34	111.91
2	D	303	OLC	O20-C1-C2	2.68	120.32	111.91
2	C	302	OLC	O20-C1-C2	2.68	120.31	111.91
2	B	303	OLC	O20-C1-C2	2.67	120.28	111.91
2	C	304	OLC	O20-C1-C2	2.63	120.16	111.91
6	C	319	RET	C7-C8-C9	-2.63	122.26	126.23
6	D	318	RET	C11-C10-C9	-2.60	123.59	127.31
6	A	321	RET	C7-C8-C9	-2.55	122.38	126.23
2	A	306	OLC	O20-C1-C2	2.54	119.89	111.91
6	E	318	RET	C7-C8-C9	-2.53	122.41	126.23
2	D	304	OLC	O20-C1-C2	2.53	119.84	111.91
6	E	318	RET	C11-C10-C9	-2.52	123.72	127.31
6	D	318	RET	C20-C13-C12	2.48	121.98	118.08
2	E	307	OLC	O20-C1-O19	-2.47	117.36	123.59
2	B	307	OLC	O20-C1-C2	2.46	119.62	111.91
2	A	304	OLC	O20-C1-O19	-2.45	117.42	123.59
6	C	319	RET	C20-C13-C12	2.44	121.93	118.08
2	E	307	OLC	O20-C1-C2	2.40	119.45	111.91
2	D	309	OLC	O20-C1-C2	2.37	119.34	111.91
6	A	321	RET	C10-C11-C12	-2.37	115.83	123.22
2	C	308	OLC	O20-C1-C2	2.35	119.29	111.91
6	B	315	RET	C20-C13-C12	2.33	121.74	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	318	RET	C19-C9-C8	2.32	121.73	118.08
2	D	307	OLC	O20-C1-C2	2.32	119.18	111.91
6	C	319	RET	C19-C9-C8	2.28	121.68	118.08
6	E	318	RET	C10-C11-C12	-2.27	116.12	123.22
6	A	321	RET	C19-C9-C8	2.27	121.66	118.08
6	B	315	RET	C10-C11-C12	-2.26	116.16	123.22
6	D	318	RET	C10-C11-C12	-2.24	116.24	123.22
6	E	318	RET	C20-C13-C12	2.23	121.59	118.08
6	A	321	RET	C20-C13-C12	2.19	121.52	118.08
2	A	302	OLC	O20-C1-O19	-2.18	118.10	123.59
2	C	304	OLC	O20-C1-O19	-2.16	118.13	123.59
2	B	305	OLC	O20-C1-O19	-2.16	118.14	123.59
6	B	315	RET	C19-C9-C8	2.15	121.46	118.08
6	D	318	RET	C19-C9-C8	2.10	121.38	118.08
2	C	301	OLC	O20-C1-O19	-2.07	118.38	123.59
6	C	319	RET	C10-C11-C12	-2.06	116.80	123.22
6	D	318	RET	C17-C1-C6	-2.04	106.99	110.30
2	D	305	OLC	O20-C1-O19	-2.04	118.46	123.59
2	D	302	OLC	O20-C1-O19	-2.03	118.48	123.59

There are no chirality outliers.

All (479) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	310	OLC	C21-C22-C24-O25
3	E	313	LFA	C17-C18-C19-C20
2	C	305	OLC	O20-C21-C22-C24
2	C	305	OLC	O20-C21-C22-O23
2	A	302	OLC	C21-C22-C24-O25
2	A	302	OLC	O23-C22-C24-O25
2	E	305	OLC	C10-C11-C12-C13
2	B	303	OLC	C21-C22-C24-O25
2	E	309	OLC	O20-C21-C22-C24
2	D	301	OLC	O20-C21-C22-C24
2	D	301	OLC	O20-C21-C22-O23
2	E	307	OLC	O20-C21-C22-O23
2	B	304	OLC	C21-C22-C24-O25
2	C	306	OLC	C21-C22-C24-O25
2	A	305	OLC	O20-C21-C22-C24
2	A	305	OLC	O20-C21-C22-O23
2	D	306	OLC	C1-C2-C3-C4
2	D	303	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
2	D	309	OLC	C21-C22-C24-O25
3	C	314	LFA	C17-C18-C19-C20
2	B	305	OLC	C10-C11-C12-C13
2	B	305	OLC	C21-C22-C24-O25
2	C	307	OLC	C21-C22-C24-O25
2	A	306	OLC	O20-C21-C22-C24
5	E	316	BOG	C2-C1-O1-C1'
5	E	316	BOG	O5-C1-O1-C1'
5	E	316	BOG	C2'-C1'-O1-C1
2	C	302	OLC	C21-C22-C24-O25
2	A	308	OLC	C21-C22-C24-O25
2	C	301	OLC	C10-C11-C12-C13
2	D	302	OLC	O20-C21-C22-O23
2	E	306	OLC	O20-C21-C22-O23
2	C	304	OLC	O19-C1-O20-C21
2	C	304	OLC	C2-C1-O20-C21
2	D	304	OLC	O19-C1-O20-C21
2	D	304	OLC	C2-C1-O20-C21
2	C	308	OLC	C2-C1-O20-C21
2	A	306	OLC	O19-C1-O20-C21
2	E	307	OLC	C2-C1-O20-C21
2	A	305	OLC	C2-C1-O20-C21
2	D	309	OLC	C2-C1-O20-C21
2	A	306	OLC	C2-C1-O20-C21
2	E	307	OLC	O19-C1-O20-C21
2	D	309	OLC	O19-C1-O20-C21
2	C	308	OLC	O19-C1-O20-C21
5	E	316	BOG	O5-C5-C6-O6
2	B	301	OLC	C2-C1-O20-C21
2	A	303	OLC	C2-C1-O20-C21
2	D	301	OLC	C2-C1-O20-C21
2	A	304	OLC	O20-C21-C22-O23
2	D	303	OLC	O20-C21-C22-O23
2	A	306	OLC	O20-C21-C22-O23
2	C	308	OLC	O20-C21-C22-O23
2	C	302	OLC	O20-C21-C22-O23
2	A	303	OLC	O19-C1-O20-C21
2	A	303	OLC	C6-C7-C8-C9
2	D	301	OLC	O19-C1-O20-C21
2	B	301	OLC	O19-C1-O20-C21
2	A	305	OLC	O19-C1-O20-C21
2	B	305	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	D	305	OLC	C2-C1-O20-C21
2	B	305	OLC	O19-C1-O20-C21
2	B	307	OLC	C2-C1-O20-C21
2	D	302	OLC	C2-C1-O20-C21
5	E	316	BOG	C4-C5-C6-O6
2	C	308	OLC	O20-C21-C22-C24
2	E	304	OLC	C4-C5-C6-C7
2	E	309	OLC	O20-C21-C22-O23
2	D	301	OLC	C1-C2-C3-C4
2	B	307	OLC	O19-C1-O20-C21
2	D	307	OLC	O23-C22-C24-O25
2	E	307	OLC	O23-C22-C24-O25
2	D	307	OLC	C1-C2-C3-C4
2	E	310	OLC	C1-C2-C3-C4
2	A	303	OLC	C1-C2-C3-C4
2	E	301	OLC	C1-C2-C3-C4
2	C	301	OLC	C1-C2-C3-C4
2	D	302	OLC	O19-C1-O20-C21
5	B	314	BOG	O5-C5-C6-O6
2	D	305	OLC	O19-C1-O20-C21
2	E	310	OLC	O20-C21-C22-O23
2	E	305	OLC	O20-C21-C22-O23
2	C	301	OLC	O20-C21-C22-O23
5	B	314	BOG	C4-C5-C6-O6
2	A	318	OLC	C2-C3-C4-C5
3	D	313	LFA	C5-C6-C7-C8
2	A	318	OLC	C5-C6-C7-C8
2	A	302	OLC	C3-C4-C5-C6
3	B	309	LFA	C14-C15-C16-C17
3	A	311	LFA	C16-C17-C18-C19
2	E	309	OLC	C11-C12-C13-C14
2	B	306	OLC	C2-C3-C4-C5
2	C	301	OLC	C5-C6-C7-C8
2	E	310	OLC	O20-C21-C22-C24
2	C	301	OLC	O20-C21-C22-C24
2	D	302	OLC	O20-C21-C22-C24
2	E	306	OLC	O20-C21-C22-C24
2	A	318	OLC	C11-C12-C13-C14
2	A	318	OLC	C13-C14-C15-C16
3	D	312	LFA	C2-C3-C4-C5
3	B	309	LFA	C16-C17-C18-C19
2	B	304	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	307	OLC	C4-C5-C6-C7
3	C	311	LFA	C16-C17-C18-C19
2	E	306	OLC	C4-C5-C6-C7
2	D	309	OLC	C11-C12-C13-C14
3	A	313	LFA	C2-C3-C4-C5
3	D	310	LFA	C6-C7-C8-C9
3	B	310	LFA	C3-C4-C5-C6
2	D	304	OLC	C4-C5-C6-C7
2	E	305	OLC	C5-C6-C7-C8
3	C	315	LFA	C9-C10-C11-C12
2	B	306	OLC	C2-C1-O20-C21
2	A	305	OLC	C4-C5-C6-C7
5	E	316	BOG	C2'-C3'-C4'-C5'
3	D	313	LFA	C11-C12-C13-C14
2	E	303	OLC	C5-C6-C7-C8
3	E	312	LFA	C13-C14-C15-C16
3	B	310	LFA	C2-C3-C4-C5
3	B	302	LFA	C16-C17-C18-C19
3	A	319	LFA	C16-C17-C18-C19
2	D	309	OLC	C2-C3-C4-C5
2	C	304	OLC	C3-C4-C5-C6
3	C	315	LFA	C12-C13-C14-C15
3	A	314	LFA	C3-C4-C5-C6
2	C	301	OLC	C3-C4-C5-C6
3	C	303	LFA	C13-C14-C15-C16
2	E	305	OLC	C3-C4-C5-C6
2	D	307	OLC	C21-C22-C24-O25
2	A	303	OLC	C21-C22-C24-O25
2	E	307	OLC	C21-C22-C24-O25
2	D	303	OLC	C21-C22-C24-O25
2	B	306	OLC	C21-C22-C24-O25
2	E	301	OLC	C21-C22-C24-O25
2	B	303	OLC	O20-C21-C22-O23
2	A	318	OLC	C12-C13-C14-C15
2	C	305	OLC	C3-C4-C5-C6
2	C	304	OLC	C4-C5-C6-C7
2	A	302	OLC	C6-C7-C8-C9
2	D	301	OLC	C6-C7-C8-C9
2	A	305	OLC	C10-C11-C12-C13
2	E	304	OLC	C5-C6-C7-C8
3	E	312	LFA	C14-C15-C16-C17
3	D	310	LFA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	C	318	LFA	C2-C3-C4-C5
3	C	318	LFA	C3-C4-C5-C6
3	A	320	LFA	C3-C4-C5-C6
2	E	307	OLC	C2-C3-C4-C5
2	A	305	OLC	C11-C12-C13-C14
2	C	309	OLC	C5-C6-C7-C8
2	D	309	OLC	C13-C14-C15-C16
3	C	315	LFA	C11-C10-C9-C8
3	C	303	LFA	C2-C3-C4-C5
3	E	312	LFA	C9-C10-C11-C12
2	B	303	OLC	C4-C5-C6-C7
2	A	303	OLC	C13-C14-C15-C16
2	A	305	OLC	C13-C14-C15-C16
3	A	314	LFA	C10-C11-C12-C13
5	D	317	BOG	C1'-C2'-C3'-C4'
3	A	319	LFA	C7-C8-C9-C10
3	D	311	LFA	C11-C12-C13-C14
3	D	311	LFA	C14-C15-C16-C17
3	D	313	LFA	C7-C8-C9-C10
3	C	318	LFA	C4-C5-C6-C7
2	D	306	OLC	C2-C3-C4-C5
2	C	308	OLC	C3-C4-C5-C6
3	E	302	LFA	C7-C8-C9-C10
3	A	314	LFA	C4-C5-C6-C7
3	D	314	LFA	C15-C16-C17-C18
2	A	305	OLC	C3-C4-C5-C6
2	D	305	OLC	C5-C6-C7-C8
3	D	310	LFA	C3-C4-C5-C6
2	E	310	OLC	O23-C22-C24-O25
2	B	304	OLC	O23-C22-C24-O25
2	C	306	OLC	O23-C22-C24-O25
2	D	309	OLC	O23-C22-C24-O25
2	C	307	OLC	O23-C22-C24-O25
2	A	308	OLC	O23-C22-C24-O25
3	D	314	LFA	C16-C17-C18-C19
2	B	301	OLC	C10-C11-C12-C13
2	A	317	OLC	C6-C7-C8-C9
2	D	309	OLC	C12-C13-C14-C15
2	C	301	OLC	C4-C5-C6-C7
2	B	306	OLC	O19-C1-O20-C21
3	B	311	LFA	C5-C6-C7-C8
2	C	302	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	B	314	BOG	C1'-C2'-C3'-C4'
3	D	313	LFA	C3-C4-C5-C6
5	A	316	BOG	C1'-C2'-C3'-C4'
2	D	304	OLC	C3-C4-C5-C6
3	C	315	LFA	C10-C11-C12-C13
2	E	310	OLC	C6-C7-C8-C9
2	A	302	OLC	C10-C11-C12-C13
2	B	303	OLC	C10-C11-C12-C13
2	A	301	OLC	C10-C11-C12-C13
2	E	301	OLC	C10-C11-C12-C13
2	B	303	OLC	C1-C2-C3-C4
2	B	303	OLC	C3-C4-C5-C6
3	C	312	LFA	C12-C13-C14-C15
5	E	316	BOG	O1-C1'-C2'-C3'
2	B	301	OLC	O20-C21-C22-C24
2	B	303	OLC	O20-C21-C22-C24
2	E	307	OLC	O20-C21-C22-C24
3	C	310	LFA	C2-C3-C4-C5
2	B	304	OLC	C4-C5-C6-C7
3	C	303	LFA	C7-C8-C9-C10
5	D	317	BOG	C4-C5-C6-O6
3	E	312	LFA	C15-C16-C17-C18
5	E	316	BOG	C1'-C2'-C3'-C4'
3	C	311	LFA	C15-C16-C17-C18
3	B	312	LFA	C15-C16-C17-C18
2	B	303	OLC	C14-C15-C16-C17
3	A	320	LFA	C4-C5-C6-C7
2	E	305	OLC	C4-C5-C6-C7
3	B	302	LFA	C11-C10-C9-C8
2	A	305	OLC	C6-C7-C8-C9
2	D	306	OLC	C10-C11-C12-C13
2	C	307	OLC	C6-C7-C8-C9
2	C	308	OLC	C4-C5-C6-C7
3	A	314	LFA	C7-C8-C9-C10
2	A	317	OLC	C13-C14-C15-C16
3	D	311	LFA	C13-C14-C15-C16
3	E	302	LFA	C11-C10-C9-C8
3	C	303	LFA	C3-C4-C5-C6
3	D	312	LFA	C4-C5-C6-C7
2	A	302	OLC	C4-C5-C6-C7
2	A	303	OLC	C2-C3-C4-C5
2	E	301	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	D	317	BOG	O5-C5-C6-O6
3	C	312	LFA	C15-C16-C17-C18
2	E	301	OLC	C5-C6-C7-C8
5	C	317	BOG	C1'-C2'-C3'-C4'
3	A	310	LFA	C4-C5-C6-C7
2	E	310	OLC	C4-C5-C6-C7
3	C	312	LFA	C13-C14-C15-C16
2	A	317	OLC	C3-C4-C5-C6
2	C	306	OLC	C6-C7-C8-C9
2	D	307	OLC	C2-C3-C4-C5
3	D	310	LFA	C4-C5-C6-C7
2	E	301	OLC	C14-C15-C16-C17
2	E	309	OLC	C1-C2-C3-C4
2	B	303	OLC	C13-C14-C15-C16
3	D	311	LFA	C4-C5-C6-C7
2	C	309	OLC	C6-C7-C8-C9
2	A	317	OLC	C11-C12-C13-C14
3	D	310	LFA	C11-C10-C9-C8
3	D	313	LFA	C13-C14-C15-C16
2	D	303	OLC	O23-C22-C24-O25
2	B	305	OLC	O23-C22-C24-O25
2	C	302	OLC	O23-C22-C24-O25
2	D	309	OLC	C10-C11-C12-C13
2	C	304	OLC	C10-C11-C12-C13
2	B	306	OLC	C10-C11-C12-C13
2	A	305	OLC	C2-C3-C4-C5
2	C	307	OLC	C2-C3-C4-C5
3	C	303	LFA	C12-C13-C14-C15
3	C	311	LFA	C17-C18-C19-C20
3	D	313	LFA	C14-C15-C16-C17
3	D	311	LFA	C1-C2-C3-C4
3	D	311	LFA	C10-C11-C12-C13
3	D	311	LFA	C12-C13-C14-C15
2	A	308	OLC	C1-C2-C3-C4
3	A	319	LFA	C13-C14-C15-C16
3	D	311	LFA	C3-C4-C5-C6
2	E	310	OLC	C5-C6-C7-C8
3	B	311	LFA	C7-C8-C9-C10
2	C	305	OLC	C1-C2-C3-C4
2	B	308	OLC	C4-C5-C6-C7
2	A	303	OLC	C14-C15-C16-C17
5	C	317	BOG	C5'-C6'-C7'-C8'

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Mol	Chain	Res	Type	Atoms
3	C	312	LFA	C9-C10-C11-C12
2	E	307	OLC	C3-C4-C5-C6
5	B	314	BOG	C5'-C6'-C7'-C8'
2	D	309	OLC	C4-C5-C6-C7
2	B	301	OLC	C5-C6-C7-C8
2	D	304	OLC	C15-C16-C17-C18
2	C	301	OLC	C2-C1-O20-C21
2	A	307	OLC	C6-C7-C8-C9
3	A	314	LFA	C11-C12-C13-C14
2	C	307	OLC	C4-C5-C6-C7
3	D	313	LFA	C6-C7-C8-C9
3	C	303	LFA	C16-C17-C18-C19
2	E	310	OLC	C3-C4-C5-C6
5	B	314	BOG	C3'-C4'-C5'-C6'
2	A	317	OLC	C14-C15-C16-C17
5	A	316	BOG	C5'-C6'-C7'-C8'
3	B	302	LFA	C6-C7-C8-C9
3	D	312	LFA	C5-C6-C7-C8
2	A	306	OLC	C5-C6-C7-C8
3	C	311	LFA	C13-C14-C15-C16
2	B	304	OLC	C1-C2-C3-C4
3	A	314	LFA	C5-C6-C7-C8
2	A	302	OLC	O20-C21-C22-C24
2	D	304	OLC	O20-C21-C22-C24
2	B	306	OLC	O20-C21-C22-C24
2	B	301	OLC	O20-C21-C22-O23
2	E	309	OLC	C4-C5-C6-C7
3	A	319	LFA	C6-C7-C8-C9
3	D	314	LFA	C14-C15-C16-C17
2	D	302	OLC	C5-C6-C7-C8
2	B	303	OLC	O23-C22-C24-O25
2	A	303	OLC	O23-C22-C24-O25
2	B	306	OLC	O23-C22-C24-O25
3	C	312	LFA	C14-C15-C16-C17
2	C	307	OLC	C11-C12-C13-C14
2	A	308	OLC	C2-C1-O20-C21
3	C	310	LFA	C4-C5-C6-C7
2	B	307	OLC	C5-C6-C7-C8
2	D	308	OLC	C2-C3-C4-C5
2	C	301	OLC	O19-C1-O20-C21
3	E	311	LFA	C16-C17-C18-C19
2	A	302	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	D	302	OLC	C6-C7-C8-C9
2	A	303	OLC	C15-C16-C17-C18
2	C	307	OLC	C1-C2-C3-C4
2	A	305	OLC	C12-C13-C14-C15
3	E	314	LFA	C17-C18-C19-C20
2	D	304	OLC	C13-C14-C15-C16
2	A	301	OLC	C11-C12-C13-C14
2	C	304	OLC	C12-C13-C14-C15
3	A	310	LFA	C1-C2-C3-C4
2	D	309	OLC	C1-C2-C3-C4
2	A	303	OLC	O20-C21-C22-C24
2	D	301	OLC	C7-C8-C9-C10
2	D	301	OLC	C2-C3-C4-C5
3	C	303	LFA	C15-C16-C17-C18
3	A	309	LFA	C15-C16-C17-C18
2	B	306	OLC	C5-C6-C7-C8
3	A	314	LFA	C13-C14-C15-C16
3	C	312	LFA	C4-C5-C6-C7
3	B	302	LFA	C9-C10-C11-C12
2	B	306	OLC	C4-C5-C6-C7
2	A	308	OLC	O19-C1-O20-C21
2	E	301	OLC	O23-C22-C24-O25
2	C	301	OLC	C6-C7-C8-C9
3	A	311	LFA	C15-C16-C17-C18
2	D	304	OLC	C2-C3-C4-C5
2	E	301	OLC	C3-C4-C5-C6
5	E	316	BOG	C5'-C6'-C7'-C8'
2	D	304	OLC	O20-C21-C22-O23
3	A	319	LFA	C11-C12-C13-C14
2	C	306	OLC	C5-C6-C7-C8
2	A	317	OLC	C12-C13-C14-C15
3	C	312	LFA	C10-C11-C12-C13
2	E	304	OLC	C13-C14-C15-C16
2	D	309	OLC	C5-C6-C7-C8
2	D	303	OLC	C1-C2-C3-C4
3	C	312	LFA	C11-C10-C9-C8
2	D	302	OLC	C4-C5-C6-C7
2	B	304	OLC	C3-C4-C5-C6
2	C	304	OLC	C5-C6-C7-C8
3	C	303	LFA	C1-C2-C3-C4
3	D	310	LFA	C17-C18-C19-C20
3	C	315	LFA	C4-C5-C6-C7

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

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Mol	Chain	Res	Type	Atoms
2	B	304	OLC	C10-C11-C12-C13
3	C	303	LFA	C4-C5-C6-C7
2	C	304	OLC	C7-C8-C9-C10
2	C	308	OLC	C6-C7-C8-C9
2	D	303	OLC	C2-C3-C4-C5
3	A	319	LFA	C12-C13-C14-C15
3	C	312	LFA	C6-C7-C8-C9
3	D	310	LFA	C16-C17-C18-C19
3	E	302	LFA	C9-C10-C11-C12
2	E	306	OLC	C5-C6-C7-C8
3	C	318	LFA	C6-C7-C8-C9
3	C	303	LFA	C14-C15-C16-C17
3	A	314	LFA	C9-C10-C11-C12
2	A	304	OLC	O20-C21-C22-C24
2	E	301	OLC	C13-C14-C15-C16
2	A	303	OLC	C9-C10-C11-C12
5	A	316	BOG	C4-C5-C6-O6
2	E	304	OLC	C12-C13-C14-C15
3	D	313	LFA	C2-C3-C4-C5
3	D	311	LFA	C5-C6-C7-C8
2	A	318	OLC	C10-C11-C12-C13
2	B	303	OLC	C7-C8-C9-C10
3	A	319	LFA	C14-C15-C16-C17
3	C	315	LFA	C3-C4-C5-C6
3	C	312	LFA	C3-C4-C5-C6
3	A	319	LFA	C11-C10-C9-C8
3	A	309	LFA	C17-C18-C19-C20
2	D	306	OLC	C7-C8-C9-C10
2	A	306	OLC	C21-C22-C24-O25
3	D	310	LFA	C11-C12-C13-C14
2	C	305	OLC	C7-C8-C9-C10
3	E	311	LFA	C17-C18-C19-C20
2	B	304	OLC	C11-C12-C13-C14
2	C	306	OLC	C4-C5-C6-C7
2	A	303	OLC	C5-C6-C7-C8
3	A	320	LFA	C2-C3-C4-C5
2	C	307	OLC	C3-C4-C5-C6
2	E	304	OLC	C11-C12-C13-C14
2	A	317	OLC	C5-C6-C7-C8
2	A	302	OLC	C9-C10-C11-C12
2	C	304	OLC	C9-C10-C11-C12
2	E	301	OLC	C7-C8-C9-C10

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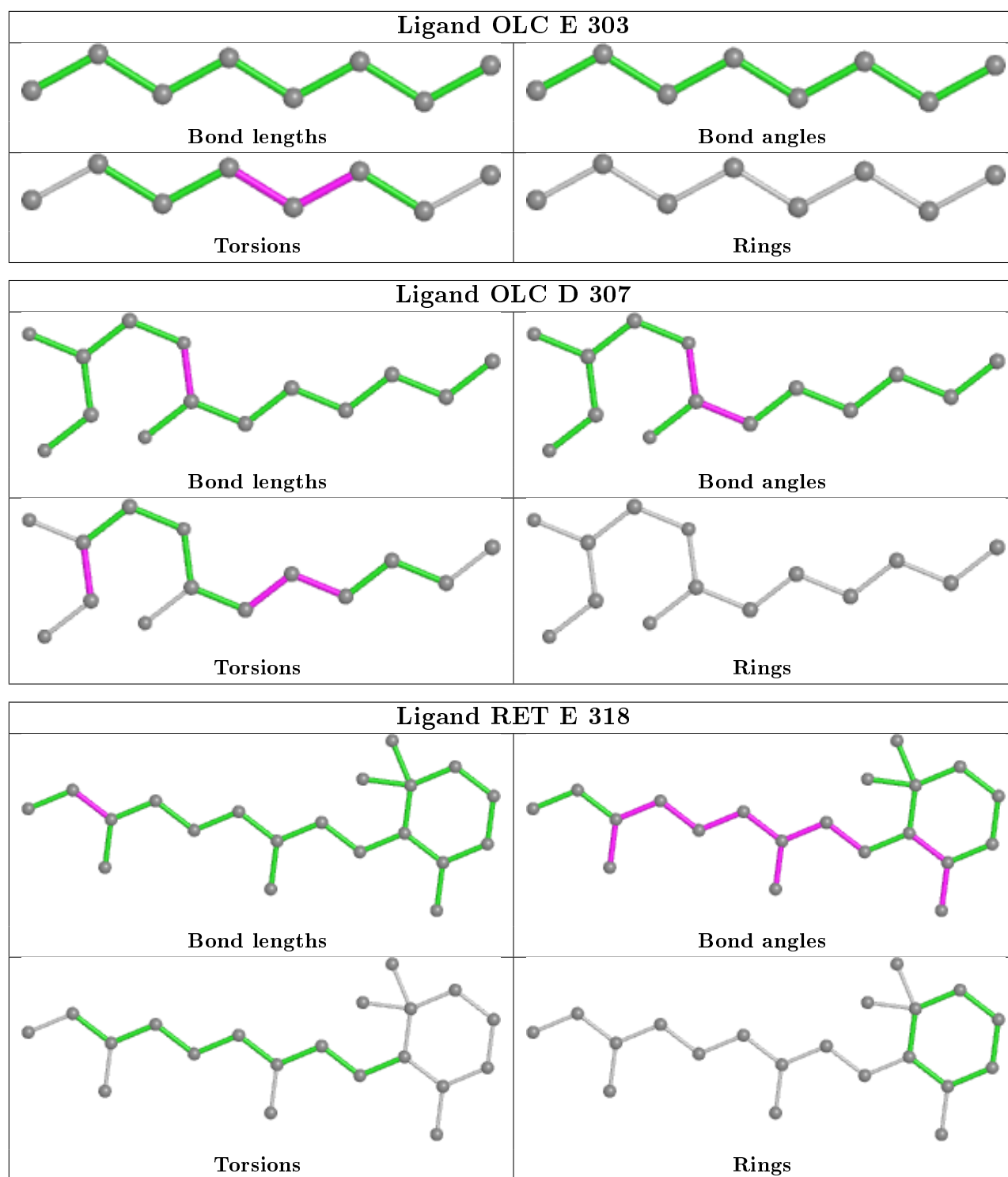
Mol	Chain	Res	Type	Atoms
2	B	303	OLC	C15-C16-C17-C18
2	E	301	OLC	C15-C16-C17-C18
2	A	318	OLC	C9-C10-C11-C12
2	E	309	OLC	C7-C8-C9-C10
2	B	306	OLC	C7-C8-C9-C10
2	B	306	OLC	O20-C21-C22-O23
2	A	318	OLC	C7-C8-C9-C10
2	E	304	OLC	C7-C8-C9-C10
5	A	316	BOG	O5-C5-C6-O6
3	E	302	LFA	C5-C6-C7-C8
2	E	307	OLC	C1-C2-C3-C4
2	A	303	OLC	O20-C1-C2-C3
5	D	317	BOG	C5'-C6'-C7'-C8'
2	A	303	OLC	C12-C13-C14-C15
3	E	302	LFA	C4-C5-C6-C7
2	E	304	OLC	C9-C10-C11-C12
2	A	301	OLC	C9-C10-C11-C12
2	B	301	OLC	C7-C8-C9-C10
2	A	303	OLC	C7-C8-C9-C10
2	B	304	OLC	C7-C8-C9-C10
5	A	316	BOG	C3'-C4'-C5'-C6'
3	C	312	LFA	C7-C8-C9-C10
3	B	311	LFA	C1-C2-C3-C4
2	D	306	OLC	C4-C5-C6-C7
3	A	310	LFA	C5-C6-C7-C8
3	A	319	LFA	C15-C16-C17-C18
2	A	302	OLC	O20-C21-C22-O23
2	B	305	OLC	C9-C10-C11-C12
2	E	301	OLC	O20-C1-C2-C3
3	B	302	LFA	C7-C8-C9-C10
3	D	313	LFA	C11-C10-C9-C8
3	A	311	LFA	C17-C18-C19-C20
3	A	319	LFA	C10-C11-C12-C13
2	B	303	OLC	C9-C10-C11-C12
3	B	309	LFA	C15-C16-C17-C18
3	A	314	LFA	C11-C10-C9-C8
2	E	301	OLC	O19-C1-C2-C3
2	D	305	OLC	O20-C21-C22-O23
3	B	311	LFA	C2-C3-C4-C5
2	A	303	OLC	O19-C1-C2-C3
2	C	301	OLC	C9-C10-C11-C12

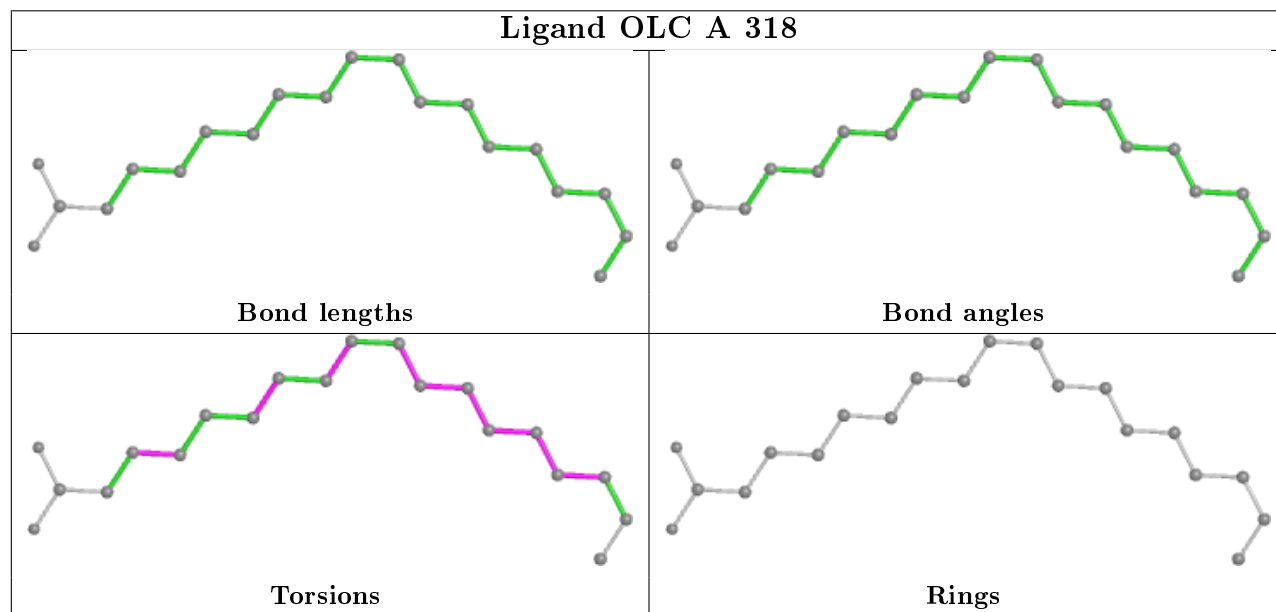
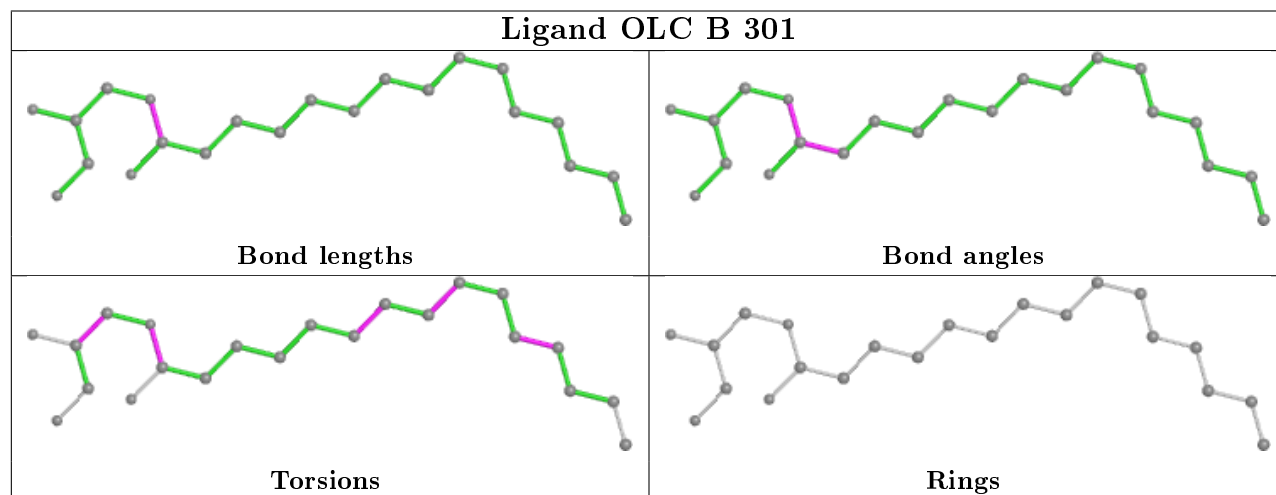
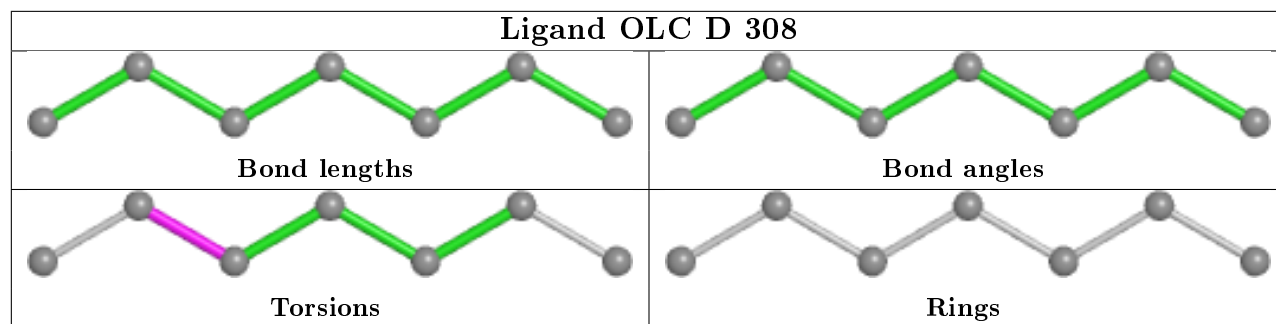
There are no ring outliers.

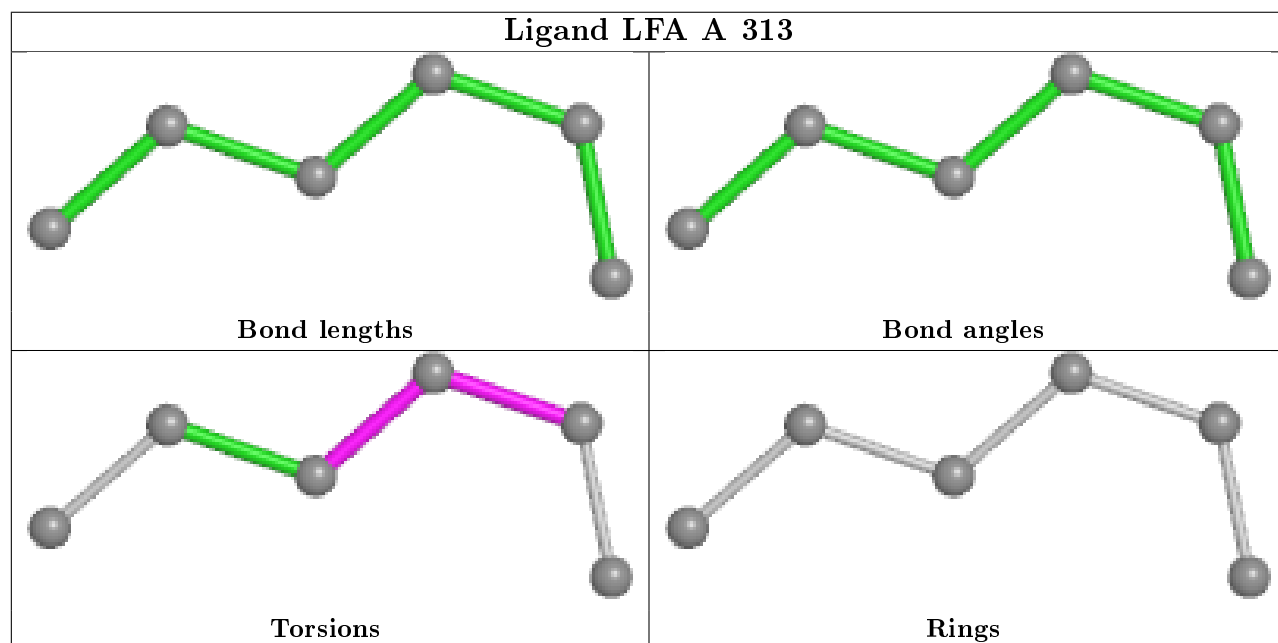
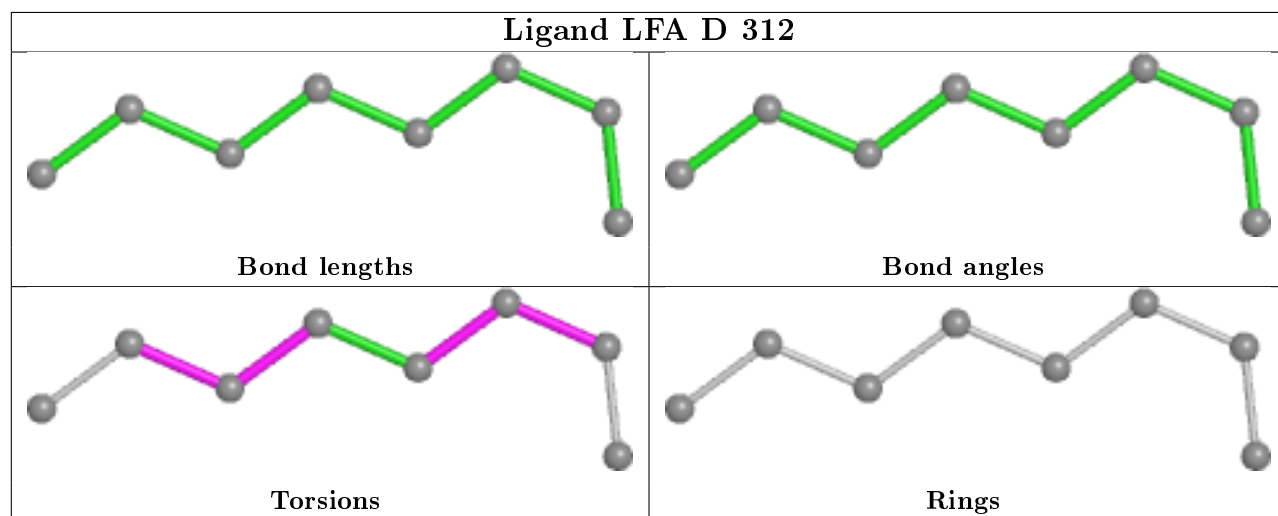
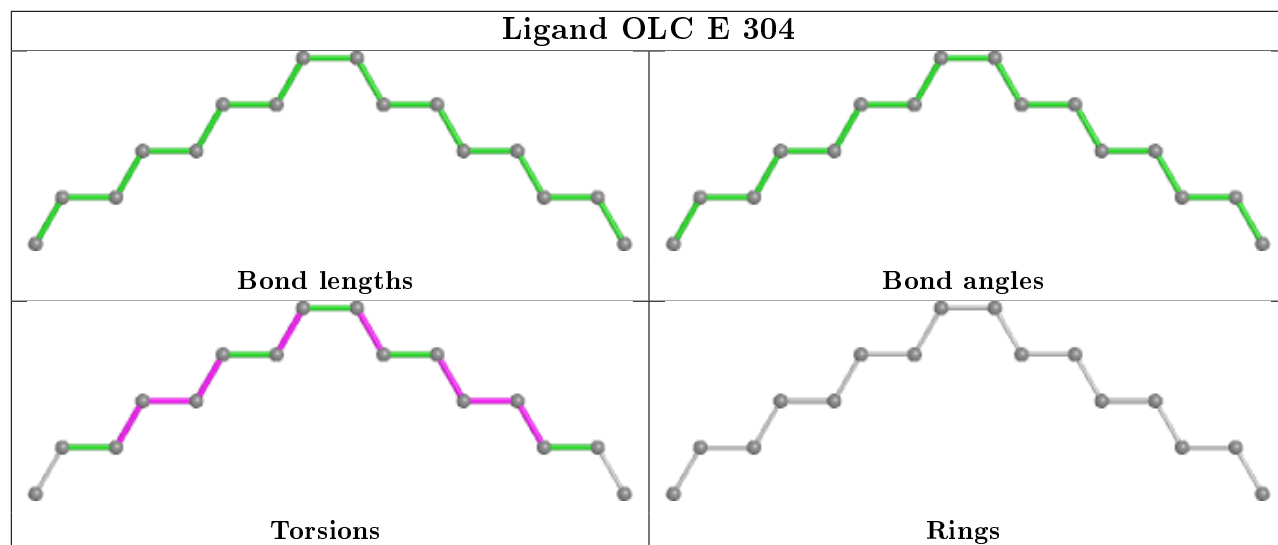
29 monomers are involved in 56 short contacts:

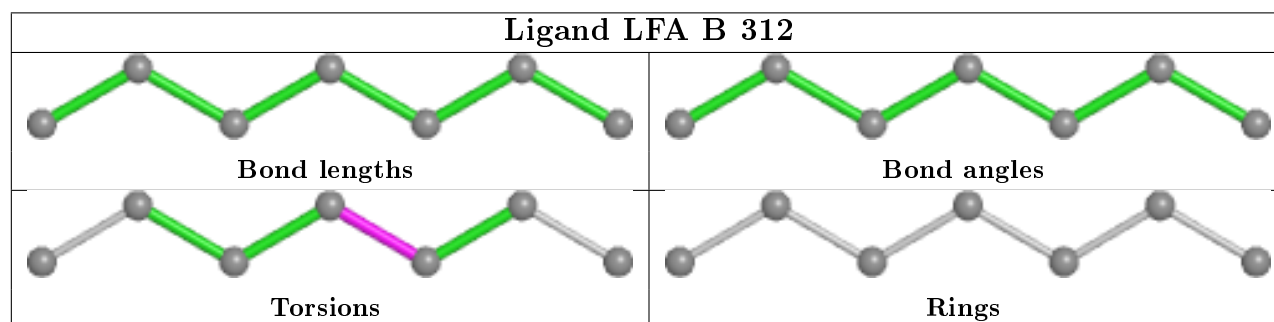
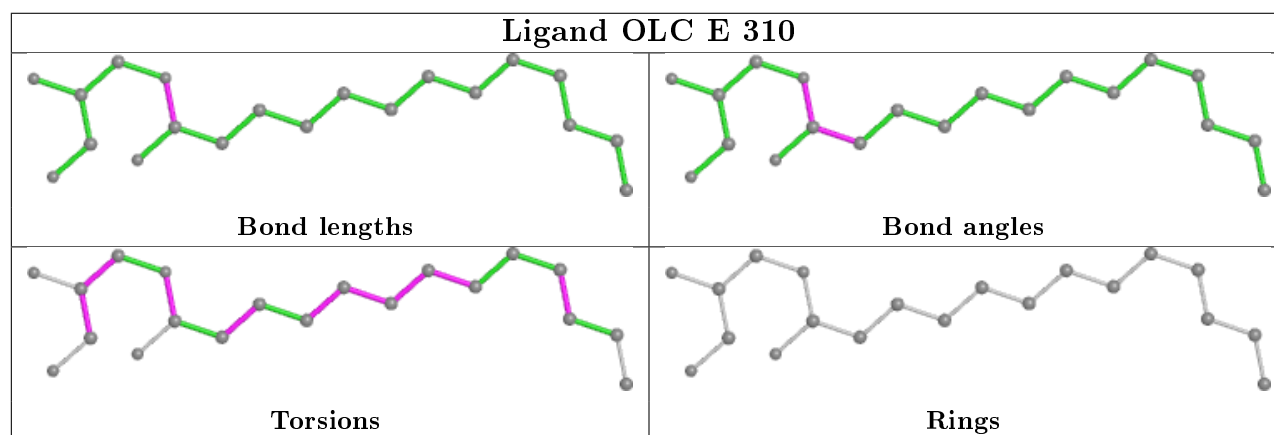
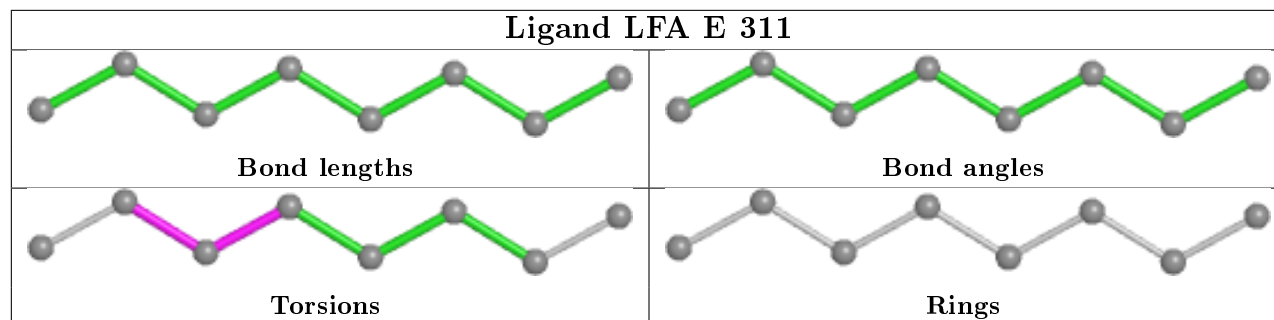
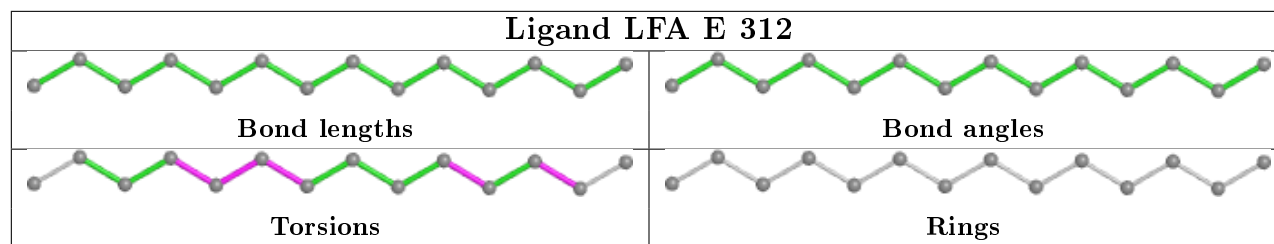
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	318	RET	6	0
2	B	301	OLC	2	0
2	E	304	OLC	1	0
3	E	312	LFA	1	0
2	E	310	OLC	1	0
3	E	313	LFA	1	0
6	C	319	RET	5	0
3	B	309	LFA	2	0
6	D	318	RET	5	0
5	D	317	BOG	1	0
2	A	303	OLC	2	0
3	C	312	LFA	1	0
2	D	301	OLC	1	0
3	C	310	LFA	4	0
2	C	306	OLC	1	0
2	C	309	OLC	1	0
2	D	309	OLC	1	0
6	B	315	RET	4	0
2	C	304	OLC	2	0
5	B	314	BOG	3	0
5	A	316	BOG	2	0
5	C	317	BOG	2	0
5	E	316	BOG	4	0
2	C	308	OLC	2	0
2	C	301	OLC	1	0
2	D	302	OLC	1	0
6	A	321	RET	4	0
3	D	313	LFA	1	0
3	C	303	LFA	1	0

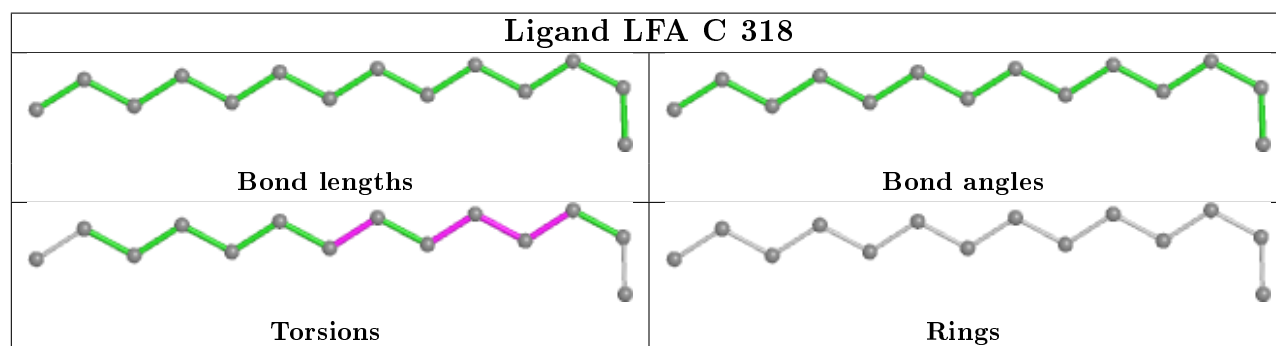
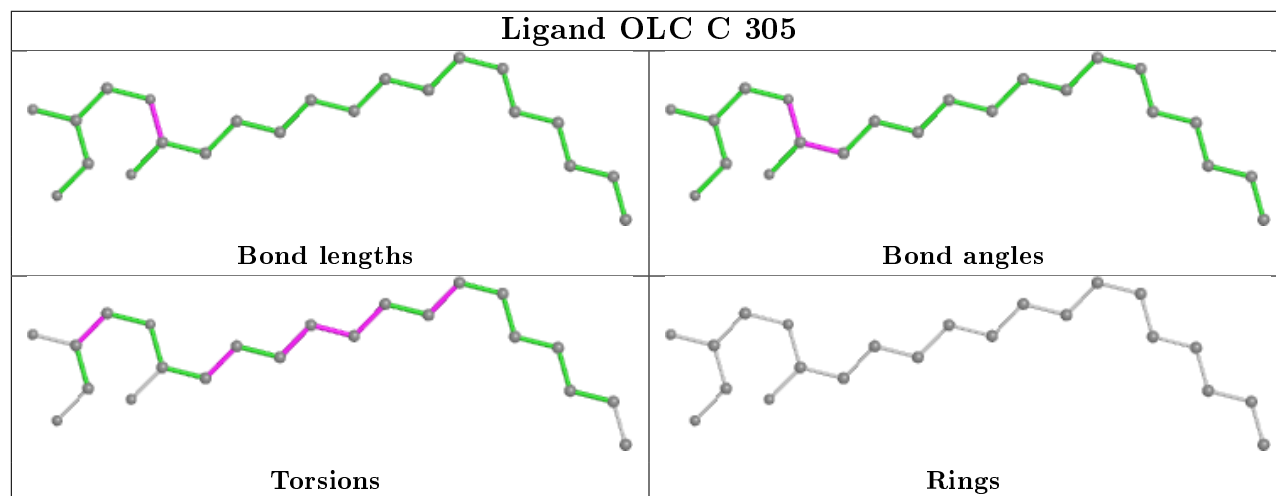
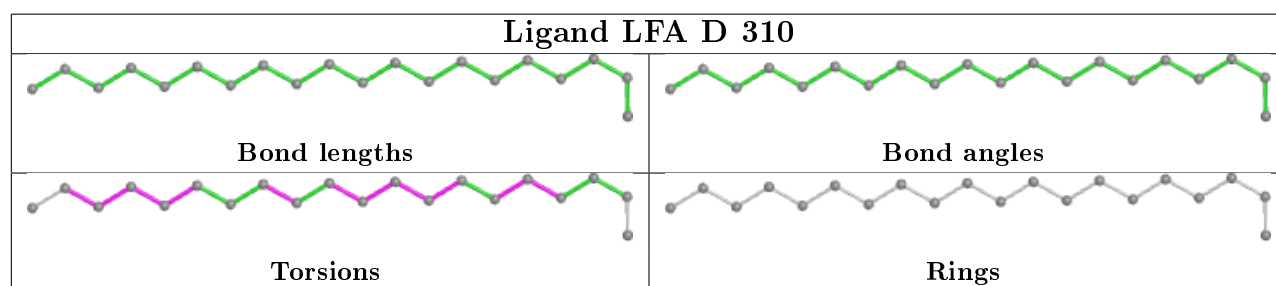
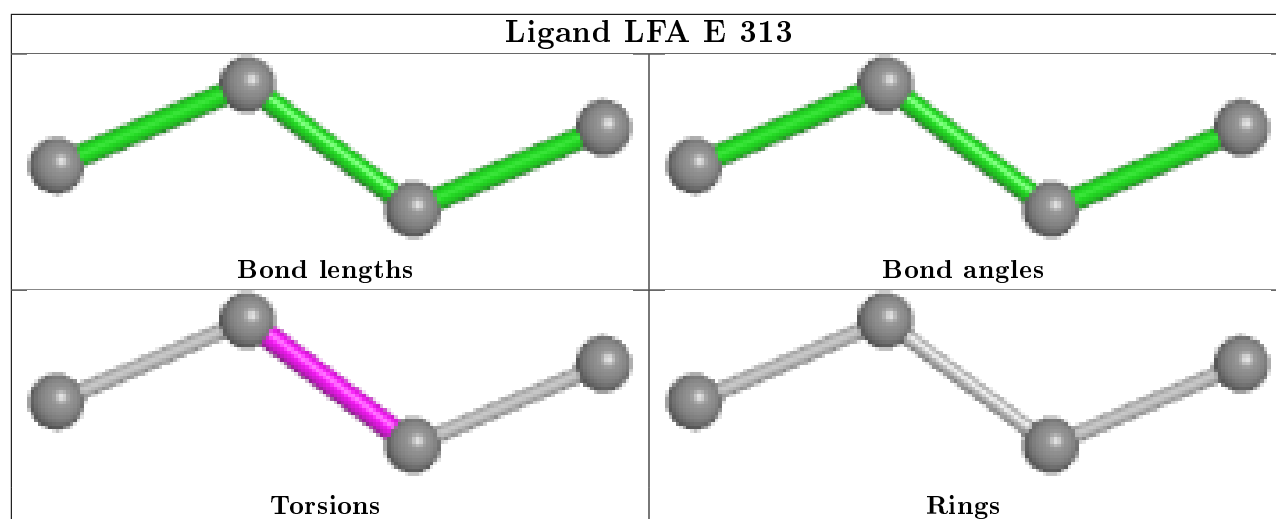
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

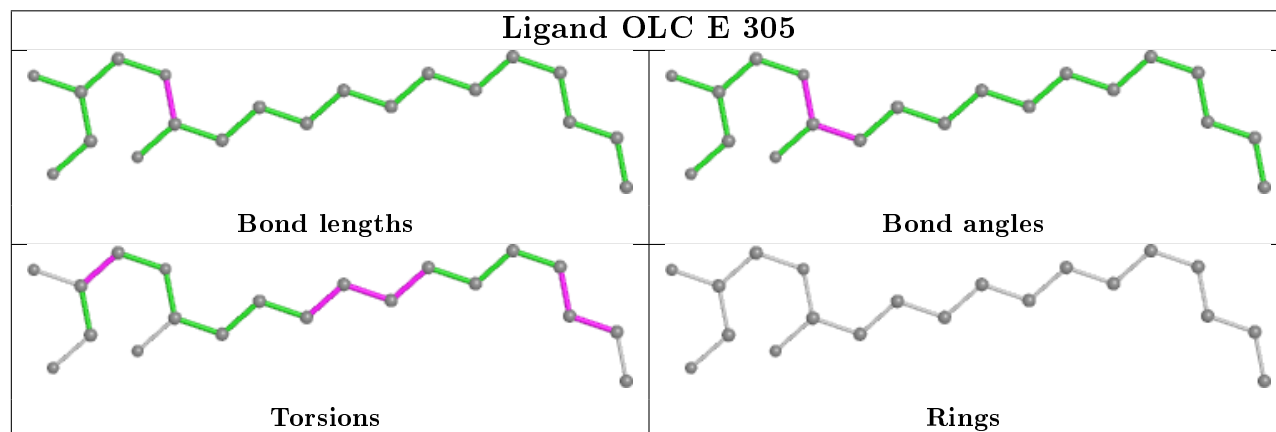
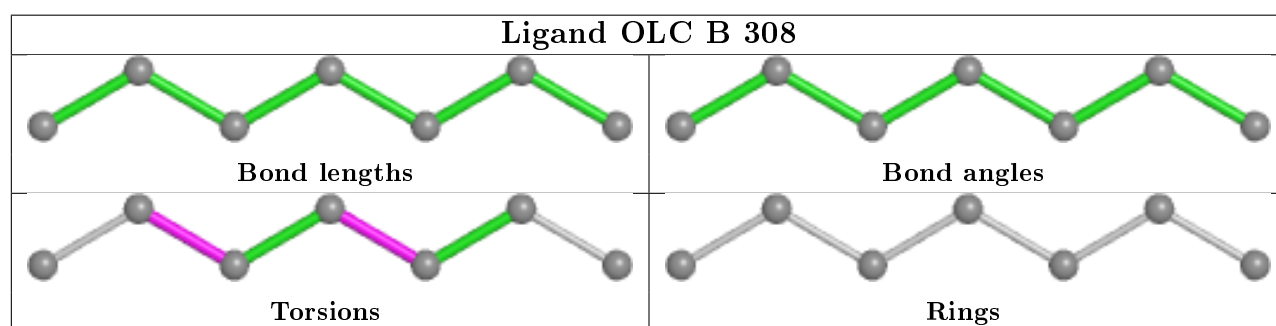
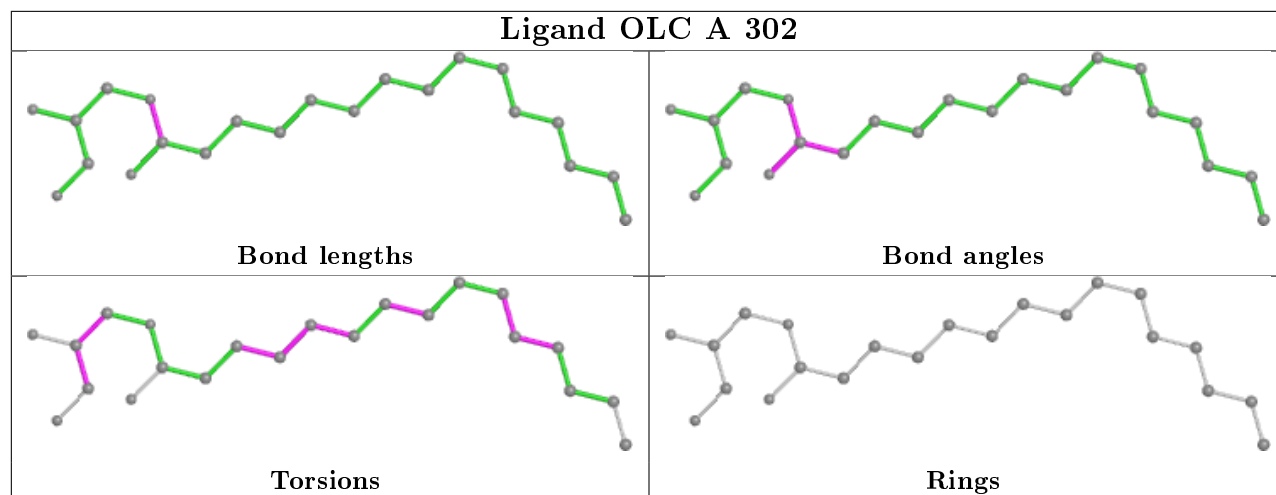


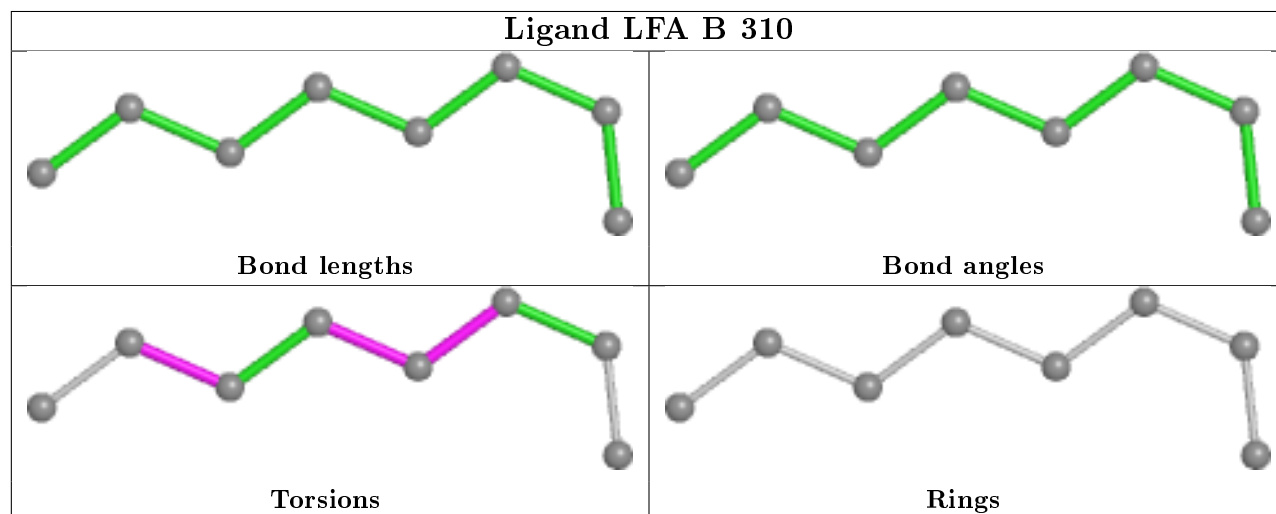
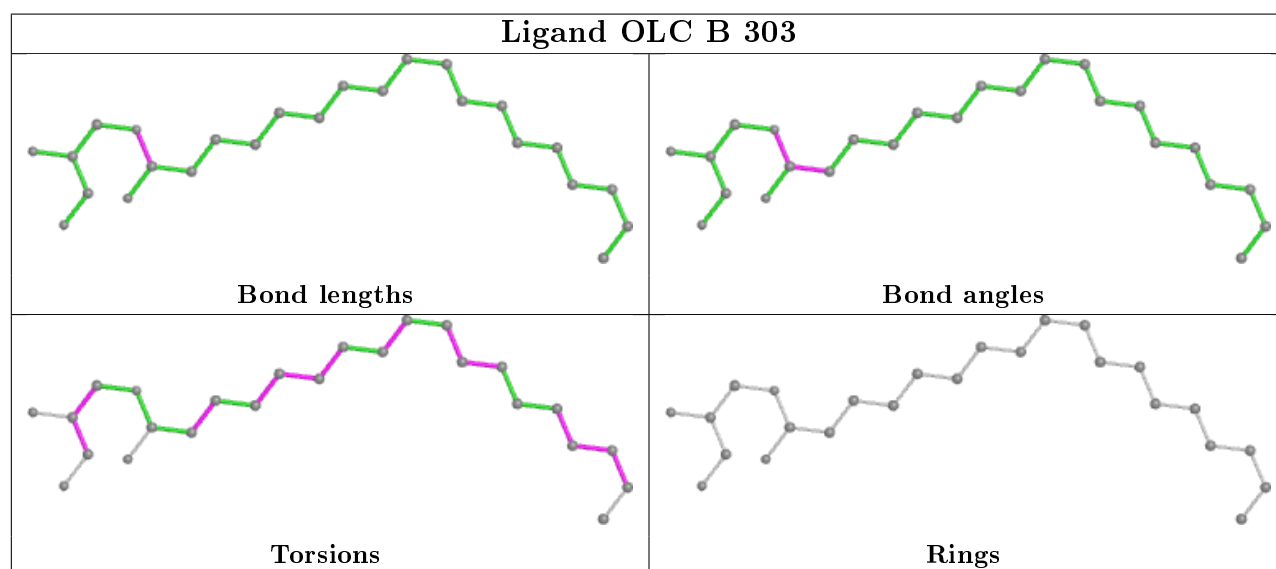
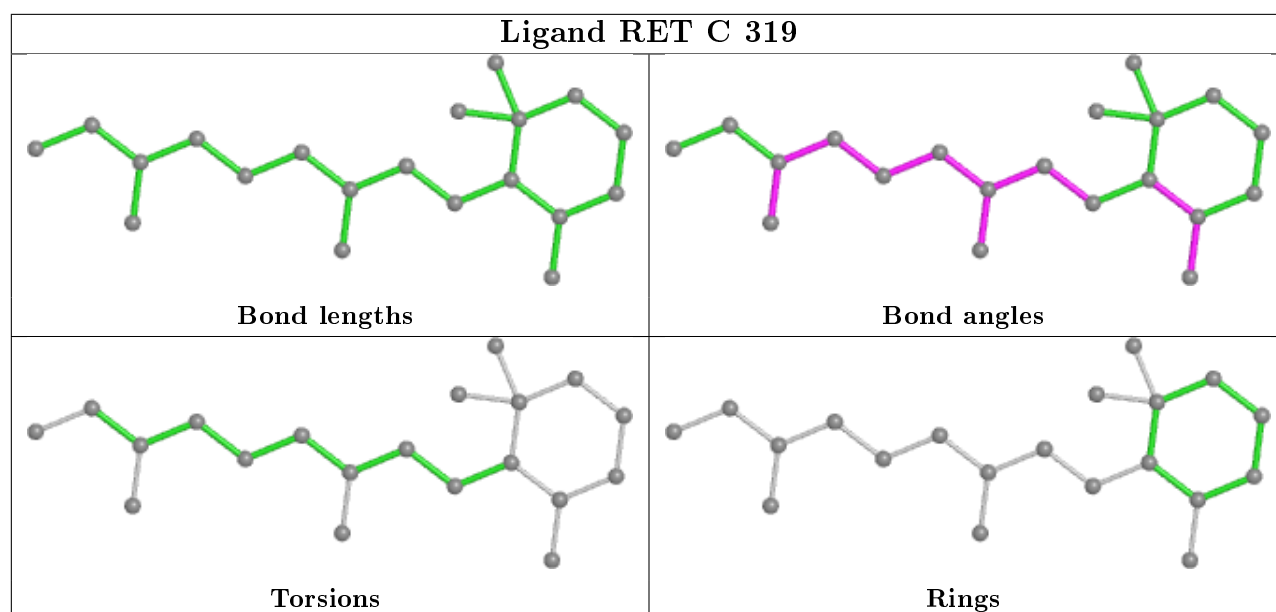


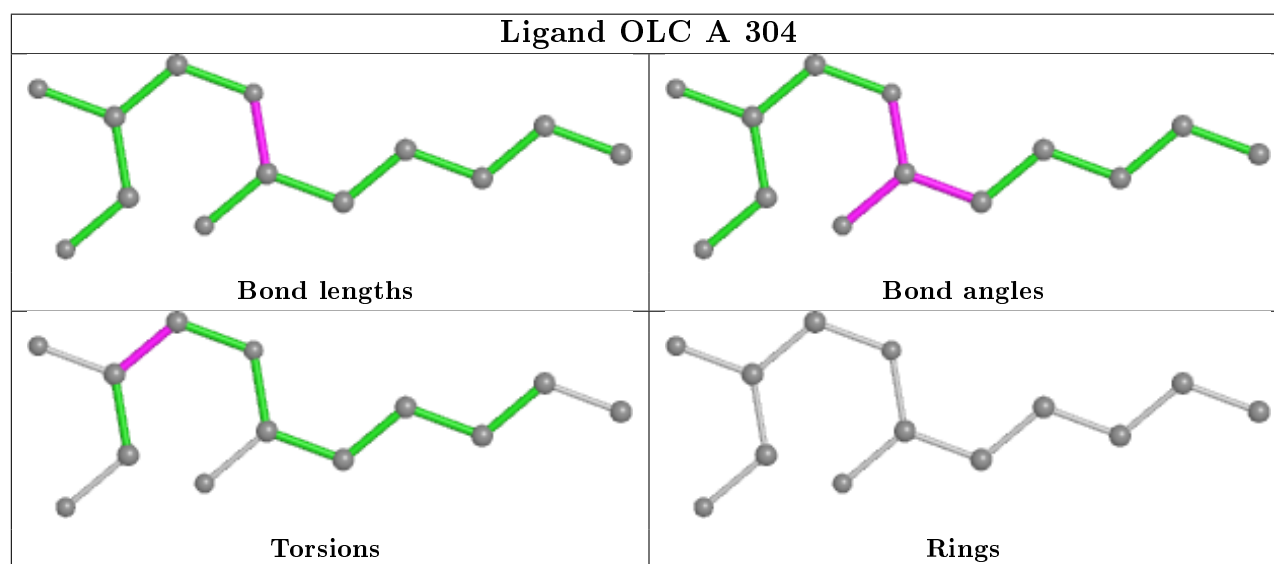
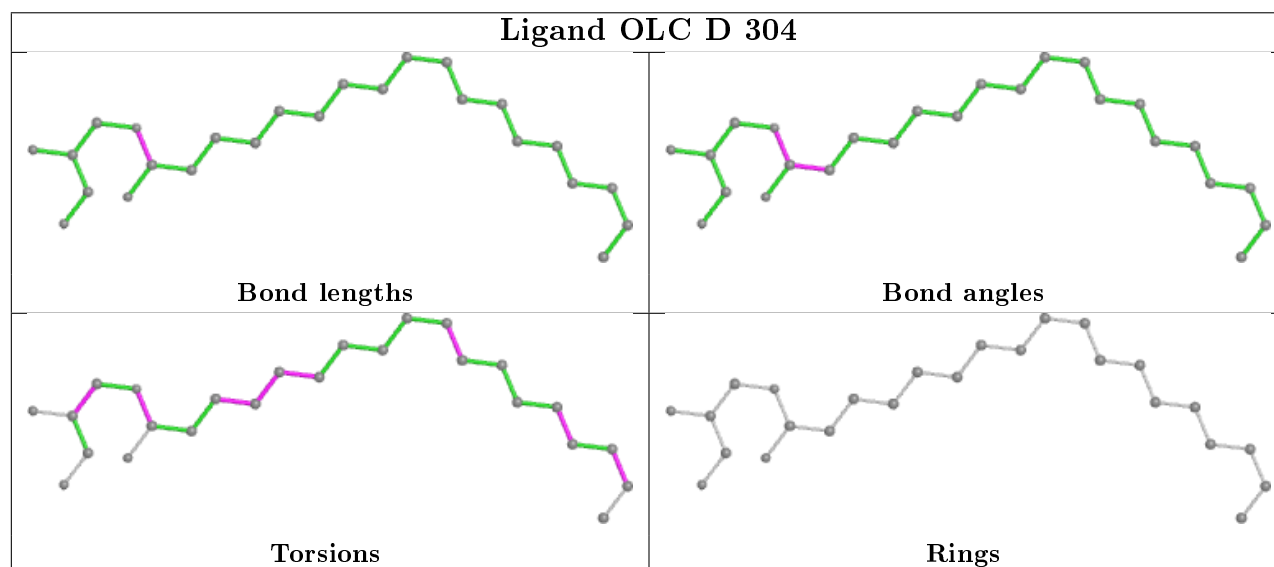
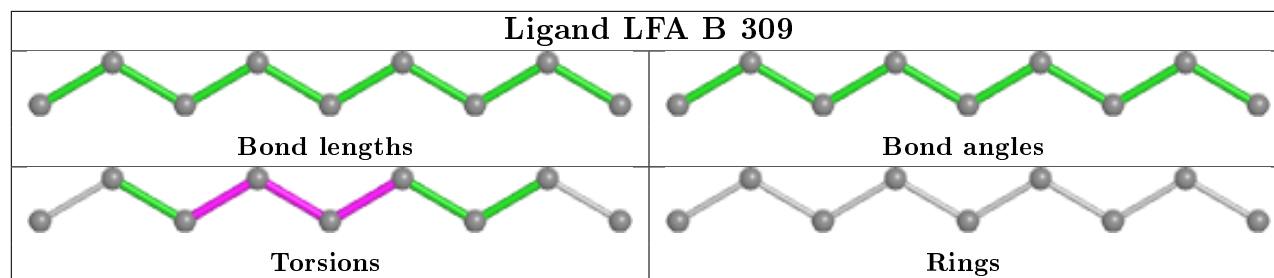


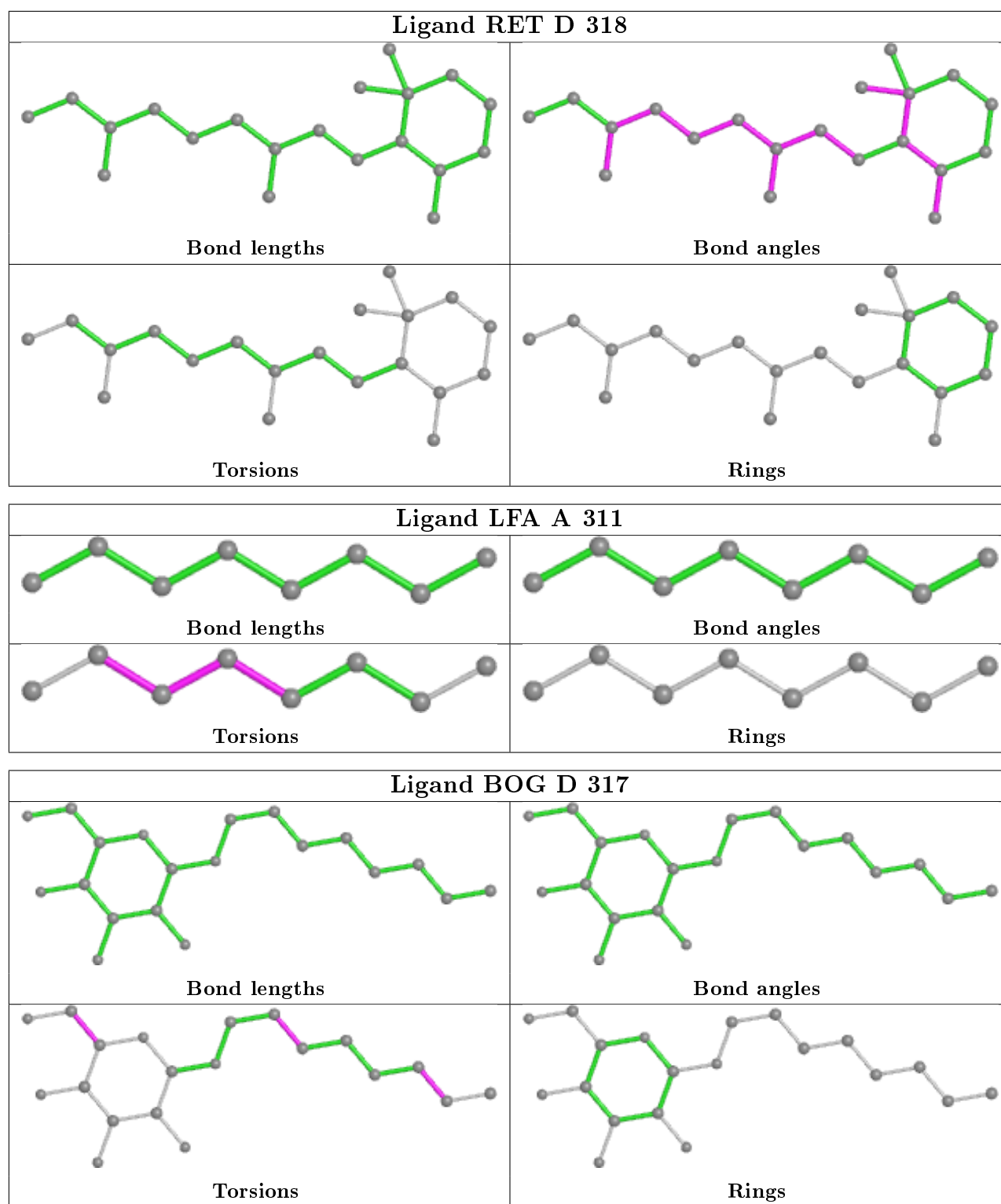


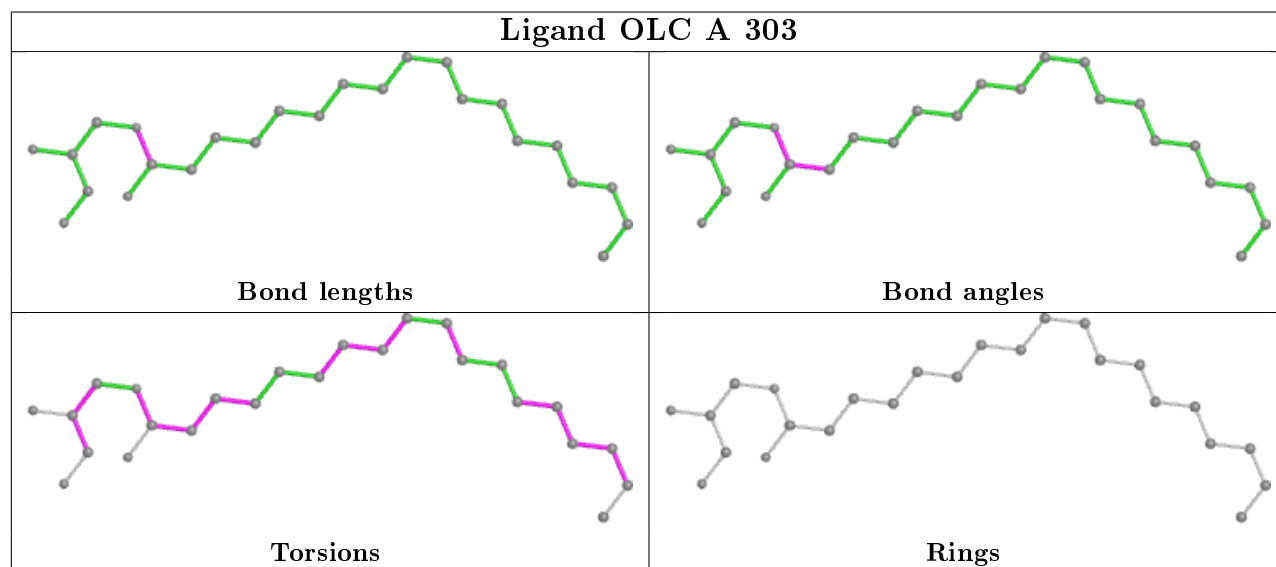
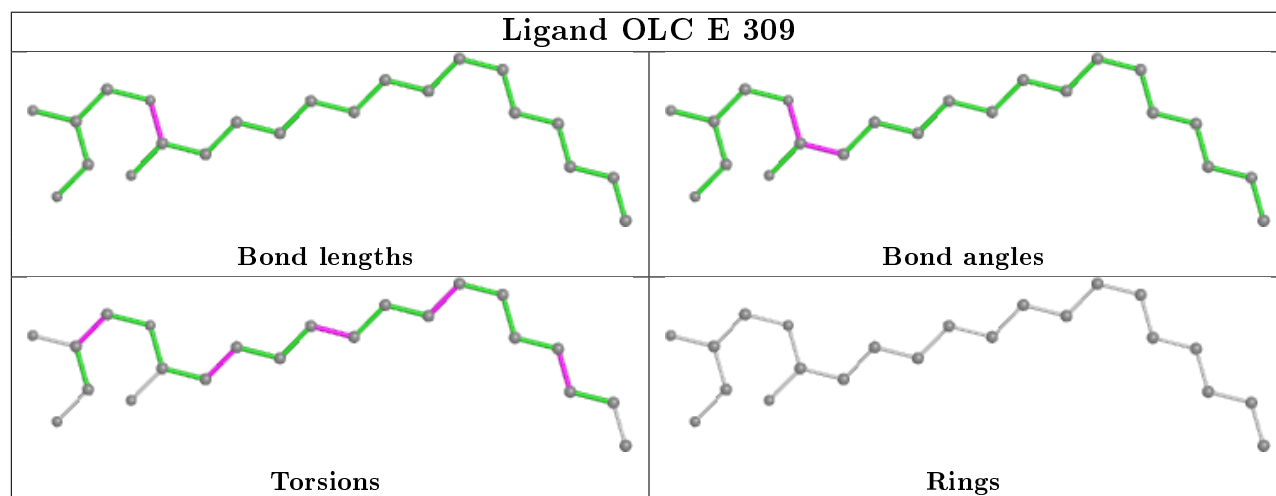
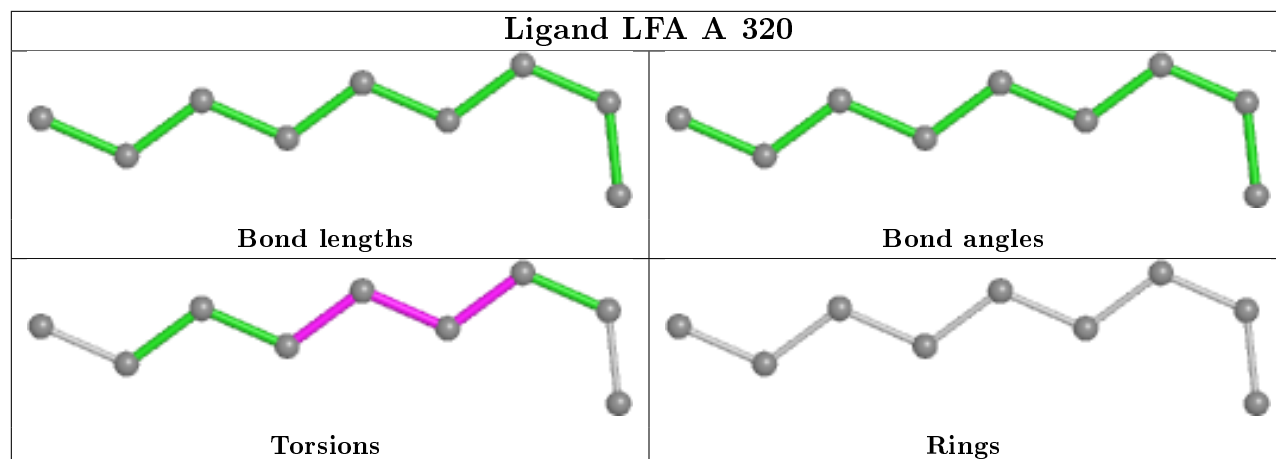


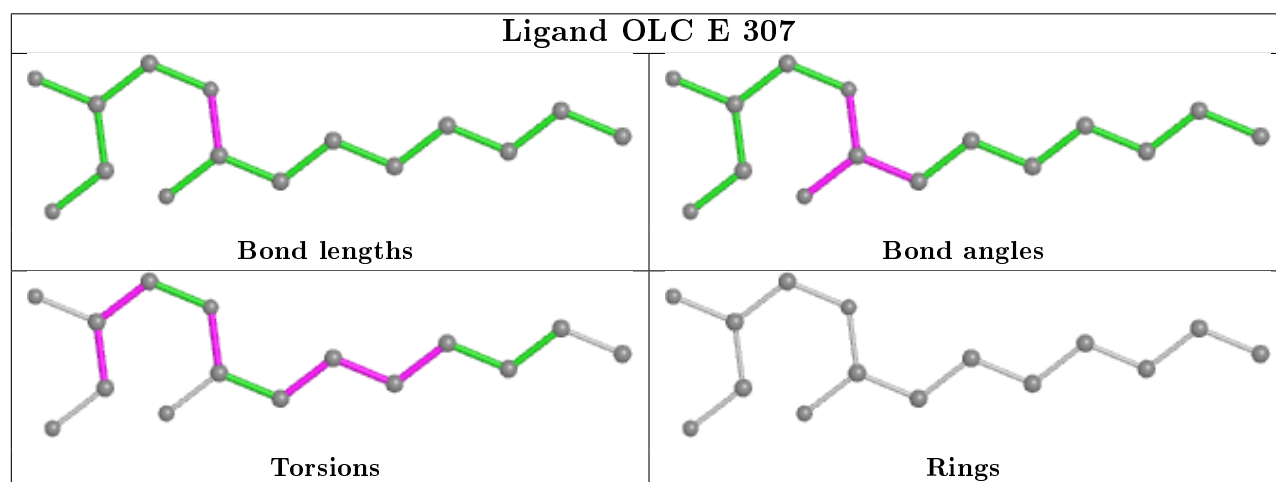
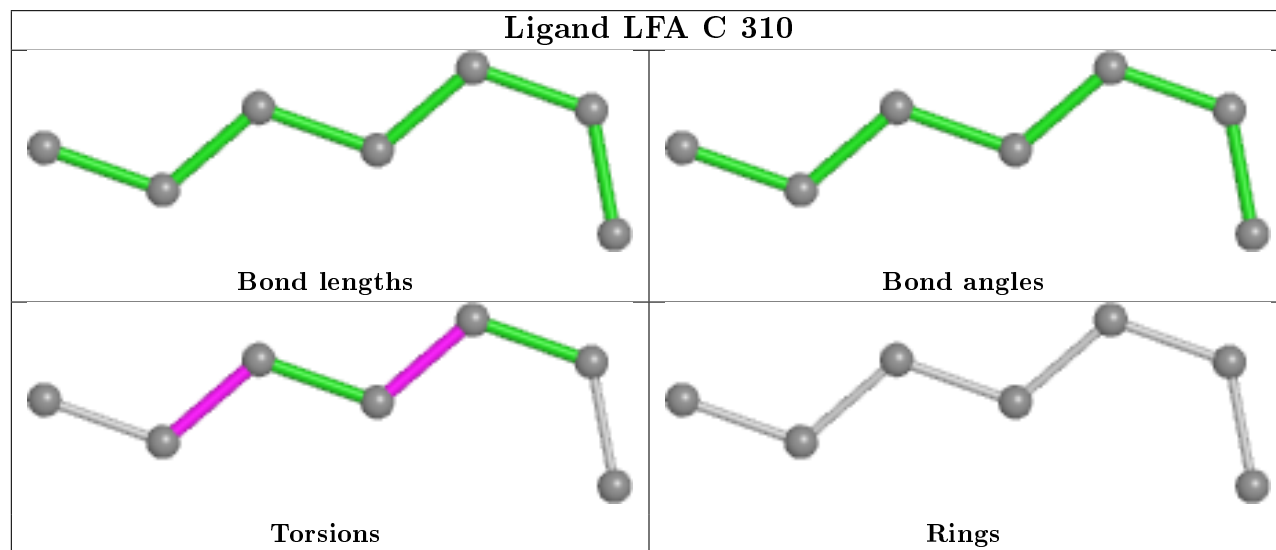
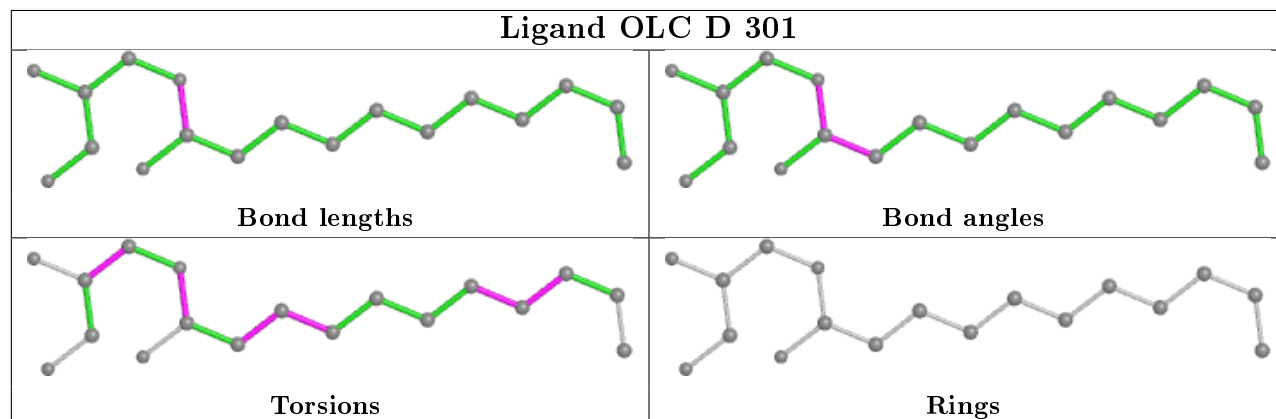
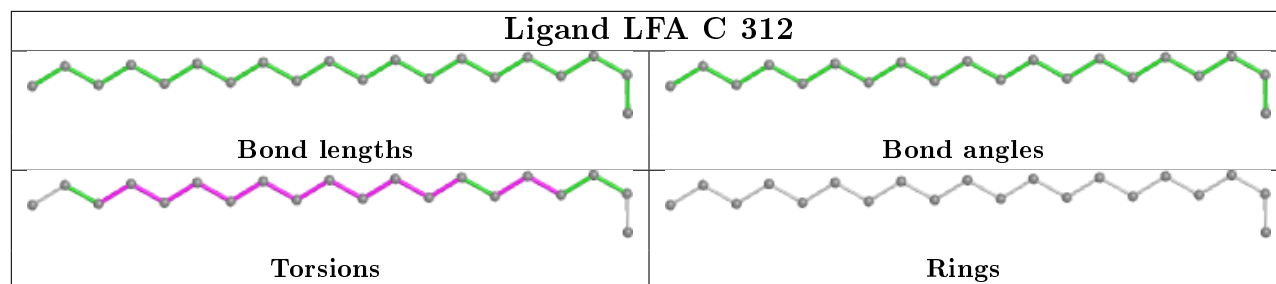


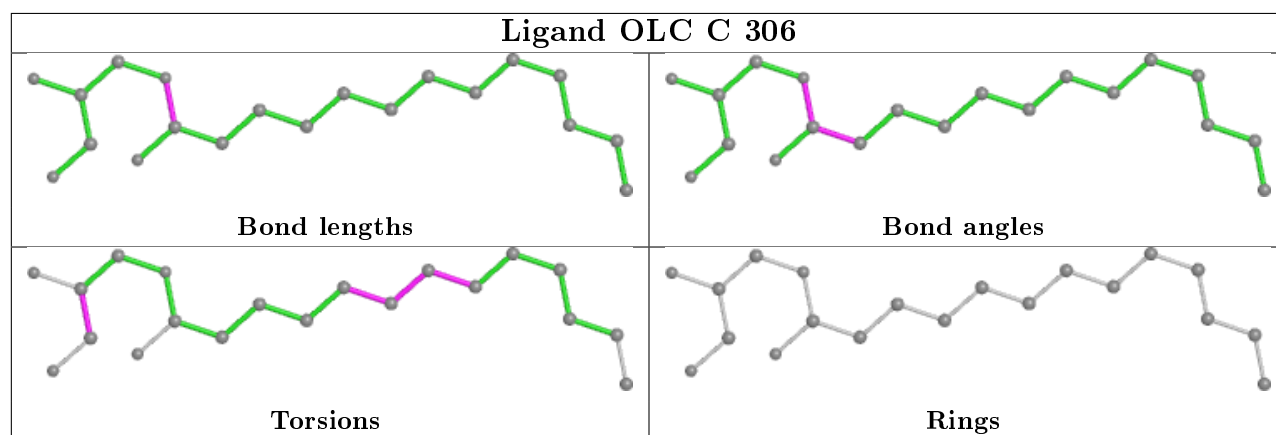
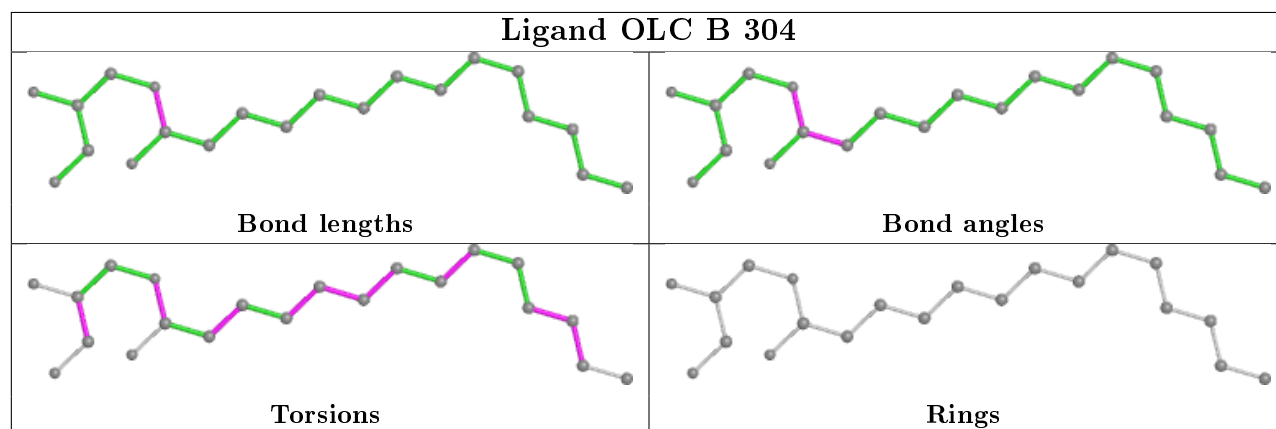
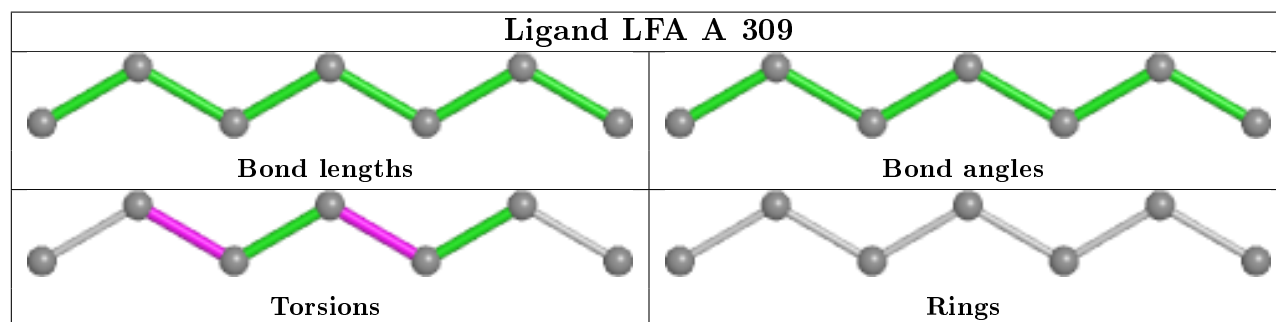
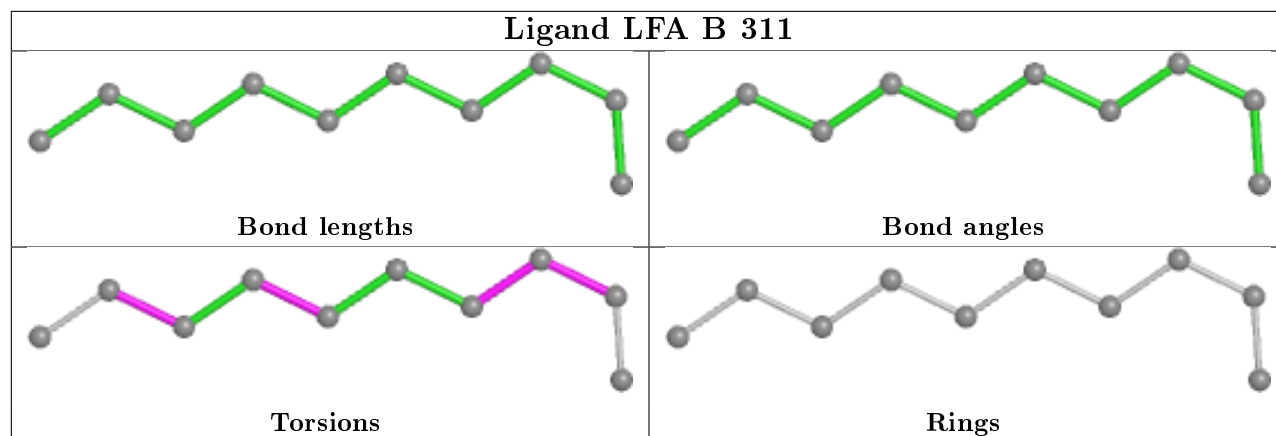


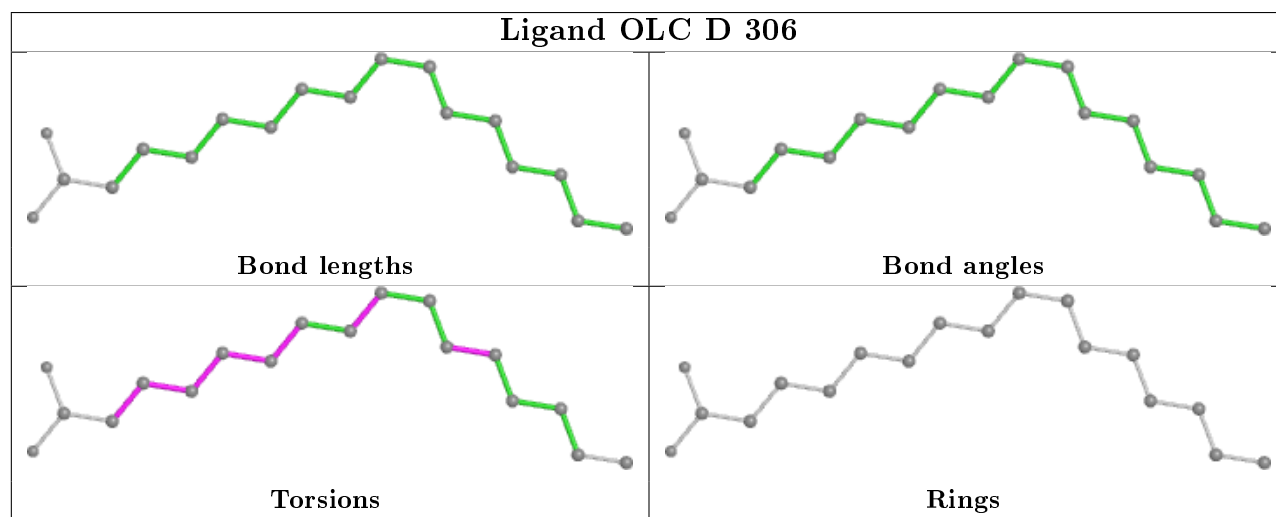
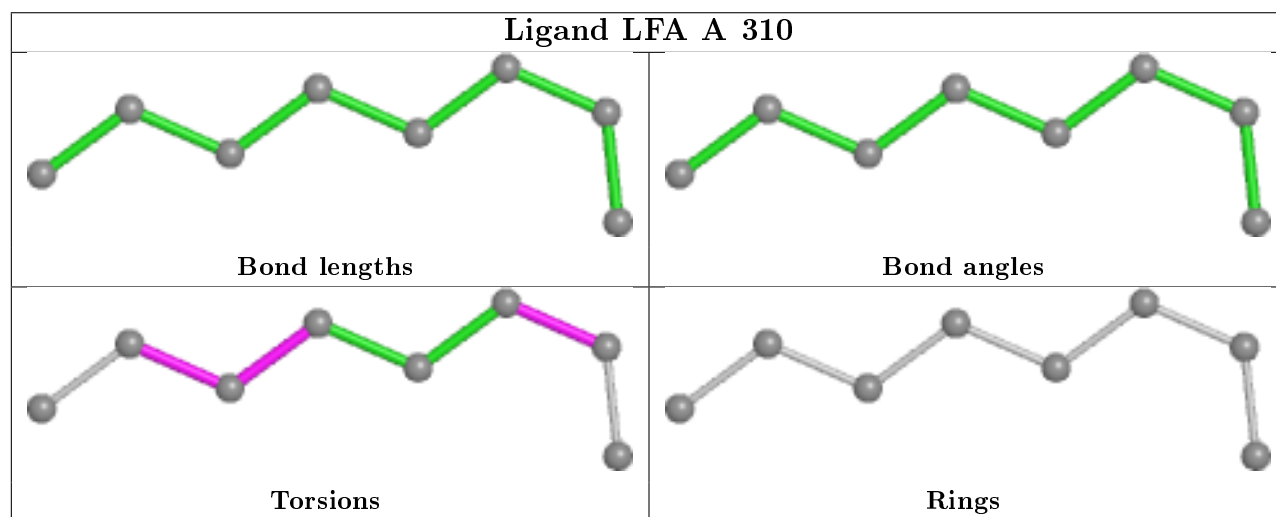
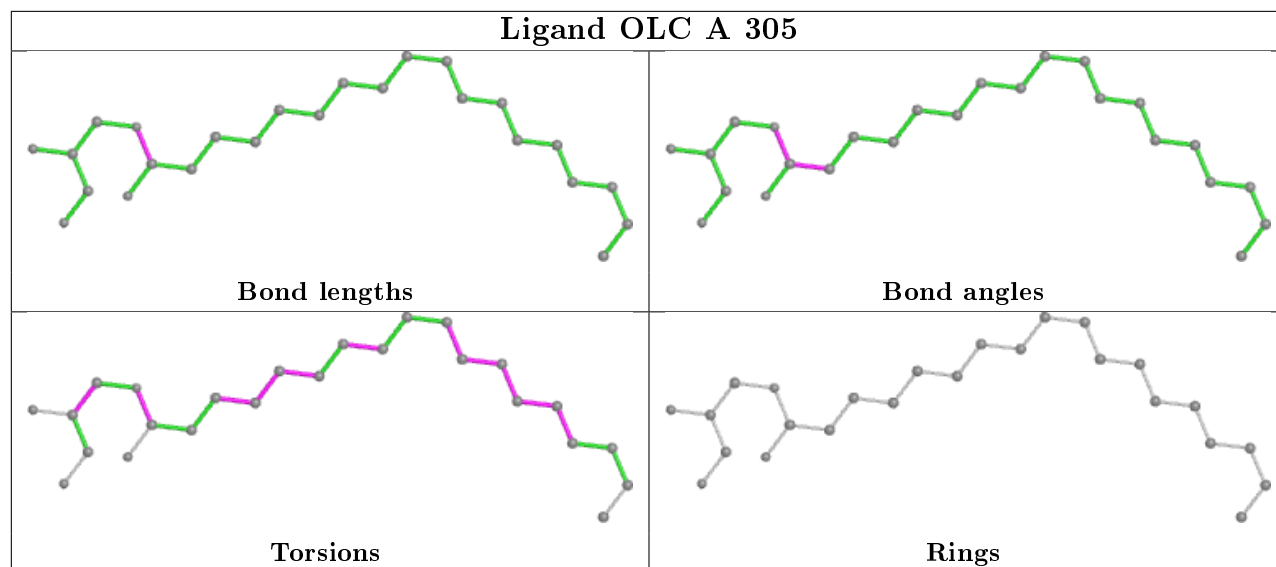


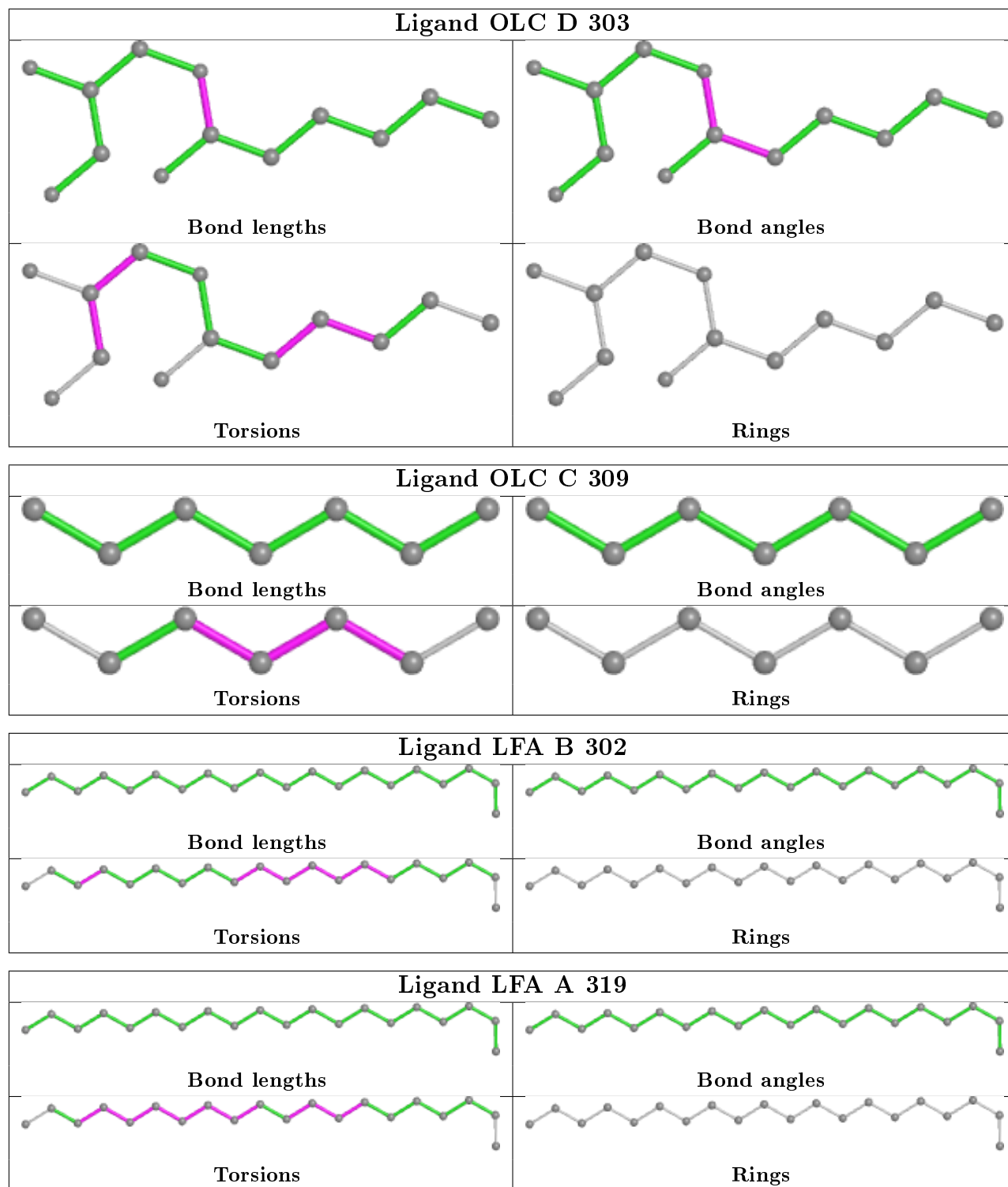


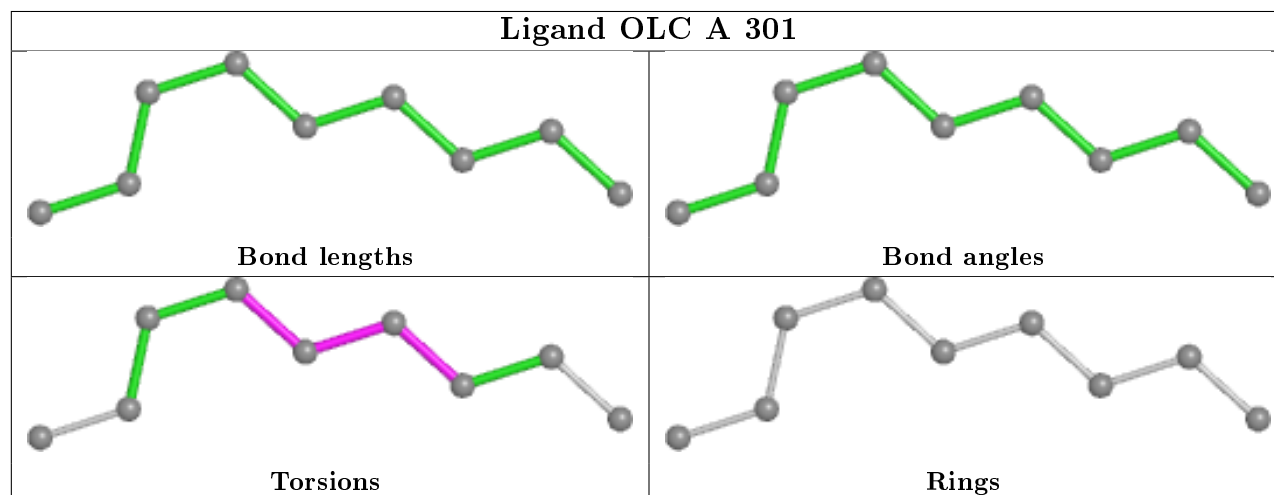
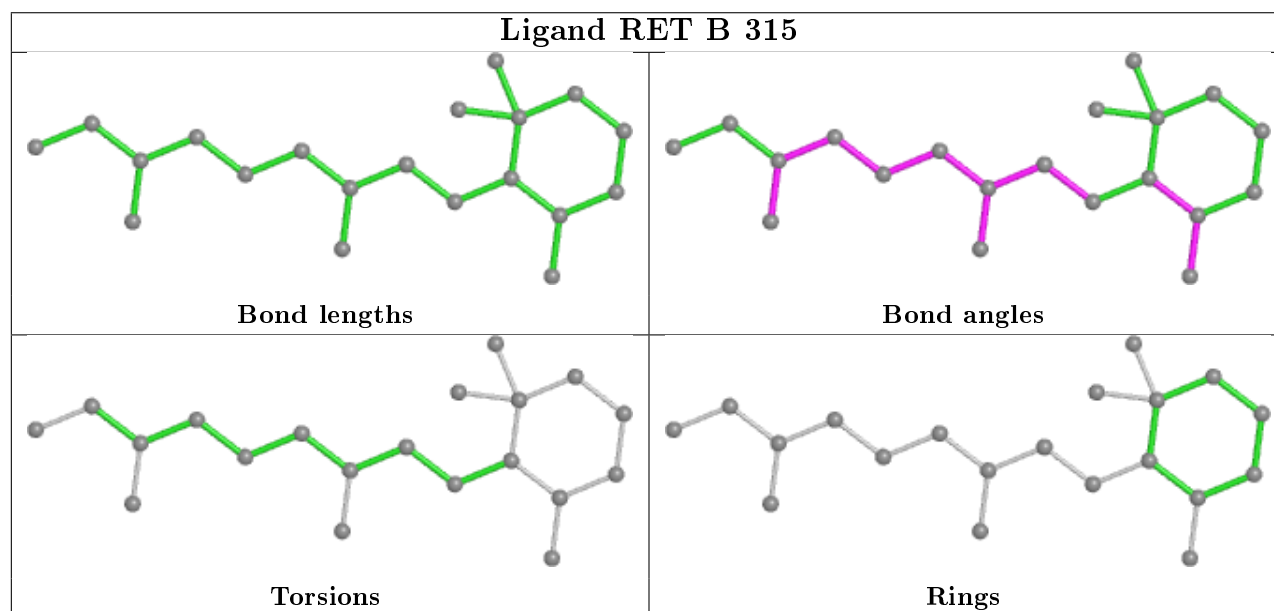
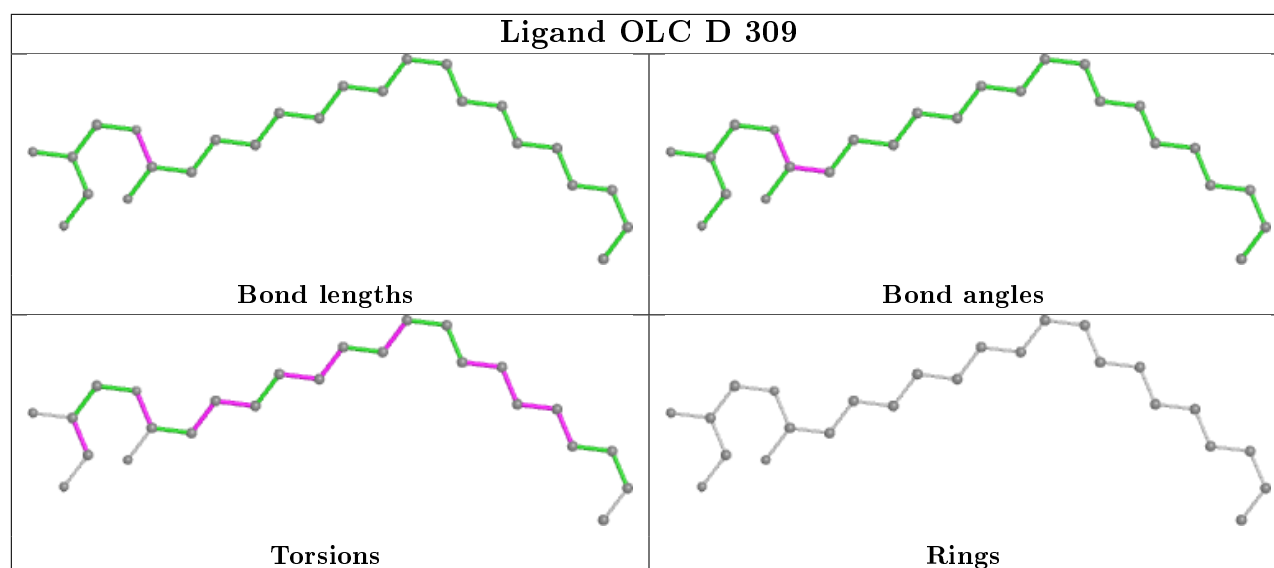


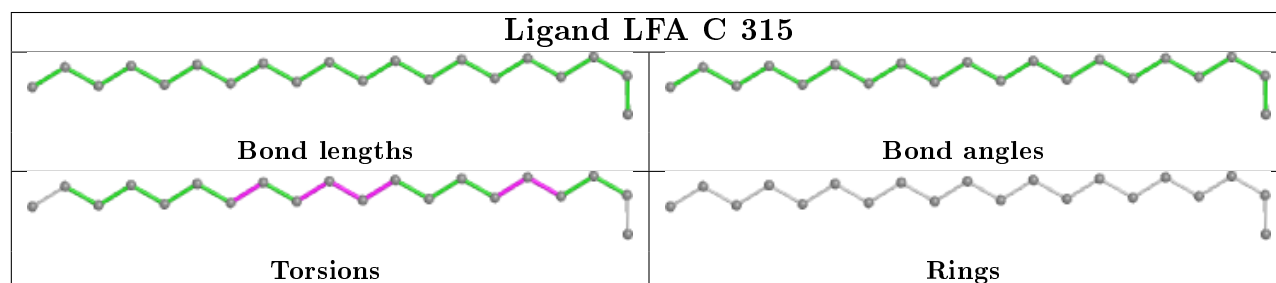
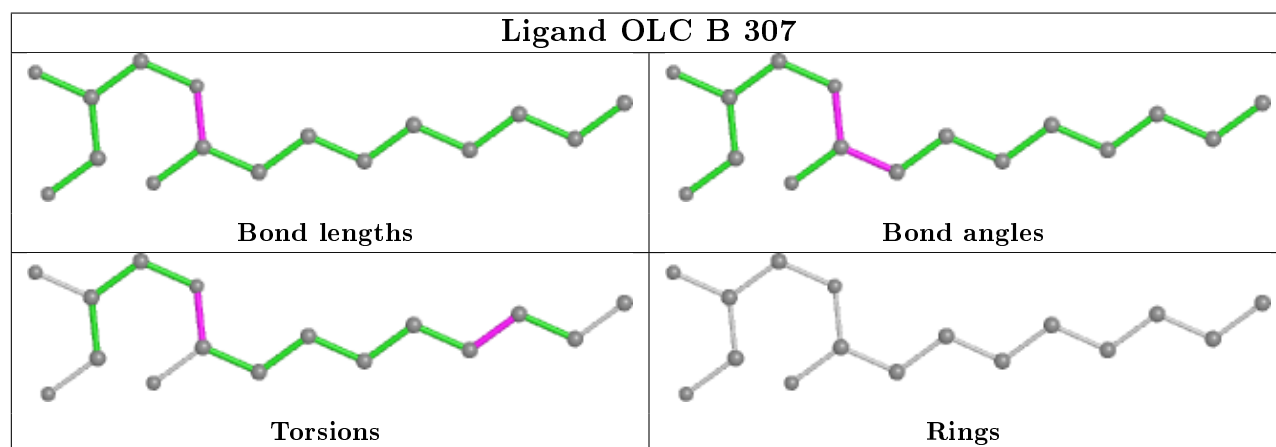
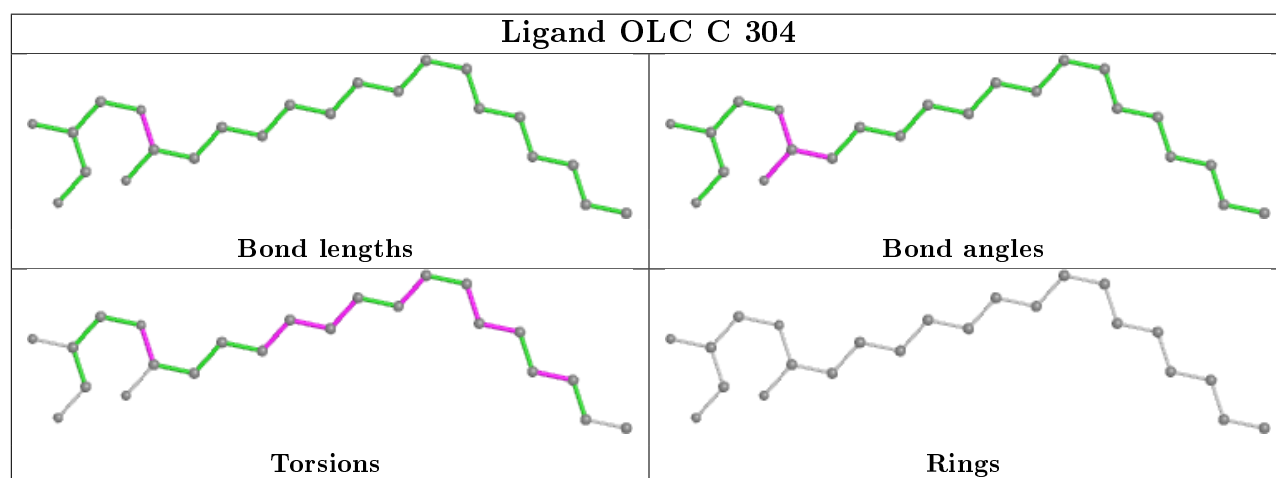
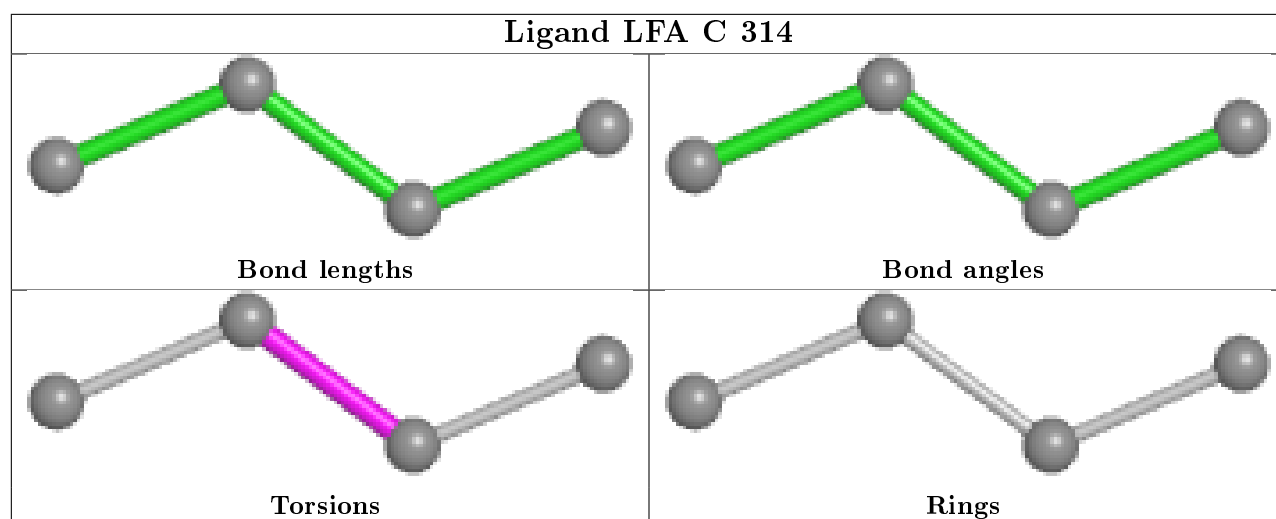


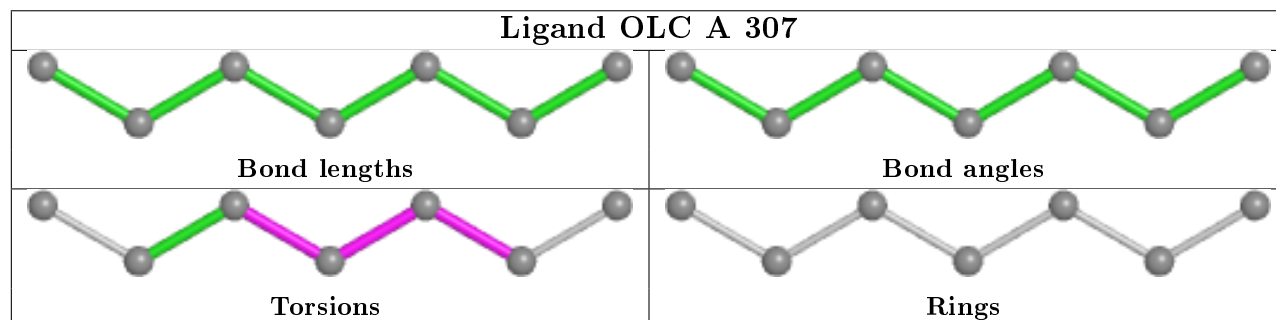
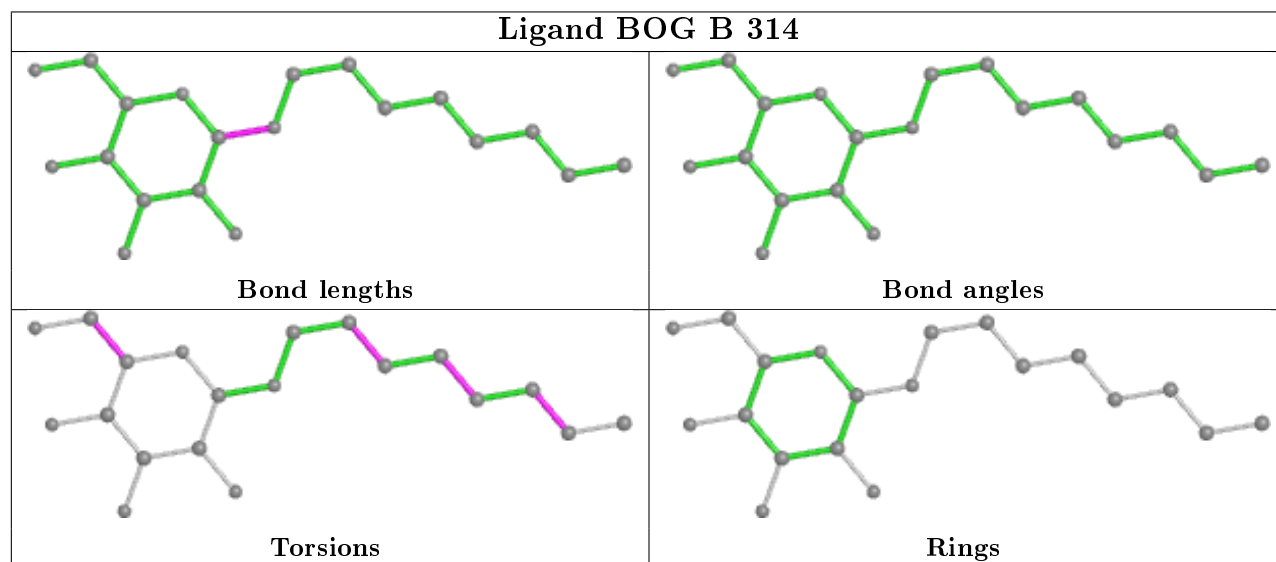
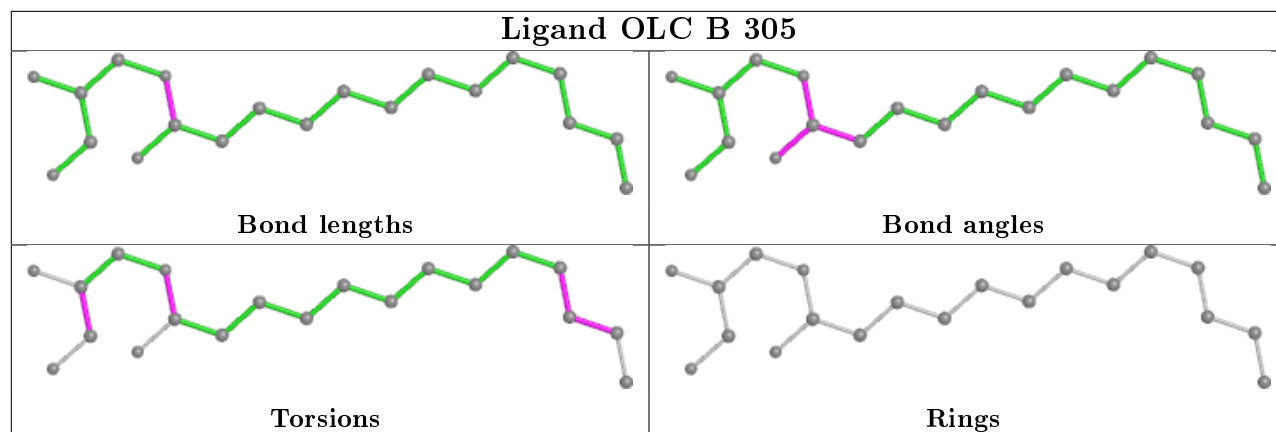


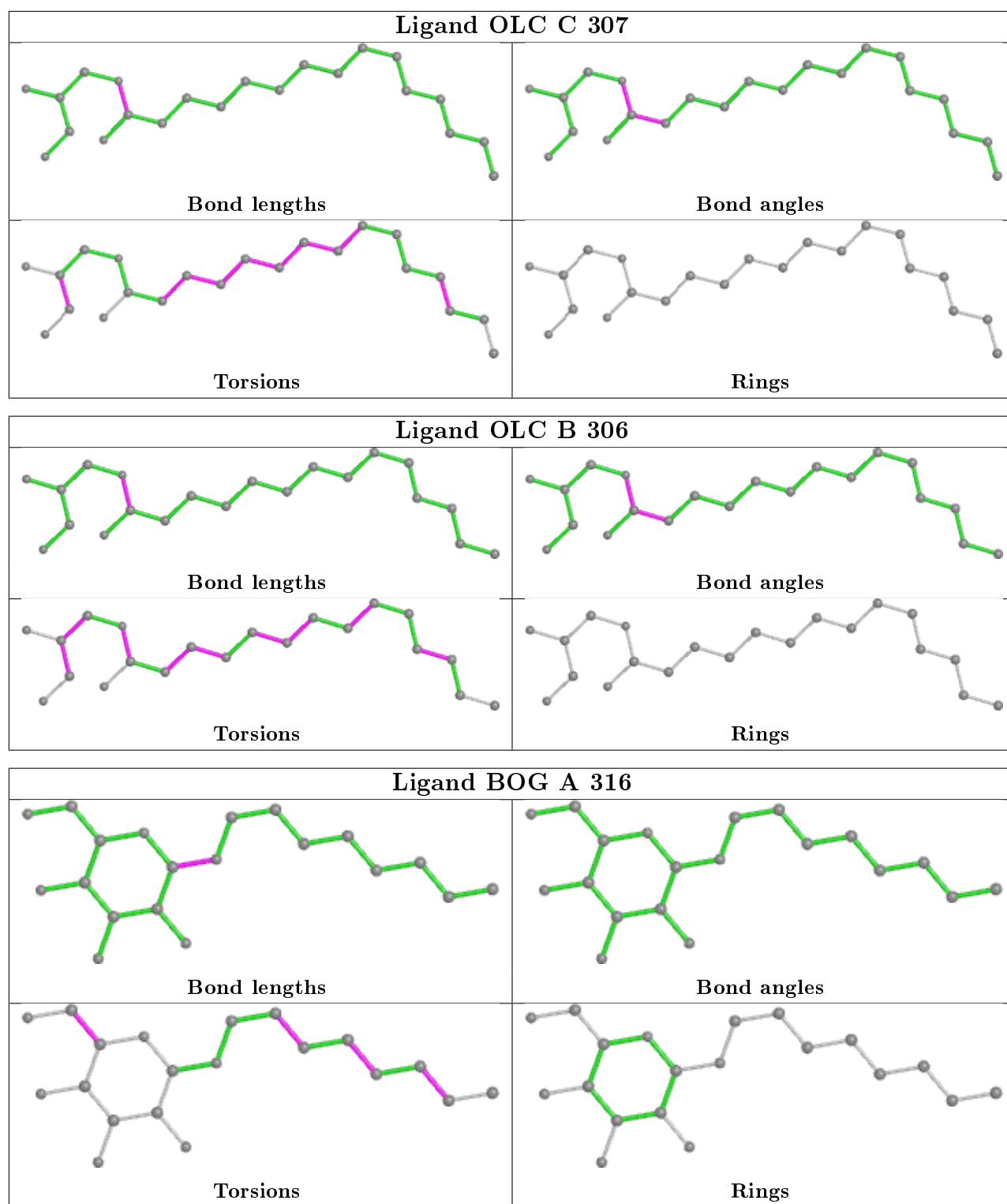


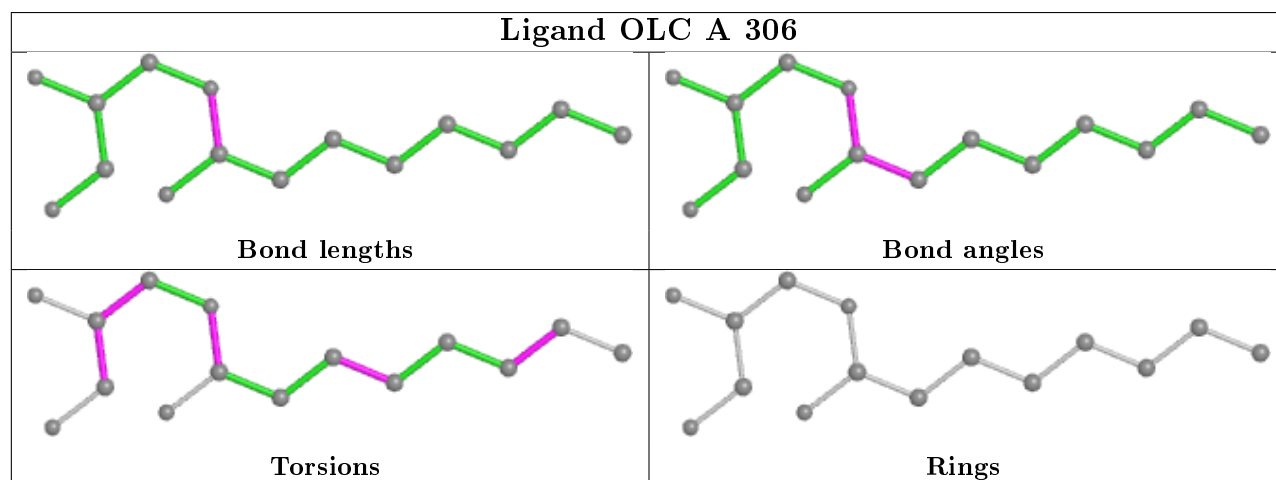
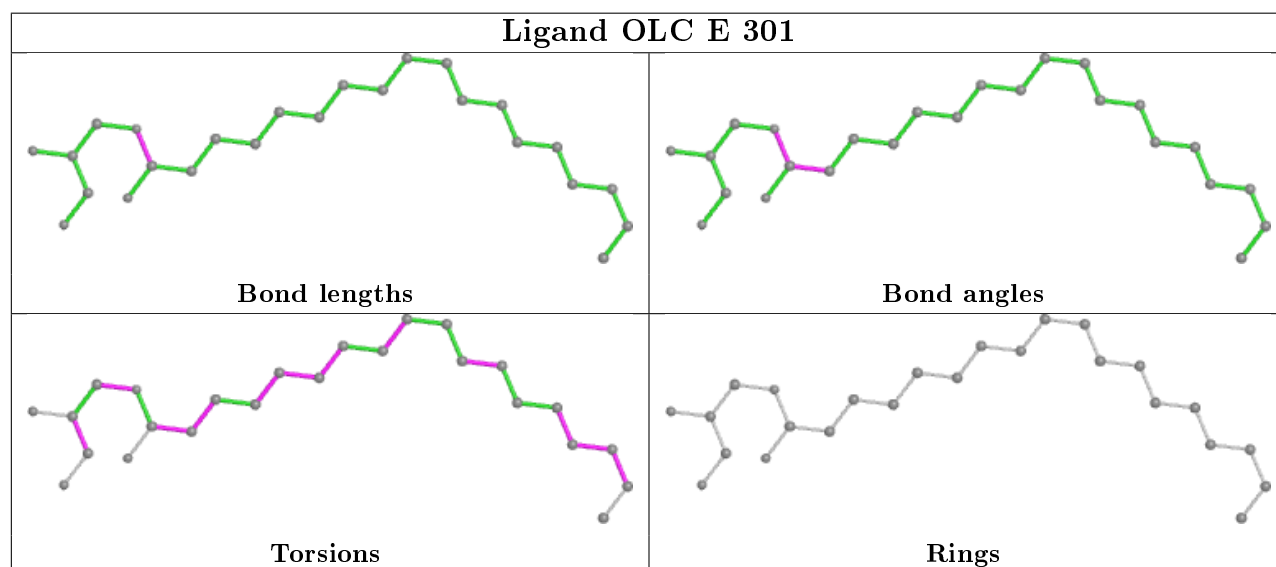
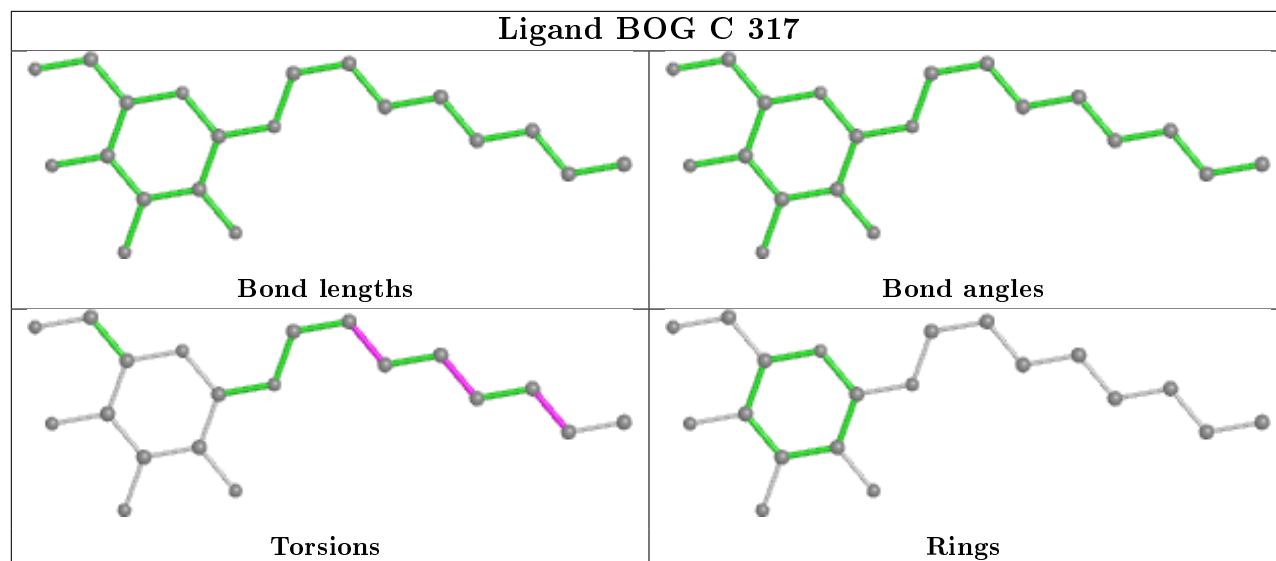


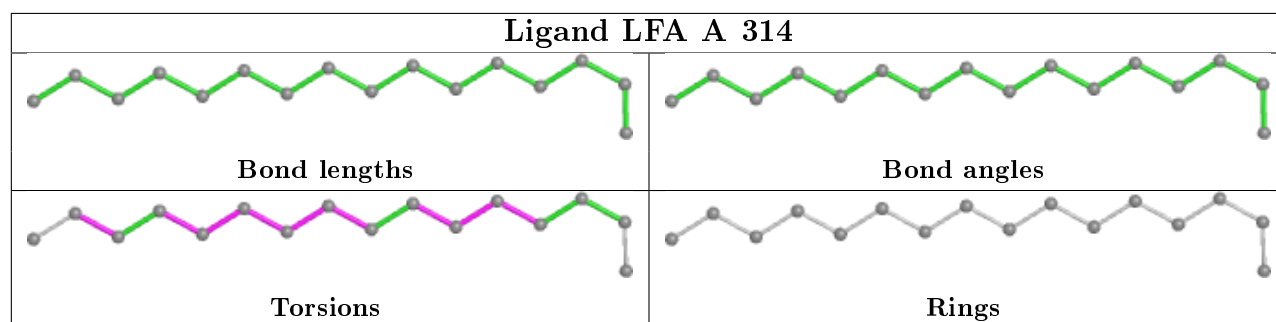
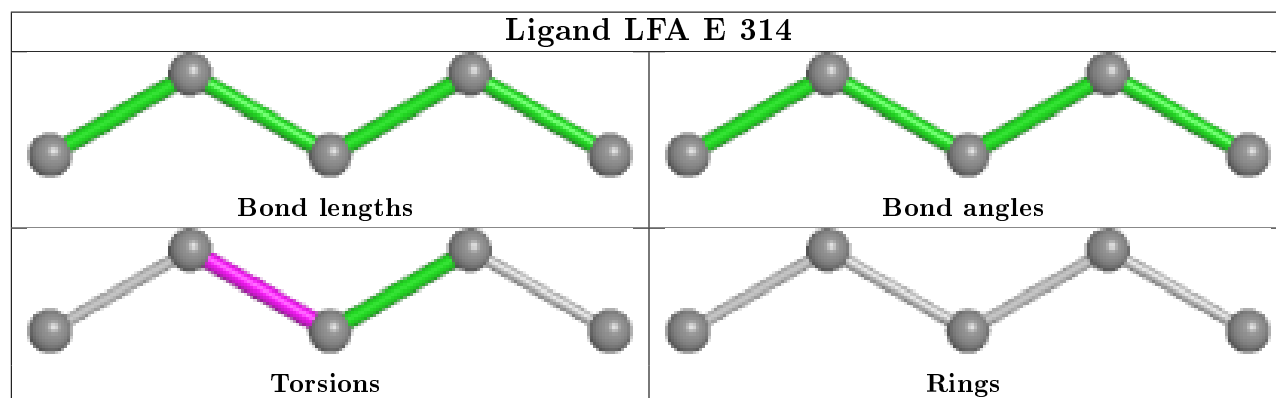
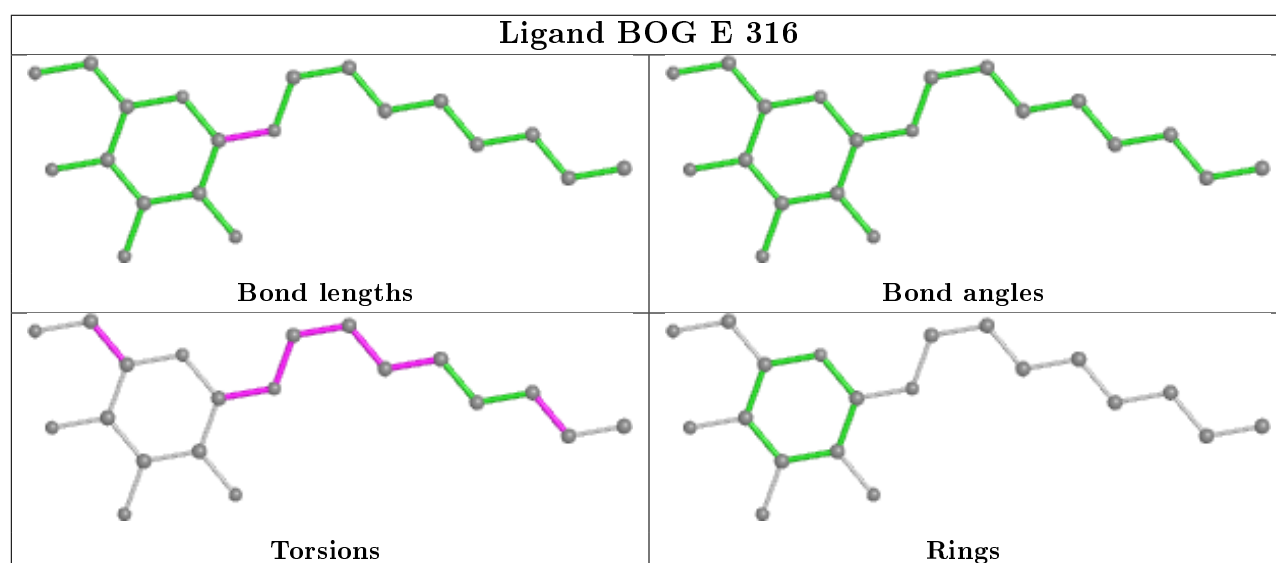
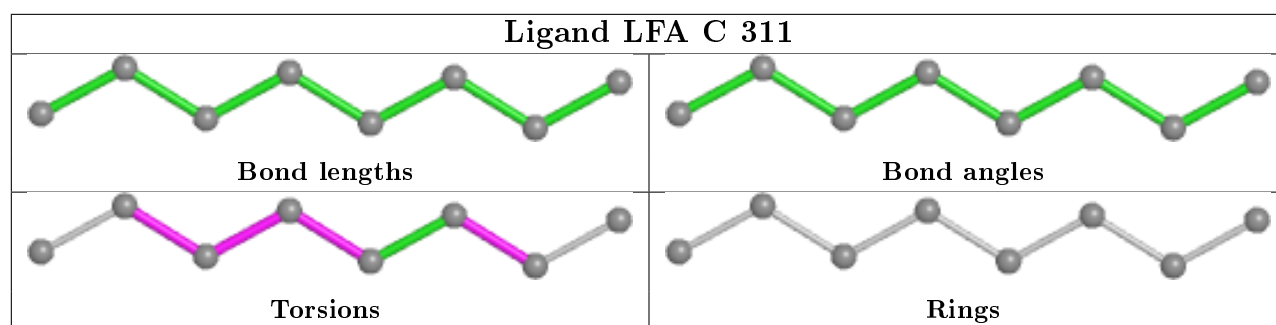


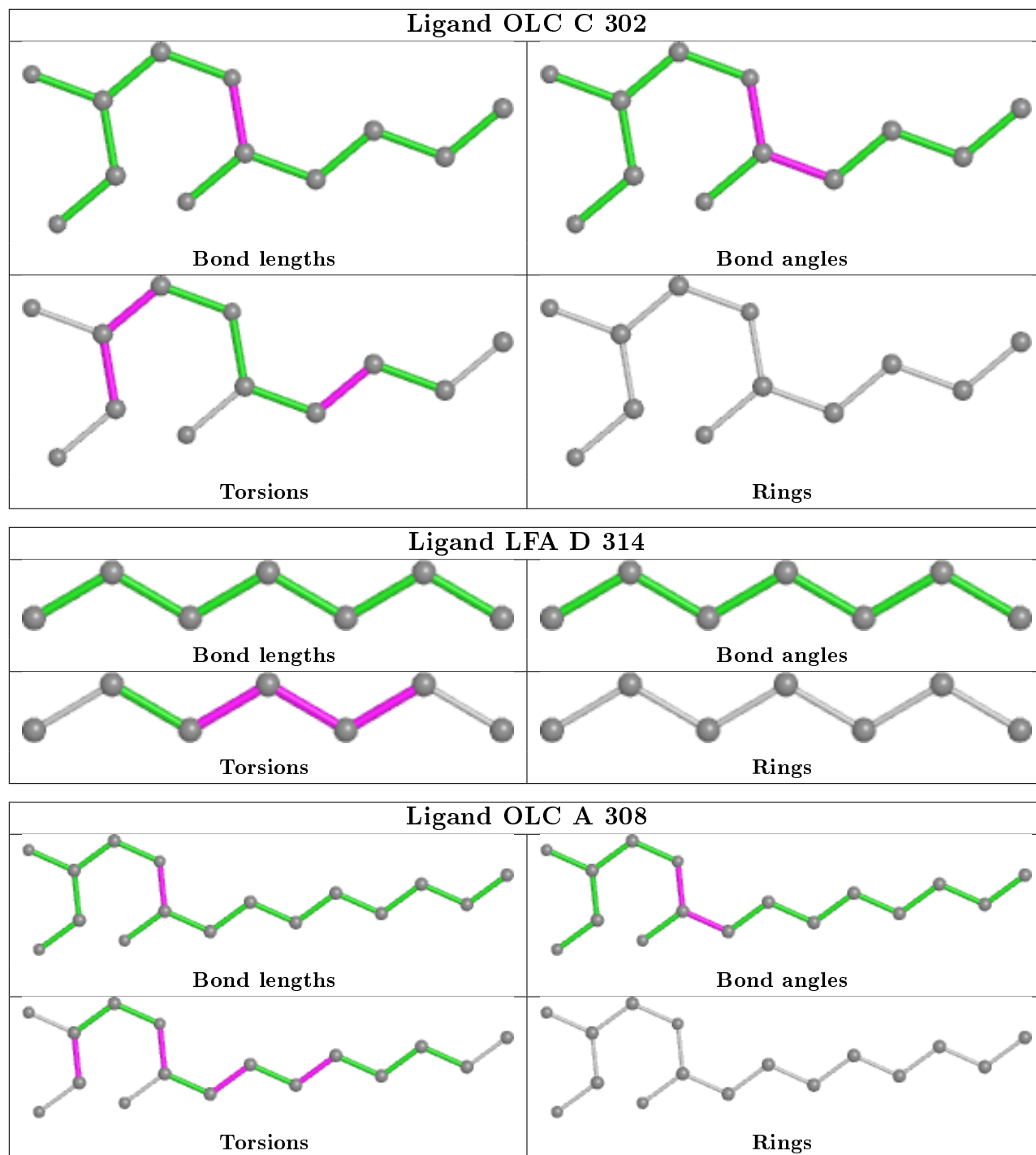


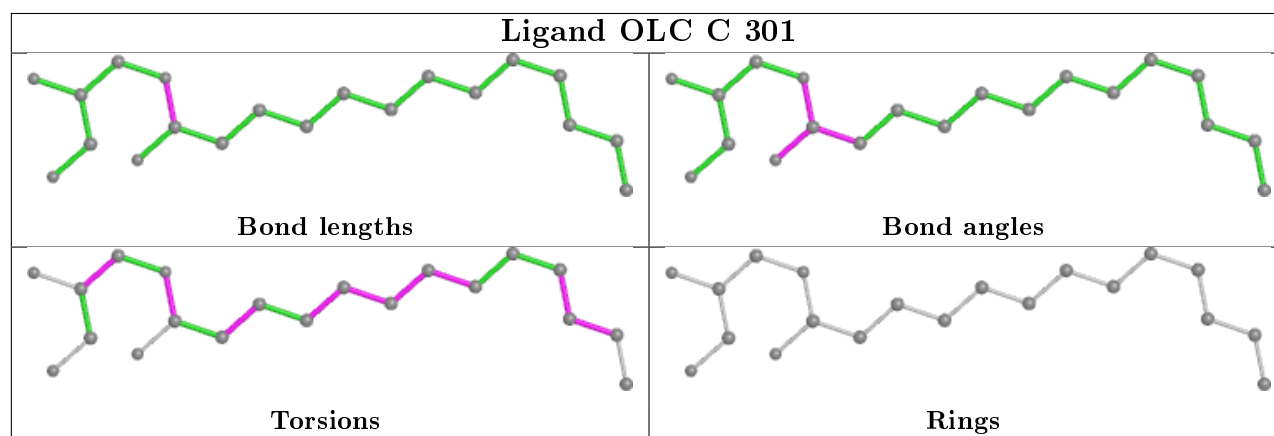
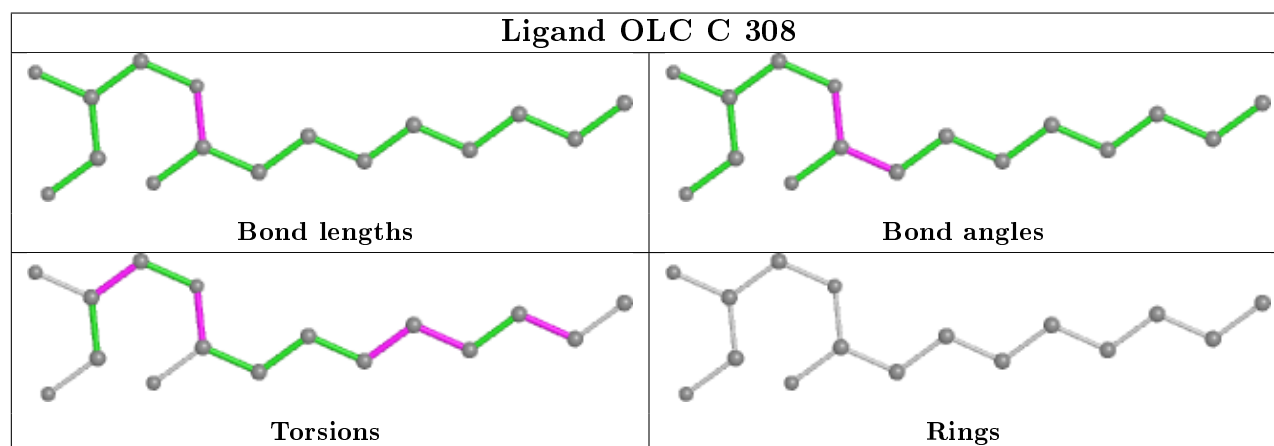
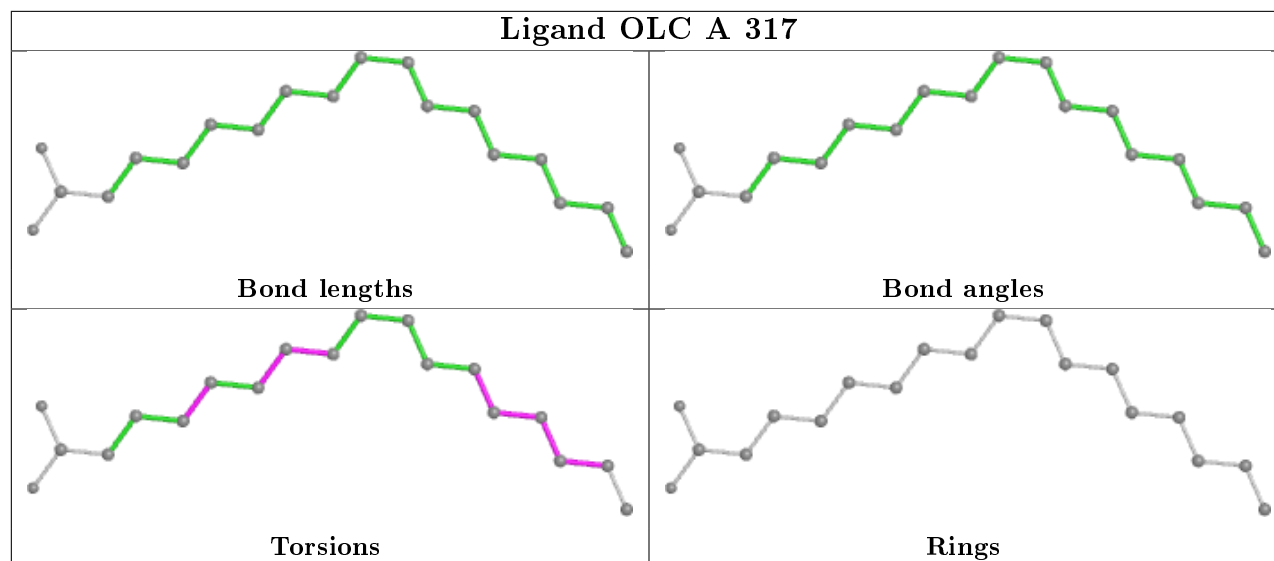


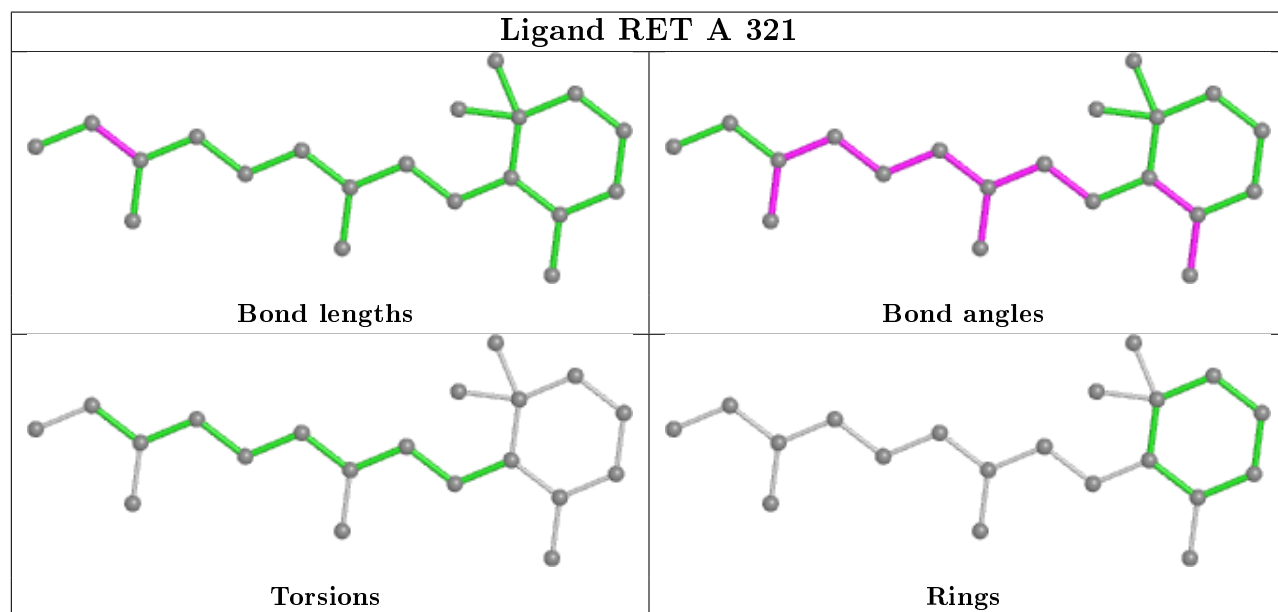
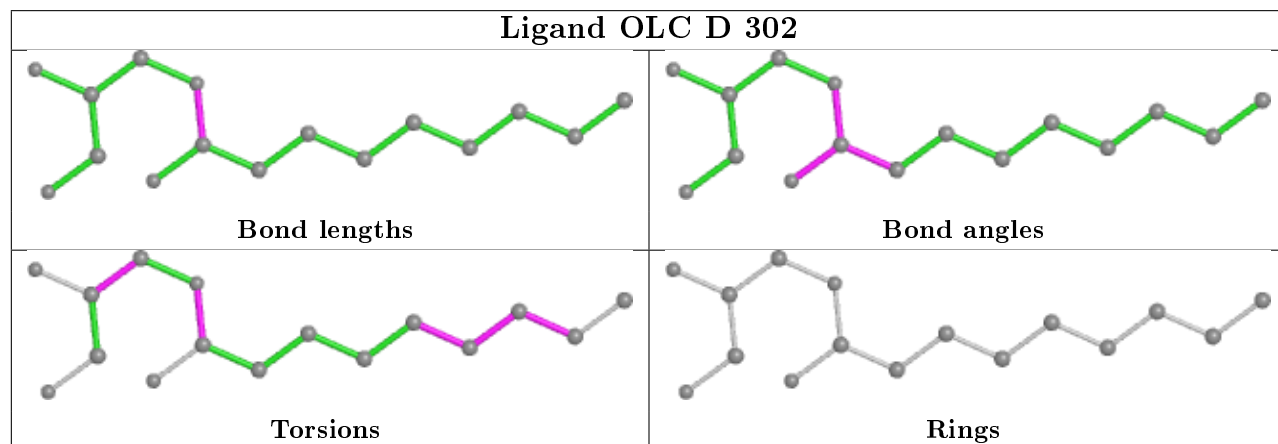
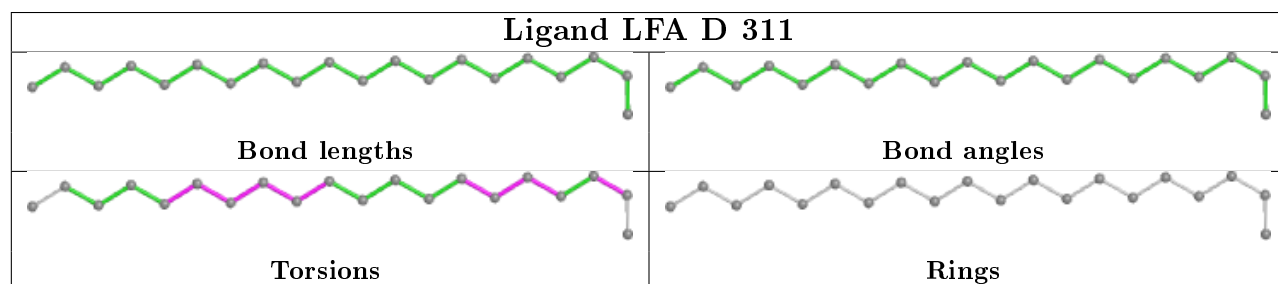
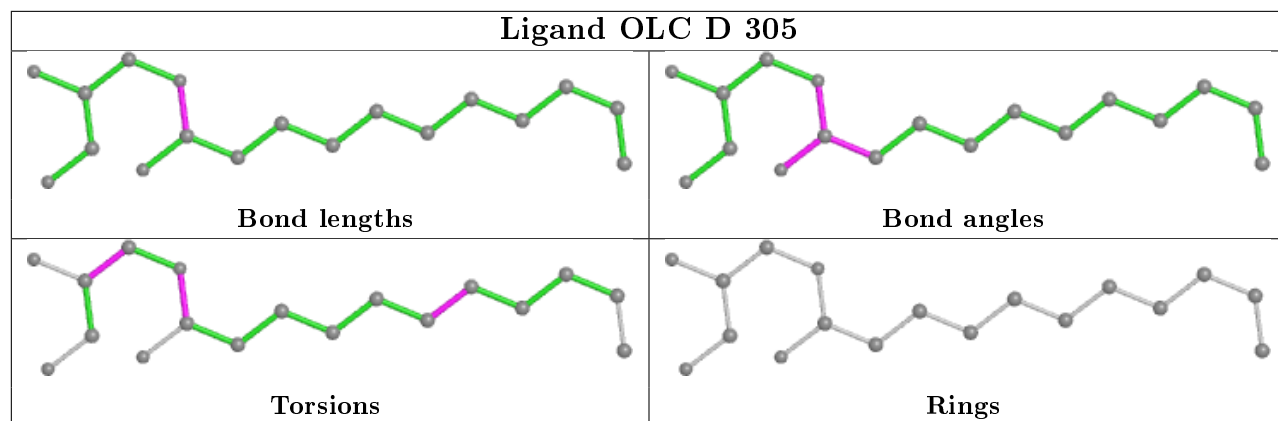


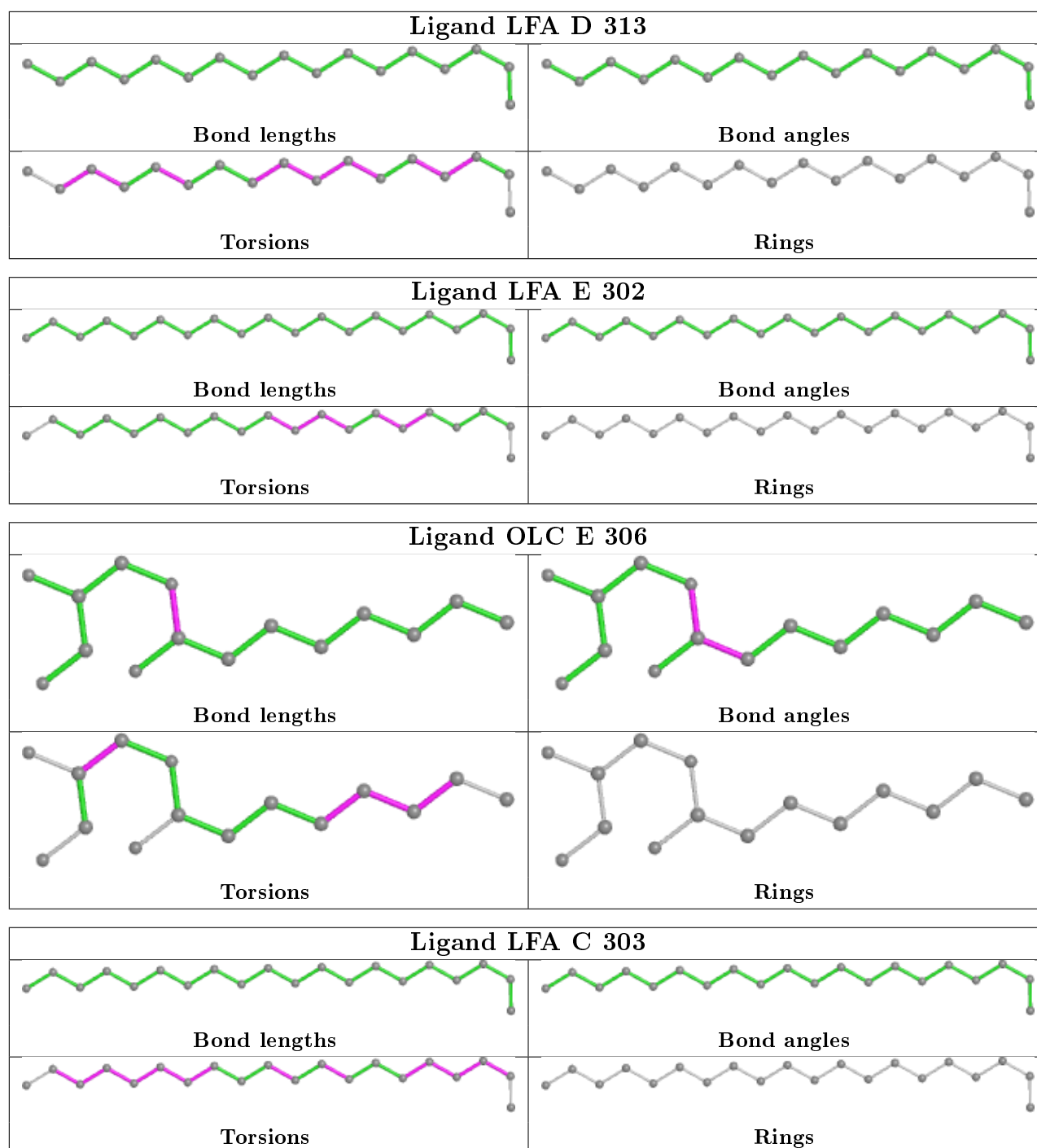












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	273/273 (100%)	-0.18	17 (6%) 20 19	22, 31, 55, 130	0
1	B	273/273 (100%)	-0.19	12 (4%) 34 32	23, 31, 55, 111	0
1	C	273/273 (100%)	-0.16	17 (6%) 20 19	22, 31, 55, 126	0
1	D	273/273 (100%)	-0.03	23 (8%) 11 9	22, 32, 59, 130	0
1	E	273/273 (100%)	-0.22	15 (5%) 25 24	22, 31, 56, 122	0
All	All	1365/1365 (100%)	-0.15	84 (6%) 20 19	22, 31, 56, 130	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	275	LEU	8.9
1	C	275	LEU	6.4
1	E	274	GLU	5.7
1	A	274	GLU	5.5
1	A	272	ASN	5.5
1	A	275	LEU	5.2
1	C	230	VAL	4.8
1	B	272	ASN	4.6
1	C	273	LYS	4.5
1	D	273	LYS	4.3
1	E	273	LYS	4.3
1	A	271	LYS	4.3
1	D	272	ASN	4.3
1	A	273	LYS	4.2
1	C	196	ILE	4.1
1	D	274	GLU	4.0
1	B	275	LEU	4.0
1	B	273	LYS	3.9
1	B	230	VAL	3.9
1	E	275	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	274	GLU	3.8
1	E	44	LEU	3.7
1	C	272	ASN	3.6
1	D	230	VAL	3.5
1	E	272	ASN	3.5
1	D	271	LYS	3.4
1	B	3	GLN	3.3
1	D	132	THR	3.3
1	C	195	GLY	3.2
1	A	270	SER	3.2
1	C	231	ASP	3.2
1	D	43	LEU	3.1
1	A	73	LEU	3.0
1	B	274	GLU	3.0
1	A	43	LEU	3.0
1	B	195	GLY	3.0
1	D	131	THR	3.0
1	B	231	ASP	2.9
1	E	3	GLN	2.8
1	B	271	LYS	2.8
1	A	3	GLN	2.8
1	E	43	LEU	2.8
1	D	40	LEU	2.7
1	B	44	LEU	2.7
1	C	44	LEU	2.6
1	A	69	VAL	2.6
1	E	40	LEU	2.6
1	A	132	THR	2.5
1	D	44	LEU	2.5
1	C	3	GLN	2.5
1	D	194	GLU	2.5
1	D	231	ASP	2.5
1	D	195	GLY	2.5
1	C	4	GLU	2.5
1	A	40	LEU	2.4
1	C	271	LYS	2.4
1	E	131	THR	2.4
1	D	3	GLN	2.4
1	D	73	LEU	2.3
1	E	73	LEU	2.3
1	D	197	SER	2.3
1	D	130	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	198	PRO	2.3
1	E	76	TYR	2.3
1	D	69	VAL	2.3
1	C	40	LEU	2.2
1	E	47	ILE	2.2
1	B	73	LEU	2.2
1	B	40	LEU	2.2
1	C	76	TYR	2.1
1	E	69	VAL	2.1
1	E	72	PHE	2.1
1	A	230	VAL	2.1
1	D	233	PHE	2.1
1	E	198	PRO	2.1
1	A	195	GLY	2.1
1	A	194	GLU	2.1
1	A	76	TYR	2.1
1	D	41	ALA	2.1
1	A	44	LEU	2.1
1	C	73	LEU	2.1
1	D	47	ILE	2.0
1	C	69	VAL	2.0
1	C	43	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	LFA	B	311	10/20	0.61	0.24	66,83,86,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	A	305	25/25	0.61	0.27	73,90,103,114	0
2	OLC	A	303	25/25	0.65	0.29	67,86,100,106	0
5	BOG	A	316	20/20	0.65	0.40	66,88,96,98	0
2	OLC	E	304	16/25	0.66	0.21	73,86,95,97	0
2	OLC	C	307	22/25	0.68	0.30	45,82,101,110	0
2	OLC	D	308	7/25	0.69	0.21	60,63,68,72	0
3	LFA	C	310	7/20	0.69	0.24	67,73,87,87	0
5	BOG	E	316	20/20	0.69	0.33	61,77,89,94	0
2	OLC	E	308	6/25	0.70	0.19	53,66,72,72	0
3	LFA	C	313	6/20	0.70	0.24	53,62,79,80	0
2	OLC	E	309	22/25	0.71	0.30	59,77,104,108	0
2	OLC	D	303	13/25	0.71	0.31	99,109,119,133	0
3	LFA	D	314	7/20	0.71	0.20	71,78,85,87	0
2	OLC	D	302	16/25	0.71	0.29	58,73,87,100	0
3	LFA	A	314	16/20	0.72	0.26	73,89,105,105	0
3	LFA	C	314	4/20	0.72	0.31	79,79,80,84	0
2	OLC	C	302	12/25	0.72	0.29	57,74,96,115	0
3	LFA	D	315	6/20	0.72	0.17	71,81,88,95	0
5	BOG	B	314	20/20	0.72	0.43	67,81,92,92	0
2	OLC	D	304	25/25	0.73	0.23	72,93,107,115	0
3	LFA	E	311	8/20	0.73	0.20	64,82,86,90	0
2	OLC	B	303	25/25	0.73	0.20	66,88,100,103	0
3	LFA	A	311	8/20	0.74	0.25	61,81,95,98	0
2	OLC	E	310	20/25	0.74	0.33	50,96,121,123	0
3	LFA	E	302	20/20	0.74	0.81	43,59,70,80	0
3	LFA	D	310	20/20	0.75	0.21	76,84,96,97	0
2	OLC	E	306	15/25	0.75	0.33	68,84,106,106	0
3	LFA	A	310	8/20	0.76	0.23	69,76,85,85	0
3	LFA	B	309	9/20	0.76	0.25	71,86,92,92	0
2	OLC	B	305	20/25	0.76	0.16	57,79,100,101	0
5	BOG	C	317	20/20	0.76	0.37	57,74,86,89	0
2	OLC	C	305	22/25	0.77	0.19	66,88,104,106	0
3	LFA	A	309	7/20	0.77	0.22	67,71,79,81	0
3	LFA	B	312	7/20	0.77	0.23	61,67,89,94	0
2	OLC	E	301	25/25	0.77	0.23	54,75,122,134	0
2	OLC	C	309	7/25	0.78	0.26	52,63,78,85	0
2	OLC	D	309	25/25	0.78	0.27	55,73,95,104	0
3	LFA	D	312	8/20	0.78	0.18	62,78,88,91	0
3	LFA	A	320	9/20	0.79	0.21	66,70,87,87	0
3	LFA	C	311	8/20	0.80	0.21	67,75,78,79	0
3	LFA	B	302	20/20	0.80	0.80	41,59,71,85	0
3	LFA	E	312	14/20	0.80	0.19	68,82,94,95	0

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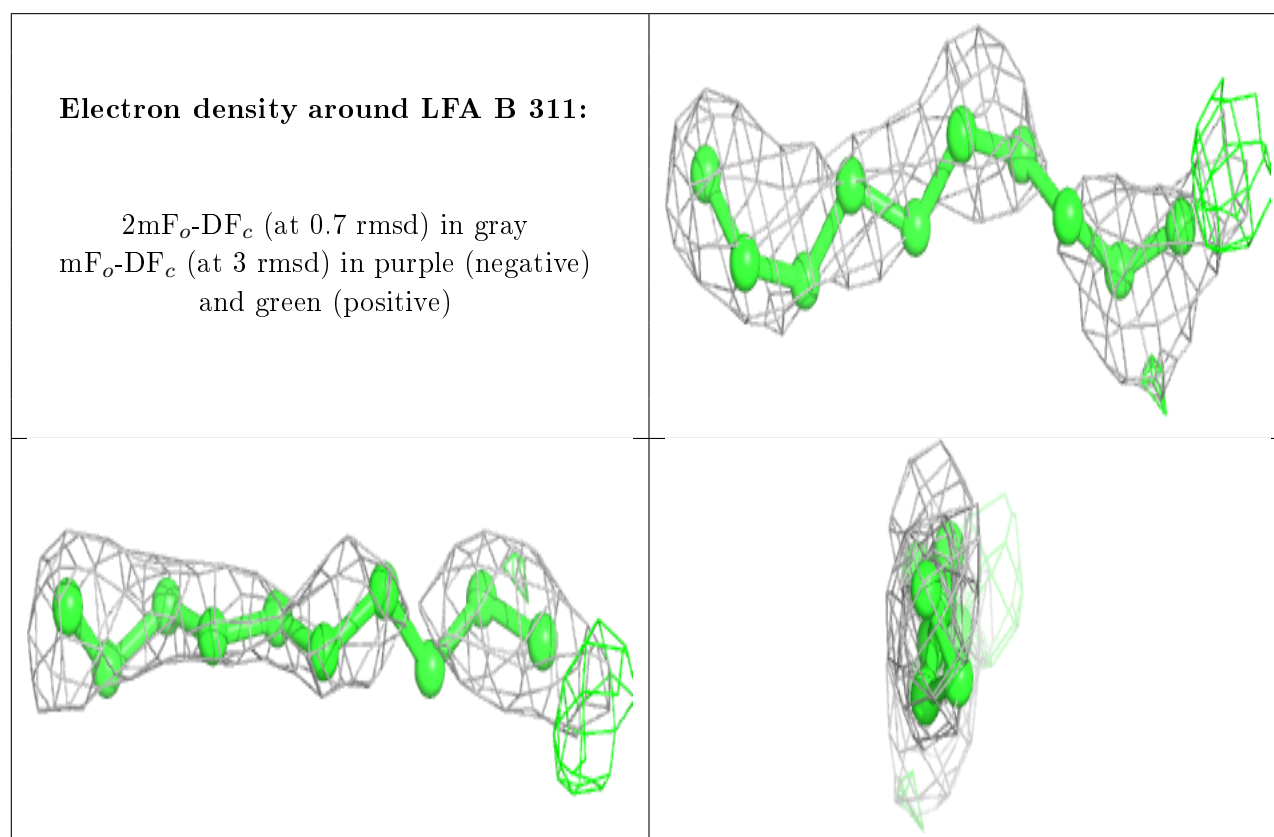
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	D	306	18/25	0.81	0.16	47,78,88,90	0
3	LFA	C	315	20/20	0.81	0.81	45,59,76,79	0
2	OLC	A	318	20/25	0.81	0.21	61,70,87,91	0
5	BOG	D	317	20/20	0.81	0.36	59,72,84,84	0
3	LFA	B	310	8/20	0.81	0.20	63,76,82,87	0
2	OLC	B	306	21/25	0.81	0.28	45,81,101,114	0
2	OLC	A	308	16/25	0.81	0.24	57,74,117,124	0
3	LFA	A	319	20/20	0.81	0.71	43,55,65,68	0
2	OLC	E	303	8/25	0.81	0.20	56,58,77,77	0
2	OLC	B	308	7/25	0.81	0.17	56,68,73,74	0
2	OLC	A	307	7/25	0.82	0.19	63,71,78,79	0
3	LFA	E	314	5/20	0.82	0.18	75,78,80,85	0
2	OLC	D	305	18/25	0.82	0.20	68,86,108,110	0
2	OLC	C	306	20/25	0.83	0.17	57,80,100,102	0
3	LFA	C	303	20/20	0.83	0.78	45,58,69,73	0
2	OLC	C	301	20/25	0.84	0.20	61,74,86,91	0
2	OLC	E	305	20/25	0.84	0.21	62,79,100,105	0
2	OLC	A	301	9/25	0.85	0.19	63,71,83,83	0
3	LFA	C	312	20/20	0.85	0.17	60,78,103,104	0
2	OLC	C	304	23/25	0.85	0.24	40,55,99,108	0
3	LFA	E	317	4/20	0.85	1.50	58,63,66,71	0
3	LFA	D	311	20/20	0.86	0.17	67,85,96,96	0
2	OLC	A	304	13/25	0.86	0.17	57,68,76,85	0
2	OLC	A	306	15/25	0.86	0.19	51,69,86,97	0
2	OLC	D	301	18/25	0.86	0.19	59,70,83,90	0
3	LFA	C	318	14/20	0.86	1.18	77,84,93,95	0
2	OLC	B	301	22/25	0.88	0.14	60,72,86,89	0
2	OLC	C	308	16/25	0.88	0.17	52,72,85,88	0
3	LFA	A	312	4/20	0.88	0.23	72,73,75,76	0
2	OLC	A	302	22/25	0.89	0.21	36,53,97,104	0
2	OLC	E	307	15/25	0.90	0.20	52,66,80,81	0
3	LFA	E	313	4/20	0.91	0.20	55,63,63,69	0
2	OLC	B	304	21/25	0.92	0.22	39,51,73,85	0
2	OLC	B	307	16/25	0.92	0.19	51,73,85,106	0
3	LFA	A	313	6/20	0.92	0.14	49,59,66,70	0
2	OLC	A	317	19/25	0.93	0.23	37,49,62,69	0
3	LFA	D	313	17/20	0.94	0.36	44,46,68,73	0
2	OLC	D	307	14/25	0.94	0.13	49,68,79,93	0
6	RET	E	318	20/21	0.95	0.10	24,27,31,31	0
6	RET	A	321	20/21	0.95	0.10	24,27,31,31	0
6	RET	D	318	20/21	0.95	0.10	25,29,33,35	0
6	RET	B	315	20/21	0.96	0.10	23,28,32,34	0

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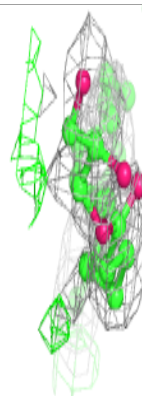
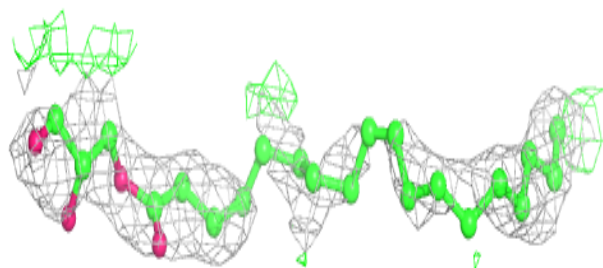
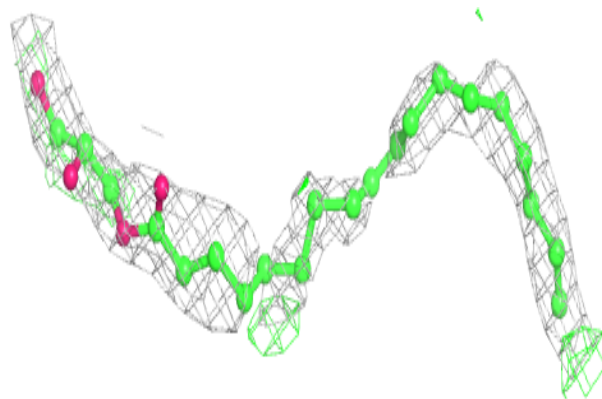
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	RET	C	319	20/21	0.96	0.09	25,29,34,36	0
4	NA	E	315	1/1	0.97	0.07	25,25,25,25	0
4	NA	A	315	1/1	0.98	0.04	26,26,26,26	0
4	NA	D	316	1/1	0.98	0.06	25,25,25,25	0
4	NA	B	313	1/1	0.98	0.05	24,24,24,24	0
4	NA	C	316	1/1	1.00	0.05	26,26,26,26	0

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

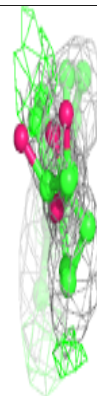
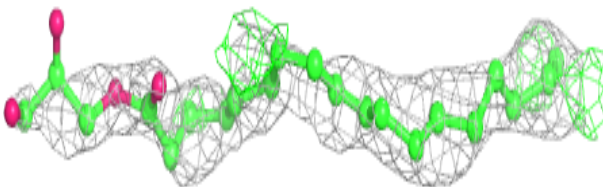
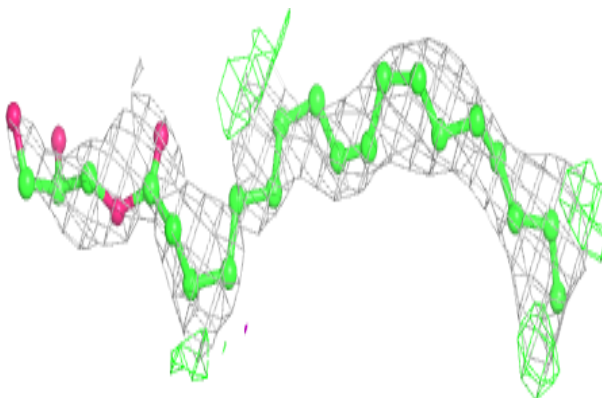


Electron density around OLC A 305:

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

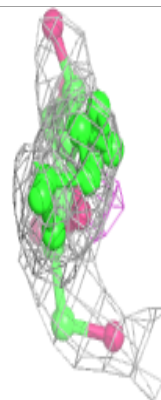
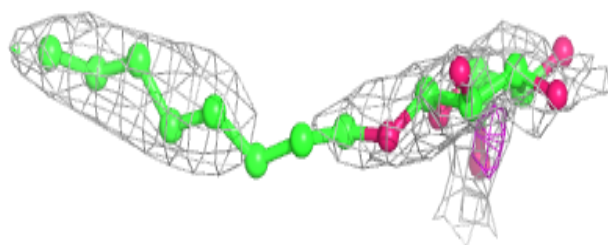
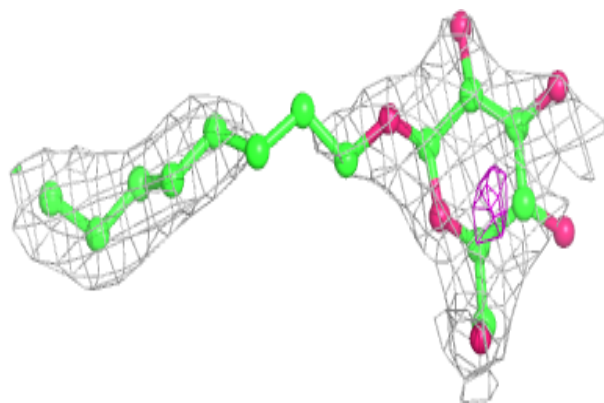
**Electron density around OLC A 303:**

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

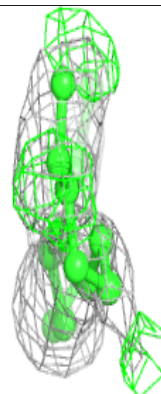
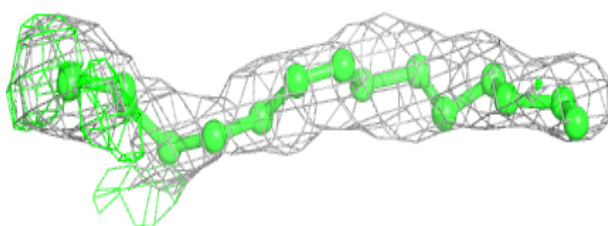
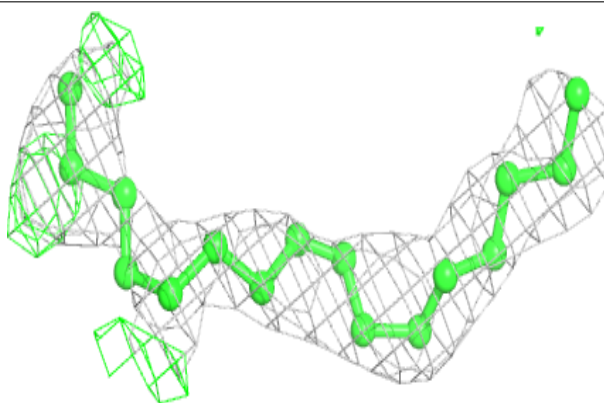


Electron density around BOG A 316:

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

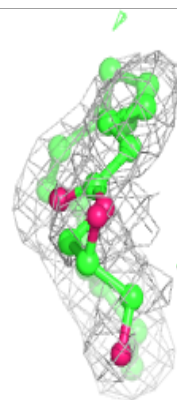
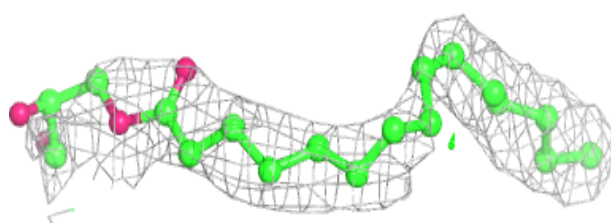
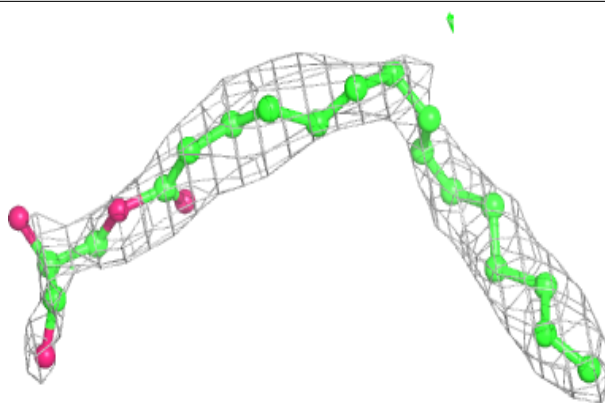
**Electron density around OLC E 304:**

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

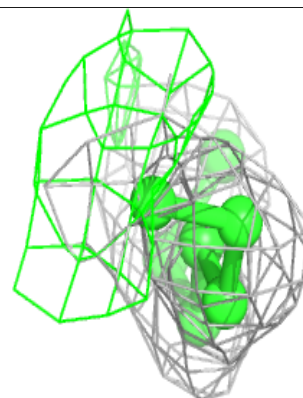
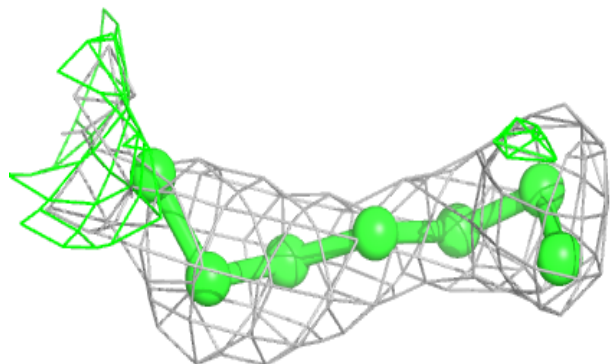
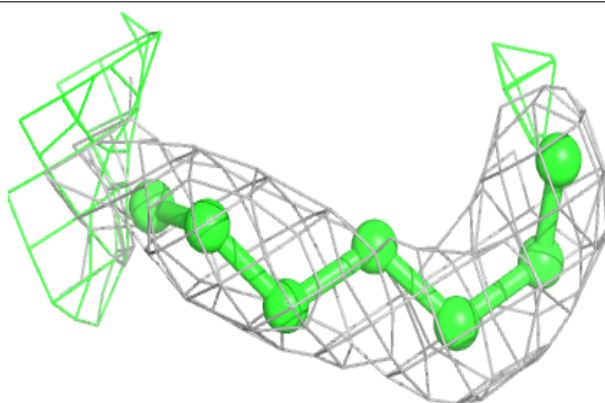


Electron density around OLC C 307:

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

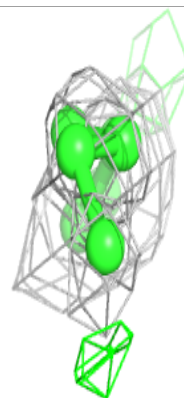
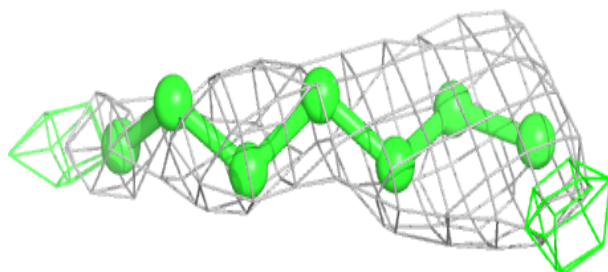
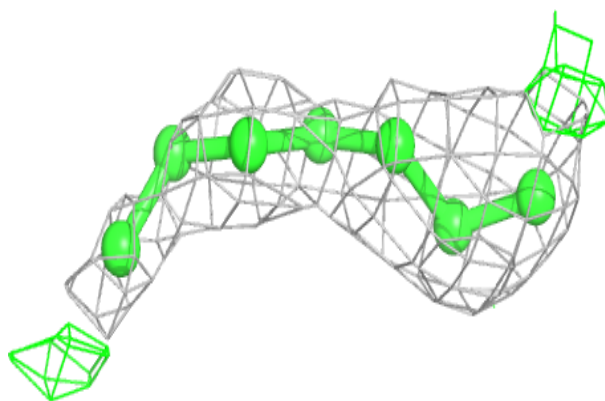
**Electron density around OLC D 308:**

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

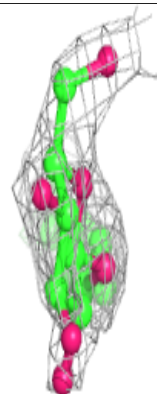
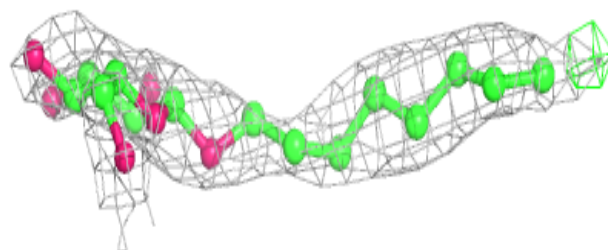
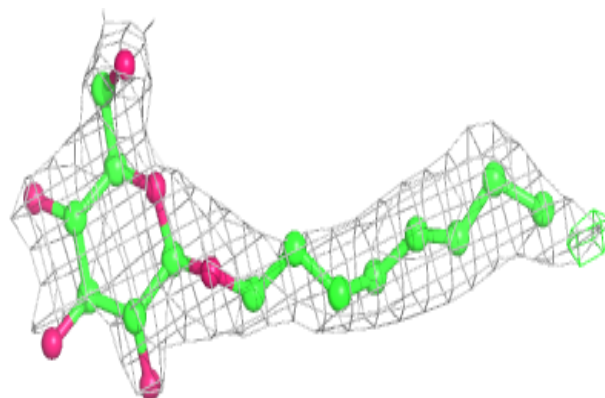


Electron density around LFA C 310:

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

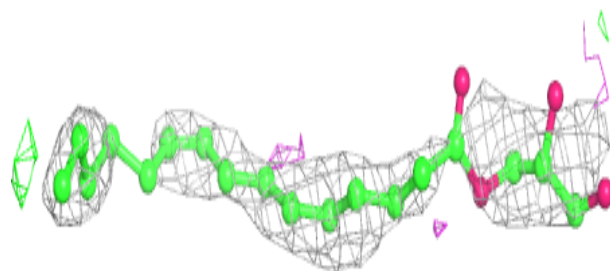
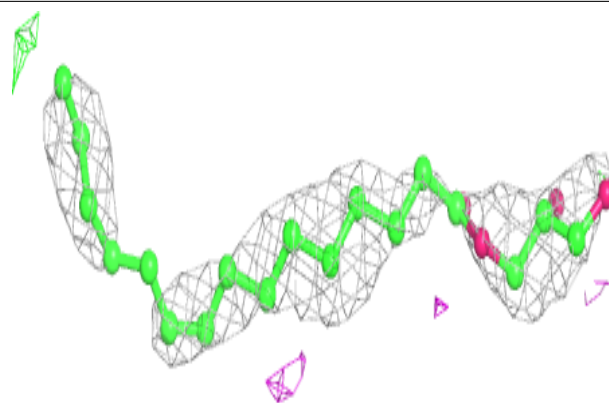
**Electron density around BOG E 316:**

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

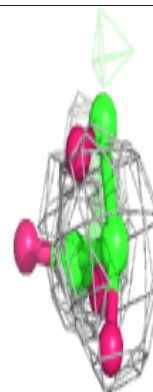
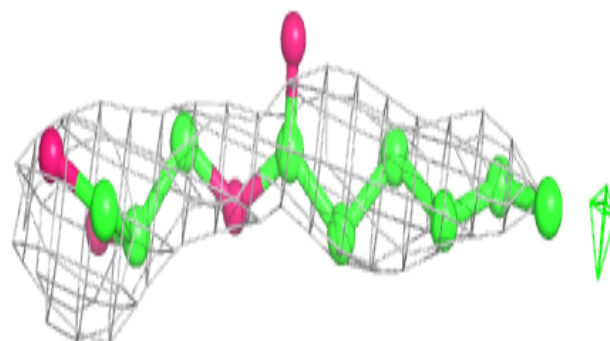
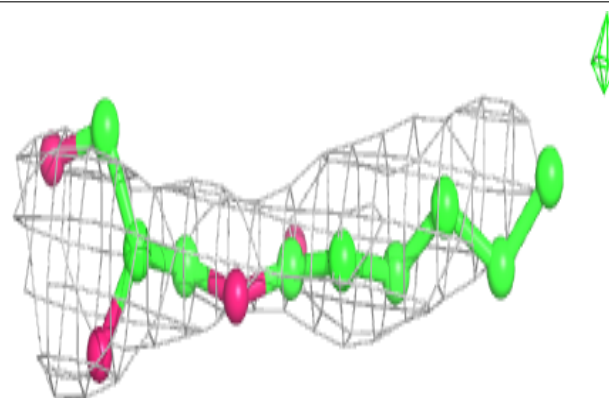


Electron density around OLC E 309:

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

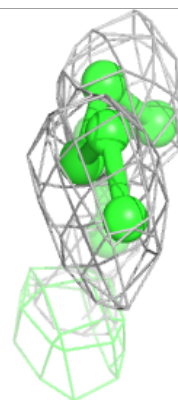
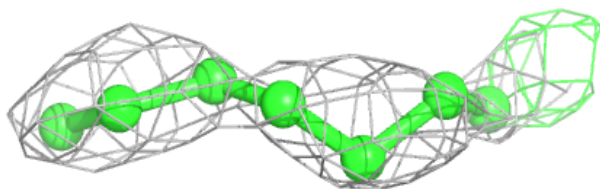
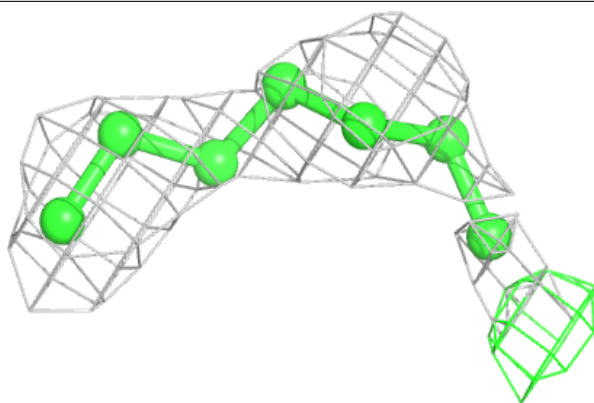
**Electron density around OLC D 303:**

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

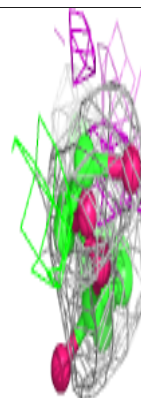
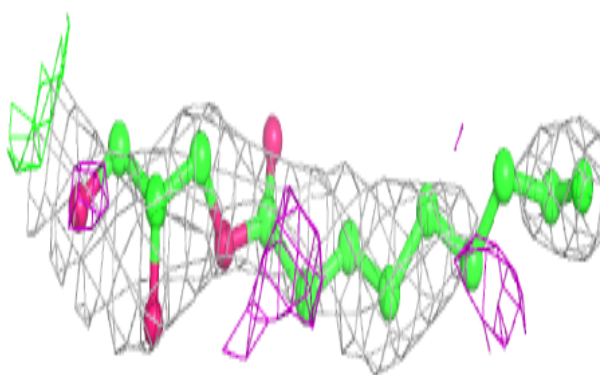
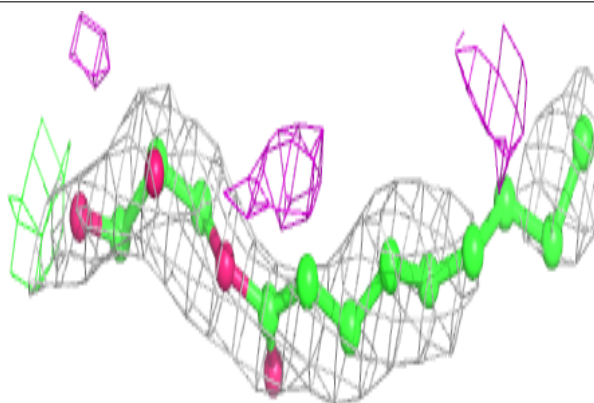


Electron density around LFA D 314:

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

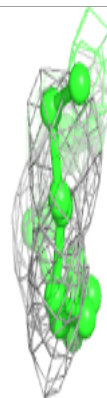
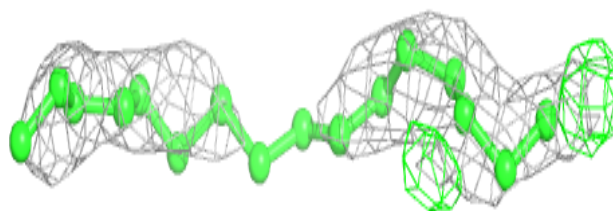
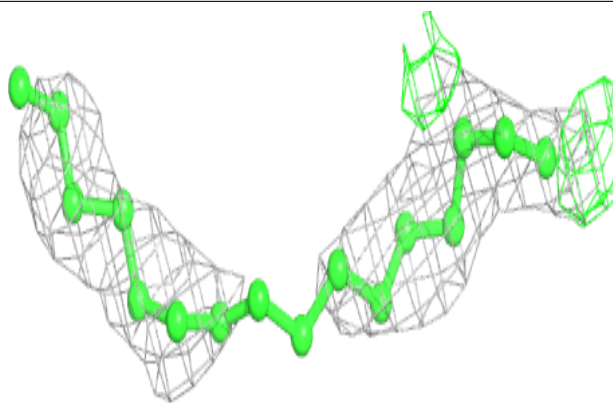
**Electron density around OLC D 302:**

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



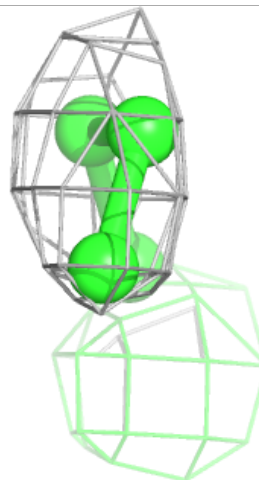
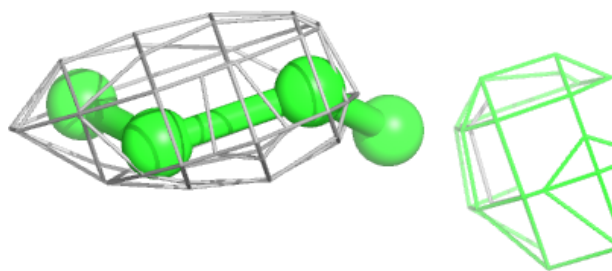
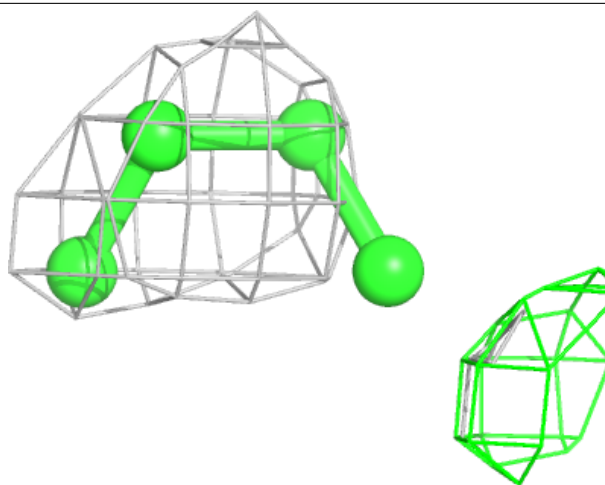
Electron density around LFA A 314:

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



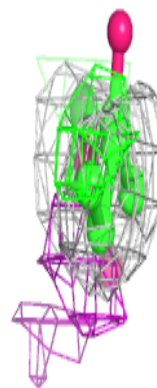
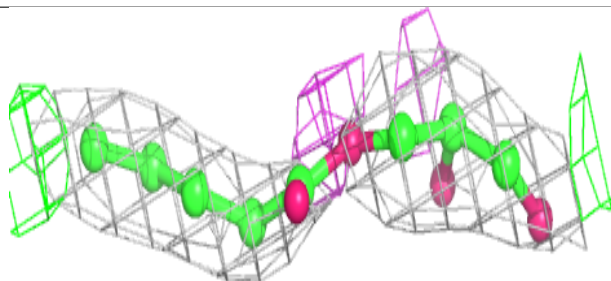
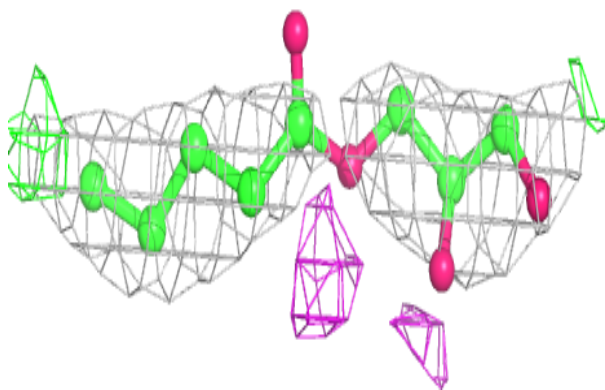
Electron density around LFA C 314:

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

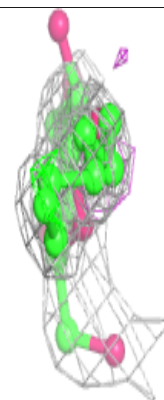
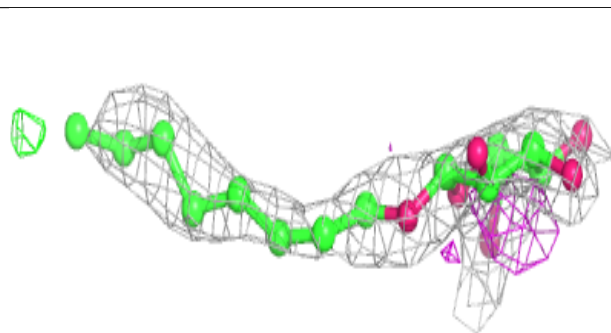
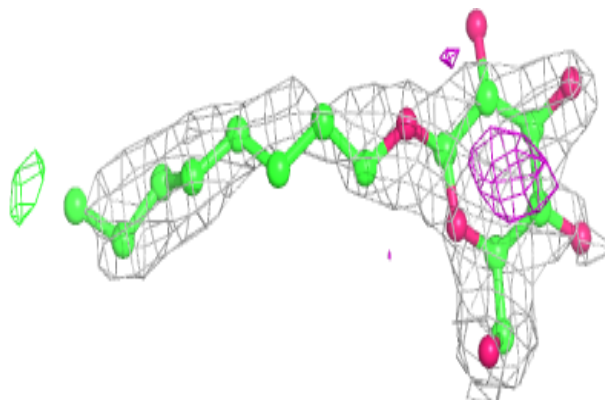


Electron density around OLC C 302:

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

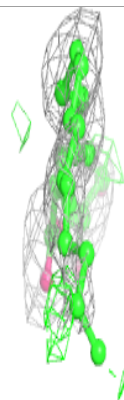
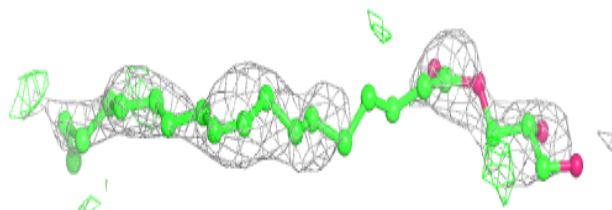
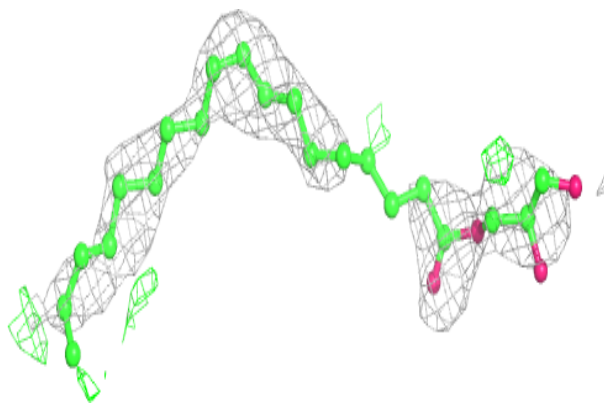
**Electron density around BOG B 314:**

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

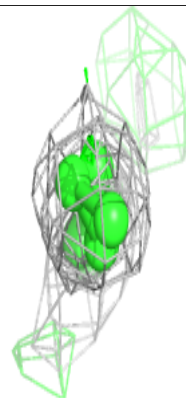
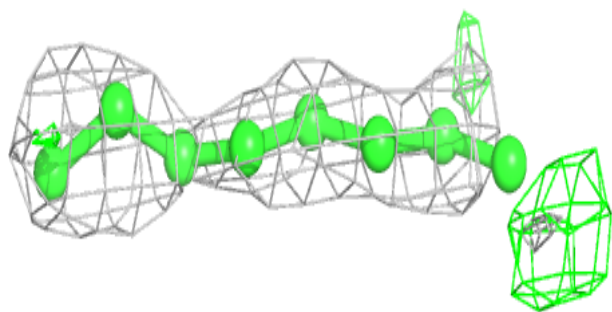
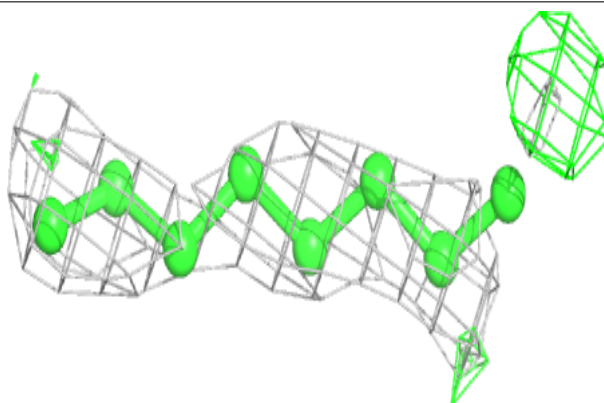


Electron density around OLC D 304:

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

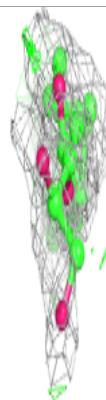
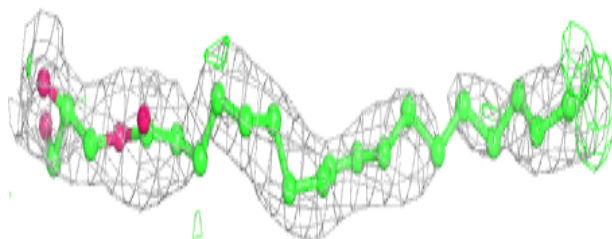
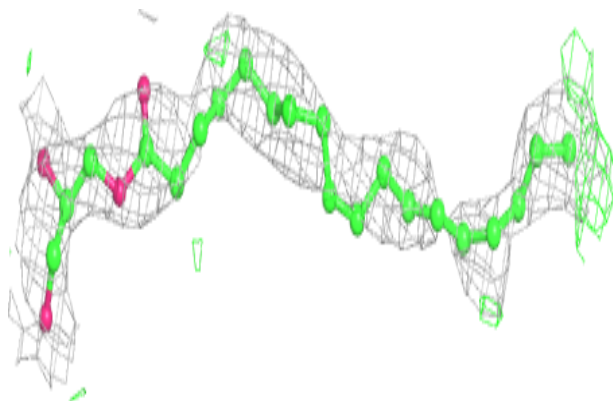
**Electron density around LFA E 311:**

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

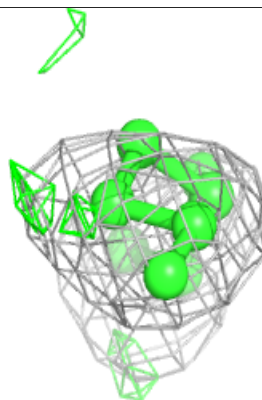
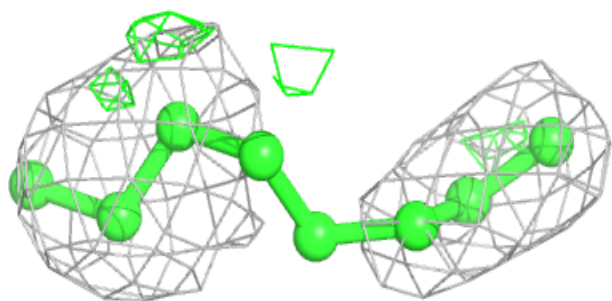
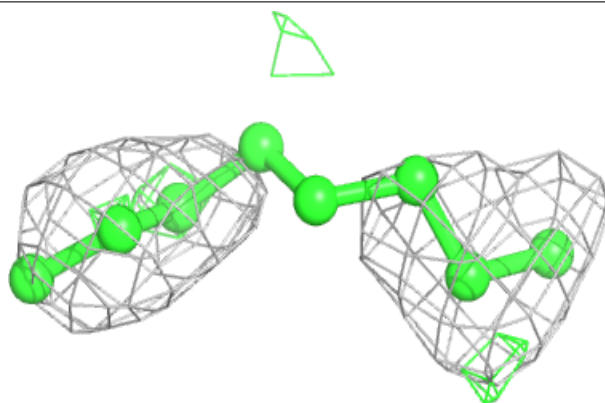


Electron density around OLC B 303:

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

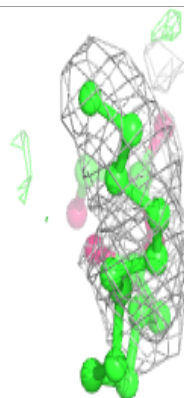
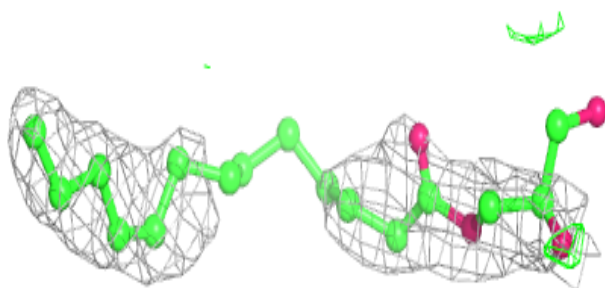
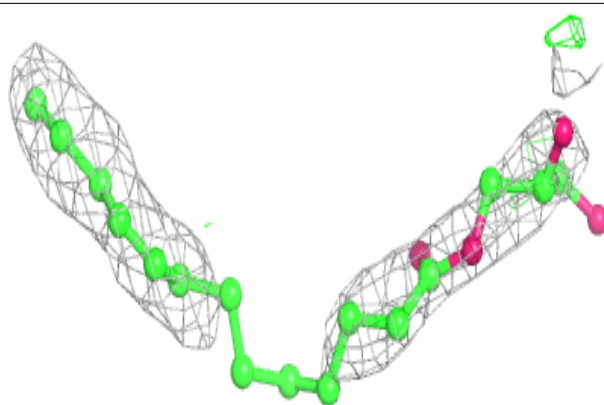
**Electron density around LFA A 311:**

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

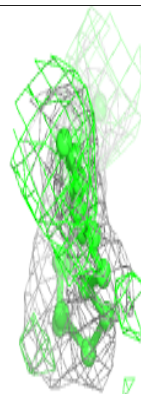
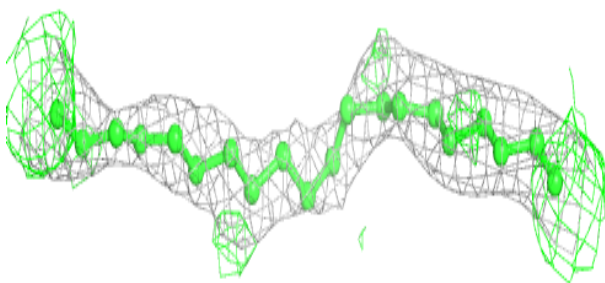
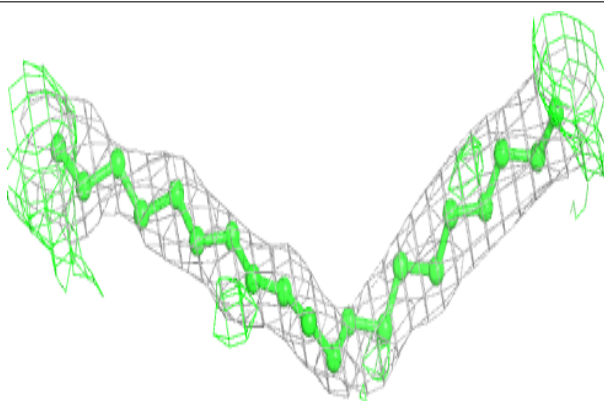


Electron density around OLC E 310:

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

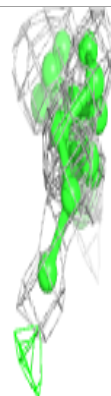
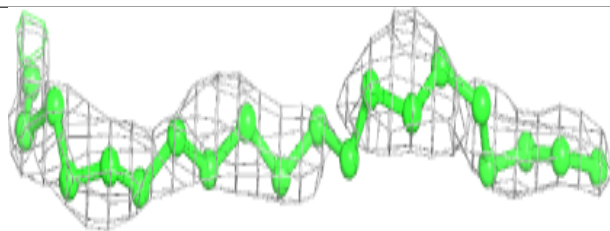
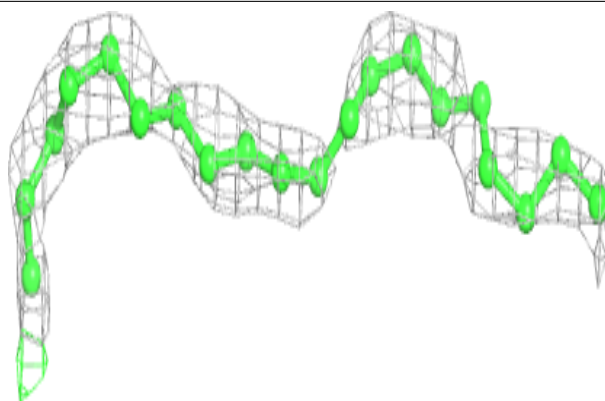
**Electron density around LFA E 302:**

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

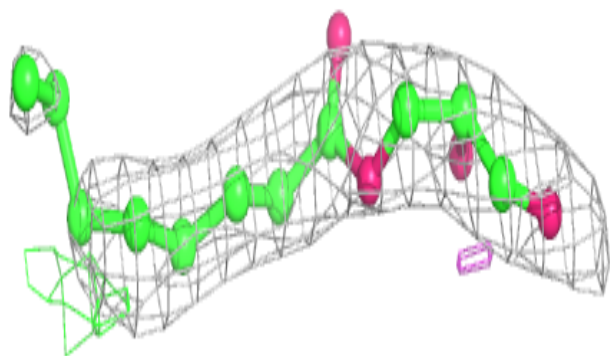
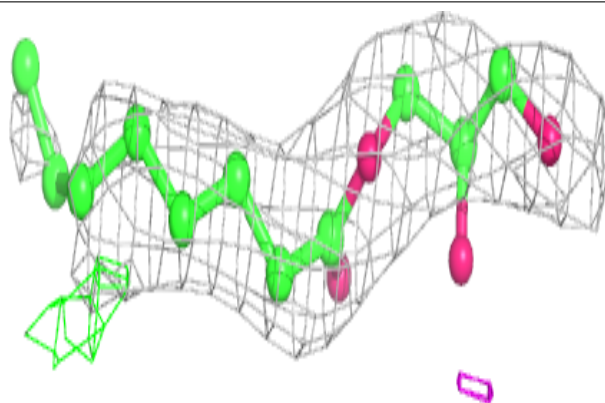


Electron density around LFA D 310:

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

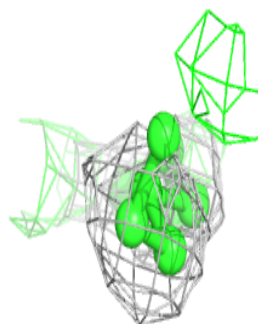
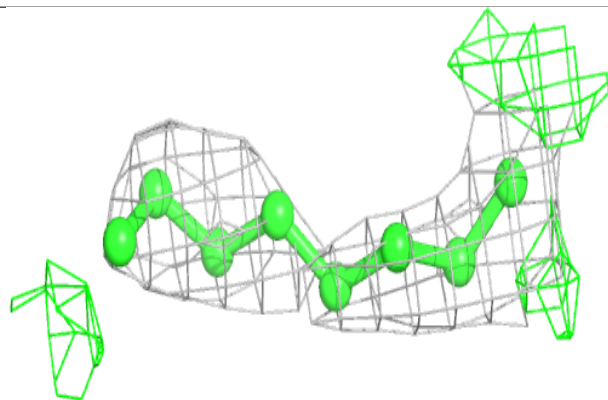
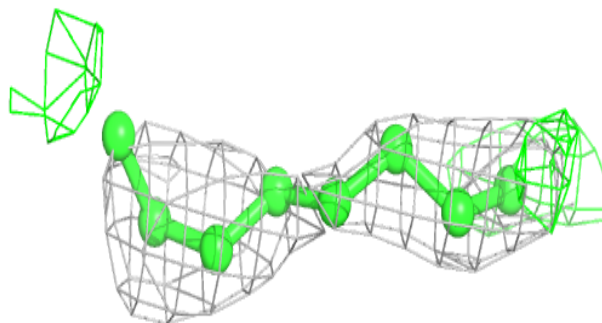
**Electron density around OLC E 306:**

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

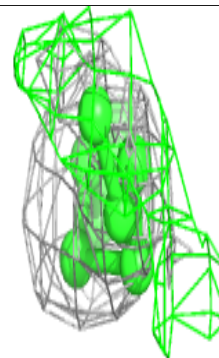
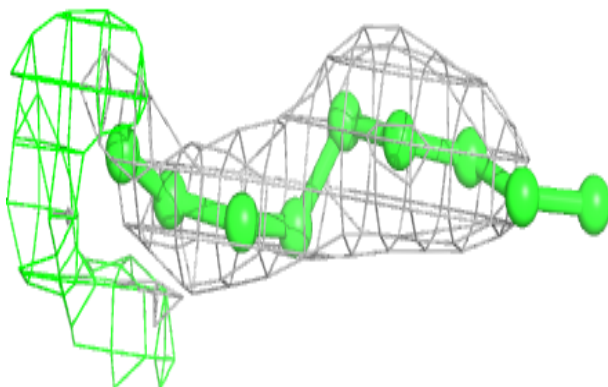
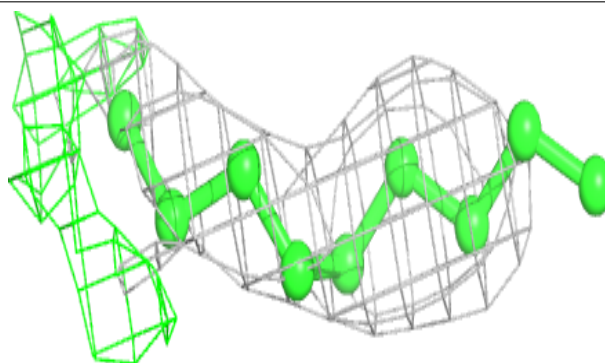


Electron density around LFA A 310:

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

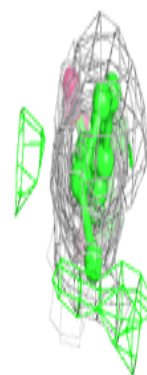
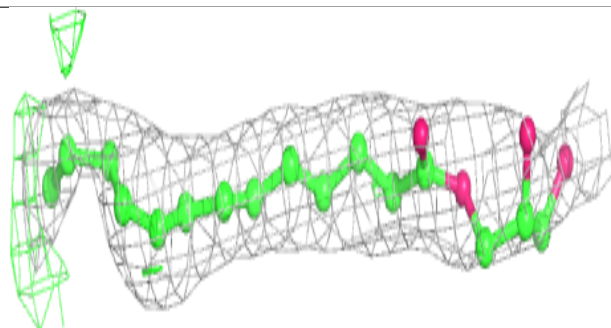
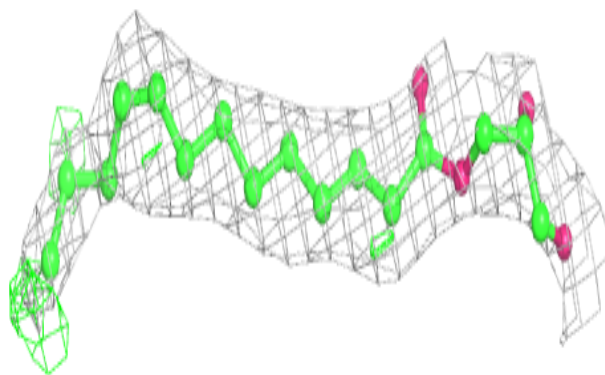
**Electron density around LFA B 309:**

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

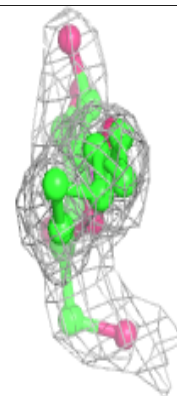
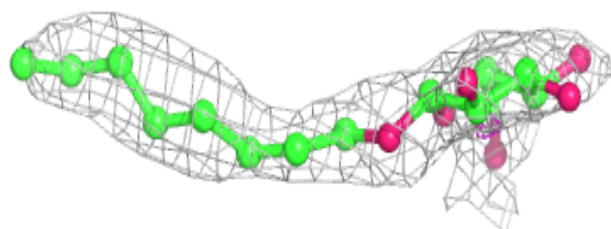
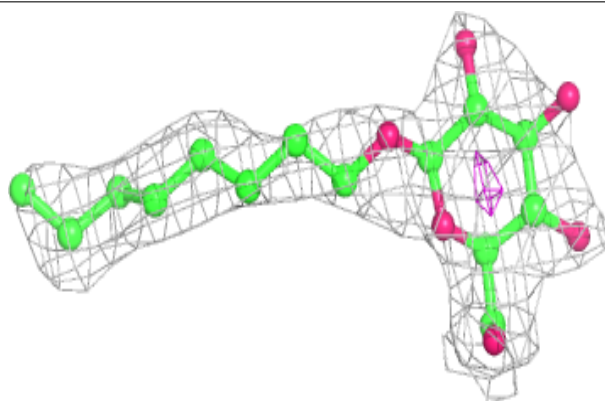


Electron density around OLC B 305:

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

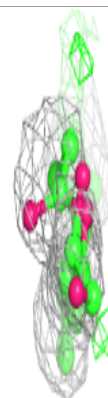
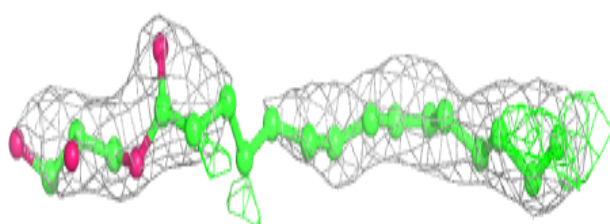
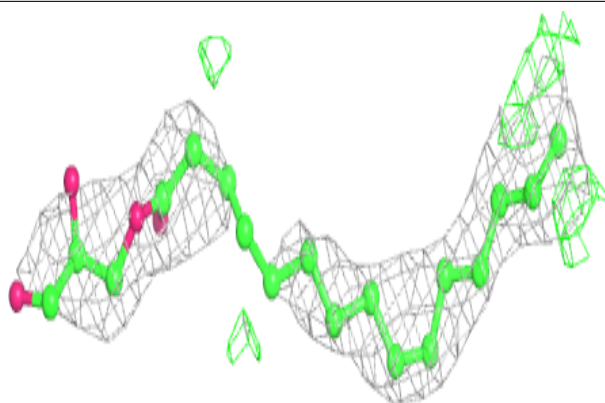
**Electron density around BOG C 317:**

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

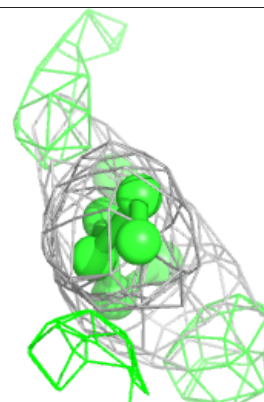
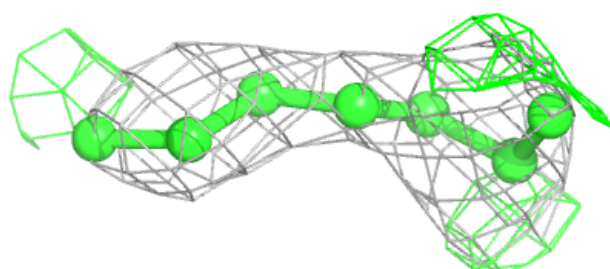
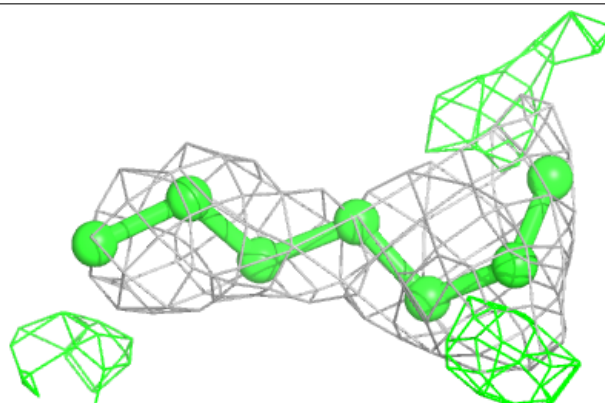


Electron density around OLC C 305:

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

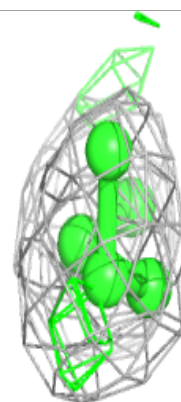
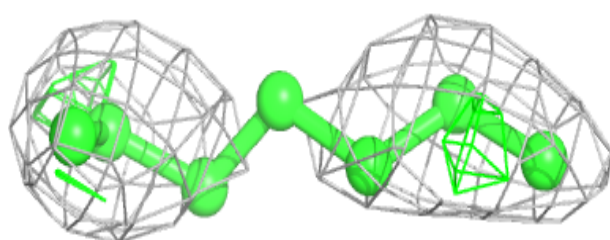
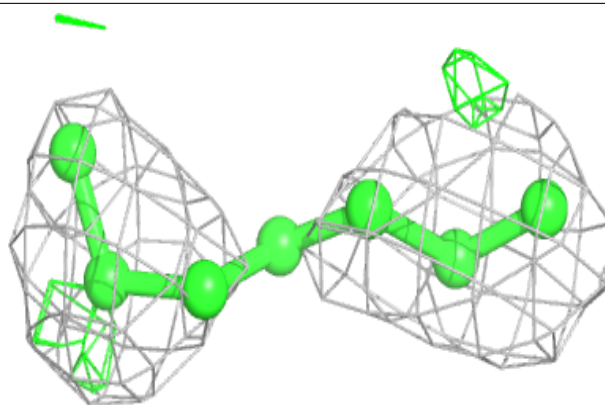
**Electron density around LFA A 309:**

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

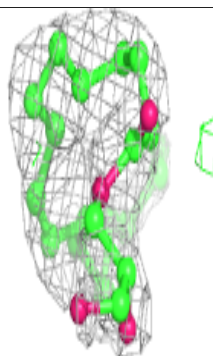
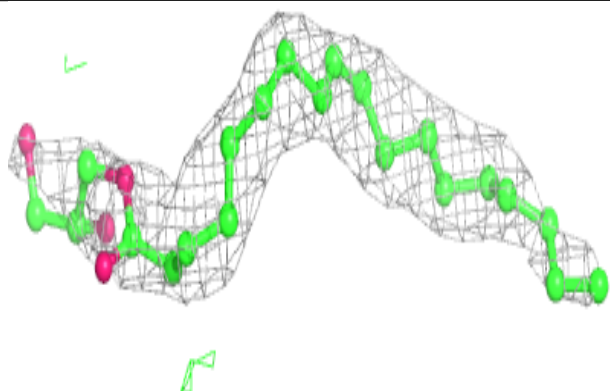
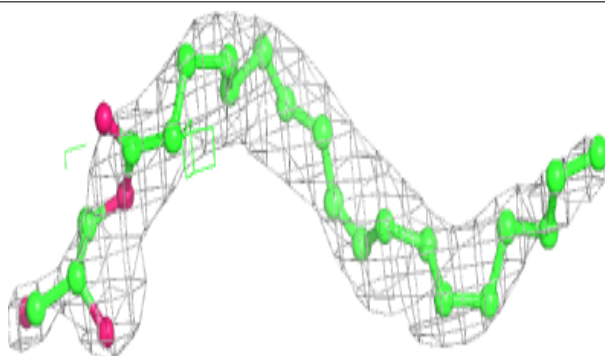


Electron density around LFA B 312:

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

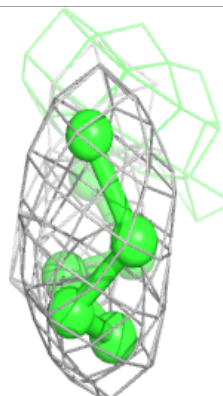
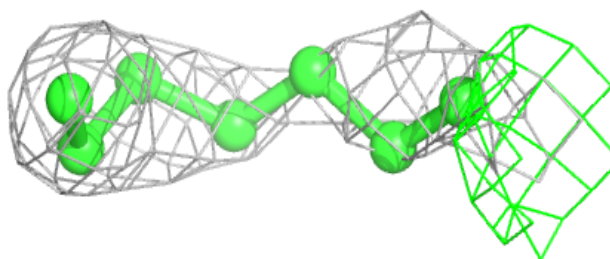
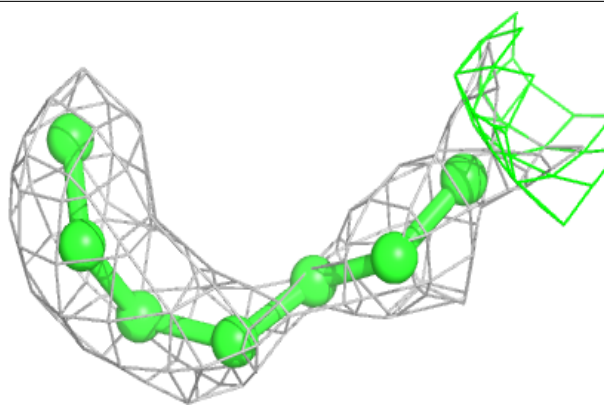
**Electron density around OLC E 301:**

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

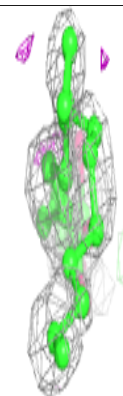
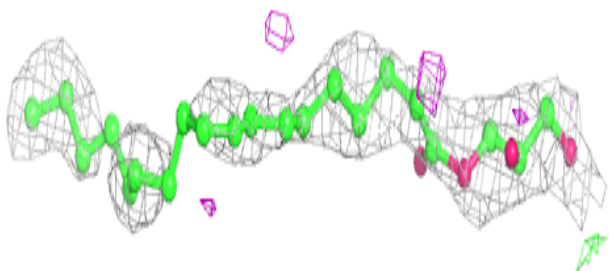
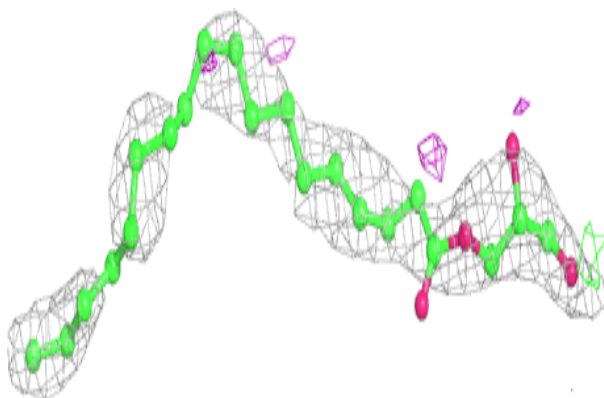


Electron density around OLC C 309:

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

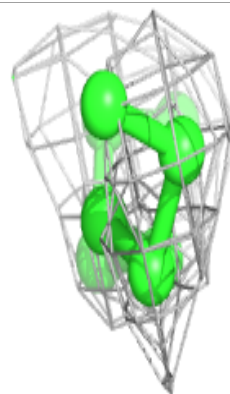
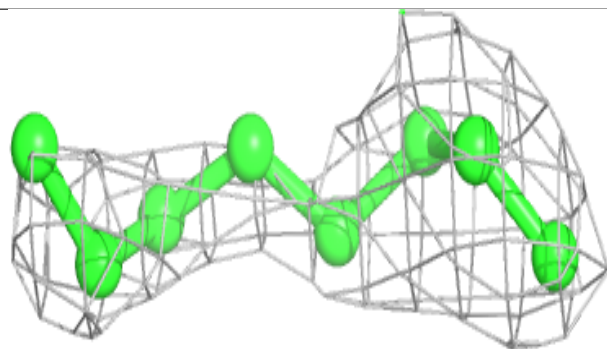
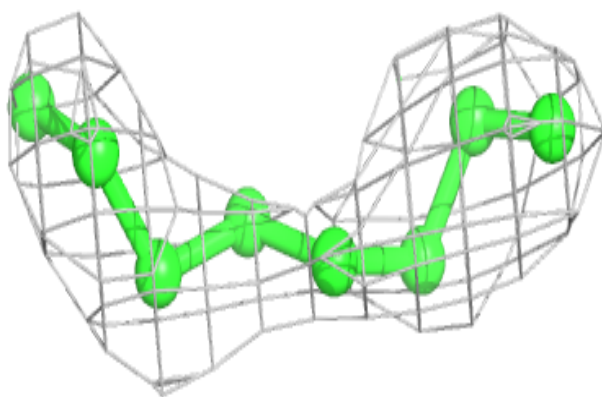
**Electron density around OLC D 309:**

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

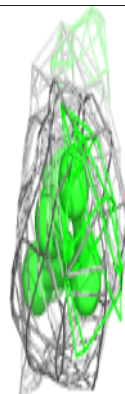
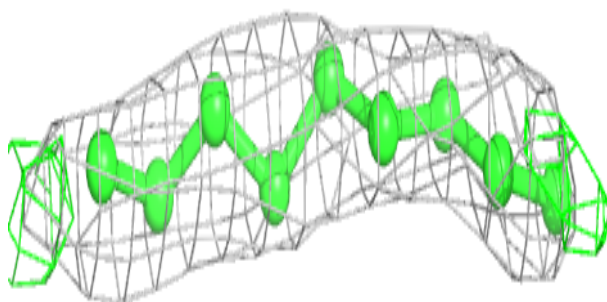
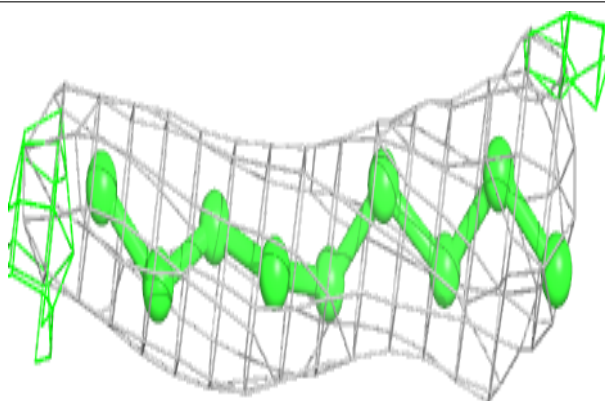


Electron density around LFA D 312:

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

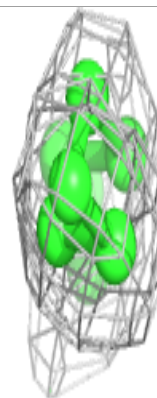
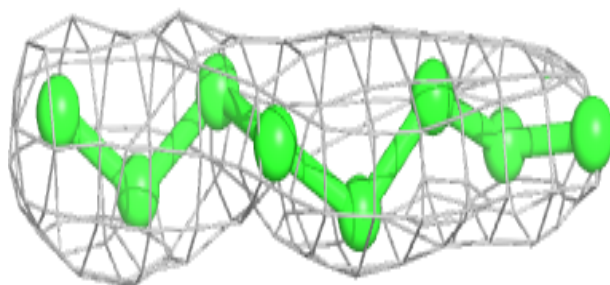
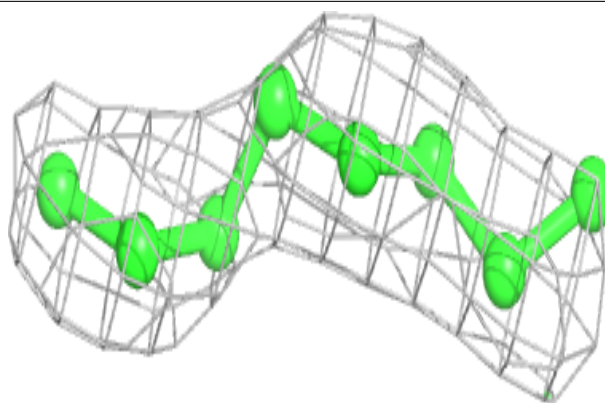
**Electron density around LFA A 320:**

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

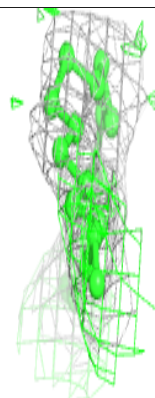
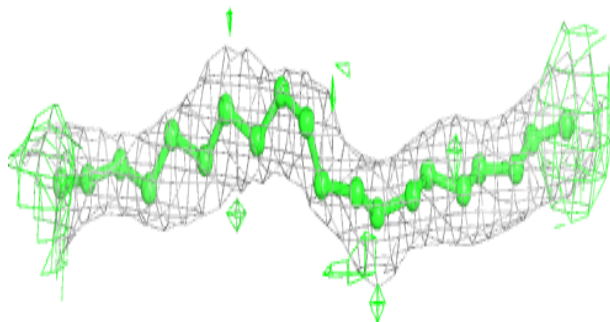
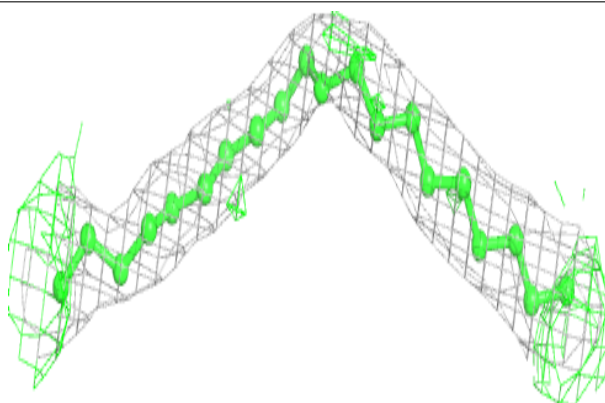


Electron density around LFA C 311:

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

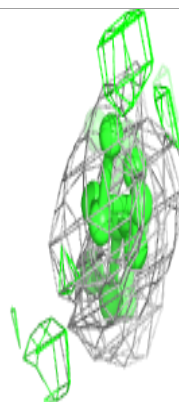
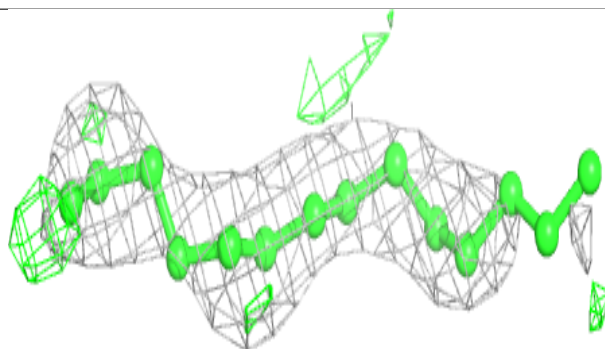
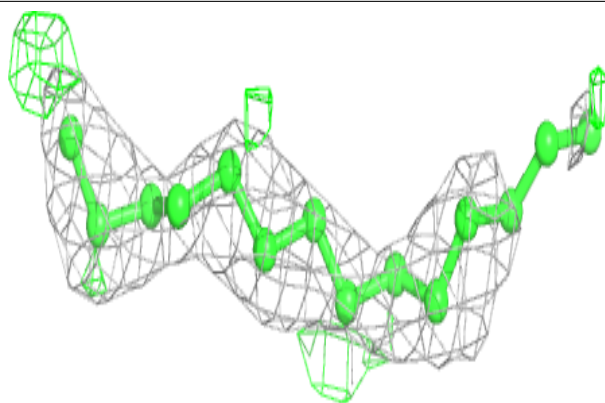
**Electron density around LFA B 302:**

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

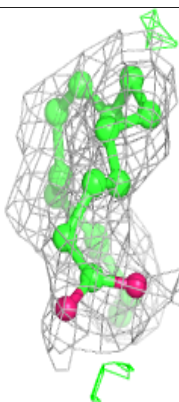
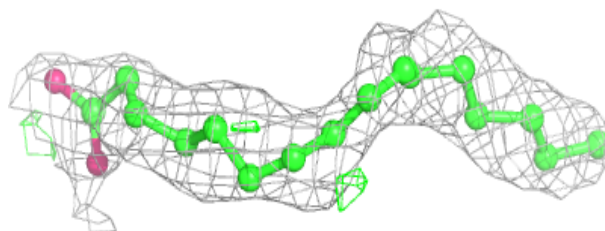


Electron density around LFA E 312:

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

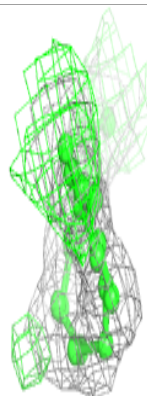
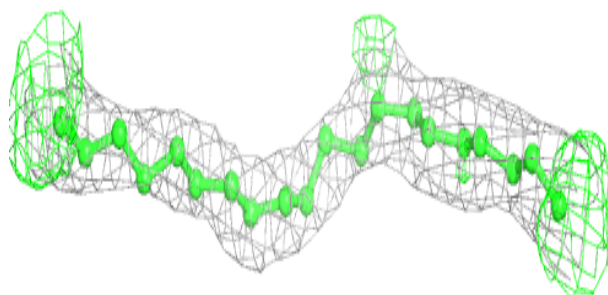
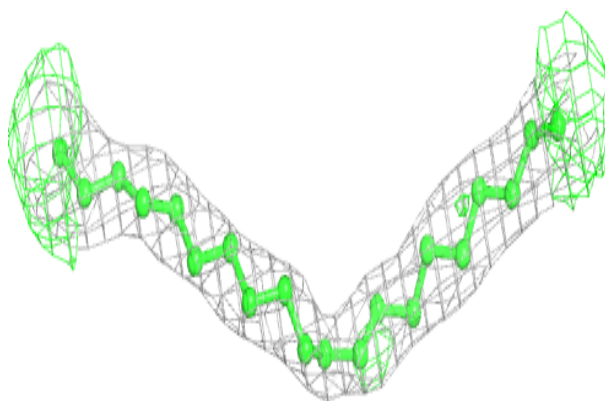
**Electron density around OLC D 306:**

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

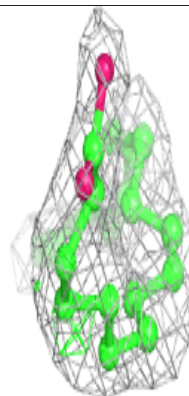
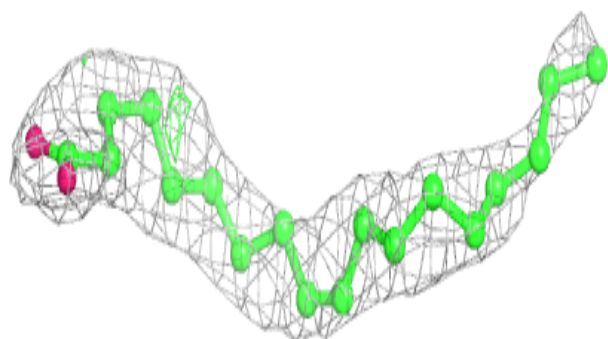
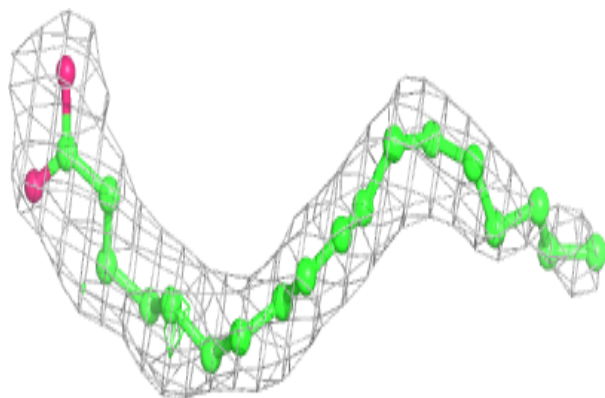


Electron density around LFA C 315:

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

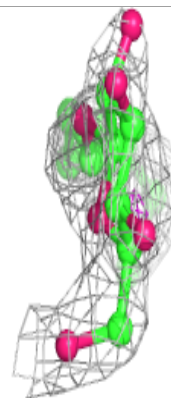
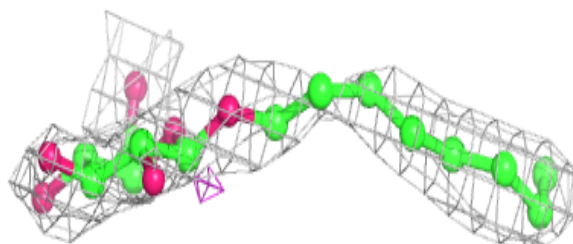
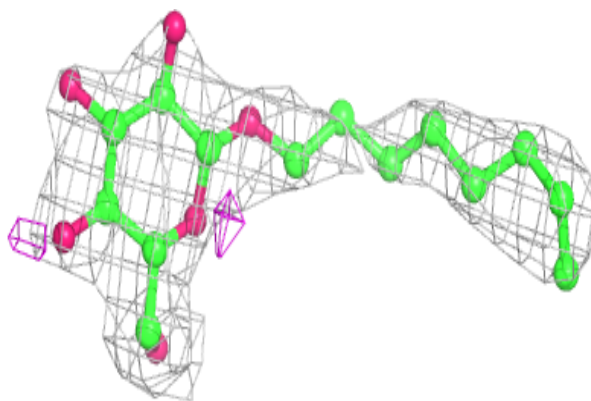
**Electron density around OLC A 318:**

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

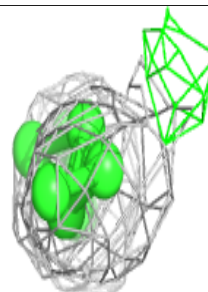
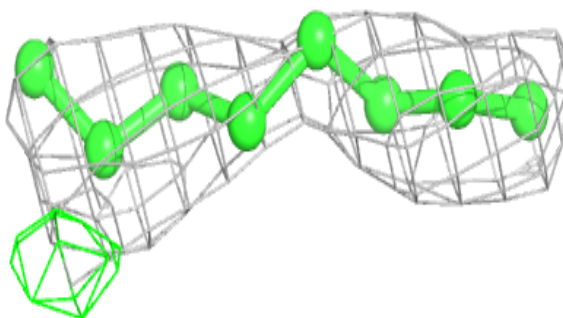
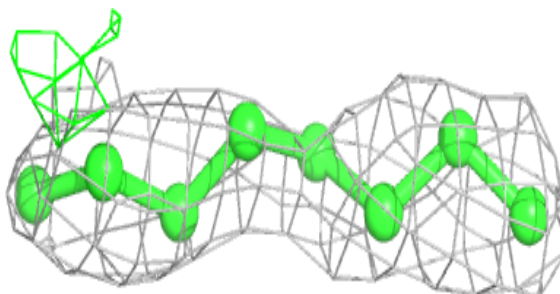


Electron density around BOG D 317:

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

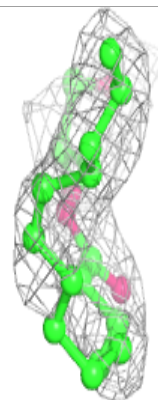
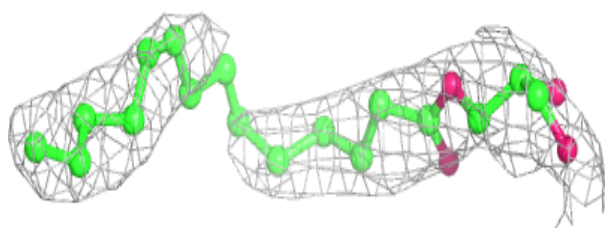
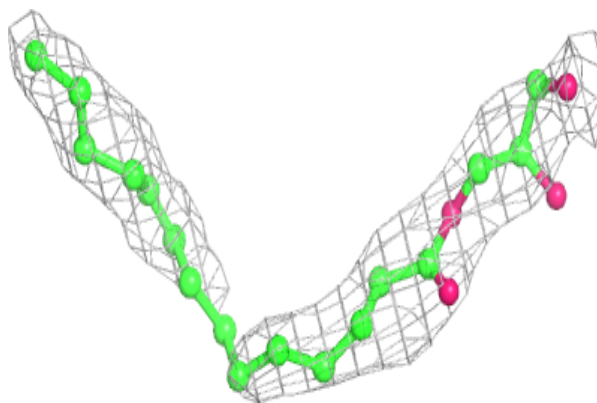
**Electron density around LFA B 310:**

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

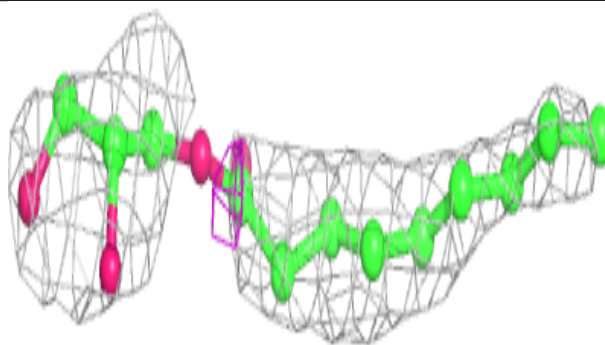
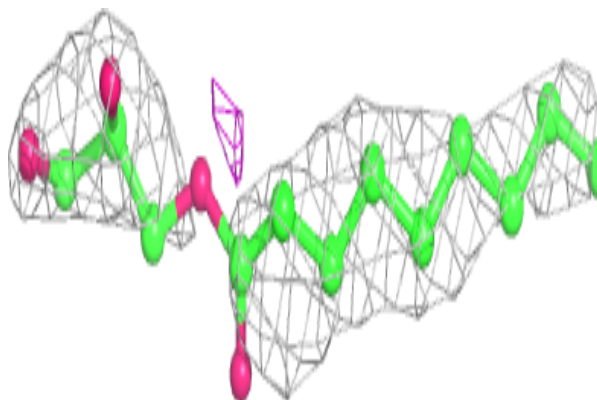


Electron density around OLC B 306:

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

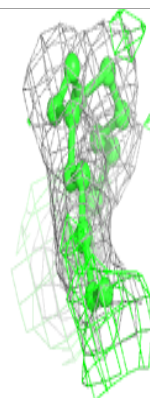
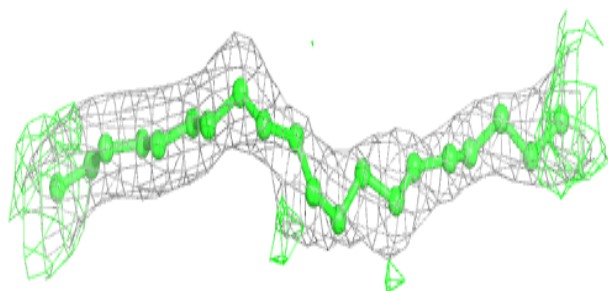
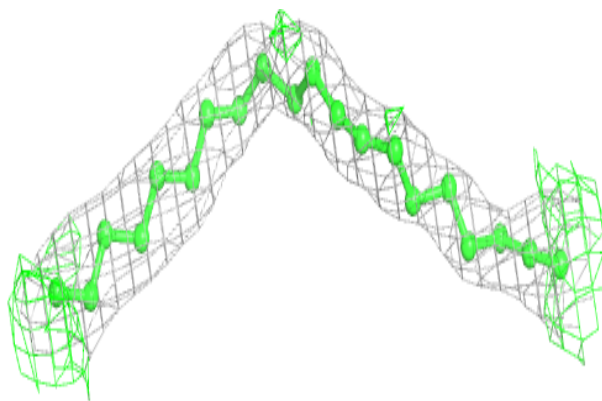
**Electron density around OLC A 308:**

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

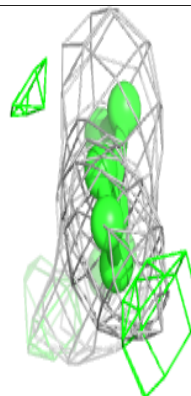
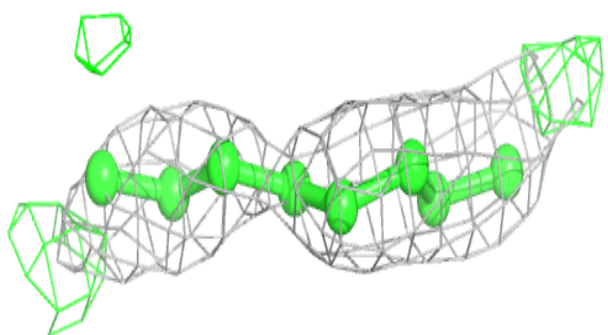
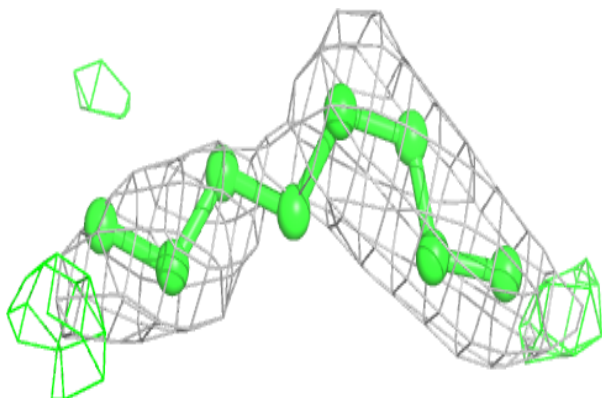


Electron density around LFA A 319:

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

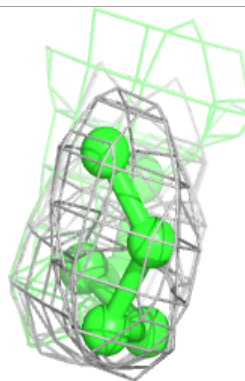
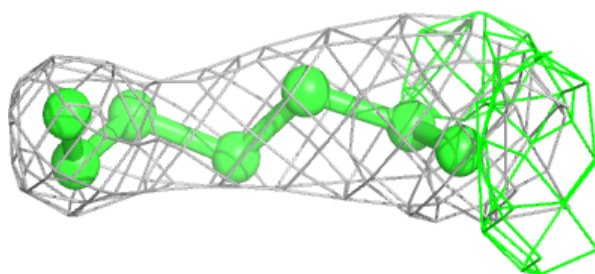
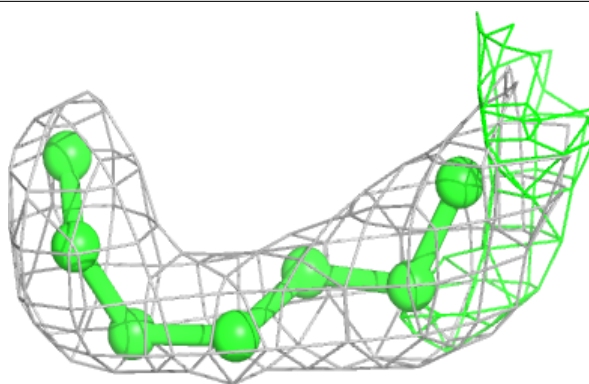
**Electron density around OLC E 303:**

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



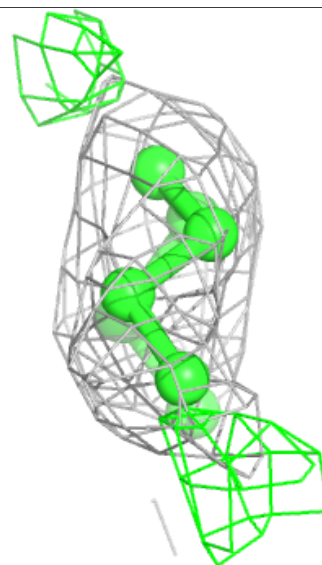
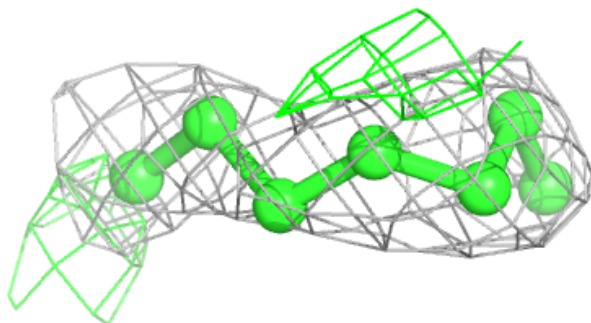
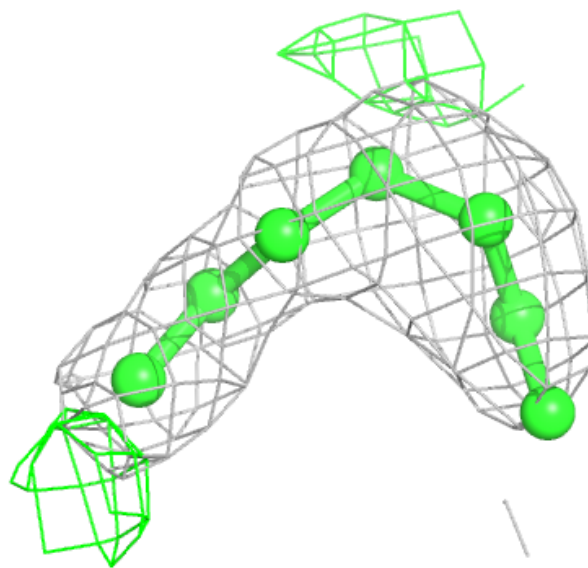
Electron density around OLC B 308:

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



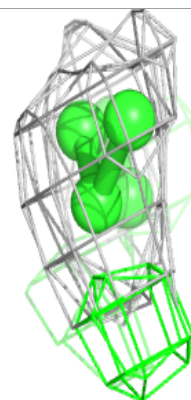
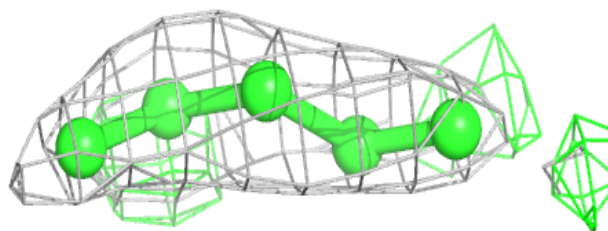
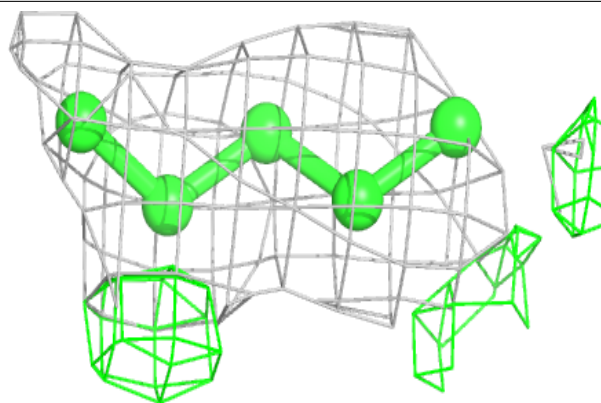
Electron density around OLC A 307:

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

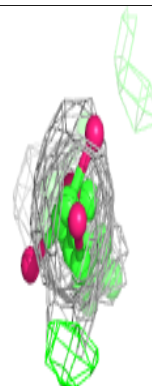
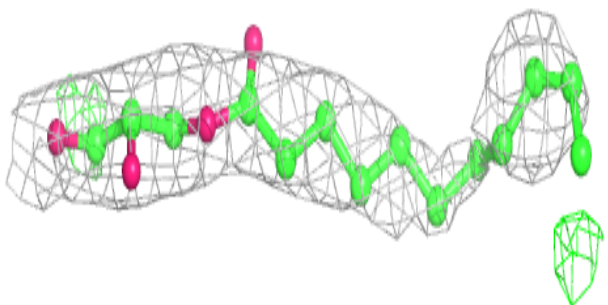
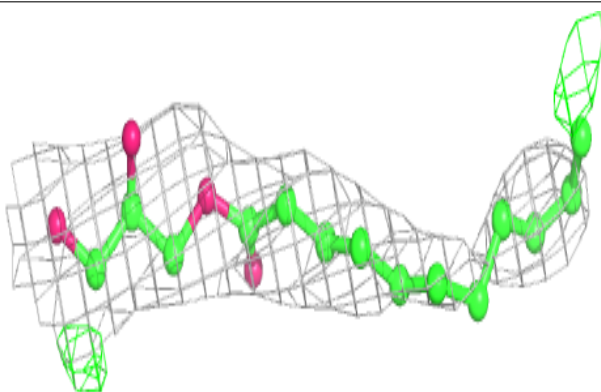


Electron density around LFA E 314:

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

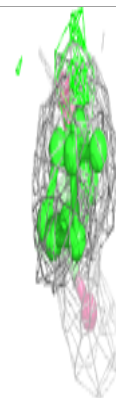
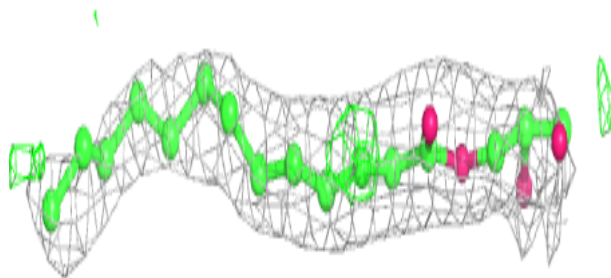
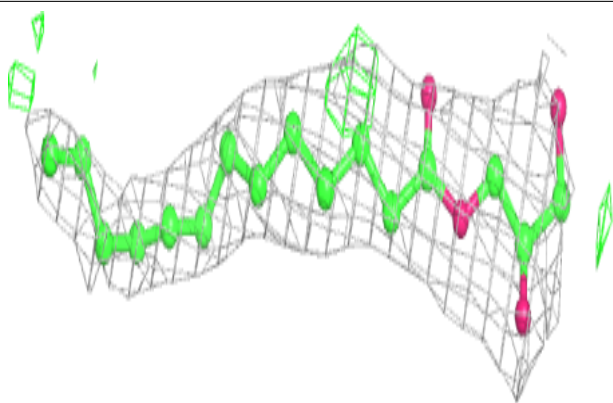
**Electron density around OLC D 305:**

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

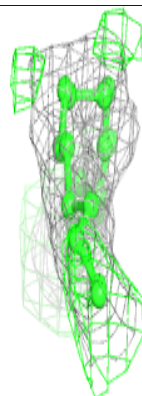
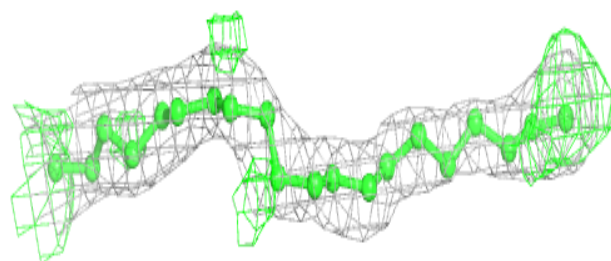
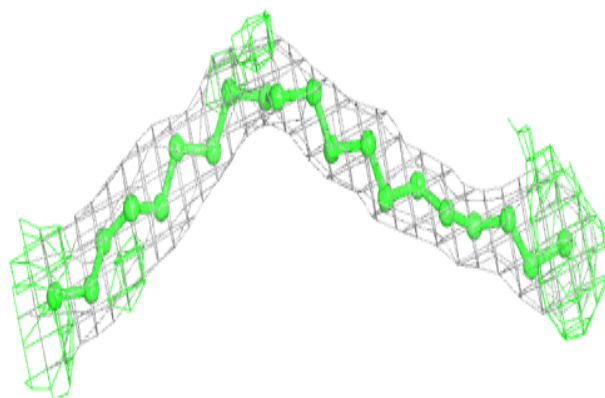


Electron density around OLC C 306:

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

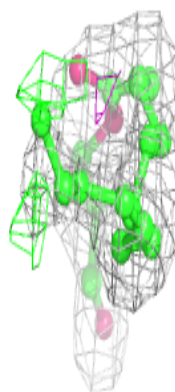
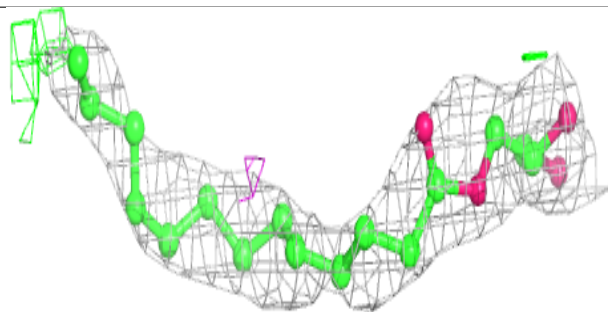
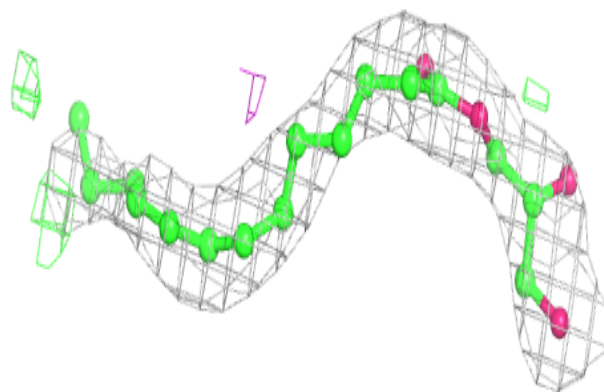
**Electron density around LFA C 303:**

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

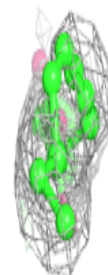
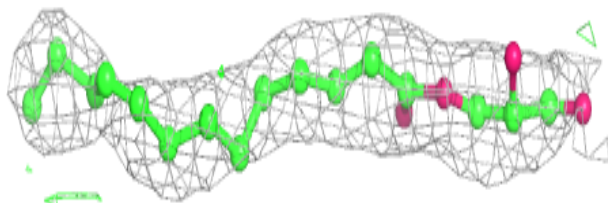
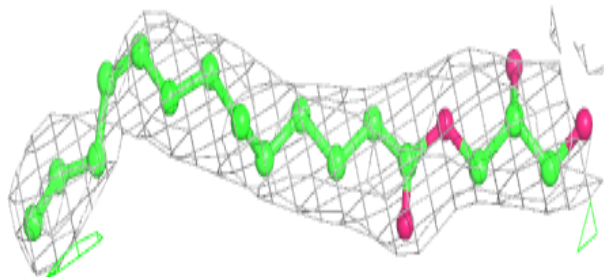


Electron density around OLC C 301:

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

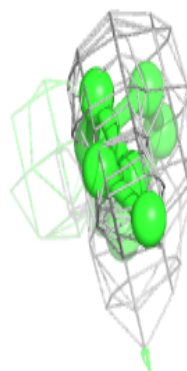
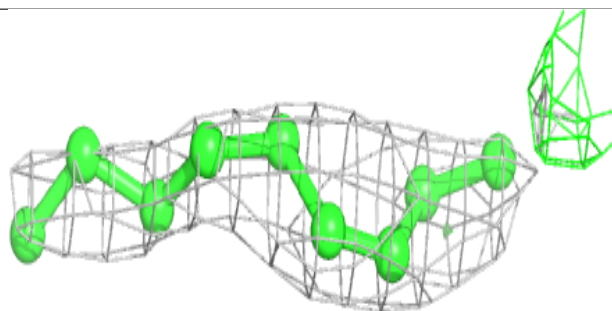
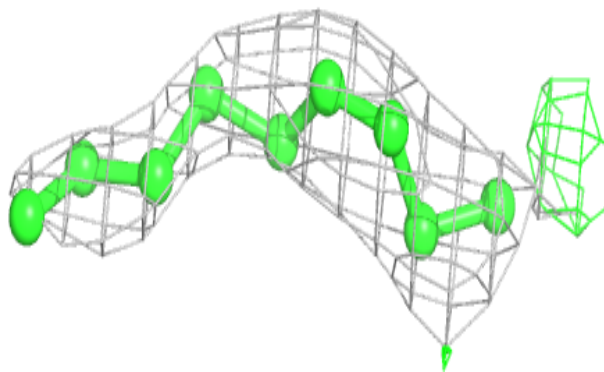
**Electron density around OLC E 305:**

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

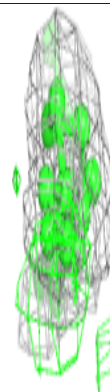
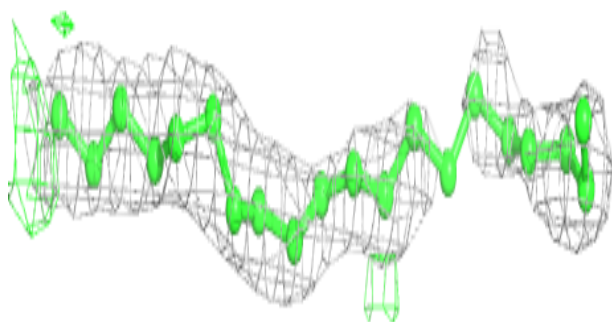
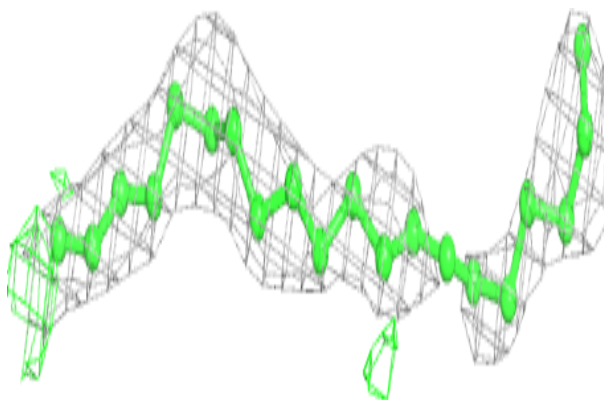


Electron density around OLC A 301:

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

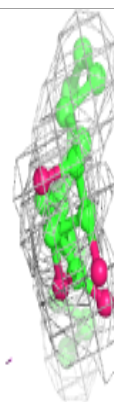
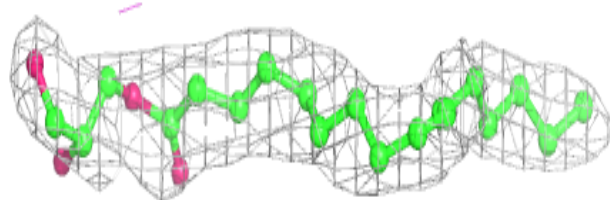
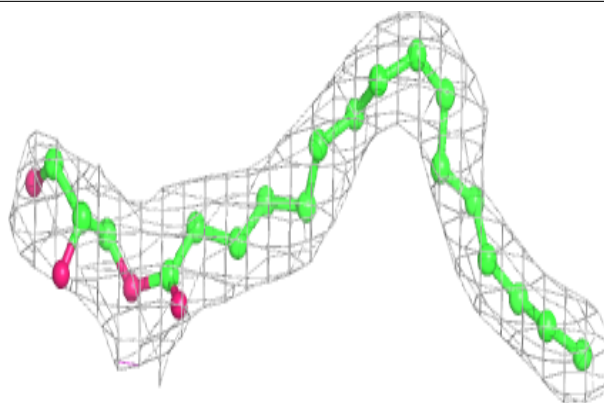
**Electron density around LFA C 312:**

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

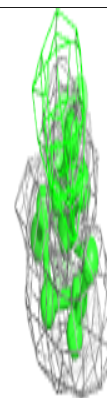
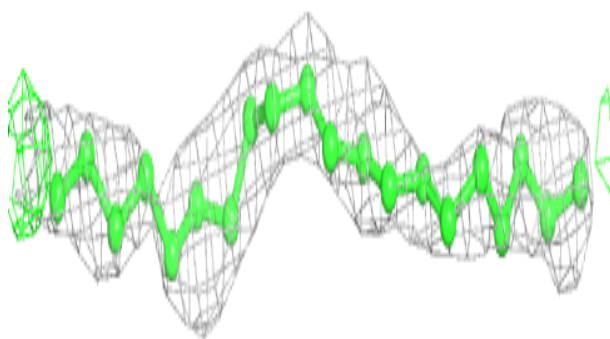
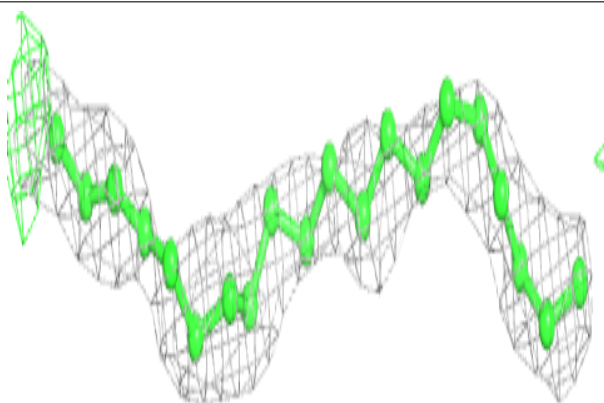


Electron density around OLC C 304:

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

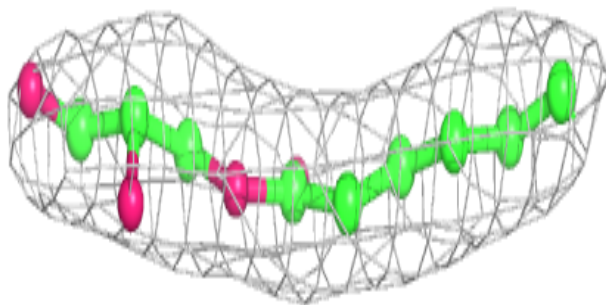
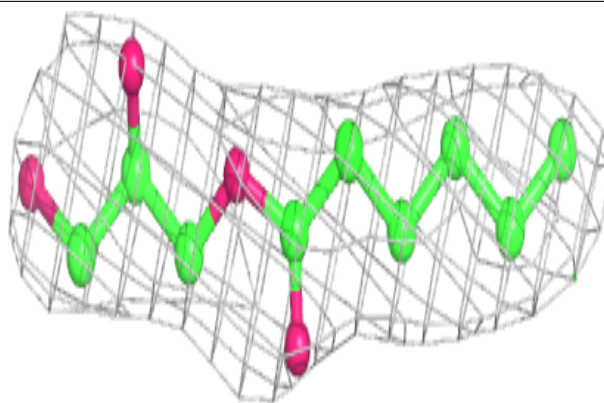
**Electron density around LFA D 311:**

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

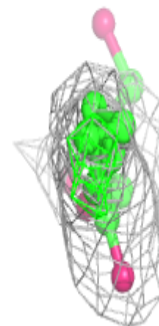
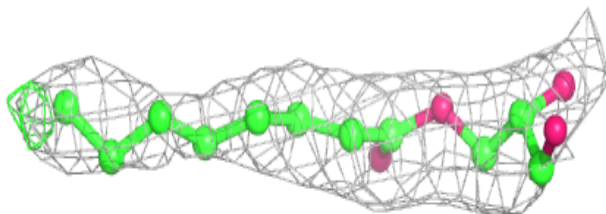
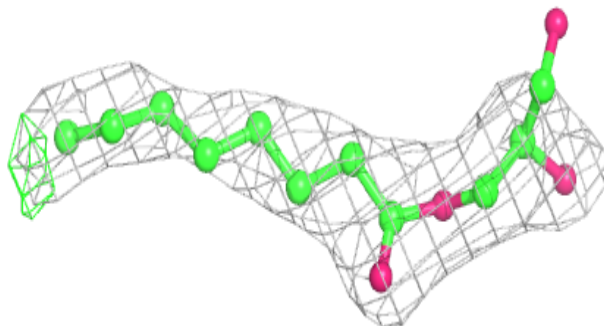


Electron density around OLC A 304:

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

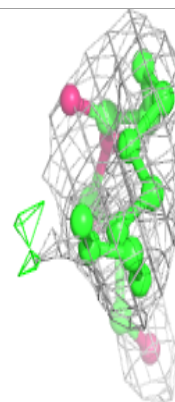
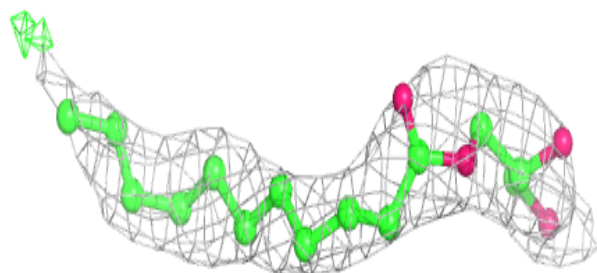
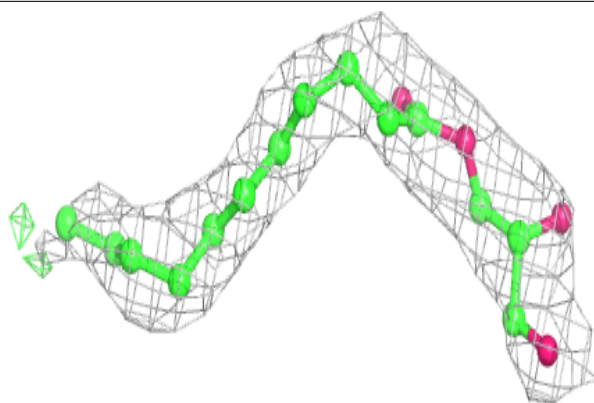
**Electron density around OLC A 306:**

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

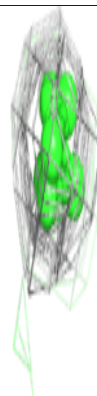
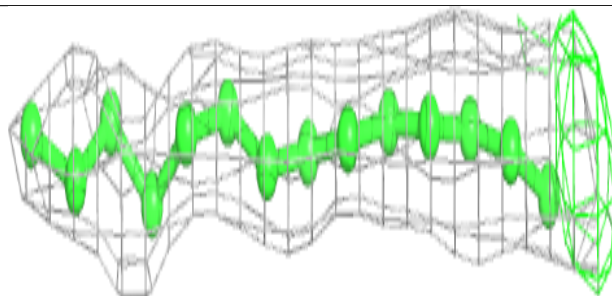
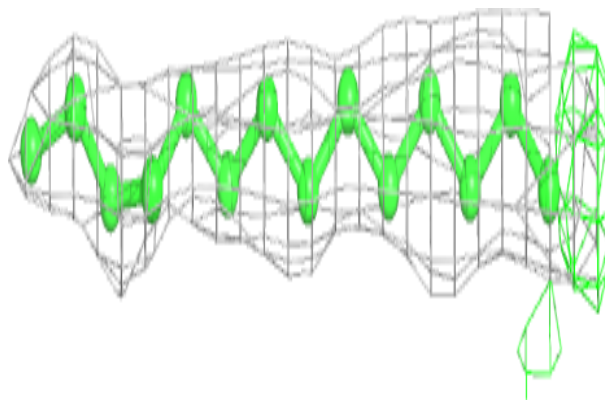


Electron density around OLC D 301:

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

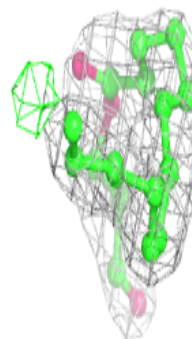
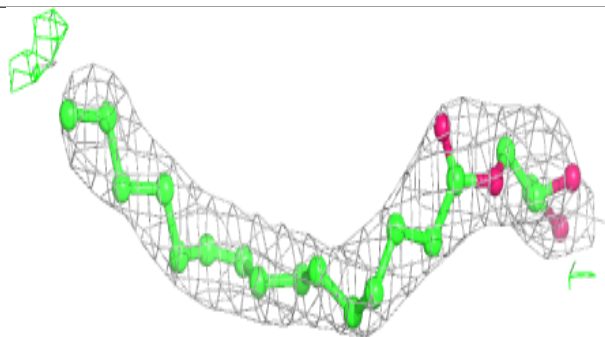
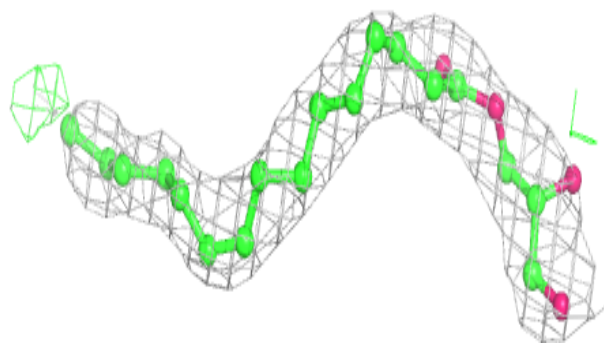
**Electron density around LFA C 318:**

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

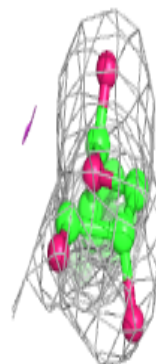
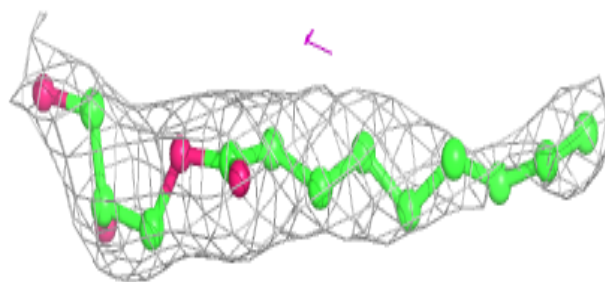
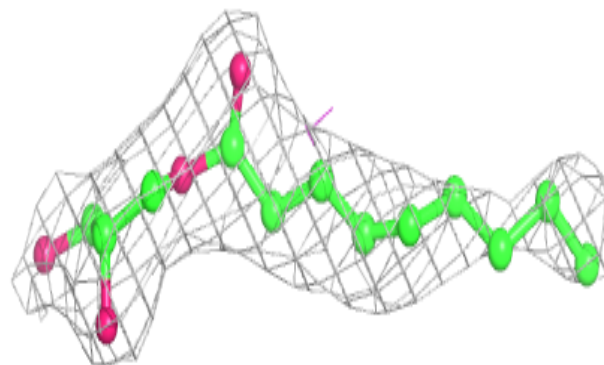


Electron density around OLC B 301:

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

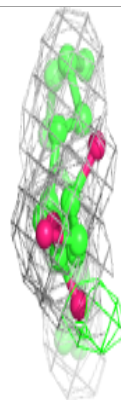
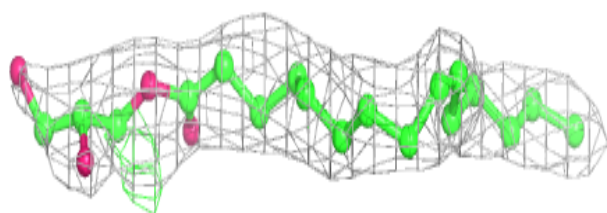
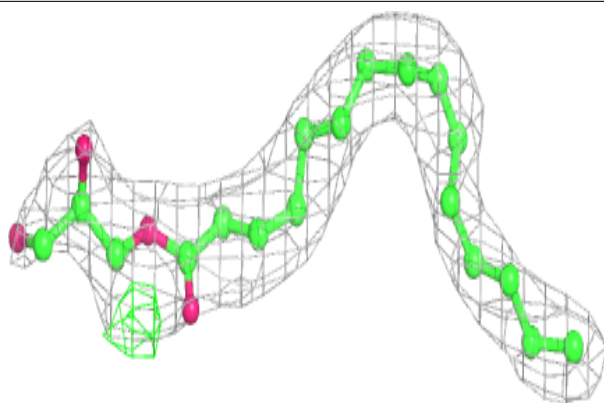
**Electron density around OLC C 308:**

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

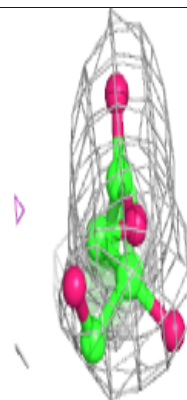
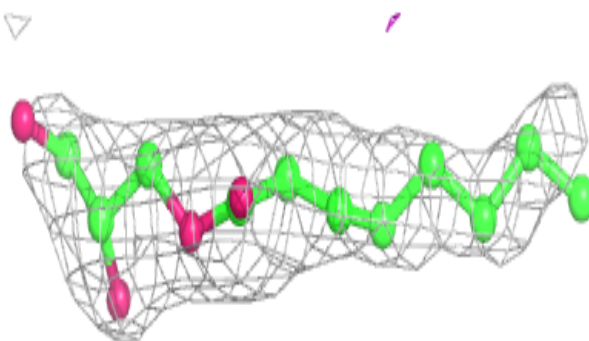
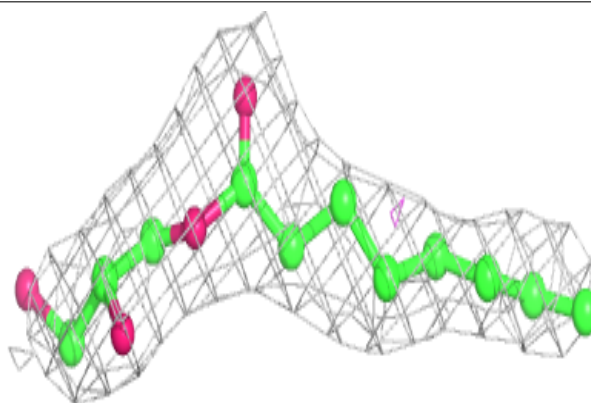


Electron density around OLC A 302:

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

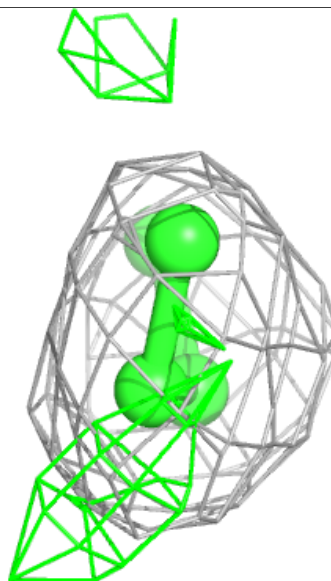
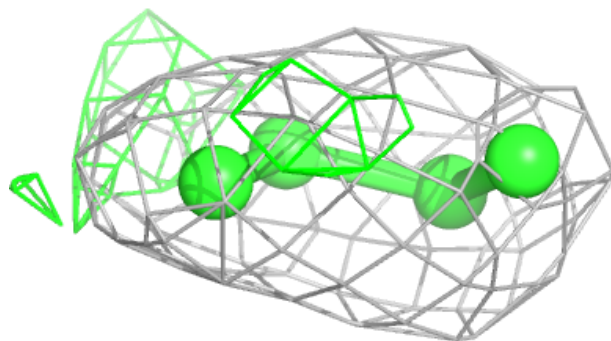
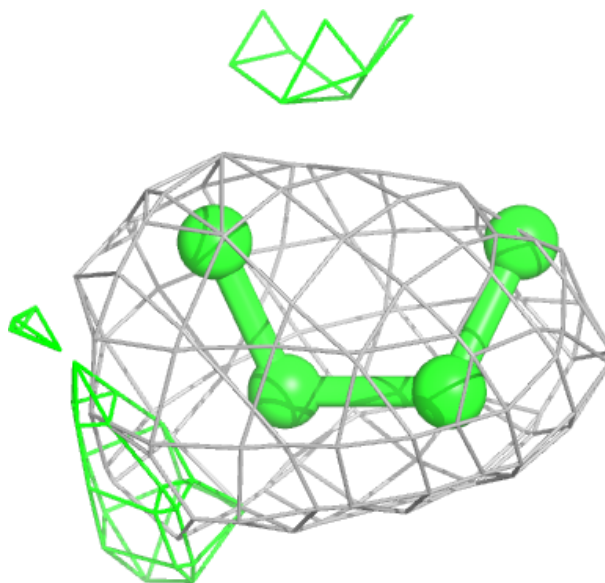
**Electron density around OLC E 307:**

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



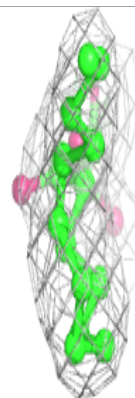
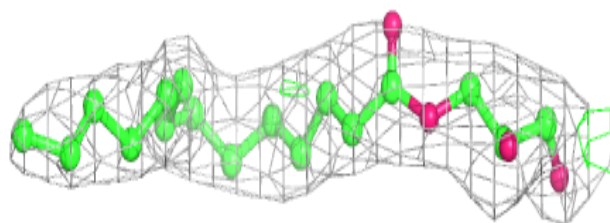
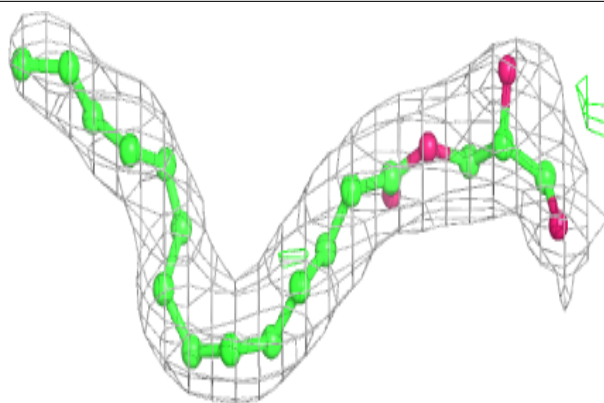
Electron density around LFA E 313:

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

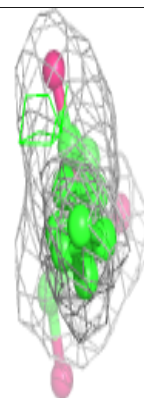
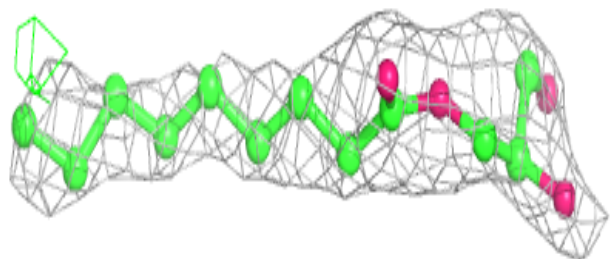
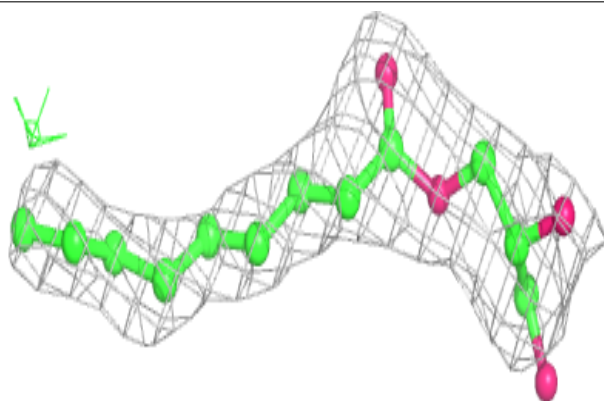


Electron density around OLC B 304:

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

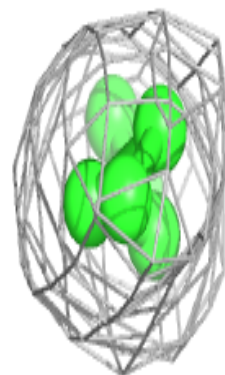
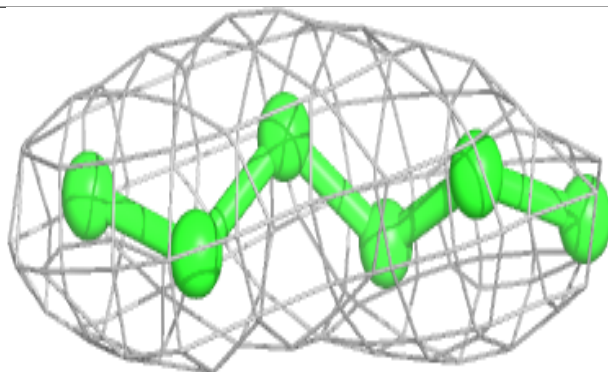
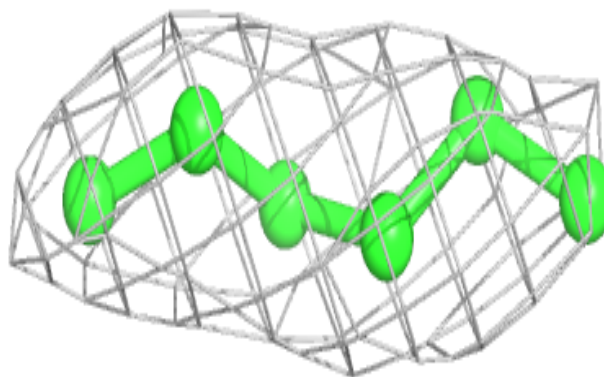
**Electron density around OLC B 307:**

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

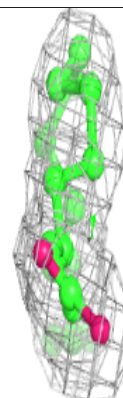
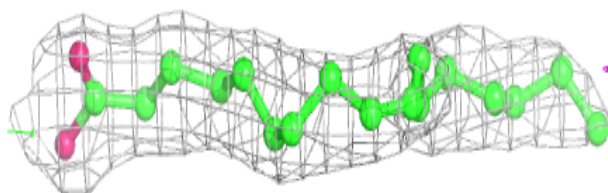
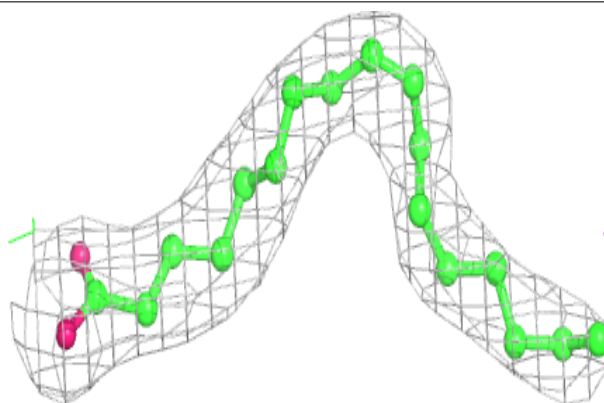


Electron density around LFA A 313:

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

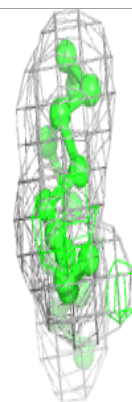
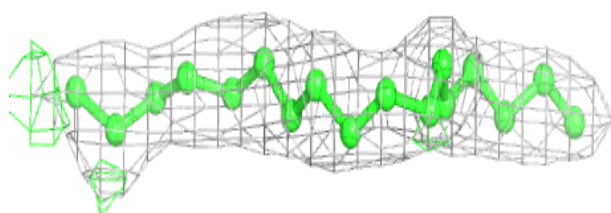
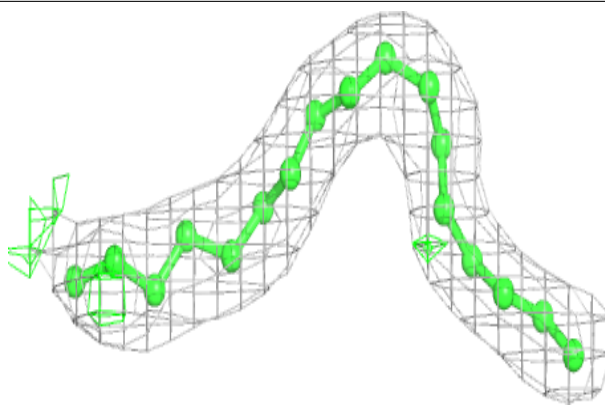
**Electron density around OLC A 317:**

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

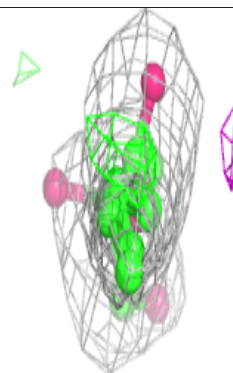
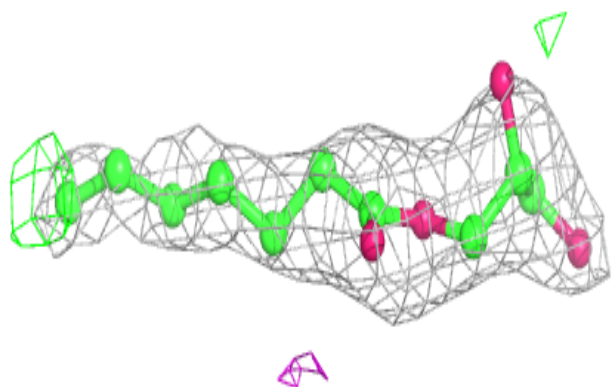
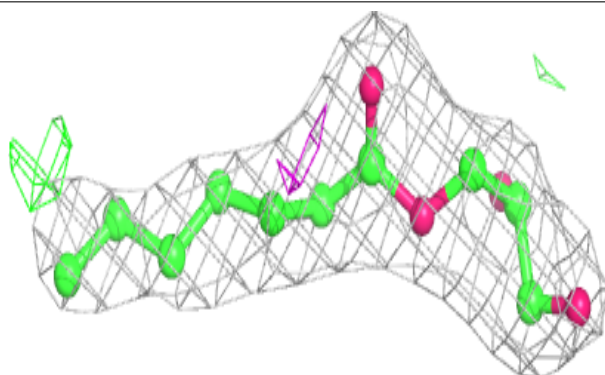


Electron density around LFA D 313:

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

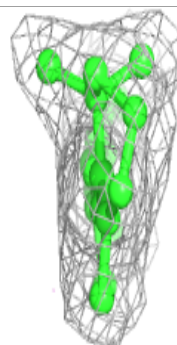
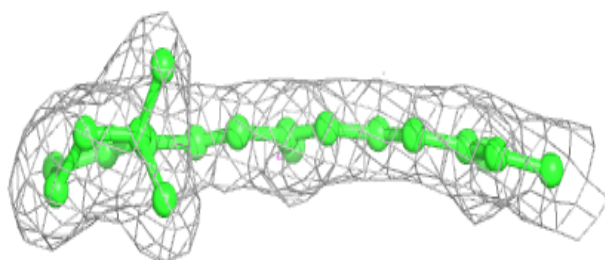
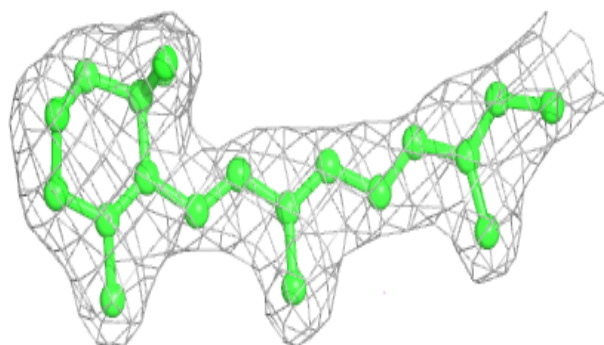
**Electron density around OLC D 307:**

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

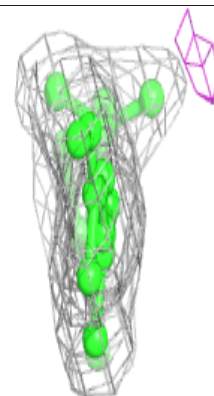
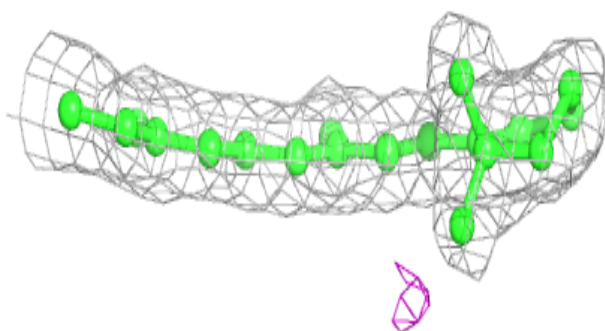
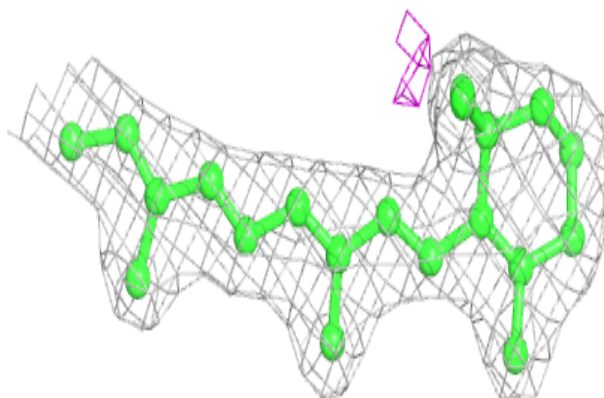


Electron density around RET E 318:

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

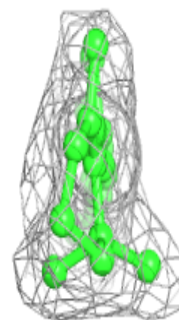
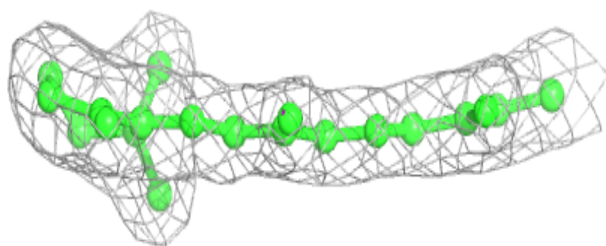
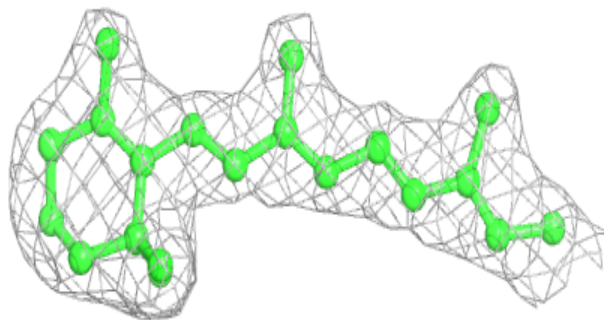
**Electron density around RET A 321:**

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

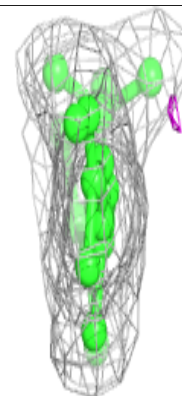
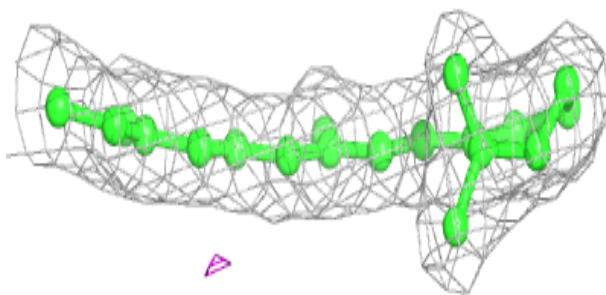
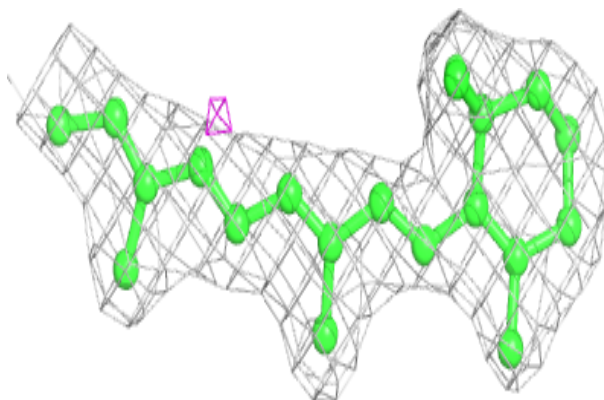


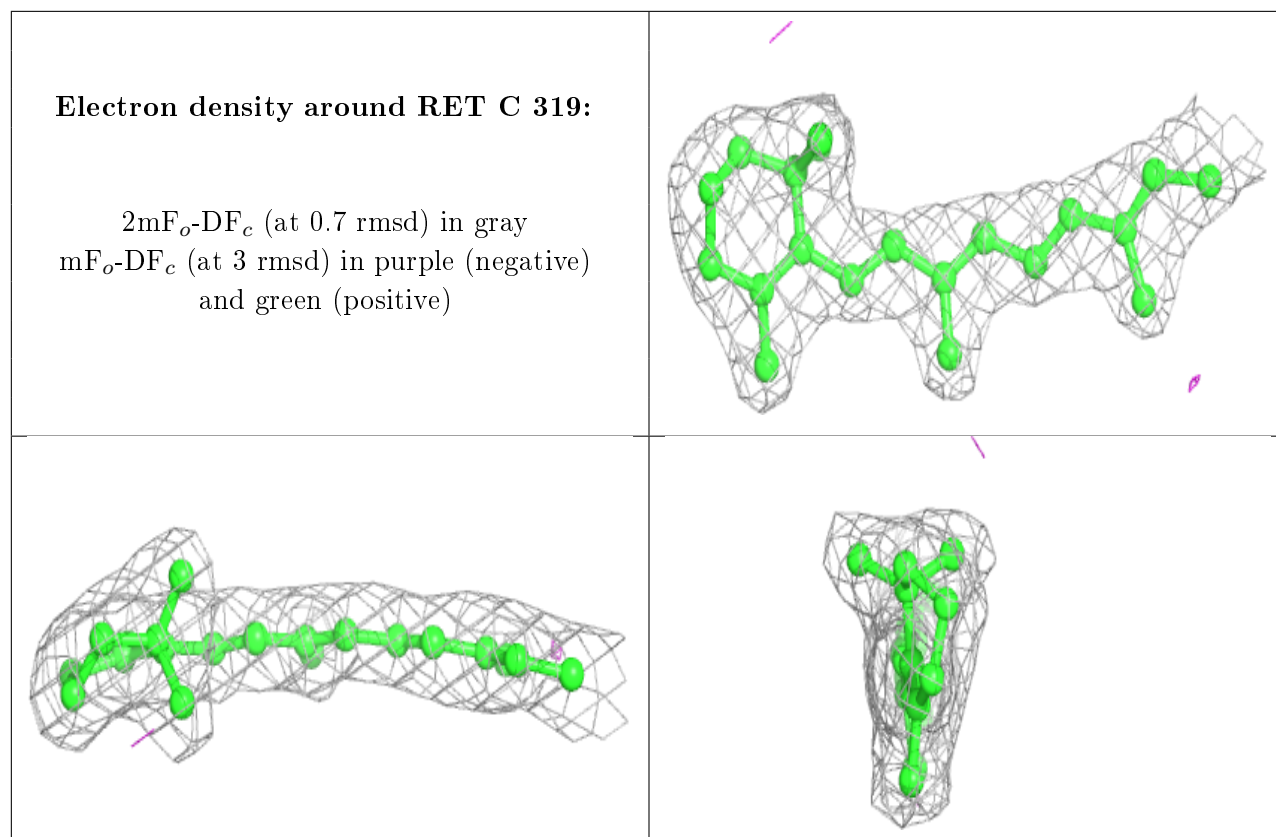
Electron density around RET D 318:

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

**Electron density around RET 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.