



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 09:14 AM EDT

PDB ID : 6SQG  
Title : Crystal structure of viral rhodopsin OLPVRII  
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Deposited on : 2019-09-03  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

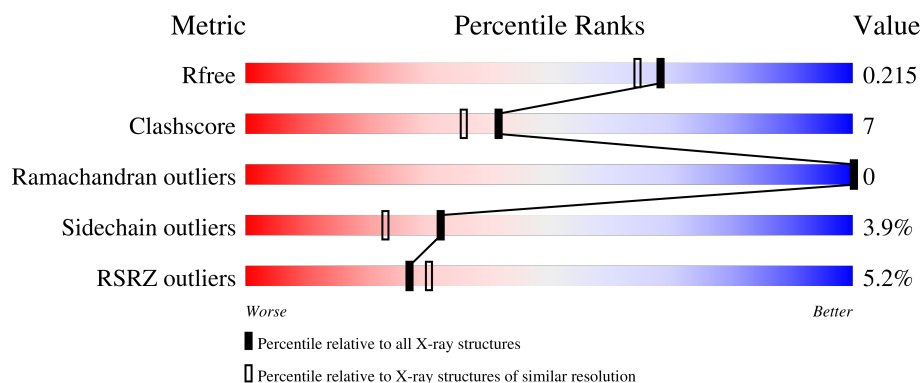
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	<div> <div>4%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	211	<div> <div>9%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	C	211	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	D	211	<div> <div>5%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	E	219	<div> <div>5%</div> <div>87%</div> <div>9%</div> <div>..</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	D	302	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9499 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 viral rhodopsin OLPVR11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	3	0
			1702	1143	259	289	11			
1	B	210	Total	C	N	O	S	0	2	0
			1707	1145	259	292	11			
1	C	209	Total	C	N	O	S	0	3	0
			1695	1141	254	288	12			
1	D	210	Total	C	N	O	S	0	2	0
			1691	1133	256	292	10			

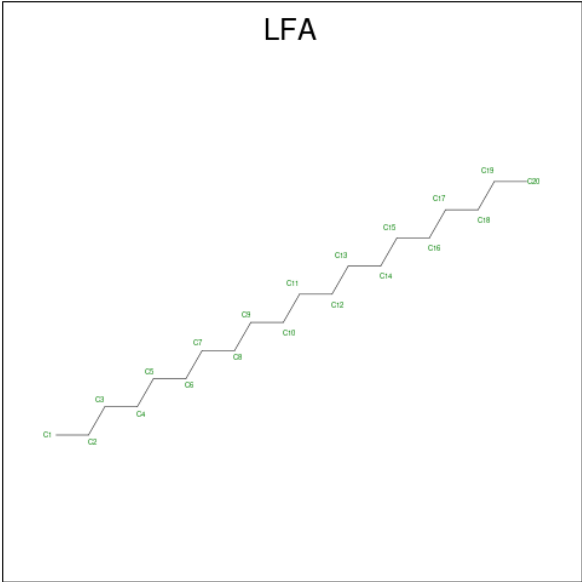
- Molecule 2 is a protein called viral rhodopsin OLPVR11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	212	Total	C	N	O	S	0	3	0
			1718	1157	257	292	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	212	LEU	-	expression tag	UNP F2Y2Z0
E	213	GLU	-	expression tag	UNP F2Y2Z0
E	214	HIS	-	expression tag	UNP F2Y2Z0
E	215	HIS	-	expression tag	UNP F2Y2Z0
E	216	HIS	-	expression tag	UNP F2Y2Z0
E	217	HIS	-	expression tag	UNP F2Y2Z0
E	218	HIS	-	expression tag	UNP F2Y2Z0
E	219	HIS	-	expression tag	UNP F2Y2Z0

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			12	12		
3	A	1	Total	C	0	0
			10	10		
3	A	1	Total	C	0	0
			12	12		
3	A	1	Total	C	0	0
			12	12		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			5	5		
3	A	1	Total	C	0	0
			16	16		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			16	16		
3	A	1	Total	C	0	0
			7	7		
3	A	1	Total	C	0	0
			12	12		
3	A	1	Total	C	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 5 5	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C 5 5	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 14 14	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 5 5	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 16 16	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 5 5	0	0
3	B	1	Total C 5 5	0	0
3	B	1	Total C 5 5	0	0
3	C	1	Total C 14 14	0	0
3	C	1	Total C 5 5	0	0
3	C	1	Total C 8 8	0	0

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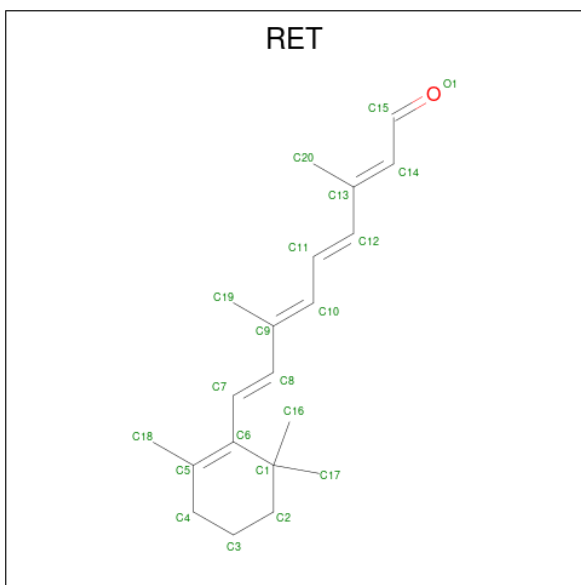
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 12 12	0	0
3	C	1	Total C 12 12	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 10 10	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 10 10	0	0
3	C	1	Total C 5 5	0	0
3	C	1	Total C 5 5	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 5 5	0	0
3	C	1	Total C 8 8	0	0
3	D	1	Total C 12 12	0	0
3	D	1	Total C 12 12	0	0
3	D	1	Total C 10 10	0	0
3	D	1	Total C 12 12	0	0
3	D	1	Total C 12 12	0	0
3	D	1	Total C 14 14	0	0
3	D	1	Total C 10 10	0	0
3	D	1	Total C 10 10	0	0
3	D	1	Total C 14 14	0	0
3	D	1	Total C 6 6	0	0

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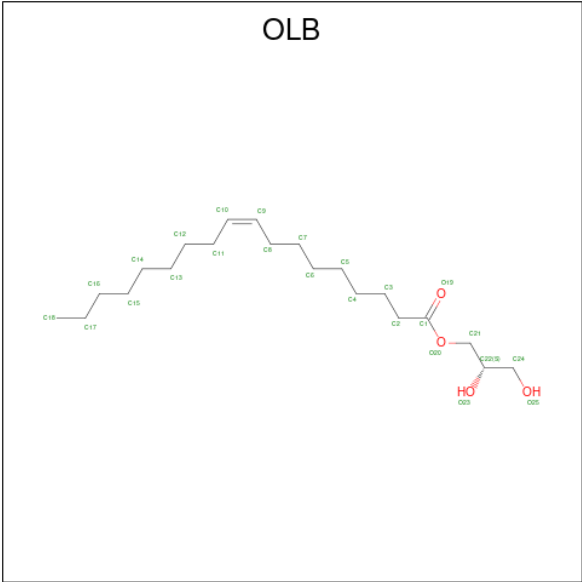
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C 5 5	0	0
3	E	1	Total C 9 9	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 12 12	0	0
3	E	1	Total C 6 6	0	0
3	E	1	Total C 5 5	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 10 10	0	0
3	E	1	Total C 6 6	0	0
3	E	1	Total C 16 16	0	0
3	E	1	Total C 16 16	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 8 8	0	0

- Molecule 4 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



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

- Molecule 5 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			16	12	4		
5	E	1	Total	C	O	0	0
			16	12	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		
6	B	42	Total	O	0	0
			42	42		
6	C	46	Total	O	0	0
			46	46		
6	D	38	Total	O	0	0
			38	38		
6	E	45	Total	O	0	0
			45	45		

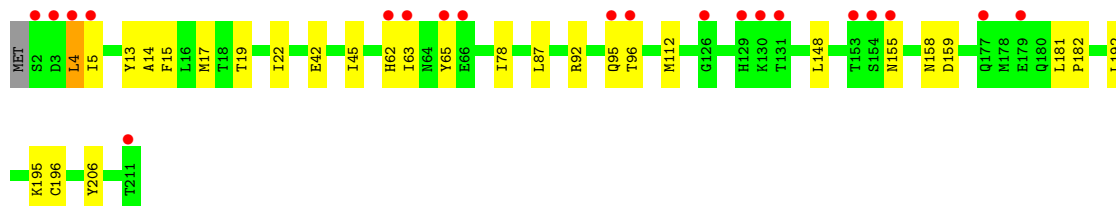
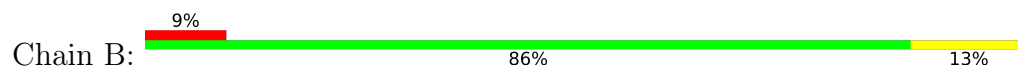
### 3 Residue-property plots [i](#)

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.

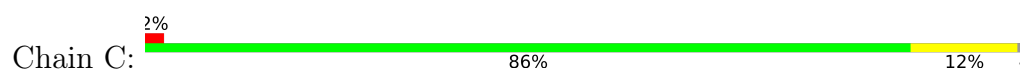
- Molecule 1: viral rhodopsin OLPVRII



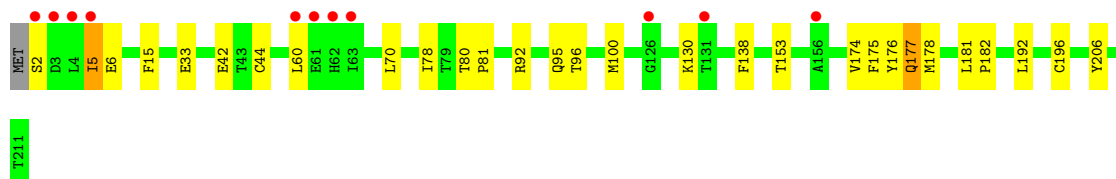
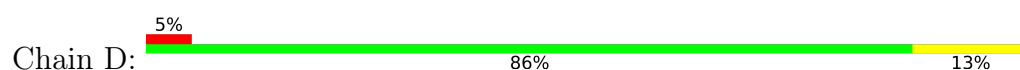
- Molecule 1: viral rhodopsin OLPVRII



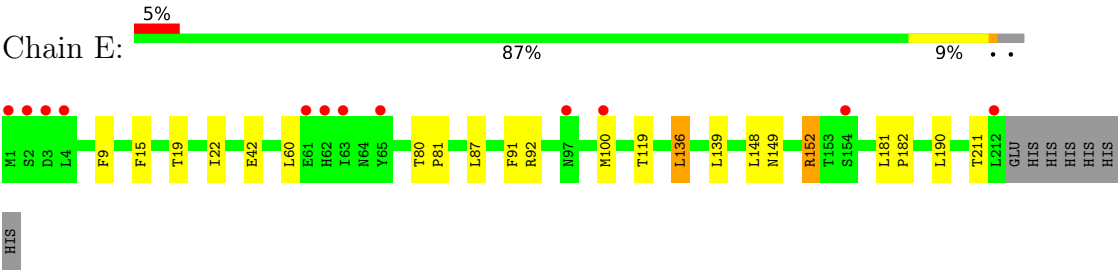
- Molecule 1: viral rhodopsin OLPVRII



- Molecule 1: viral rhodopsin OLPVRII



- Molecule 2: viral rhodopsin OLPVRII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.58Å 99.70Å 82.96Å 90.00° 117.17° 90.00°	Depositor
Resolution (Å)	41.37 – 1.90 41.37 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (41.37-1.90) 98.7 (41.37-1.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.171 , 0.210 0.181 , 0.215	Depositor DCC
$R_{free}$ test set	4363 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9499	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: LFA, OLB, RET

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	0.34	0/1757	0.49	0/2385
1	B	0.31	0/1759	0.47	0/2388
1	C	0.36	0/1750	0.50	0/2376
1	D	0.32	0/1742	0.48	0/2367
2	E	0.34	0/1773	0.47	0/2406
All	All	0.33	0/8781	0.48	0/11922

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1702	0	1687	19	0
1	B	1707	0	1693	23	0
1	C	1695	0	1676	16	0
1	D	1691	0	1656	25	0
2	E	1718	0	1705	15	0
3	A	149	0	281	6	0
3	B	128	0	238	4	0
3	C	115	0	213	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	117	0	217	7	0
3	E	128	0	239	4	0
4	A	20	0	27	6	0
4	B	20	0	27	4	0
4	C	20	0	27	5	0
4	D	20	0	27	6	0
4	E	20	0	27	6	0
5	D	16	0	21	2	0
5	E	16	0	21	0	0
6	A	46	0	0	3	0
6	B	42	0	0	5	0
6	C	46	0	0	2	0
6	D	38	0	0	3	0
6	E	45	0	0	2	0
All	All	9499	0	9782	134	0

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

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:307:LFA:C3	3:D:308:LFA:C10	1.84	1.54
3:A:312:LFA:H11	3:A:316:LFA:C5	1.77	1.13
3:A:312:LFA:C1	3:A:316:LFA:C5	2.35	1.04
1:A:44:CYS:SG	2:E:22[B]:ILE:HG13	2.01	1.00
1:B:22[B]:ILE:HG13	1:D:44:CYS:SG	2.05	0.96
4:C:315:RET:H8	4:C:315:RET:H171	1.48	0.96
1:A:44:CYS:SG	2:E:22[B]:ILE:CG1	2.53	0.95
3:D:307:LFA:C3	3:D:308:LFA:C9	2.48	0.92
3:A:309:LFA:H22	6:A:443:HOH:O	1.73	0.85
3:A:311:LFA:H101	3:A:317:LFA:H11	1.59	0.83
3:C:303:LFA:C2	3:C:306:LFA:C6	2.59	0.80
1:D:174:VAL:O	1:D:177:GLN:HG2	1.84	0.78
1:B:159:ASP:OD1	6:B:401:HOH:O	2.01	0.78
1:B:112:MET:HE3	3:B:309:LFA:H62	1.68	0.76
1:B:22[B]:ILE:CG1	1:D:44:CYS:SG	2.75	0.75
1:B:181:LEU:HB3	1:B:182:PRO:HD3	1.68	0.75
4:A:318:RET:H171	4:A:318:RET:H8	1.68	0.73
1:B:95:GLN:HG3	1:B:96:THR:HG23	1.72	0.71
4:D:313:RET:H8	4:D:313:RET:H171	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:316:RET:H171	4:B:316:RET:H8	1.71	0.71
4:C:315:RET:H171	4:C:315:RET:C8	2.16	0.71
1:A:178:MET:HE3	1:A:182:PRO:HB2	1.73	0.70
1:B:22[B]:ILE:HG13	1:D:44:CYS:HG	1.57	0.69
2:E:119:THR:HG21	2:E:136:LEU:HB3	1.74	0.69
3:D:307:LFA:C3	3:D:308:LFA:H91	2.22	0.68
1:A:44:CYS:SG	2:E:22[B]:ILE:HG12	2.32	0.68
3:A:312:LFA:H12	3:A:316:LFA:C5	2.24	0.68
1:A:149:ASN:OD1	1:A:152:ARG:NH2	2.28	0.66
2:E:149:ASN:OD1	2:E:152:ARG:NH2	2.26	0.65
1:D:42:GLU:OE1	6:D:401:HOH:O	2.15	0.64
1:D:181:LEU:HB3	1:D:182:PRO:HD3	1.79	0.63
1:D:174:VAL:HG22	3:D:309:LFA:H51	1.79	0.63
1:B:42:GLU:OE1	6:B:402:HOH:O	2.16	0.63
3:C:303:LFA:H22	3:C:306:LFA:C6	2.28	0.62
1:D:174:VAL:HG22	3:D:309:LFA:C5	2.29	0.62
1:D:2:SER:O	1:D:5:ILE:HG23	2.00	0.61
3:B:305:LFA:H11	3:C:308:LFA:C7	2.30	0.61
4:A:318:RET:H171	4:A:318:RET:C8	2.31	0.60
3:C:303:LFA:H11	3:C:306:LFA:C6	2.31	0.60
4:D:313:RET:H171	4:D:313:RET:C8	2.32	0.60
4:E:316:RET:H8	4:E:316:RET:H161	1.83	0.60
1:C:131:THR:HG23	6:C:443:HOH:O	2.02	0.60
4:B:316:RET:H171	4:B:316:RET:C8	2.31	0.59
3:E:303:LFA:H11	3:E:305:LFA:H11	1.84	0.58
1:B:63:ILE:CD1	1:B:65:TYR:CE1	2.86	0.58
1:D:2:SER:O	1:D:5:ILE:CG2	2.52	0.58
1:A:59:LYS:HG3	6:A:422:HOH:O	2.04	0.57
4:E:316:RET:H8	4:E:316:RET:H171	1.86	0.57
1:D:95:GLN:HE21	1:D:153:THR:CB	2.20	0.55
3:C:303:LFA:H21	3:C:306:LFA:C6	2.35	0.55
1:B:63:ILE:HD11	1:B:65:TYR:CE1	2.41	0.55
1:B:14:ALA:HB3	1:D:78:ILE:CD1	2.38	0.53
1:C:5:ILE:HD11	1:C:9:PHE:HE2	1.73	0.53
1:D:92:ARG:HG3	1:D:100:MET:O	2.07	0.53
2:E:181:LEU:HB3	2:E:182:PRO:CD	2.39	0.53
1:A:42:GLU:OE1	6:A:401:HOH:O	2.19	0.53
2:E:181:LEU:HB3	2:E:182:PRO:HD3	1.91	0.52
1:B:155:ASN:HB3	1:B:158:ASN:HB2	1.90	0.52
1:B:206:TYR:OH	6:B:403:HOH:O	2.17	0.52
1:B:78:ILE:CD1	1:C:14:ALA:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:LEU:C	2:E:181:LEU:HD23	2.30	0.52
3:C:303:LFA:C1	3:C:306:LFA:C6	2.88	0.51
1:C:164:ALA:HA	3:C:301:LFA:H102	1.92	0.51
2:E:92:ARG:HG3	2:E:100:MET:O	2.10	0.51
1:B:63:ILE:HD13	1:B:65:TYR:CE1	2.46	0.51
1:C:92:ARG:HG2	1:C:100:MET:O	2.10	0.50
1:A:175:PHE:HD1	1:A:178:MET:HE2	1.77	0.50
2:E:9[B]:PHE:CD2	2:E:60:LEU:HD21	2.47	0.50
4:A:318:RET:H8	4:A:318:RET:H161	1.92	0.49
4:E:316:RET:H161	4:E:316:RET:C8	2.42	0.49
1:A:178:MET:CE	1:A:182:PRO:HB2	2.40	0.49
4:E:316:RET:H171	4:E:316:RET:C8	2.42	0.49
1:A:75:ASP:OD1	1:A:75:ASP:C	2.51	0.49
4:D:313:RET:H8	4:D:313:RET:H161	1.94	0.49
1:B:42:GLU:HA	1:B:45:ILE:HD12	1.93	0.49
1:A:192:LEU:O	1:A:196:CYS:HB2	2.12	0.49
1:D:175:PHE:HA	1:D:178:MET:HG3	1.94	0.48
2:E:91:PHE:CZ	2:E:152:ARG:HG3	2.49	0.48
1:D:6:GLU:HG3	1:D:60:LEU:HD13	1.97	0.47
3:C:309:LFA:C1	3:C:311:LFA:C5	2.93	0.47
5:D:301:OLB:H24A	6:D:428:HOH:O	2.14	0.47
1:B:192:LEU:O	1:B:196:CYS:HB2	2.15	0.47
1:D:95:GLN:HE21	1:D:153:THR:HB	1.80	0.47
1:A:22[B]:ILE:CG1	1:C:44:CYS:SG	3.03	0.46
1:D:6:GLU:CG	1:D:60:LEU:HD13	2.46	0.46
1:D:130:LYS:NZ	1:D:176:TYR:O	2.48	0.46
4:C:315:RET:H181	4:C:315:RET:H7	1.60	0.46
4:D:313:RET:H181	4:D:313:RET:H7	1.64	0.46
2:E:80:THR:N	2:E:81:PRO:HD2	2.31	0.45
4:E:316:RET:H7	4:E:316:RET:H181	1.63	0.45
1:B:195:LYS:NZ	6:B:406:HOH:O	2.49	0.45
1:A:63:ILE:HG13	1:A:67:GLU:CB	2.47	0.45
2:E:42:GLU:OE1	6:E:401:HOH:O	2.21	0.45
1:D:138:PHE:CE1	3:D:309:LFA:H91	2.52	0.45
1:D:96:THR:HG22	1:D:96:THR:O	2.17	0.44
1:D:174:VAL:HG22	3:D:309:LFA:H52	1.98	0.44
1:C:4:LEU:HA	1:C:7:TYR:HB2	1.99	0.44
4:B:316:RET:H7	4:B:316:RET:H181	1.54	0.44
2:E:91:PHE:CE1	2:E:152:ARG:HG3	2.53	0.44
4:C:315:RET:H11	4:C:315:RET:H191	1.86	0.44
1:A:18:THR:O	1:A:22[B]:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:316:RET:H8	4:B:316:RET:H161	2.00	0.43
1:A:22[B]:ILE:HG13	1:C:44:CYS:SG	2.59	0.43
1:D:192:LEU:O	1:D:196:CYS:HB2	2.18	0.43
1:B:4:LEU:HD23	3:B:310:LFA:H62	1.99	0.43
4:A:318:RET:C8	4:A:318:RET:H161	2.48	0.43
1:C:3:ASP:O	1:C:6:GLU:N	2.51	0.43
4:A:318:RET:H11	4:A:318:RET:H191	1.84	0.43
3:A:314:LFA:H52	3:E:309:LFA:H41	2.01	0.42
4:D:313:RET:C8	4:D:313:RET:H161	2.49	0.42
1:A:63:ILE:CG1	1:A:67:GLU:CB	2.96	0.42
2:E:19:THR:HG22	6:E:403:HOH:O	2.19	0.42
5:D:301:OLB:C9	3:E:306:LFA:H12	2.50	0.42
1:B:13:TYR:CZ	1:B:17[B]:MET:CE	3.02	0.42
4:D:313:RET:H11	4:D:313:RET:H191	1.92	0.42
1:C:29:ARG:NE	6:C:408:HOH:O	2.51	0.42
1:C:75:ASP:OD1	1:C:75:ASP:C	2.58	0.42
1:C:175[B]:PHE:HA	1:C:178[B]:MET:HE2	2.01	0.42
1:C:181:LEU:HB3	1:C:182:PRO:CD	2.50	0.42
1:D:181:LEU:C	1:D:181:LEU:HD23	2.40	0.42
1:C:124:ASP:OD1	1:C:130:LYS:NZ	2.53	0.41
1:A:22[B]:ILE:HG12	1:C:44:CYS:SG	2.61	0.41
1:B:19:THR:HG22	6:B:411:HOH:O	2.21	0.41
1:B:181:LEU:HB3	1:B:182:PRO:CD	2.43	0.41
1:D:80:THR:N	1:D:81:PRO:HD2	2.35	0.41
1:D:206:TYR:OH	6:D:402:HOH:O	2.21	0.41
4:C:315:RET:C8	4:C:315:RET:C17	2.88	0.41
1:C:80:THR:N	1:C:81:PRO:HD2	2.36	0.41
1:A:181:LEU:HD23	1:A:181:LEU:C	2.41	0.41
3:E:302:LFA:C10	3:E:303:LFA:H13	2.51	0.41
1:A:85:LEU:HG	1:A:89:LEU:HD22	2.02	0.40
1:B:112:MET:CE	3:B:309:LFA:H62	2.46	0.40
4:A:318:RET:H7	4:A:318:RET:H181	1.63	0.40
4:E:316:RET:H191	4:E:316:RET:H11	1.78	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	211/211 (100%)	211 (100%)	0	0	100	100
1	B	210/211 (100%)	208 (99%)	2 (1%)	0	100	100
1	C	210/211 (100%)	206 (98%)	4 (2%)	0	100	100
1	D	210/211 (100%)	209 (100%)	1 (0%)	0	100	100
2	E	213/219 (97%)	211 (99%)	2 (1%)	0	100	100
All	All	1054/1063 (99%)	1045 (99%)	9 (1%)	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	177/183 (97%)	168 (95%)	9 (5%)	24	14
1	B	179/183 (98%)	172 (96%)	7 (4%)	32	23
1	C	176/183 (96%)	170 (97%)	6 (3%)	37	28
1	D	174/183 (95%)	168 (97%)	6 (3%)	37	28
2	E	178/191 (93%)	170 (96%)	8 (4%)	27	18
All	All	884/923 (96%)	848 (96%)	36 (4%)	32	21

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	22[A]	ILE
1	A	22[B]	ILE
1	A	61	GLU
1	A	87	LEU
1	A	89	LEU
1	A	148	LEU
1	A	154	SER
1	A	190	LEU
1	B	4	LEU
1	B	5	ILE
1	B	15	PHE
1	B	62	HIS
1	B	87	LEU
1	B	92	ARG
1	B	148	LEU
1	C	5	ILE
1	C	15	PHE
1	C	148	LEU
1	C	151	LEU
1	C	209	ILE
1	C	211	THR
1	D	5	ILE
1	D	15	PHE
1	D	33[A]	GLU
1	D	33[B]	GLU
1	D	70	LEU
1	D	177	GLN
2	E	15	PHE
2	E	87	LEU
2	E	136	LEU
2	E	139	LEU
2	E	148	LEU
2	E	152	ARG
2	E	190	LEU
2	E	211	THR

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

Mol	Chain	Res	Type
1	A	71	ASN
1	A	95	GLN
1	A	155	ASN

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Mol	Chain	Res	Type
1	B	71	ASN
1	C	113	ASN
1	C	177	GLN
1	D	95	GLN
1	D	177	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

78 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	LFA	C	309	-	9,9,19	0.26	0	8,8,18	0.48	0
3	LFA	C	302	-	4,4,19	0.28	0	3,3,18	0.38	0
3	LFA	E	309	-	5,5,19	0.23	0	4,4,18	0.35	0
3	LFA	B	307	-	6,6,19	0.26	0	5,5,18	0.41	0
3	LFA	E	305	-	5,5,19	0.24	0	4,4,18	0.37	0
3	LFA	C	307	-	9,9,19	0.30	0	8,8,18	0.40	0
3	LFA	B	310	-	7,7,19	0.25	0	6,6,18	0.48	0
3	LFA	A	302	-	9,9,19	0.27	0	8,8,18	0.46	0
3	LFA	C	303	-	7,7,19	0.22	0	6,6,18	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	OLB	E	301	-	15,15,24	1.15	1 (6%)	16,16,25	0.96	1 (6%)
3	LFA	E	308	-	9,9,19	0.28	0	8,8,18	0.45	0
3	LFA	B	309	-	6,6,19	0.25	0	5,5,18	0.44	0
3	LFA	A	315	-	4,4,19	0.28	0	3,3,18	0.40	0
3	LFA	A	312	-	6,6,19	0.22	0	5,5,18	0.50	0
4	RET	B	316	1	20,20,21	2.44	4 (20%)	27,27,28	1.94	9 (33%)
3	LFA	D	302	-	11,11,19	0.27	0	10,10,18	0.49	0
3	LFA	C	301	-	13,13,19	0.31	0	12,12,18	0.45	0
3	LFA	D	303	-	11,11,19	0.29	0	10,10,18	0.49	0
3	LFA	B	306	-	11,11,19	0.28	0	10,10,18	0.43	0
3	LFA	A	310	-	5,5,19	0.29	0	4,4,18	0.36	0
3	LFA	D	304	-	9,9,19	0.30	0	8,8,18	0.49	0
3	LFA	B	302	-	7,7,19	0.25	0	6,6,18	0.50	0
3	LFA	A	317	-	4,4,19	0.27	0	3,3,18	0.43	0
3	LFA	D	307	-	13,13,19	0.26	0	12,12,18	0.62	0
3	LFA	E	302	-	8,8,19	0.22	0	7,7,18	0.56	0
3	LFA	E	304	-	11,11,19	0.27	0	10,10,18	0.48	0
3	LFA	A	311	-	15,15,19	0.27	0	14,14,18	0.52	0
3	LFA	E	312	-	7,7,19	0.27	0	6,6,18	0.48	0
3	LFA	C	312	-	7,7,19	0.23	0	6,6,18	0.54	0
3	LFA	A	304	-	11,11,19	0.22	0	10,10,18	0.66	0
4	RET	D	313	1	20,20,21	2.44	4 (20%)	27,27,28	1.97	6 (22%)
3	LFA	C	314	-	7,7,19	0.29	0	6,6,18	0.40	0
4	RET	E	316	2	20,20,21	2.32	4 (20%)	27,27,28	2.12	7 (25%)
3	LFA	E	313	-	7,7,19	0.28	0	6,6,18	0.51	0
3	LFA	A	313	-	11,11,19	0.26	0	10,10,18	0.48	0
3	LFA	C	305	-	11,11,19	0.28	0	10,10,18	0.45	0
3	LFA	E	314	-	7,7,19	0.26	0	6,6,18	0.45	0
3	LFA	D	311	-	5,5,19	0.27	0	4,4,18	0.36	0
3	LFA	E	307	-	7,7,19	0.24	0	6,6,18	0.45	0
3	LFA	A	316	-	4,4,19	0.25	0	3,3,18	0.42	0
3	LFA	D	312	-	4,4,19	0.29	0	3,3,18	0.35	0
3	LFA	E	303	-	7,7,19	0.23	0	6,6,18	0.75	0
3	LFA	B	312	-	5,5,19	0.29	0	4,4,18	0.32	0
3	LFA	A	305	-	7,7,19	0.25	0	6,6,18	0.47	0
3	LFA	C	308	-	6,6,19	0.27	0	5,5,18	0.45	0
3	LFA	E	310	-	15,15,19	0.30	0	14,14,18	0.53	0
3	LFA	B	314	-	4,4,19	0.27	0	3,3,18	0.37	0
3	LFA	A	309	-	15,15,19	0.31	0	14,14,18	0.45	0
3	LFA	D	305	-	11,11,19	0.20	0	10,10,18	0.63	0
3	LFA	A	308	-	4,4,19	0.25	0	3,3,18	0.37	0
3	LFA	D	309	-	9,9,19	0.28	0	8,8,18	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LFA	B	305	-	4,4,19	0.28	0	3,3,18	0.35	0
3	LFA	A	303	-	11,11,19	0.24	0	10,10,18	0.50	0
3	LFA	C	304	-	11,11,19	0.25	0	10,10,18	0.55	0
4	RET	C	315	1	20,20,21	2.25	3 (15%)	27,27,28	1.92	5 (18%)
3	LFA	B	303	-	13,13,19	0.25	0	12,12,18	0.52	0
3	LFA	C	306	-	5,5,19	0.22	0	4,4,18	0.36	0
3	LFA	D	310	-	13,13,19	0.25	0	12,12,18	0.56	0
3	LFA	E	315	-	7,7,19	0.26	0	6,6,18	0.49	0
4	RET	A	318	1	20,20,21	2.49	3 (15%)	27,27,28	1.89	6 (22%)
3	LFA	A	301	-	11,11,19	0.30	0	10,10,18	0.52	0
3	LFA	B	301	-	7,7,19	0.18	0	6,6,18	0.50	0
3	LFA	D	306	-	11,11,19	0.23	0	10,10,18	0.58	0
3	LFA	B	315	-	4,4,19	0.27	0	3,3,18	0.40	0
3	LFA	A	306	-	5,5,19	0.23	0	4,4,18	0.40	0
3	LFA	D	308	-	9,9,19	0.22	0	8,8,18	0.49	0
3	LFA	C	310	-	4,4,19	0.31	0	3,3,18	0.35	0
3	LFA	B	308	-	9,9,19	0.23	0	8,8,18	0.57	0
3	LFA	B	313	-	4,4,19	0.27	0	3,3,18	0.35	0
3	LFA	A	314	-	5,5,19	0.26	0	4,4,18	0.35	0
3	LFA	C	313	-	4,4,19	0.25	0	3,3,18	0.34	0
3	LFA	E	311	-	15,15,19	0.29	0	14,14,18	0.49	0
3	LFA	B	311	-	15,15,19	0.26	0	14,14,18	0.53	0
3	LFA	B	304	-	11,11,19	0.30	0	10,10,18	0.41	0
3	LFA	C	311	-	4,4,19	0.28	0	3,3,18	0.39	0
3	LFA	A	307	-	5,5,19	0.26	0	4,4,18	0.39	0
3	LFA	E	306	-	4,4,19	0.28	0	3,3,18	0.43	0
5	OLB	D	301	-	15,15,24	1.20	1 (6%)	16,16,25	1.02	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	C	309	-	-	6/7/7/17	-
3	LFA	C	302	-	-	1/2/2/17	-
3	LFA	E	309	-	-	2/3/3/17	-
3	LFA	B	307	-	-	2/4/4/17	-
3	LFA	E	305	-	-	1/3/3/17	-
3	LFA	C	307	-	-	5/7/7/17	-
3	LFA	B	310	-	-	4/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	302	-	-	1/7/7/17	-
3	LFA	C	303	-	-	1/5/5/17	-
5	OLB	E	301	-	-	9/15/15/24	-
3	LFA	E	308	-	-	4/7/7/17	-
3	LFA	B	309	-	-	3/4/4/17	-
3	LFA	A	315	-	-	1/2/2/17	-
3	LFA	A	312	-	-	1/4/4/17	-
4	RET	B	316	1	-	0/13/30/31	0/1/1/1
3	LFA	D	302	-	-	7/9/9/17	-
3	LFA	C	301	-	-	9/11/11/17	-
3	LFA	D	303	-	-	5/9/9/17	-
3	LFA	B	306	-	-	6/9/9/17	-
3	LFA	A	310	-	-	1/3/3/17	-
3	LFA	D	304	-	-	2/7/7/17	-
3	LFA	B	302	-	-	3/5/5/17	-
3	LFA	A	317	-	-	0/2/2/17	-
3	LFA	D	307	-	-	2/11/11/17	-
3	LFA	E	302	-	-	2/6/6/17	-
3	LFA	E	304	-	-	3/9/9/17	-
3	LFA	A	311	-	-	9/13/13/17	-
3	LFA	E	312	-	-	3/5/5/17	-
3	LFA	C	312	-	-	2/5/5/17	-
3	LFA	A	304	-	-	6/9/9/17	-
4	RET	D	313	1	-	0/13/30/31	0/1/1/1
3	LFA	C	314	-	-	3/5/5/17	-
4	RET	E	316	2	-	0/13/30/31	0/1/1/1
3	LFA	E	313	-	-	2/5/5/17	-
3	LFA	A	313	-	-	7/9/9/17	-
3	LFA	C	305	-	-	4/9/9/17	-
3	LFA	E	314	-	-	2/5/5/17	-
3	LFA	D	311	-	-	3/3/3/17	-
3	LFA	E	307	-	-	4/5/5/17	-
3	LFA	A	316	-	-	1/2/2/17	-
3	LFA	D	312	-	-	0/2/2/17	-
3	LFA	E	303	-	-	0/5/5/17	-
3	LFA	B	312	-	-	2/3/3/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	305	-	-	3/5/5/17	-
3	LFA	C	308	-	-	1/4/4/17	-
3	LFA	E	310	-	-	5/13/13/17	-
3	LFA	B	314	-	-	0/2/2/17	-
3	LFA	A	309	-	-	8/13/13/17	-
3	LFA	D	305	-	-	4/9/9/17	-
3	LFA	A	308	-	-	2/2/2/17	-
3	LFA	D	309	-	-	3/7/7/17	-
3	LFA	B	305	-	-	2/2/2/17	-
3	LFA	A	303	-	-	6/9/9/17	-
3	LFA	C	304	-	-	6/9/9/17	-
4	RET	C	315	1	-	0/13/30/31	0/1/1/1
3	LFA	B	303	-	-	8/11/11/17	-
3	LFA	C	306	-	-	2/3/3/17	-
3	LFA	D	310	-	-	7/11/11/17	-
3	LFA	E	315	-	-	1/5/5/17	-
4	RET	A	318	1	-	0/13/30/31	0/1/1/1
3	LFA	A	301	-	-	6/9/9/17	-
3	LFA	B	301	-	-	2/5/5/17	-
3	LFA	D	306	-	-	5/9/9/17	-
3	LFA	B	315	-	-	1/2/2/17	-
3	LFA	A	306	-	-	1/3/3/17	-
3	LFA	D	308	-	-	3/7/7/17	-
3	LFA	C	310	-	-	0/2/2/17	-
3	LFA	B	308	-	-	1/7/7/17	-
3	LFA	B	313	-	-	1/2/2/17	-
3	LFA	A	314	-	-	1/3/3/17	-
3	LFA	C	313	-	-	1/2/2/17	-
3	LFA	E	311	-	-	4/13/13/17	-
3	LFA	B	311	-	-	8/13/13/17	-
3	LFA	B	304	-	-	5/9/9/17	-
3	LFA	C	311	-	-	0/2/2/17	-
3	LFA	A	307	-	-	1/3/3/17	-
3	LFA	E	306	-	-	1/2/2/17	-
5	OLB	D	301	-	-	6/15/15/24	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	318	RET	C14-C13	9.40	1.41	1.33
4	D	313	RET	C14-C13	8.97	1.40	1.33
4	B	316	RET	C14-C13	8.91	1.40	1.33
4	E	316	RET	C14-C13	8.56	1.40	1.33
4	C	315	RET	C14-C13	8.22	1.40	1.33
5	D	301	OLB	O20-C1	4.41	1.46	1.33
5	E	301	OLB	O20-C1	4.25	1.45	1.33
4	D	313	RET	C10-C9	3.52	1.40	1.35
4	B	316	RET	C10-C9	3.14	1.39	1.35
4	A	318	RET	C15-C14	-2.87	1.38	1.49
4	E	316	RET	C10-C9	2.86	1.39	1.35
4	B	316	RET	C15-C14	-2.72	1.39	1.49
4	C	315	RET	C10-C9	2.65	1.39	1.35
4	A	318	RET	C10-C9	2.65	1.39	1.35
4	E	316	RET	C15-C14	-2.63	1.39	1.49
4	C	315	RET	C15-C14	-2.61	1.39	1.49
4	D	313	RET	C15-C14	-2.60	1.39	1.49
4	E	316	RET	C11-C12	2.27	1.40	1.34
4	D	313	RET	C11-C12	2.17	1.40	1.34
4	B	316	RET	C11-C12	2.01	1.39	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	316	RET	C18-C5-C6	-5.01	118.90	124.53
4	C	315	RET	C7-C8-C9	-4.57	119.32	126.23
4	D	313	RET	C7-C8-C9	-4.56	119.34	126.23
4	C	315	RET	C18-C5-C6	-4.43	119.56	124.53
4	E	316	RET	C18-C5-C6	-4.43	119.56	124.53
4	B	316	RET	C7-C8-C9	-4.42	119.56	126.23
4	D	313	RET	C18-C5-C6	-4.35	119.65	124.53
4	A	318	RET	C18-C5-C6	-4.31	119.69	124.53
4	E	316	RET	C7-C8-C9	-4.21	119.87	126.23
4	E	316	RET	C19-C9-C10	-4.18	117.07	122.92
4	A	318	RET	C7-C8-C9	-4.08	120.07	126.23
4	C	315	RET	C11-C10-C9	-3.59	122.19	127.31
4	E	316	RET	C11-C10-C9	-3.51	122.30	127.31
4	C	315	RET	C10-C11-C12	-3.49	112.32	123.22
4	A	318	RET	C11-C10-C9	-3.43	122.41	127.31
4	D	313	RET	C3-C4-C5	-3.38	108.04	114.08
4	E	316	RET	C10-C11-C12	-3.28	112.99	123.22
4	A	318	RET	C19-C9-C10	-3.24	118.38	122.92
4	B	316	RET	C10-C11-C12	-3.20	113.24	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	316	RET	C3-C4-C5	-3.10	108.54	114.08
4	D	313	RET	C10-C11-C12	-3.09	113.57	123.22
4	A	318	RET	C10-C11-C12	-2.99	113.88	123.22
5	D	301	OLB	O20-C1-C2	2.74	120.52	111.91
4	D	313	RET	C19-C9-C10	-2.73	119.11	122.92
4	C	315	RET	C19-C9-C10	-2.71	119.13	122.92
4	D	313	RET	C11-C10-C9	-2.66	123.51	127.31
4	B	316	RET	C19-C9-C10	-2.65	119.22	122.92
5	E	301	OLB	O20-C1-C2	2.60	120.06	111.91
4	B	316	RET	C3-C4-C5	-2.57	109.49	114.08
4	A	318	RET	C3-C4-C5	-2.55	109.52	114.08
4	B	316	RET	C17-C1-C6	-2.25	106.66	110.30
4	E	316	RET	C8-C9-C10	2.15	122.24	118.94
4	B	316	RET	C1-C6-C7	2.12	121.78	115.78
4	B	316	RET	C7-C6-C5	-2.04	116.51	121.46
4	B	316	RET	C11-C10-C9	-2.01	124.44	127.31

There are no chirality outliers.

All (234) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	301	OLB	O20-C21-C22-C24
5	D	301	OLB	C2-C1-O20-C21
5	E	301	OLB	C2-C1-O20-C21
5	E	301	OLB	O19-C1-O20-C21
5	D	301	OLB	O19-C1-O20-C21
5	E	301	OLB	O20-C21-C22-O23
3	B	306	LFA	C5-C6-C7-C8
3	A	303	LFA	C2-C3-C4-C5
3	A	313	LFA	C7-C8-C9-C10
5	D	301	OLB	O20-C21-C22-O23
3	C	304	LFA	C6-C7-C8-C9
3	B	311	LFA	C11-C12-C13-C14
3	D	308	LFA	C6-C7-C8-C9
3	E	310	LFA	C11-C10-C9-C8
3	E	310	LFA	C11-C12-C13-C14
5	D	301	OLB	O20-C21-C22-C24
3	A	311	LFA	C4-C5-C6-C7
3	B	311	LFA	C11-C10-C9-C8
3	C	305	LFA	C7-C8-C9-C10
3	D	303	LFA	C11-C10-C9-C8
3	E	308	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	302	LFA	C4-C5-C6-C7
3	B	311	LFA	C7-C8-C9-C10
3	A	304	LFA	C6-C7-C8-C9
3	A	313	LFA	C6-C7-C8-C9
3	C	305	LFA	C3-C4-C5-C6
3	C	309	LFA	C2-C3-C4-C5
3	B	306	LFA	C10-C11-C12-C13
3	D	304	LFA	C7-C8-C9-C10
3	D	308	LFA	C5-C6-C7-C8
3	D	303	LFA	C5-C6-C7-C8
3	E	311	LFA	C4-C5-C6-C7
3	A	303	LFA	C5-C6-C7-C8
3	A	309	LFA	C10-C11-C12-C13
3	A	314	LFA	C2-C3-C4-C5
3	B	311	LFA	C10-C11-C12-C13
3	D	303	LFA	C2-C3-C4-C5
3	C	301	LFA	C4-C5-C6-C7
3	B	312	LFA	C2-C3-C4-C5
3	C	301	LFA	C7-C8-C9-C10
3	C	308	LFA	C2-C3-C4-C5
3	D	302	LFA	C3-C4-C5-C6
3	E	308	LFA	C2-C3-C4-C5
3	E	311	LFA	C7-C8-C9-C10
5	E	301	OLB	C3-C4-C5-C6
3	A	309	LFA	C11-C12-C13-C14
3	B	304	LFA	C5-C6-C7-C8
3	B	310	LFA	C2-C3-C4-C5
3	D	302	LFA	C5-C6-C7-C8
3	D	305	LFA	C6-C7-C8-C9
3	B	303	LFA	C3-C4-C5-C6
3	E	304	LFA	C6-C7-C8-C9
3	A	301	LFA	C4-C5-C6-C7
3	D	310	LFA	C3-C4-C5-C6
3	C	304	LFA	C4-C5-C6-C7
3	D	309	LFA	C4-C5-C6-C7
3	E	304	LFA	C11-C10-C9-C8
3	A	303	LFA	C11-C10-C9-C8
3	B	302	LFA	C2-C3-C4-C5
3	B	304	LFA	C6-C7-C8-C9
3	B	303	LFA	C9-C10-C11-C12
3	B	311	LFA	C5-C6-C7-C8
3	C	301	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	310	LFA	C4-C5-C6-C7
3	E	315	LFA	C3-C4-C5-C6
3	B	307	LFA	C4-C5-C6-C7
3	C	314	LFA	C3-C4-C5-C6
3	E	311	LFA	C12-C13-C14-C15
3	D	305	LFA	C2-C3-C4-C5
3	D	310	LFA	C7-C8-C9-C10
3	C	307	LFA	C2-C3-C4-C5
3	C	305	LFA	C2-C3-C4-C5
3	D	302	LFA	C4-C5-C6-C7
3	C	301	LFA	C5-C6-C7-C8
3	B	311	LFA	C2-C3-C4-C5
3	B	303	LFA	C6-C7-C8-C9
3	C	301	LFA	C2-C3-C4-C5
3	C	314	LFA	C2-C3-C4-C5
3	A	311	LFA	C10-C11-C12-C13
5	E	301	OLB	C4-C5-C6-C7
3	E	307	LFA	C2-C3-C4-C5
3	D	311	LFA	C2-C3-C4-C5
3	A	304	LFA	C7-C8-C9-C10
3	B	306	LFA	C11-C12-C13-C14
3	C	301	LFA	C11-C12-C13-C14
3	E	305	LFA	C1-C2-C3-C4
3	A	309	LFA	C7-C8-C9-C10
3	A	311	LFA	C9-C10-C11-C12
3	B	304	LFA	C7-C8-C9-C10
3	A	305	LFA	C4-C5-C6-C7
3	B	310	LFA	C3-C4-C5-C6
5	D	301	OLB	C6-C7-C8-C9
3	A	307	LFA	C3-C4-C5-C6
3	A	310	LFA	C3-C4-C5-C6
3	D	306	LFA	C7-C8-C9-C10
3	E	310	LFA	C9-C10-C11-C12
3	A	301	LFA	C2-C3-C4-C5
3	A	309	LFA	C1-C2-C3-C4
3	C	303	LFA	C5-C6-C7-C8
3	B	308	LFA	C7-C8-C9-C10
3	E	307	LFA	C1-C2-C3-C4
3	E	302	LFA	C2-C3-C4-C5
3	C	307	LFA	C7-C8-C9-C10
3	C	312	LFA	C1-C2-C3-C4
3	D	302	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	D	309	LFA	C3-C4-C5-C6
3	C	305	LFA	C9-C10-C11-C12
3	A	308	LFA	C1-C2-C3-C4
3	A	304	LFA	C3-C4-C5-C6
3	D	305	LFA	C9-C10-C11-C12
3	D	311	LFA	C1-C2-C3-C4
3	B	305	LFA	C1-C2-C3-C4
5	E	301	OLB	C6-C7-C8-C9
5	E	301	OLB	C1-C2-C3-C4
3	D	310	LFA	C5-C6-C7-C8
3	A	313	LFA	C9-C10-C11-C12
3	E	313	LFA	C3-C4-C5-C6
3	B	303	LFA	C2-C3-C4-C5
3	D	306	LFA	C1-C2-C3-C4
3	A	309	LFA	C9-C10-C11-C12
3	B	309	LFA	C3-C4-C5-C6
3	C	301	LFA	C1-C2-C3-C4
3	D	306	LFA	C9-C10-C11-C12
3	A	301	LFA	C1-C2-C3-C4
3	D	308	LFA	C7-C8-C9-C10
3	E	306	LFA	C1-C2-C3-C4
3	E	311	LFA	C11-C10-C9-C8
3	A	306	LFA	C1-C2-C3-C4
3	A	309	LFA	C12-C13-C14-C15
3	B	303	LFA	C11-C12-C13-C14
3	C	306	LFA	C1-C2-C3-C4
3	A	303	LFA	C6-C7-C8-C9
3	B	311	LFA	C4-C5-C6-C7
3	C	309	LFA	C1-C2-C3-C4
3	B	304	LFA	C2-C3-C4-C5
3	D	306	LFA	C4-C5-C6-C7
3	D	304	LFA	C6-C7-C8-C9
3	A	312	LFA	C3-C4-C5-C6
3	C	306	LFA	C3-C4-C5-C6
5	E	301	OLB	C2-C3-C4-C5
3	E	307	LFA	C3-C4-C5-C6
3	A	313	LFA	C3-C4-C5-C6
3	C	312	LFA	C4-C5-C6-C7
3	D	303	LFA	C9-C10-C11-C12
3	B	304	LFA	C1-C2-C3-C4
3	E	310	LFA	C13-C14-C15-C16
3	A	301	LFA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	A	313	LFA	C1-C2-C3-C4
3	D	302	LFA	C11-C10-C9-C8
3	A	303	LFA	C3-C4-C5-C6
3	E	310	LFA	C6-C7-C8-C9
3	B	306	LFA	C3-C4-C5-C6
3	E	309	LFA	C1-C2-C3-C4
3	C	313	LFA	C2-C3-C4-C5
3	C	307	LFA	C3-C4-C5-C6
3	A	311	LFA	C13-C14-C15-C16
3	B	309	LFA	C1-C2-C3-C4
3	B	313	LFA	C1-C2-C3-C4
3	B	302	LFA	C5-C6-C7-C8
3	E	312	LFA	C3-C4-C5-C6
3	B	303	LFA	C11-C10-C9-C8
3	E	307	LFA	C4-C5-C6-C7
3	C	302	LFA	C2-C3-C4-C5
3	B	302	LFA	C1-C2-C3-C4
3	C	314	LFA	C4-C5-C6-C7
3	E	304	LFA	C4-C5-C6-C7
3	B	312	LFA	C3-C4-C5-C6
3	A	311	LFA	C12-C13-C14-C15
3	D	306	LFA	C2-C3-C4-C5
3	A	309	LFA	C2-C3-C4-C5
3	A	305	LFA	C2-C3-C4-C5
3	D	303	LFA	C4-C5-C6-C7
3	D	302	LFA	C1-C2-C3-C4
3	E	313	LFA	C2-C3-C4-C5
3	A	311	LFA	C11-C10-C9-C8
3	A	301	LFA	C3-C4-C5-C6
3	D	307	LFA	C12-C13-C14-C15
3	C	304	LFA	C3-C4-C5-C6
3	E	312	LFA	C4-C5-C6-C7
5	D	301	OLB	C2-C3-C4-C5
3	C	309	LFA	C5-C6-C7-C8
3	A	313	LFA	C5-C6-C7-C8
3	C	309	LFA	C6-C7-C8-C9
3	D	305	LFA	C1-C2-C3-C4
3	A	301	LFA	C5-C6-C7-C8
3	B	301	LFA	C3-C4-C5-C6
3	D	310	LFA	C9-C10-C11-C12
3	A	308	LFA	C2-C3-C4-C5
3	B	310	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	C	304	LFA	C5-C6-C7-C8
3	C	307	LFA	C5-C6-C7-C8
3	D	302	LFA	C7-C8-C9-C10
3	A	311	LFA	C6-C7-C8-C9
3	B	311	LFA	C6-C7-C8-C9
3	B	307	LFA	C2-C3-C4-C5
3	E	308	LFA	C3-C4-C5-C6
3	A	311	LFA	C1-C2-C3-C4
3	B	303	LFA	C1-C2-C3-C4
3	C	301	LFA	C9-C10-C11-C12
3	B	301	LFA	C2-C3-C4-C5
3	B	309	LFA	C2-C3-C4-C5
3	B	315	LFA	C1-C2-C3-C4
3	D	311	LFA	C3-C4-C5-C6
3	C	309	LFA	C7-C8-C9-C10
3	A	304	LFA	C4-C5-C6-C7
3	C	304	LFA	C9-C10-C11-C12
3	D	310	LFA	C10-C11-C12-C13
3	A	311	LFA	C3-C4-C5-C6
3	B	306	LFA	C7-C8-C9-C10
3	E	309	LFA	C2-C3-C4-C5
3	A	315	LFA	C2-C3-C4-C5
3	D	310	LFA	C1-C2-C3-C4
3	A	303	LFA	C9-C10-C11-C12
3	B	306	LFA	C9-C10-C11-C12
3	D	309	LFA	C1-C2-C3-C4
3	D	307	LFA	C3-C4-C5-C6
3	E	308	LFA	C7-C8-C9-C10
3	B	303	LFA	C5-C6-C7-C8
3	C	309	LFA	C4-C5-C6-C7
3	E	314	LFA	C4-C5-C6-C7
3	A	305	LFA	C5-C6-C7-C8
3	E	312	LFA	C5-C6-C7-C8
3	A	313	LFA	C11-C10-C9-C8
3	A	309	LFA	C11-C10-C9-C8
3	A	304	LFA	C2-C3-C4-C5
3	B	305	LFA	C2-C3-C4-C5
3	C	301	LFA	C10-C11-C12-C13
3	E	314	LFA	C3-C4-C5-C6
3	E	302	LFA	C5-C6-C7-C8
3	A	316	LFA	C2-C3-C4-C5
3	C	307	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	C	304	LFA	C1-C2-C3-C4
3	D	310	LFA	C11-C10-C9-C8
3	A	304	LFA	C9-C10-C11-C12

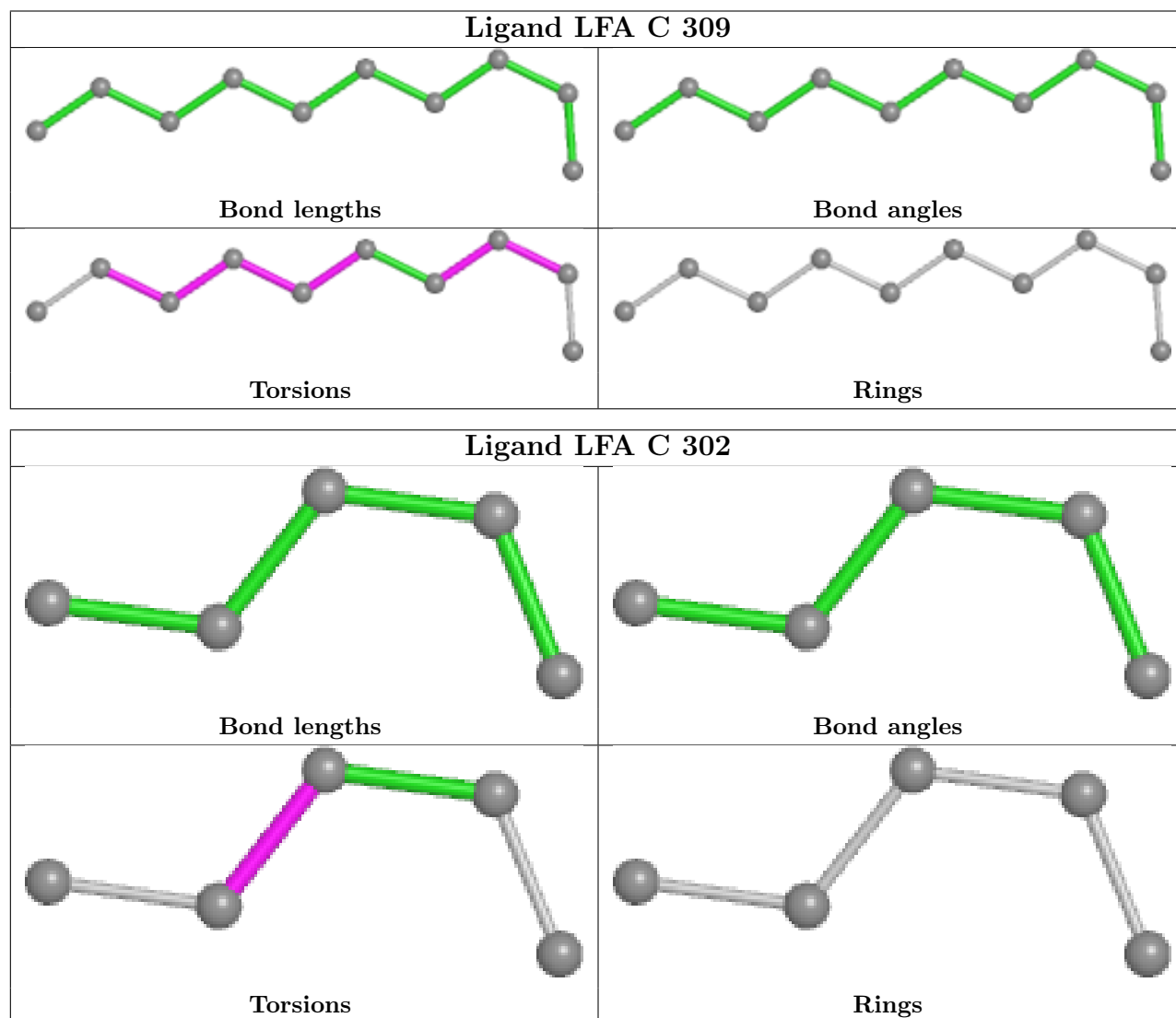
There are no ring outliers.

29 monomers are involved in 55 short contacts:

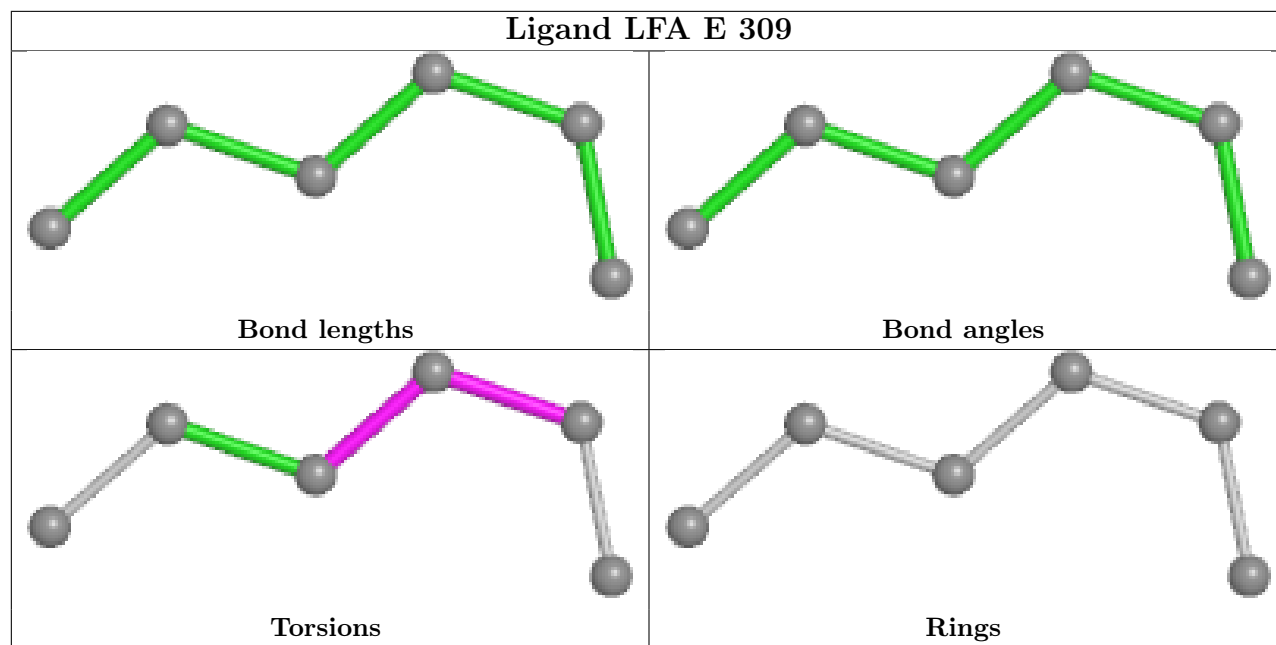
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	309	LFA	1	0
3	E	309	LFA	1	0
3	E	305	LFA	1	0
3	B	310	LFA	1	0
3	C	303	LFA	5	0
3	B	309	LFA	2	0
3	A	312	LFA	3	0
4	B	316	RET	4	0
3	C	301	LFA	1	0
3	A	317	LFA	1	0
3	D	307	LFA	3	0
3	E	302	LFA	1	0
3	A	311	LFA	1	0
4	D	313	RET	6	0
4	E	316	RET	6	0
3	A	316	LFA	3	0
3	E	303	LFA	2	0
3	C	308	LFA	1	0
3	A	309	LFA	1	0
3	D	309	LFA	4	0
3	B	305	LFA	1	0
4	C	315	RET	5	0
3	C	306	LFA	5	0
4	A	318	RET	6	0
3	D	308	LFA	3	0
3	A	314	LFA	1	0
3	C	311	LFA	1	0
3	E	306	LFA	1	0
5	D	301	OLB	2	0

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

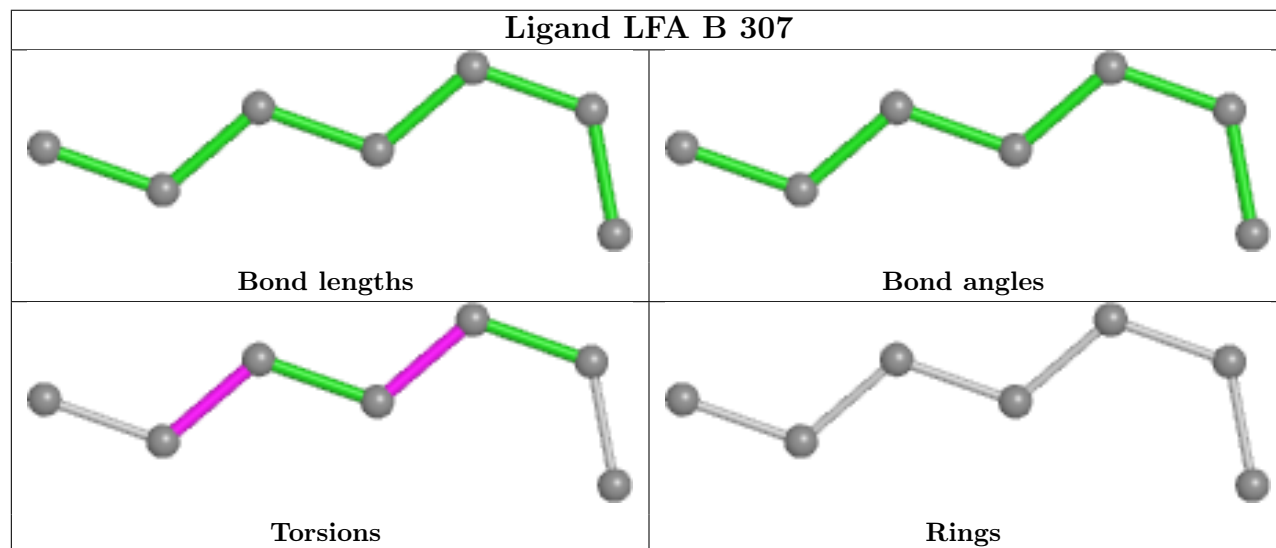
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

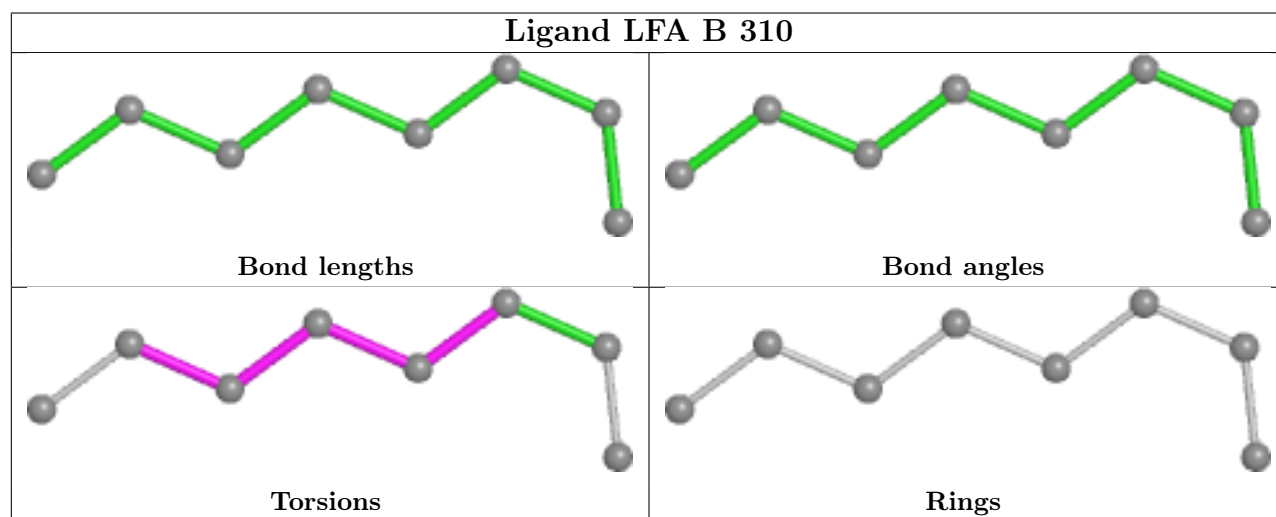
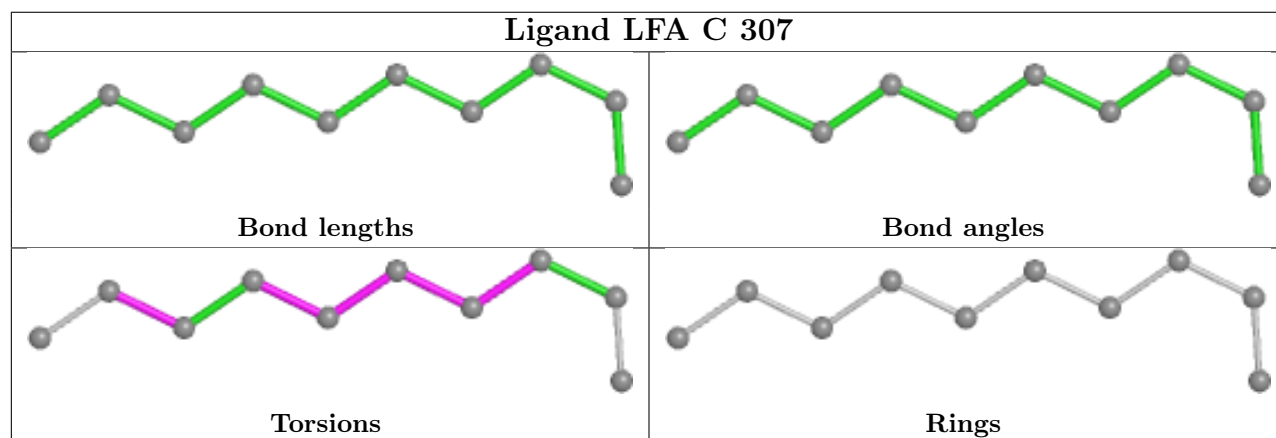
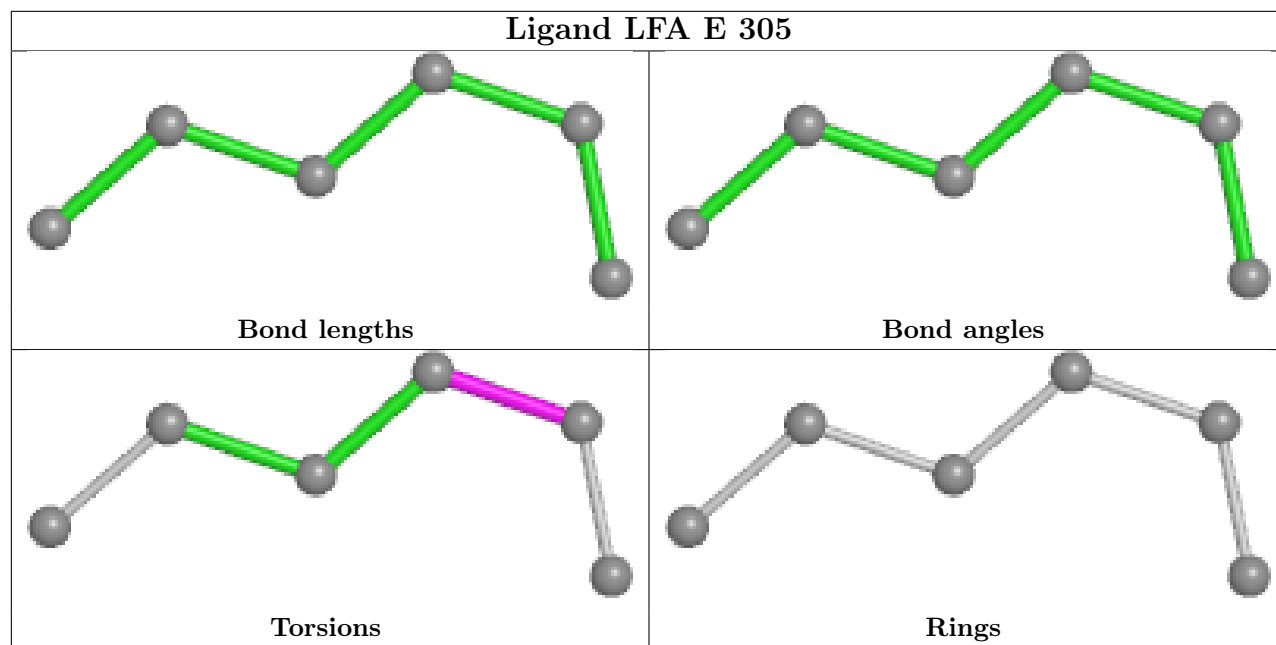


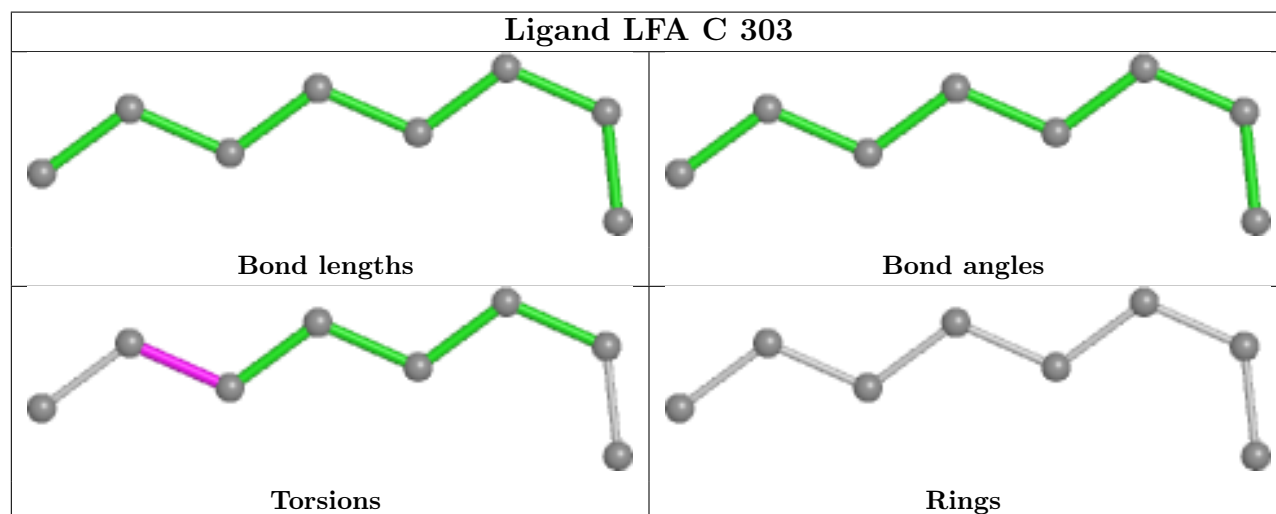
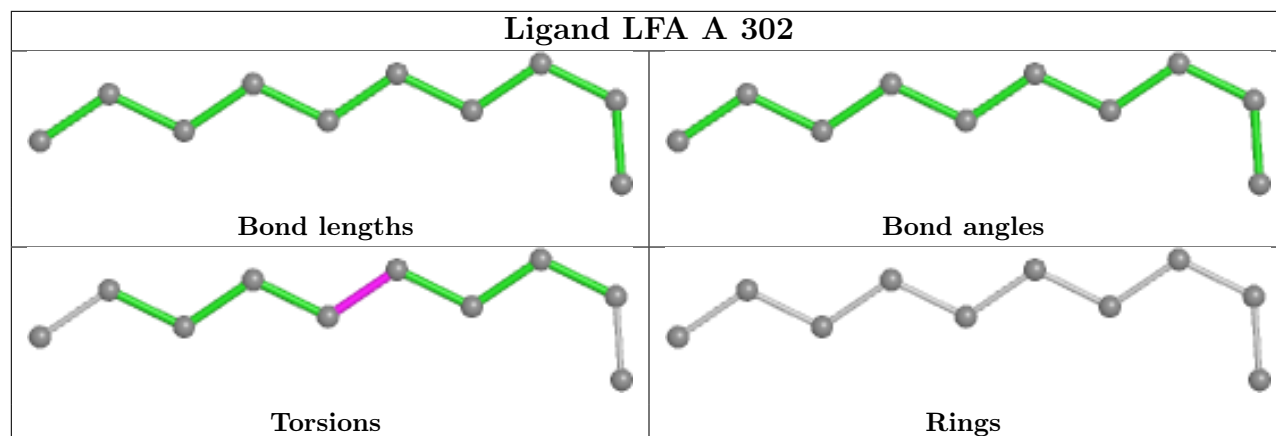
## Ligand LFA E 309



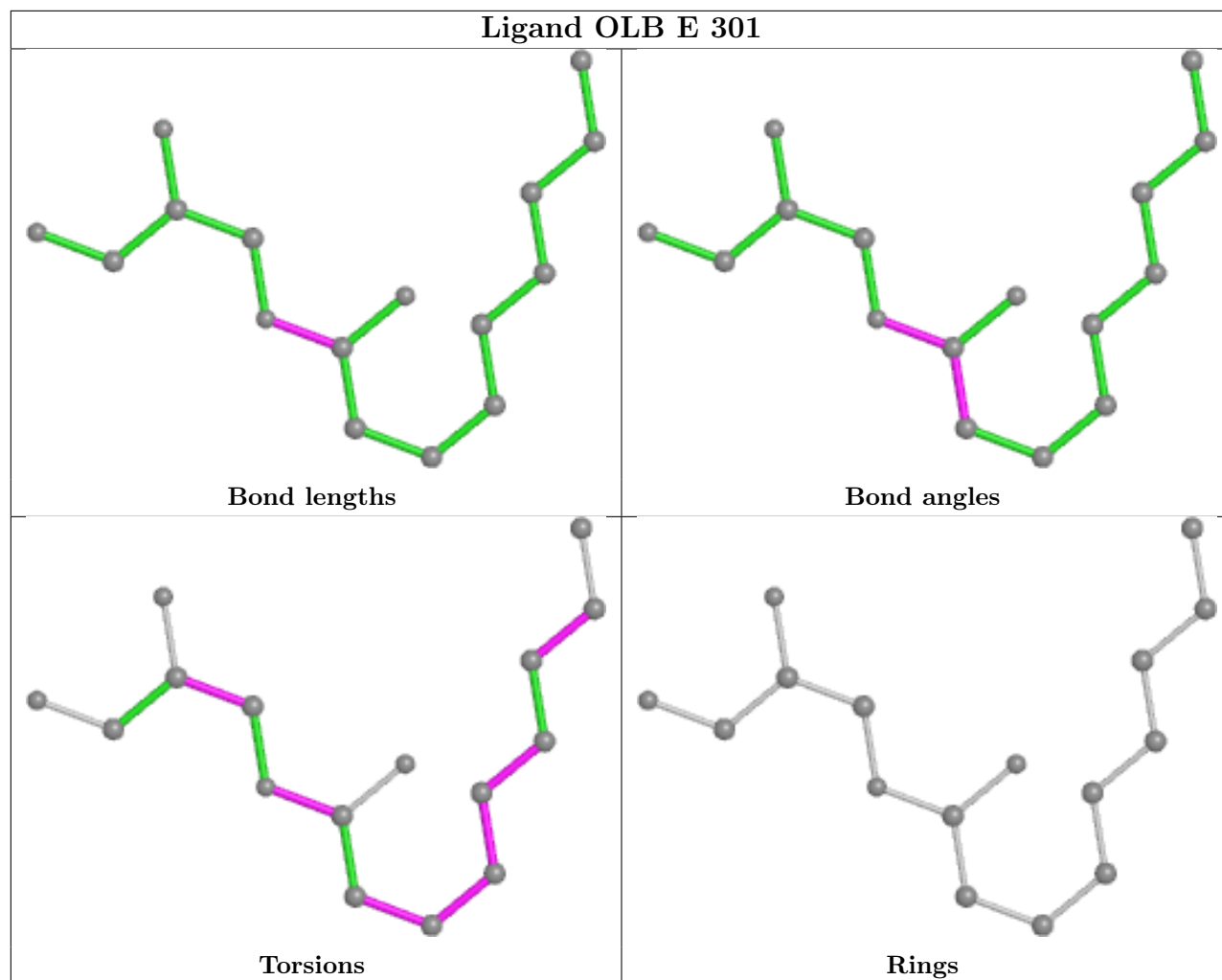
## Ligand LFA B 307



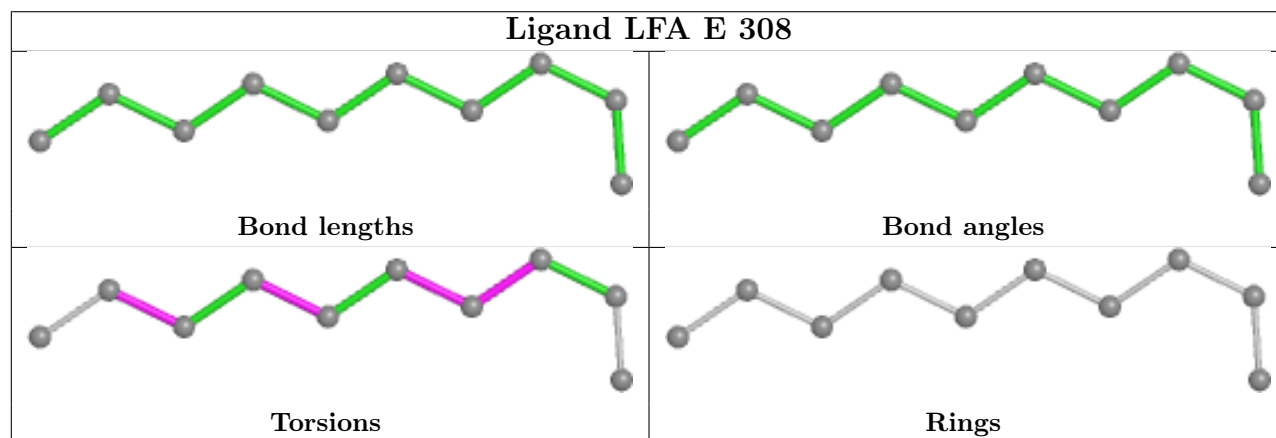


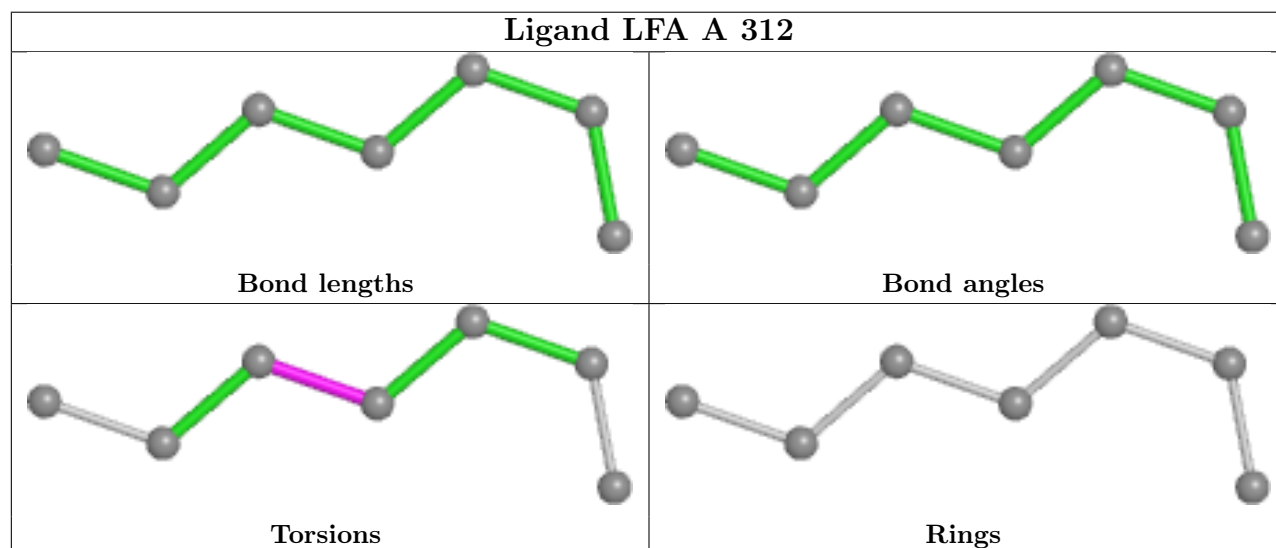
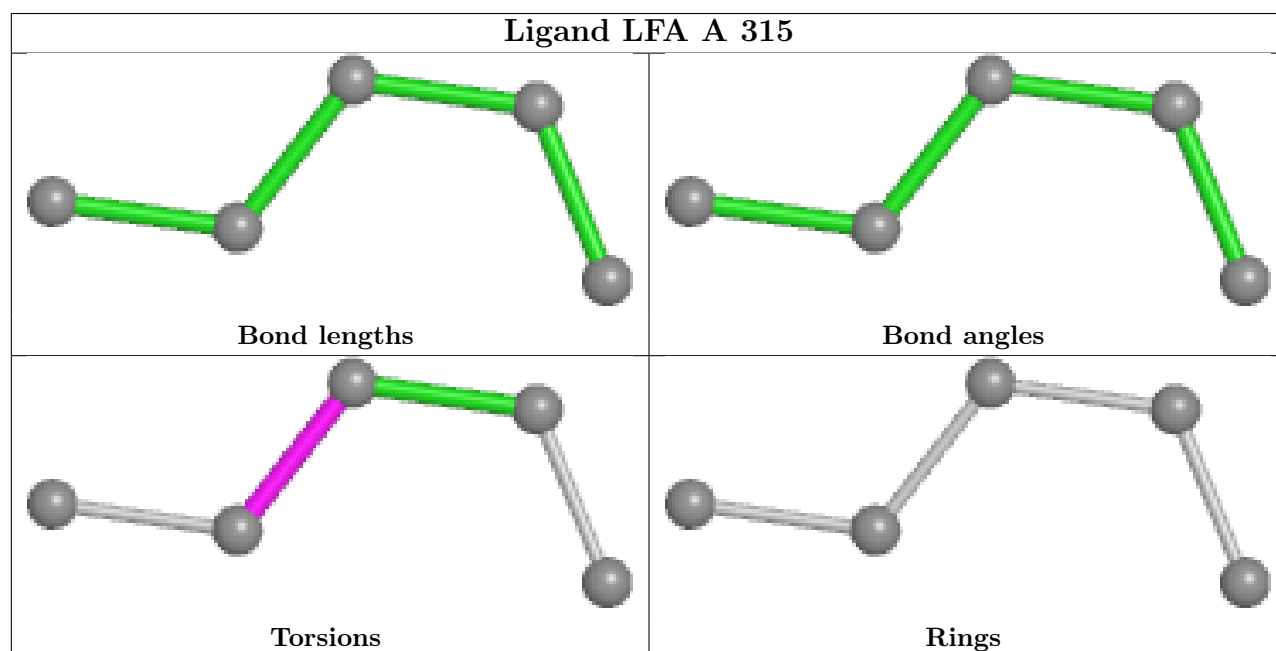
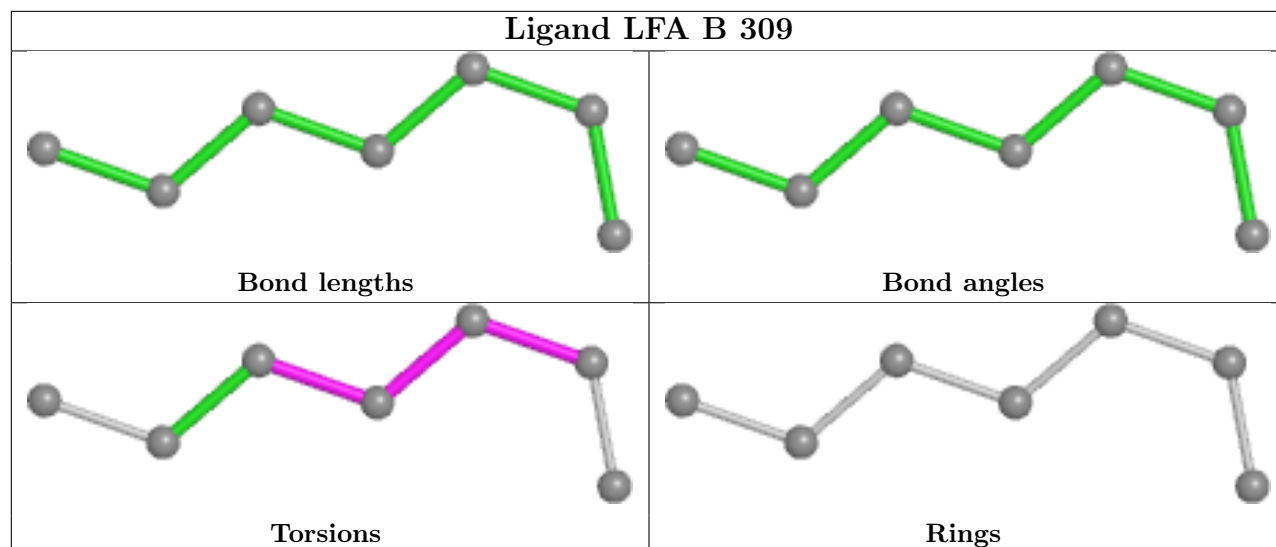


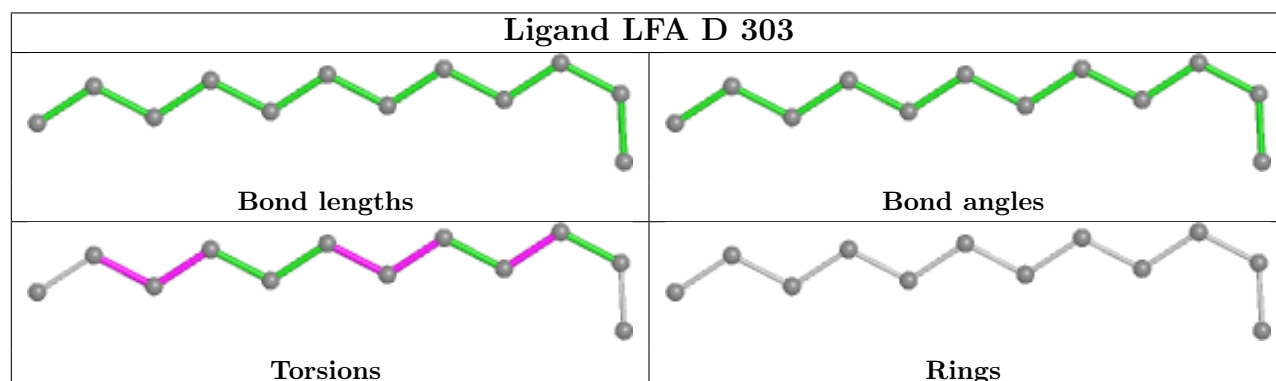
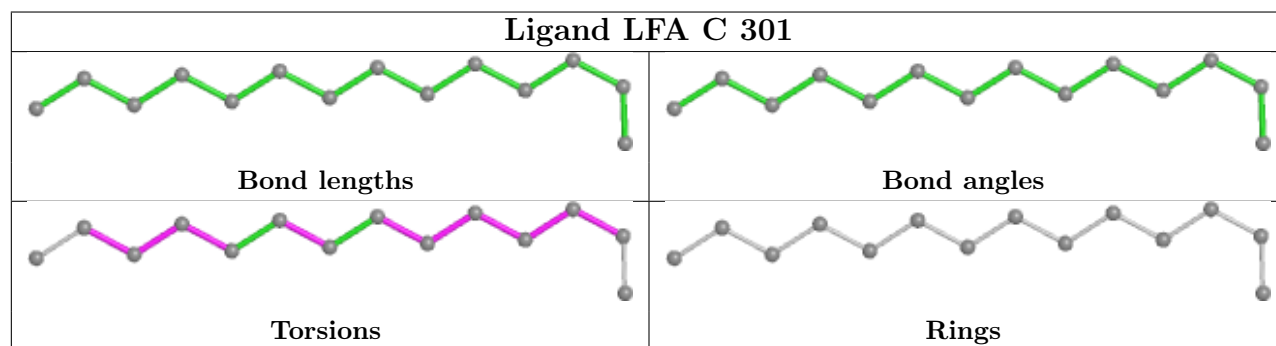
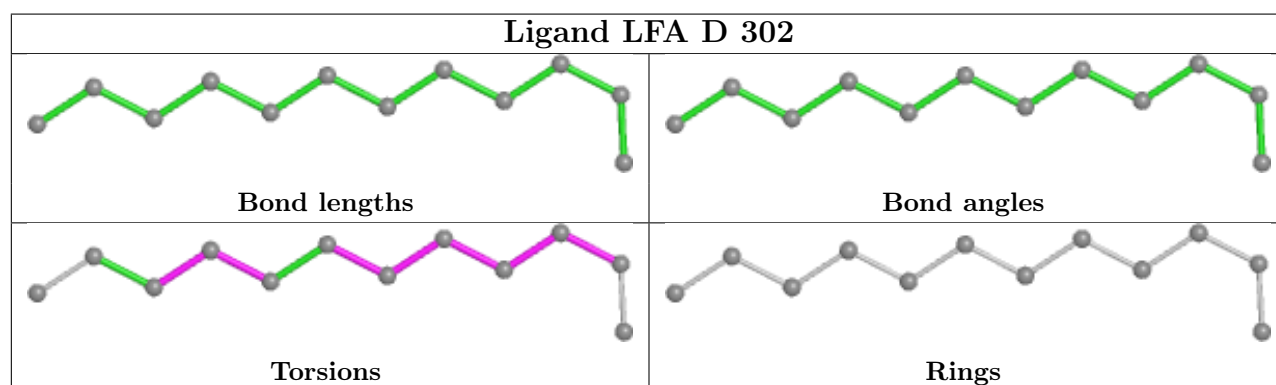
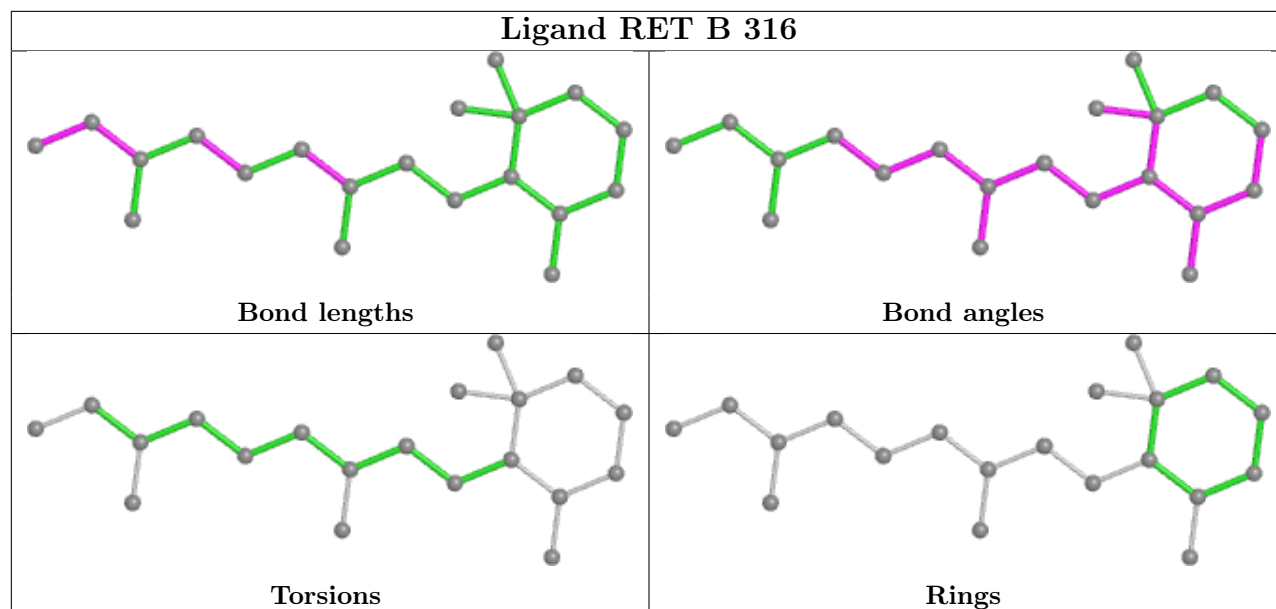
## Ligand OLB E 301

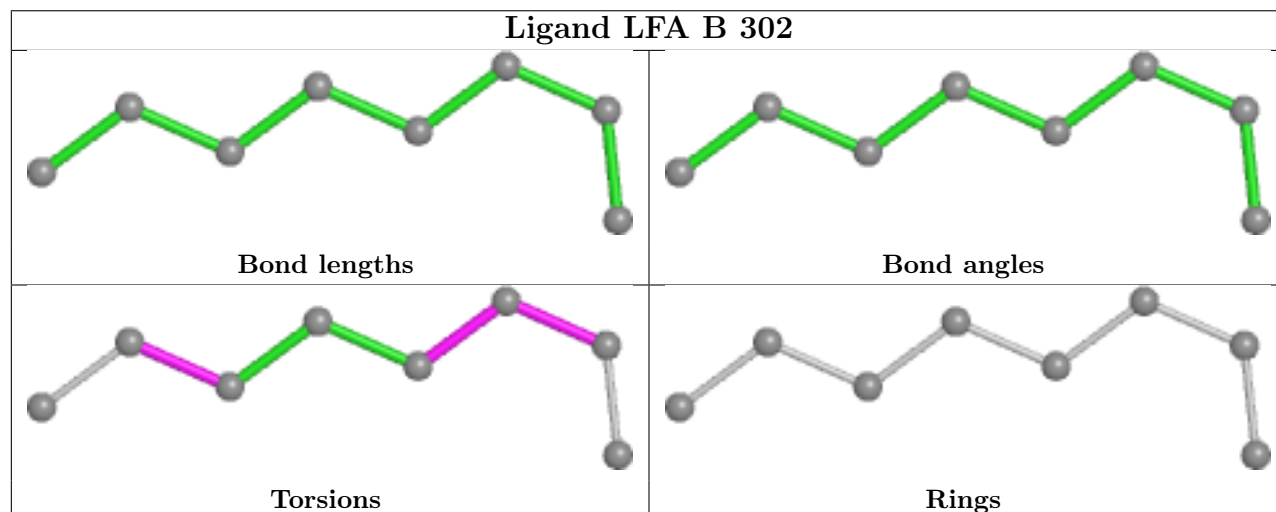
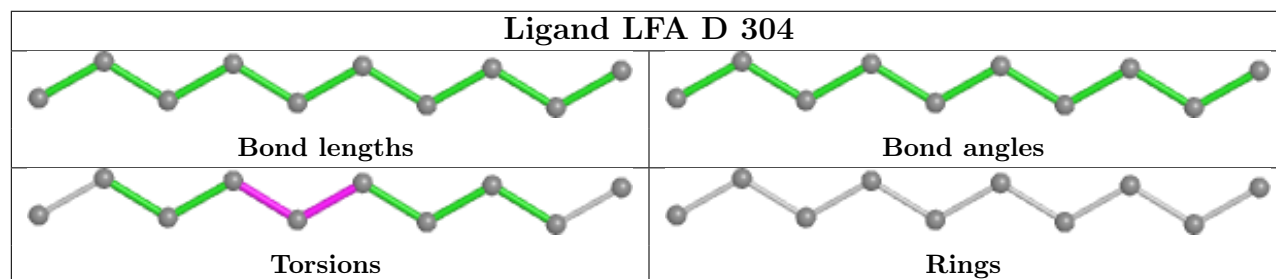
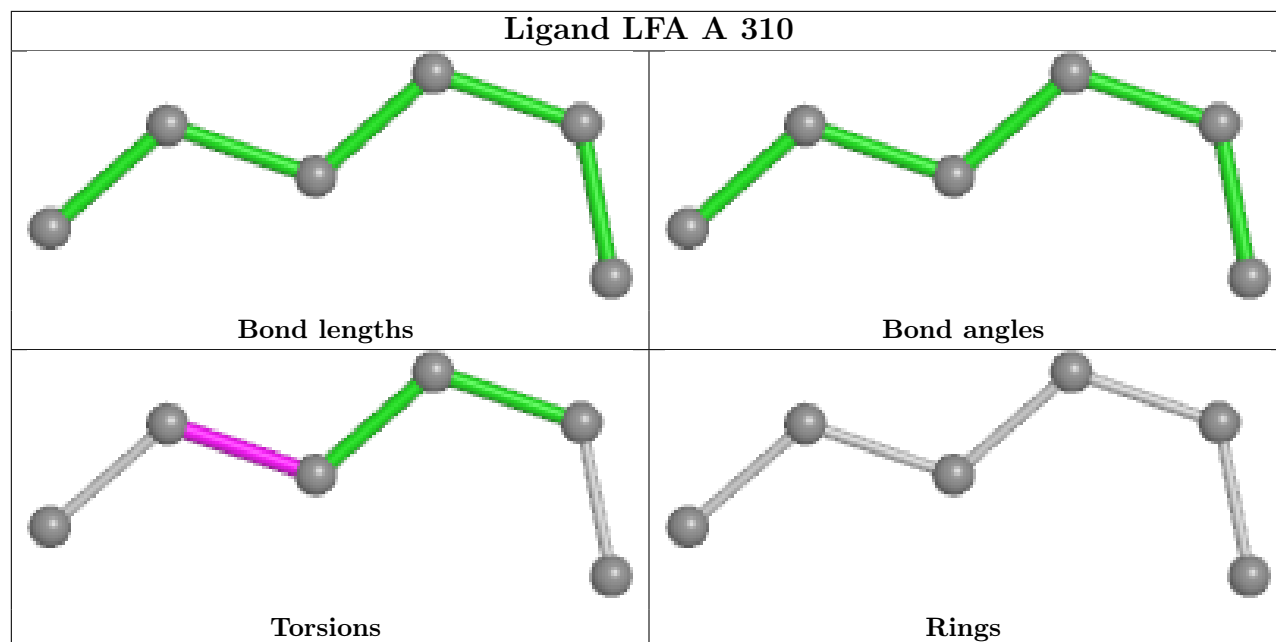
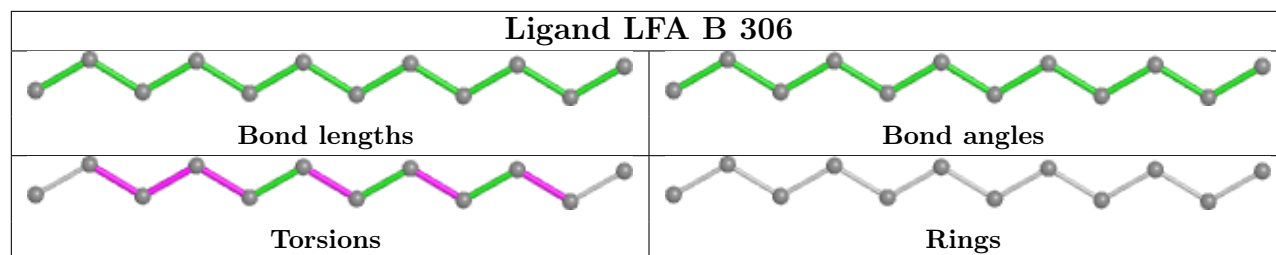


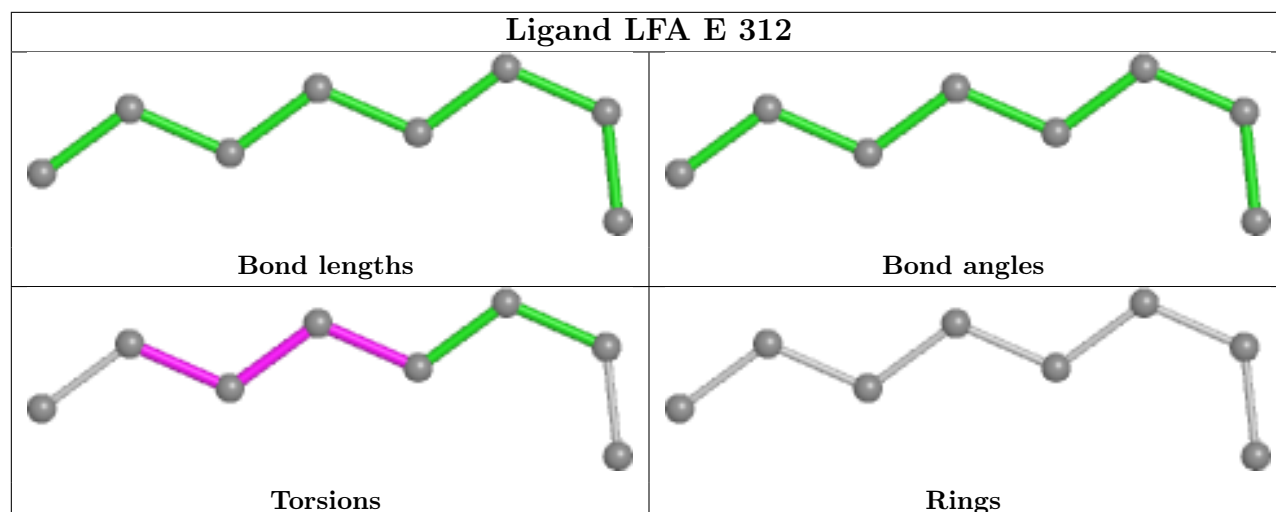
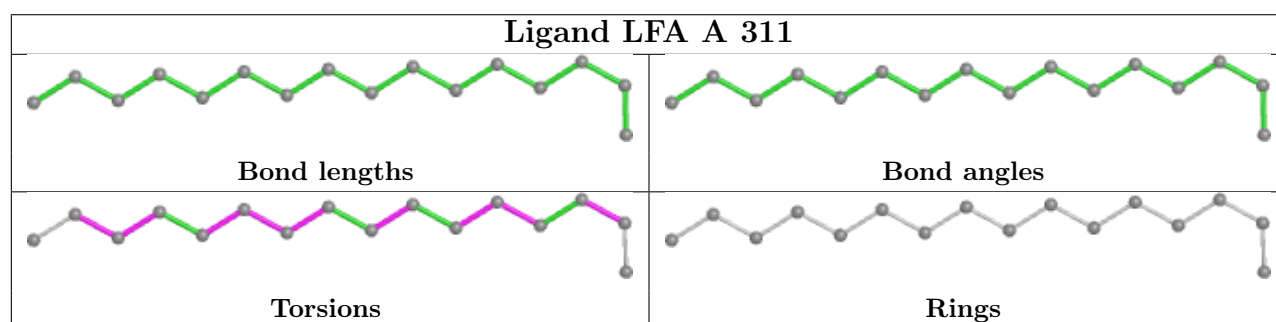
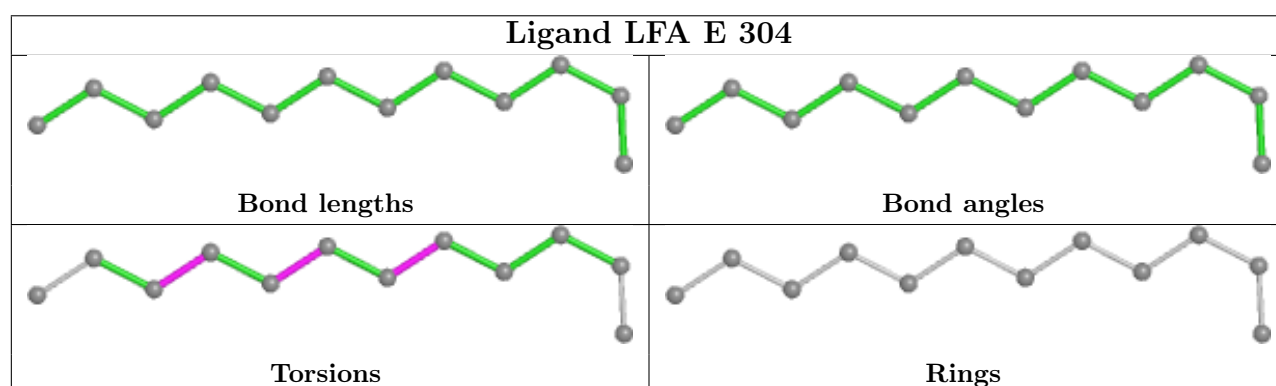
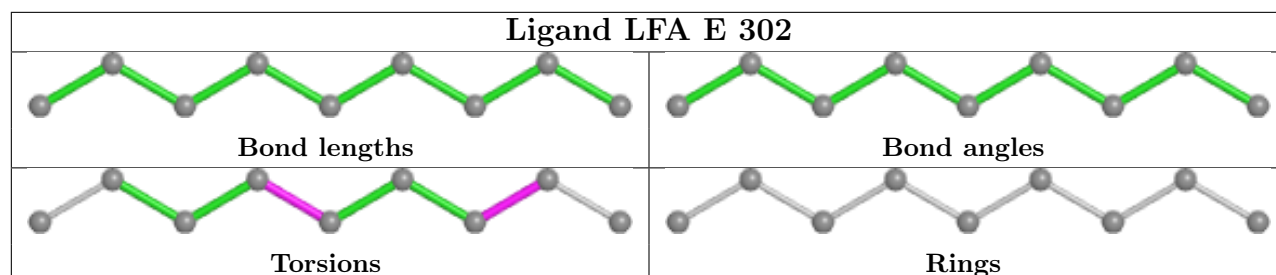
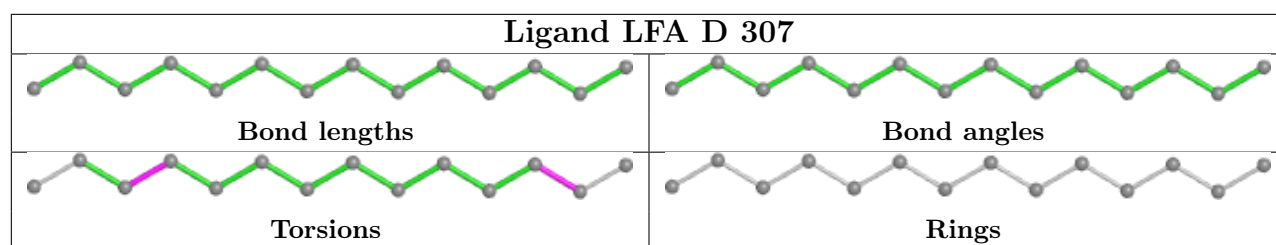
## Ligand LFA E 308

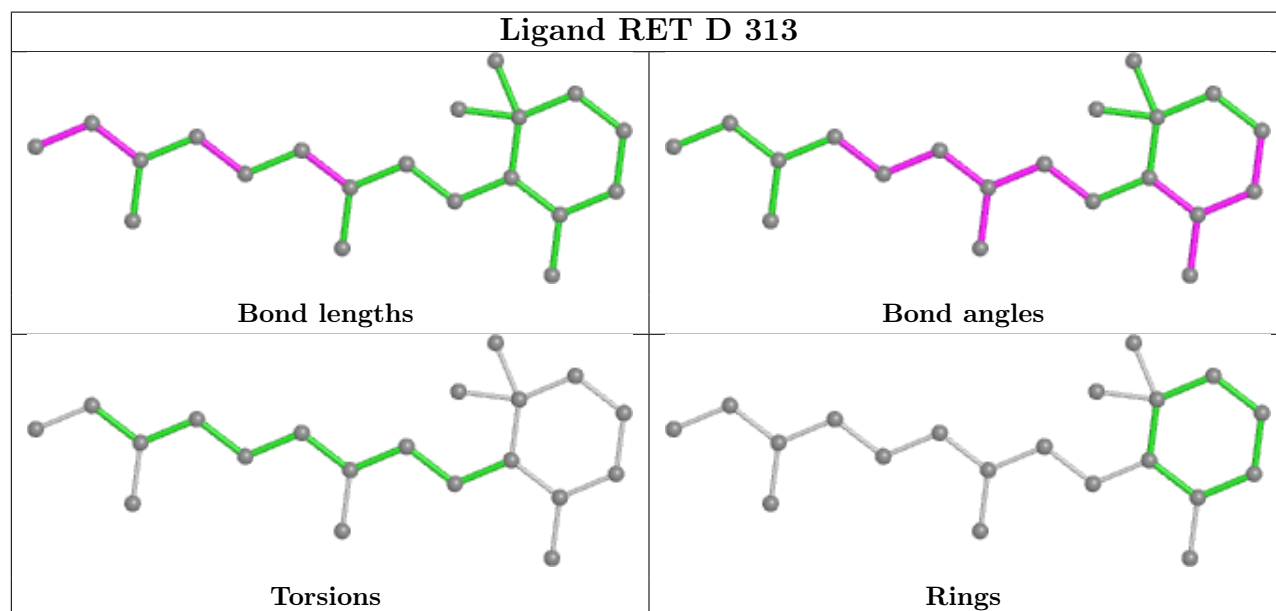
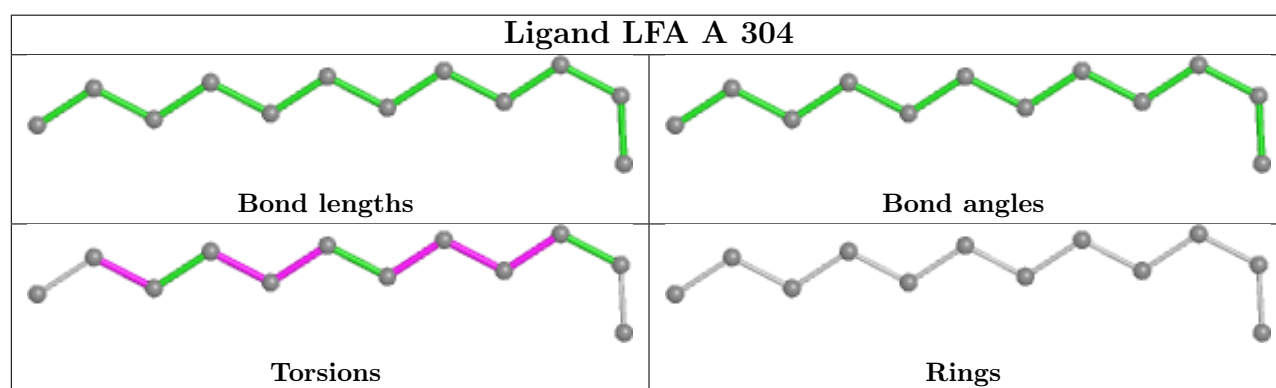
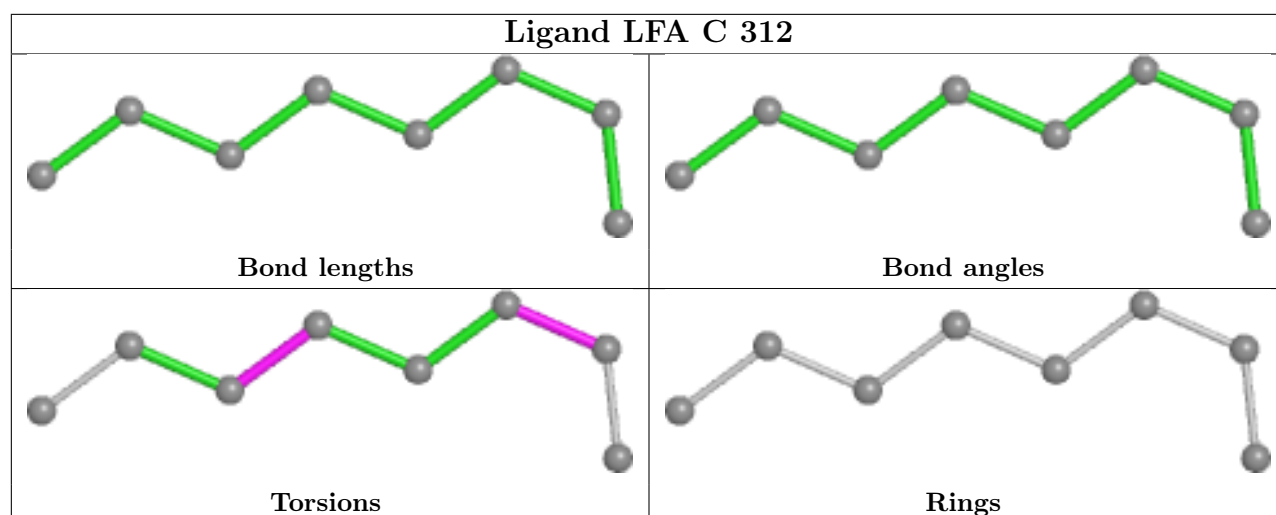


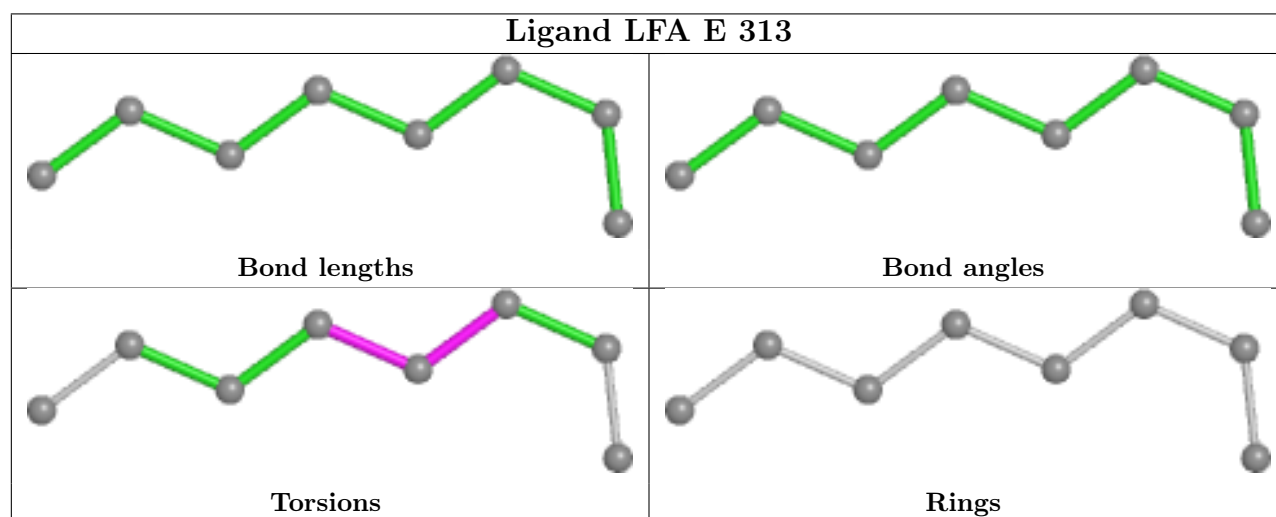
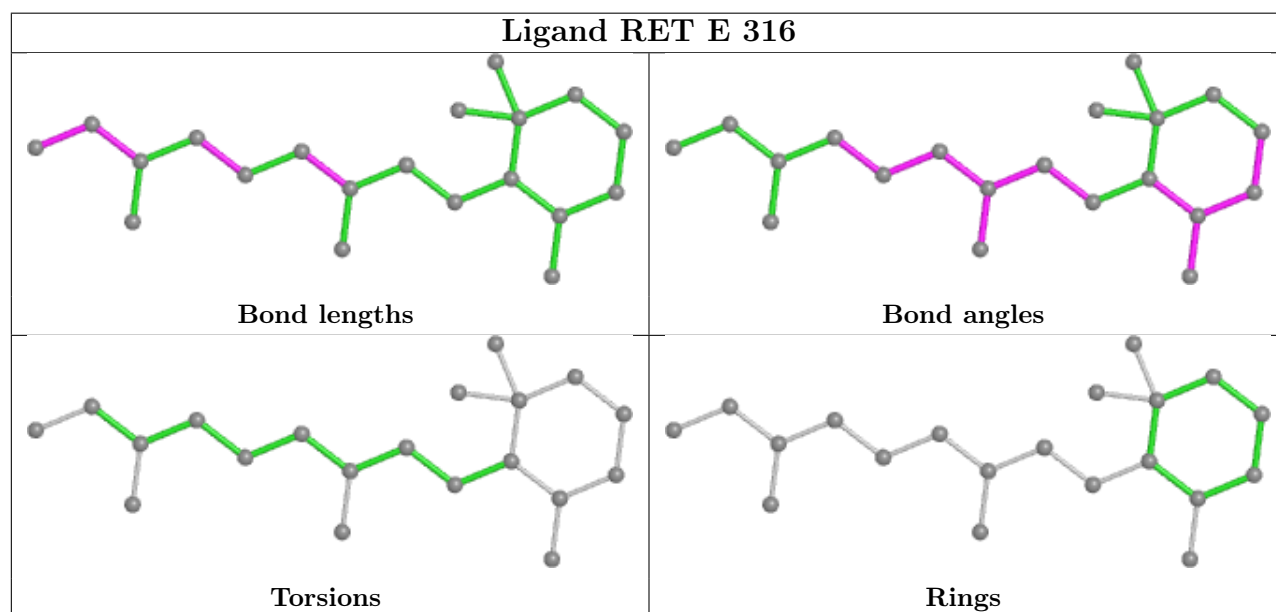
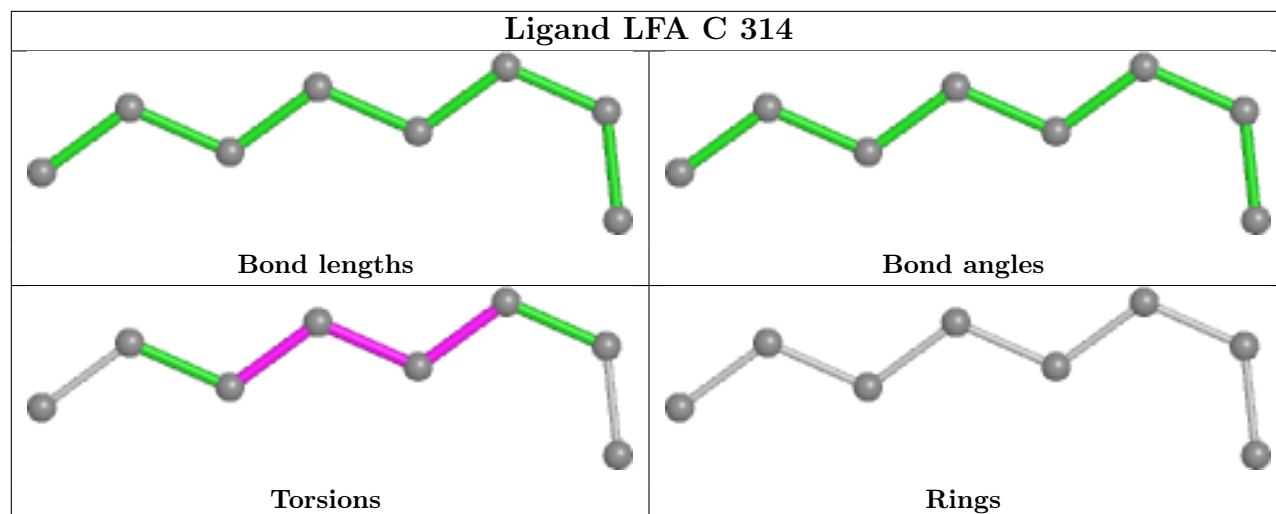


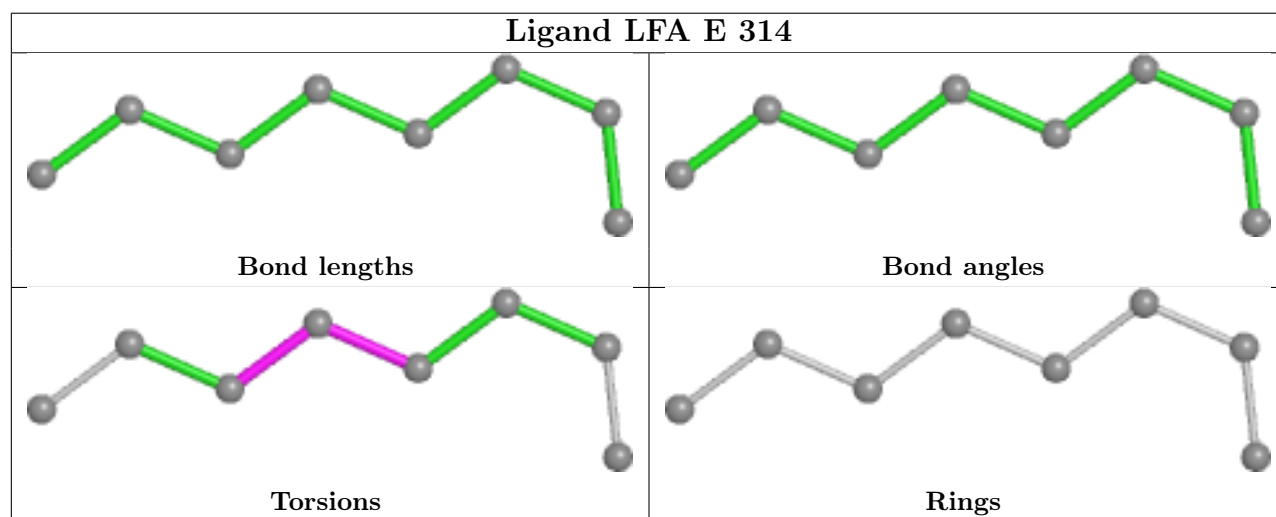
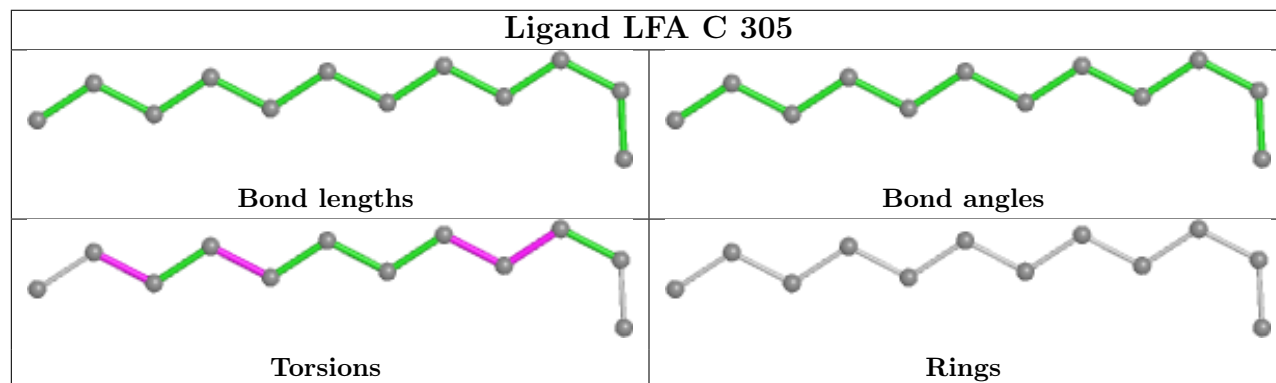
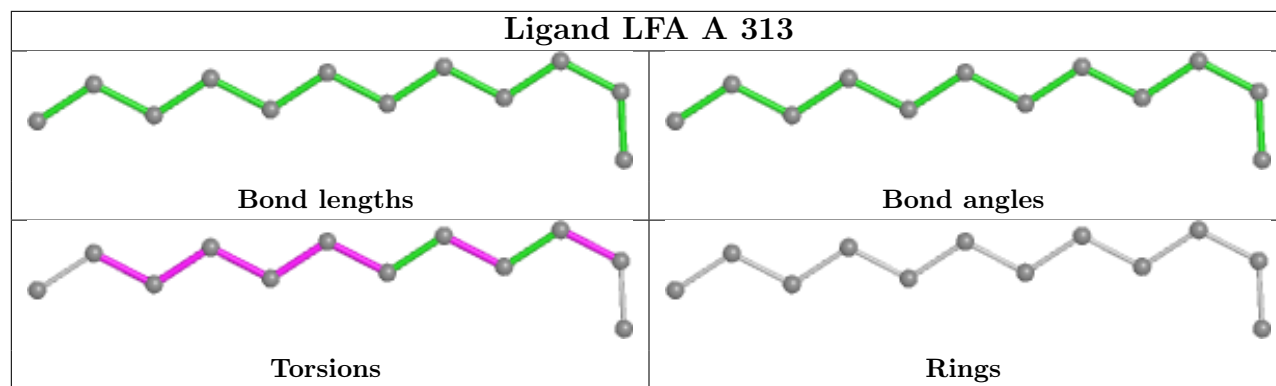


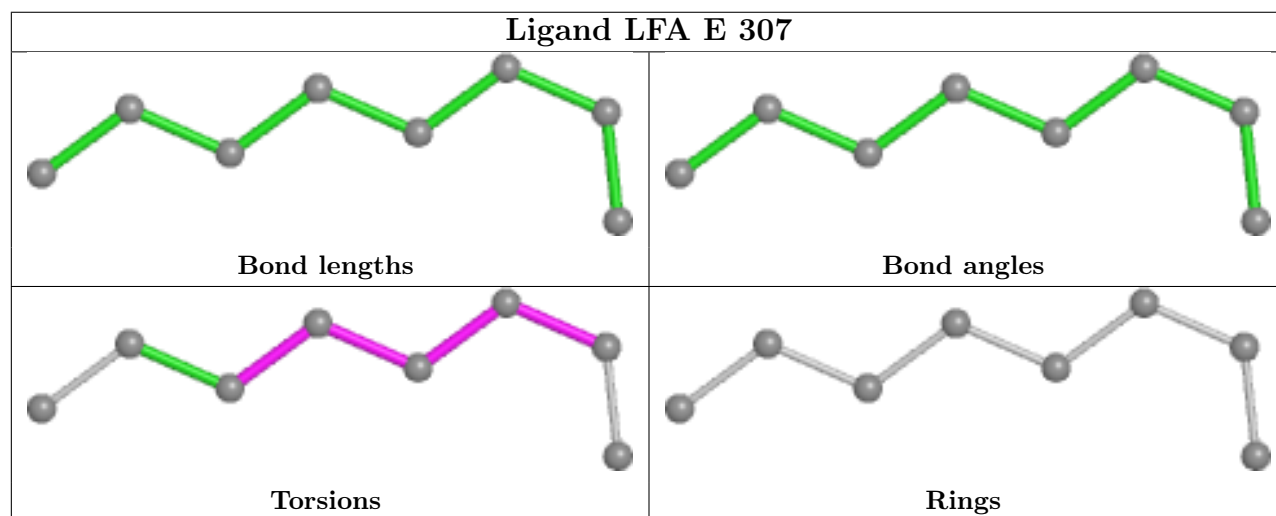
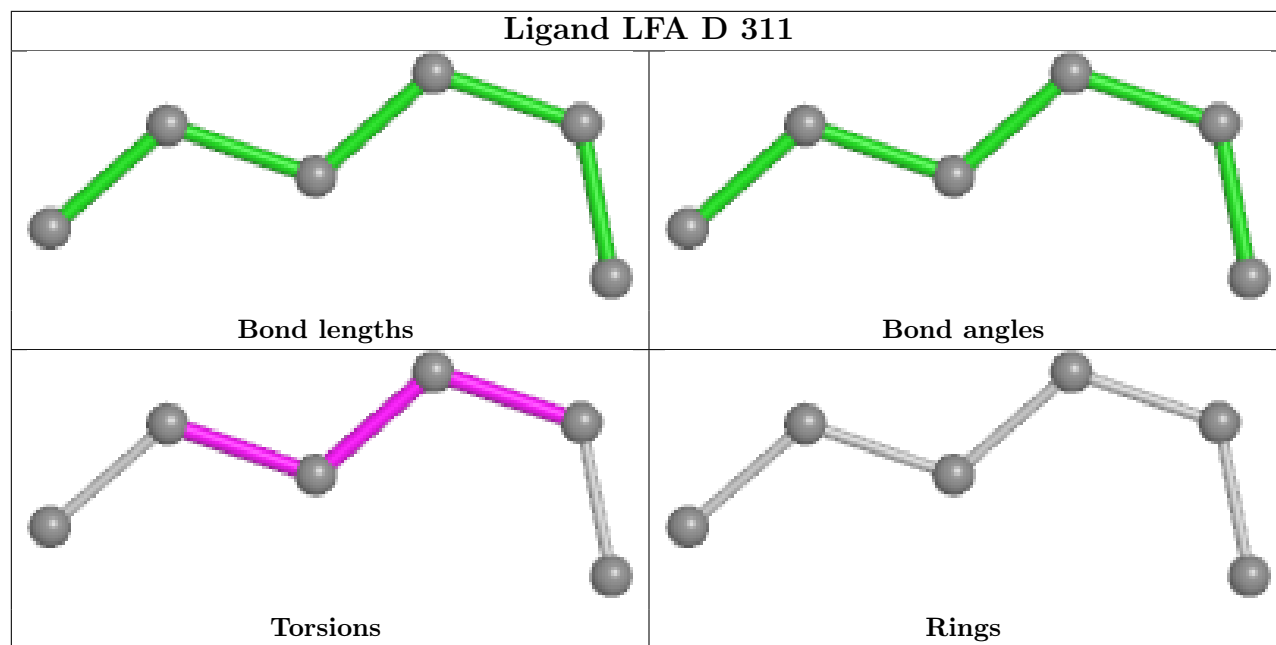


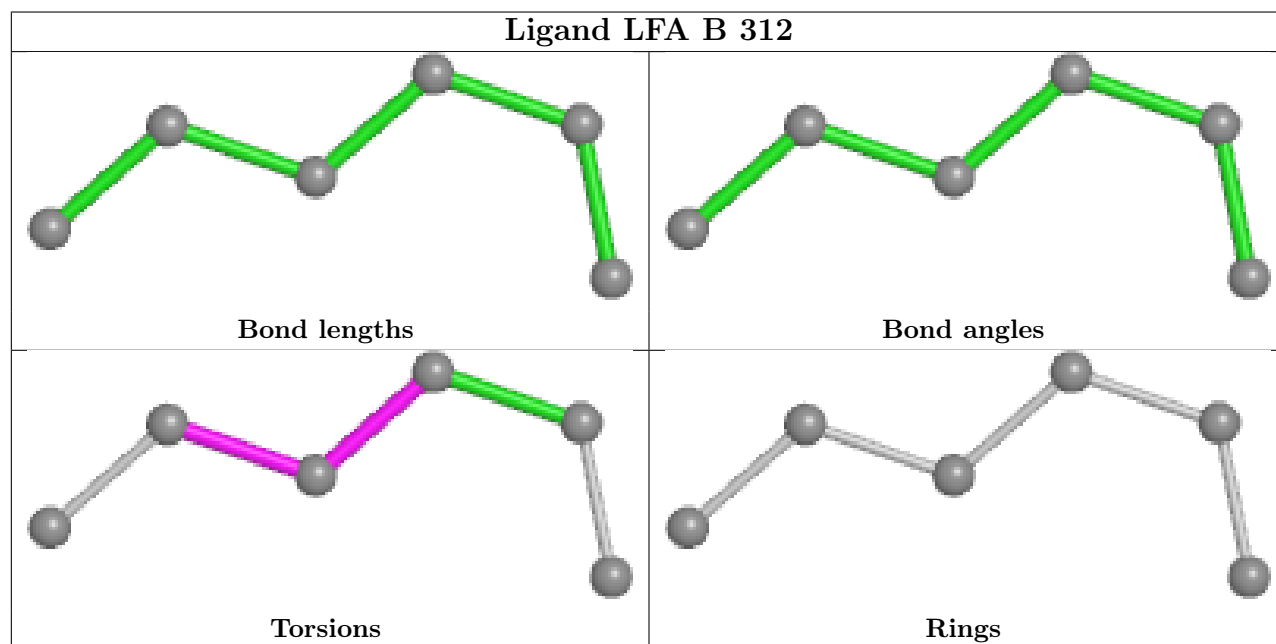
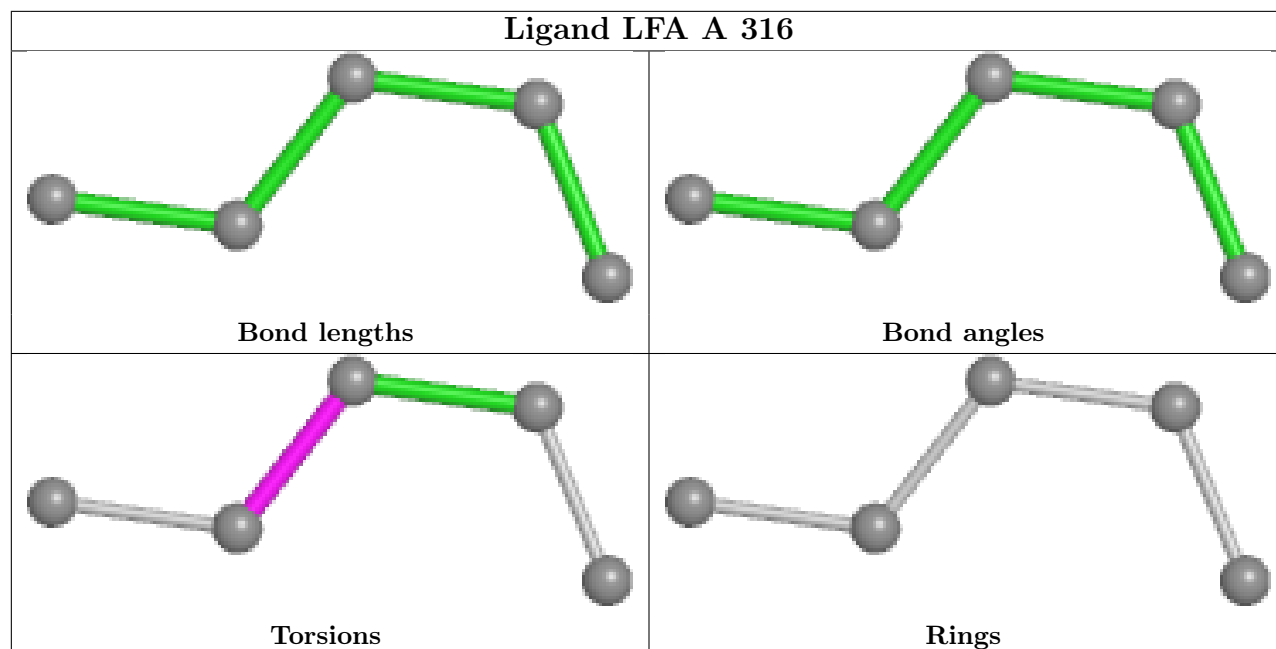


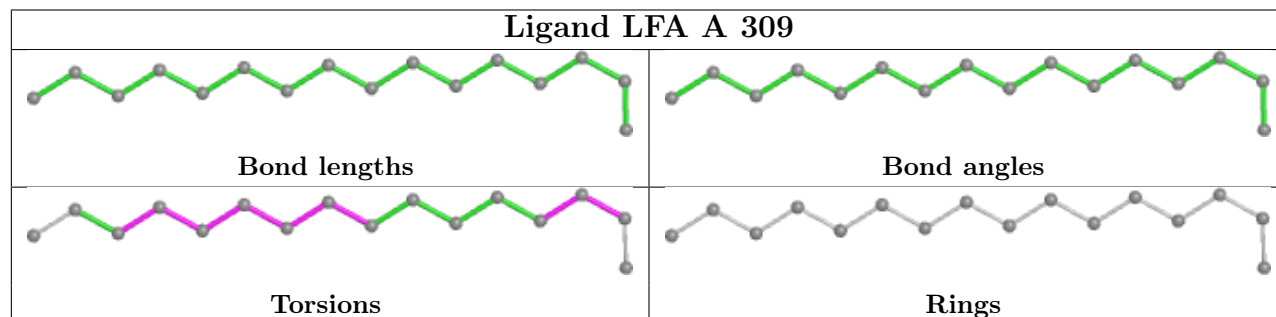
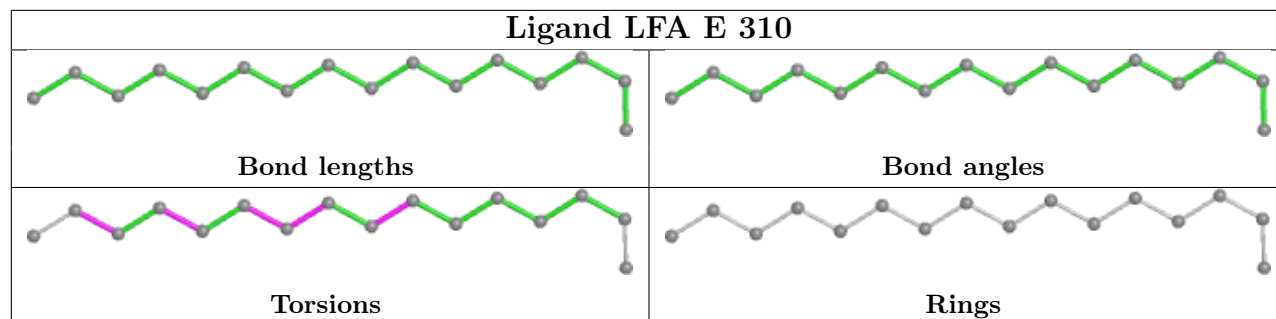
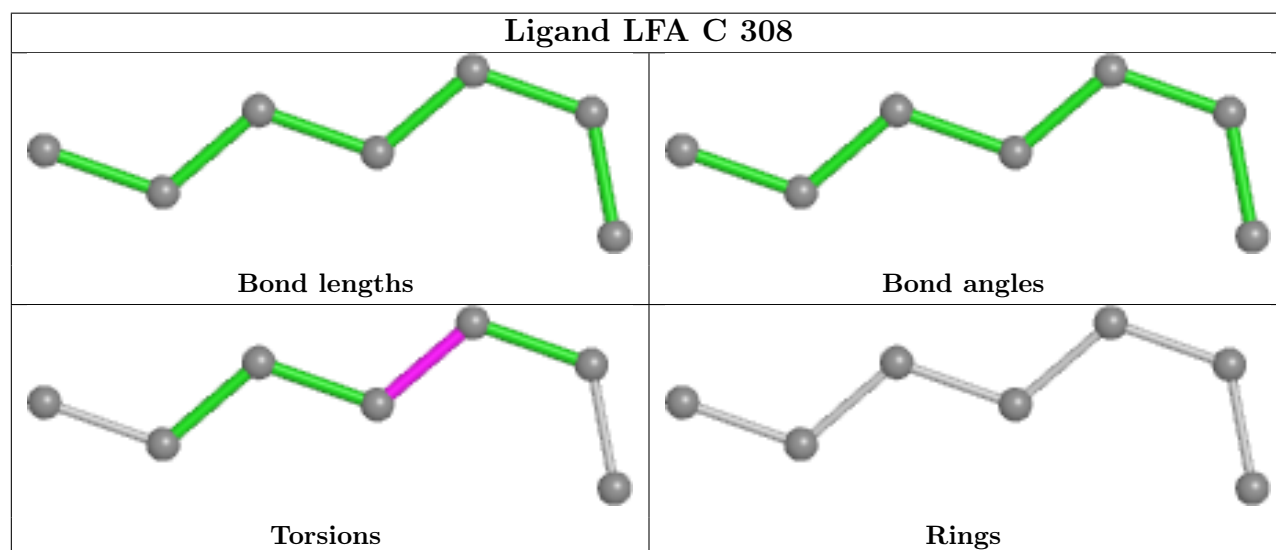
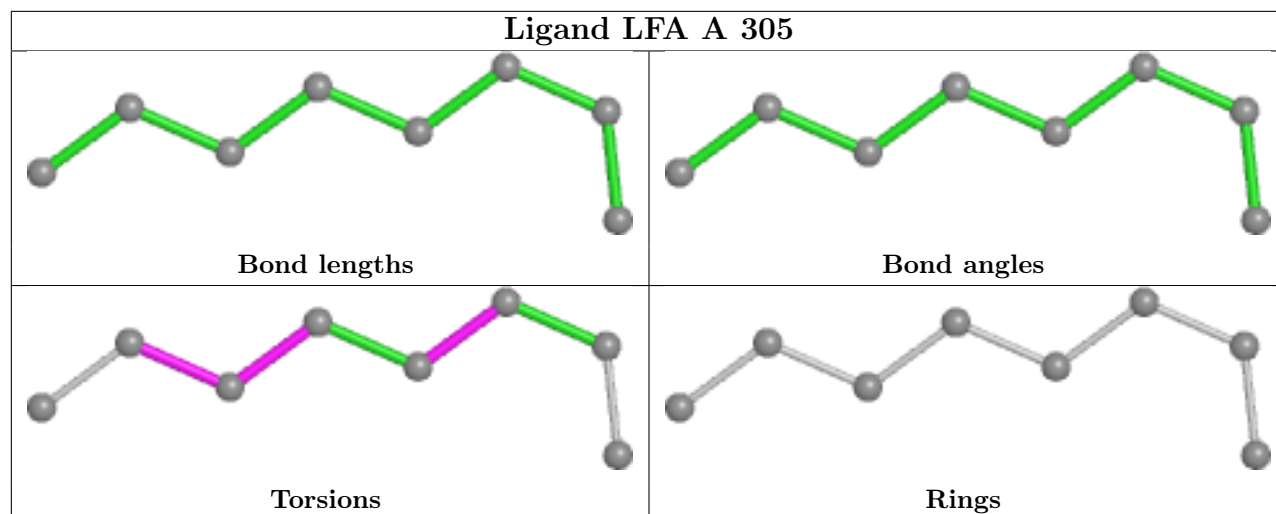




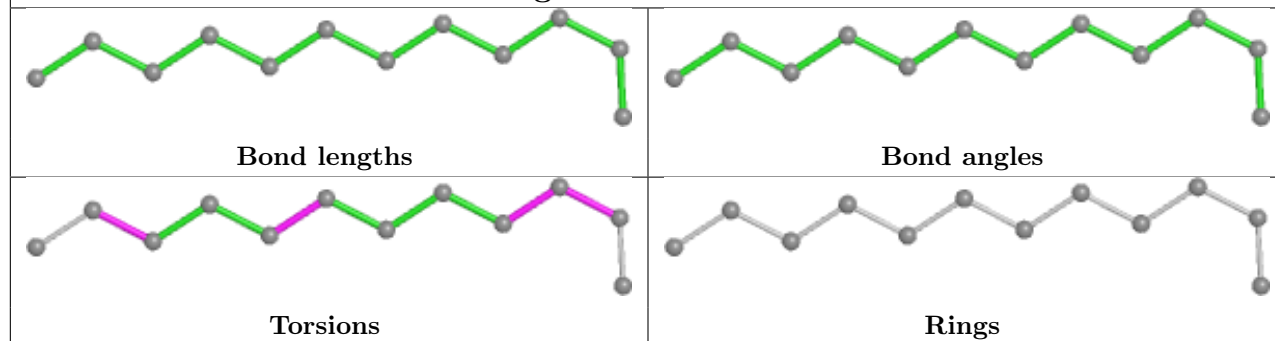




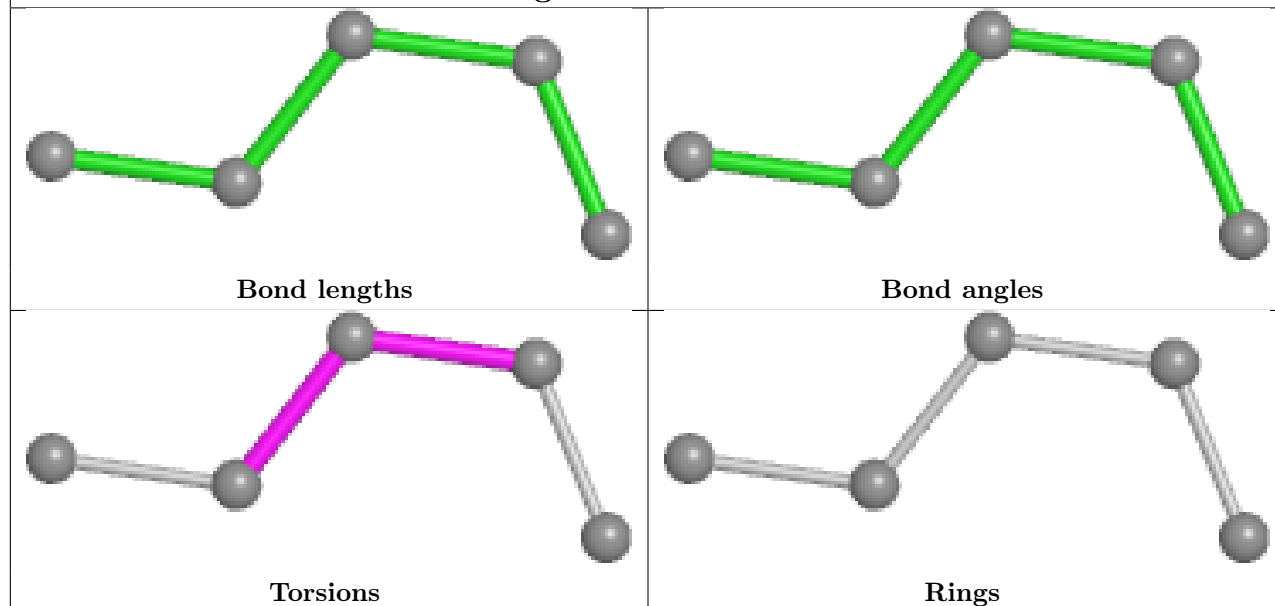




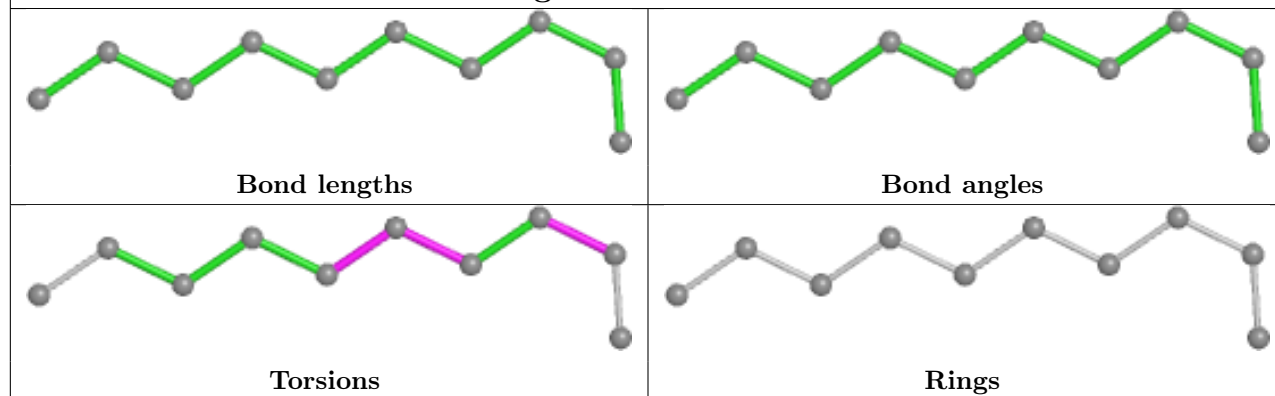
## Ligand LFA D 305

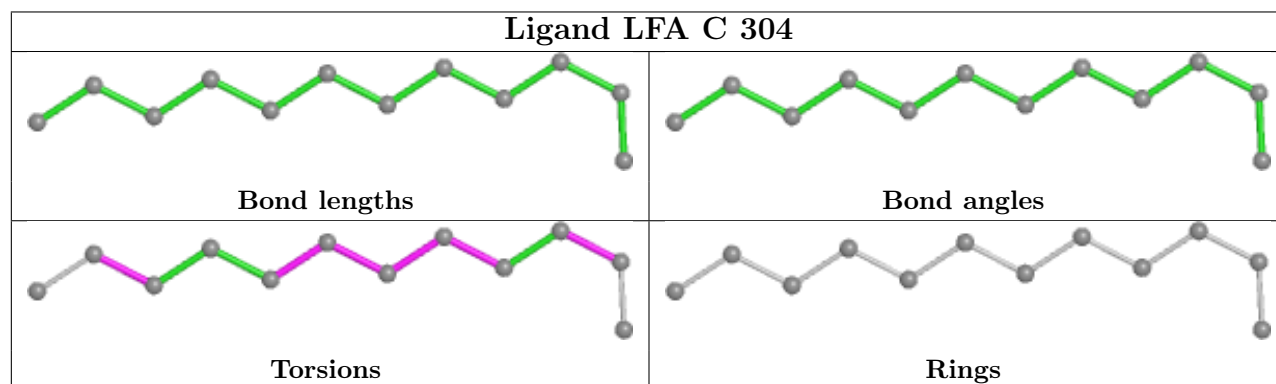
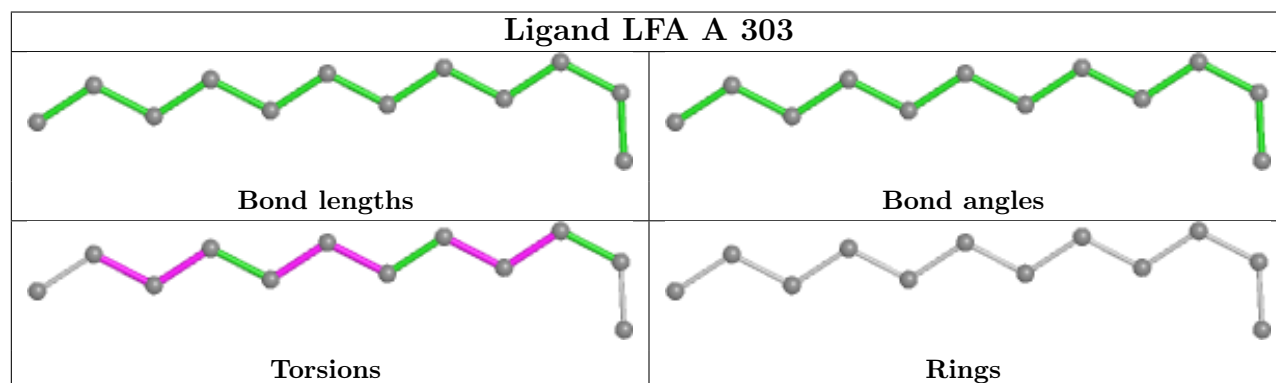
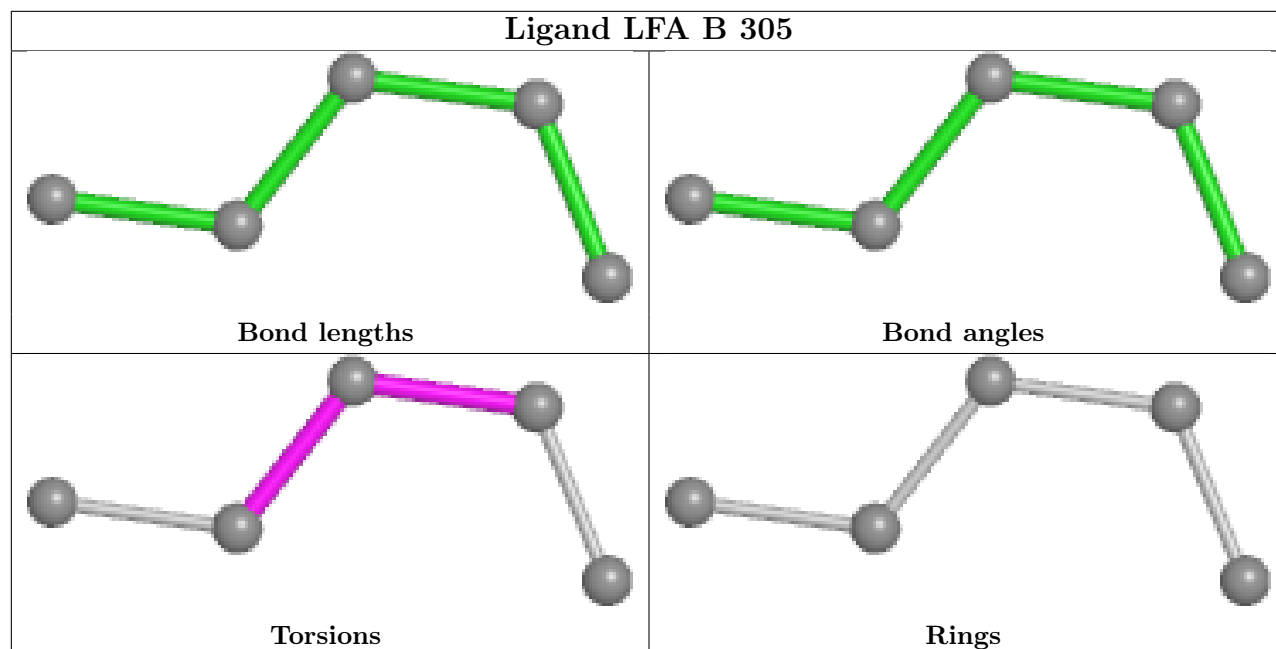


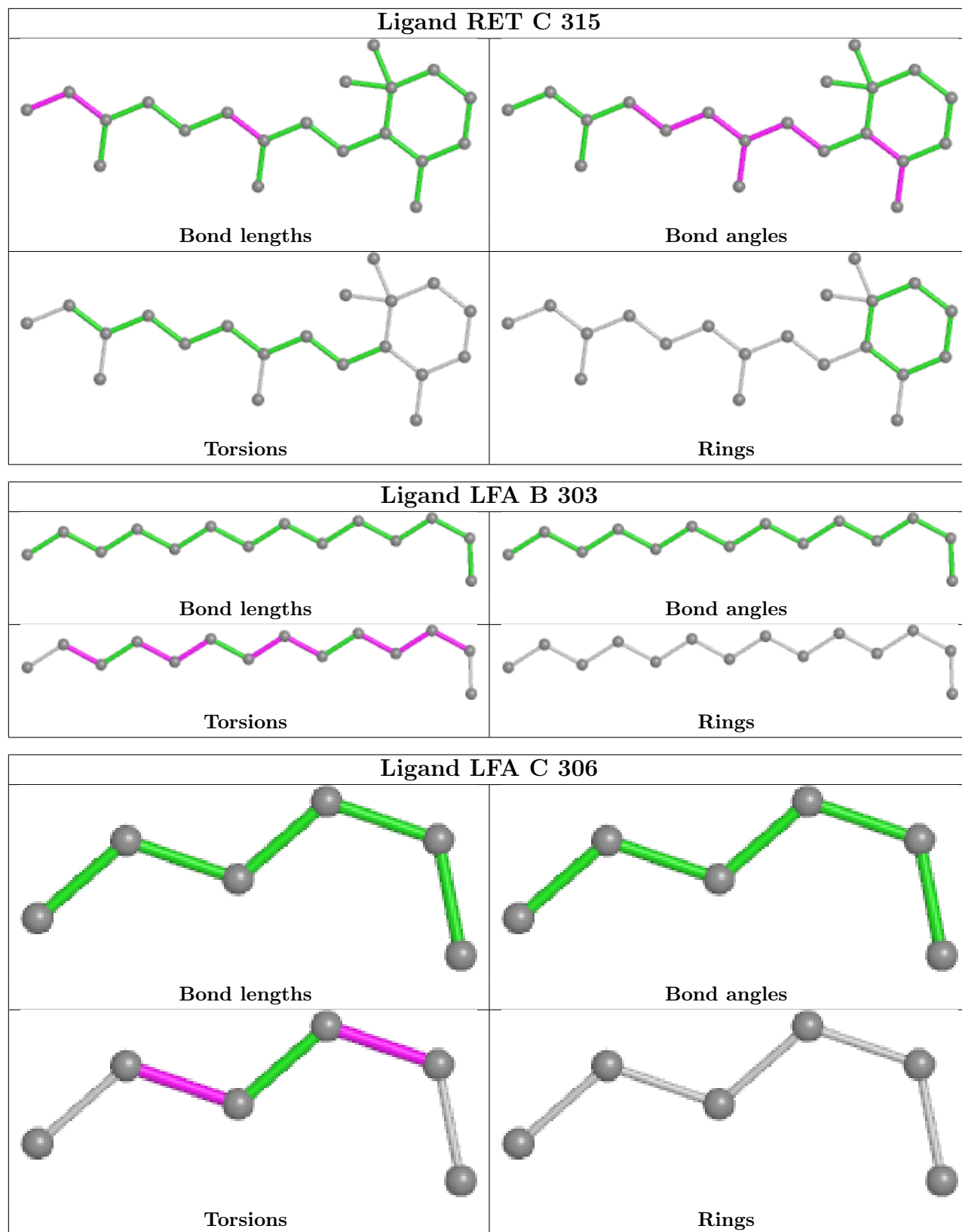
## Ligand LFA A 308

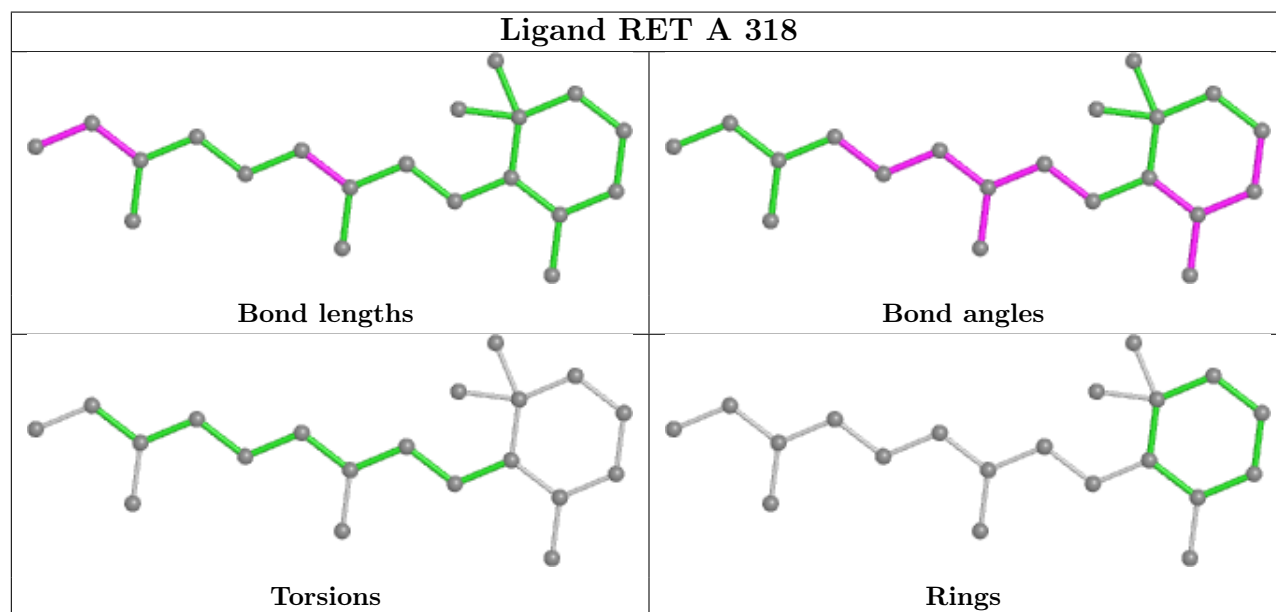
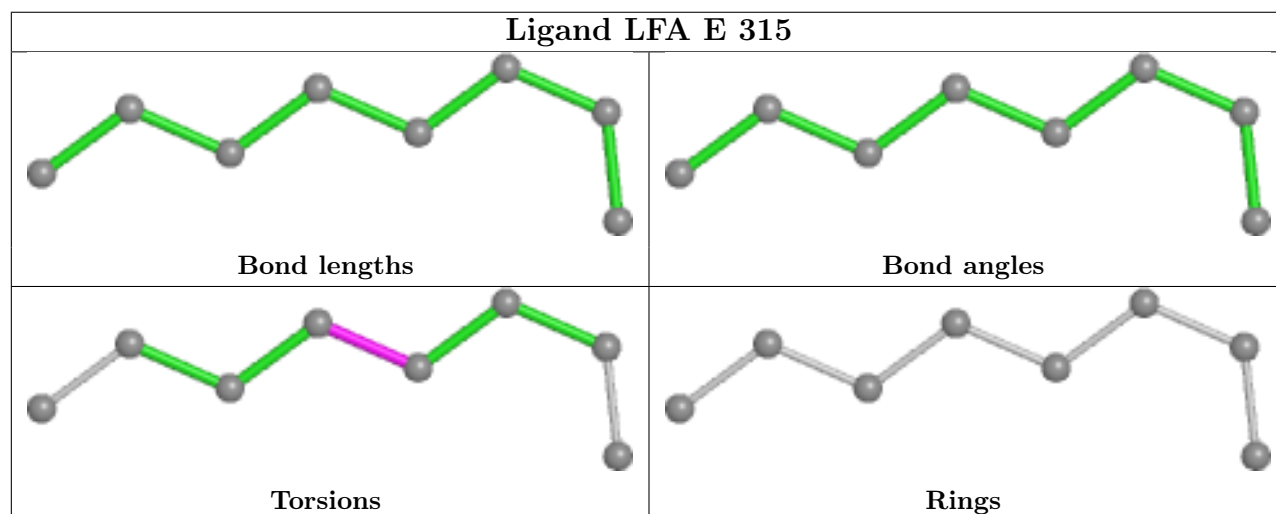
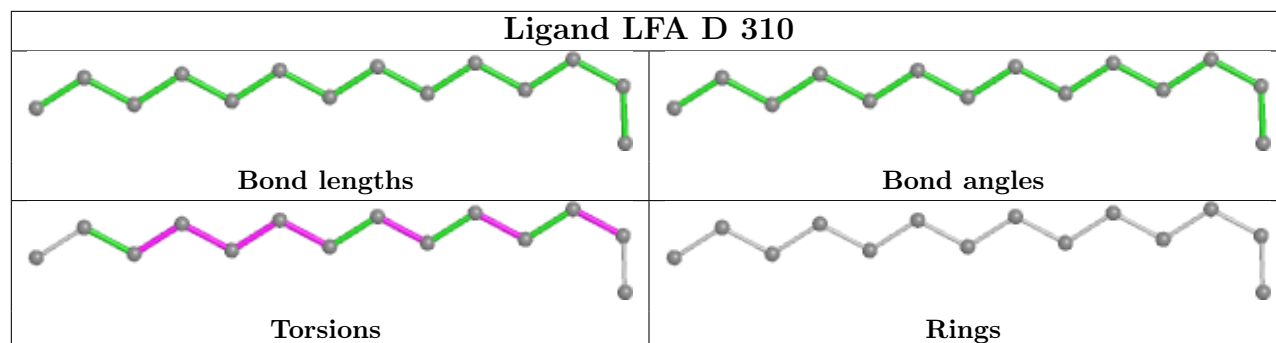


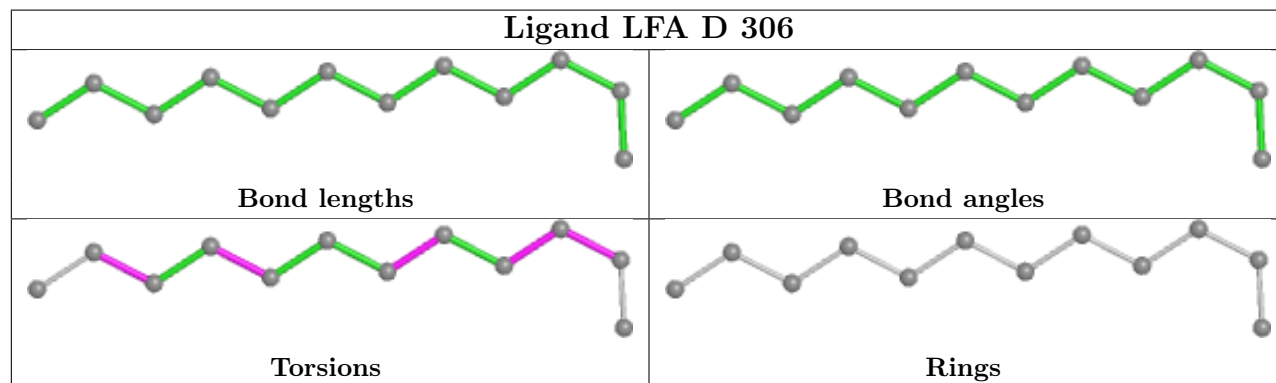
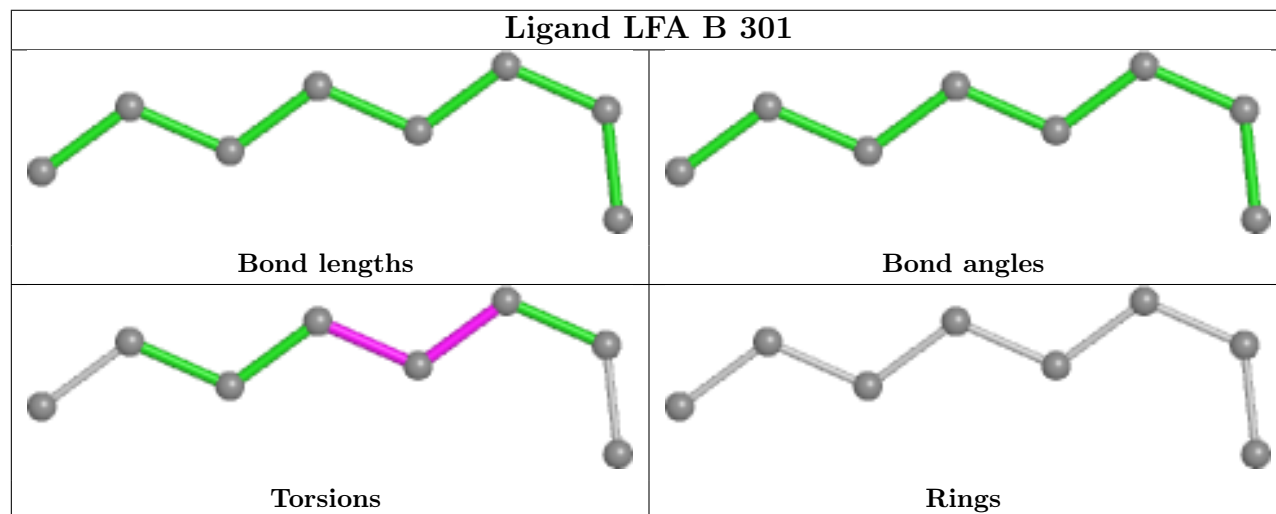
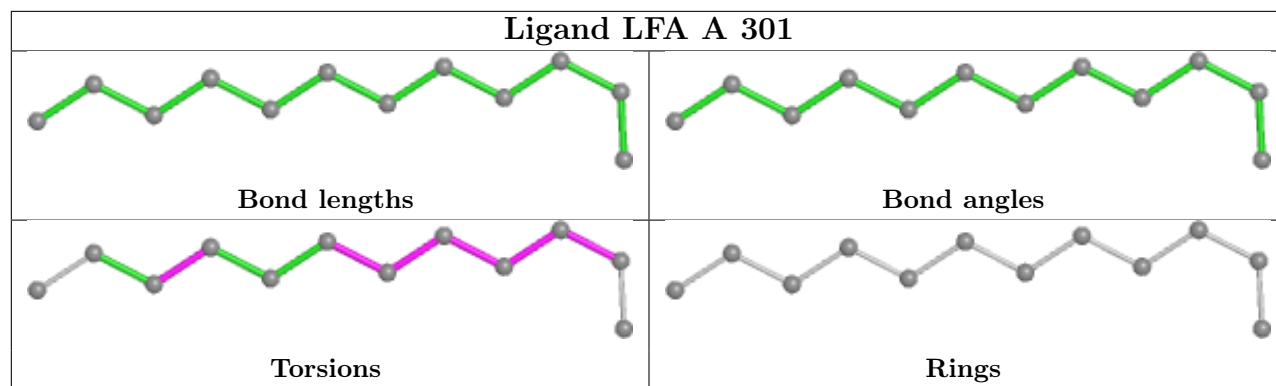
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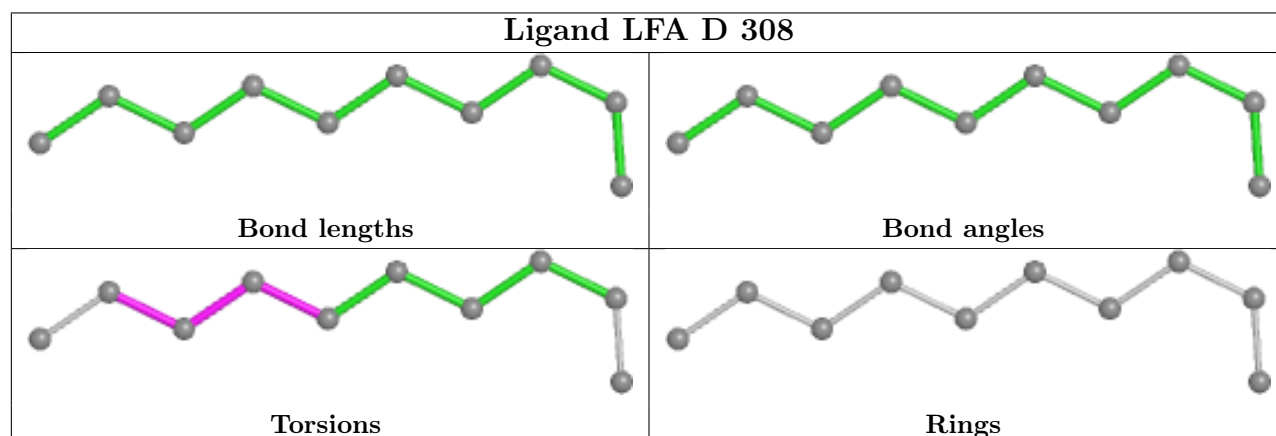
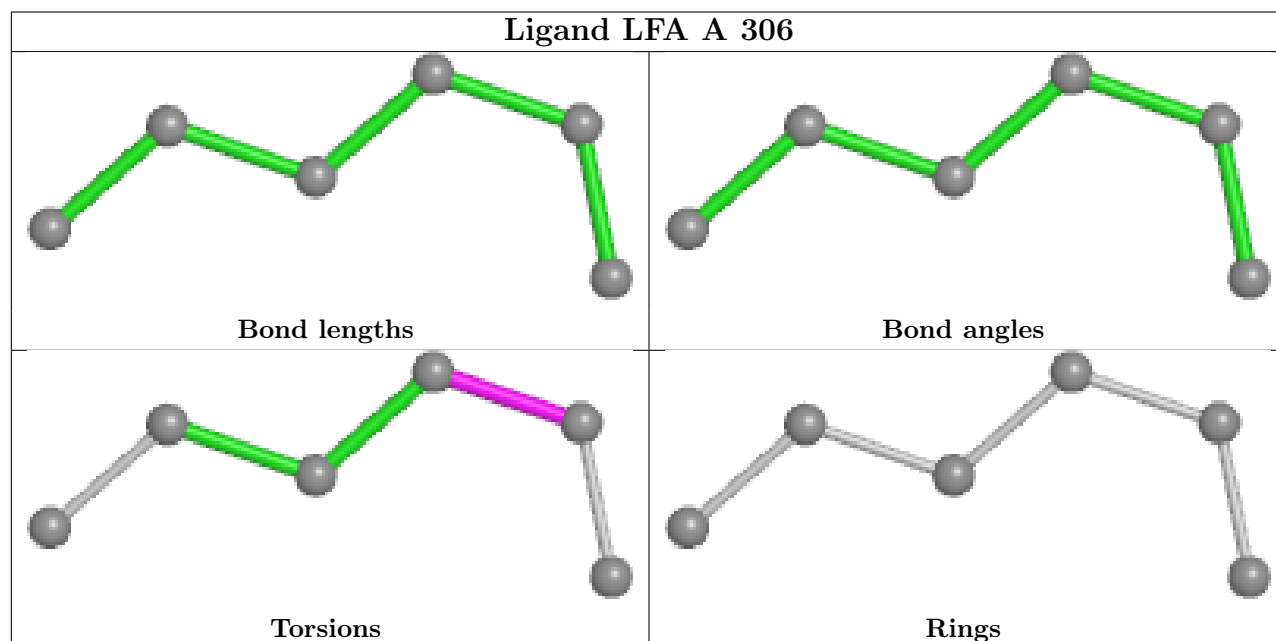
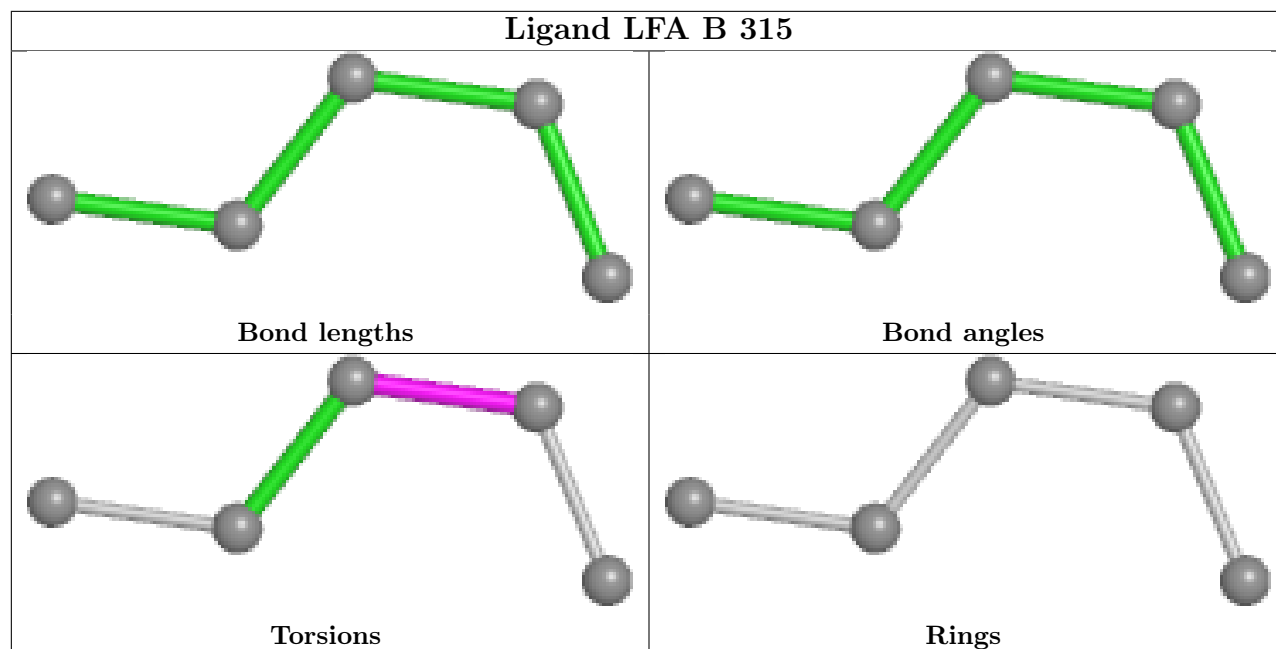


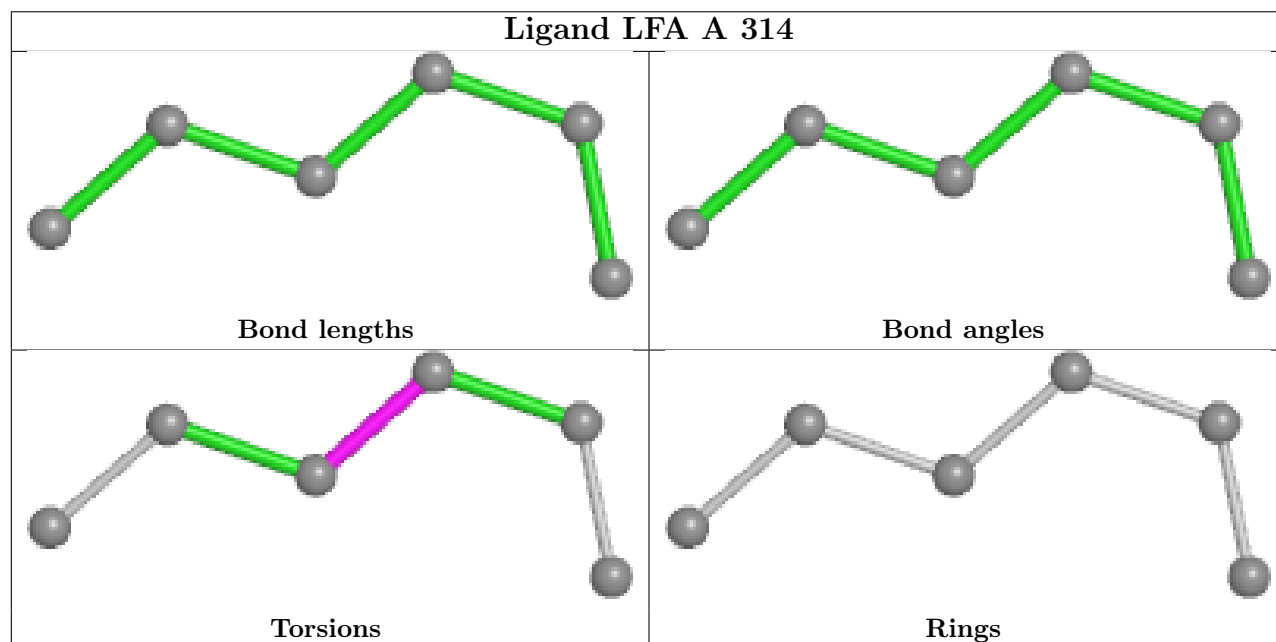
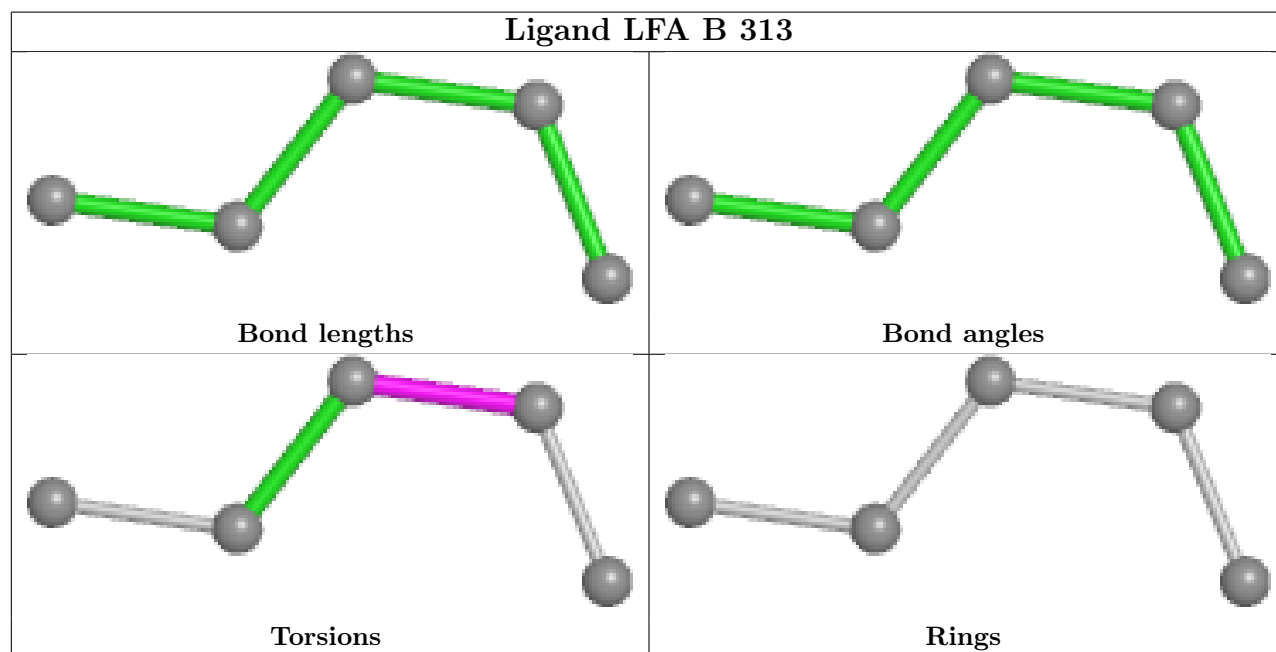
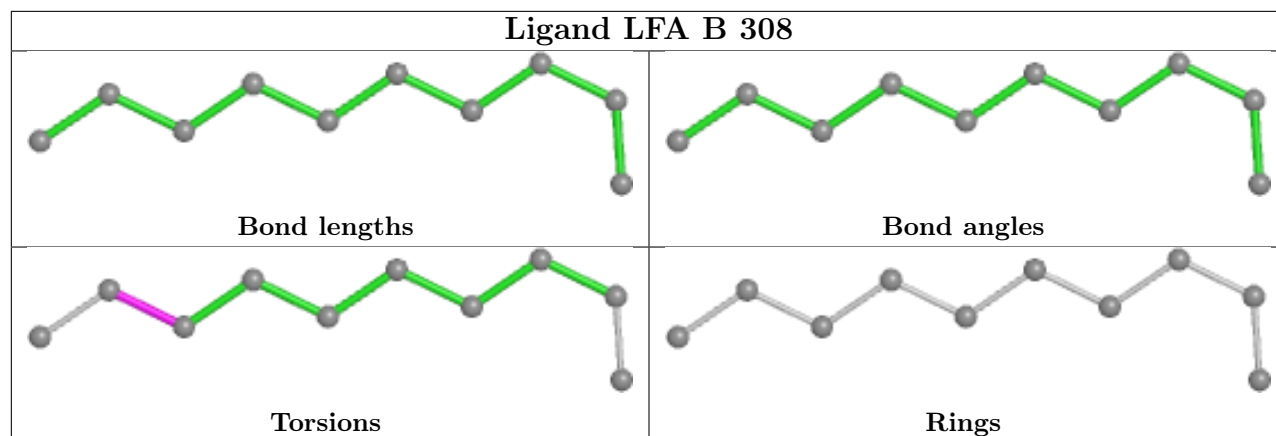


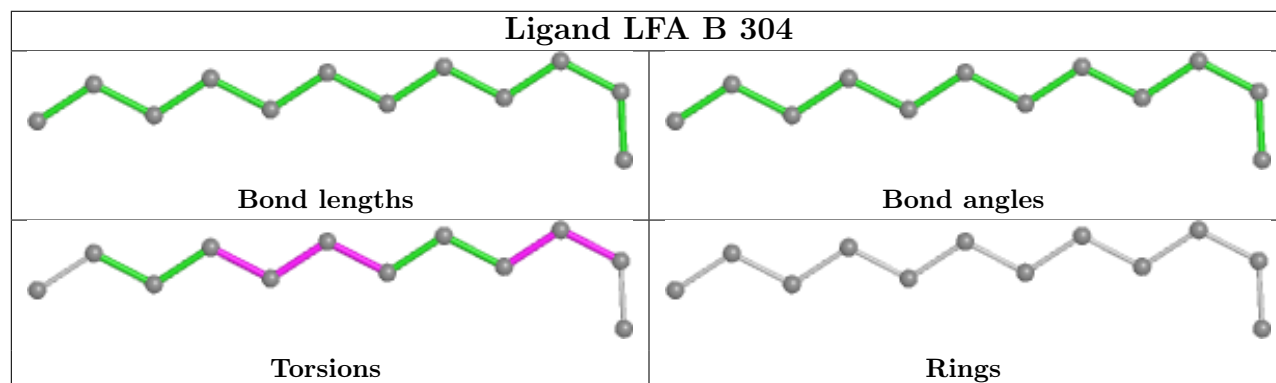
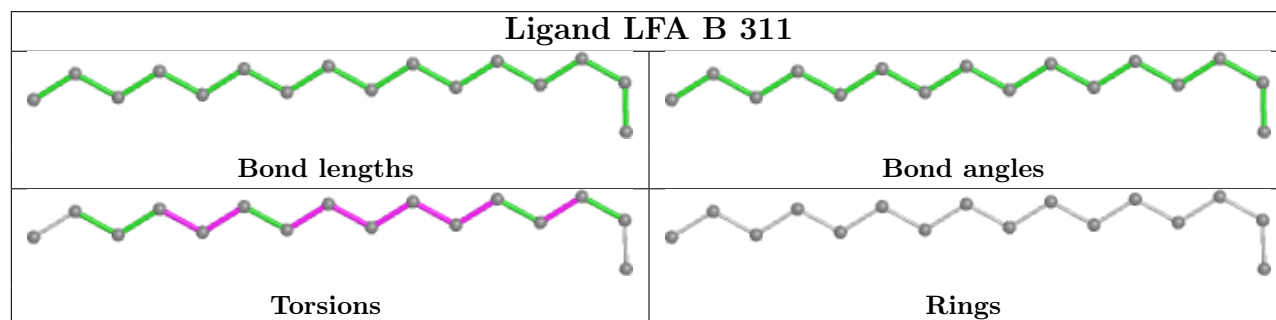
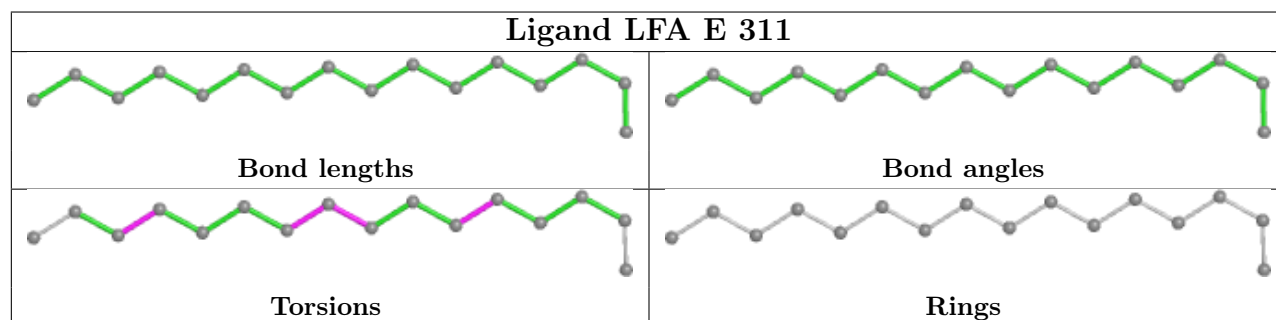
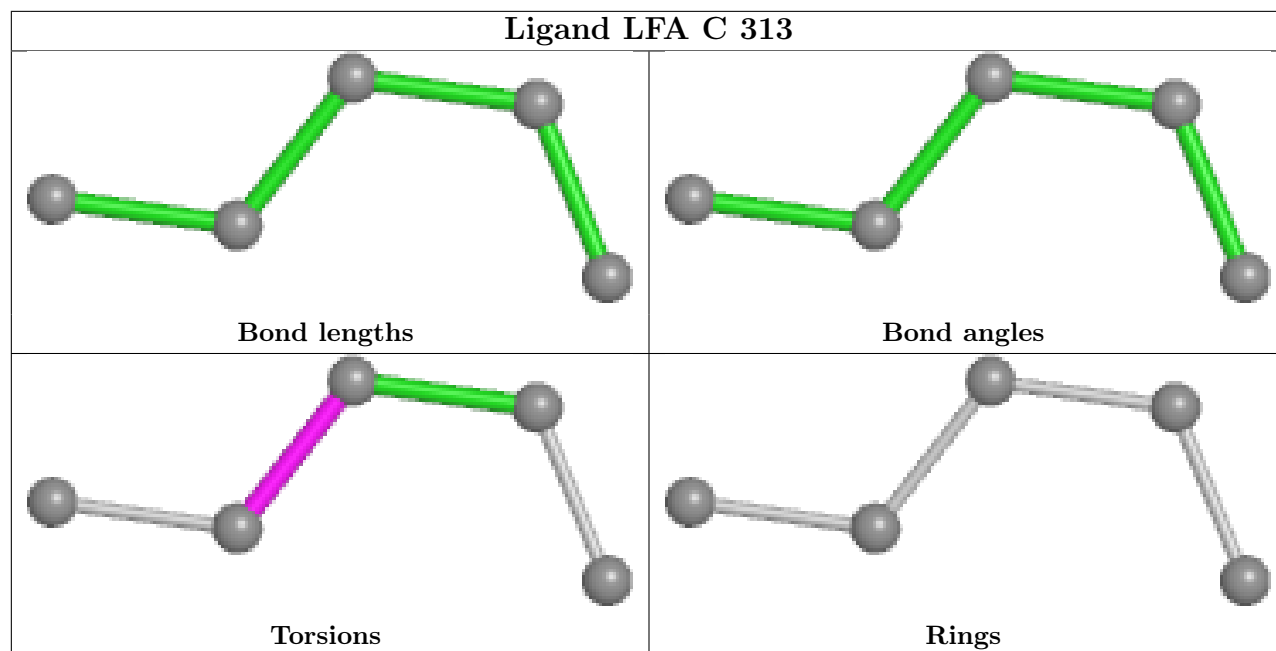


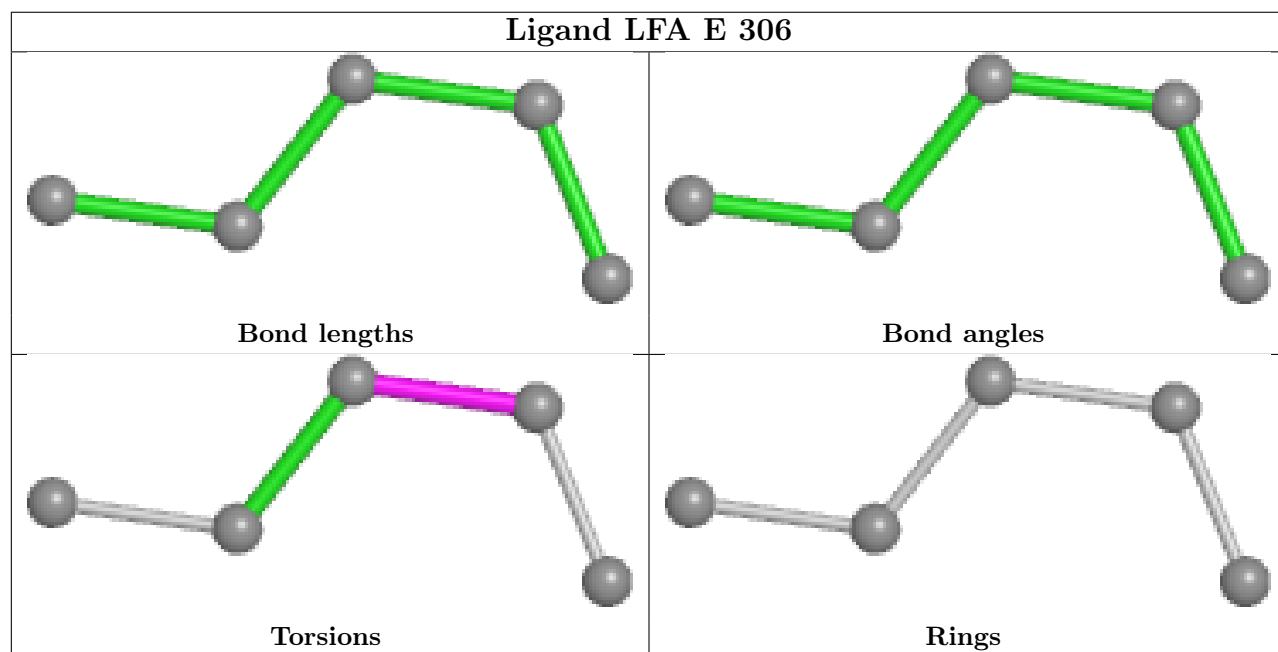
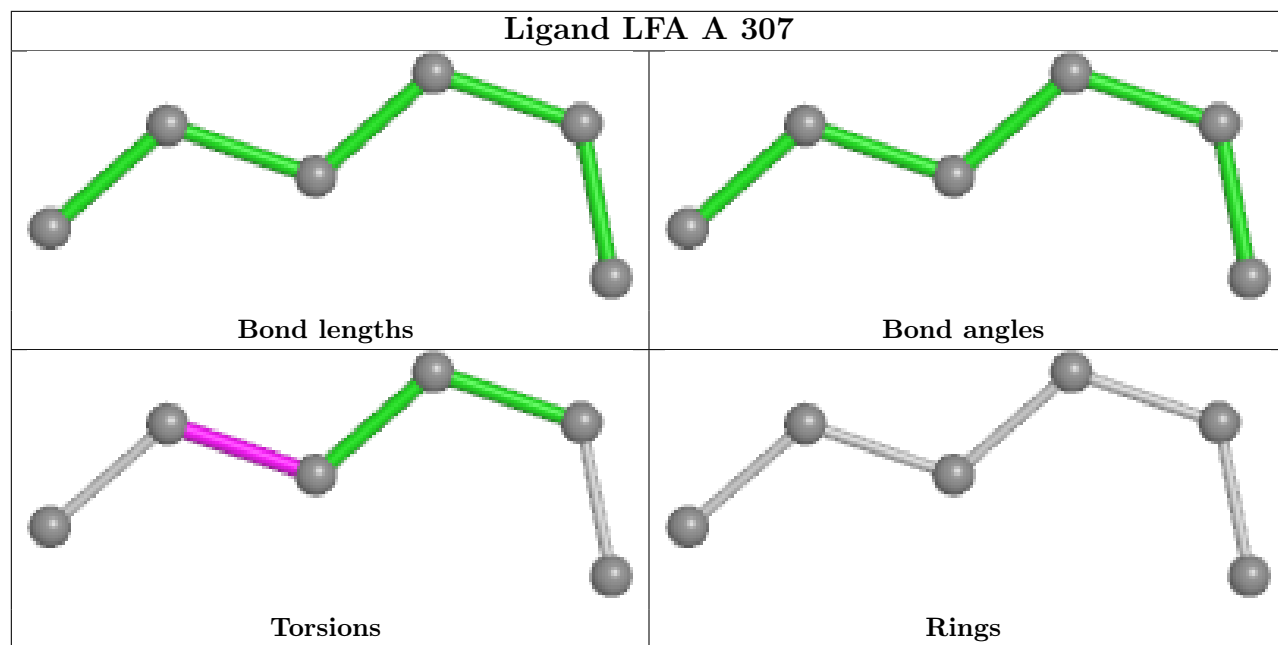


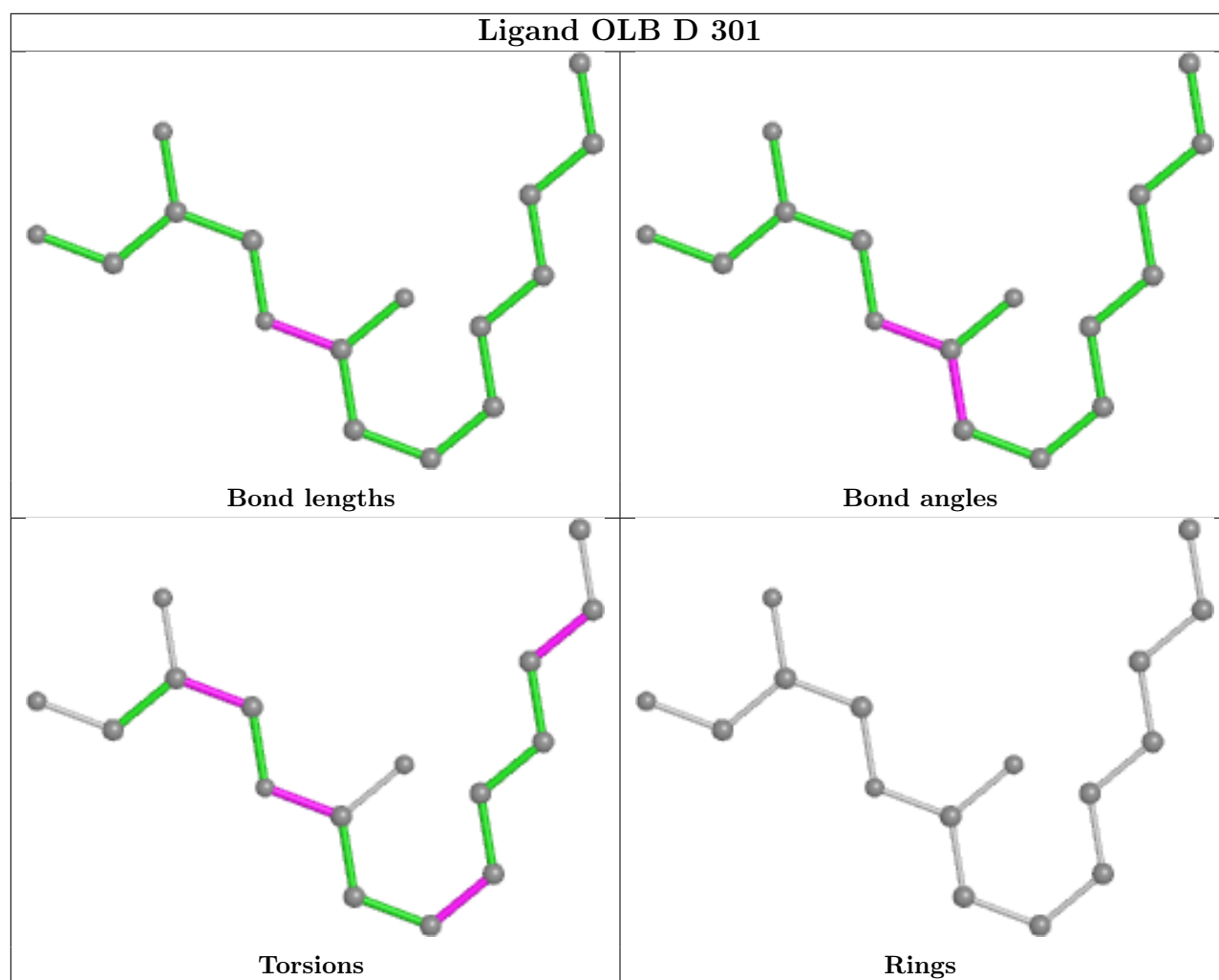












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	210/211 (99%)	-0.08	8 (3%) 40 43	23, 32, 54, 77	0
1	B	210/211 (99%)	0.27	20 (9%) 8 9	24, 37, 63, 78	0
1	C	209/211 (99%)	-0.06	4 (1%) 66 69	23, 31, 55, 82	0
1	D	210/211 (99%)	0.21	11 (5%) 27 30	26, 40, 69, 89	0
2	E	212/219 (96%)	0.02	12 (5%) 23 26	24, 34, 59, 94	0
All	All	1051/1063 (98%)	0.07	55 (5%) 27 30	23, 35, 62, 94	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	ILE	7.3
1	D	4	LEU	7.0
1	D	2	SER	6.8
1	D	3	ASP	6.3
1	D	131	THR	6.2
1	B	4	LEU	4.8
1	D	126	GLY	4.7
1	C	4	LEU	4.1
1	B	65	TYR	4.1
2	E	62	HIS	4.0
1	D	63	ILE	4.0
1	B	154	SER	3.9
1	A	2	SER	3.8
2	E	1	MET	3.8
1	B	2	SER	3.7
1	A	154	SER	3.6
2	E	154	SER	3.5
1	D	156	ALA	3.5
1	D	5	ILE	3.5
2	E	97	ASN	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	E	63	ILE	3.2
1	B	177	GLN	3.1
1	B	155	ASN	3.1
2	E	2	SER	3.0
1	C	62	HIS	3.0
1	C	63	ILE	2.9
1	A	211	THR	2.8
1	D	60	LEU	2.8
1	D	61	GLU	2.7
2	E	61	GLU	2.7
1	A	63	ILE	2.7
1	B	5	ILE	2.7
1	B	211	THR	2.6
2	E	65	TYR	2.6
1	A	3	ASP	2.6
1	B	179	GLU	2.4
1	D	62	HIS	2.4
1	B	3	ASP	2.4
1	A	62	HIS	2.4
1	A	61	GLU	2.3
1	B	96	THR	2.3
1	A	4	LEU	2.2
1	B	130	LYS	2.2
2	E	4	LEU	2.2
1	B	131	THR	2.2
2	E	3	ASP	2.1
1	B	129	HIS	2.1
1	B	153	THR	2.1
1	B	95	GLN	2.1
2	E	100	MET	2.0
1	B	66	GLU	2.0
1	C	211	THR	2.0
1	B	126	GLY	2.0
2	E	212	LEU	2.0
1	B	62	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	OLB	D	301	16/25	0.42	0.33	58,69,81,91	0
3	LFA	D	312	5/20	0.43	0.30	54,57,63,66	0
5	OLB	E	301	16/25	0.44	0.35	57,82,97,110	0
3	LFA	C	314	8/20	0.56	0.18	62,68,72,76	0
3	LFA	C	311	5/20	0.59	0.29	53,59,63,63	0
3	LFA	B	313	5/20	0.62	0.22	55,57,60,65	0
3	LFA	E	310	16/20	0.64	0.27	46,59,69,75	0
3	LFA	A	309	16/20	0.65	0.21	56,75,96,97	0
3	LFA	E	312	8/20	0.68	0.29	52,60,69,70	0
3	LFA	E	308	10/20	0.68	0.21	52,62,65,66	0
3	LFA	A	317	5/20	0.68	0.24	57,63,71,74	0
3	LFA	B	312	6/20	0.70	0.18	58,65,68,69	0
3	LFA	C	305	12/20	0.70	0.23	61,68,80,81	0
3	LFA	A	301	12/20	0.72	0.20	58,66,77,80	0
3	LFA	E	314	8/20	0.74	0.37	56,65,67,70	0
3	LFA	A	311	16/20	0.75	0.21	48,60,85,90	0
3	LFA	B	303	14/20	0.75	0.21	49,59,74,75	0
3	LFA	A	313	12/20	0.76	0.22	41,57,65,69	0
3	LFA	E	315	8/20	0.76	0.35	58,63,68,69	0
3	LFA	D	302	12/20	0.76	0.43	51,57,64,68	0
3	LFA	B	315	5/20	0.76	0.15	56,57,63,64	0
3	LFA	D	303	12/20	0.77	0.16	45,66,73,76	0
3	LFA	D	310	14/20	0.77	0.33	63,77,94,98	0
3	LFA	B	304	12/20	0.78	0.24	50,67,76,78	0
3	LFA	E	313	8/20	0.78	0.24	56,65,68,69	0
3	LFA	E	311	16/20	0.78	0.24	51,67,74,74	0
3	LFA	C	307	10/20	0.79	0.21	51,58,67,75	0
3	LFA	C	313	5/20	0.79	0.16	54,54,58,59	0
3	LFA	B	306	12/20	0.80	0.16	53,61,66,67	0
3	LFA	E	305	6/20	0.80	0.22	43,49,50,51	0
3	LFA	B	308	10/20	0.80	0.24	54,68,75,76	0
3	LFA	B	309	7/20	0.80	0.14	63,75,80,82	0

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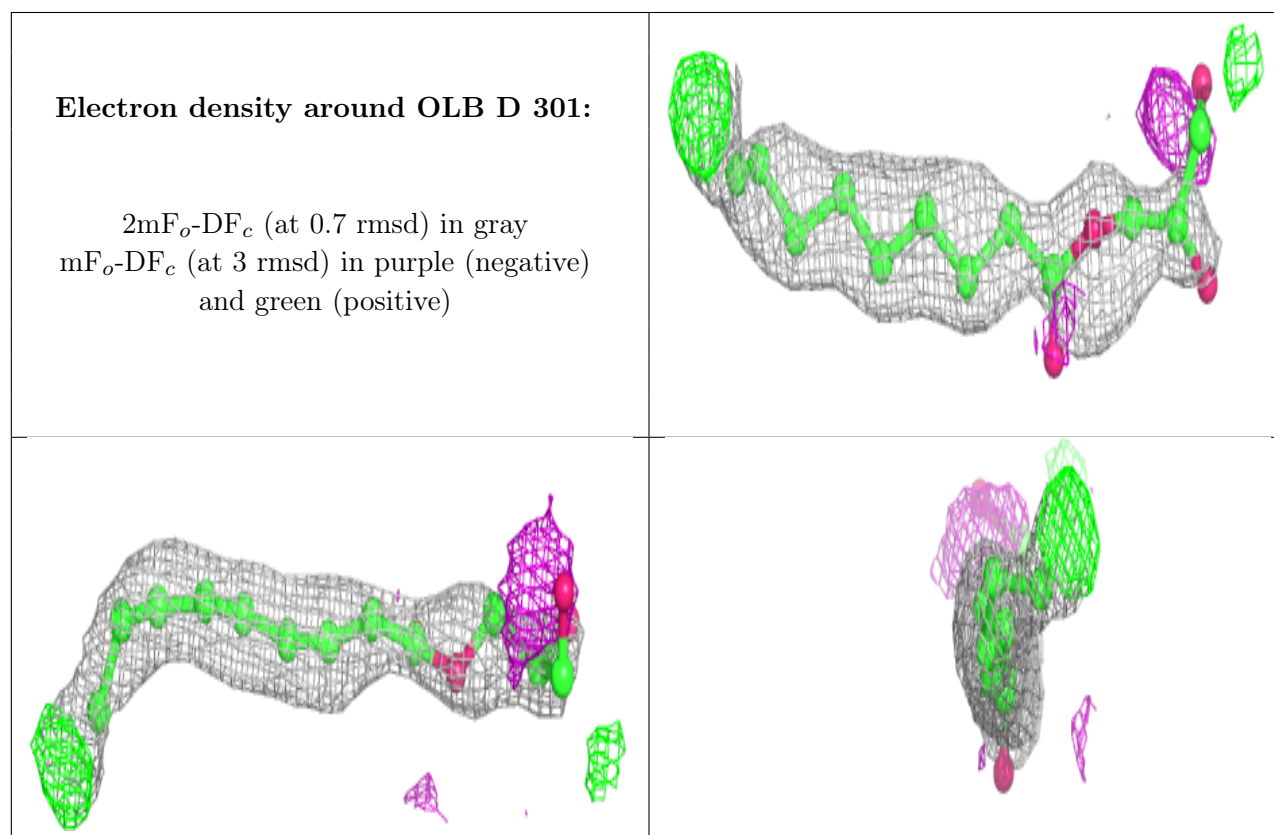
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	B	310	8/20	0.80	0.26	54,61,65,71	0
3	LFA	B	311	16/20	0.80	0.23	55,62,75,77	0
3	LFA	B	302	8/20	0.80	0.61	49,52,54,62	0
3	LFA	A	310	6/20	0.80	0.17	47,51,52,53	0
3	LFA	D	307	14/20	0.80	0.19	52,59,65,67	0
3	LFA	D	309	10/20	0.80	0.24	48,69,81,86	0
3	LFA	A	302	10/20	0.80	0.21	65,71,83,83	0
3	LFA	B	305	5/20	0.81	0.23	47,53,57,57	0
3	LFA	C	312	8/20	0.81	0.21	50,57,60,60	0
3	LFA	A	316	5/20	0.81	0.12	59,59,65,67	0
3	LFA	B	307	7/20	0.81	0.21	53,57,63,64	0
3	LFA	C	308	7/20	0.82	0.26	50,55,66,69	0
3	LFA	A	312	7/20	0.83	0.18	52,52,66,69	0
3	LFA	E	304	12/20	0.83	0.13	58,62,68,69	0
3	LFA	D	304	10/20	0.83	0.28	54,69,72,74	0
3	LFA	D	305	12/20	0.83	0.29	48,53,59,61	0
3	LFA	C	304	12/20	0.84	0.12	56,67,73,77	0
3	LFA	A	314	6/20	0.84	0.27	60,68,76,79	0
3	LFA	C	301	14/20	0.84	0.19	45,57,70,71	0
3	LFA	C	302	5/20	0.85	0.17	49,51,58,59	0
3	LFA	E	309	6/20	0.85	0.27	61,63,74,76	0
3	LFA	D	311	6/20	0.86	0.15	54,64,71,79	0
3	LFA	E	307	8/20	0.86	0.21	49,54,55,56	0
3	LFA	A	304	12/20	0.86	0.41	40,48,56,62	0
3	LFA	D	308	10/20	0.86	0.23	46,51,64,67	0
3	LFA	E	306	5/20	0.87	0.15	45,47,51,54	0
3	LFA	C	310	5/20	0.87	0.11	50,53,57,58	0
3	LFA	E	303	8/20	0.87	0.17	49,53,62,70	0
3	LFA	A	315	5/20	0.88	0.19	46,49,59,59	0
3	LFA	A	307	6/20	0.88	0.17	49,50,52,55	0
3	LFA	C	309	10/20	0.88	0.13	53,56,60,61	0
3	LFA	A	308	5/20	0.89	0.27	47,49,53,53	0
3	LFA	B	314	5/20	0.89	0.12	55,58,59,62	0
3	LFA	A	306	6/20	0.89	0.24	47,54,59,69	0
3	LFA	D	306	12/20	0.89	0.23	50,63,86,87	0
3	LFA	A	303	12/20	0.89	0.37	46,52,64,69	0
3	LFA	C	303	8/20	0.90	0.17	41,49,59,64	0
3	LFA	C	306	6/20	0.90	0.12	48,53,57,58	0
3	LFA	A	305	8/20	0.92	0.14	50,58,65,67	0
4	RET	B	316	20/21	0.92	0.09	28,33,38,43	0
4	RET	D	313	20/21	0.93	0.11	32,38,49,51	0
4	RET	A	318	20/21	0.93	0.12	24,27,32,34	0

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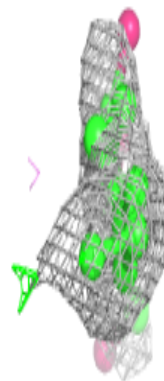
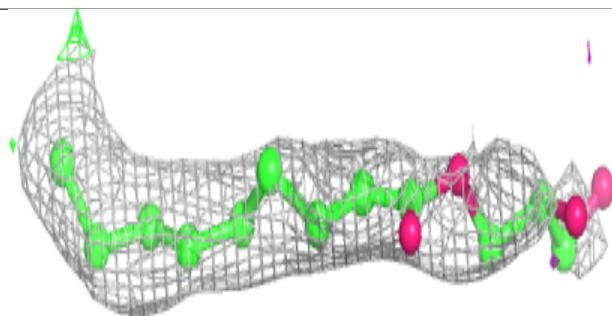
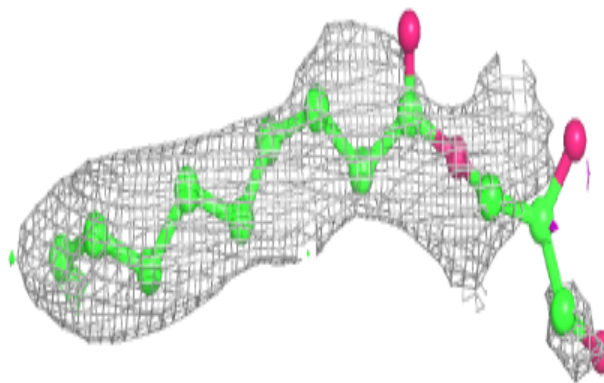
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	E	302	9/20	0.93	0.16	35,39,48,50	0
3	LFA	B	301	8/20	0.95	0.38	39,46,59,59	0
4	RET	E	316	20/21	0.95	0.09	25,29,38,39	0
4	RET	C	315	20/21	0.96	0.08	20,25,32,36	0

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.

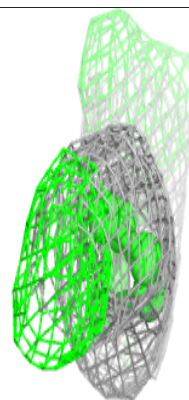
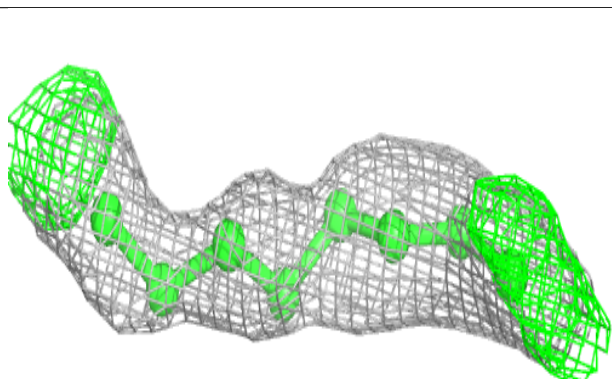
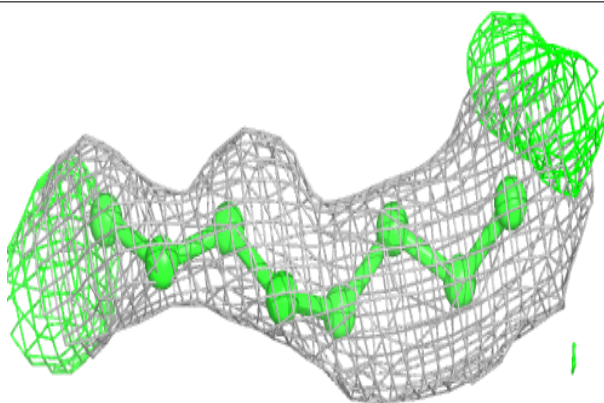


**Electron density around OLB E 301:**

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

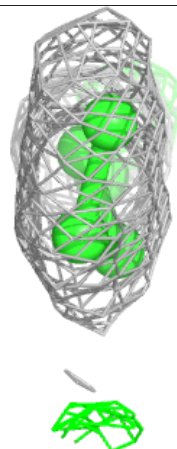
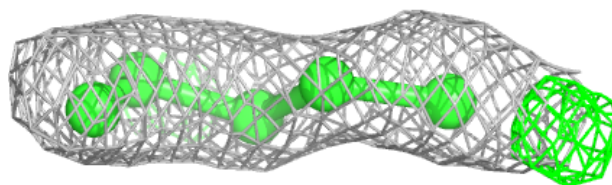
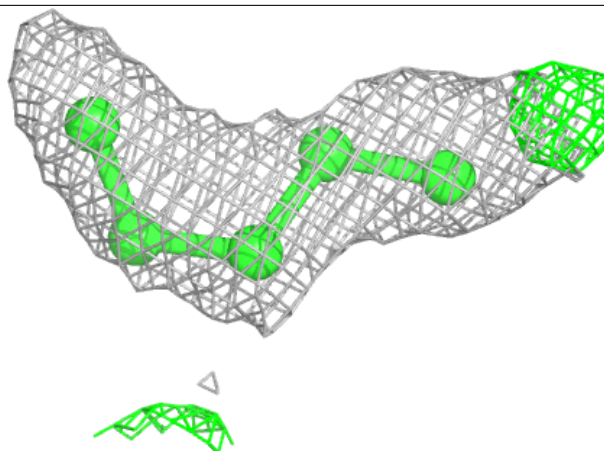
**Electron density around LFA C 314:**

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



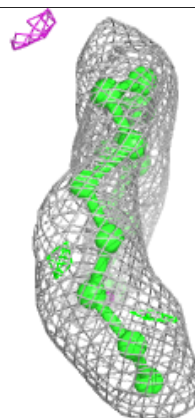
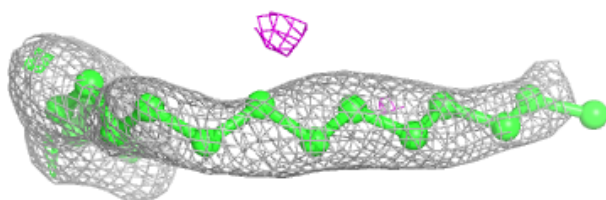
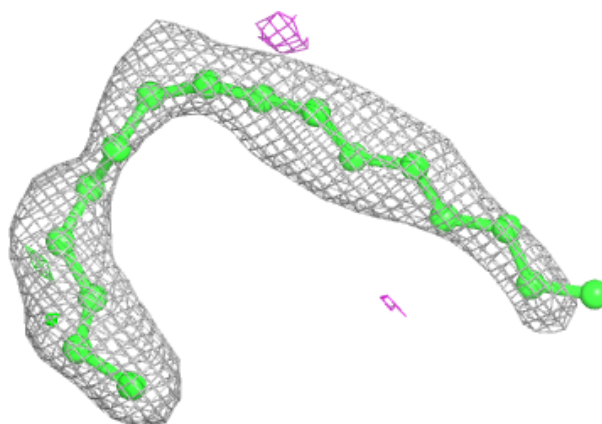
**Electron density around LFA B 313:**

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

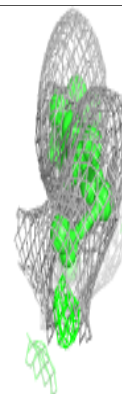
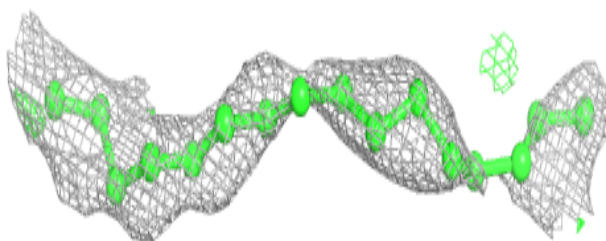
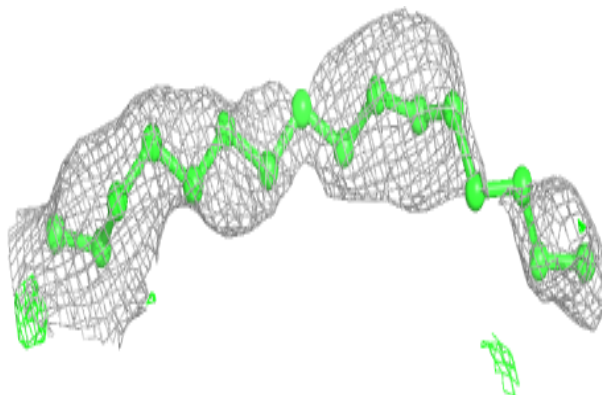


**Electron density around LFA E 310:**

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

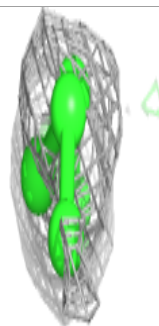
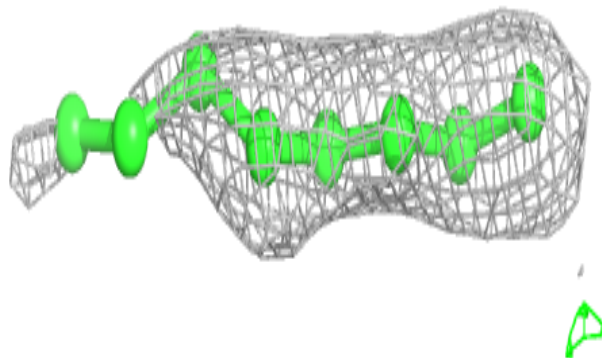
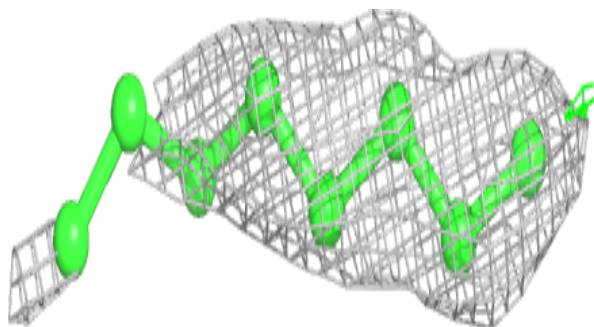
**Electron density around LFA A 309:**

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

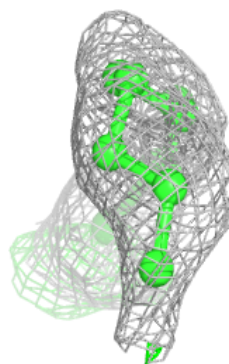
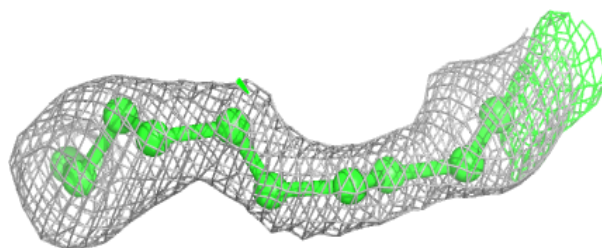
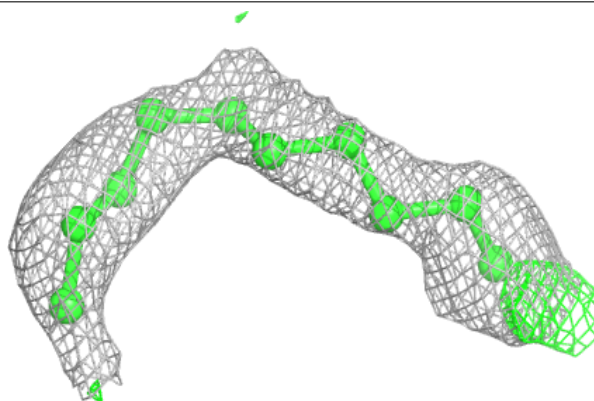


**Electron density around LFA E 312:**

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

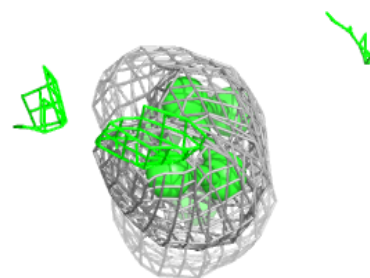
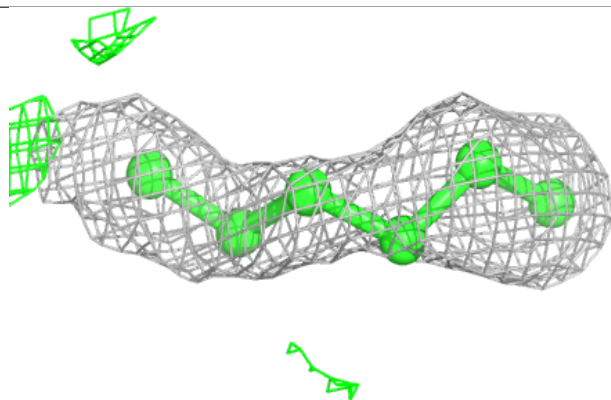
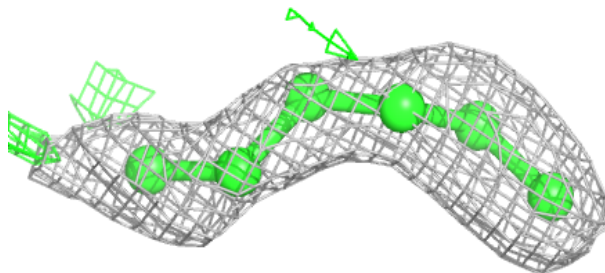
**Electron density around LFA E 308:**

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

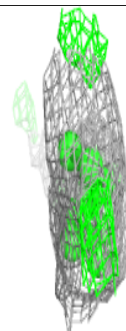
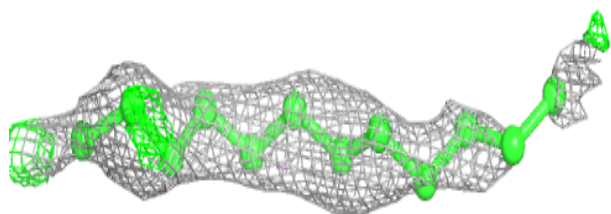
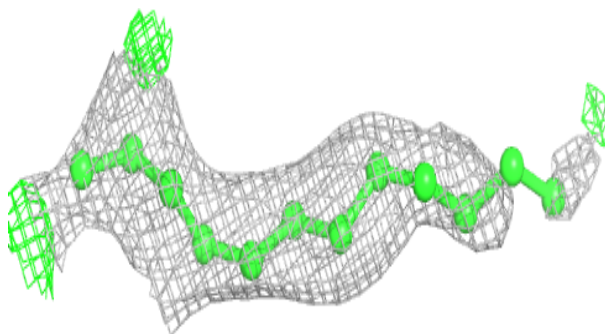


**Electron density around LFA B 312:**

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

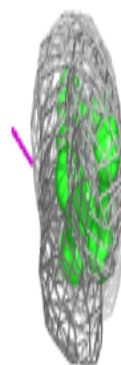
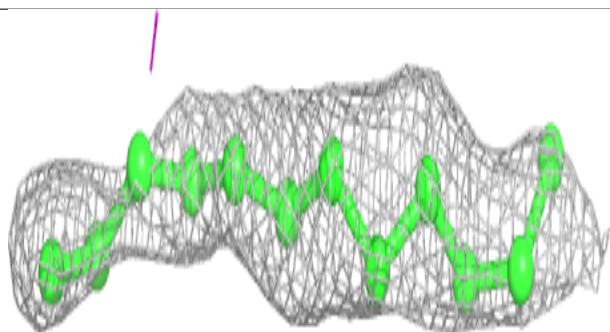
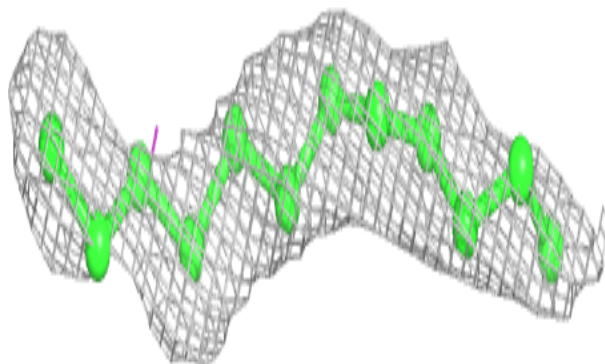
**Electron density around LFA C 305:**

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

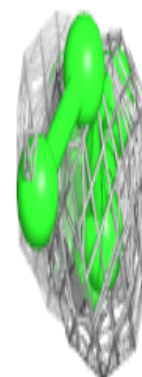
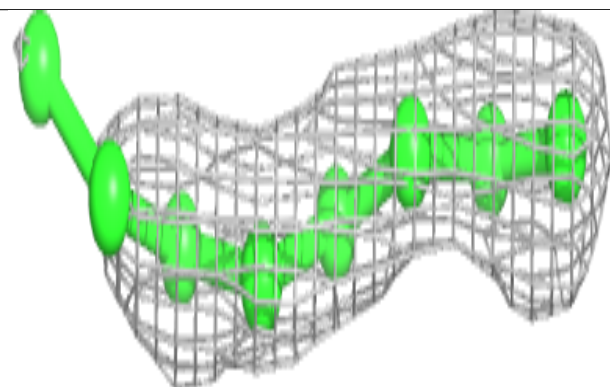
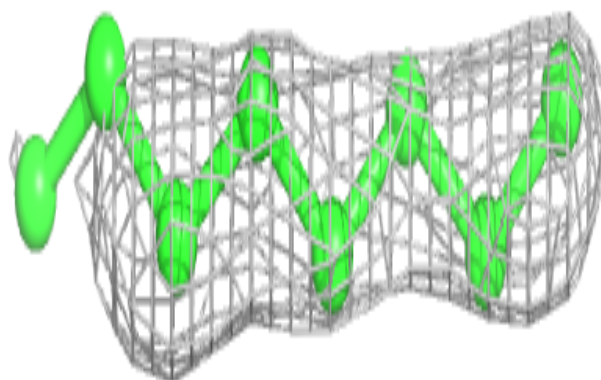


**Electron density around LFA A 301:**

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

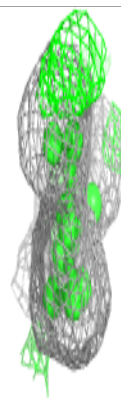
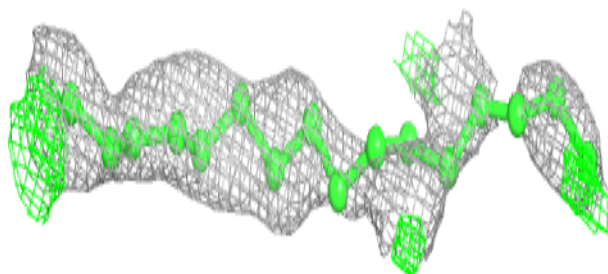
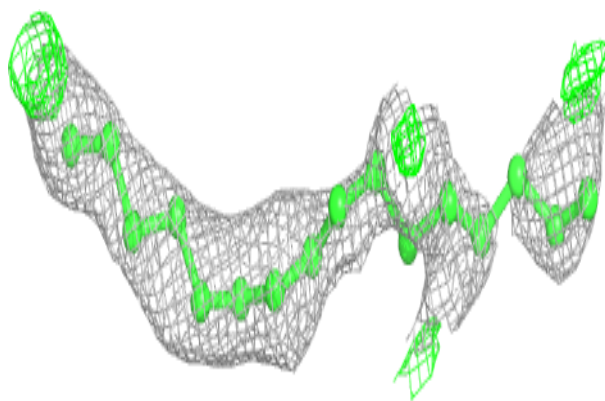
**Electron density around LFA E 314:**

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



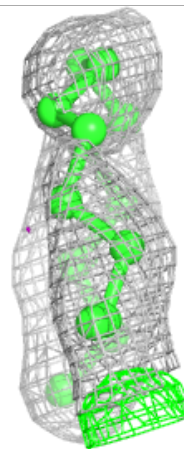
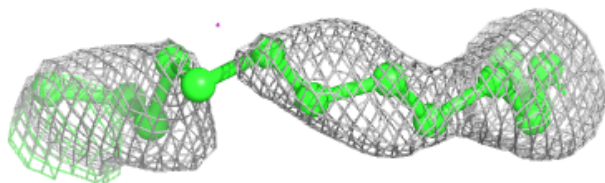
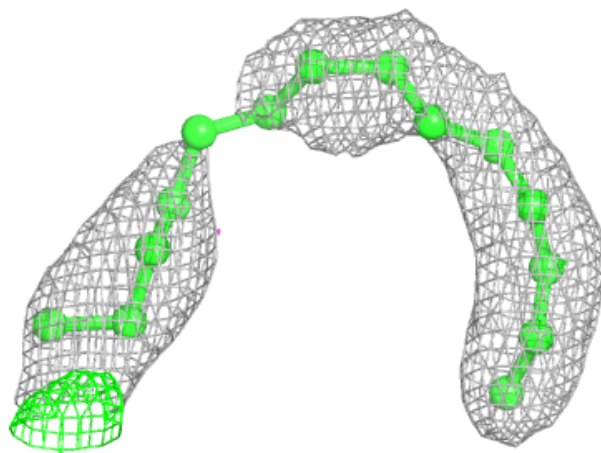
**Electron density around LFA A 311:**

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



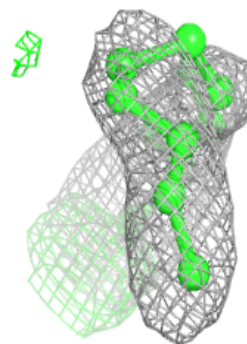
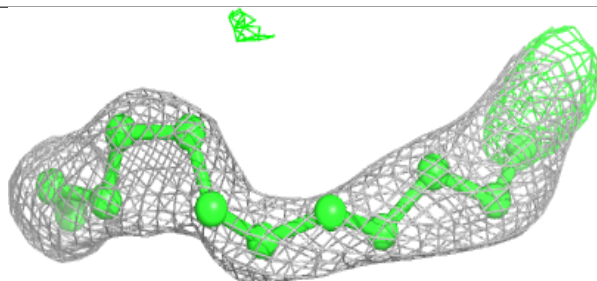
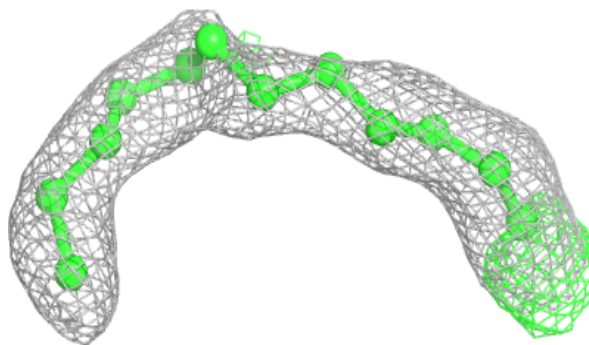
**Electron density around LFA B 303:**

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

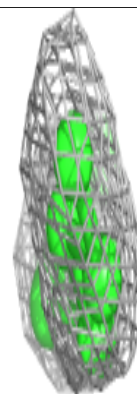
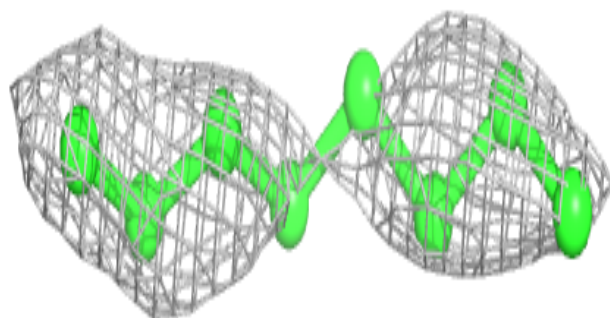
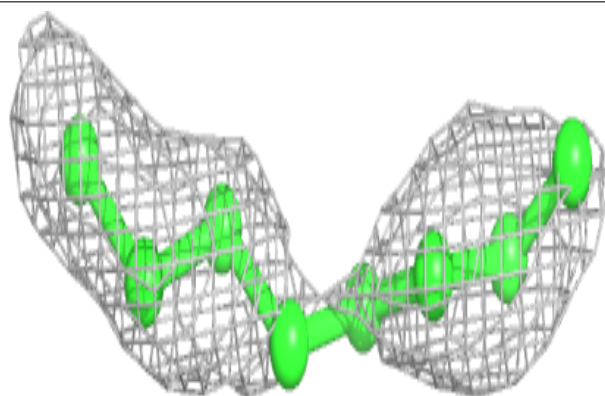


**Electron density around LFA A 313:**

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

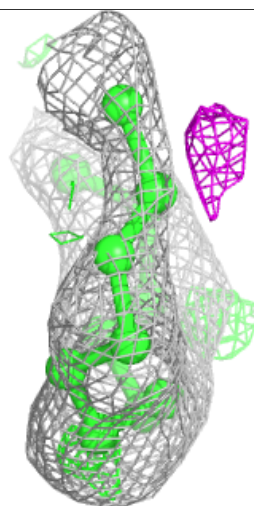
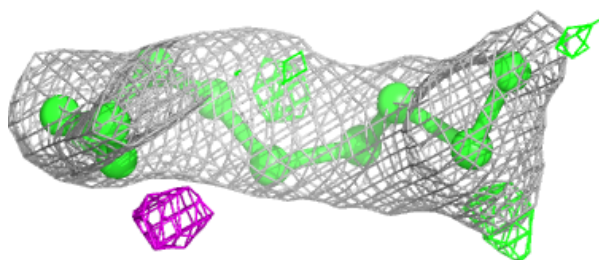
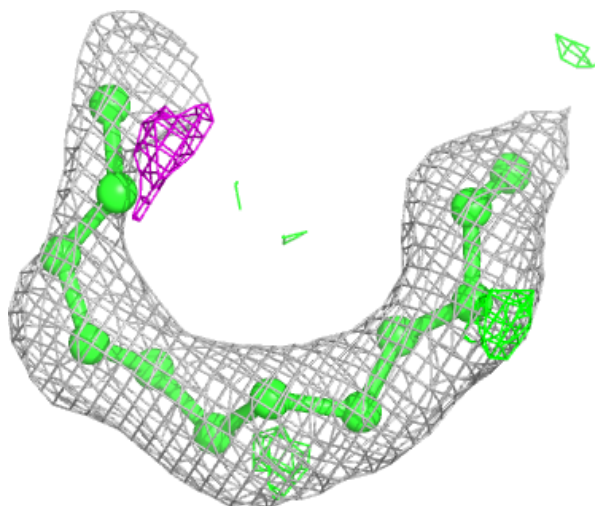
**Electron density around LFA E 315:**

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



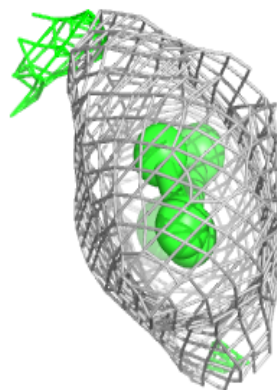
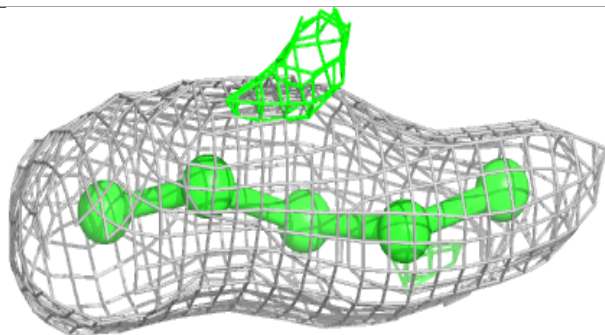
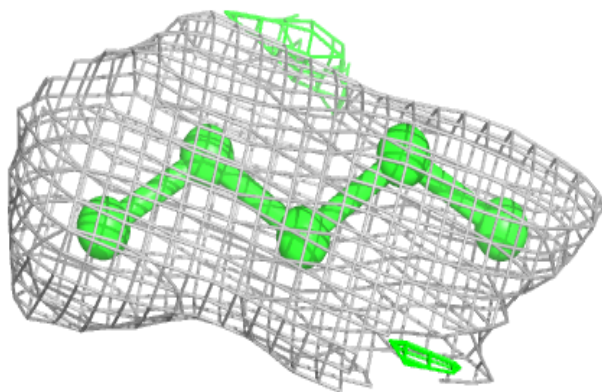
**Electron density around LFA D 302:**

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



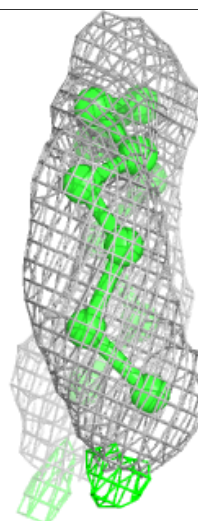
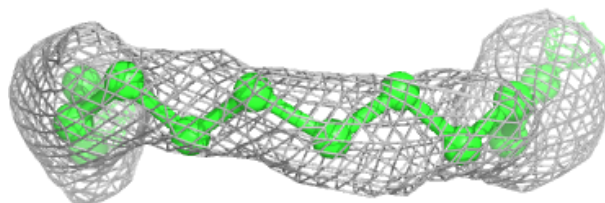
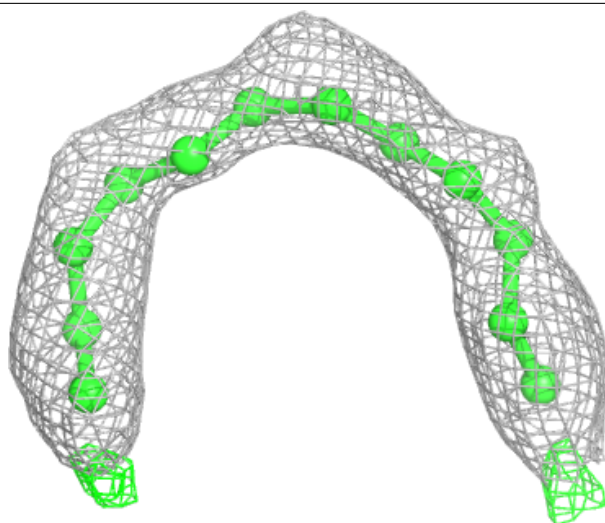
**Electron density around LFA B 315:**

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



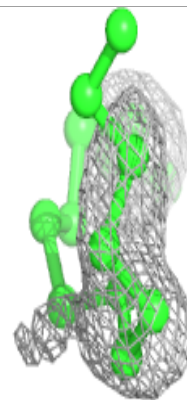
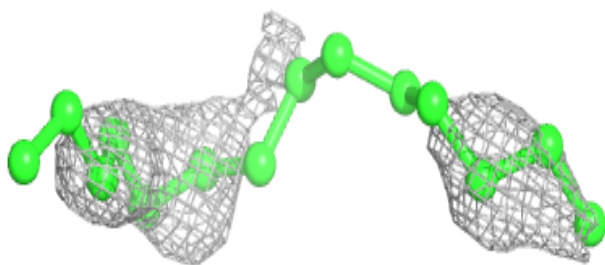
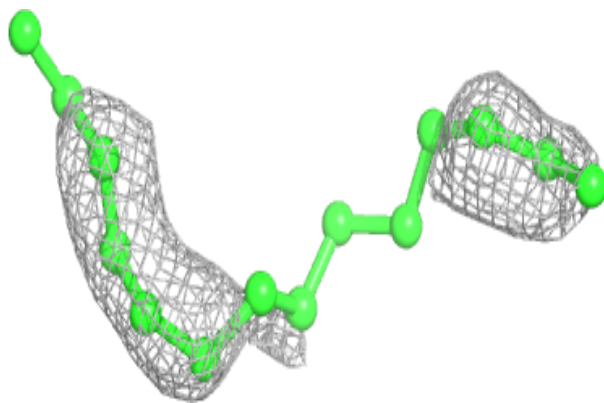
**Electron density around LFA D 303:**

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

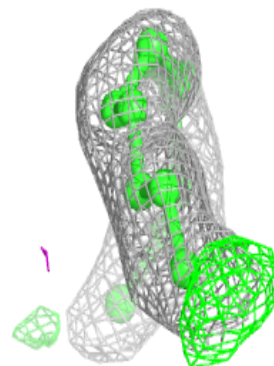
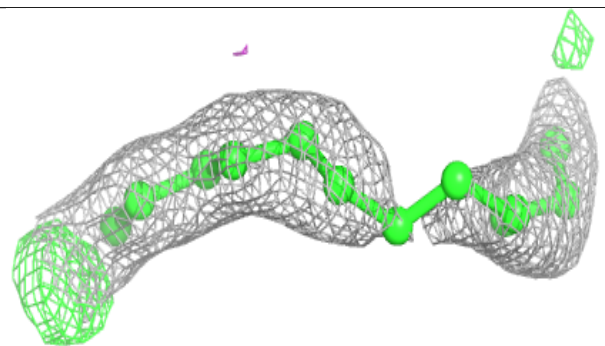
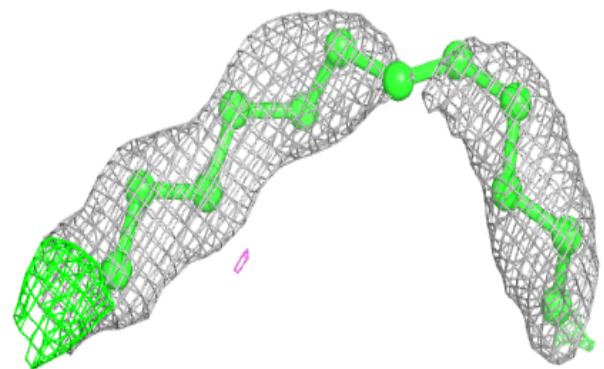


**Electron density around LFA D 310:**

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

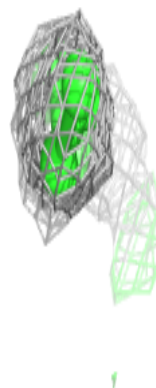
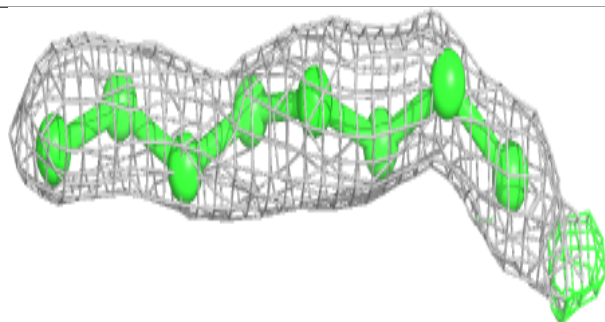
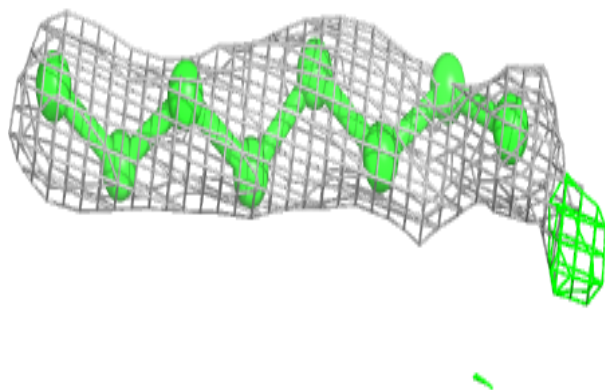
**Electron density around LFA B 304:**

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

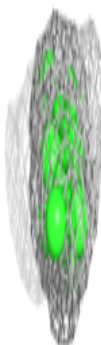
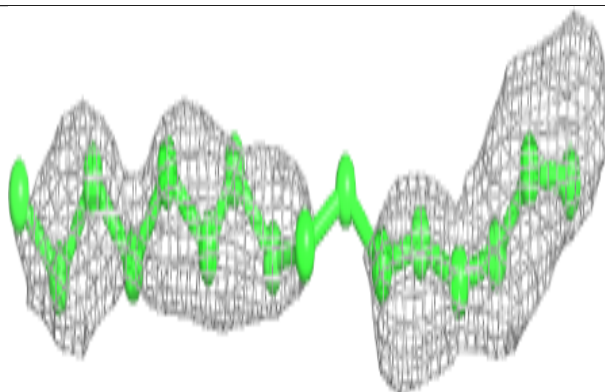
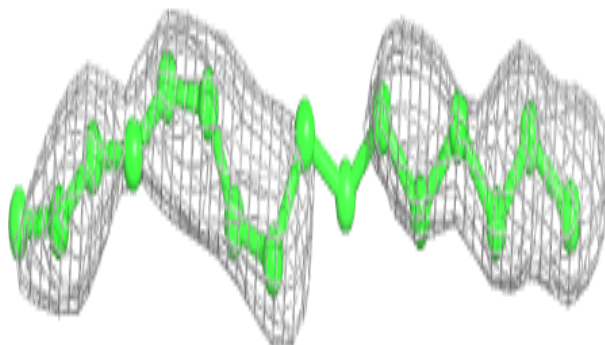


**Electron density around LFA E 313:**

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

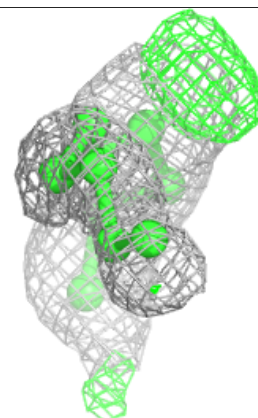
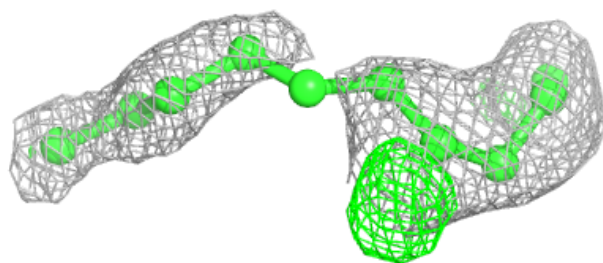
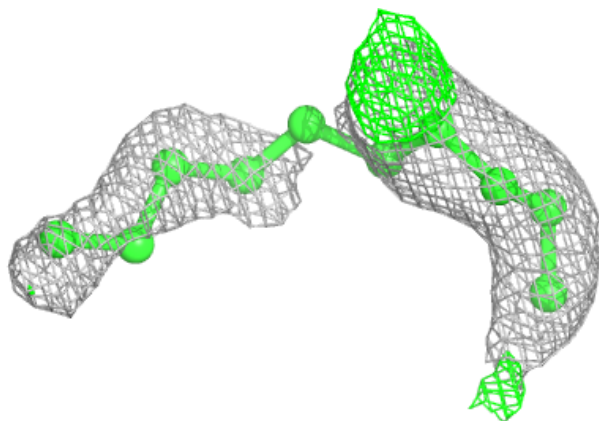
**Electron density around LFA E 311:**

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

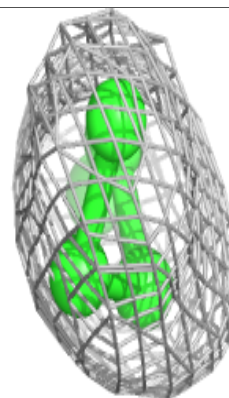
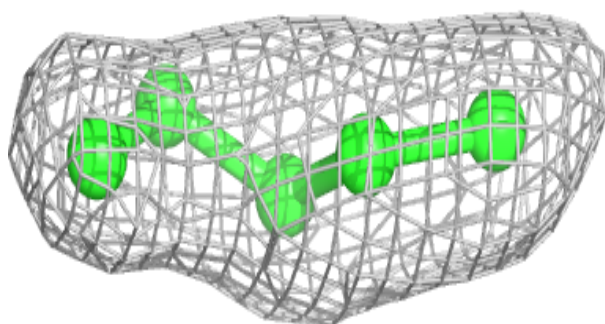
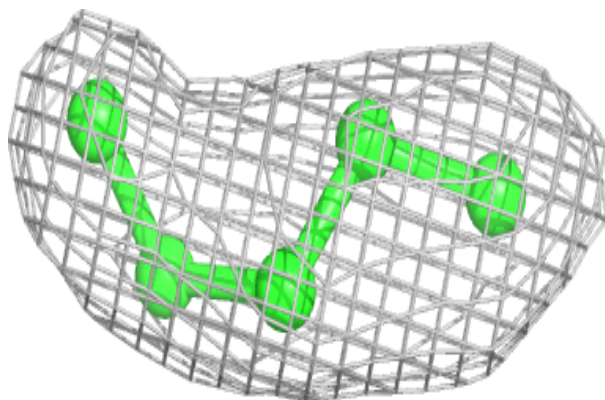


**Electron density around LFA C 307:**

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

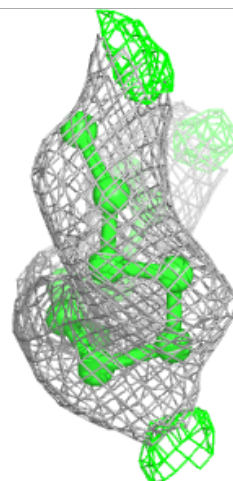
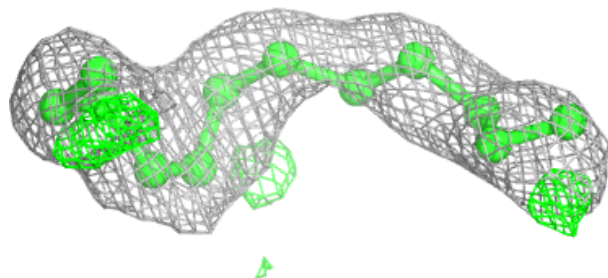
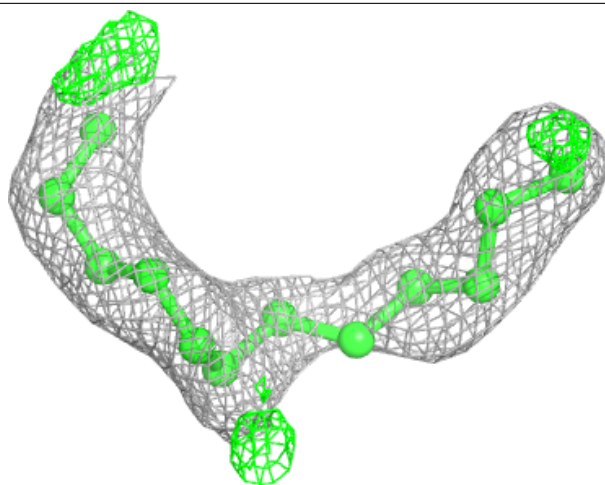
**Electron density around LFA C 313:**

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



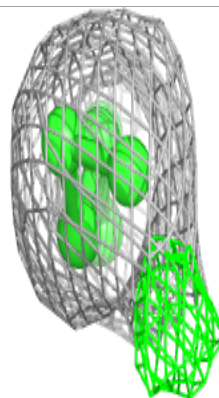
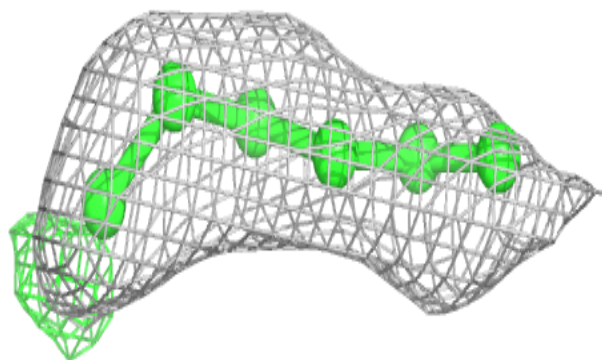
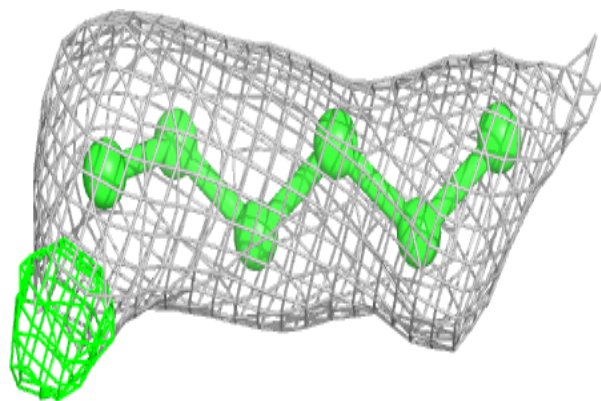
**Electron density around LFA B 306:**

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

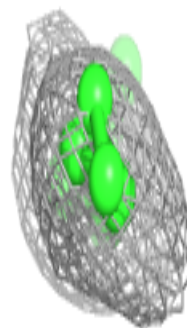
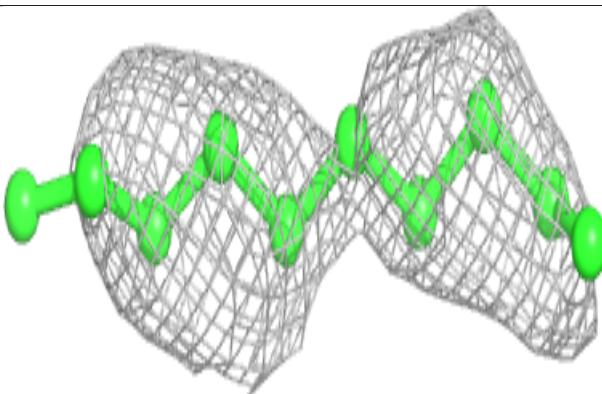
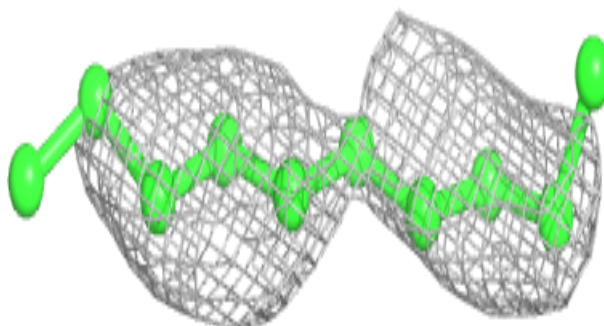


**Electron density around LFA E 305:**

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

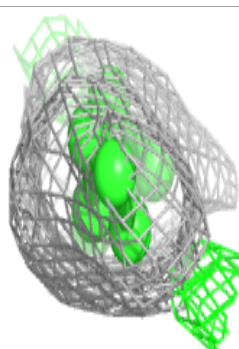
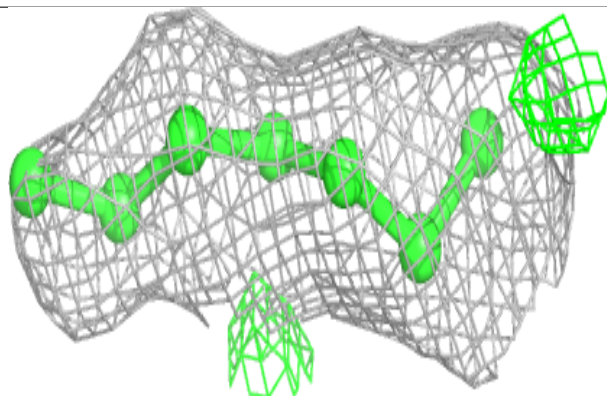
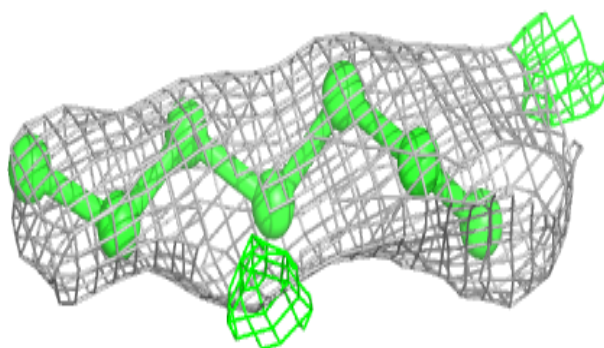
**Electron density around LFA B 308:**

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

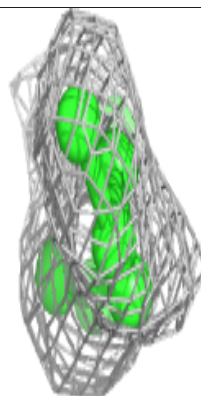
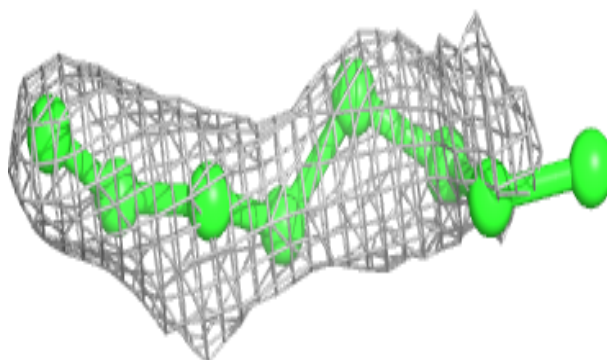
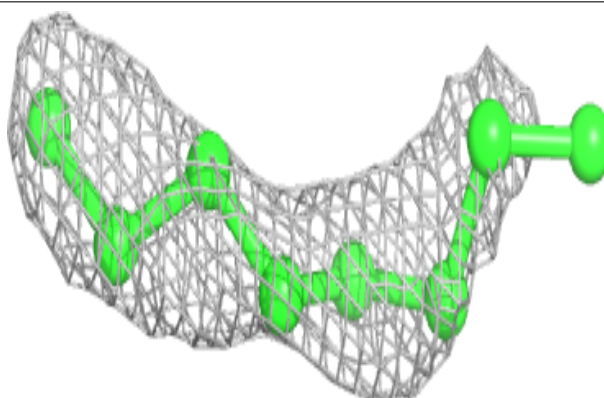


**Electron density around LFA B 309:**

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

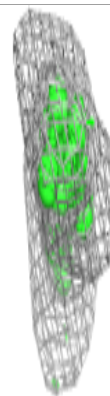
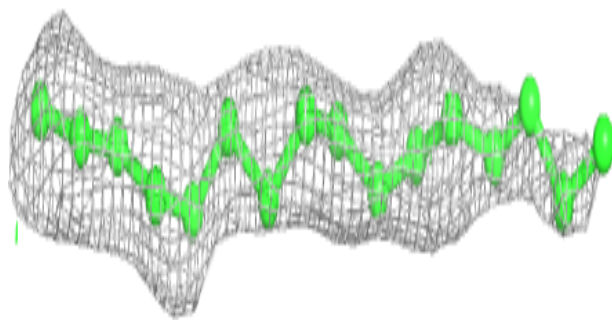
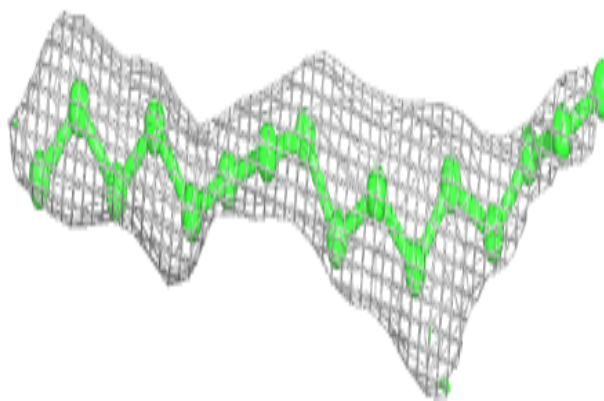
**Electron density around LFA B 310:**

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

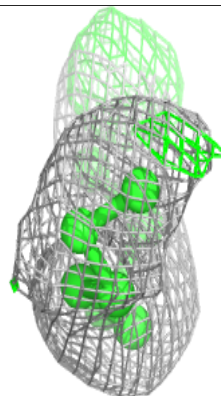
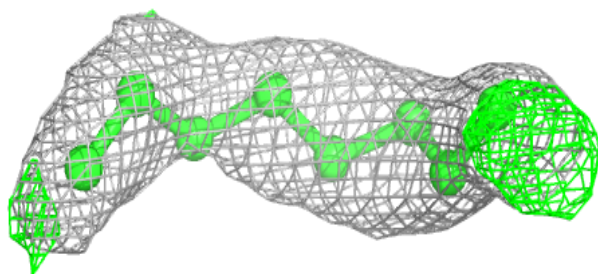
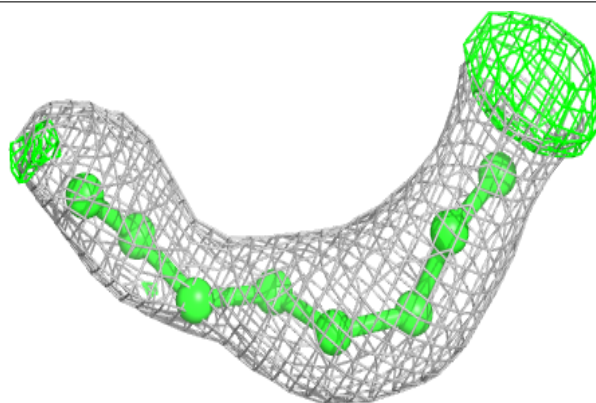


**Electron density around LFA B 311:**

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

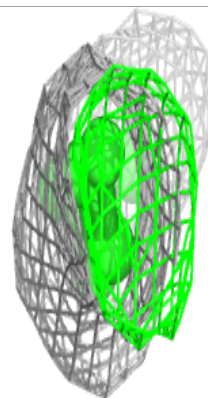
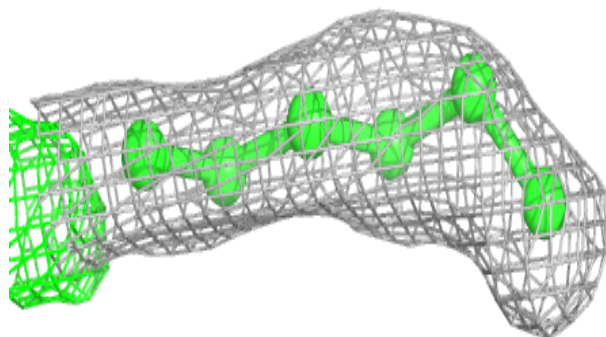
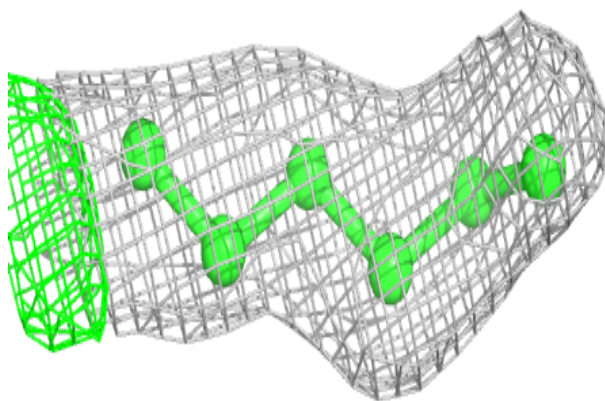
**Electron density around LFA B 302:**

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

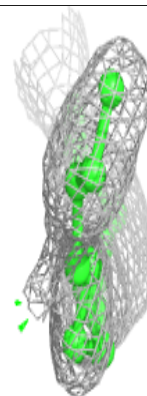
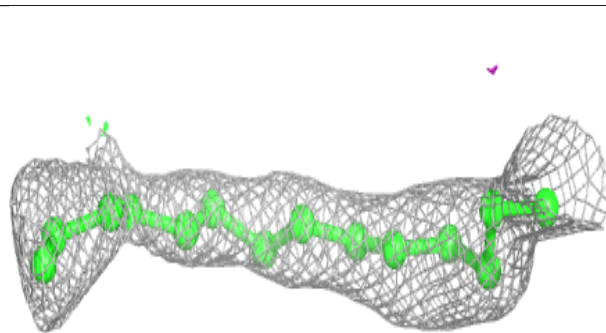
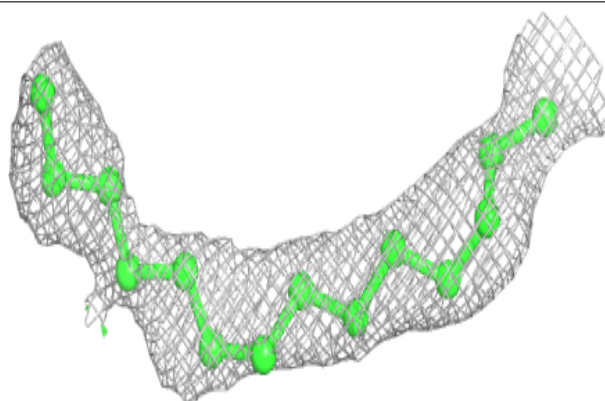


**Electron density around LFA A 310:**

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

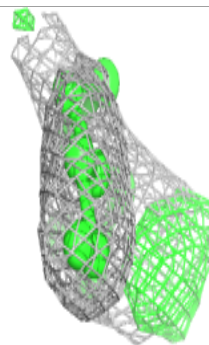
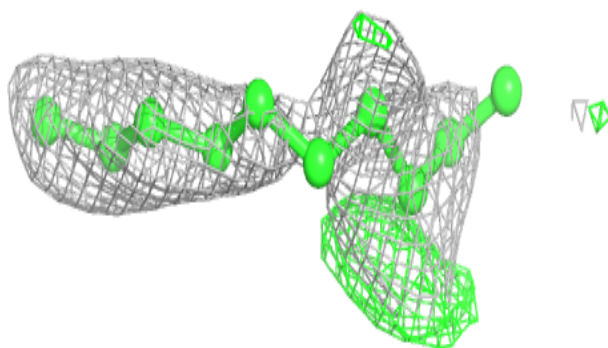
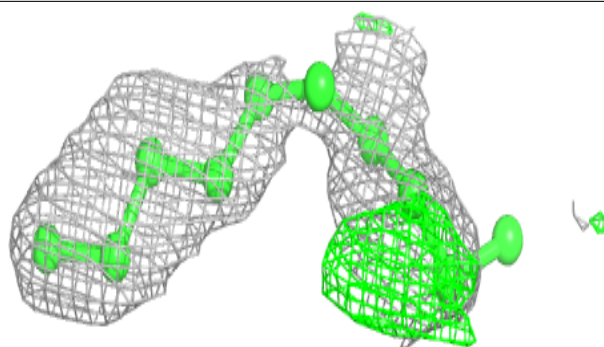
**Electron density around LFA D 307:**

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

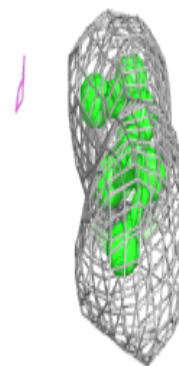
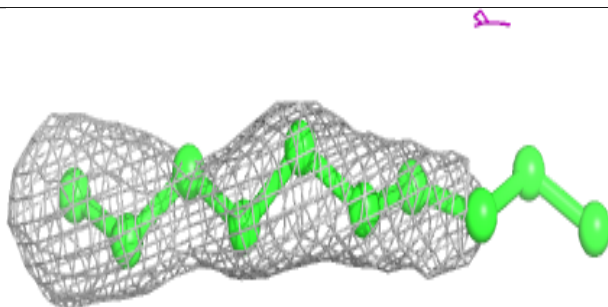
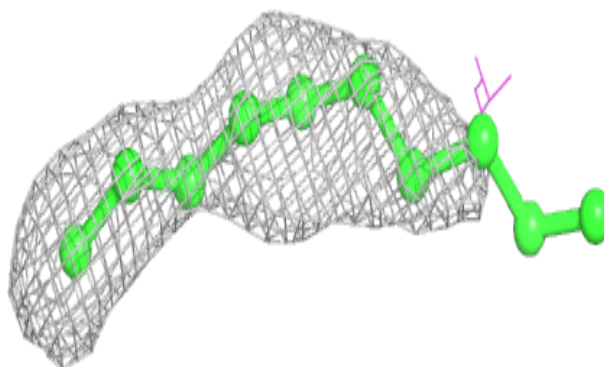


**Electron density around LFA D 309:**

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

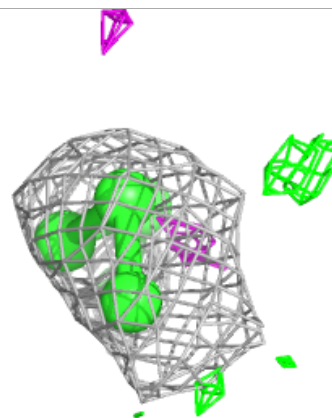
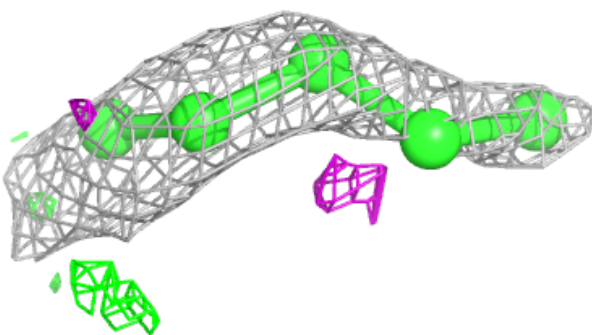
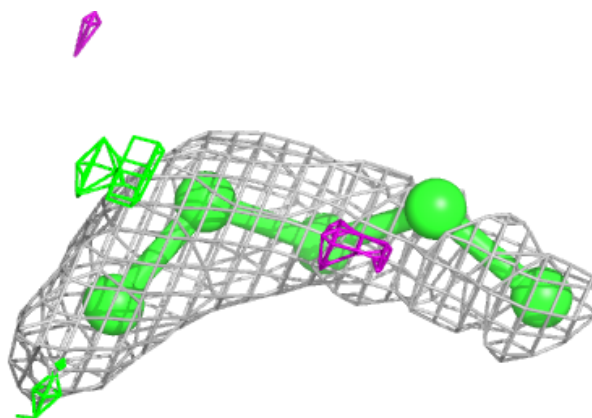
**Electron density around LFA A 302:**

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



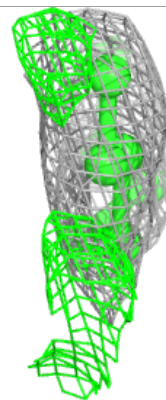
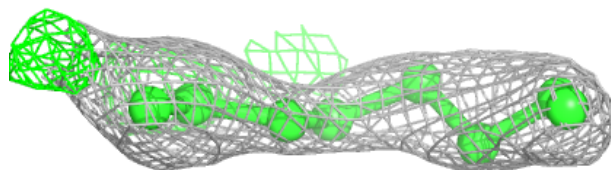
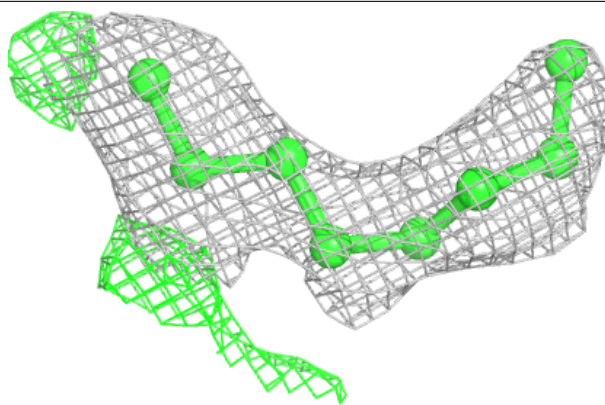
**Electron density around LFA B 305:**

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

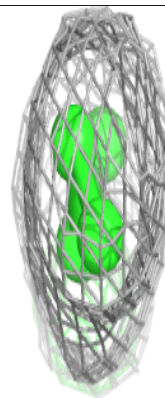
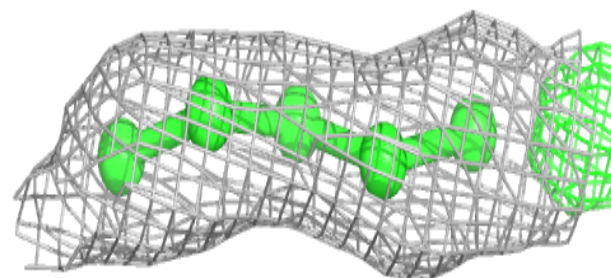
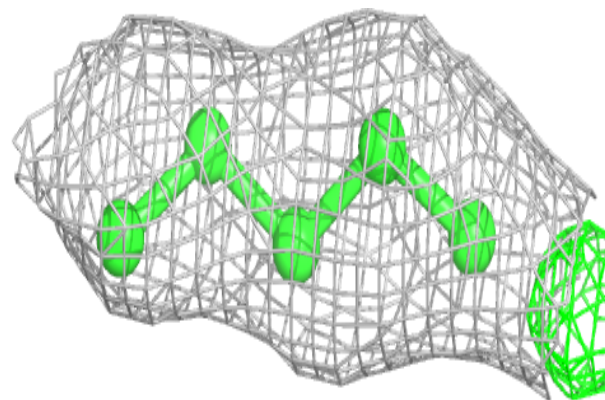


**Electron density around LFA C 312:**

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

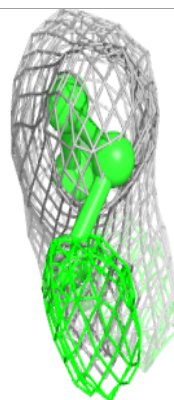
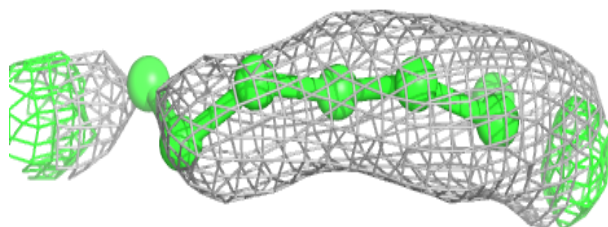
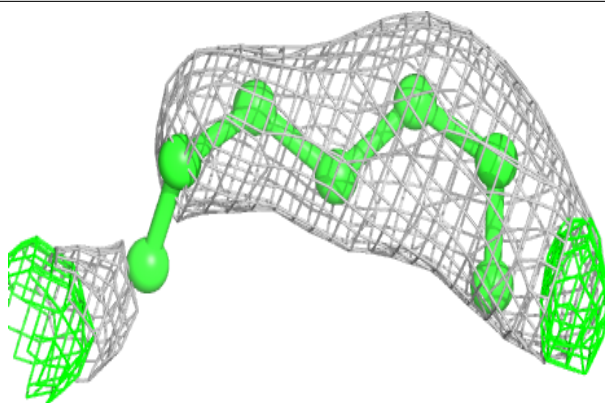
**Electron density around LFA A 316:**

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

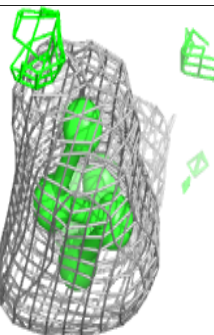
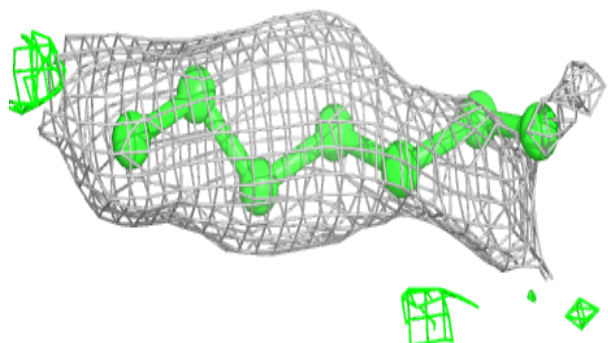
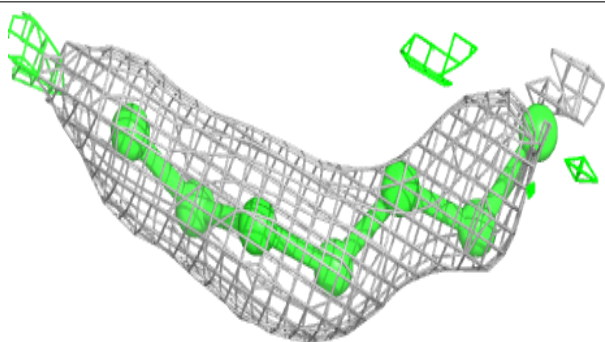


**Electron density around LFA B 307:**

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

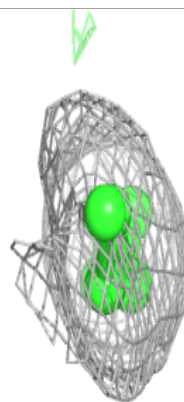
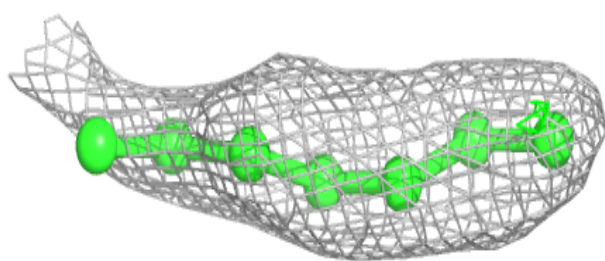
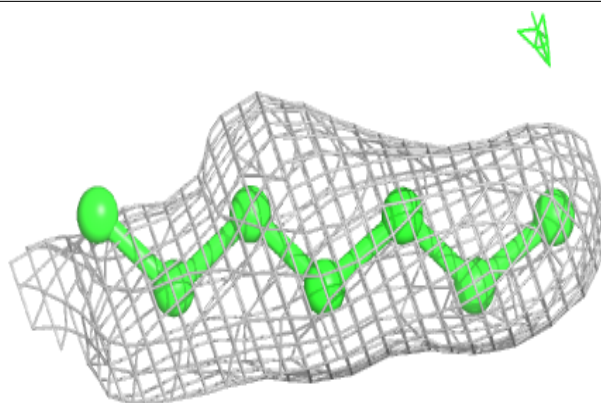
**Electron density around LFA C 308:**

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

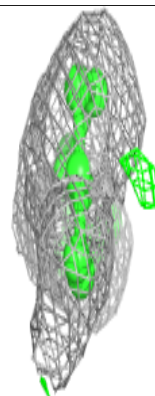
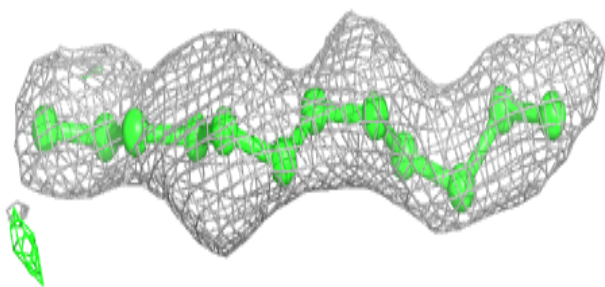
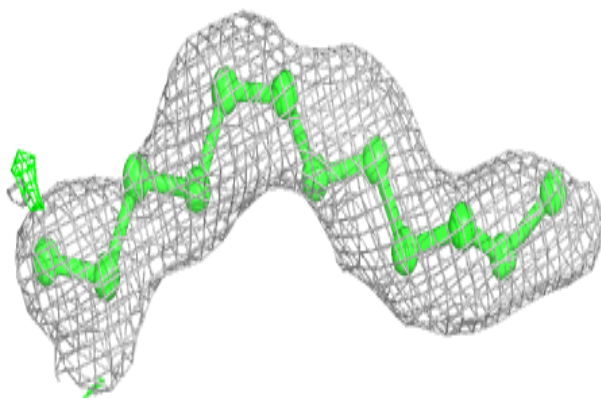


**Electron density around LFA A 312:**

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

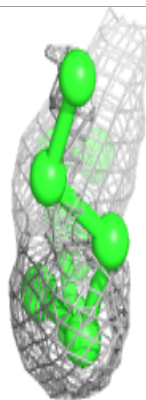
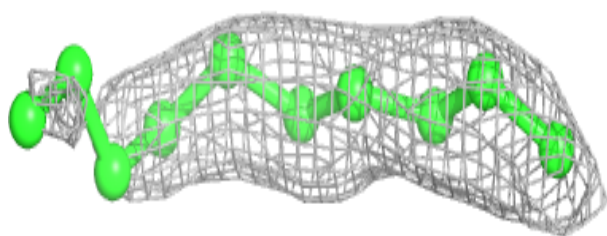
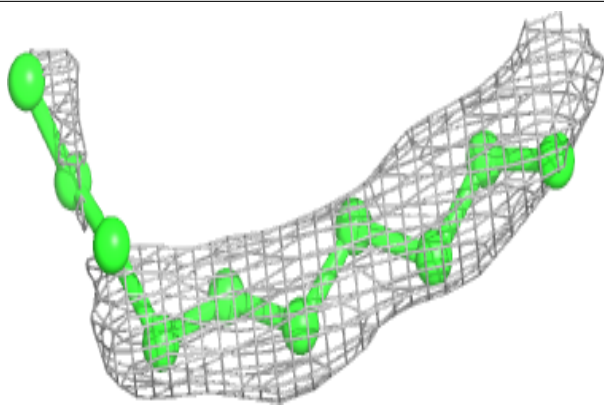
**Electron density around LFA E 304:**

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

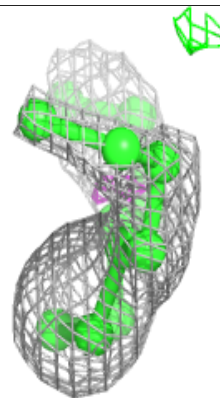
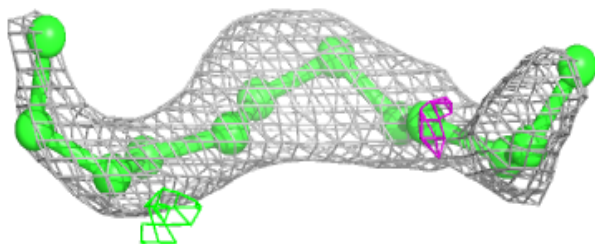
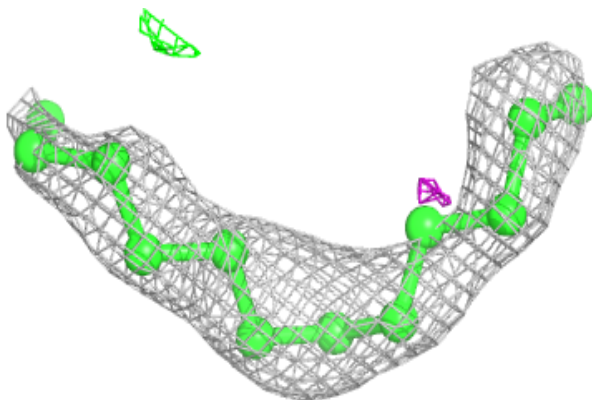


**Electron density around LFA D 304:**

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

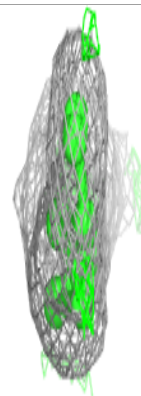
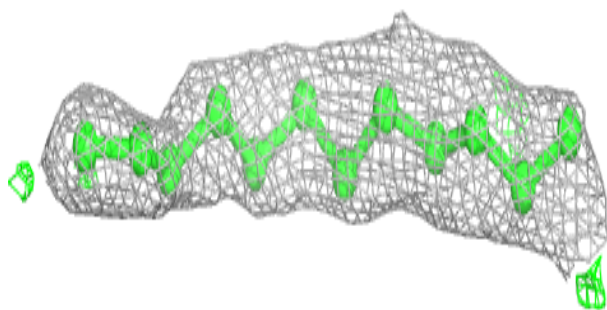
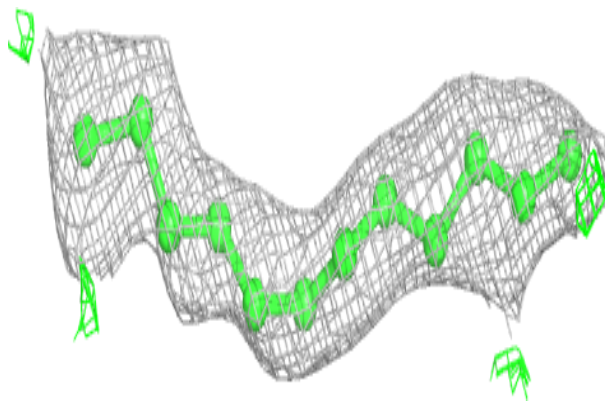
**Electron density around LFA D 305:**

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

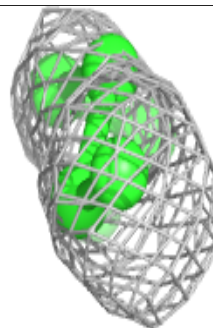
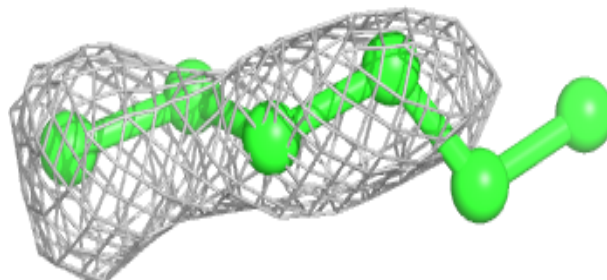
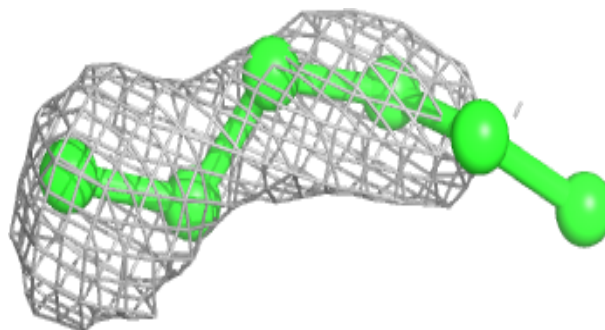


**Electron density around LFA C 304:**

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

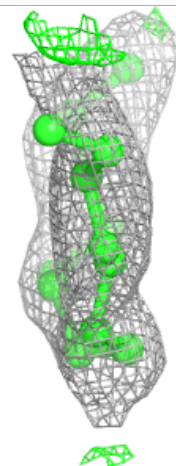
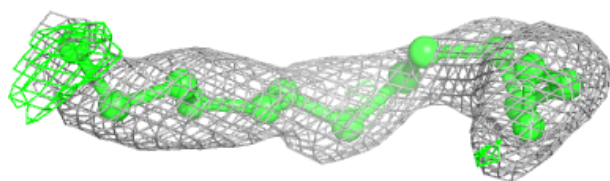
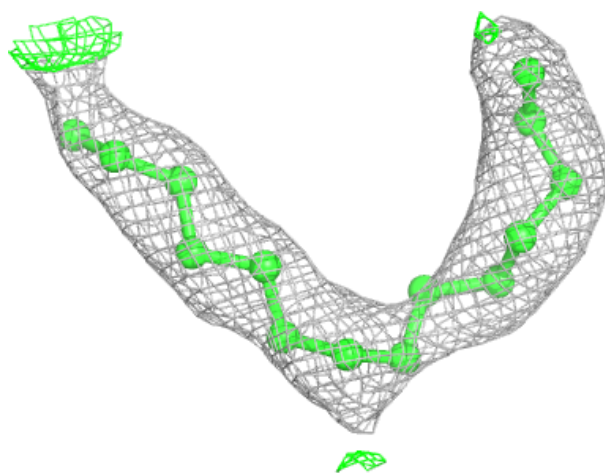
**Electron density around LFA A 314:**

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



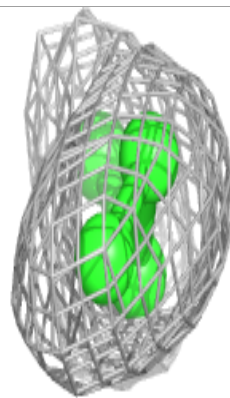
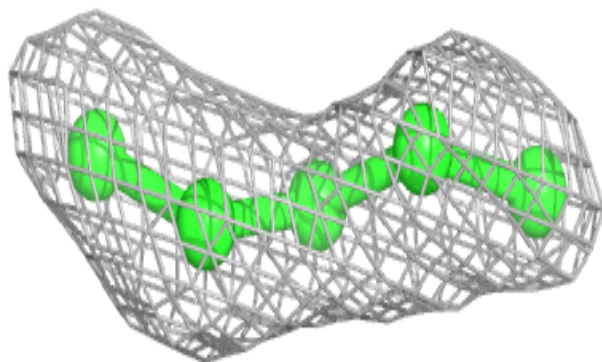
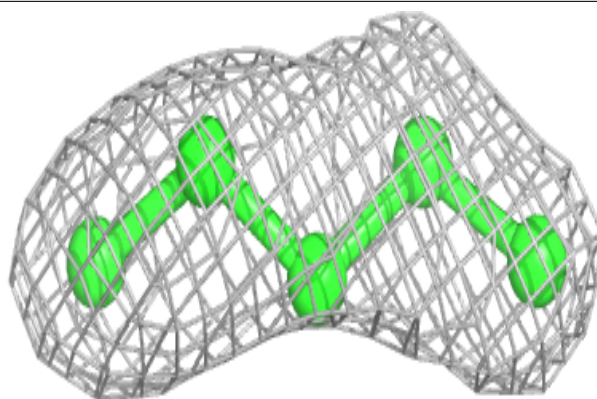
**Electron density around LFA C 301:**

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

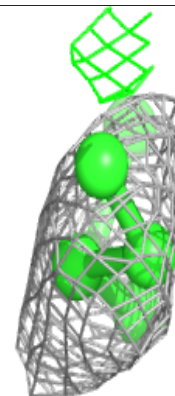
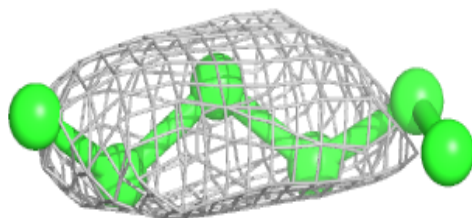
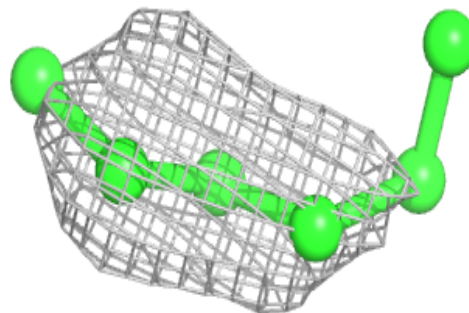


**Electron density around LFA C 302:**

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

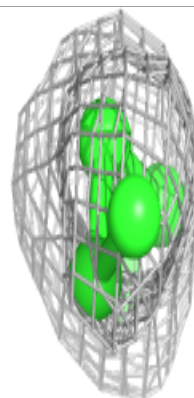
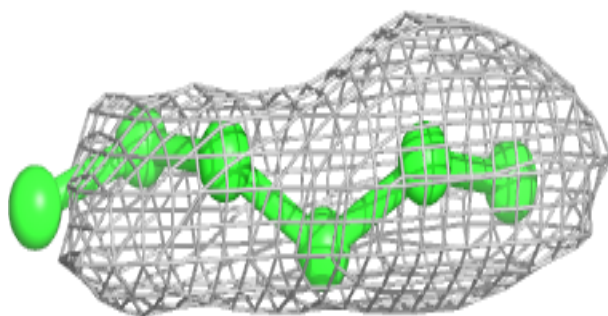
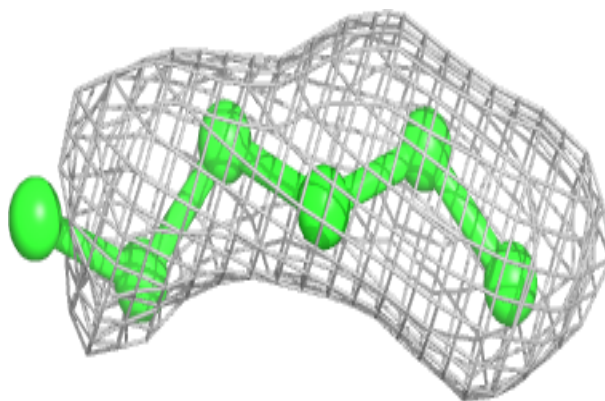
**Electron density around LFA E 309:**

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

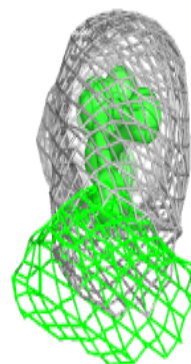
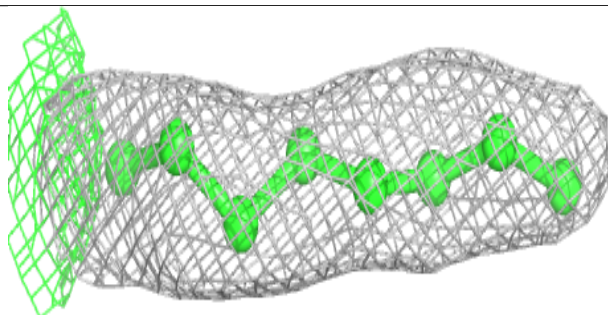
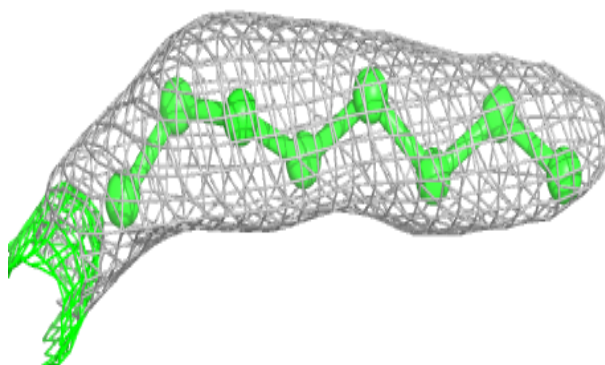


**Electron density around LFA D 311:**

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

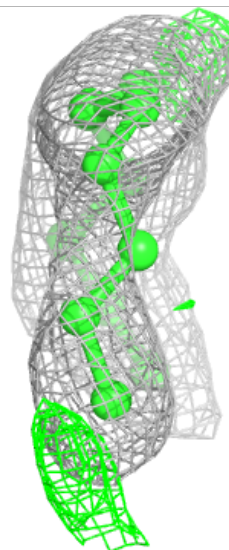
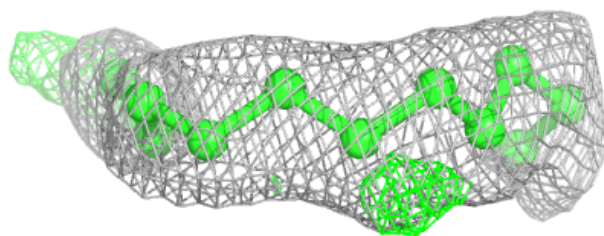
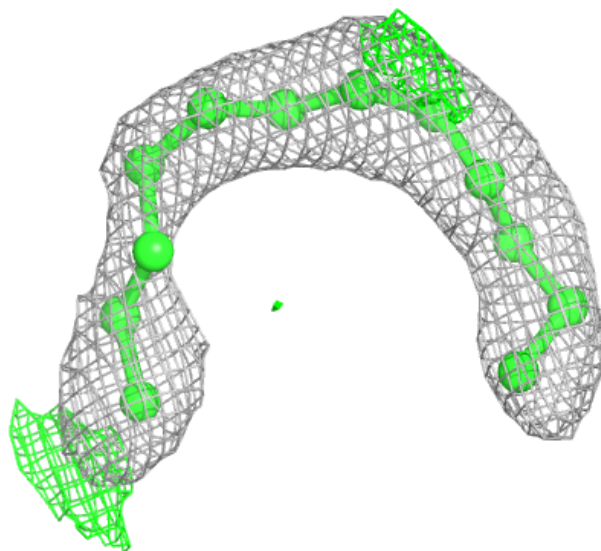
**Electron density around LFA E 307:**

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



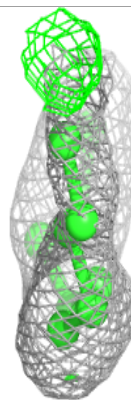
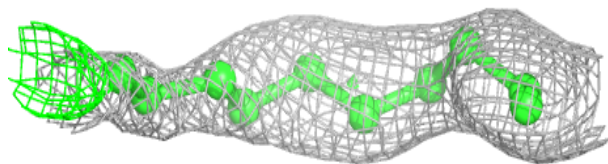
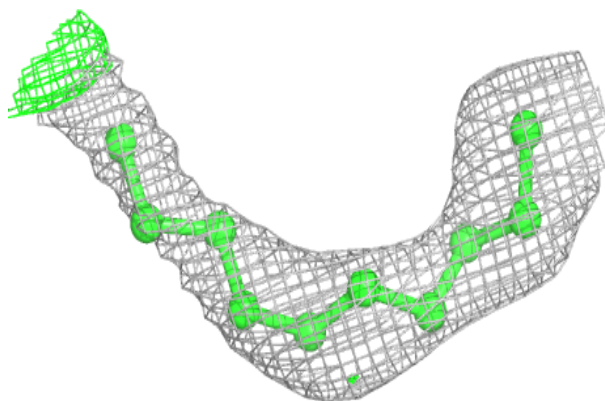
**Electron density around LFA A 304:**

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

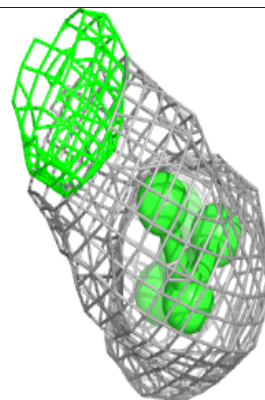
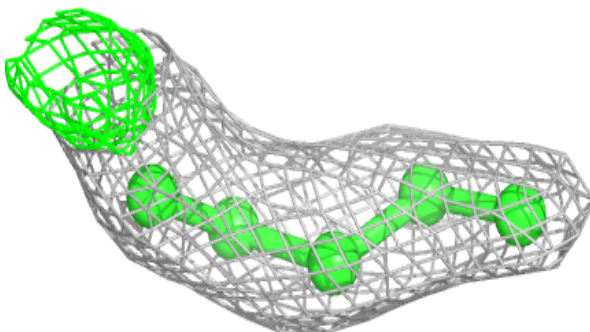
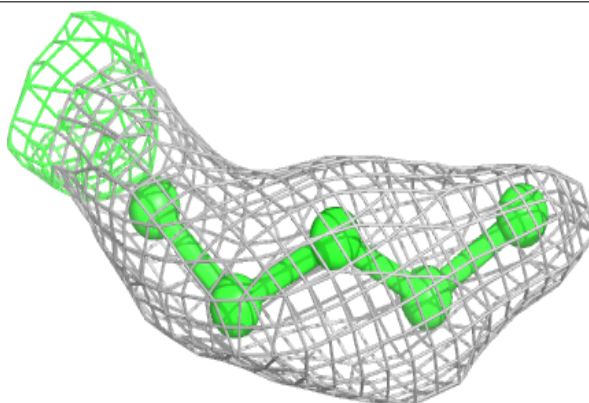


**Electron density around LFA D 308:**

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

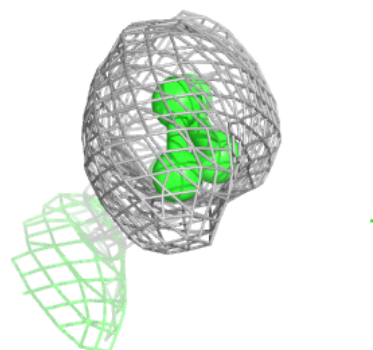
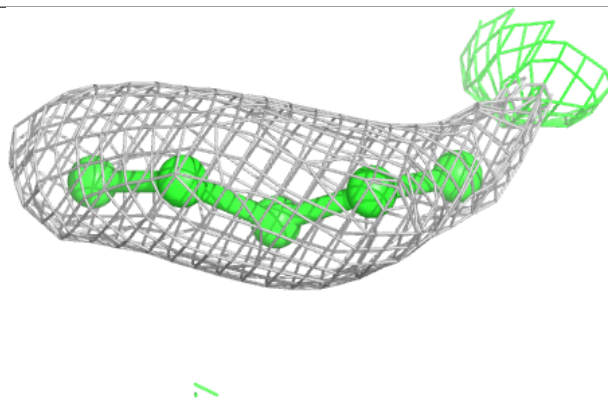
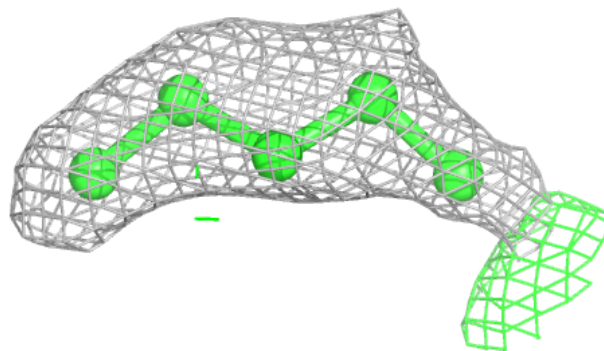
**Electron density around LFA E 306:**

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

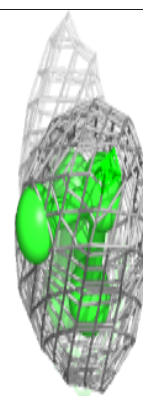
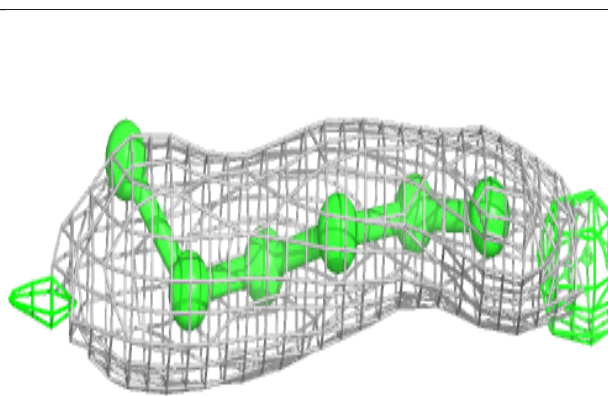
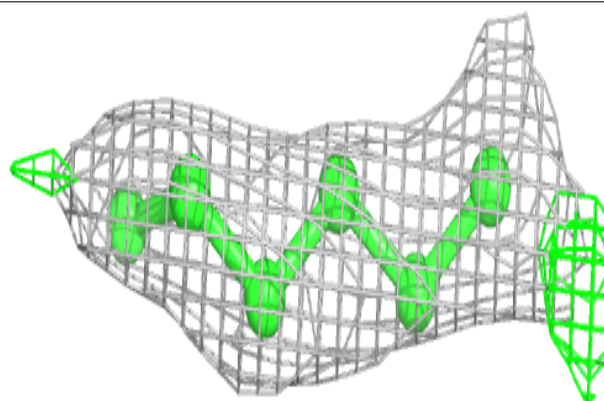


**Electron density around LFA A 315:**

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

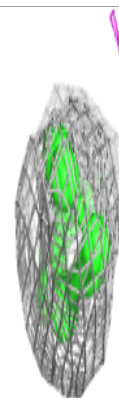
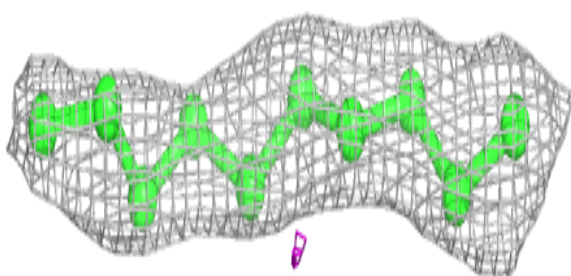
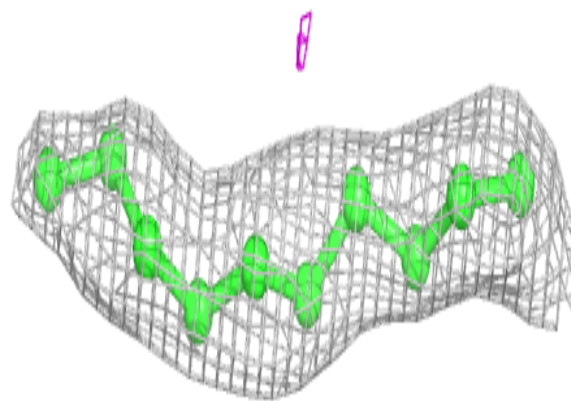
**Electron density around LFA A 307:**

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

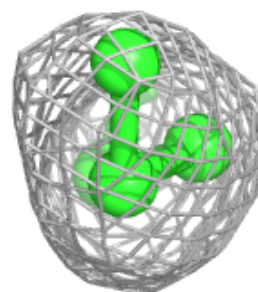
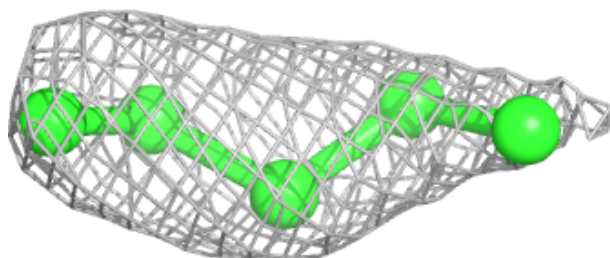
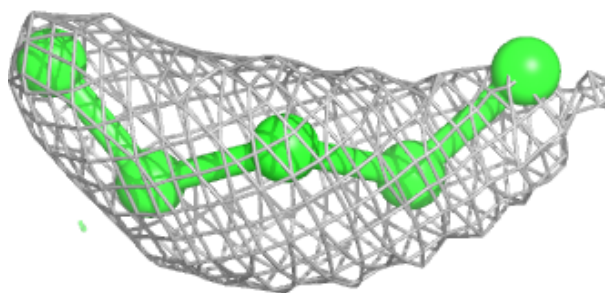


**Electron density around LFA C 309:**

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

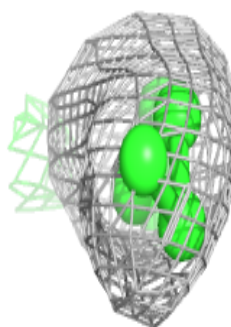
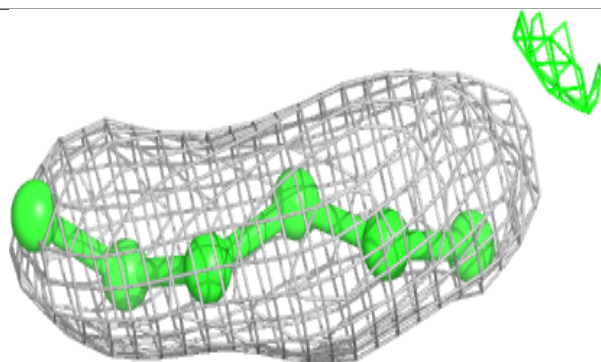
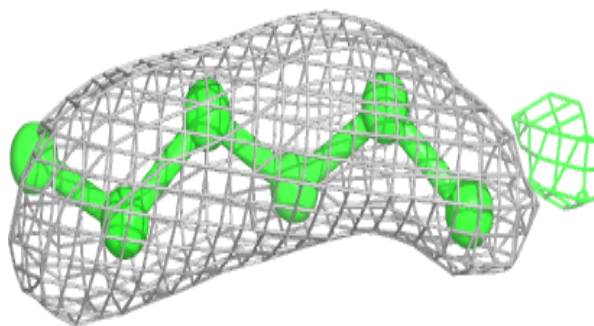
**Electron density around LFA A 308:**

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

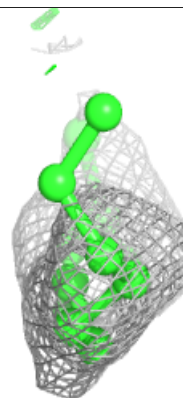
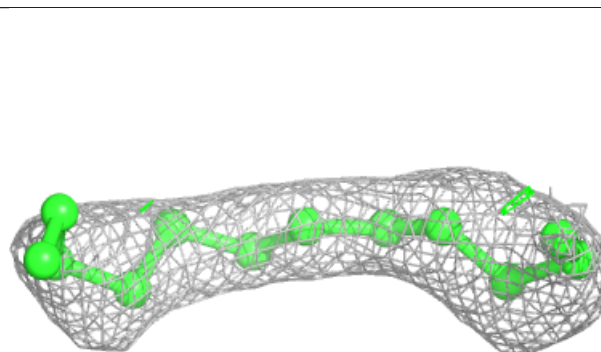
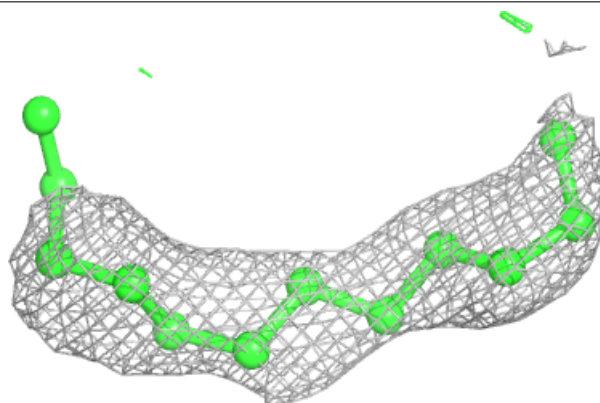


**Electron density around LFA A 306:**

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

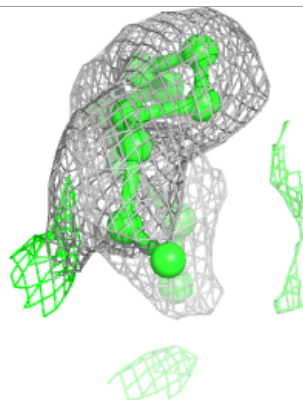
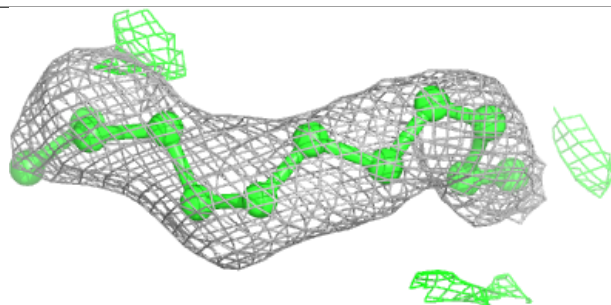
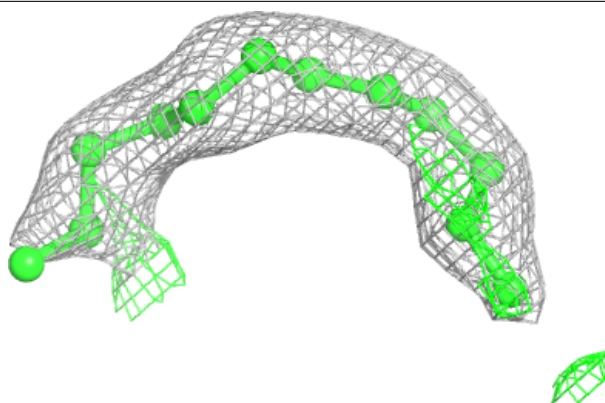
**Electron density around LFA D 306:**

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

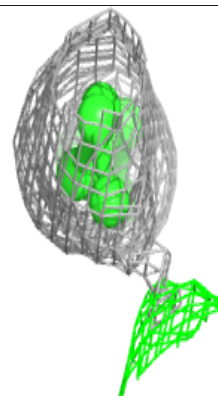
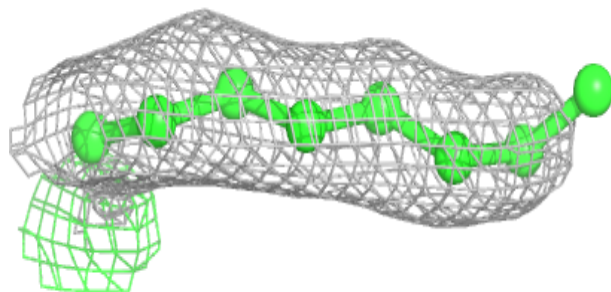
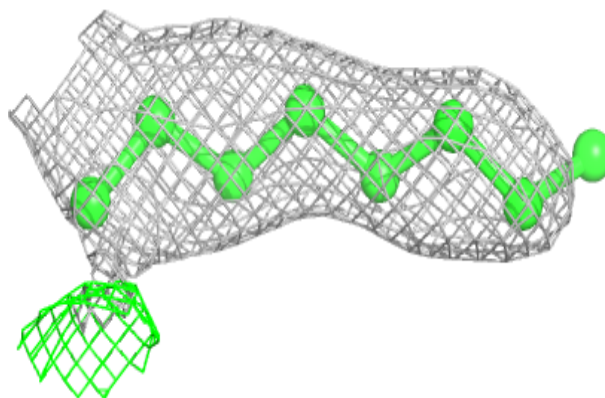


**Electron density around LFA A 303:**

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

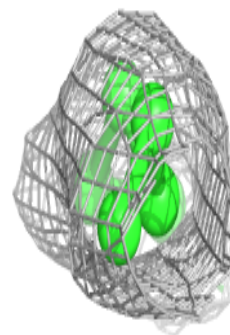
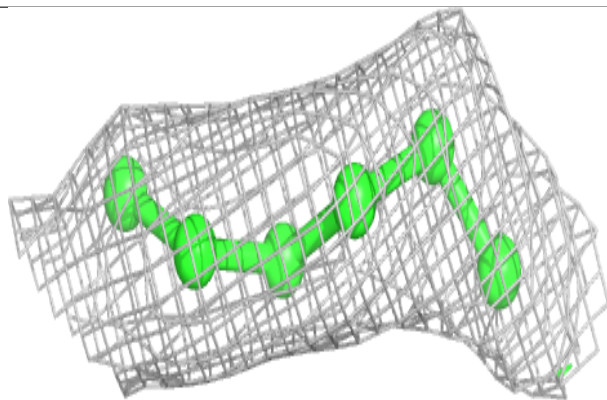
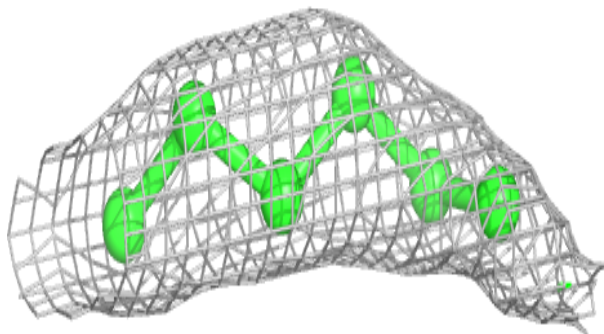
**Electron density around LFA C 303:**

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

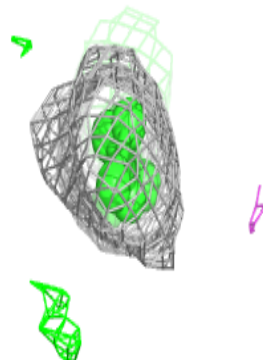
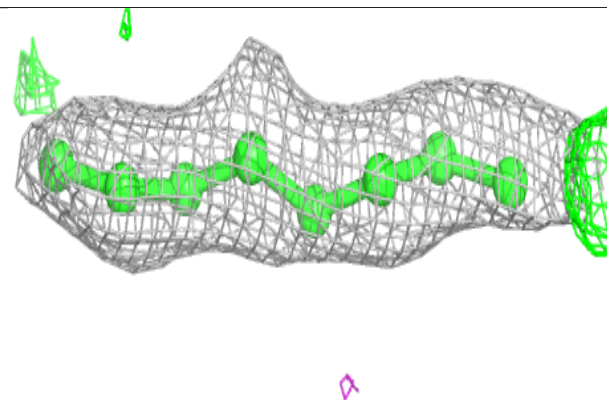
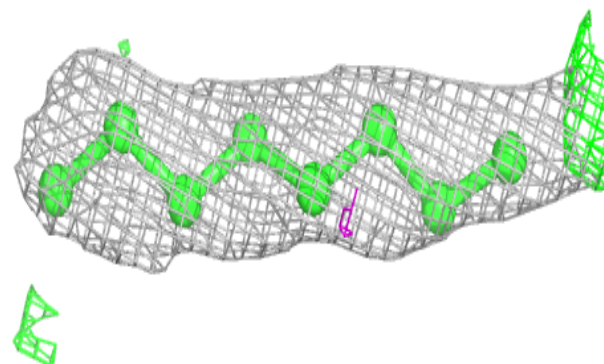


**Electron density around LFA C 306:**

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

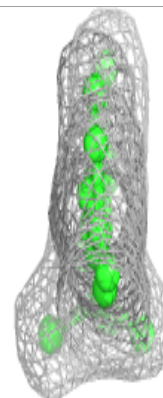
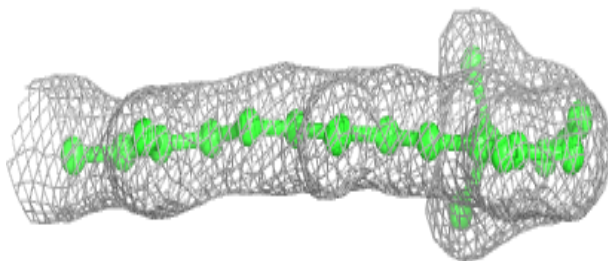
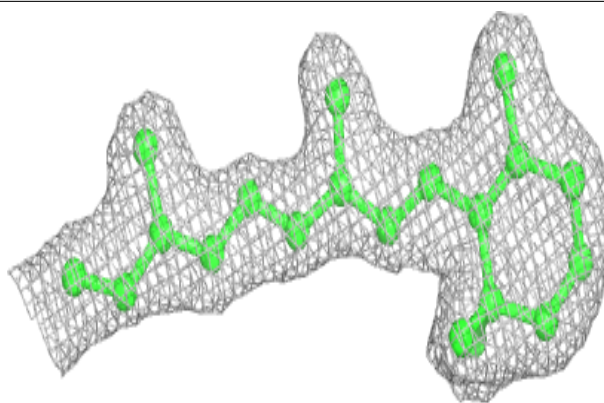
**Electron density around LFA A 305:**

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

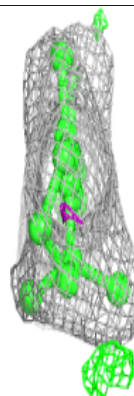
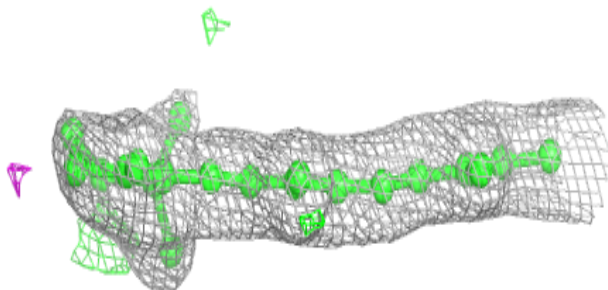
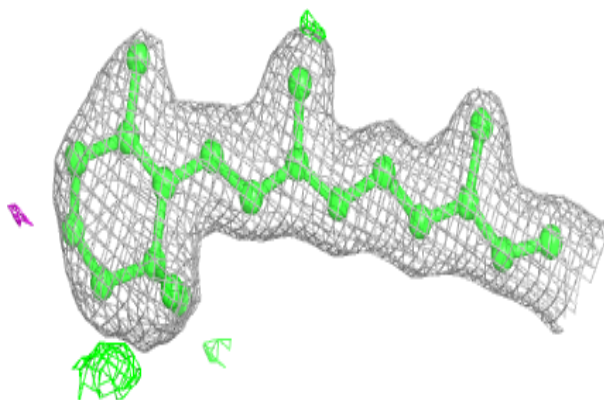


**Electron density around RET B 316:**

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

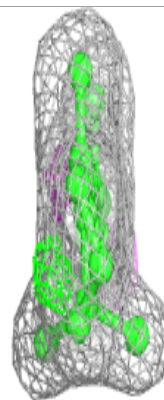
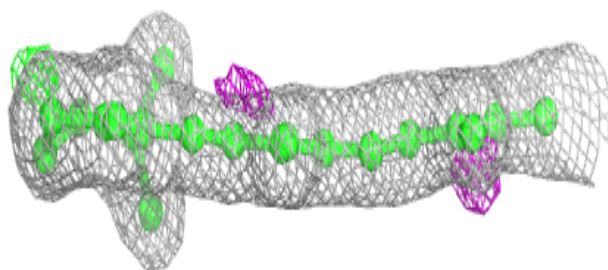
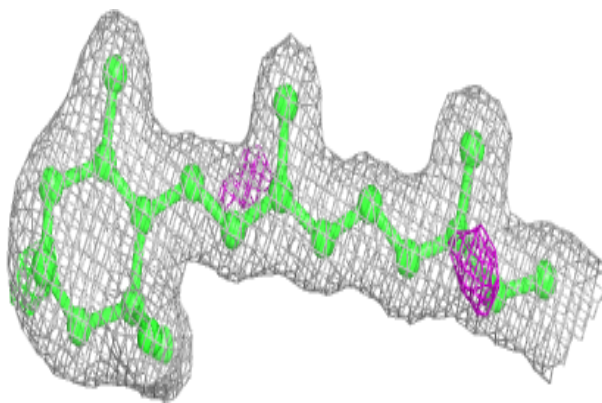
**Electron density around RET D 313:**

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

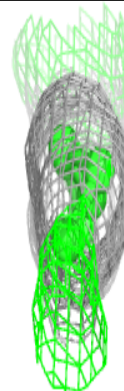
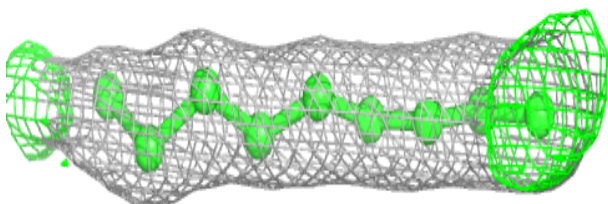
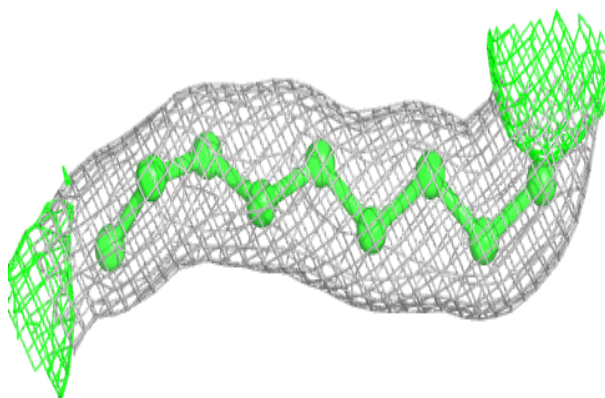


**Electron density around RET A 318:**

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

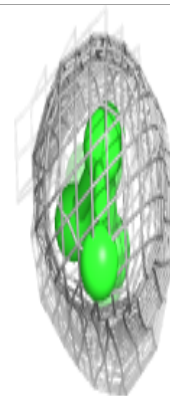
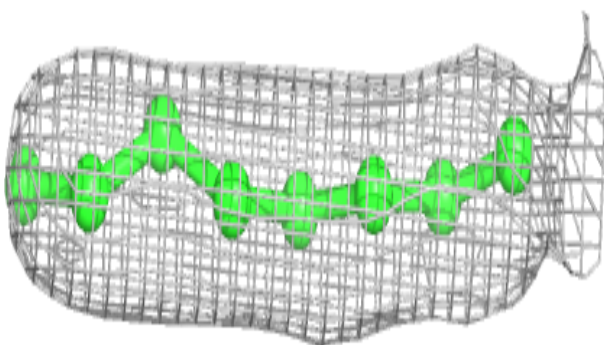
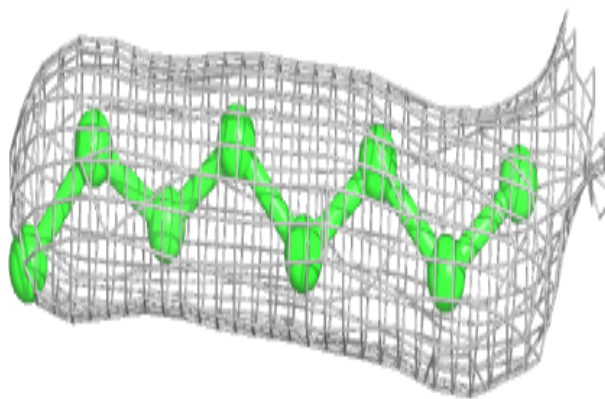
**Electron density around LFA E 302:**

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

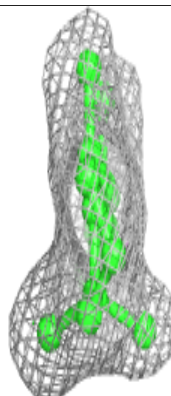
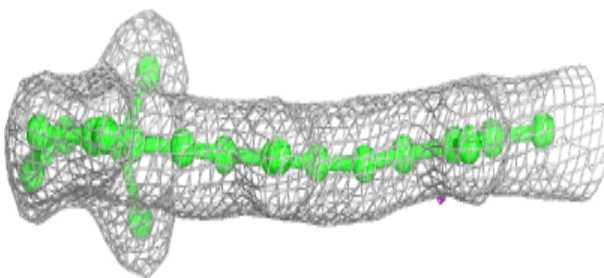
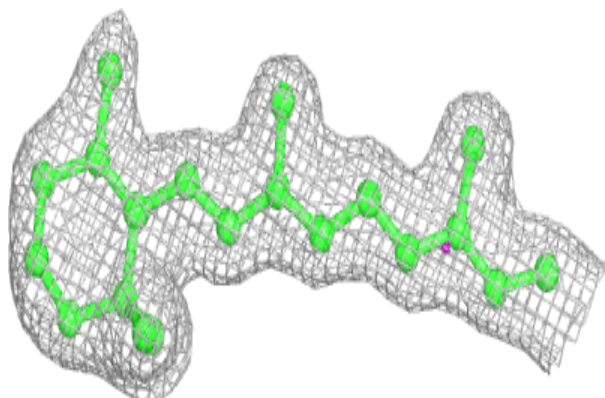


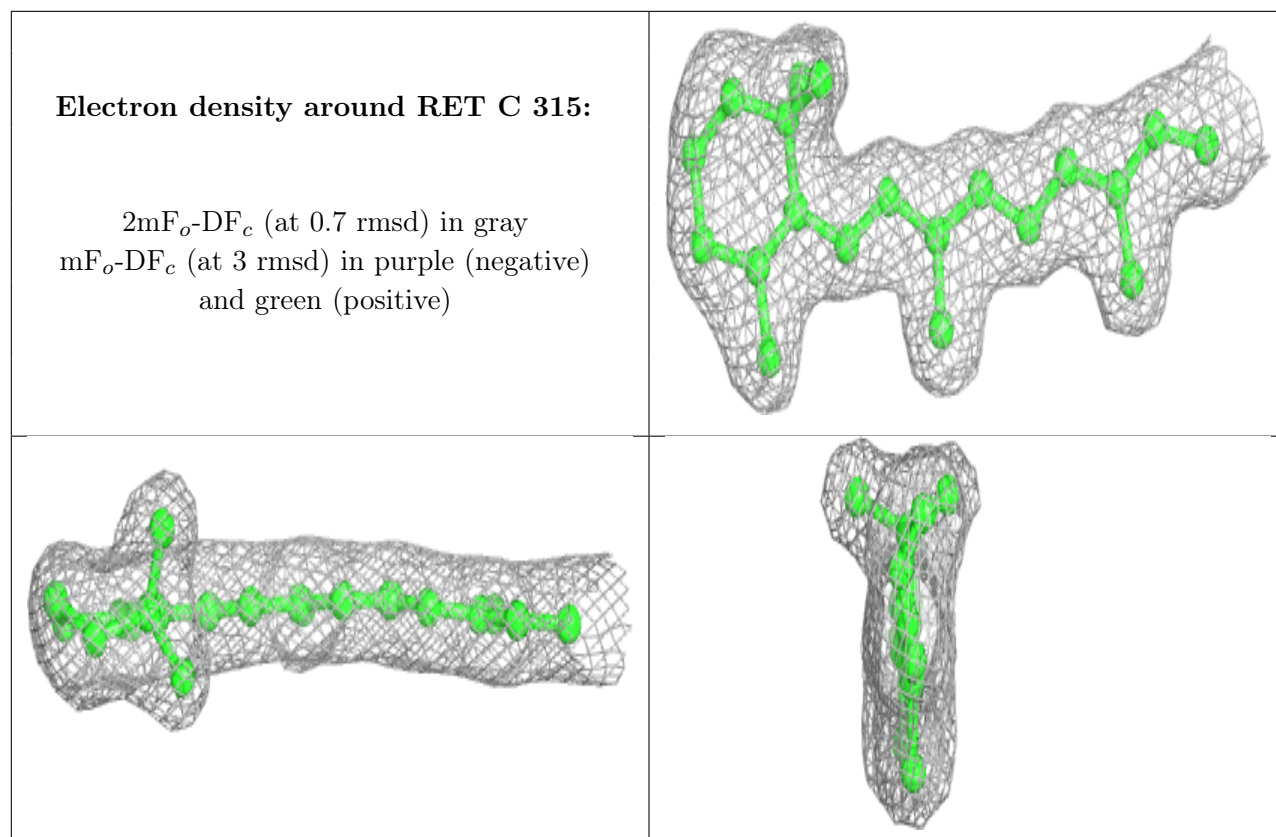
**Electron density around LFA B 301:**

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

**Electron density around RET 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.