



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:51 PM BST

PDB ID : 6REX  
Title : Crystal structure of the light-driven sodium pump KR2 in the pentameric form, pH 6.0  
Authors : Kovalev, K.; Polovinkin, V.; Gushchin, I.; Borshchevskiy, V.; Gordeliy, V.  
Deposited on : 2019-04-12  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

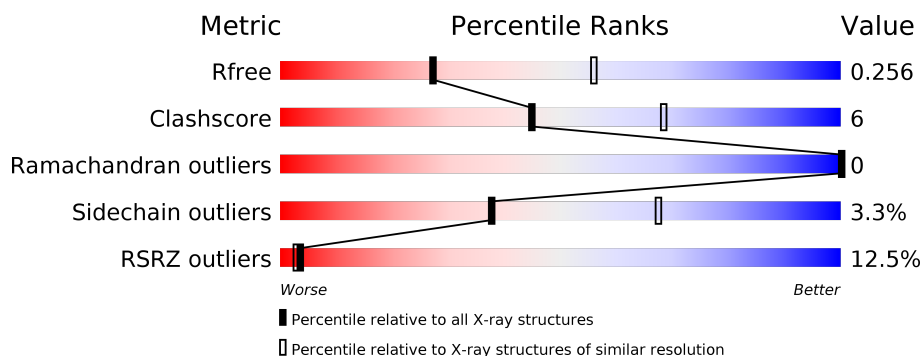
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	273	<div> <div>11%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	273	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
1	C	273	<div> <div>14%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> </div>
1	D	273	<div> <div>13%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
1	E	273	<div> <div>16%</div> <div> <div></div> <div>86%</div> <div>13%</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
2	OLC	B	305	-	-	-	X
2	OLC	C	303	-	-	-	X
2	OLC	C	309	-	-	-	X
2	OLC	D	303	-	-	-	X
2	OLC	D	305	-	-	-	X
2	OLC	E	304	-	-	-	X
3	LFA	A	311	-	-	-	X
3	LFA	B	302	-	-	-	X
3	LFA	B	306	-	-	-	X
3	LFA	C	313	-	-	-	X
3	LFA	C	314	-	-	-	X
3	LFA	D	306	-	-	-	X
3	LFA	D	312	-	-	-	X
5	BOG	A	310	-	-	-	X
5	BOG	B	312	-	-	-	X
5	BOG	C	317	-	-	-	X
5	BOG	D	314	-	-	-	X
5	BOG	E	312	-	-	-	X

## 2 Entry composition [i](#)

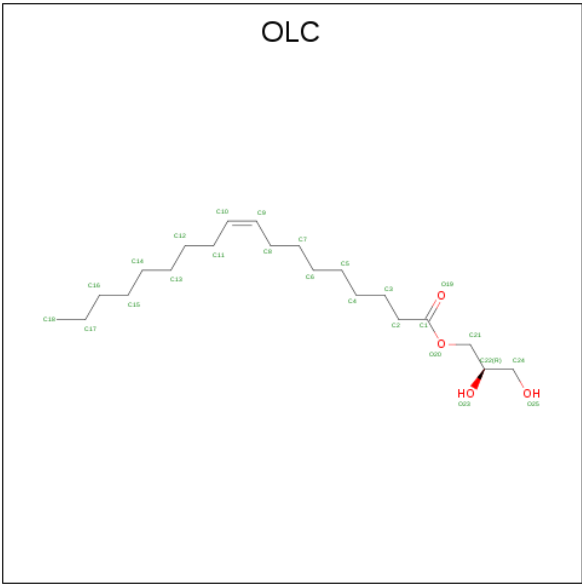
There are 7 unique types of molecules in this entry. The entry contains 12192 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	1	0
			2179	1451	330	389	9			
1	B	273	Total	C	N	O	S	0	1	0
			2173	1446	331	387	9			
1	C	273	Total	C	N	O	S	0	1	0
			2178	1450	330	389	9			
1	D	273	Total	C	N	O	S	0	1	0
			2170	1445	330	386	9			
1	E	273	Total	C	N	O	S	0	1	0
			2172	1447	330	386	9			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	18	4		

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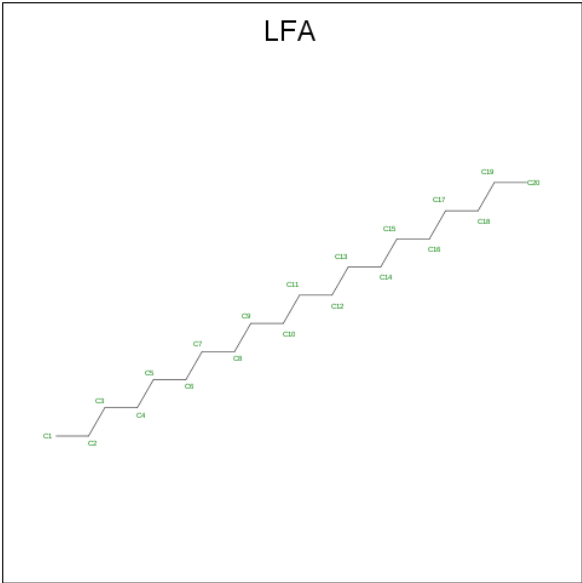
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	9	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			16	12	4		
2	B	1	Total	C	O	0	0
			17	13	4		
2	C	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			23	19	4		
2	C	1	Total	C	O	0	0
			18	14	4		
2	C	1	Total	C	O	0	0
			15	11	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			16	12	4		
2	D	1	Total	C	O	0	0
			25	21	4		
2	D	1	Total	C	O	0	0
			18	14	4		
2	D	1	Total	C	O	0	0
			14	10	4		
2	D	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			24	20	4		
2	E	1	Total	C	O	0	0
			25	21	4		
2	E	1	Total	C	O	0	0
			15	11	4		

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

- 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
			8	8		
3	A	1	Total	C	0	0
			5	5		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			4	4		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			20	20		
3	B	1	Total	C	0	0
			20	20		
3	B	1	Total	C	0	0
			9	9		
3	B	1	Total	C	0	0
			5	5		
3	B	1	Total	C	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 7 7	0	0
3	B	1	Total C 6 6	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 12 12	0	0
3	C	1	Total C 11 11	0	0
3	C	1	Total C 4 4	0	0
3	C	1	Total C 6 6	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 20 20	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 6 6	0	0
3	E	1	Total C 14 14	0	0
3	E	1	Total C 4 4	0	0

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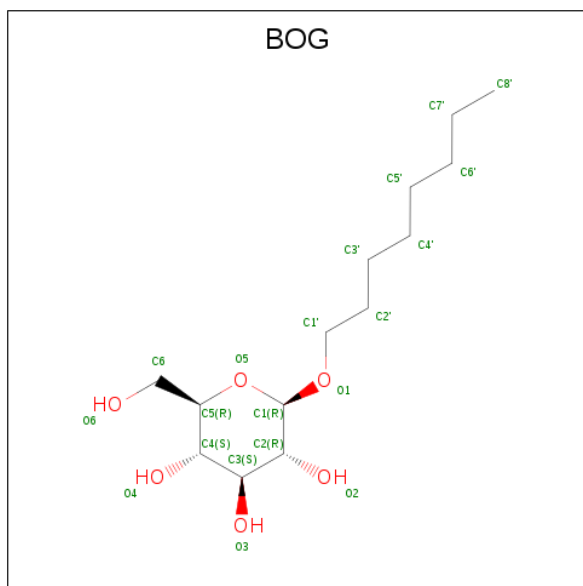
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 5 5	0	0
3	E	1	Total C 6 6	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 14 14	0	0

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

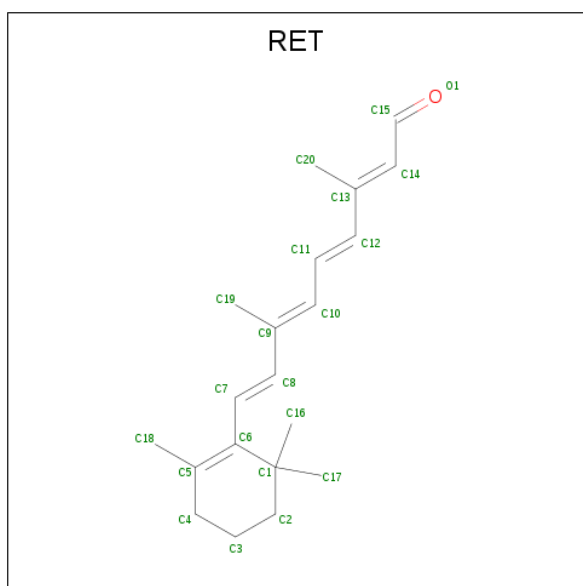
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



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

- Molecule 6 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



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

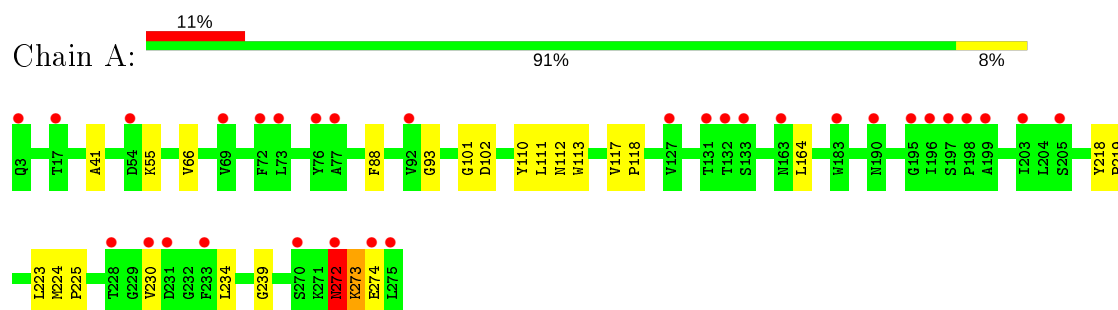
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	64	Total 64	O 64	0	0
7	B	66	Total 66	O 66	0	0
7	C	76	Total 76	O 76	0	0
7	D	41	Total 41	O 41	0	0
7	E	69	Total 69	O 69	0	0

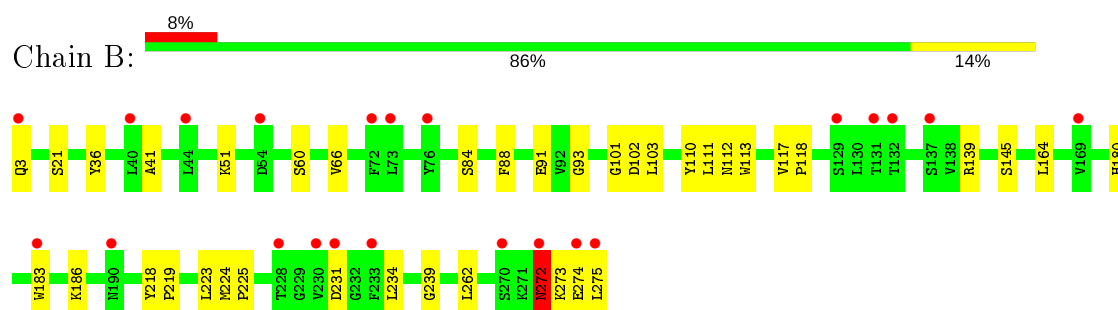
### 3 Residue-property plots [i](#)

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

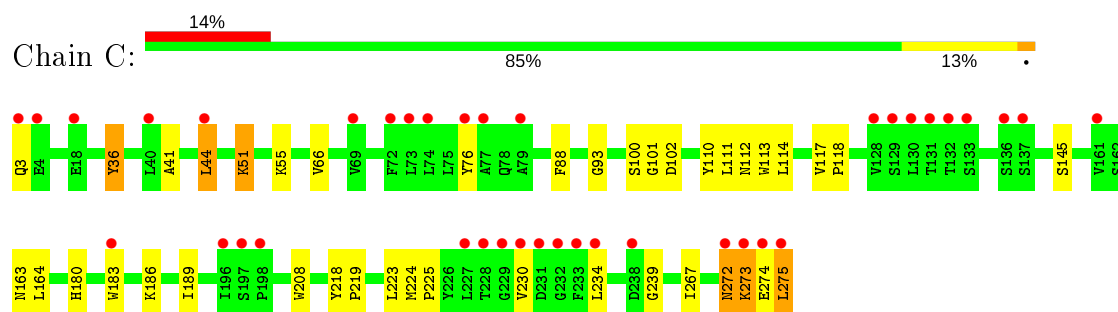
- Molecule 1: Sodium pumping rhodopsin



- Molecule 1: Sodium pumping rhodopsin

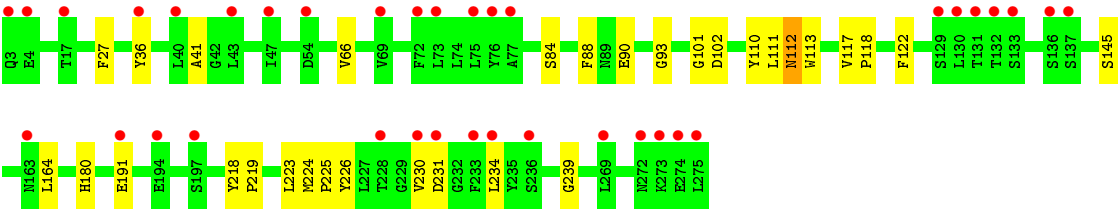


- Molecule 1: Sodium pumping rhodopsin

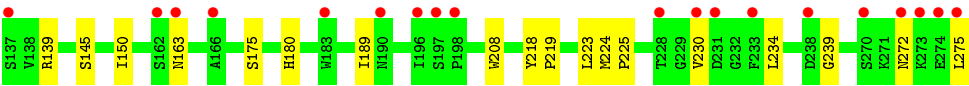
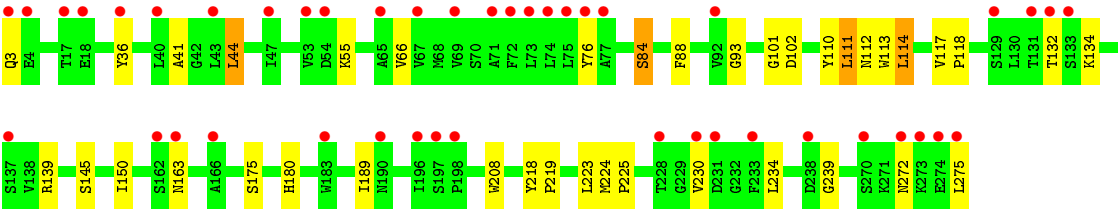
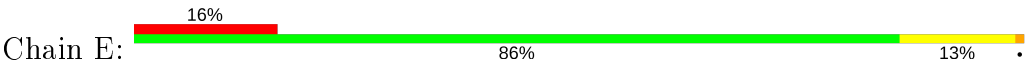


- Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.43Å 240.79Å 135.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.70 48.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.26-2.70) 96.5 (48.21-2.70)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.223 , 0.250 0.232 , 0.256	Depositor DCC
$R_{free}$ test set	2803 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/2237	0.41	0/3041
1	B	0.27	0/2231	0.41	0/3034
1	C	0.26	0/2236	0.41	0/3040
1	D	0.26	0/2228	0.41	0/3029
1	E	0.26	0/2230	0.41	0/3032
All	All	0.27	0/11162	0.41	0/15176

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	E	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	ASN	Peptide
1	B	272	ASN	Peptide
1	C	272	ASN	Peptide
1	E	139	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	272	ASN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2179	0	2154	19	0
1	B	2173	0	2149	34	0
1	C	2178	0	2152	28	0
1	D	2170	0	2142	23	0
1	E	2172	0	2150	24	0
2	A	50	0	65	0	0
2	B	78	0	110	4	0
2	C	145	0	194	6	0
2	D	82	0	120	4	0
2	E	89	0	134	1	0
3	A	51	0	99	0	0
3	B	57	0	111	3	0
3	C	68	0	132	5	0
3	D	118	0	240	1	0
3	E	61	0	114	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	20	0	28	2	0
5	B	20	0	28	2	0
5	C	20	0	28	1	0
5	D	20	0	28	4	0
5	E	20	0	28	0	0
6	A	20	0	27	5	0
6	B	20	0	27	4	0
6	C	20	0	27	5	0
6	D	20	0	27	5	0
6	E	20	0	27	6	0
7	A	64	0	0	1	0
7	B	66	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	76	0	0	5	0
7	D	41	0	0	2	0
7	E	69	0	0	1	0
All	All	12192	0	12341	157	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:N	1:B:272:ASN:HD22	1.66	0.90
1:A:272:ASN:HD22	1:A:272:ASN:N	1.69	0.89
6:E:315:RET:H161	6:E:315:RET:H8	1.59	0.85
6:D:315:RET:H8	6:D:315:RET:H161	1.60	0.84
6:A:312:RET:H161	6:A:312:RET:H8	1.60	0.83
6:C:318:RET:H8	6:C:318:RET:H161	1.61	0.82
6:B:313:RET:H161	6:B:313:RET:H8	1.59	0.81
1:B:273:LYS:O	7:B:401:HOH:O	2.03	0.77
2:B:305:OLC:H2	2:C:303:OLC:H24A	1.69	0.75
1:E:175:SER:OG	3:E:310:LFA:H202	1.87	0.75
1:B:231:ASP:N	5:B:312:BOG:O6	2.13	0.74
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.74	0.69
1:A:272:ASN:ND2	1:A:272:ASN:N	2.43	0.67
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.76	0.67
1:B:231:ASP:H	5:B:312:BOG:HO6	1.39	0.66
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.77	0.66
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.76	0.66
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.77	0.66
1:D:191:GLU:O	7:D:401:HOH:O	2.15	0.64
6:E:315:RET:H161	6:E:315:RET:C8	2.28	0.64
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.79	0.64
6:D:315:RET:C8	6:D:315:RET:H161	2.27	0.63
1:B:272:ASN:N	1:B:272:ASN:ND2	2.41	0.62
1:C:189:ILE:HD12	1:C:208:TRP:HB2	1.82	0.62
6:C:318:RET:H161	6:C:318:RET:C8	2.28	0.62
6:B:313:RET:H161	6:B:313:RET:C8	2.28	0.61
1:D:112:ASN:HB3	7:D:410:HOH:O	2.01	0.60
1:A:164:LEU:HD21	5:A:310:BOG:H2'1	1.83	0.60
1:E:189:ILE:HD12	1:E:208:TRP:HB2	1.83	0.60
1:A:272:ASN:HD22	1:A:272:ASN:H	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:H	1:B:272:ASN:HD22	1.48	0.59
1:E:224:MET:N	1:E:225:PRO:HD2	2.18	0.58
1:C:55:LYS:NZ	7:C:402:HOH:O	2.37	0.58
1:C:224:MET:N	1:C:225:PRO:HD2	2.18	0.58
1:A:224:MET:N	1:A:225:PRO:HD2	2.19	0.57
1:B:224:MET:N	1:B:225:PRO:HD2	2.19	0.57
1:E:145:SER:OG	1:E:180:HIS:HD2	1.88	0.57
1:D:224:MET:N	1:D:225:PRO:HD2	2.20	0.57
6:A:312:RET:H161	6:A:312:RET:C8	2.28	0.56
1:C:145:SER:OG	1:C:180:HIS:HD2	1.89	0.56
1:D:145:SER:OG	1:D:180:HIS:HD2	1.89	0.56
1:B:145:SER:OG	1:B:180:HIS:HD2	1.89	0.56
1:C:186:LYS:HG2	3:C:310:LFA:H52	1.87	0.56
1:C:234:LEU:O	1:C:239:GLY:HA3	2.06	0.56
2:B:305:OLC:H21A	7:C:452:HOH:O	2.06	0.56
2:C:305:OLC:H13	2:C:306:OLC:H4A	1.87	0.55
6:C:318:RET:H171	6:C:318:RET:H8	1.89	0.55
1:D:234:LEU:O	1:D:239:GLY:HA3	2.06	0.55
6:D:315:RET:H8	6:D:315:RET:H171	1.88	0.55
1:E:234:LEU:O	1:E:239:GLY:HA3	2.05	0.55
6:A:312:RET:H171	6:A:312:RET:H8	1.89	0.55
1:B:234:LEU:O	1:B:239:GLY:HA3	2.07	0.54
1:A:234:LEU:O	1:A:239:GLY:HA3	2.07	0.54
1:D:231:ASP:H	5:D:314:BOG:HO6	1.53	0.54
1:A:272:ASN:HB2	1:A:273:LYS:HE2	1.90	0.54
1:D:90:GLU:OE2	1:E:3:GLN:NE2	2.41	0.54
1:C:183:TRP:CE3	3:C:310:LFA:H41	2.42	0.54
6:E:315:RET:H8	6:E:315:RET:H171	1.90	0.53
1:B:139:ARG:NH1	2:B:301:OLC:H24	2.23	0.52
6:B:313:RET:H171	6:B:313:RET:H8	1.91	0.52
7:A:408:HOH:O	1:B:3:GLN:HG3	2.09	0.52
1:E:163:ASN:HD22	2:E:304:OLC:H22	1.75	0.52
1:B:274:GLU:O	1:B:275:LEU:CB	2.58	0.52
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.92	0.52
1:D:226:TYR:HB3	5:D:314:BOG:H5'2	1.92	0.52
1:B:223:LEU:C	1:B:225:PRO:HD2	2.31	0.51
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.93	0.51
1:A:223:LEU:C	1:A:225:PRO:HD2	2.30	0.51
1:B:275:LEU:HD23	1:B:275:LEU:O	2.11	0.51
1:E:223:LEU:C	1:E:225:PRO:HD2	2.31	0.51
1:D:223:LEU:C	1:D:225:PRO:HD2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LEU:C	1:C:225:PRO:HD2	2.31	0.50
1:C:164:LEU:HD21	5:C:317:BOG:H2'1	1.93	0.50
3:C:304:LFA:H172	3:D:301:LFA:H61	1.93	0.50
1:C:114:LEU:HD22	2:C:302:OLC:H10	1.94	0.49
1:C:163:ASN:HD22	2:C:308:OLC:C24	2.26	0.49
1:C:110:TYR:O	1:C:113:TRP:HB2	2.14	0.48
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.95	0.48
6:D:315:RET:C8	6:D:315:RET:H171	2.44	0.48
1:B:183:TRP:CZ3	3:B:306:LFA:H182	2.49	0.48
1:C:272:ASN:HB2	1:C:273:LYS:HD3	1.95	0.47
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.94	0.47
2:D:302:OLC:H18A	2:D:305:OLC:H6	1.96	0.47
6:A:312:RET:H171	6:A:312:RET:C8	2.44	0.47
1:C:51:LYS:HD3	7:C:448:HOH:O	2.14	0.47
1:E:101:GLY:O	1:E:102:ASP:HB2	2.14	0.47
1:C:101:GLY:O	1:C:102:ASP:HB2	2.13	0.47
6:C:318:RET:H171	6:C:318:RET:C8	2.45	0.47
1:B:110:TYR:O	1:B:113:TRP:HB2	2.15	0.47
1:B:60:SER:HB3	7:B:441:HOH:O	2.15	0.47
1:A:101:GLY:O	1:A:102:ASP:HB2	2.15	0.47
3:E:307:LFA:H141	3:E:308:LFA:H201	1.97	0.46
1:A:110:TYR:O	1:A:113:TRP:HB2	2.15	0.46
1:C:267:ILE:HG21	1:C:275:LEU:HB3	1.98	0.46
6:B:313:RET:H171	6:B:313:RET:C8	2.45	0.46
1:E:110:TYR:O	1:E:113:TRP:HB2	2.15	0.46
2:D:302:OLC:H11A	2:D:305:OLC:H17	1.98	0.46
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.51	0.46
1:C:100:SER:HB2	7:C:469:HOH:O	2.16	0.45
1:B:101:GLY:O	1:B:102:ASP:HB2	2.16	0.45
1:D:164:LEU:HD21	5:D:314:BOG:H2'1	1.99	0.45
1:D:110:TYR:O	1:D:113:TRP:HB2	2.15	0.45
6:E:315:RET:C8	6:E:315:RET:H171	2.46	0.45
1:E:218:TYR:N	1:E:219:PRO:HD2	2.32	0.44
1:E:224:MET:N	1:E:225:PRO:CD	2.81	0.44
1:B:218:TYR:N	1:B:219:PRO:HD2	2.32	0.44
2:C:307:OLC:H2A	2:C:308:OLC:H21A	1.99	0.44
1:D:27:PHE:HE1	2:D:305:OLC:H2	1.82	0.44
1:B:21:SER:OG	2:B:305:OLC:H24	2.17	0.44
1:C:218:TYR:N	1:C:219:PRO:HD2	2.32	0.44
3:C:304:LFA:H32	3:E:314:LFA:H102	1.99	0.44
1:B:110:TYR:HA	1:B:113:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:HB2	1:B:273:LYS:HD3	2.00	0.44
1:D:101:GLY:O	1:D:102:ASP:HB2	2.16	0.44
1:D:110:TYR:HA	1:D:113:TRP:CE3	2.53	0.44
1:D:218:TYR:N	1:D:219:PRO:HD2	2.32	0.44
1:A:224:MET:N	1:A:225:PRO:CD	2.81	0.43
1:B:51:LYS:HB2	7:C:402:HOH:O	2.18	0.43
1:C:110:TYR:HA	1:C:113:TRP:CE3	2.53	0.43
1:E:84[B]:SER:HB3	7:E:436:HOH:O	2.18	0.43
1:A:110:TYR:HA	1:A:113:TRP:CE3	2.53	0.43
1:A:218:TYR:N	1:A:219:PRO:HD2	2.34	0.43
1:B:117:VAL:CB	1:B:118:PRO:HD3	2.47	0.43
1:E:44:LEU:HA	1:E:44:LEU:HD23	1.80	0.43
6:C:318:RET:H181	6:C:318:RET:H7	1.77	0.43
1:B:224:MET:N	1:B:225:PRO:CD	2.82	0.42
1:D:224:MET:N	1:D:225:PRO:CD	2.82	0.42
1:E:110:TYR:HA	1:E:113:TRP:CE3	2.54	0.42
1:C:183:TRP:CZ3	3:C:310:LFA:H41	2.54	0.42
1:A:88:PHE:CZ	1:A:93:GLY:HA2	2.55	0.42
1:C:224:MET:N	1:C:225:PRO:CD	2.81	0.42
1:E:111:LEU:O	1:E:114:LEU:HB2	2.19	0.42
6:A:312:RET:H7	6:A:312:RET:H181	1.75	0.42
6:E:315:RET:H7	6:E:315:RET:H181	1.77	0.42
2:C:305:OLC:H5	2:C:306:OLC:H2A	2.01	0.42
1:D:231:ASP:N	5:D:314:BOG:O6	2.21	0.42
1:B:186:LYS:HG2	3:B:306:LFA:H192	2.01	0.41
1:B:84[B]:SER:OG	7:B:402:HOH:O	2.22	0.41
1:B:91:GLU:H	1:B:91:GLU:HG2	1.67	0.41
1:E:117:VAL:CB	1:E:118:PRO:HD3	2.45	0.41
1:A:164:LEU:HD21	5:A:310:BOG:C2'	2.50	0.41
1:B:223:LEU:HD11	3:B:310:LFA:H12	2.02	0.41
1:B:262:LEU:HA	1:B:262:LEU:HD23	1.95	0.41
1:C:88:PHE:CZ	1:C:93:GLY:HA2	2.55	0.41
1:B:88:PHE:CZ	1:B:93:GLY:HA2	2.55	0.41
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.79	0.41
6:E:315:RET:H11	6:E:315:RET:H191	1.95	0.41
1:E:114:LEU:HD12	1:E:114:LEU:HA	1.78	0.41
1:D:27:PHE:CE1	2:D:305:OLC:H2	2.55	0.41
1:D:41:ALA:HB1	1:E:66:VAL:HG13	2.03	0.41
1:C:117:VAL:CB	1:C:118:PRO:HD3	2.50	0.40
6:D:315:RET:H191	6:D:315:RET:H11	1.93	0.40
1:E:36:TYR:CD2	1:E:76:TYR:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:CB	1:A:118:PRO:HD3	2.48	0.40
1:C:36:TYR:CD2	1:C:76:TYR:HA	2.57	0.40
1:D:118:PRO:O	1:D:122:PHE:HB2	2.22	0.40
1:D:88:PHE:CZ	1:D:93:GLY:HA2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/273 (100%)	266 (98%)	6 (2%)	0	100	100
1	B	272/273 (100%)	264 (97%)	8 (3%)	0	100	100
1	C	272/273 (100%)	267 (98%)	5 (2%)	0	100	100
1	D	272/273 (100%)	266 (98%)	6 (2%)	0	100	100
1	E	272/273 (100%)	267 (98%)	5 (2%)	0	100	100
All	All	1360/1365 (100%)	1330 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/234 (99%)	224 (97%)	7 (3%)	41	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	231/234 (99%)	225 (97%)	6 (3%)	46	75
1	C	231/234 (99%)	221 (96%)	10 (4%)	29	57
1	D	229/234 (98%)	223 (97%)	6 (3%)	46	75
1	E	230/234 (98%)	219 (95%)	11 (5%)	25	53
All	All	1152/1170 (98%)	1112 (96%)	40 (4%)	38	65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	111	LEU
1	A	112	ASN
1	A	230	VAL
1	A	272	ASN
1	A	273	LYS
1	A	274	GLU
1	B	36	TYR
1	B	103	LEU
1	B	111	LEU
1	B	112	ASN
1	B	164	LEU
1	B	272	ASN
1	C	3	GLN
1	C	36	TYR
1	C	44	LEU
1	C	51	LYS
1	C	111	LEU
1	C	112	ASN
1	C	230	VAL
1	C	273	LYS
1	C	274	GLU
1	C	275	LEU
1	D	36	TYR
1	D	84[A]	SER
1	D	84[B]	SER
1	D	111	LEU
1	D	112	ASN
1	D	230	VAL
1	E	44	LEU
1	E	55	LYS
1	E	84[A]	SER

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Mol	Chain	Res	Type
1	E	84[B]	SER
1	E	111	LEU
1	E	112	ASN
1	E	114	LEU
1	E	132	THR
1	E	134	LYS
1	E	230	VAL
1	E	275	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 5 are monoatomic - leaving 68 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	C	303	-	15,15,24	1.23	1 (6%)	16,16,25	1.02	1 (6%)
3	LFA	A	307	-	3,3,19	0.38	0	2,2,18	0.58	0
3	LFA	D	312	-	19,19,19	0.38	0	18,18,18	0.35	0
3	LFA	A	308	-	5,5,19	0.29	0	4,4,18	0.32	0
2	OLC	D	305	-	24,24,24	0.94	1 (4%)	25,25,25	0.81	1 (4%)
2	OLC	B	301	-	24,24,24	0.94	1 (4%)	25,25,25	0.86	1 (4%)
3	LFA	D	311	-	5,5,19	0.32	0	4,4,18	0.31	0
3	LFA	C	315	-	5,5,19	0.31	0	4,4,18	0.30	0
5	BOG	A	310	-	20,20,20	0.59	1 (5%)	25,25,25	0.67	0
3	LFA	B	308	-	9,9,19	0.31	0	8,8,18	0.43	0
3	LFA	B	310	-	5,5,19	0.27	0	4,4,18	0.36	0
2	OLC	C	309	-	15,15,24	1.25	1 (6%)	16,16,25	1.04	1 (6%)
2	OLC	A	302	-	12,12,24	1.32	1 (8%)	13,13,25	1.23	2 (15%)
3	LFA	A	305	-	4,4,19	0.30	0	3,3,18	0.38	0
3	LFA	C	304	-	19,19,19	0.37	0	18,18,18	0.33	0
5	BOG	C	317	-	20,20,20	0.56	1 (5%)	25,25,25	0.62	0
3	LFA	E	313	-	3,3,19	0.39	0	2,2,18	0.57	0
3	LFA	E	308	-	3,3,19	0.37	0	2,2,18	0.60	0
3	LFA	E	314	-	13,13,19	0.29	0	12,12,18	0.50	0
5	BOG	E	312	-	20,20,20	0.57	1 (5%)	25,25,25	0.55	0
6	RET	A	312	1	20,20,21	0.72	0	27,27,28	1.62	4 (14%)
3	LFA	B	306	-	8,8,19	0.30	0	7,7,18	0.41	0
2	OLC	C	305	-	22,22,24	0.96	1 (4%)	23,23,25	0.87	2 (8%)
3	LFA	C	310	-	6,6,19	0.31	0	5,5,18	0.36	0
6	RET	D	315	1	20,20,21	0.71	0	27,27,28	1.59	4 (14%)
2	OLC	E	302	-	24,24,24	0.94	1 (4%)	25,25,25	0.89	1 (4%)
2	OLC	A	301	-	21,21,24	0.98	1 (4%)	22,22,25	0.87	2 (9%)
2	OLC	B	303	-	19,19,24	1.07	1 (5%)	20,20,25	0.90	1 (5%)
3	LFA	D	310	-	6,6,19	0.29	0	5,5,18	0.38	0
3	LFA	E	309	-	4,4,19	0.29	0	3,3,18	0.35	0
3	LFA	C	313	-	10,10,19	0.29	0	9,9,18	0.52	0
2	OLC	B	305	-	16,16,24	1.17	1 (6%)	17,17,25	0.97	1 (5%)
2	OLC	D	304	-	13,13,24	1.22	1 (7%)	14,14,25	1.02	2 (14%)
3	LFA	E	305	-	7,7,19	0.30	0	6,6,18	0.39	0
3	LFA	A	304	-	7,7,19	0.31	0	6,6,18	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LFA	C	314	-	3,3,19	0.37	0	2,2,18	0.59	0
3	LFA	B	309	-	6,6,19	0.27	0	5,5,18	0.42	0
5	BOG	D	314	-	20,20,20	0.53	0	25,25,25	0.68	0
2	OLC	E	304	-	24,24,24	0.94	1 (4%)	25,25,25	0.82	2 (8%)
3	LFA	A	306	-	7,7,19	0.29	0	6,6,18	0.40	0
3	LFA	D	301	-	19,19,19	0.36	0	18,18,18	0.38	0
3	LFA	E	306	-	5,5,19	0.43	0	4,4,18	0.32	0
3	LFA	D	306	-	19,19,19	0.27	0	18,18,18	0.57	0
3	LFA	C	311	-	7,7,19	0.32	0	6,6,18	0.32	0
2	OLC	C	301	-	20,20,24	1.01	1 (5%)	21,21,25	0.95	1 (4%)
6	RET	C	318	1	20,20,21	0.73	0	27,27,28	1.59	3 (11%)
2	OLC	E	301	-	23,23,24	0.96	1 (4%)	24,24,25	0.87	1 (4%)
2	OLC	C	306	-	17,17,24	1.11	1 (5%)	18,18,25	0.98	1 (5%)
2	OLC	B	304	-	15,15,24	1.14	1 (6%)	16,16,25	1.05	2 (12%)
3	LFA	C	312	-	11,11,19	0.31	0	10,10,18	0.43	0
3	LFA	B	302	-	19,19,19	0.36	0	18,18,18	0.40	0
2	OLC	C	308	-	15,15,24	1.19	1 (6%)	16,16,25	0.92	1 (6%)
3	LFA	D	308	-	7,7,19	0.31	0	6,6,18	0.34	0
2	OLC	D	303	-	17,17,24	1.16	1 (5%)	18,18,25	1.03	1 (5%)
3	LFA	D	309	-	16,16,19	0.30	0	15,15,18	0.49	0
6	RET	B	313	1	20,20,21	0.76	0	27,27,28	1.63	5 (18%)
2	OLC	D	302	-	24,24,24	0.93	1 (4%)	25,25,25	0.87	1 (4%)
3	LFA	E	307	-	13,13,19	0.27	0	12,12,18	0.54	0
3	LFA	E	310	-	5,5,19	0.31	0	4,4,18	0.35	0
6	RET	E	315	1	20,20,21	0.74	0	27,27,28	1.56	4 (14%)
3	LFA	A	311	-	19,19,19	0.36	0	18,18,18	0.38	0
3	LFA	D	307	-	19,19,19	0.27	0	18,18,18	0.55	0
2	OLC	C	307	-	14,14,24	1.23	1 (7%)	15,15,25	1.01	1 (6%)
2	OLC	C	302	-	19,19,24	1.05	1 (5%)	20,20,25	0.92	2 (10%)
2	OLC	E	303	-	14,14,24	1.27	1 (7%)	15,15,25	1.05	1 (6%)
3	LFA	B	307	-	4,4,19	0.34	0	3,3,18	0.29	0
5	BOG	B	312	-	20,20,20	0.55	0	25,25,25	0.64	0
2	OLC	A	303	-	14,14,24	1.19	1 (7%)	15,15,25	1.05	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	303	-	-	7/15/15/24	-
3	LFA	A	307	-	-	0/1/1/17	-
3	LFA	D	312	-	-	5/17/17/17	-
3	LFA	A	308	-	-	3/3/3/17	-
2	OLC	D	305	-	-	14/24/24/24	-
2	OLC	B	301	-	-	10/24/24/24	-
3	LFA	D	311	-	-	1/3/3/17	-
3	LFA	C	315	-	-	3/3/3/17	-
5	BOG	A	310	-	-	4/11/31/31	0/1/1/1
3	LFA	B	308	-	-	4/7/7/17	-
3	LFA	B	310	-	-	1/3/3/17	-
2	OLC	C	309	-	-	9/15/15/24	-
2	OLC	A	302	-	-	1/12/12/24	-
3	LFA	A	305	-	-	1/2/2/17	-
3	LFA	C	304	-	-	10/17/17/17	-
5	BOG	C	317	-	-	3/11/31/31	0/1/1/1
3	LFA	E	313	-	-	0/1/1/17	-
3	LFA	E	308	-	-	1/1/1/17	-
3	LFA	E	314	-	-	4/11/11/17	-
5	BOG	E	312	-	-	9/11/31/31	0/1/1/1
6	RET	A	312	1	-	0/13/30/31	0/1/1/1
3	LFA	B	306	-	-	3/6/6/17	-
2	OLC	C	305	-	-	9/22/22/24	-
3	LFA	C	310	-	-	2/4/4/17	-
6	RET	D	315	1	-	0/13/30/31	0/1/1/1
2	OLC	E	302	-	-	13/24/24/24	-
2	OLC	A	301	-	-	9/21/21/24	-
2	OLC	B	303	-	-	7/19/19/24	-
3	LFA	D	310	-	-	3/4/4/17	-
3	LFA	E	309	-	-	1/2/2/17	-
3	LFA	C	313	-	-	3/8/8/17	-
2	OLC	B	305	-	-	9/16/16/24	-
2	OLC	D	304	-	-	9/13/13/24	-
3	LFA	E	305	-	-	0/5/5/17	-
3	LFA	A	304	-	-	2/5/5/17	-
3	LFA	C	314	-	-	1/1/1/17	-
3	LFA	B	309	-	-	0/4/4/17	-
5	BOG	D	314	-	-	1/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	E	304	-	-	15/24/24/24	-
3	LFA	A	306	-	-	3/5/5/17	-
3	LFA	D	301	-	-	8/17/17/17	-
3	LFA	E	306	-	-	1/3/3/17	-
3	LFA	D	306	-	-	10/17/17/17	-
3	LFA	C	311	-	-	5/5/5/17	-
2	OLC	C	301	-	-	9/20/20/24	-
6	RET	C	318	1	-	0/13/30/31	0/1/1/1
2	OLC	E	301	-	-	15/23/23/24	-
2	OLC	C	306	-	-	7/17/17/24	-
2	OLC	B	304	-	-	4/15/15/24	-
3	LFA	C	312	-	-	7/9/9/17	-
3	LFA	B	302	-	-	6/17/17/17	-
2	OLC	C	308	-	-	9/15/15/24	-
3	LFA	D	308	-	-	4/5/5/17	-
2	OLC	D	303	-	-	4/17/17/24	-
3	LFA	D	309	-	-	8/14/14/17	-
6	RET	B	313	1	-	0/13/30/31	0/1/1/1
2	OLC	D	302	-	-	10/24/24/24	-
3	LFA	E	307	-	-	7/11/11/17	-
3	LFA	E	310	-	-	1/3/3/17	-
6	RET	E	315	1	-	0/13/30/31	0/1/1/1
3	LFA	A	311	-	-	9/17/17/17	-
3	LFA	D	307	-	-	8/17/17/17	-
2	OLC	C	307	-	-	4/14/14/24	-
2	OLC	C	302	-	-	11/19/19/24	-
2	OLC	E	303	-	-	5/14/14/24	-
3	LFA	B	307	-	-	2/2/2/17	-
5	BOG	B	312	-	-	7/11/31/31	0/1/1/1
2	OLC	A	303	-	-	6/14/14/24	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	309	OLC	O20-C1	4.61	1.46	1.33
2	C	303	OLC	O20-C1	4.56	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	303	OLC	O20-C1	4.56	1.46	1.33
2	D	303	OLC	O20-C1	4.51	1.46	1.33
2	C	307	OLC	O20-C1	4.43	1.46	1.33
2	A	302	OLC	O20-C1	4.42	1.46	1.33
2	B	303	OLC	O20-C1	4.39	1.46	1.33
2	C	308	OLC	O20-C1	4.37	1.46	1.33
2	E	302	OLC	O20-C1	4.36	1.46	1.33
2	D	305	OLC	O20-C1	4.35	1.46	1.33
2	B	305	OLC	O20-C1	4.34	1.46	1.33
2	C	302	OLC	O20-C1	4.33	1.46	1.33
2	B	301	OLC	O20-C1	4.32	1.46	1.33
2	D	302	OLC	O20-C1	4.32	1.46	1.33
2	C	301	OLC	O20-C1	4.29	1.45	1.33
2	E	301	OLC	O20-C1	4.29	1.45	1.33
2	C	306	OLC	O20-C1	4.28	1.45	1.33
2	E	304	OLC	O20-C1	4.23	1.45	1.33
2	A	303	OLC	O20-C1	4.22	1.45	1.33
2	B	304	OLC	O20-C1	4.20	1.45	1.33
2	D	304	OLC	O20-C1	4.19	1.45	1.33
2	C	305	OLC	O20-C1	4.18	1.45	1.33
2	A	301	OLC	O20-C1	4.17	1.45	1.33
5	A	310	BOG	O1-C1	2.07	1.43	1.40
5	E	312	BOG	O1-C1	2.02	1.43	1.40
5	C	317	BOG	O1-C1	2.01	1.43	1.40

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	312	RET	C18-C5-C6	-4.64	119.32	124.53
6	B	313	RET	C18-C5-C6	-4.44	119.54	124.53
6	D	315	RET	C18-C5-C6	-4.40	119.58	124.53
6	C	318	RET	C18-C5-C6	-4.35	119.64	124.53
6	E	315	RET	C18-C5-C6	-4.35	119.65	124.53
6	B	313	RET	C7-C8-C9	-3.30	121.25	126.23
6	D	315	RET	C7-C8-C9	-3.25	121.33	126.23
2	A	302	OLC	O20-C1-C2	3.20	121.94	111.91
6	C	318	RET	C7-C8-C9	-3.14	121.49	126.23
6	A	312	RET	C7-C8-C9	-3.09	121.57	126.23
2	C	309	OLC	O20-C1-C2	2.90	121.02	111.91
2	E	303	OLC	O20-C1-C2	2.90	121.01	111.91
6	E	315	RET	C7-C8-C9	-2.90	121.85	126.23
2	C	302	OLC	O20-C1-C2	2.89	120.96	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	OLC	O20-C1-C2	2.87	120.92	111.91
2	D	303	OLC	O20-C1-C2	2.86	120.88	111.91
2	A	303	OLC	O20-C1-C2	2.85	120.86	111.91
2	C	303	OLC	O20-C1-C2	2.84	120.82	111.91
2	C	307	OLC	O20-C1-C2	2.79	120.68	111.91
2	B	304	OLC	O20-C1-C2	2.79	120.68	111.91
2	E	302	OLC	O20-C1-C2	2.74	120.51	111.91
2	B	301	OLC	O20-C1-C2	2.72	120.44	111.91
2	C	305	OLC	O20-C1-C2	2.72	120.43	111.91
2	B	303	OLC	O20-C1-C2	2.70	120.39	111.91
2	E	301	OLC	O20-C1-C2	2.70	120.39	111.91
2	D	304	OLC	O20-C1-C2	2.70	120.38	111.91
2	C	306	OLC	O20-C1-C2	2.69	120.33	111.91
2	E	304	OLC	O20-C1-C2	2.67	120.30	111.91
2	B	305	OLC	O20-C1-C2	2.67	120.28	111.91
2	D	302	OLC	O20-C1-C2	2.65	120.23	111.91
2	A	301	OLC	O20-C1-C2	2.64	120.20	111.91
2	D	305	OLC	O20-C1-C2	2.62	120.13	111.91
6	D	315	RET	C11-C10-C9	-2.54	123.69	127.31
6	B	313	RET	C11-C10-C9	-2.53	123.70	127.31
2	C	308	OLC	O20-C1-C2	2.50	119.76	111.91
6	C	318	RET	C11-C10-C9	-2.48	123.78	127.31
2	E	304	OLC	O20-C1-O19	-2.37	117.61	123.59
6	A	312	RET	C11-C10-C9	-2.36	123.94	127.31
6	E	315	RET	C11-C10-C9	-2.24	124.11	127.31
6	B	313	RET	C10-C11-C12	-2.23	116.27	123.22
2	A	301	OLC	O20-C1-O19	-2.21	118.00	123.59
6	A	312	RET	C10-C11-C12	-2.20	116.34	123.22
2	C	305	OLC	O20-C1-O19	-2.20	118.04	123.59
6	B	313	RET	C19-C9-C8	2.16	121.48	118.08
2	A	302	OLC	O20-C1-O19	-2.16	118.15	123.59
6	D	315	RET	C10-C11-C12	-2.15	116.50	123.22
2	A	303	OLC	O20-C1-O19	-2.14	118.19	123.59
2	B	304	OLC	O20-C1-O19	-2.10	118.30	123.59
2	C	302	OLC	O20-C1-O19	-2.05	118.43	123.59
6	E	315	RET	C10-C11-C12	-2.03	116.87	123.22
2	D	304	OLC	O20-C1-O19	-2.03	118.47	123.59

There are no chirality outliers.

All (347) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	303	OLC	C21-C22-C24-O25
5	A	310	BOG	C2'-C1'-O1-C1
2	C	309	OLC	O20-C21-C22-O23
5	E	312	BOG	C2-C1-O1-C1'
5	E	312	BOG	O5-C1-O1-C1'
5	E	312	BOG	C2'-C1'-O1-C1
2	C	305	OLC	C2-C1-O20-C21
2	E	302	OLC	C21-C22-C24-O25
2	A	301	OLC	C21-C22-C24-O25
2	A	301	OLC	O23-C22-C24-O25
2	D	304	OLC	C21-C22-C24-O25
2	B	303	OLC	C10-C11-C12-C13
3	C	314	LFA	C17-C18-C19-C20
2	E	304	OLC	O20-C21-C22-C24
2	E	304	OLC	O20-C21-C22-O23
2	B	305	OLC	O20-C21-C22-C24
2	B	305	OLC	O20-C21-C22-O23
2	C	301	OLC	C21-C22-C24-O25
2	E	301	OLC	O20-C21-C22-C24
2	E	303	OLC	O20-C21-C22-O23
2	C	305	OLC	O19-C1-O20-C21
2	A	303	OLC	O19-C1-O20-C21
5	E	312	BOG	O5-C5-C6-O6
2	D	305	OLC	O19-C1-O20-C21
2	E	302	OLC	C2-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
2	E	304	OLC	O19-C1-O20-C21
2	D	305	OLC	C2-C1-O20-C21
2	E	304	OLC	C2-C1-O20-C21
2	A	303	OLC	C2-C1-O20-C21
2	B	303	OLC	C2-C1-O20-C21
2	C	308	OLC	C2-C1-O20-C21
2	B	304	OLC	C2-C1-O20-C21
2	E	302	OLC	O19-C1-O20-C21
2	B	301	OLC	O19-C1-O20-C21
2	C	305	OLC	O20-C21-C22-O23
2	C	308	OLC	O20-C21-C22-O23
2	E	301	OLC	O20-C21-C22-O23
5	E	312	BOG	C4-C5-C6-O6
2	C	308	OLC	O19-C1-O20-C21
2	B	304	OLC	O19-C1-O20-C21
2	D	303	OLC	C2-C1-O20-C21
2	B	303	OLC	O19-C1-O20-C21

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

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Mol	Chain	Res	Type	Atoms
3	E	307	LFA	C13-C14-C15-C16
2	D	305	OLC	C13-C14-C15-C16
2	D	305	OLC	C12-C13-C14-C15
3	D	301	LFA	C9-C10-C11-C12
2	D	305	OLC	C21-C22-C24-O25
2	C	307	OLC	C21-C22-C24-O25
2	E	304	OLC	C21-C22-C24-O25
2	D	305	OLC	O20-C21-C22-O23
3	C	313	LFA	C4-C5-C6-C7
2	C	308	OLC	C3-C4-C5-C6
3	D	309	LFA	C5-C6-C7-C8
2	E	304	OLC	C6-C7-C8-C9
2	E	301	OLC	C6-C7-C8-C9
3	D	306	LFA	C9-C10-C11-C12
2	C	302	OLC	C4-C5-C6-C7
2	C	302	OLC	C3-C4-C5-C6
3	D	311	LFA	C16-C17-C18-C19
3	D	307	LFA	C14-C15-C16-C17
3	C	304	LFA	C15-C16-C17-C18
2	C	305	OLC	C4-C5-C6-C7
3	C	311	LFA	C16-C17-C18-C19
3	A	311	LFA	C13-C14-C15-C16
3	D	301	LFA	C10-C11-C12-C13
3	D	301	LFA	C12-C13-C14-C15
3	D	310	LFA	C15-C16-C17-C18
3	C	304	LFA	C16-C17-C18-C19
2	D	303	OLC	C5-C6-C7-C8
3	C	304	LFA	C9-C10-C11-C12
2	D	305	OLC	O23-C22-C24-O25
2	E	302	OLC	O23-C22-C24-O25
2	D	304	OLC	O23-C22-C24-O25
2	C	307	OLC	O23-C22-C24-O25
2	E	304	OLC	O23-C22-C24-O25
2	C	301	OLC	O23-C22-C24-O25
2	B	301	OLC	C10-C11-C12-C13
2	C	309	OLC	O19-C1-O20-C21
2	E	301	OLC	O19-C1-O20-C21
3	C	311	LFA	C15-C16-C17-C18
3	D	306	LFA	C4-C5-C6-C7
3	D	307	LFA	C11-C12-C13-C14
3	A	311	LFA	C16-C17-C18-C19
5	E	312	BOG	O1-C1'-C2'-C3'

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

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Mol	Chain	Res	Type	Atoms
3	B	308	LFA	C7-C8-C9-C10
2	E	304	OLC	C12-C13-C14-C15
2	C	303	OLC	O23-C22-C24-O25
2	A	301	OLC	C10-C11-C12-C13
3	E	306	LFA	C17-C18-C19-C20
3	D	306	LFA	C11-C10-C9-C8
2	E	302	OLC	C12-C13-C14-C15
3	D	309	LFA	C14-C15-C16-C17
3	B	307	LFA	C1-C2-C3-C4
3	E	314	LFA	C4-C5-C6-C7
3	A	311	LFA	C12-C13-C14-C15
3	D	307	LFA	C4-C5-C6-C7
3	C	304	LFA	C2-C3-C4-C5
3	D	307	LFA	C1-C2-C3-C4
2	E	303	OLC	C5-C6-C7-C8
2	C	309	OLC	C4-C5-C6-C7
3	A	304	LFA	C1-C2-C3-C4
2	E	302	OLC	C11-C12-C13-C14
3	D	309	LFA	C2-C3-C4-C5
3	A	311	LFA	C7-C8-C9-C10
2	C	309	OLC	C3-C4-C5-C6
2	A	303	OLC	C5-C6-C7-C8
3	D	308	LFA	C1-C2-C3-C4
3	C	311	LFA	C17-C18-C19-C20
2	C	302	OLC	C2-C1-O20-C21
3	A	305	LFA	C16-C17-C18-C19
2	C	305	OLC	C5-C6-C7-C8
2	C	301	OLC	C4-C5-C6-C7
2	C	301	OLC	C2-C1-O20-C21
5	A	310	BOG	O1-C1'-C2'-C3'
2	E	304	OLC	C11-C12-C13-C14
5	B	312	BOG	C3'-C4'-C5'-C6'
3	B	302	LFA	C6-C7-C8-C9
3	D	307	LFA	C3-C4-C5-C6
2	C	306	OLC	C2-C3-C4-C5
3	C	311	LFA	C13-C14-C15-C16
3	D	307	LFA	C10-C11-C12-C13
3	E	307	LFA	C16-C17-C18-C19
2	E	303	OLC	O20-C21-C22-C24
5	B	312	BOG	C4-C5-C6-O6
2	E	301	OLC	C12-C13-C14-C15
2	E	304	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	D	306	LFA	C14-C15-C16-C17
3	B	310	LFA	C1-C2-C3-C4
3	A	308	LFA	C3-C4-C5-C6
2	D	304	OLC	C4-C5-C6-C7
2	C	301	OLC	C11-C12-C13-C14
2	B	301	OLC	C15-C16-C17-C18
2	B	301	OLC	C6-C7-C8-C9
2	C	303	OLC	C3-C4-C5-C6
2	E	301	OLC	C5-C6-C7-C8
2	D	302	OLC	C3-C4-C5-C6
3	D	310	LFA	C14-C15-C16-C17
5	B	312	BOG	O5-C5-C6-O6
5	A	310	BOG	C5'-C6'-C7'-C8'
3	D	301	LFA	C15-C16-C17-C18
3	D	309	LFA	C7-C8-C9-C10
2	D	302	OLC	C5-C6-C7-C8
3	C	315	LFA	C1-C2-C3-C4
2	D	305	OLC	C4-C5-C6-C7
3	C	315	LFA	C3-C4-C5-C6
2	A	303	OLC	C3-C4-C5-C6
3	D	307	LFA	C12-C13-C14-C15
2	E	302	OLC	C10-C11-C12-C13
2	C	301	OLC	C10-C11-C12-C13
3	B	302	LFA	C9-C10-C11-C12
2	C	302	OLC	O19-C1-O20-C21
2	C	301	OLC	O19-C1-O20-C21
3	C	312	LFA	C15-C16-C17-C18
2	C	309	OLC	O23-C22-C24-O25
2	E	301	OLC	O23-C22-C24-O25
2	A	301	OLC	C6-C7-C8-C9
3	C	312	LFA	C13-C14-C15-C16
3	E	307	LFA	C7-C8-C9-C10
3	A	308	LFA	C1-C2-C3-C4
2	B	304	OLC	C21-C22-C24-O25
3	A	311	LFA	C14-C15-C16-C17
2	C	303	OLC	O20-C21-C22-O23
2	D	303	OLC	C1-C2-C3-C4
3	C	304	LFA	C1-C2-C3-C4
3	A	311	LFA	C11-C12-C13-C14
2	E	302	OLC	C14-C15-C16-C17
3	B	302	LFA	C11-C12-C13-C14
2	B	303	OLC	C4-C5-C6-C7

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

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

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Mol	Chain	Res	Type	Atoms
3	E	309	LFA	C17-C18-C19-C20
2	D	304	OLC	O19-C1-C2-C3
5	B	312	BOG	C2'-C3'-C4'-C5'
2	C	308	OLC	C2-C3-C4-C5
2	D	302	OLC	O20-C1-C2-C3
2	C	302	OLC	C9-C10-C11-C12
3	D	306	LFA	C7-C8-C9-C10
3	C	304	LFA	C12-C13-C14-C15
2	C	307	OLC	C2-C3-C4-C5
3	B	308	LFA	C4-C5-C6-C7

There are no ring outliers.

29 monomers are involved in 58 short contacts:

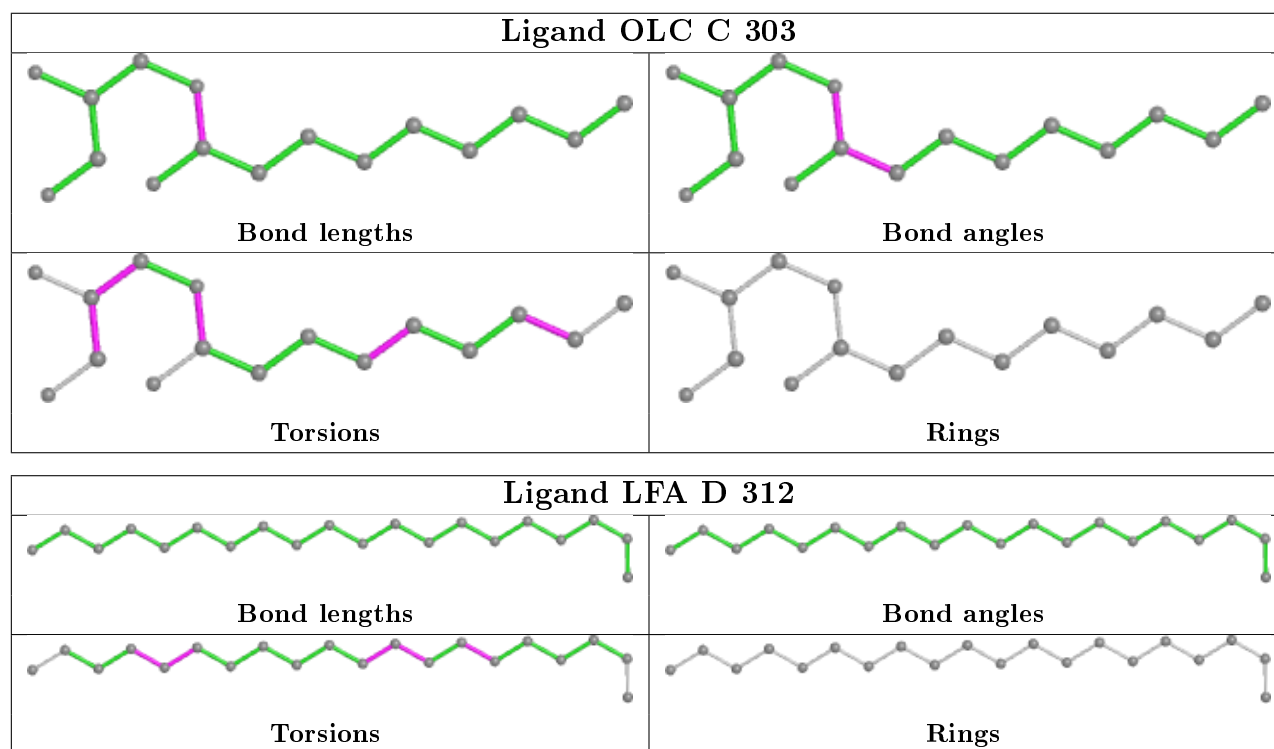
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	303	OLC	1	0
2	D	305	OLC	4	0
2	B	301	OLC	1	0
5	A	310	BOG	2	0
3	B	310	LFA	1	0
3	C	304	LFA	2	0
5	C	317	BOG	1	0
3	E	308	LFA	1	0
3	E	314	LFA	1	0
6	A	312	RET	5	0
3	B	306	LFA	2	0
2	C	305	OLC	2	0
3	C	310	LFA	3	0
6	D	315	RET	5	0
2	B	305	OLC	3	0
5	D	314	BOG	4	0
2	E	304	OLC	1	0
3	D	301	LFA	1	0
6	C	318	RET	5	0
2	C	306	OLC	2	0
2	C	308	OLC	2	0
6	B	313	RET	4	0
2	D	302	OLC	2	0
3	E	307	LFA	1	0
3	E	310	LFA	1	0
6	E	315	RET	6	0
2	C	307	OLC	1	0

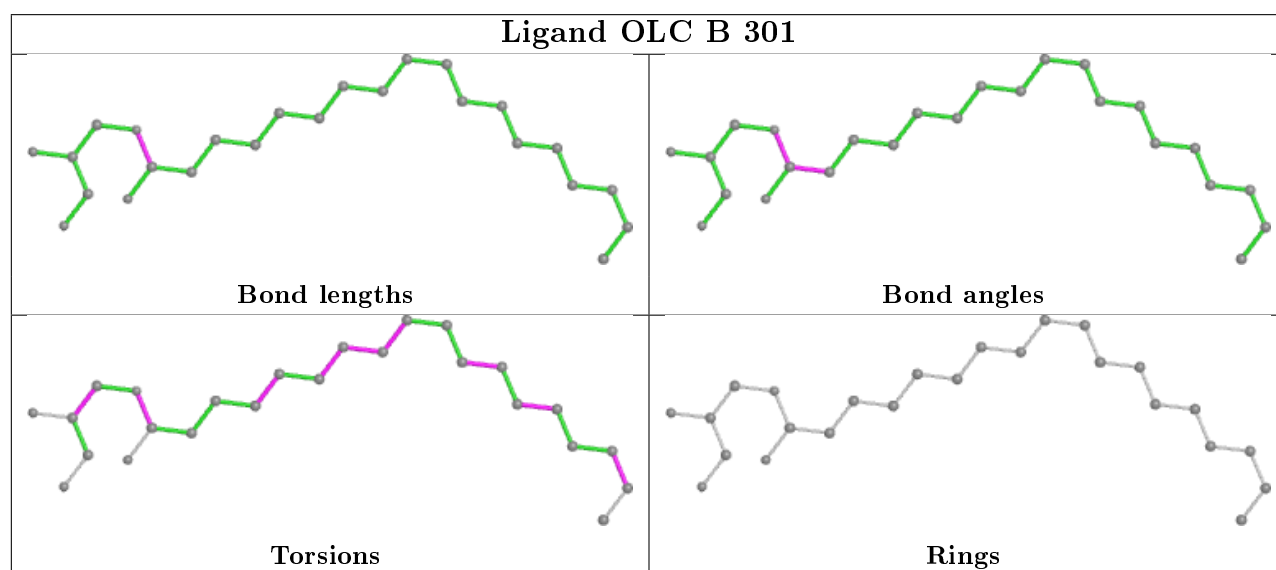
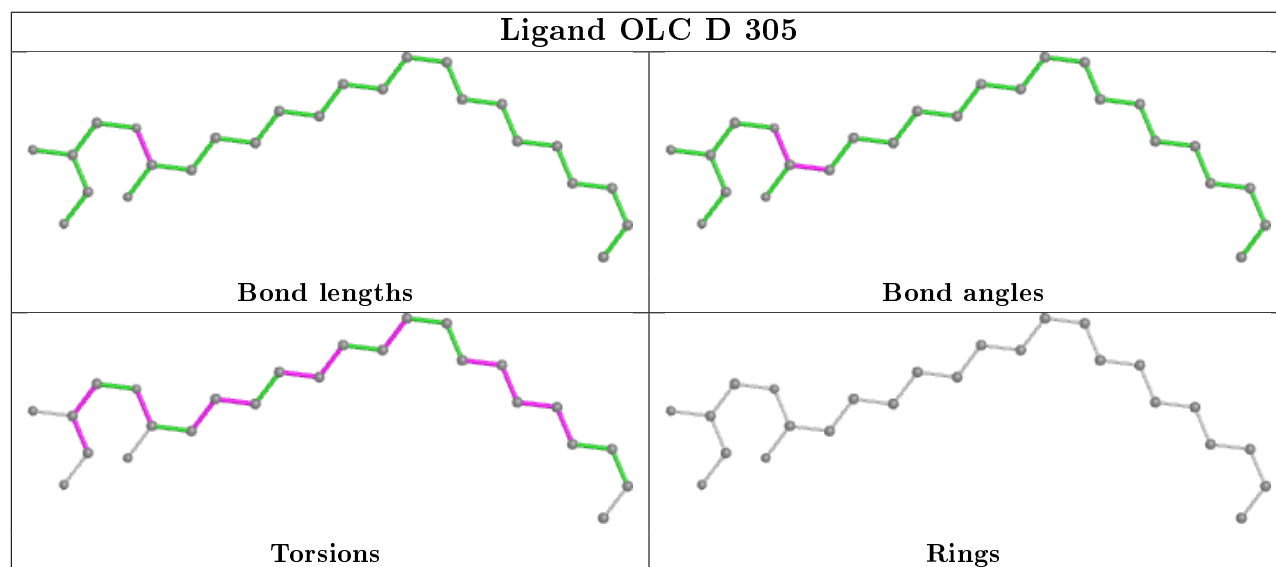
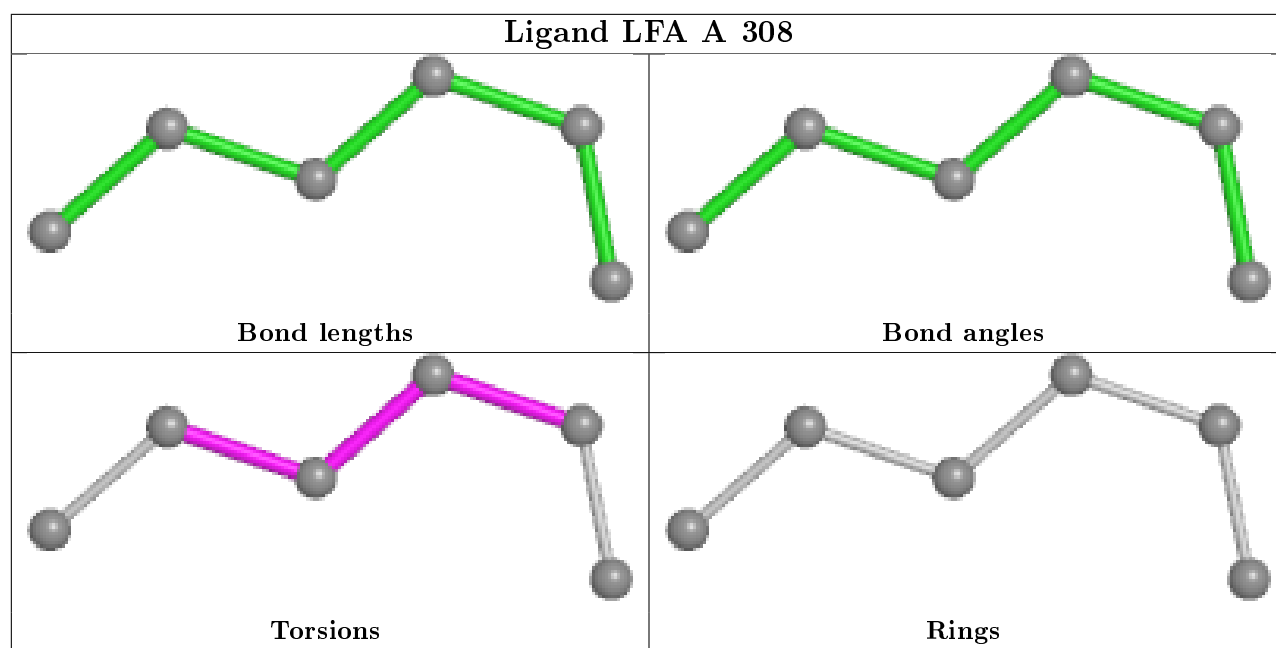
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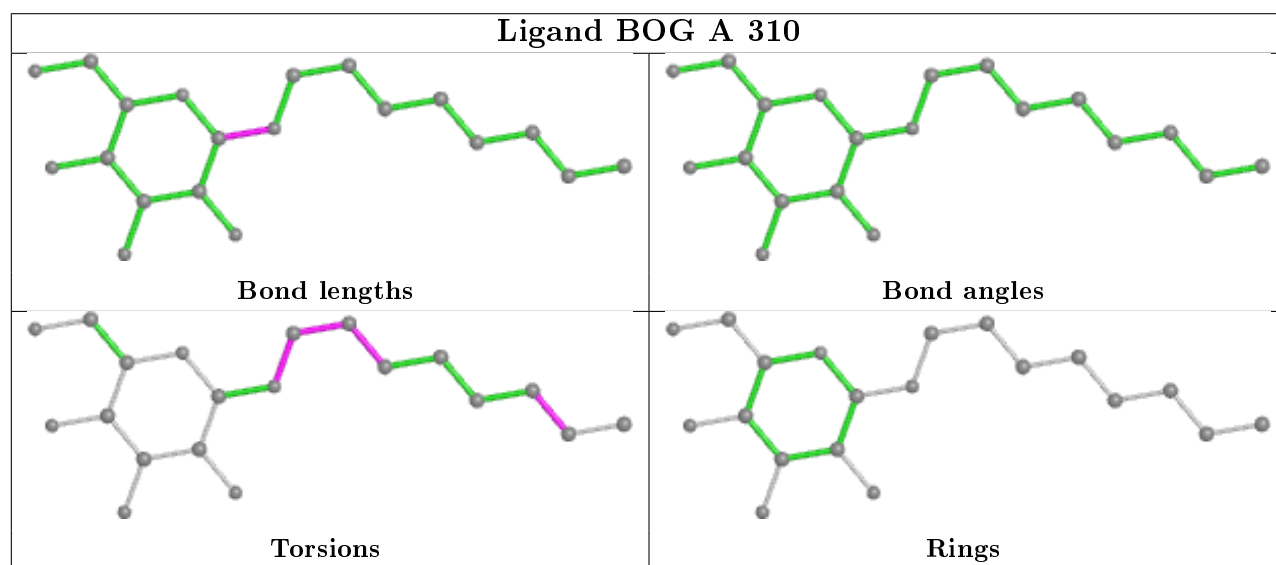
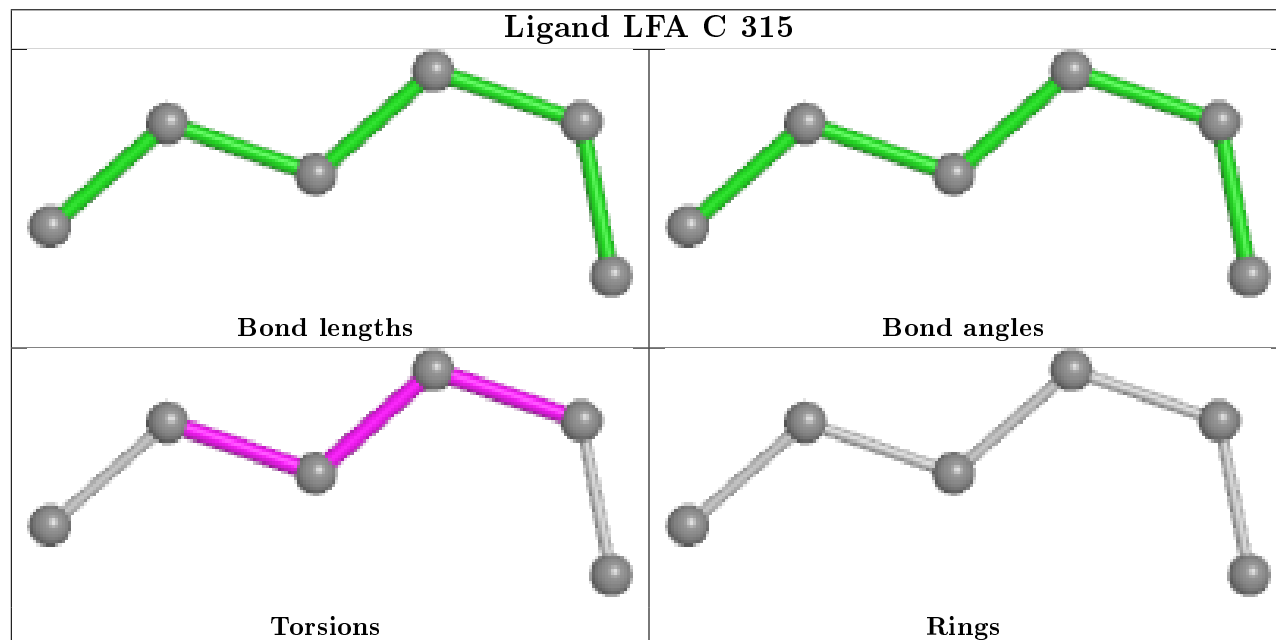
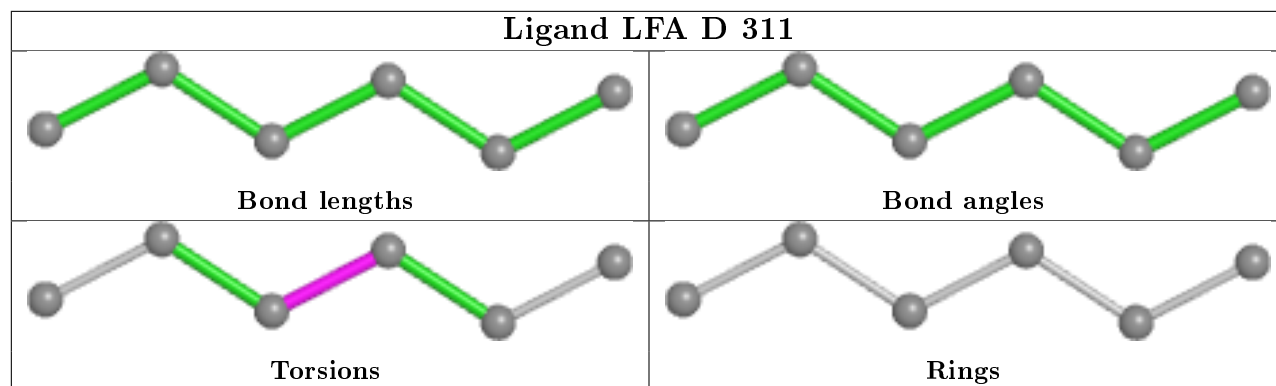
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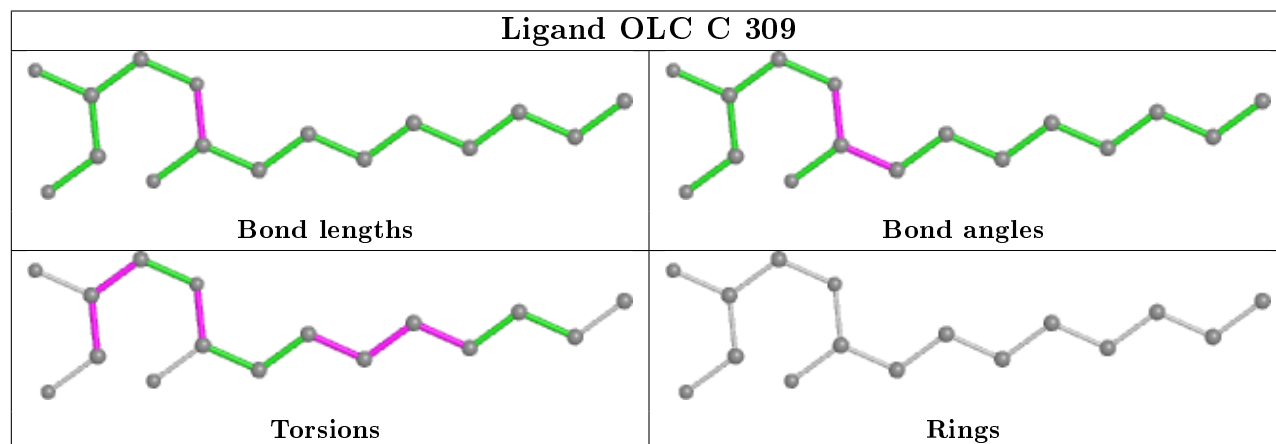
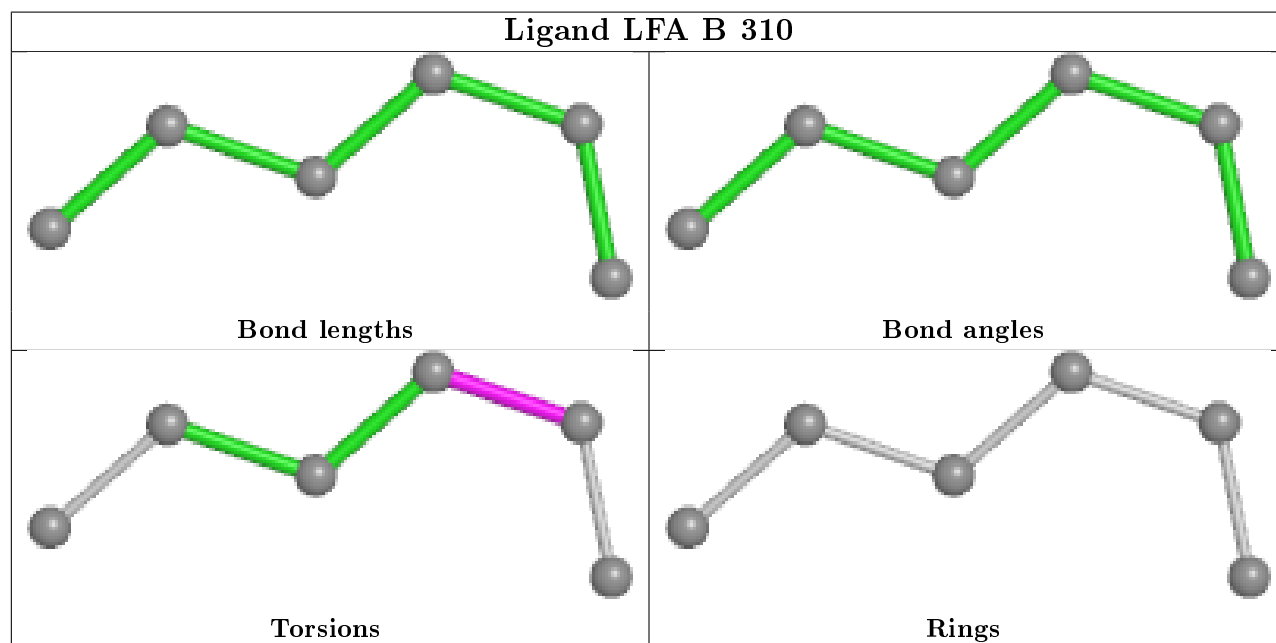
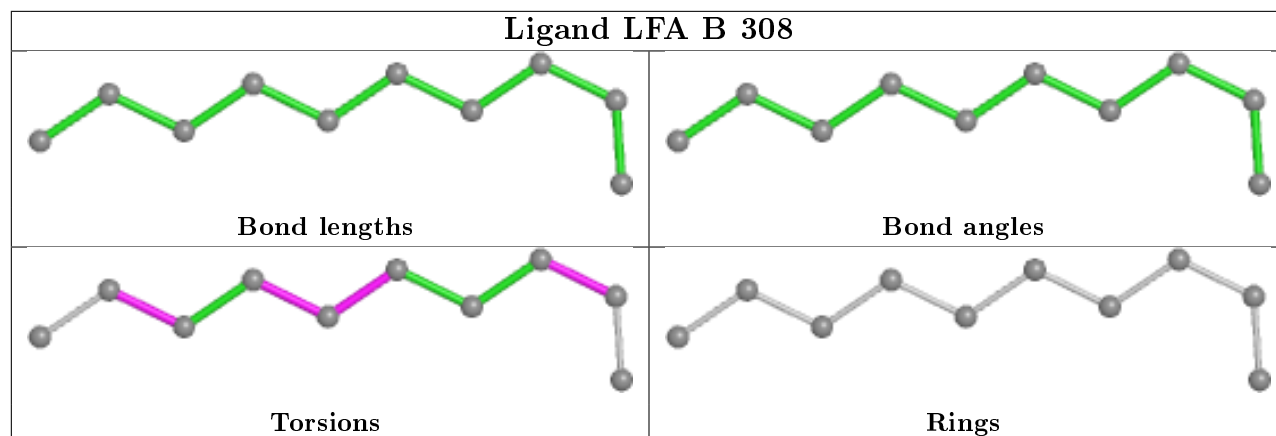
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302	OLC	1	0
5	B	312	BOG	2	0

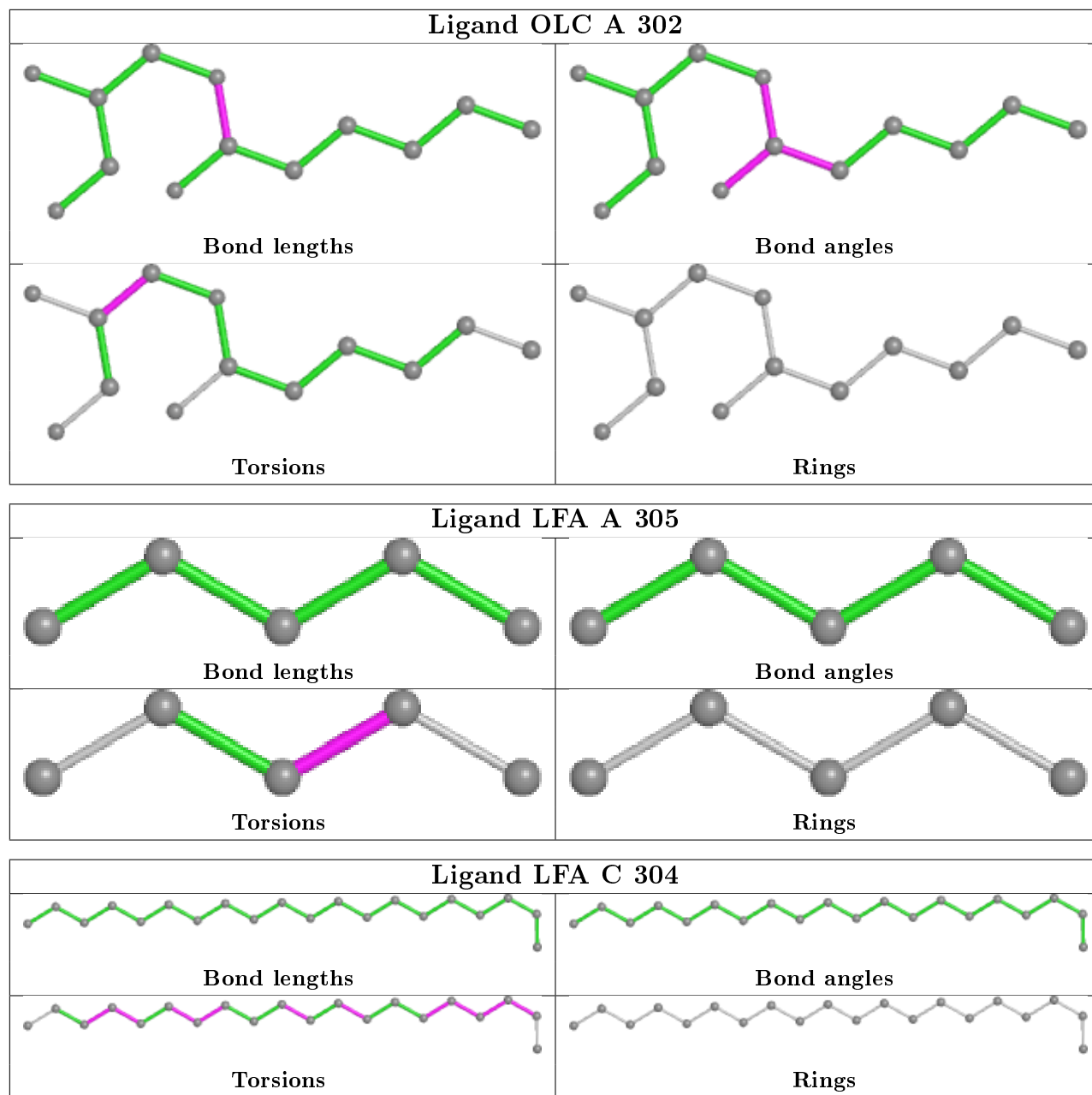
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

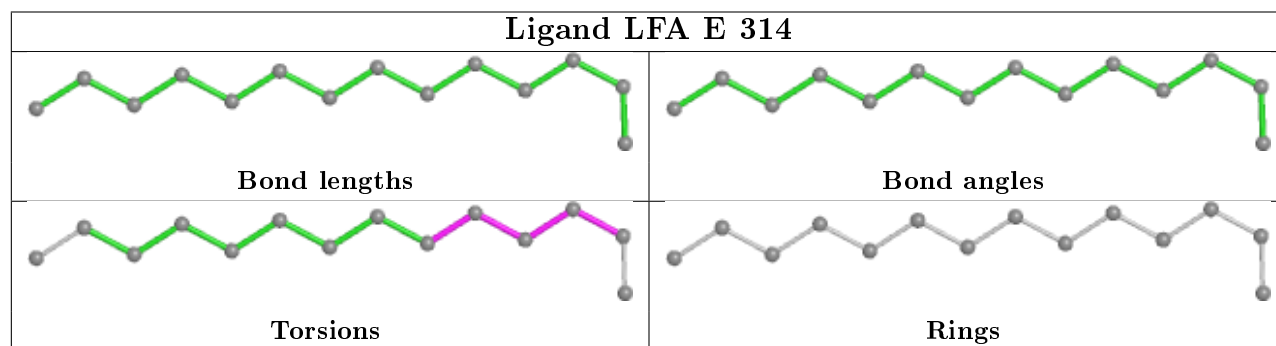
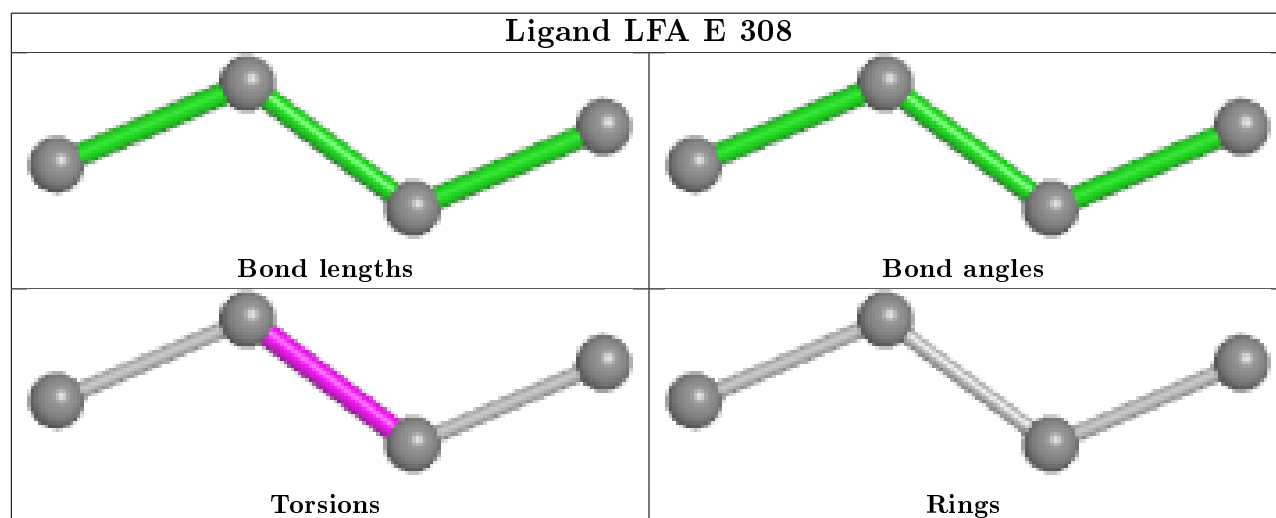
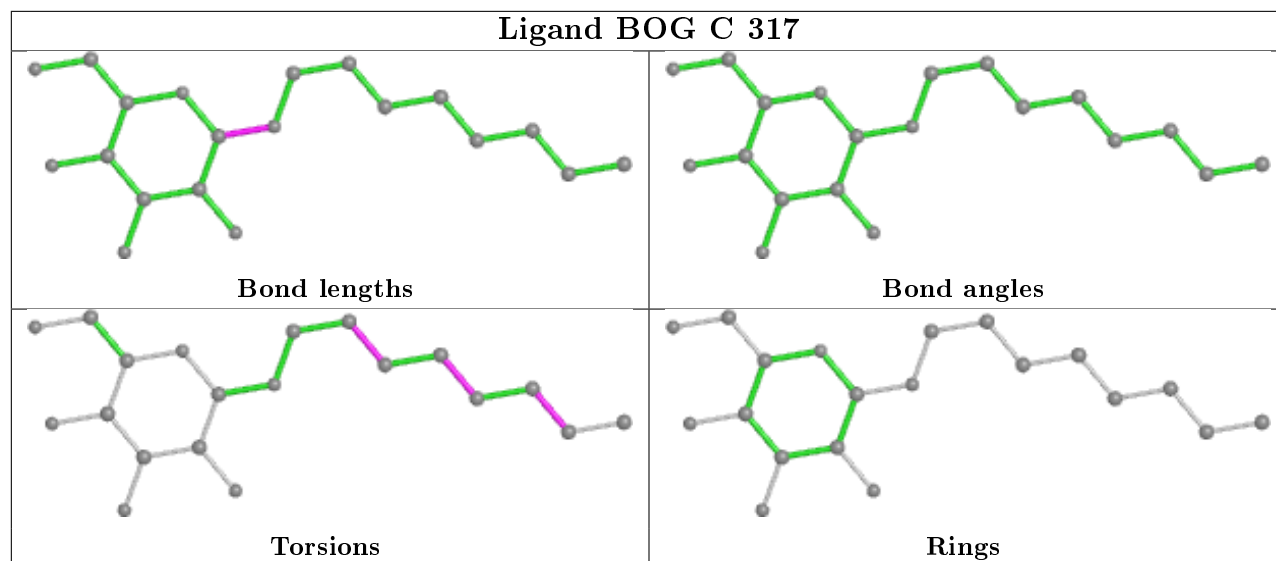


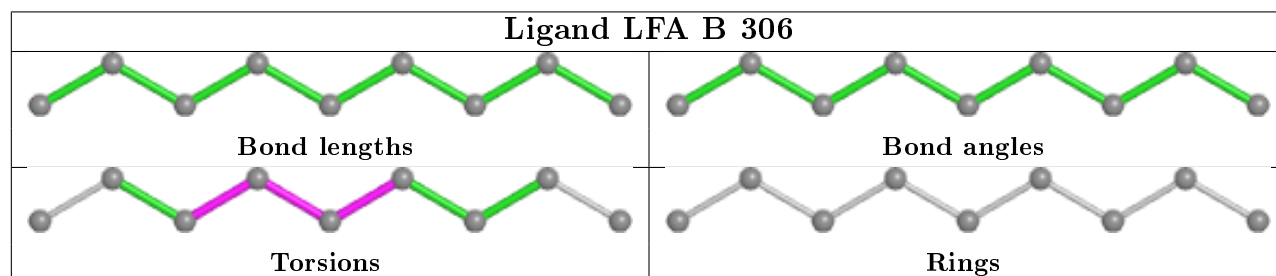
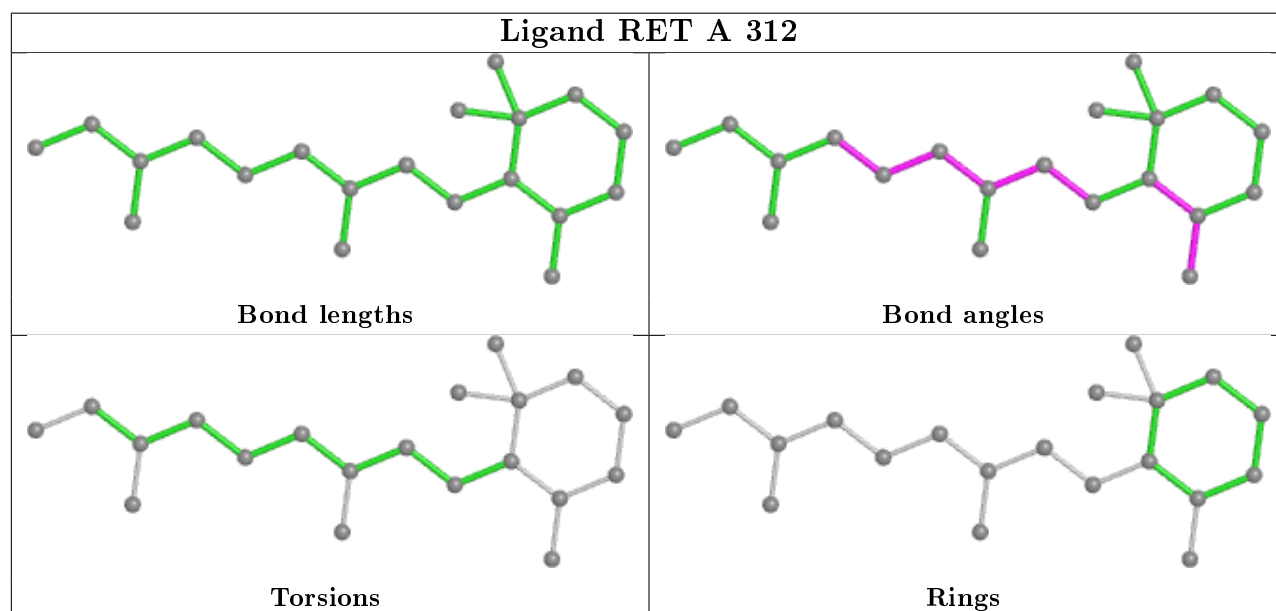
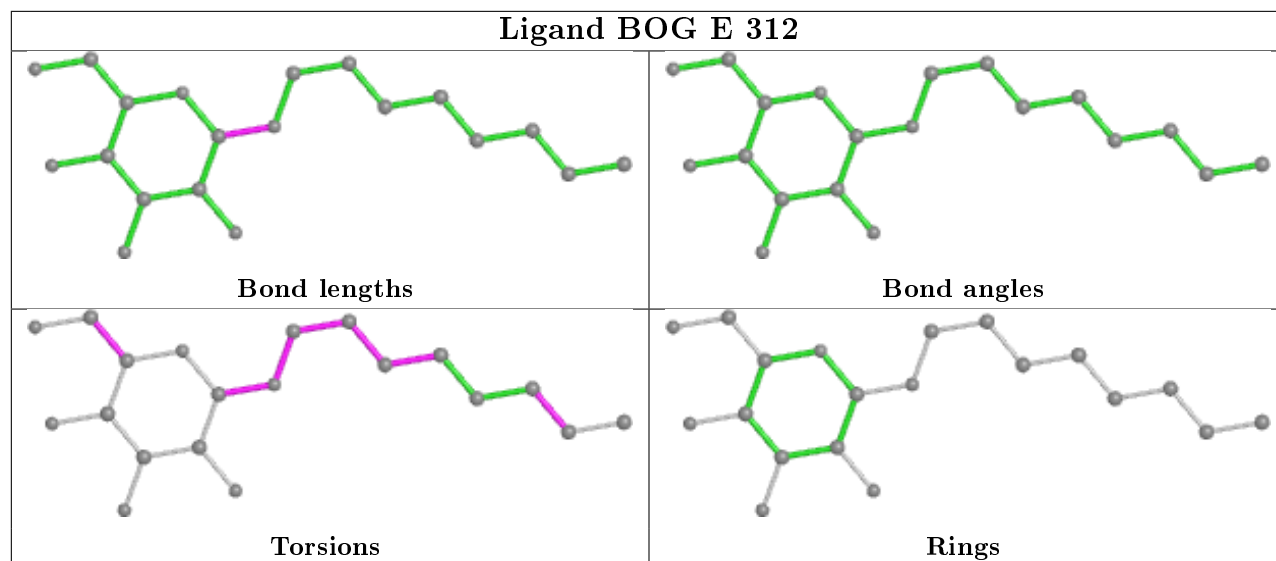




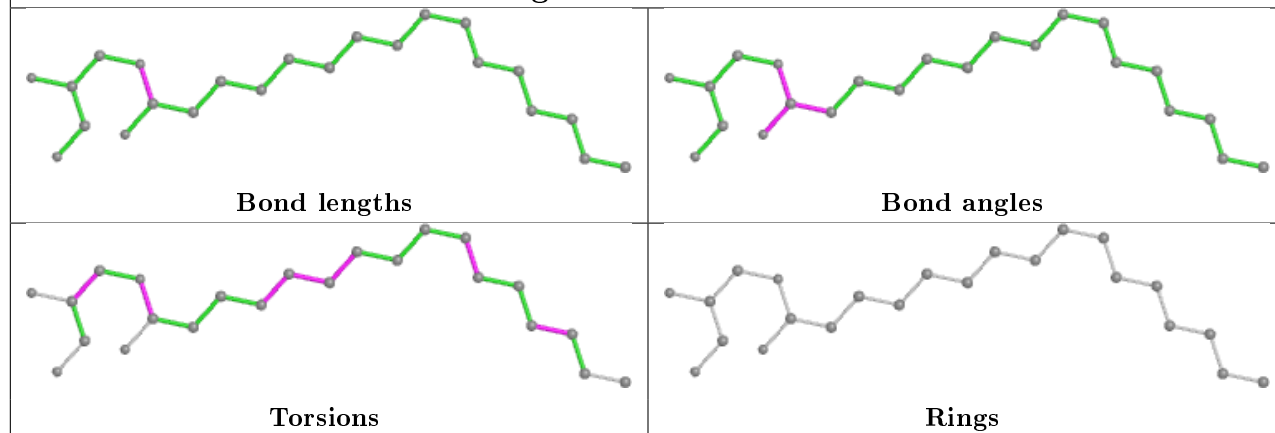




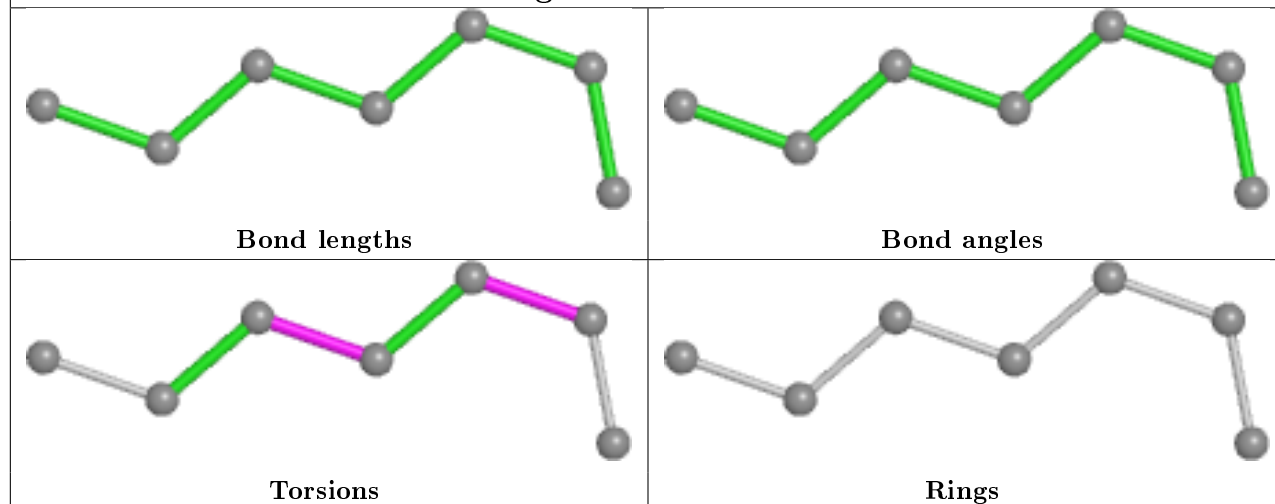




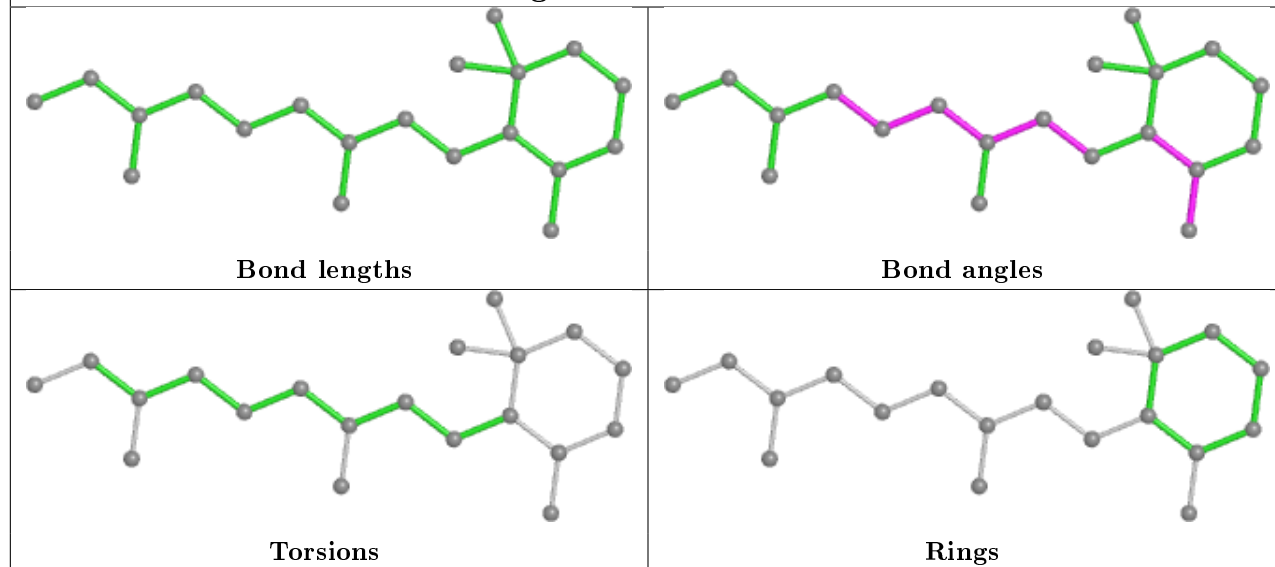
## Ligand OLC C 305

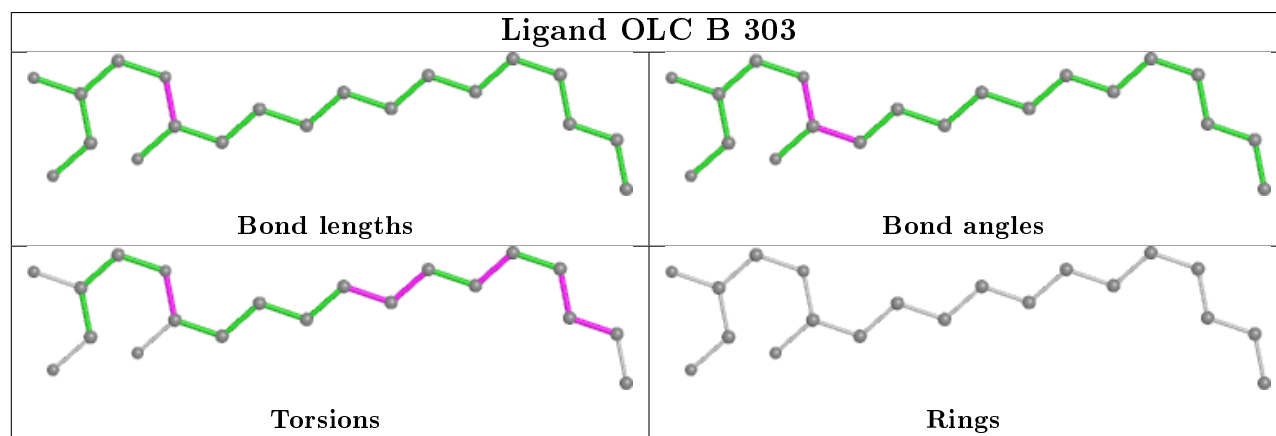
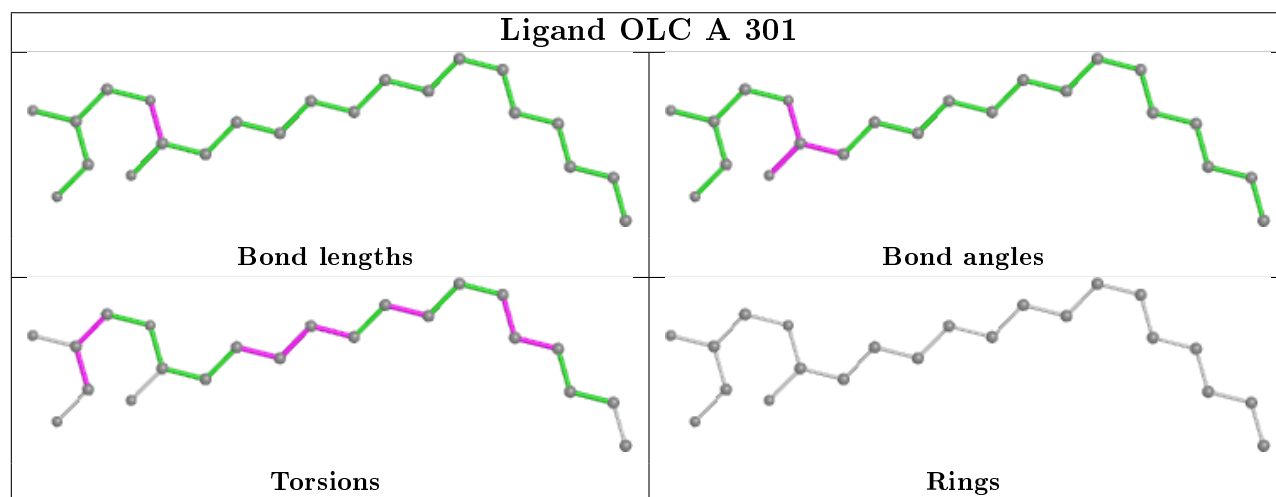
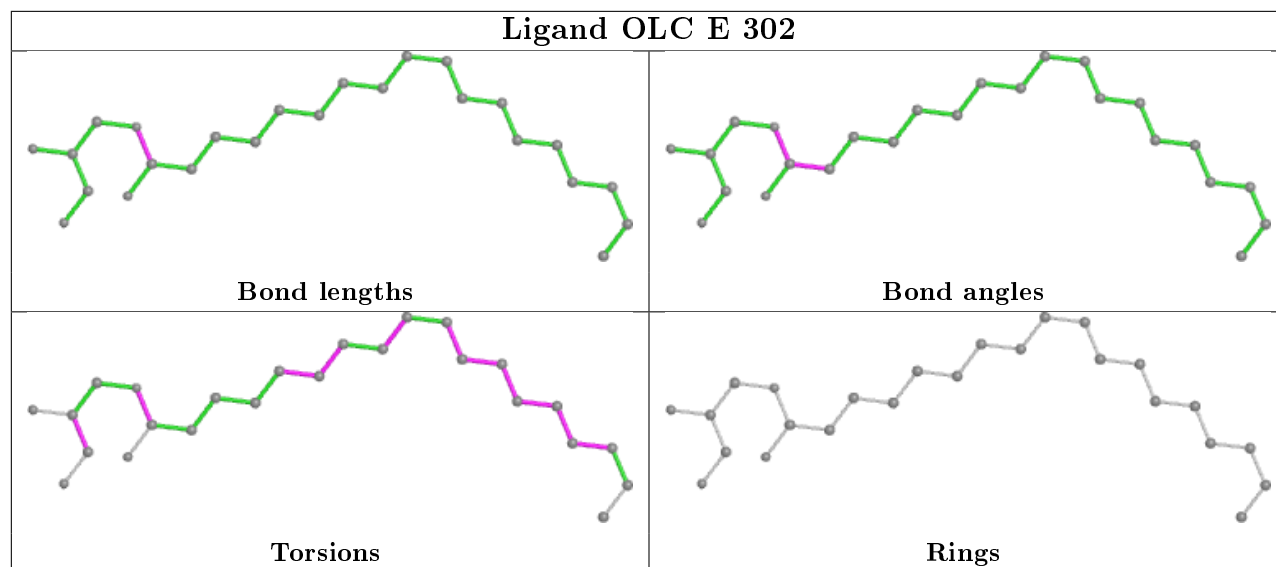


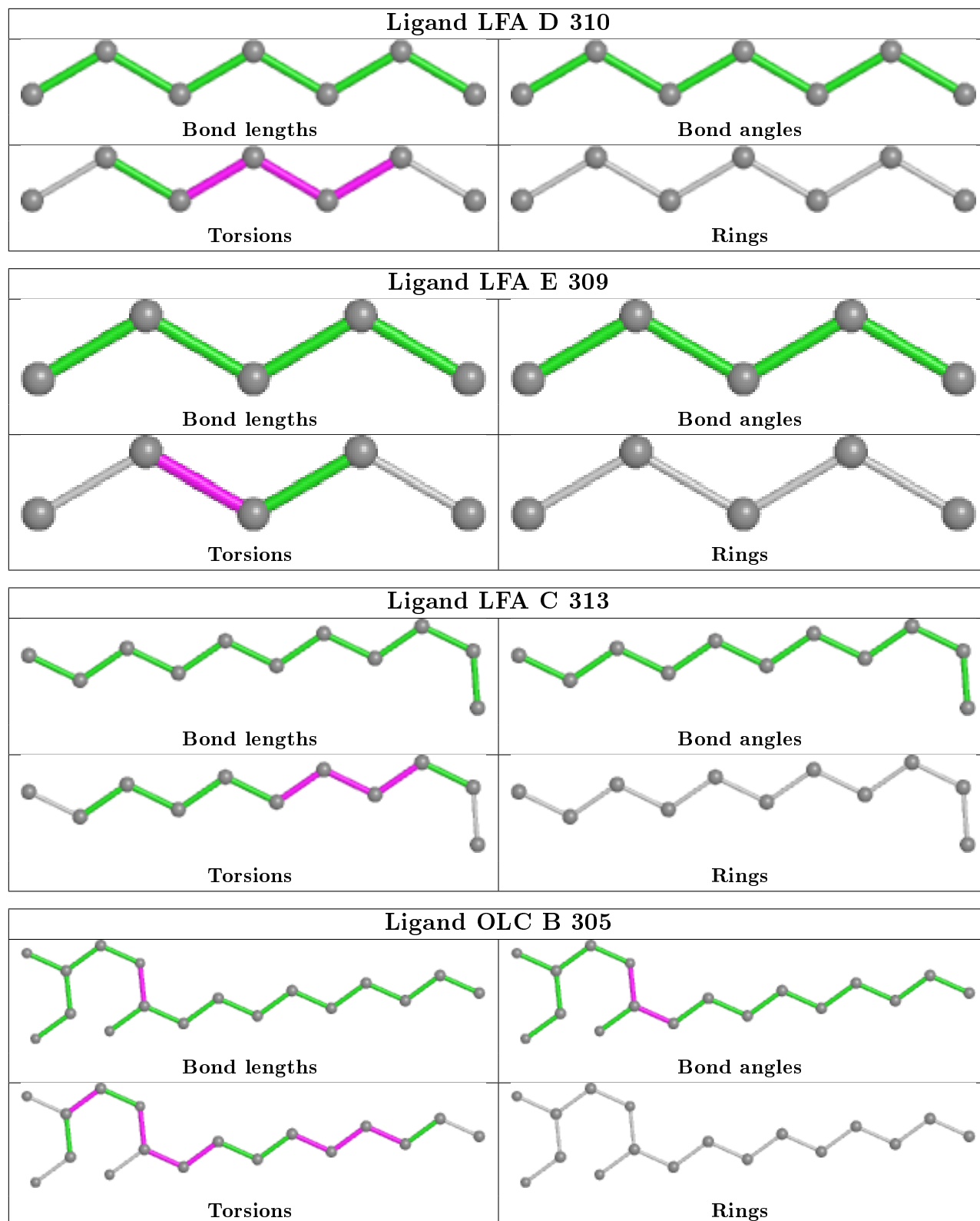
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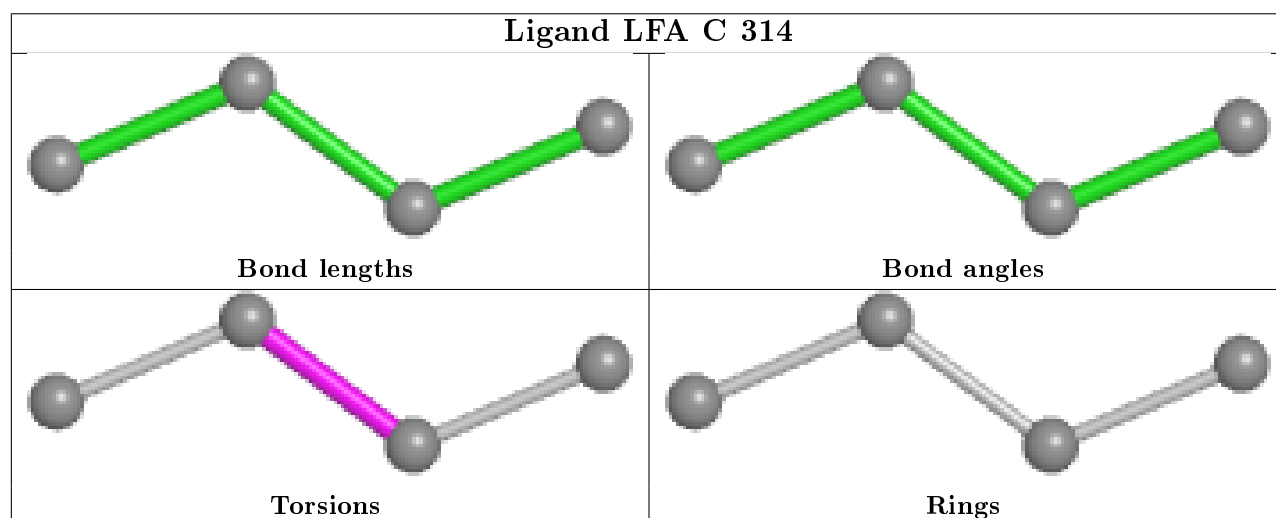
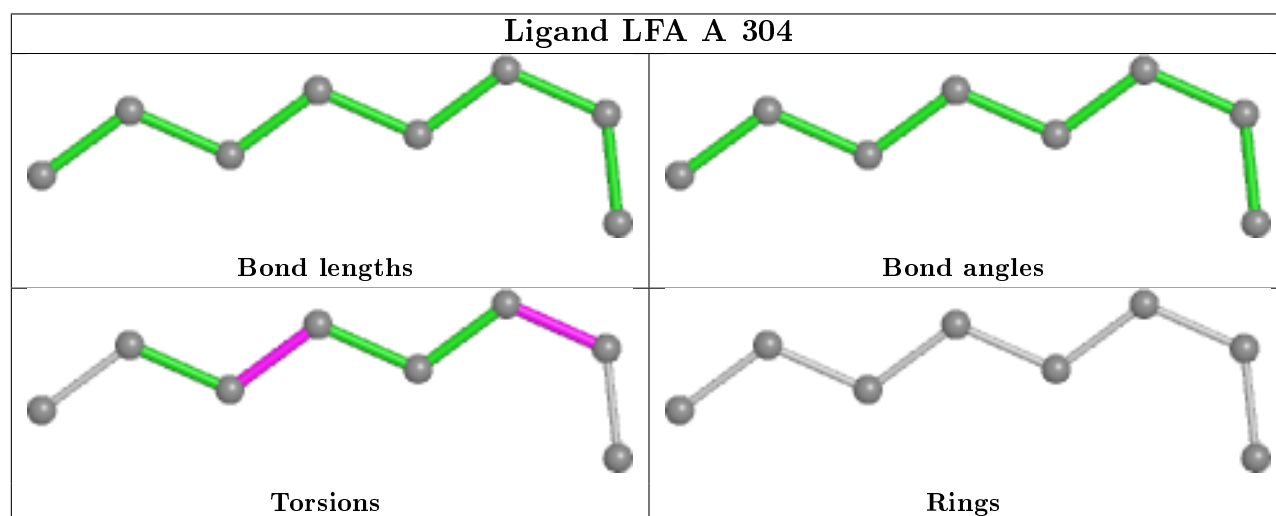
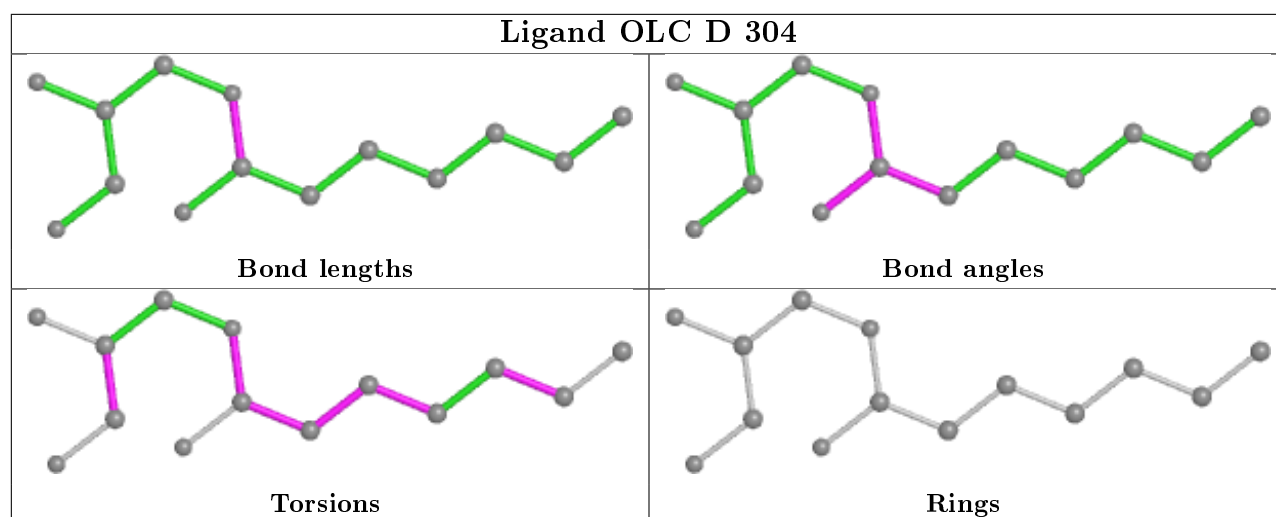


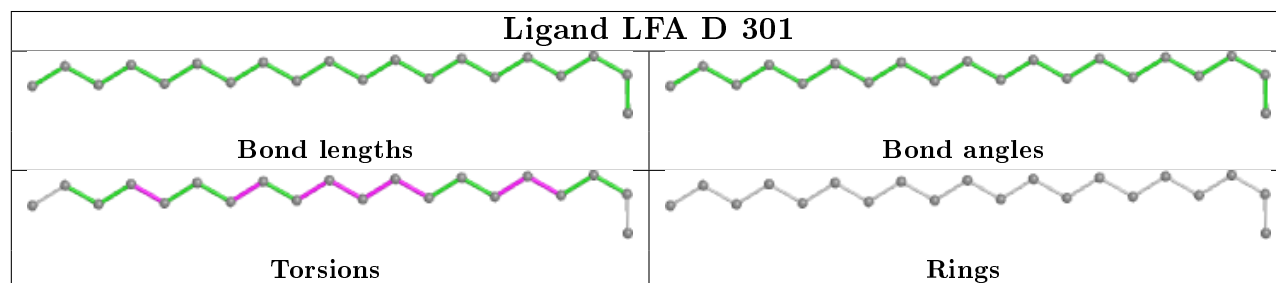
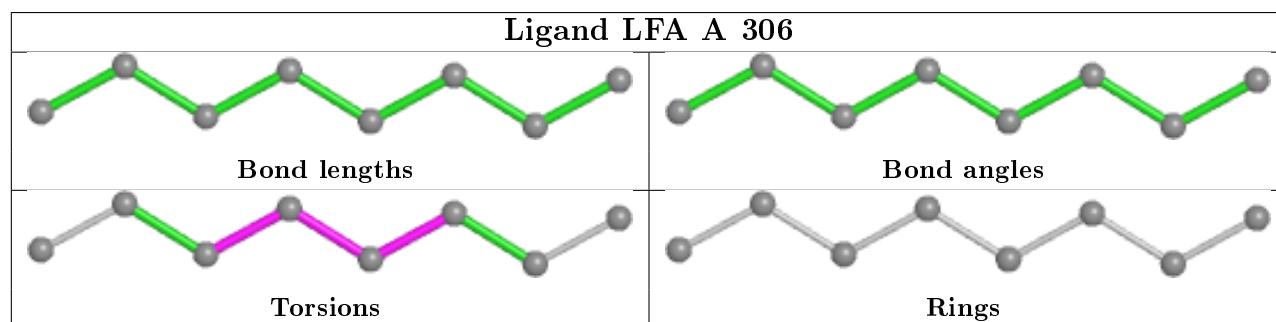
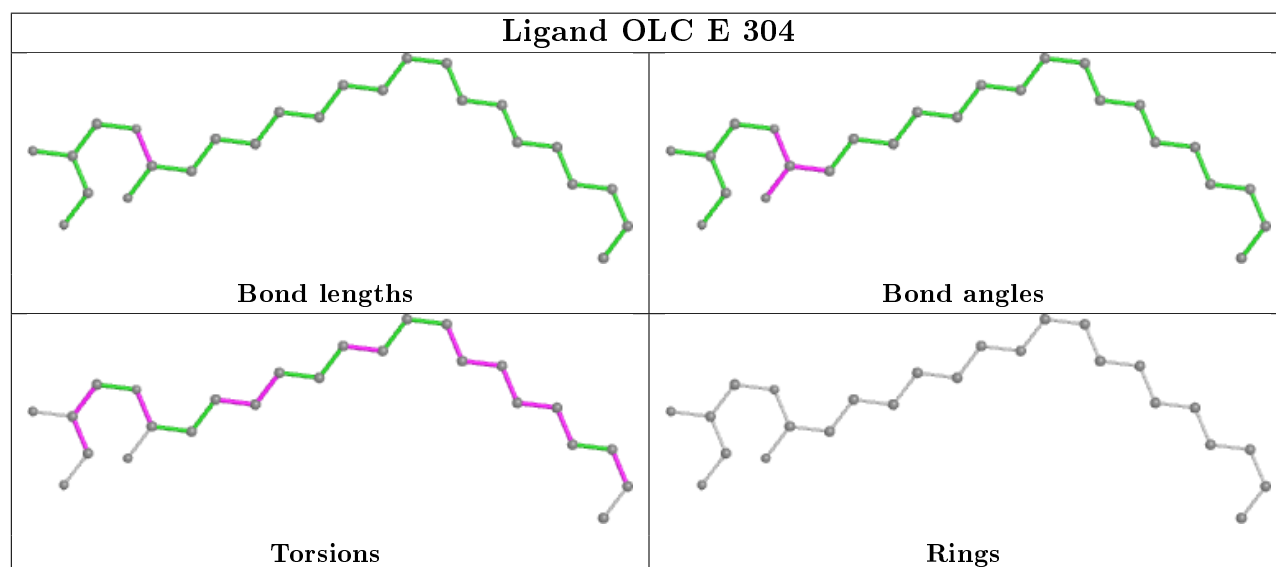
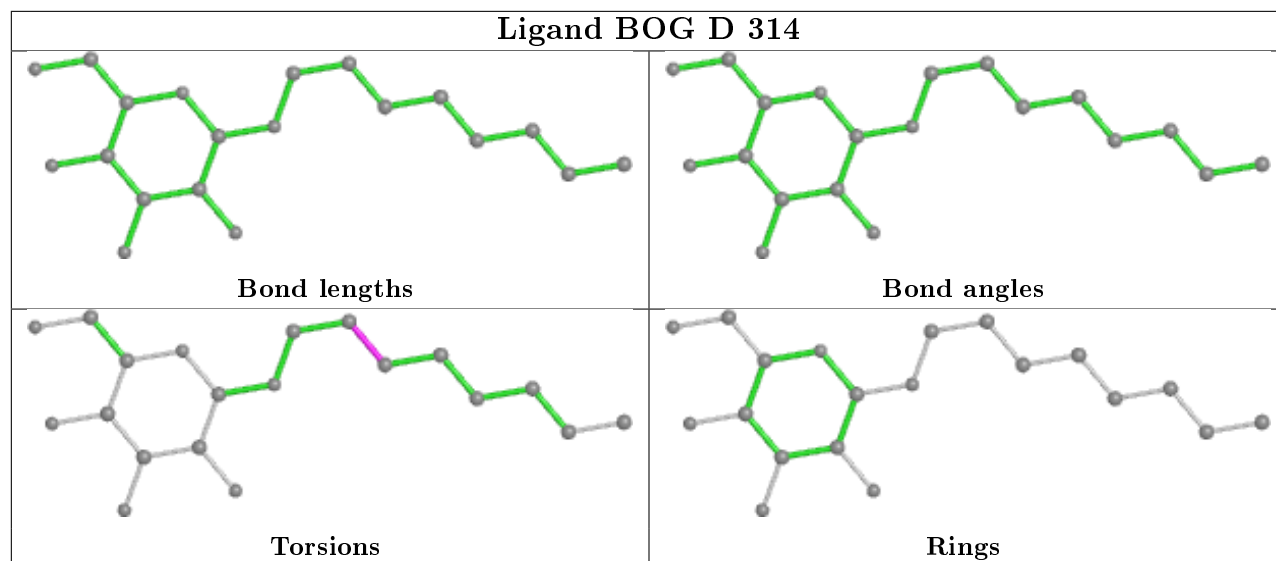
## Ligand RET D 315

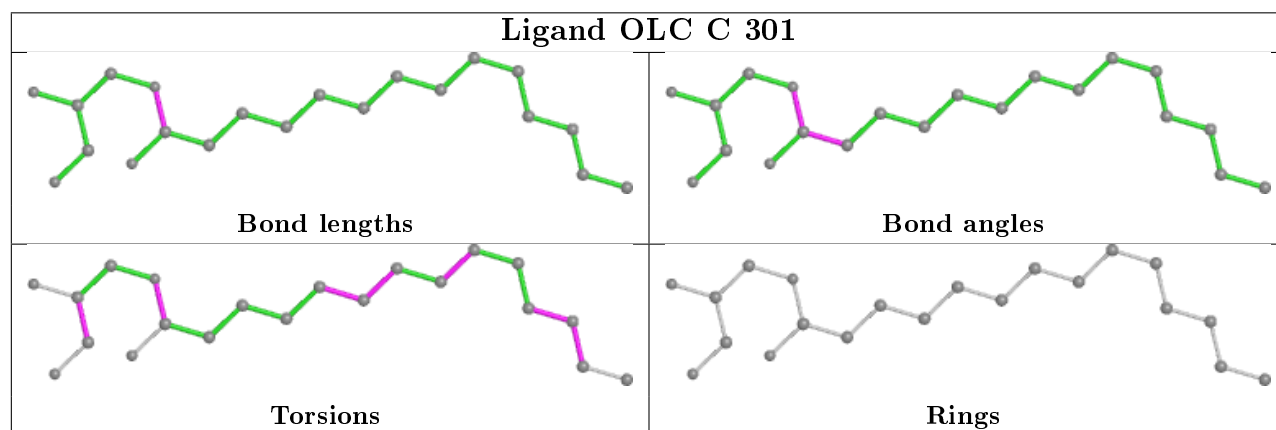
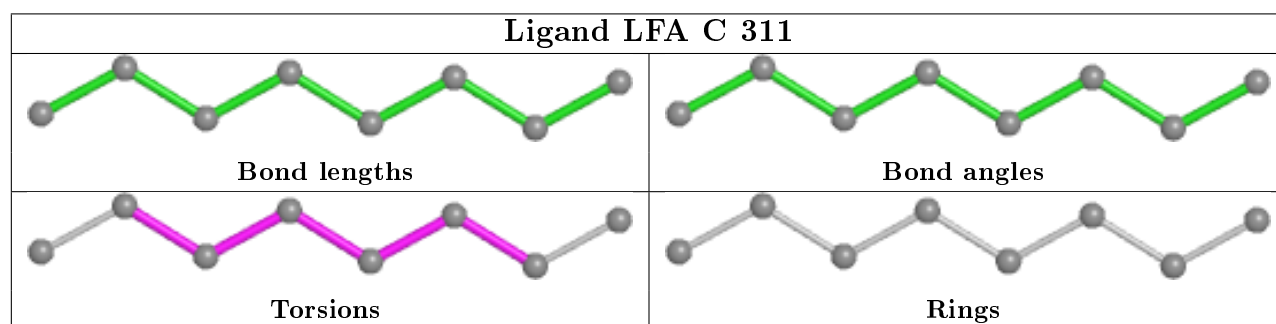
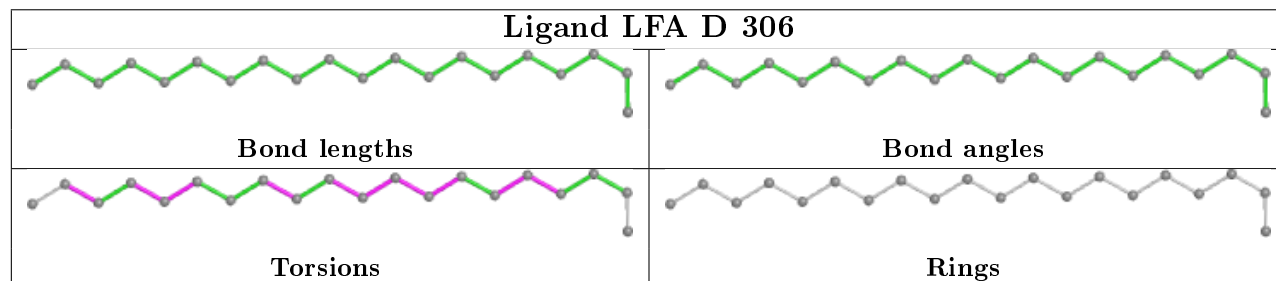
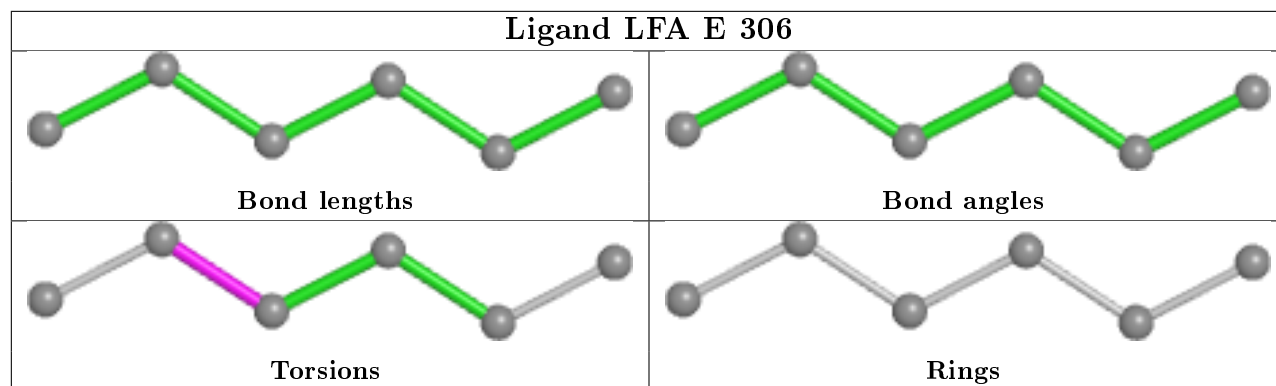


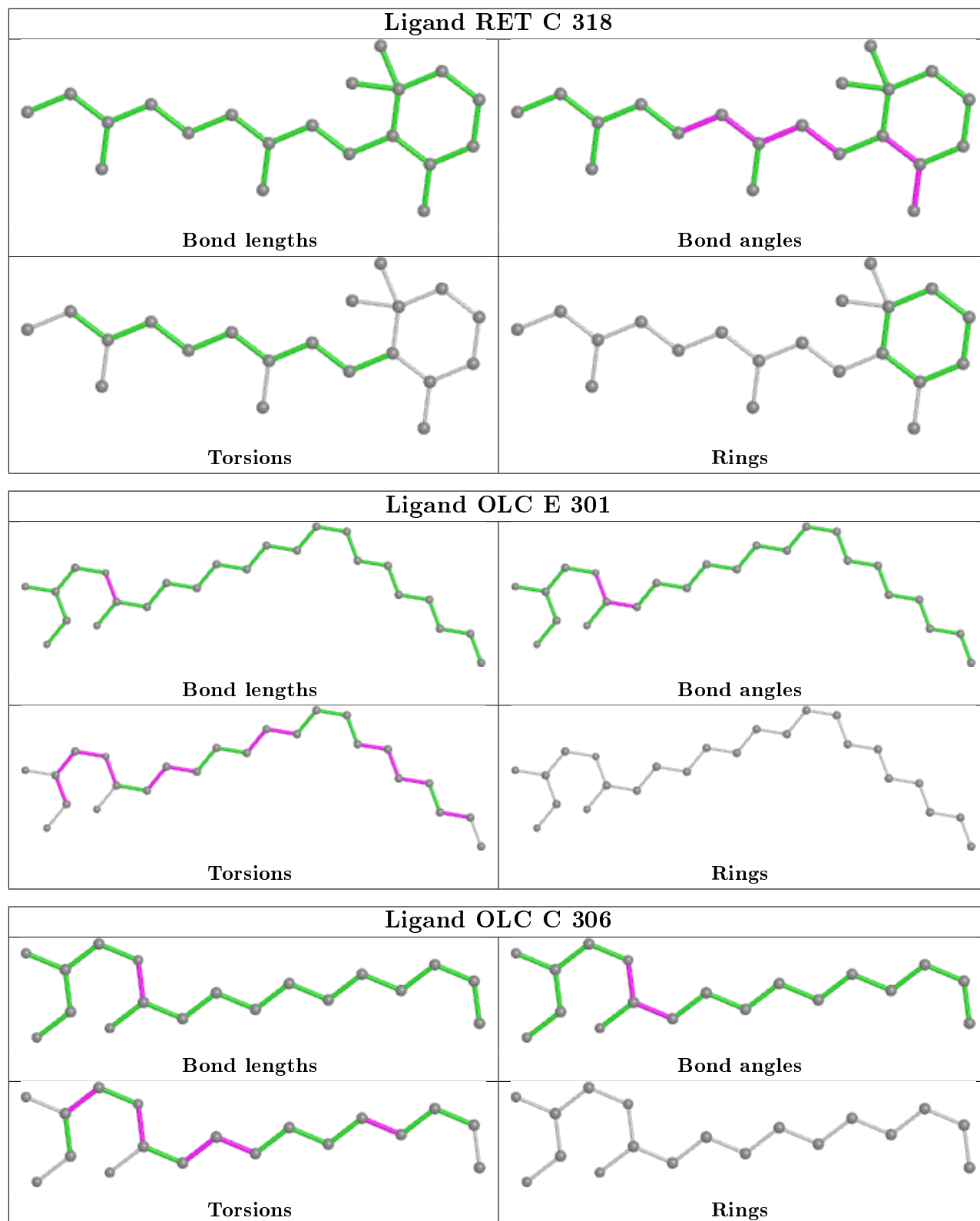


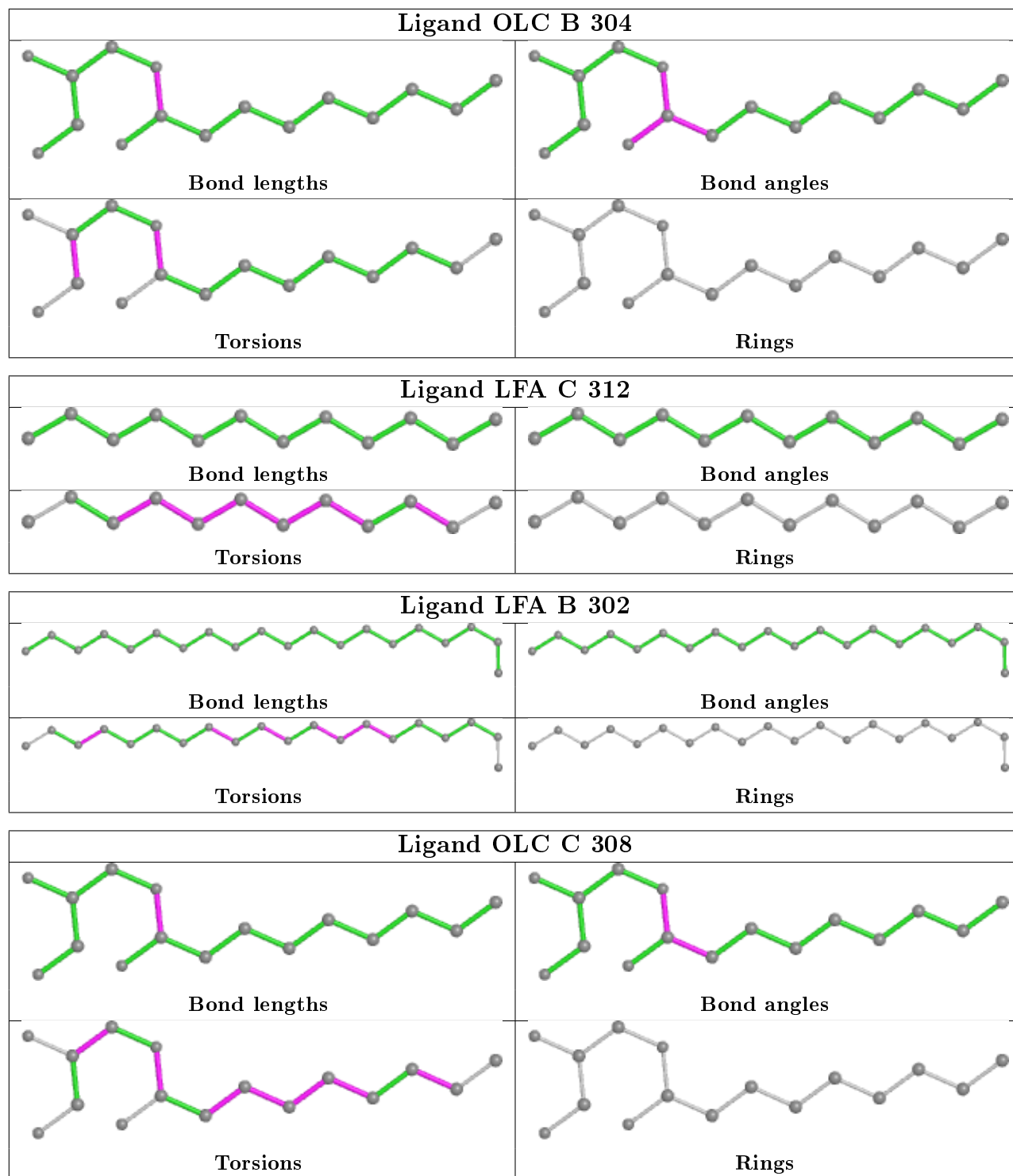


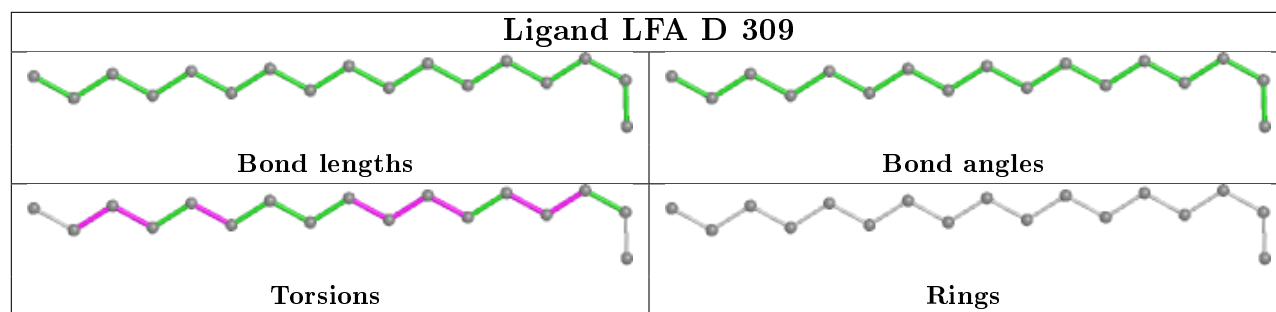
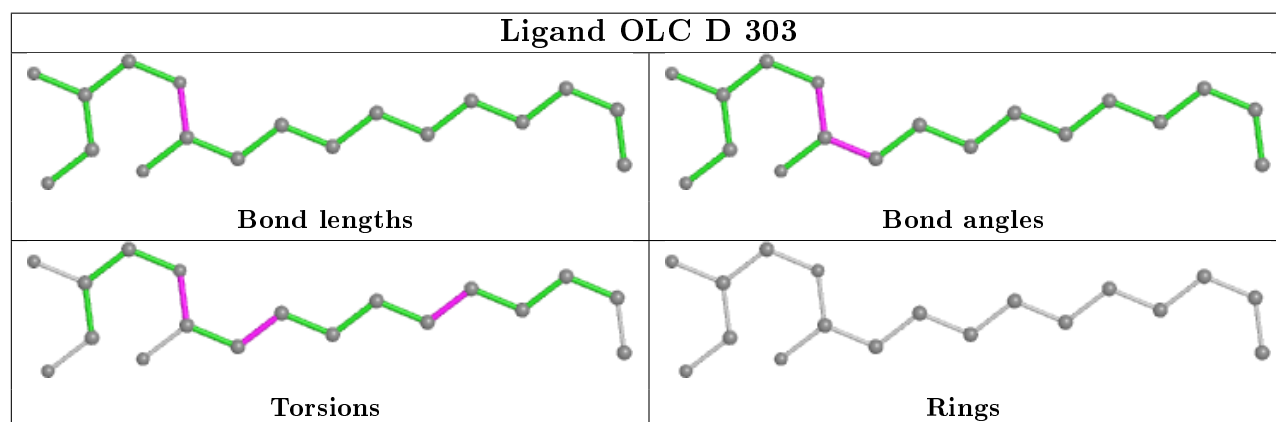
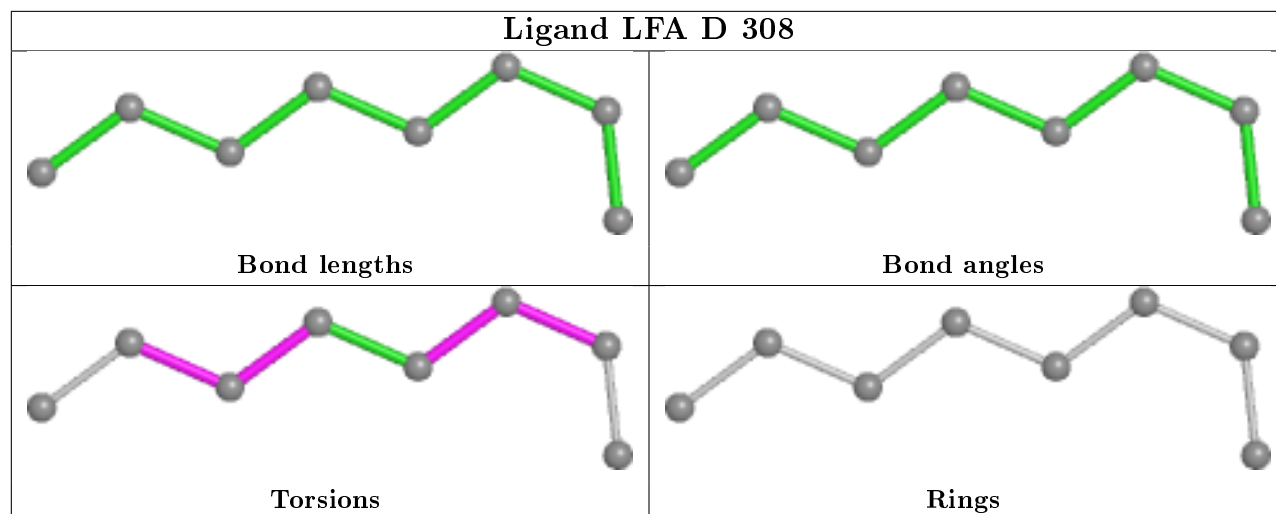


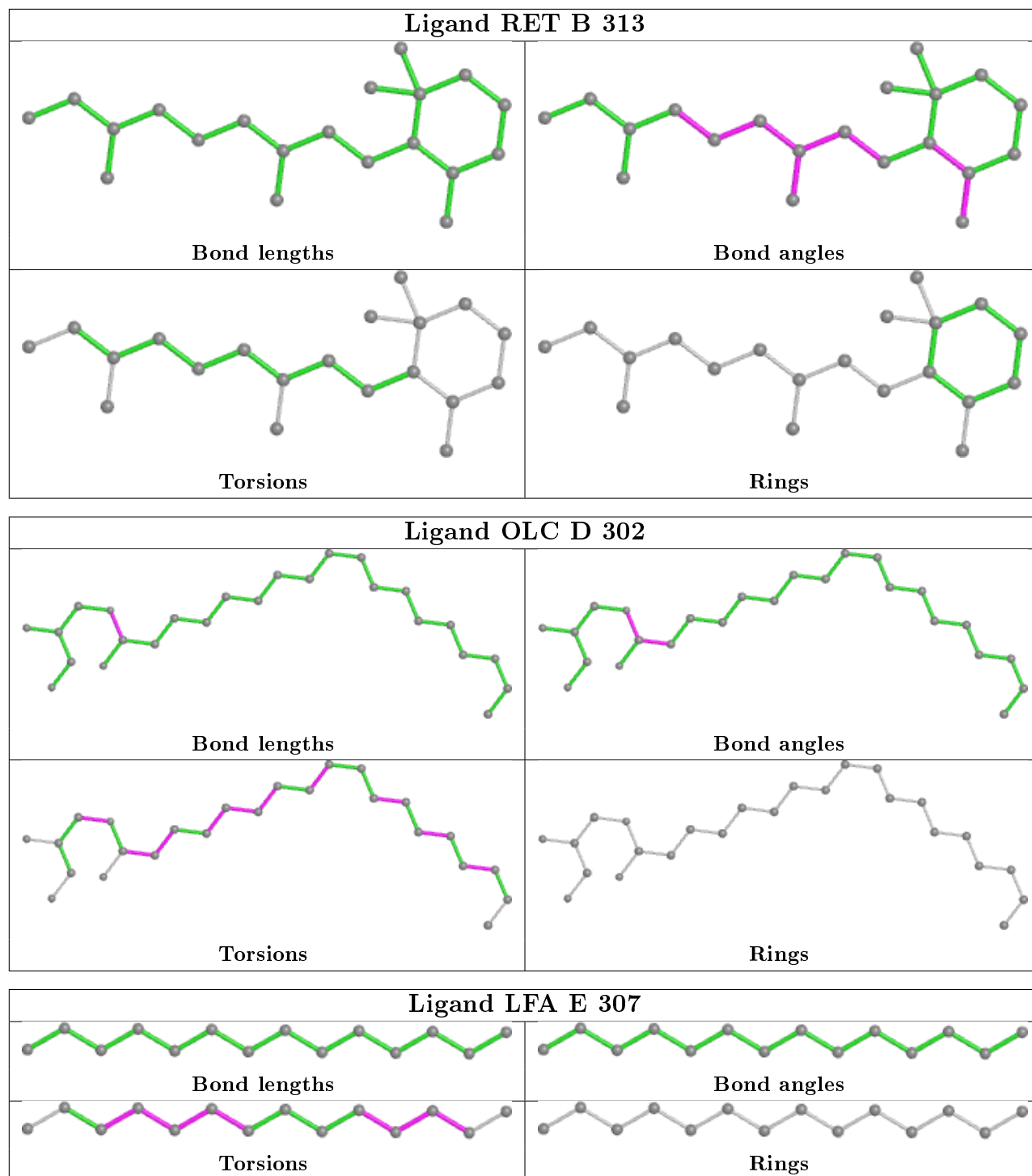


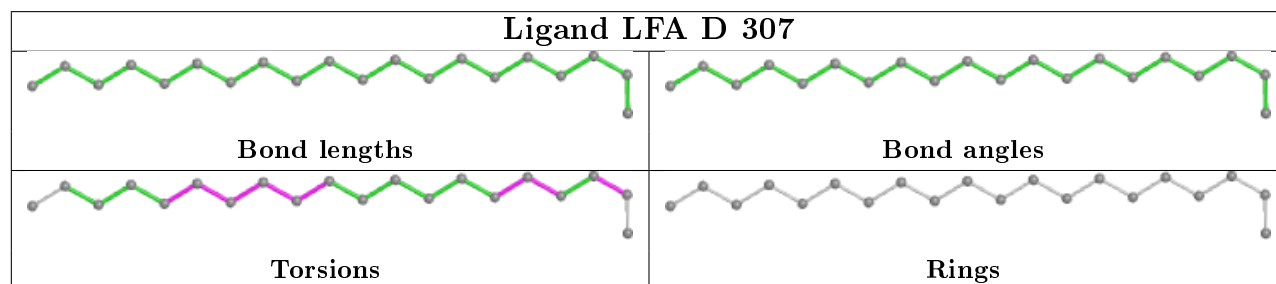
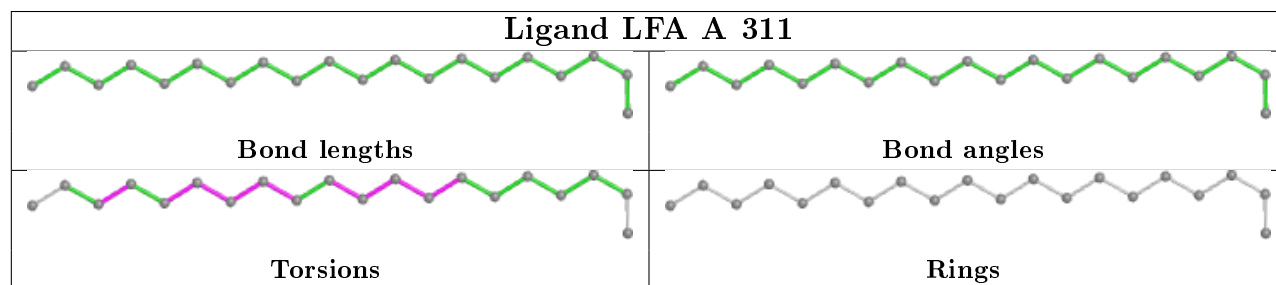
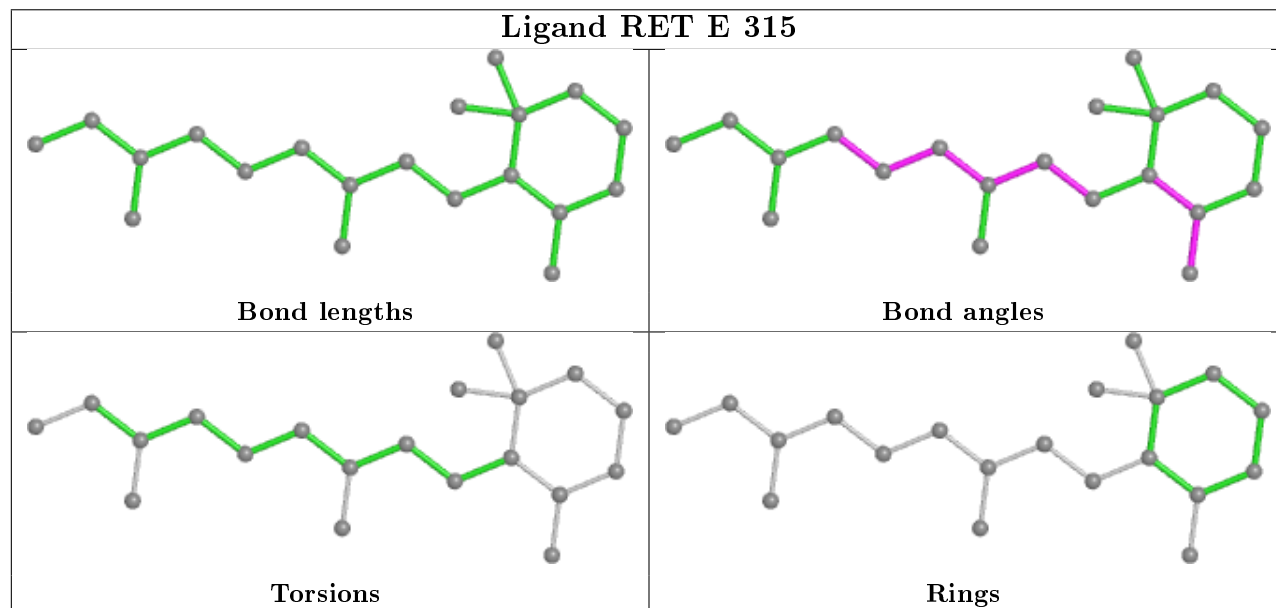
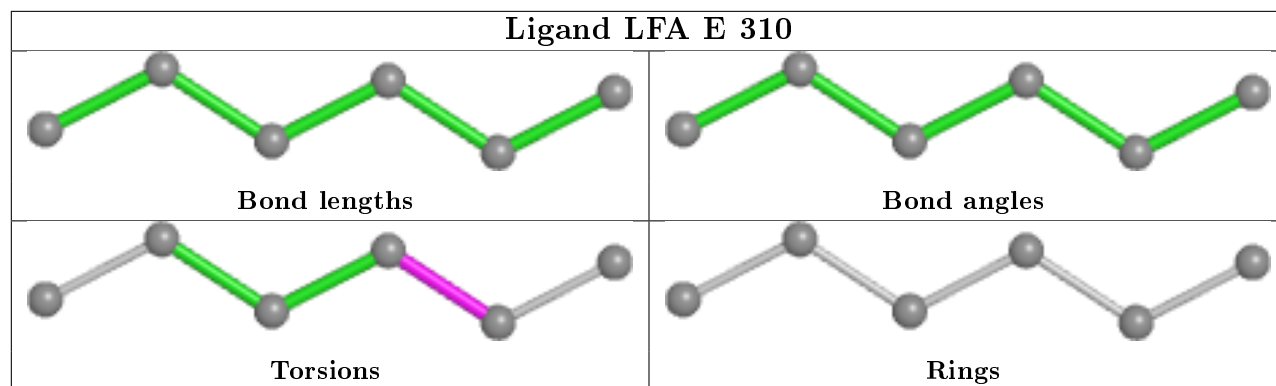


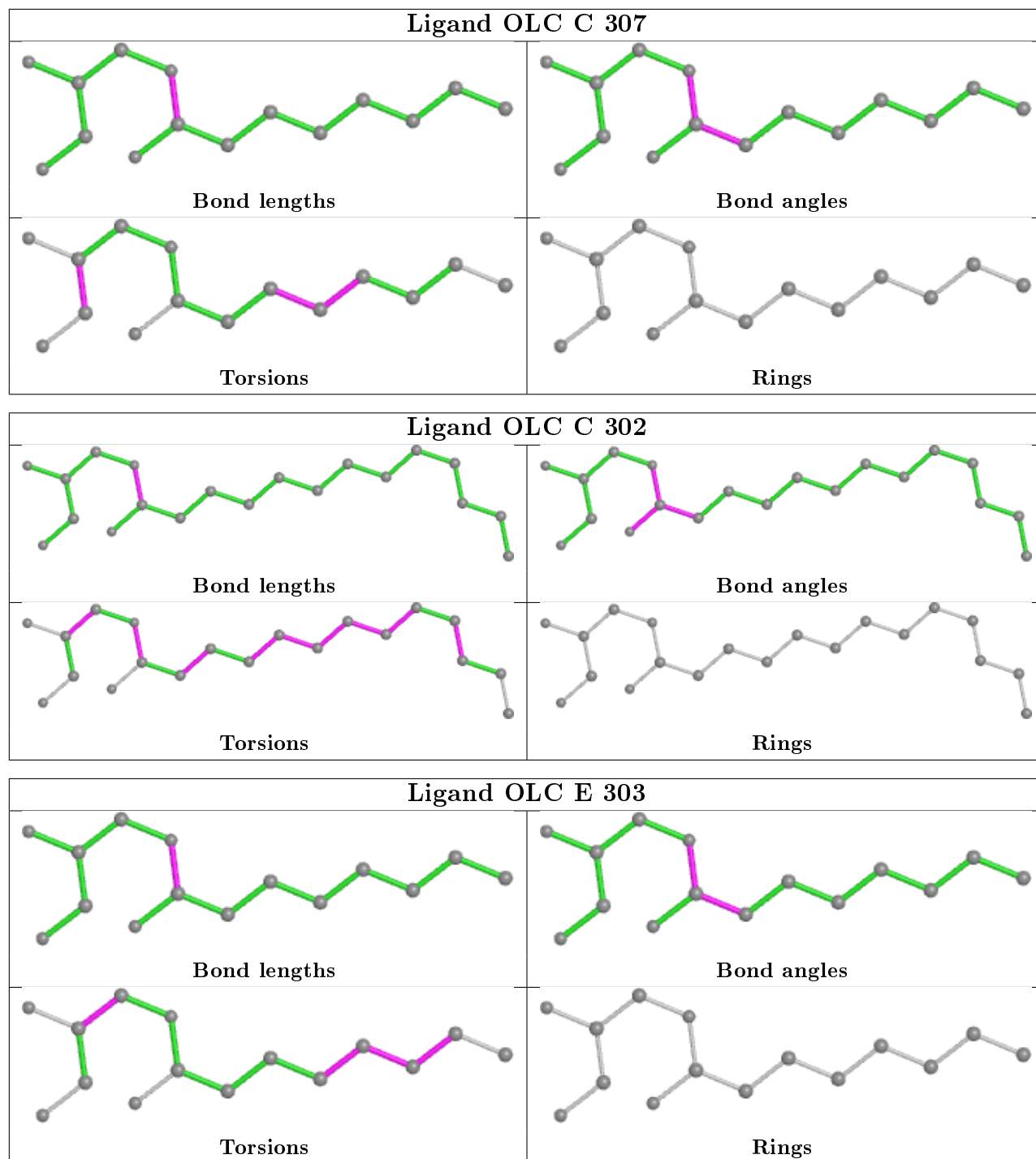


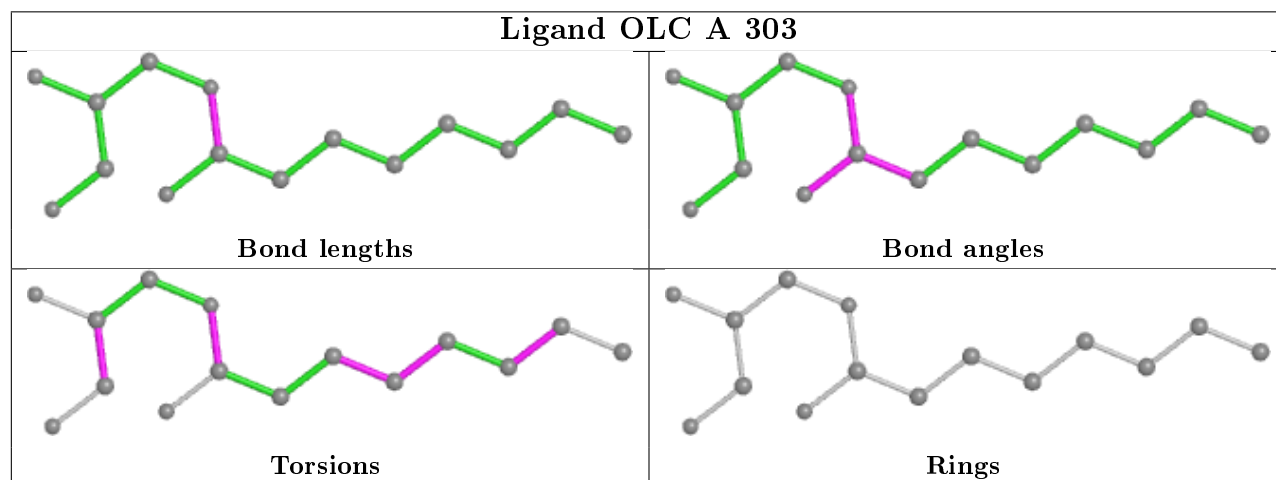
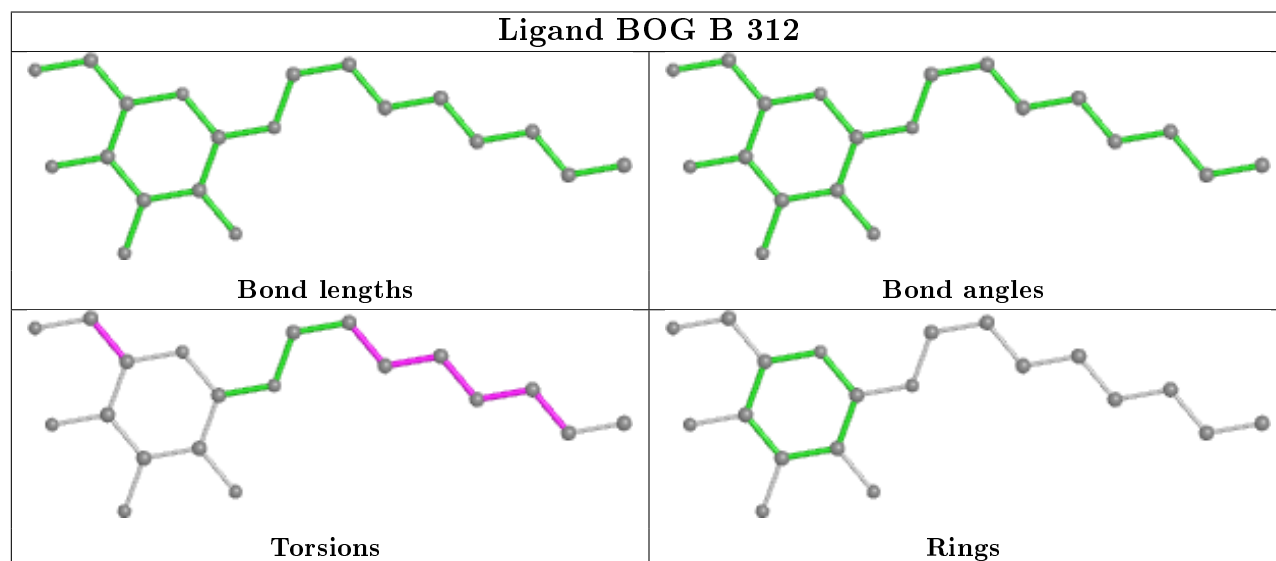
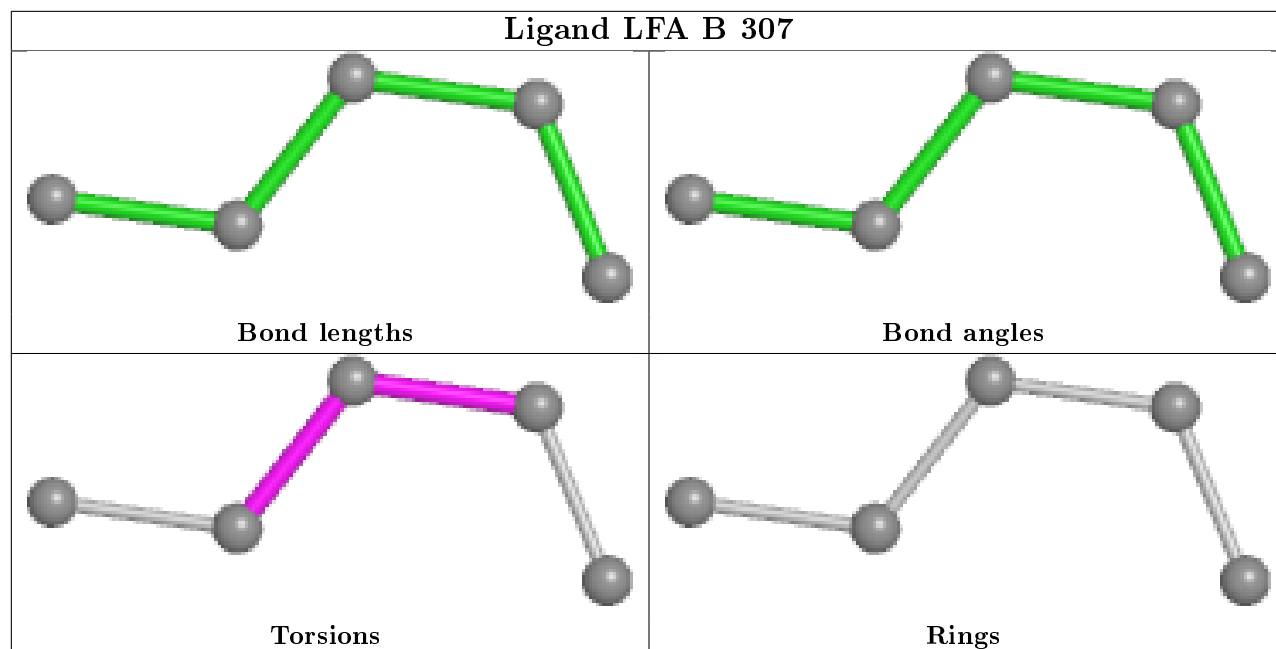












## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	273/273 (100%)	0.77	31 (11%) 5 4	23, 34, 59, 110	0
1	B	273/273 (100%)	0.69	22 (8%) 12 10	23, 35, 59, 95	0
1	C	273/273 (100%)	0.80	38 (13%) 2 2	22, 35, 58, 117	0
1	D	273/273 (100%)	0.79	36 (13%) 3 2	21, 36, 60, 140	0
1	E	273/273 (100%)	0.75	44 (16%) 1 1	22, 36, 59, 121	0
All	All	1365/1365 (100%)	0.76	171 (12%) 3 3	21, 35, 59, 140	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	274	GLU	7.7
1	D	275	LEU	7.2
1	D	131	THR	6.2
1	C	230	VAL	6.0
1	A	272	ASN	6.0
1	B	272	ASN	5.4
1	C	272	ASN	5.3
1	D	132	THR	5.2
1	B	3	GLN	5.1
1	C	3	GLN	4.7
1	A	3	GLN	4.6
1	C	228	THR	4.6
1	D	233	PHE	4.6
1	A	233	PHE	4.4
1	E	233	PHE	4.4
1	D	3	GLN	4.4
1	D	130	LEU	4.4
1	D	274	GLU	4.4
1	B	230	VAL	4.3
1	D	72	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	132	THR	4.2
1	A	275	LEU	4.2
1	B	275	LEU	4.2
1	B	274	GLU	4.0
1	C	232	GLY	3.9
1	A	163	ASN	3.8
1	E	275	LEU	3.7
1	C	183	TRP	3.7
1	D	230	VAL	3.7
1	A	73	LEU	3.6
1	A	270	SER	3.6
1	D	40	LEU	3.5
1	C	274	GLU	3.5
1	C	238	ASP	3.5
1	C	273	LYS	3.4
1	A	274	GLU	3.4
1	D	76	TYR	3.4
1	A	132	THR	3.4
1	A	196	ILE	3.3
1	E	72	PHE	3.3
1	A	230	VAL	3.3
1	D	129	SER	3.3
1	A	183	TRP	3.3
1	E	3	GLN	3.3
1	C	137	SER	3.2
1	D	133	SER	3.2
1	E	273	LYS	3.2
1	B	76	TYR	3.2
1	D	4	GLU	3.2
1	C	72	PHE	3.2
1	C	233	PHE	3.2
1	B	72	PHE	3.2
1	C	275	LEU	3.2
1	A	199	ALA	3.1
1	C	130	LEU	3.0
1	D	73	LEU	3.0
1	E	92	VAL	3.0
1	C	129	SER	3.0
1	E	230	VAL	3.0
1	D	273	LYS	3.0
1	C	131	THR	3.0
1	E	132	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	75	LEU	3.0
1	C	40	LEU	2.9
1	E	228	THR	2.9
1	C	229	GLY	2.9
1	E	133	SER	2.9
1	B	183	TRP	2.8
1	D	197	SER	2.8
1	C	73	LEU	2.8
1	E	40	LEU	2.8
1	E	74	LEU	2.8
1	D	163	ASN	2.8
1	E	18	GLU	2.7
1	E	270	SER	2.7
1	A	92	VAL	2.7
1	E	129	SER	2.7
1	E	131	THR	2.7
1	D	194	GLU	2.7
1	E	69	VAL	2.7
1	B	40	LEU	2.7
1	E	197	SER	2.7
1	A	198	PRO	2.7
1	A	72	PHE	2.7
1	C	196	ILE	2.6
1	E	76	TYR	2.6
1	D	272	ASN	2.6
1	C	128	VAL	2.6
1	B	231	ASP	2.6
1	E	73	LEU	2.6
1	E	54	ASP	2.6
1	C	136	SER	2.6
1	A	17	THR	2.5
1	B	169	VAL	2.5
1	E	183	TRP	2.5
1	C	76	TYR	2.5
1	B	233	PHE	2.5
1	C	4	GLU	2.5
1	C	161	VAL	2.5
1	C	231	ASP	2.5
1	C	197	SER	2.5
1	E	198	PRO	2.5
1	E	17	THR	2.5
1	A	205	SER	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	190	ASN	2.5
1	A	197	SER	2.4
1	D	236	SER	2.4
1	C	18	GLU	2.4
1	A	195	GLY	2.4
1	D	69	VAL	2.4
1	B	54	ASP	2.4
1	B	132	THR	2.4
1	E	166	ALA	2.4
1	B	270	SER	2.4
1	E	196	ILE	2.4
1	A	131	THR	2.4
1	E	47	ILE	2.4
1	B	131	THR	2.4
1	C	198	PRO	2.4
1	D	43	LEU	2.4
1	D	77	ALA	2.4
1	E	238	ASP	2.4
1	A	54	ASP	2.3
1	B	228	THR	2.3
1	D	228	THR	2.3
1	A	228	THR	2.3
1	A	190	ASN	2.3
1	C	227	LEU	2.3
1	A	76	TYR	2.3
1	D	54	ASP	2.3
1	E	163	ASN	2.3
1	C	77	ALA	2.2
1	A	231	ASP	2.2
1	E	65	ALA	2.2
1	E	67	VAL	2.2
1	D	137	SER	2.2
1	E	137	SER	2.2
1	E	231	ASP	2.2
1	A	77	ALA	2.2
1	E	190	ASN	2.2
1	C	69	VAL	2.2
1	C	234	LEU	2.2
1	A	127	VAL	2.2
1	B	137	SER	2.2
1	D	47	ILE	2.2
1	B	44	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	272	ASN	2.1
1	C	79	ALA	2.1
1	E	77	ALA	2.1
1	D	136	SER	2.1
1	E	75	LEU	2.1
1	A	133	SER	2.1
1	B	129	SER	2.1
1	C	133	SER	2.1
1	A	203	ILE	2.1
1	C	74	LEU	2.1
1	E	4	GLU	2.1
1	E	36	TYR	2.1
1	D	269	LEU	2.1
1	E	53	VAL	2.1
1	D	36	TYR	2.1
1	B	73	LEU	2.1
1	C	44	LEU	2.1
1	E	162	SER	2.1
1	A	69	VAL	2.0
1	D	191	GLU	2.0
1	D	234	LEU	2.0
1	E	43	LEU	2.0
1	E	71	ALA	2.0
1	D	231	ASP	2.0
1	D	17	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	OLC	C	309	16/25	0.55	0.47	55,75,96,106	0
3	LFA	A	306	8/20	0.60	0.32	49,72,86,89	0
5	BOG	A	310	20/20	0.61	0.59	53,78,98,102	0
2	OLC	D	305	25/25	0.62	0.52	63,78,95,109	0
3	LFA	B	306	9/20	0.63	0.44	71,81,86,88	0
3	LFA	C	314	4/20	0.65	0.56	64,65,68,69	0
3	LFA	C	313	11/20	0.65	0.47	58,77,93,93	0
5	BOG	E	312	20/20	0.68	0.43	50,86,110,114	0
3	LFA	B	302	20/20	0.68	1.19	43,63,75,78	0
3	LFA	C	310	7/20	0.69	0.33	51,58,67,69	0
2	OLC	C	303	16/25	0.69	0.41	63,76,93,104	0
5	BOG	B	312	20/20	0.69	0.70	66,87,108,108	0
3	LFA	D	312	20/20	0.69	1.13	42,58,75,80	0
3	LFA	B	308	10/20	0.70	0.33	54,69,81,82	0
5	BOG	C	317	20/20	0.71	0.52	57,84,95,101	0
3	LFA	D	308	8/20	0.71	0.31	55,74,88,94	0
2	OLC	C	307	15/25	0.74	0.30	48,63,81,87	0
3	LFA	C	312	12/20	0.74	0.33	60,65,76,79	0
3	LFA	E	307	14/20	0.74	0.27	47,71,88,93	0
3	LFA	A	311	20/20	0.75	1.02	34,65,78,78	0
2	OLC	E	302	25/25	0.77	0.34	62,78,114,119	0
3	LFA	C	311	8/20	0.77	0.30	42,59,64,65	0
2	OLC	D	302	25/25	0.77	0.34	55,76,110,116	0
2	OLC	B	305	17/25	0.77	0.42	49,79,102,104	0
3	LFA	E	305	8/20	0.77	0.30	61,67,71,72	0
3	LFA	D	310	7/20	0.77	0.30	53,59,69,71	0
2	OLC	A	301	22/25	0.78	0.34	38,51,92,94	0
3	LFA	D	306	20/20	0.78	0.46	64,86,95,95	0
2	OLC	D	303	18/25	0.78	0.42	47,71,84,106	0
2	OLC	E	301	24/25	0.78	0.35	41,52,91,94	0
2	OLC	B	303	20/25	0.79	0.35	46,58,87,92	0
3	LFA	B	309	7/20	0.79	0.32	56,59,73,78	0
2	OLC	C	306	18/25	0.79	0.31	57,71,86,90	0
5	BOG	D	314	20/20	0.79	0.51	66,84,88,90	0
2	OLC	E	304	25/25	0.79	0.47	42,72,104,111	0
3	LFA	E	309	5/20	0.79	0.28	61,65,69,72	0
3	LFA	C	304	20/20	0.80	0.99	34,51,62,64	0
3	LFA	E	308	4/20	0.80	0.31	62,62,63,67	0
2	OLC	E	303	15/25	0.80	0.36	56,67,75,77	0
2	OLC	C	302	20/25	0.81	0.29	55,68,73,81	0
3	LFA	D	307	20/20	0.81	0.32	56,70,85,90	0
3	LFA	A	304	8/20	0.81	0.30	52,58,66,67	0

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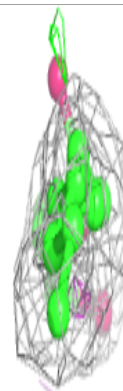
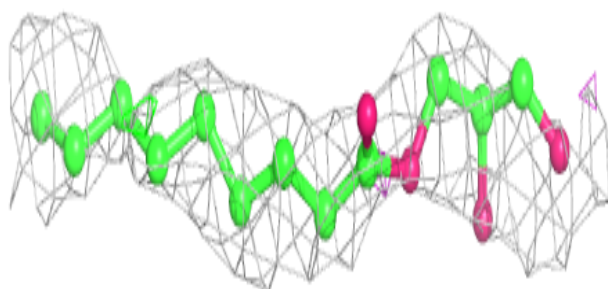
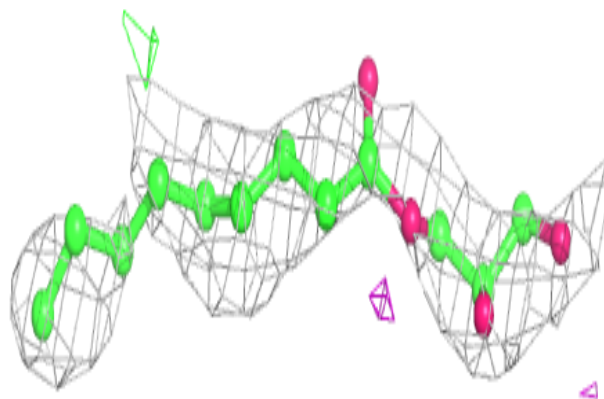
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	C	305	23/25	0.82	0.36	34,45,95,121	0
3	LFA	D	301	20/20	0.82	0.91	34,53,63,65	0
4	NA	E	311	1/1	0.82	0.20	34,34,34,34	0
3	LFA	B	307	5/20	0.83	0.23	30,35,40,42	0
3	LFA	E	314	14/20	0.83	1.30	86,97,101,105	0
3	LFA	A	307	4/20	0.84	0.35	52,58,59,63	0
3	LFA	B	310	6/20	0.84	0.34	49,51,53,54	0
2	OLC	C	301	21/25	0.84	0.33	39,46,63,83	0
3	LFA	E	306	6/20	0.85	0.51	53,58,61,61	0
3	LFA	A	305	5/20	0.85	0.29	50,51,56,57	0
2	OLC	A	302	13/25	0.85	0.36	47,59,65,79	0
3	LFA	D	311	6/20	0.86	0.26	37,41,44,47	0
2	OLC	A	303	15/25	0.86	0.30	50,56,78,81	0
2	OLC	B	301	25/25	0.87	0.29	60,77,94,100	0
2	OLC	B	304	16/25	0.87	0.31	54,61,67,71	0
3	LFA	E	313	4/20	0.88	1.65	59,63,67,70	0
2	OLC	D	304	14/25	0.89	0.30	46,68,75,77	0
3	LFA	D	309	17/20	0.89	0.39	37,45,50,50	0
3	LFA	C	315	6/20	0.89	0.32	39,42,45,45	0
6	RET	A	312	20/21	0.90	0.21	26,31,36,40	0
6	RET	E	315	20/21	0.90	0.22	24,28,38,38	0
2	OLC	C	308	16/25	0.90	0.25	41,58,71,77	0
6	RET	B	313	20/21	0.91	0.22	25,32,35,40	0
3	LFA	A	308	6/20	0.91	0.24	43,44,45,47	0
4	NA	B	311	1/1	0.91	0.13	33,33,33,33	0
6	RET	C	318	20/21	0.92	0.22	27,31,38,38	0
3	LFA	E	310	6/20	0.93	0.20	46,50,51,55	0
6	RET	D	315	20/21	0.93	0.19	29,34,40,41	0
4	NA	A	309	1/1	0.94	0.20	36,36,36,36	0
4	NA	D	313	1/1	0.96	0.09	34,34,34,34	0
4	NA	C	316	1/1	0.97	0.07	25,25,25,25	0

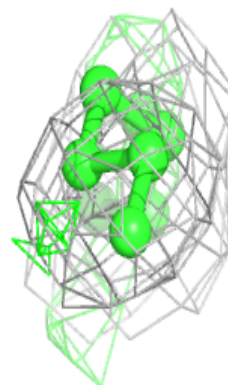
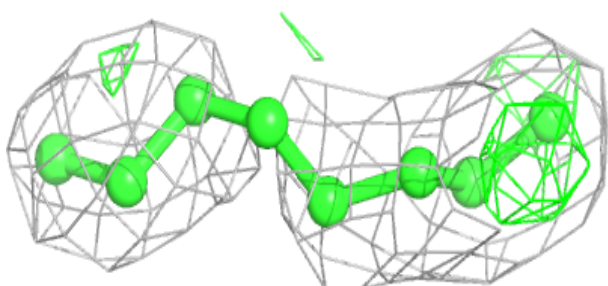
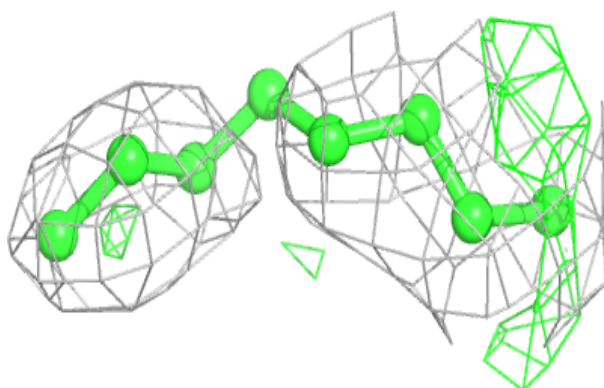
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC C 309:**

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

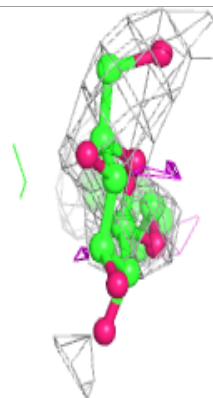
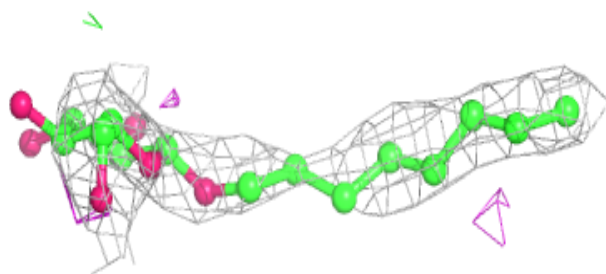
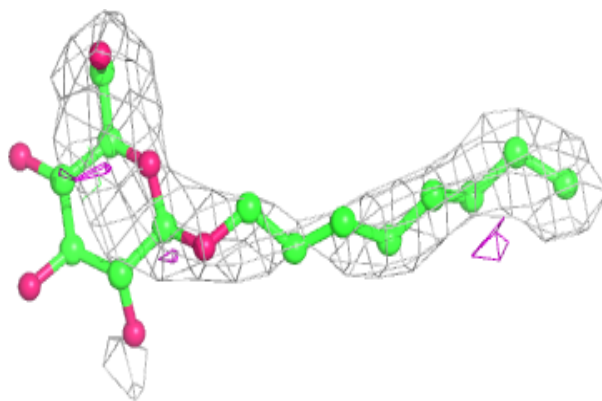
**Electron density around LFA A 306:**

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

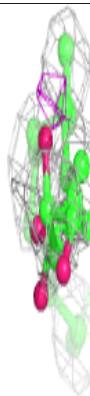
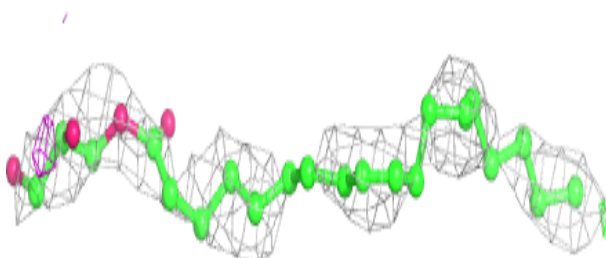
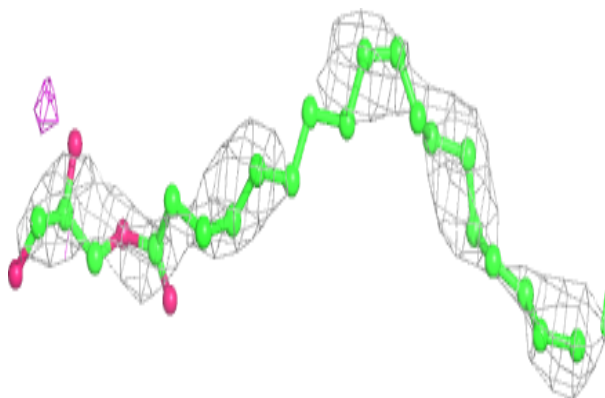


**Electron density around BOG A 310:**

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

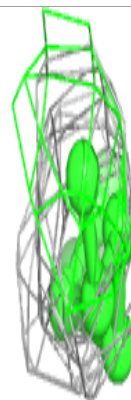
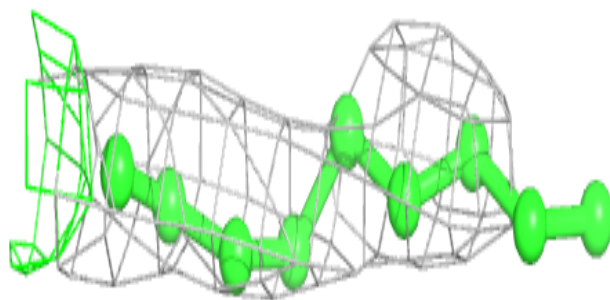
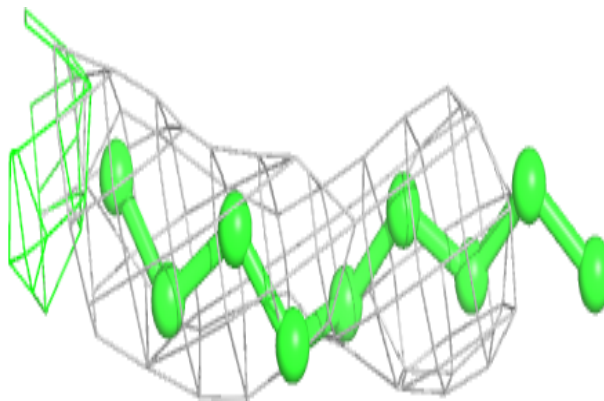
**Electron density around OLC D 305:**

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



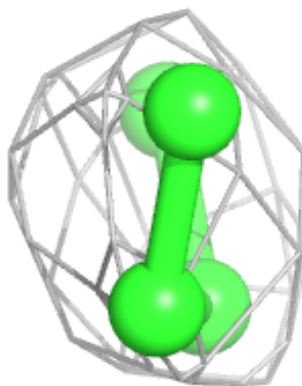
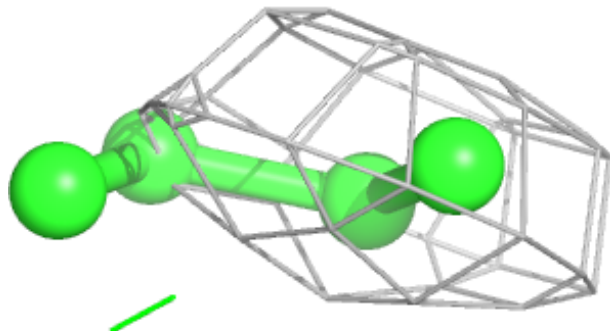
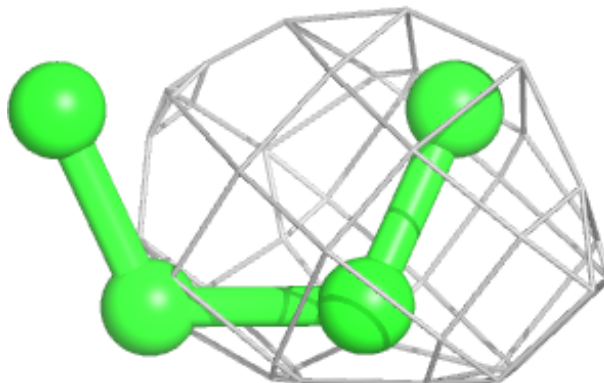
**Electron density around LFA B 306:**

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



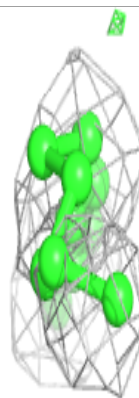
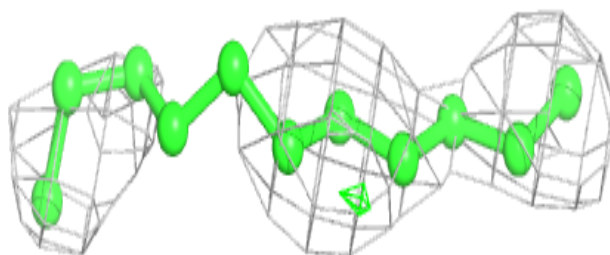
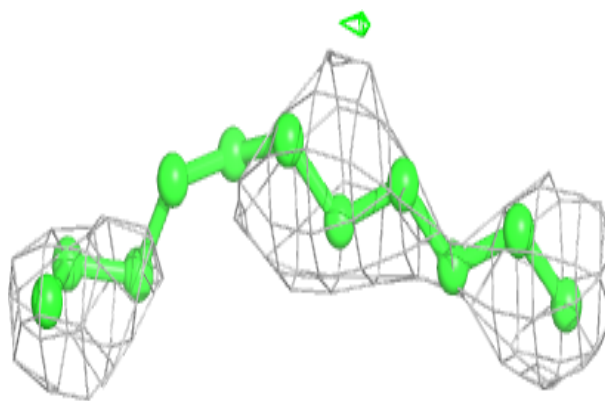
**Electron density around LFA C 314:**

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

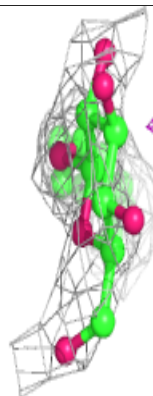
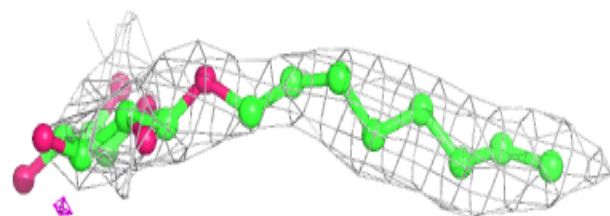
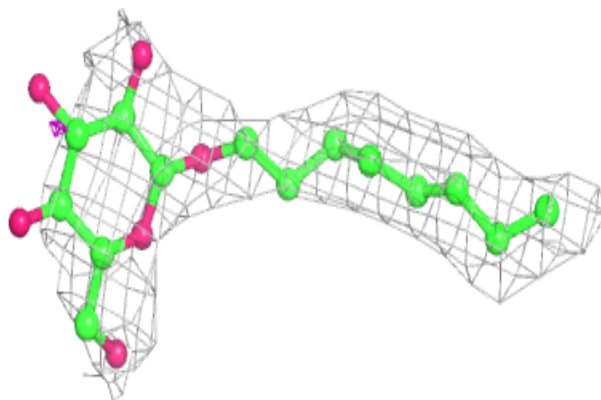


**Electron density around LFA C 313:**

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

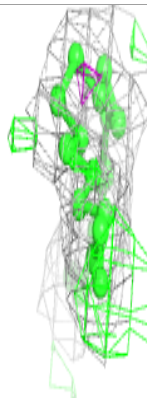
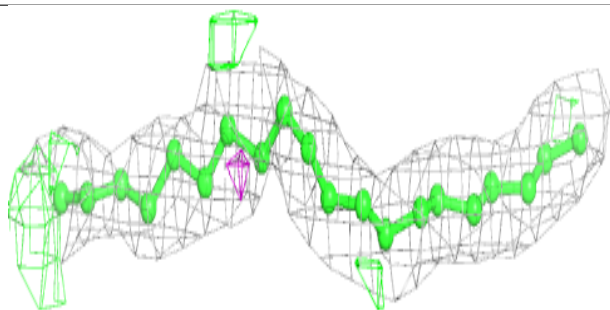
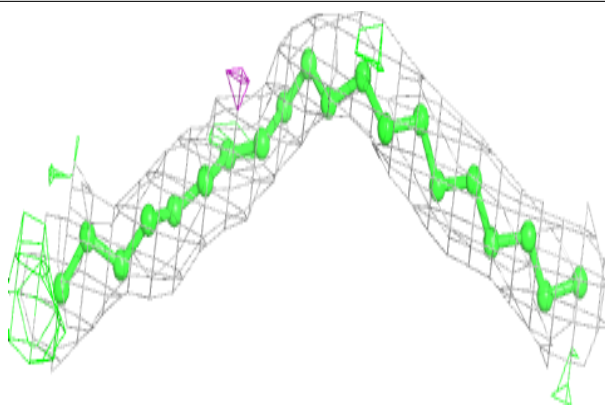
**Electron density around BOG E 312:**

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

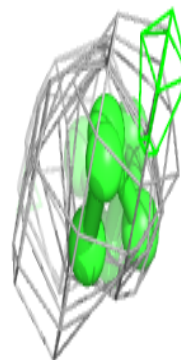
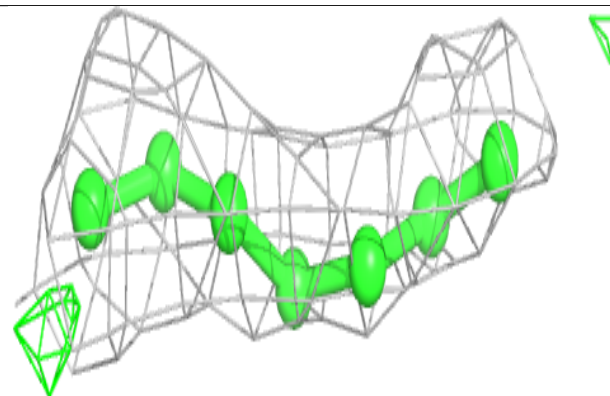
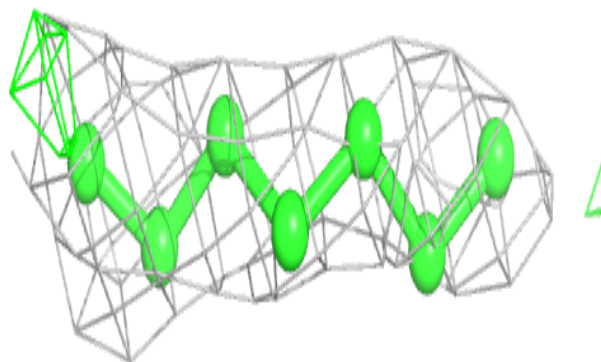


**Electron density around LFA B 302:**

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

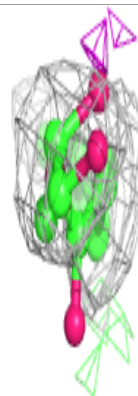
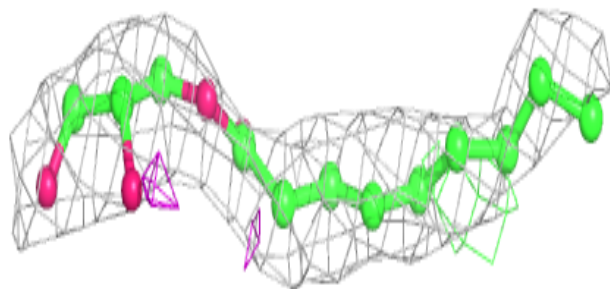
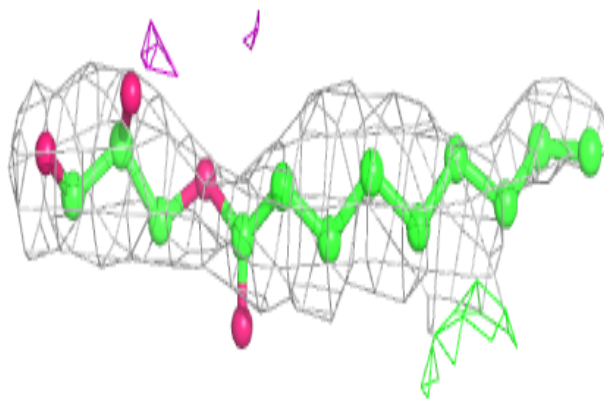
**Electron density around LFA C 310:**

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

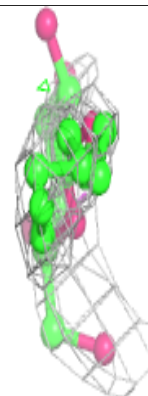
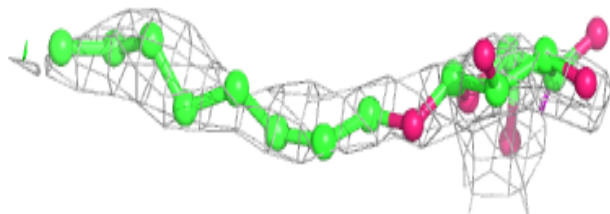
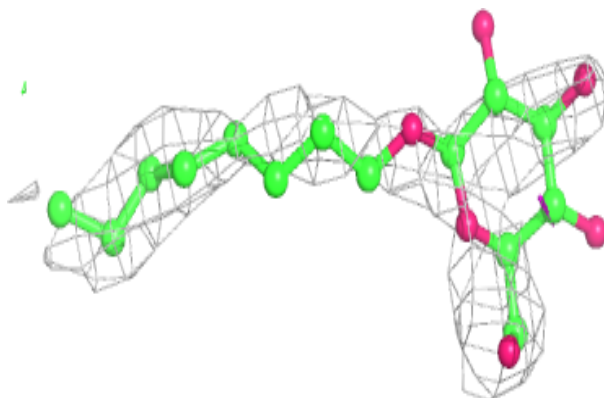


**Electron density around OLC C 303:**

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

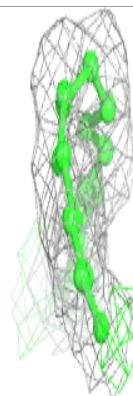
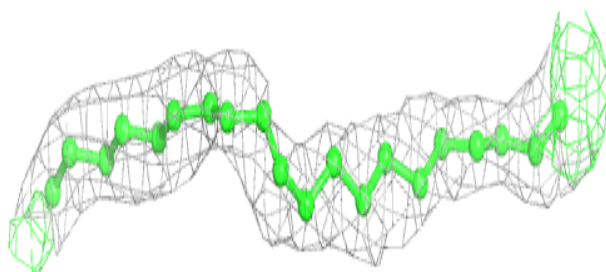
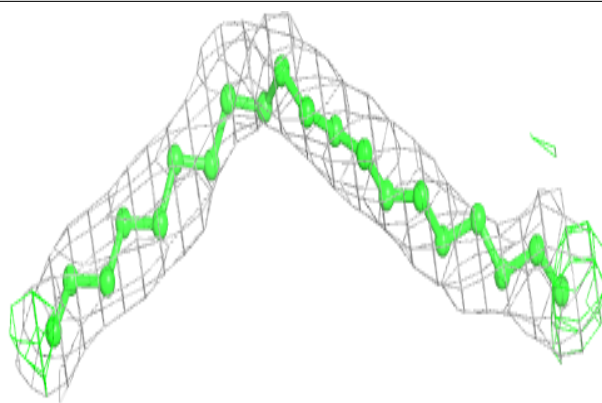
**Electron density around BOG B 312:**

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

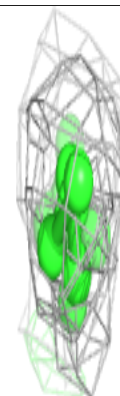
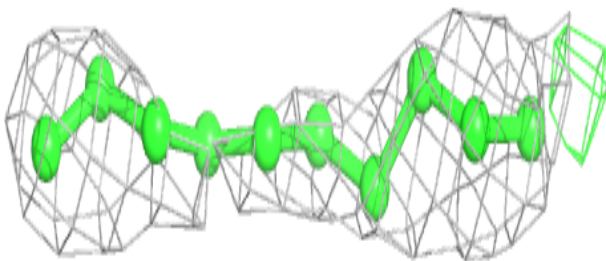
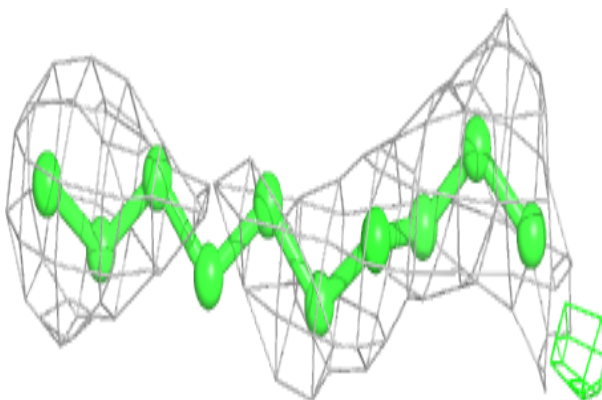


**Electron density around LFA D 312:**

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

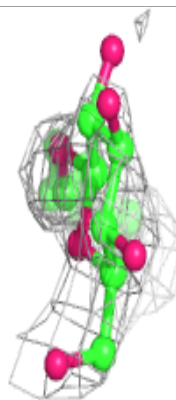
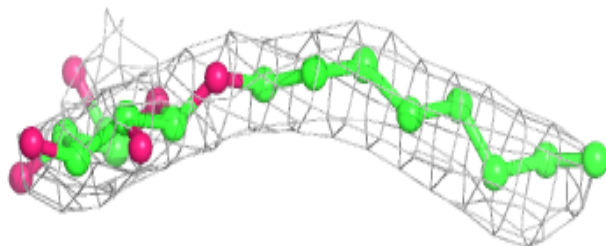
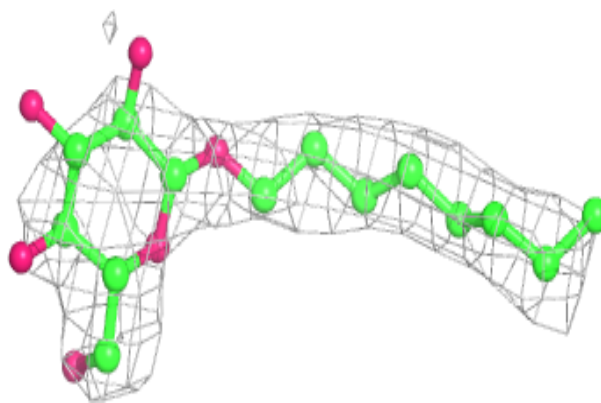
**Electron density around LFA B 308:**

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

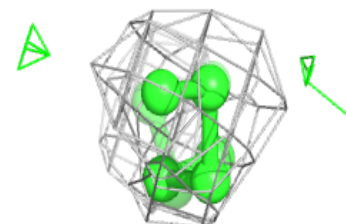
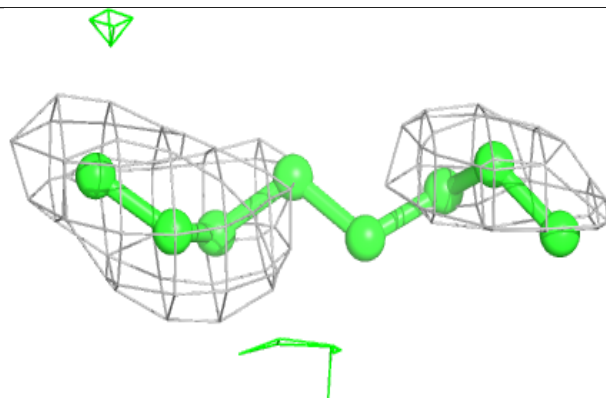
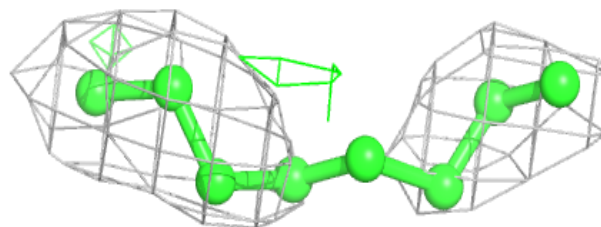


**Electron density around BOG C 317:**

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

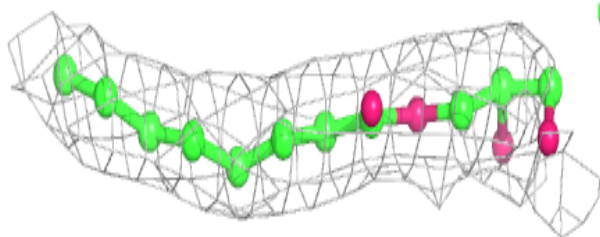
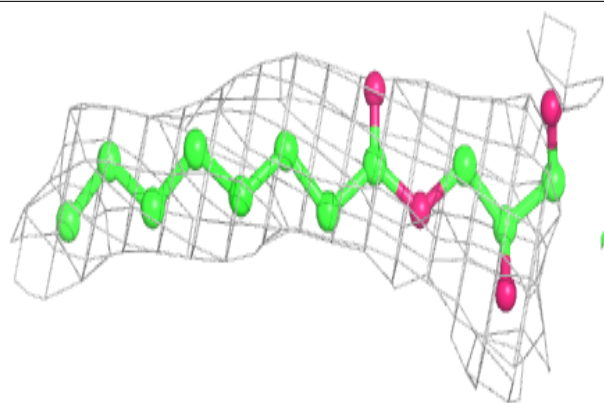
**Electron density around LFA D 308:**

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

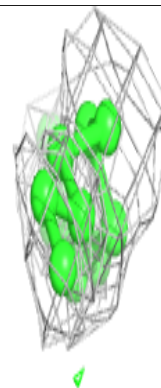
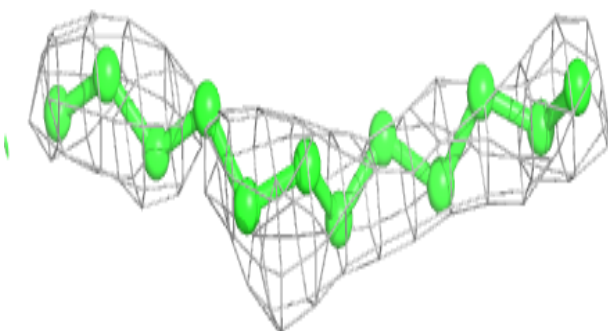
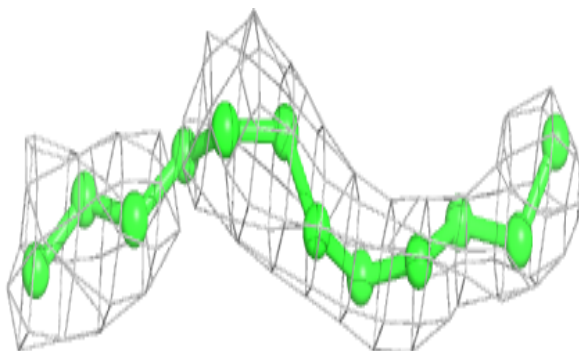


**Electron density around OLC C 307:**

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

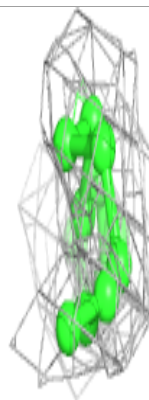
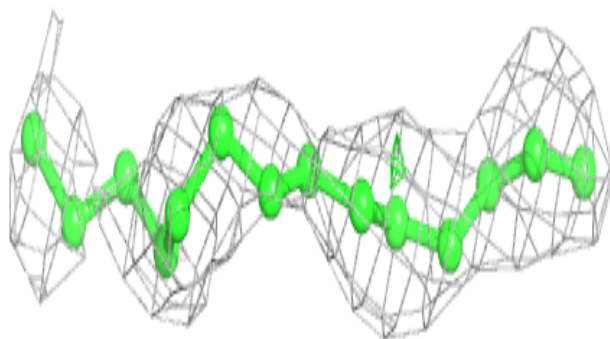
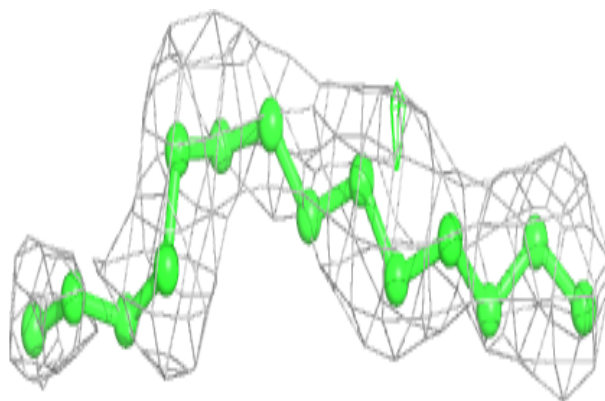
**Electron density around LFA C 312:**

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

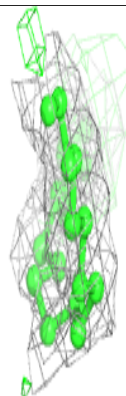
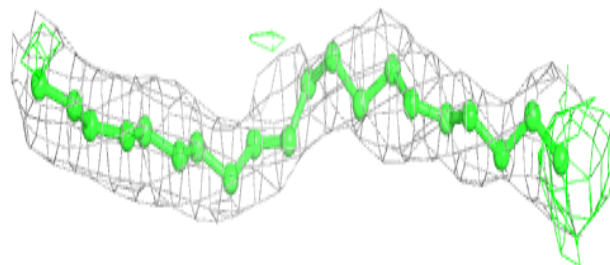
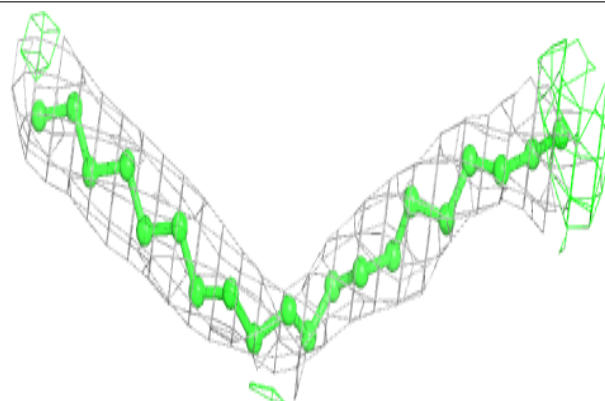


**Electron density around LFA E 307:**

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

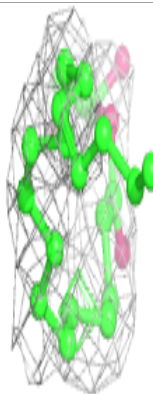
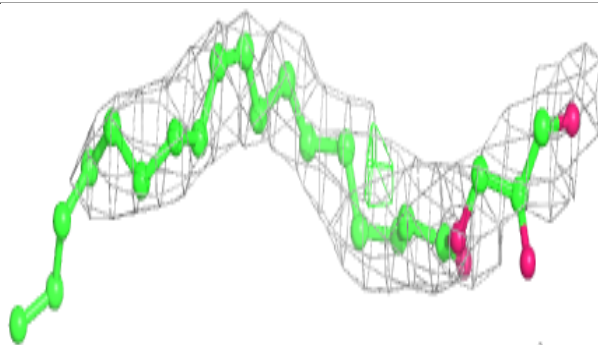
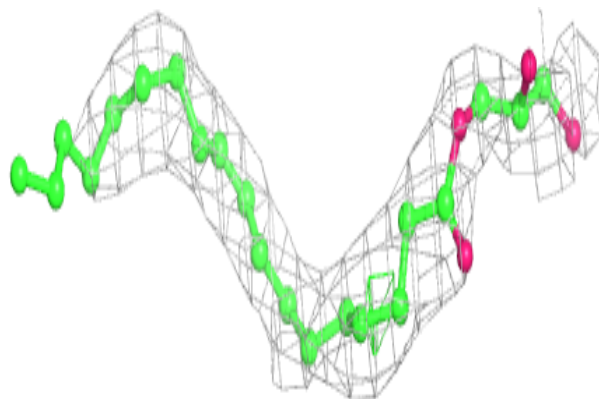
**Electron density around LFA A 311:**

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

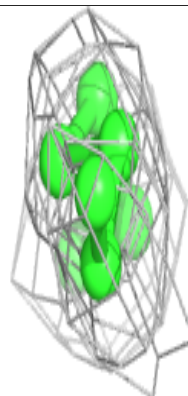
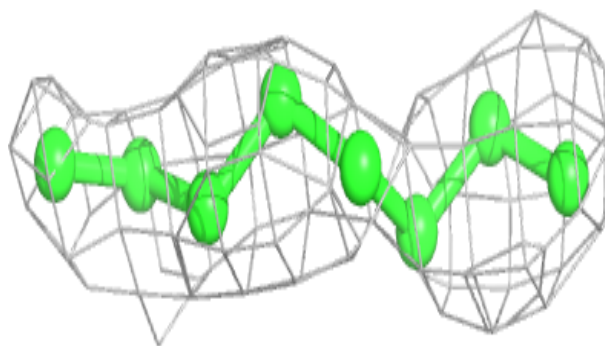
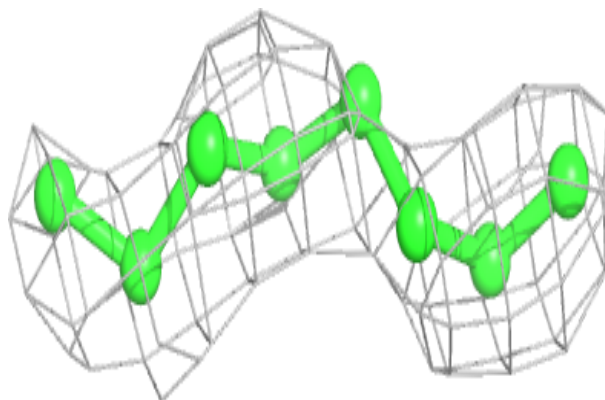


**Electron density around OLC E 302:**

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

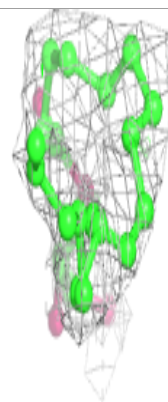
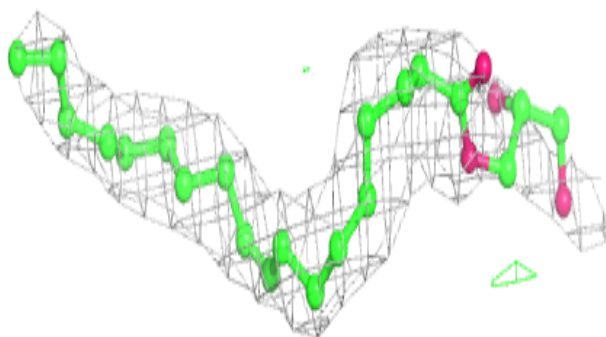
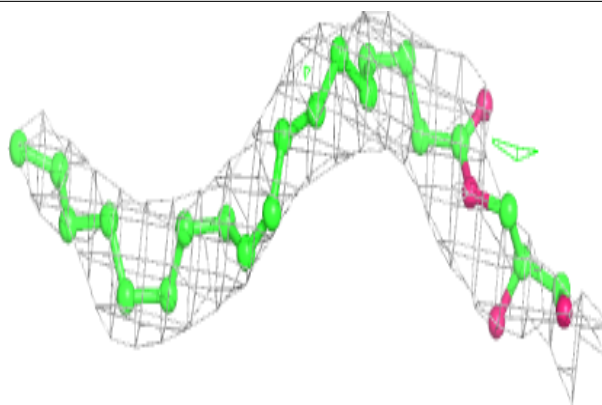
**Electron density around LFA C 311:**

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

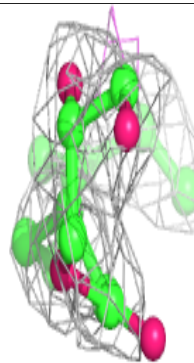
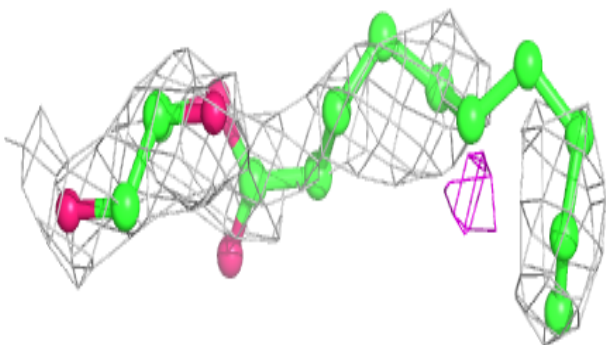
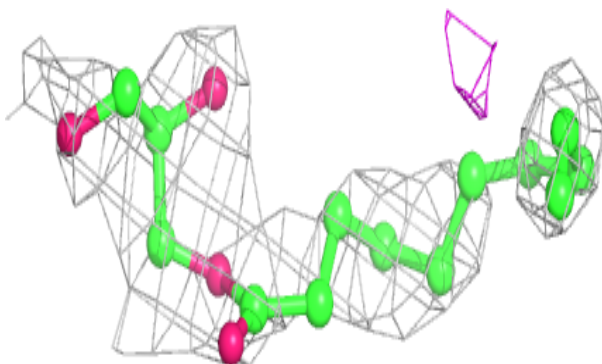


**Electron density around OLC D 302:**

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

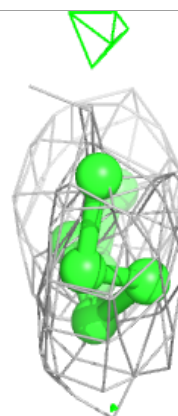
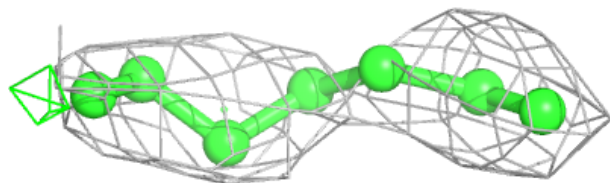
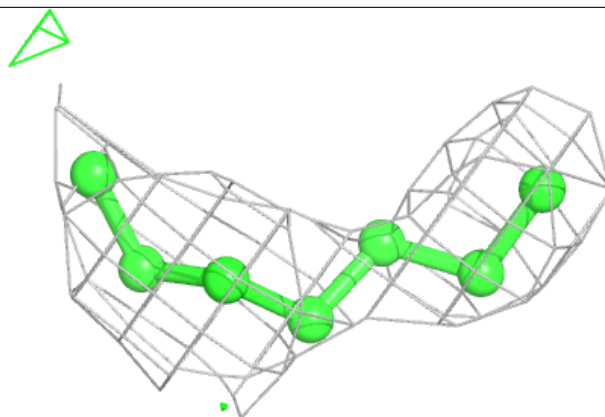
**Electron density around OLC B 305:**

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

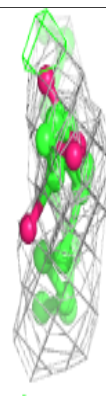
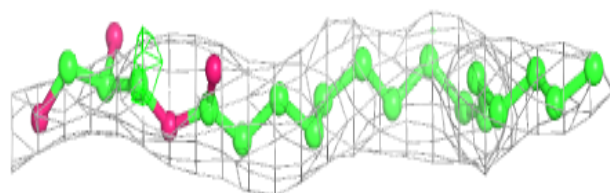
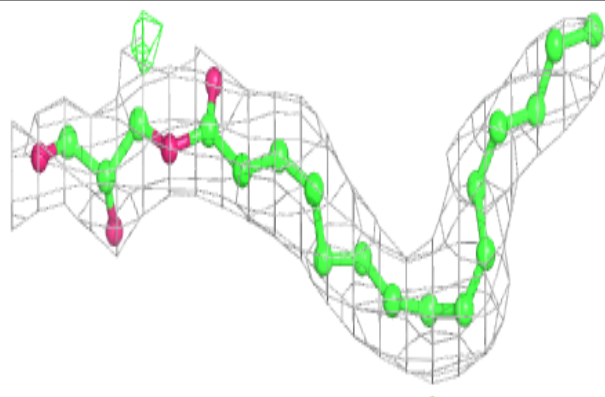


**Electron density around LFA D 310:**

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

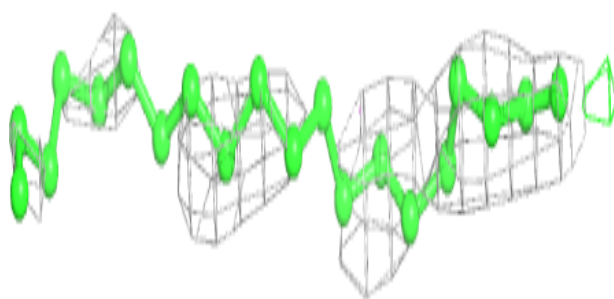
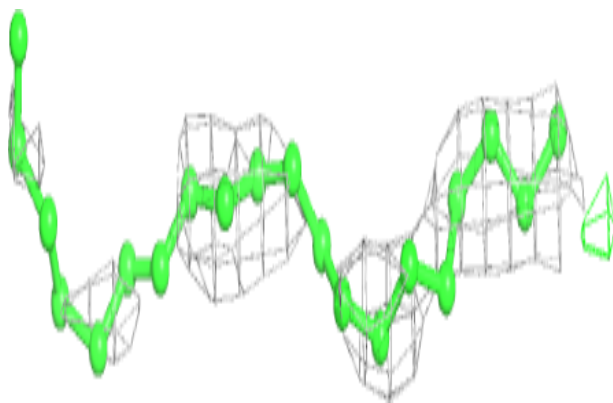
**Electron density around OLC A 301:**

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

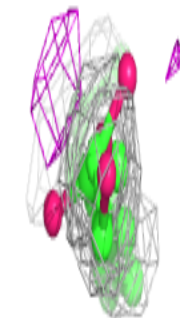
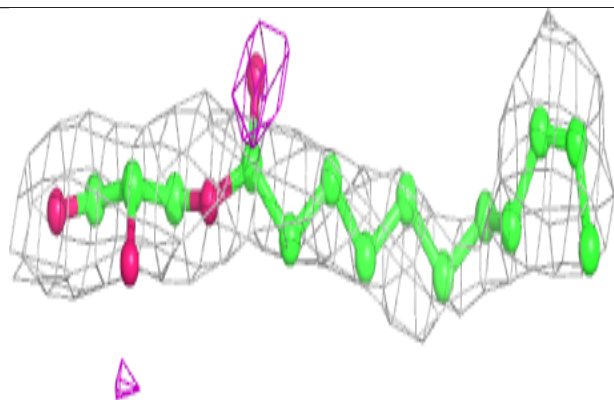
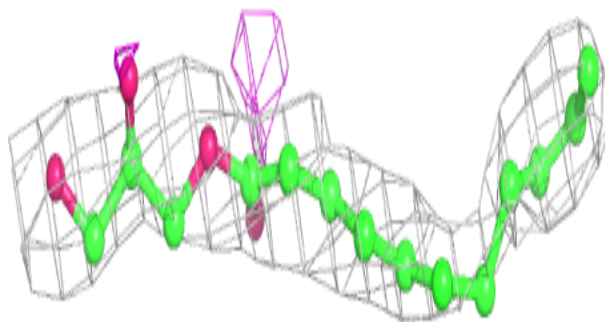


**Electron density around LFA D 306:**

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

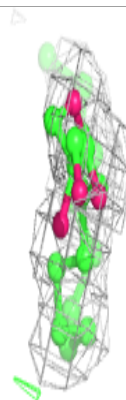
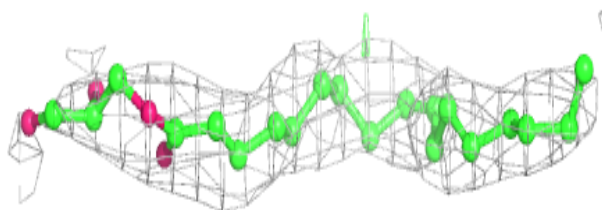
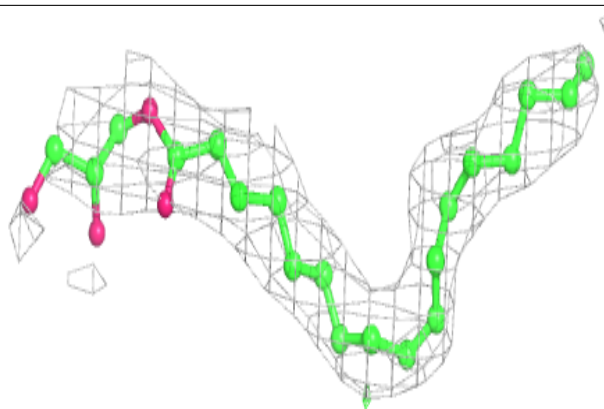
**Electron density around OLC D 303:**

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

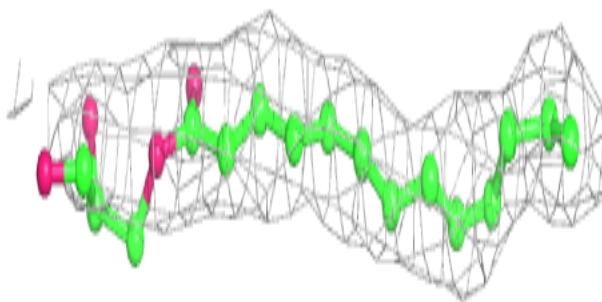
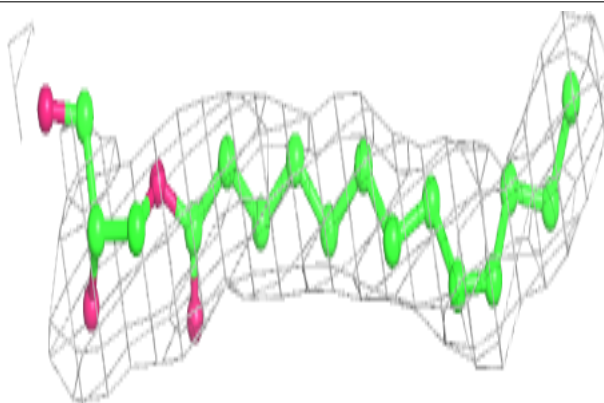


**Electron density around OLC E 301:**

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

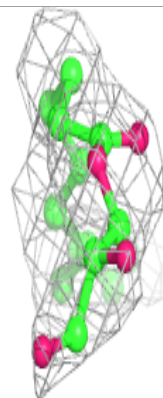
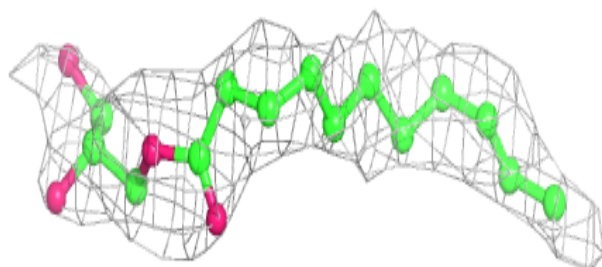
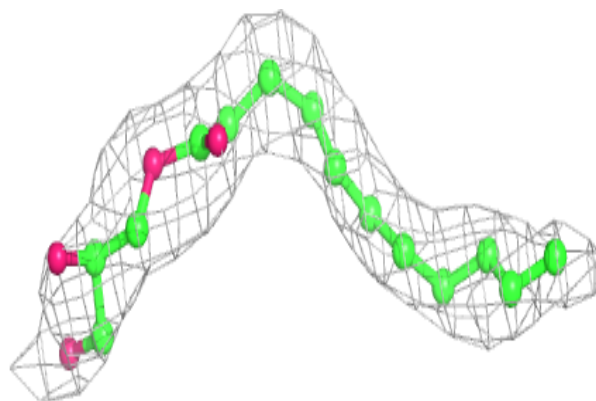
**Electron density around OLC B 303:**

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

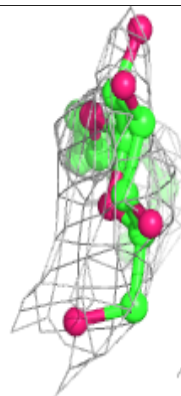
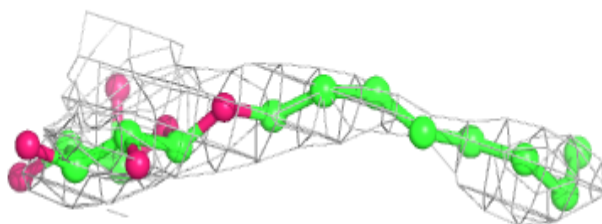
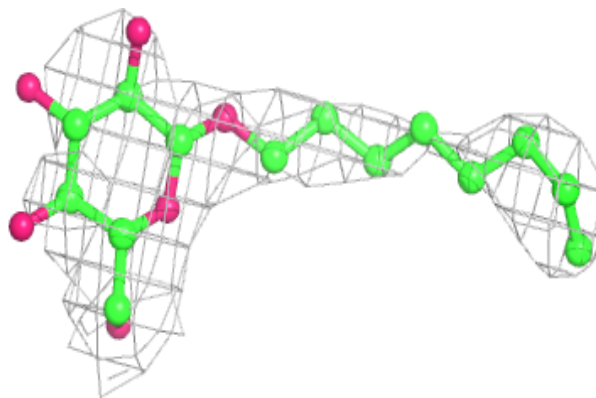


**Electron density around OLC C 306:**

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

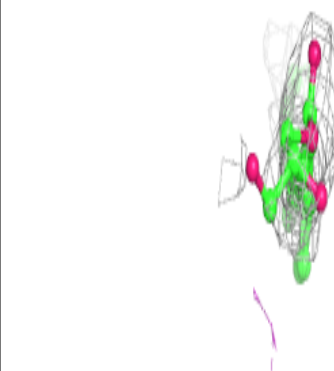
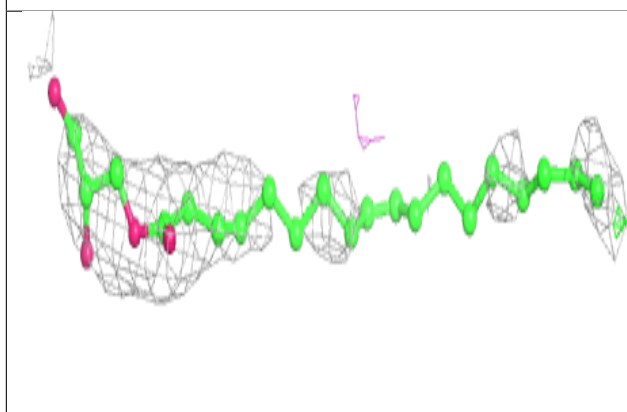
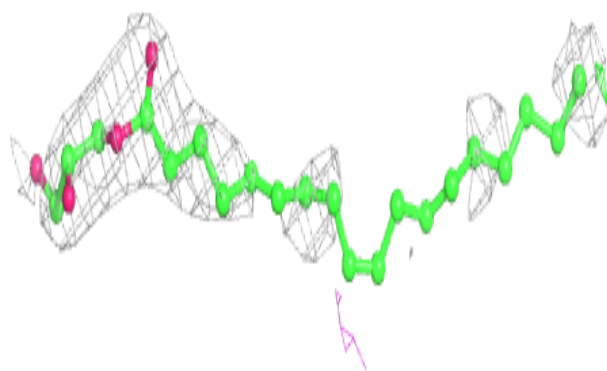
**Electron density around BOG D 314:**

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

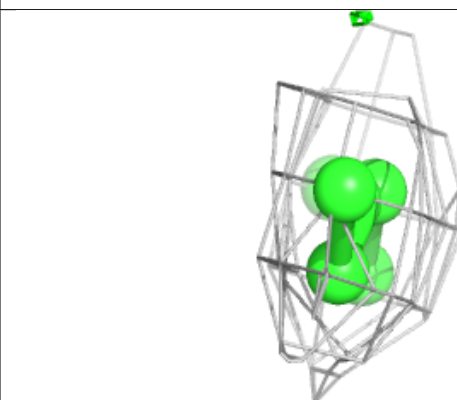
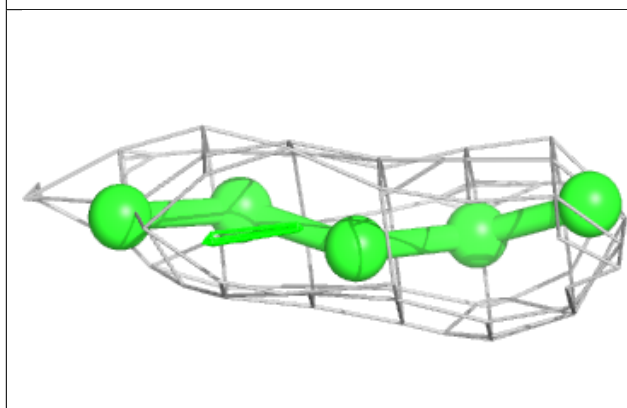
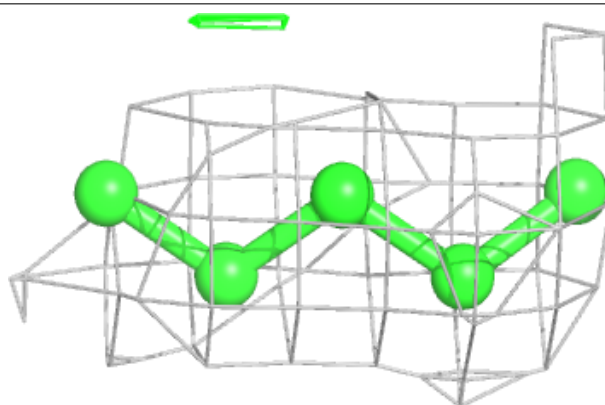


**Electron density around OLC E 304:**

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

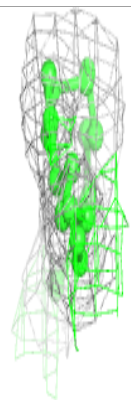
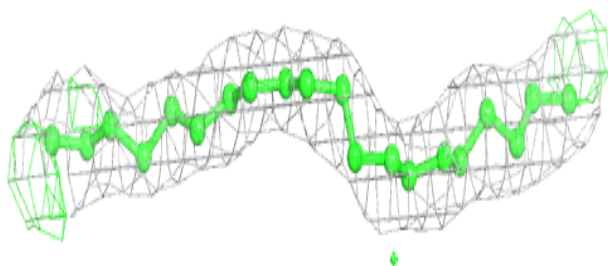
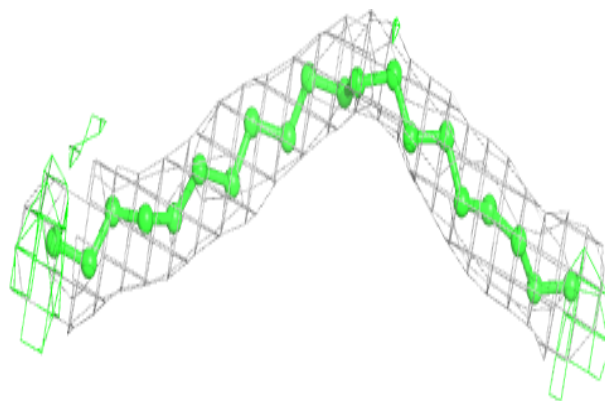
**Electron density around LFA E 309:**

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

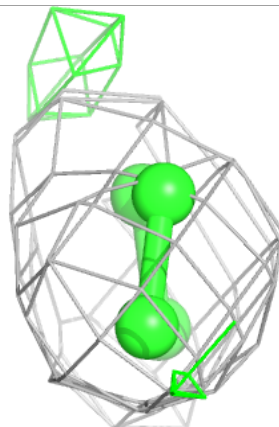
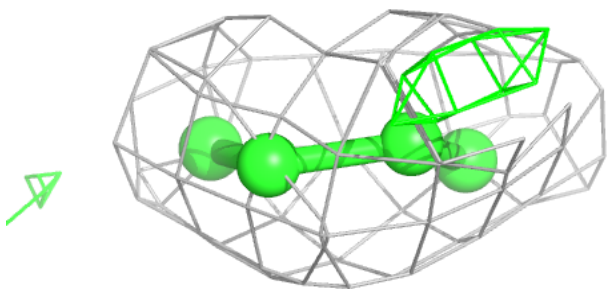
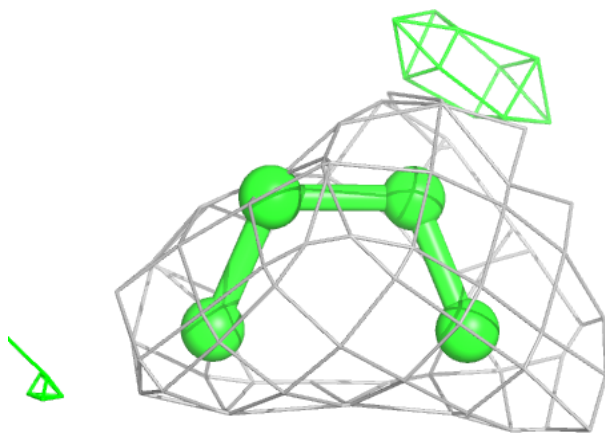


**Electron density around LFA C 304:**

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

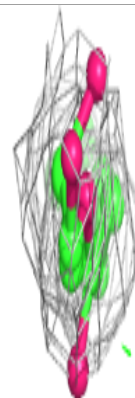
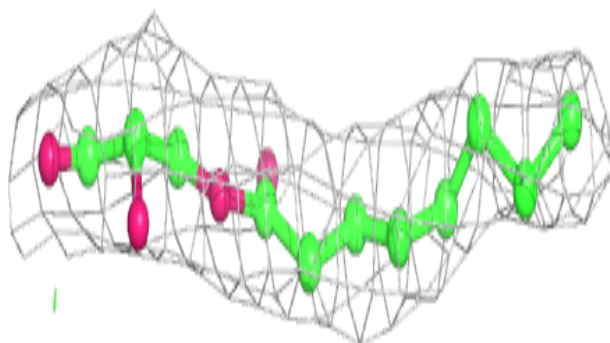
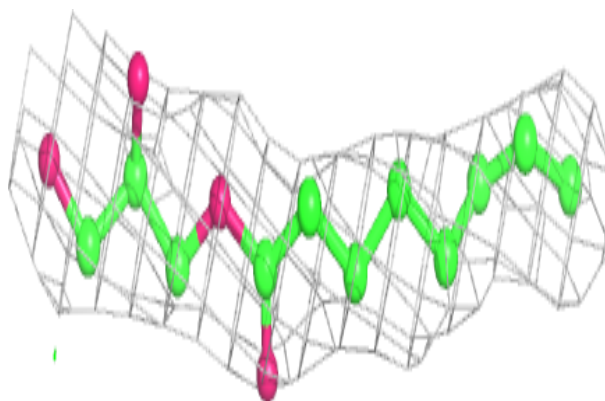
**Electron density around LFA E 308:**

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

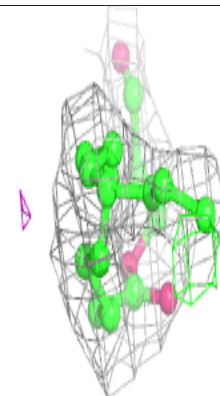
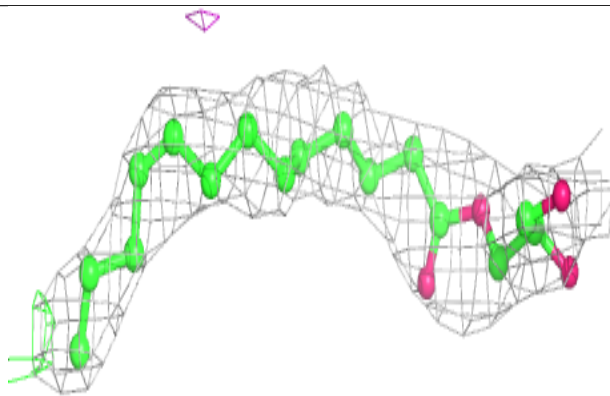
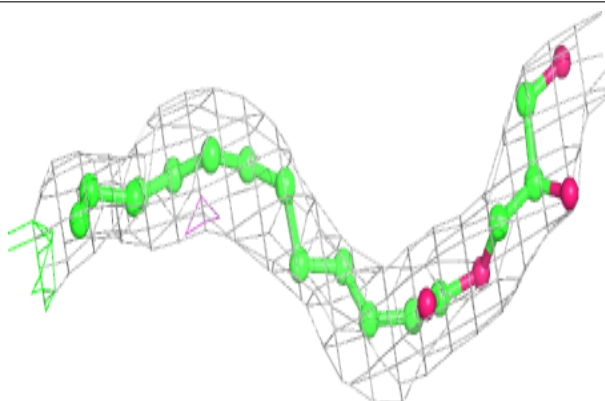


**Electron density around OLC E 303:**

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

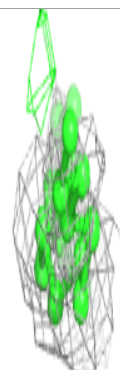
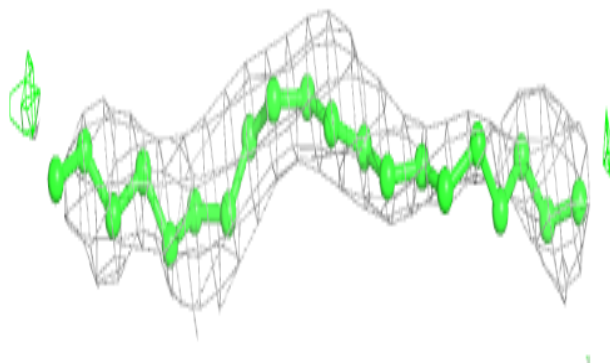
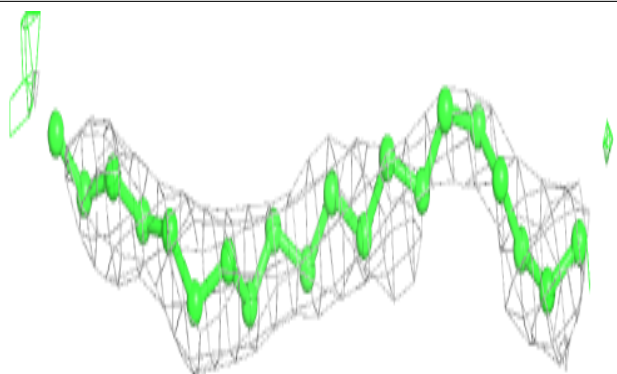
**Electron density around OLC C 302:**

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

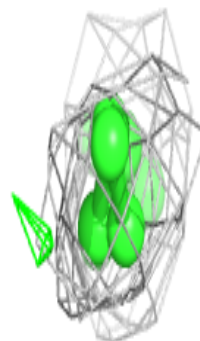
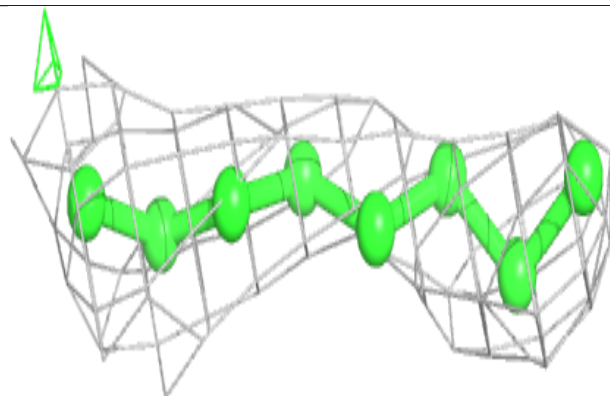
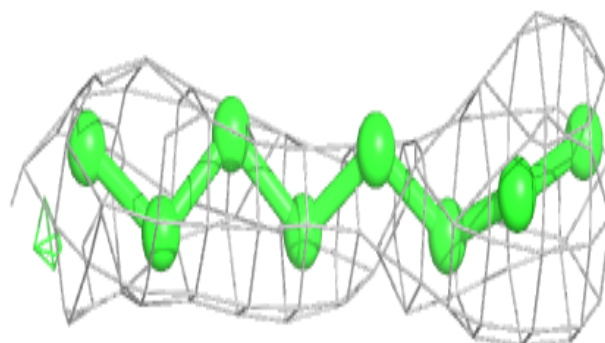


**Electron density around LFA D 307:**

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

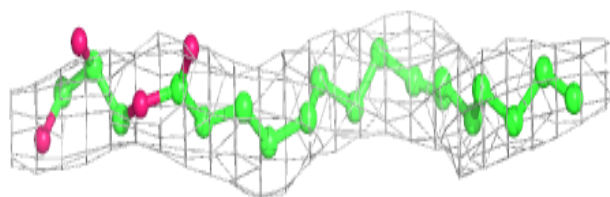
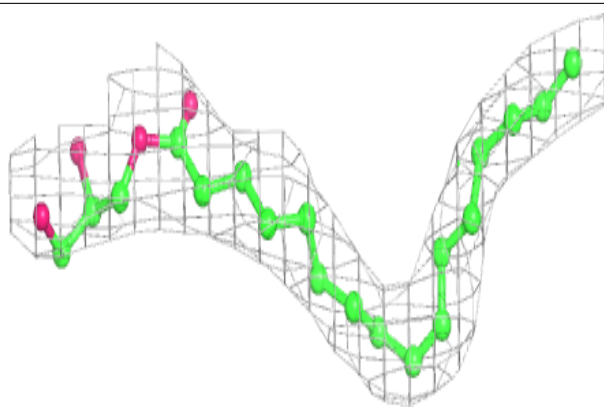
**Electron density around LFA A 304:**

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

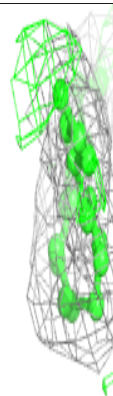
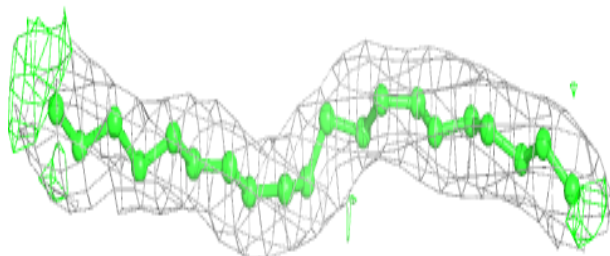
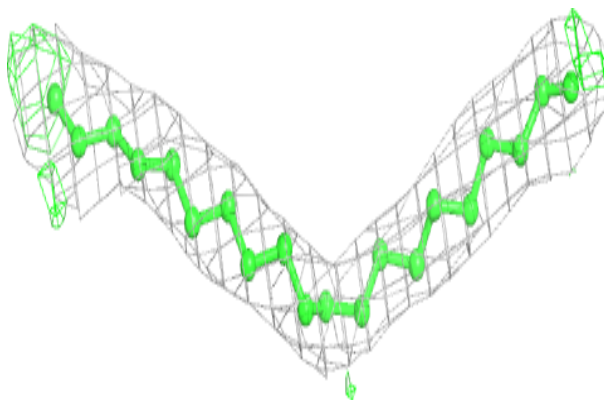


**Electron density around OLC C 305:**

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

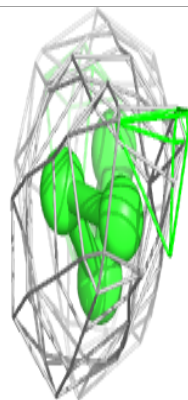
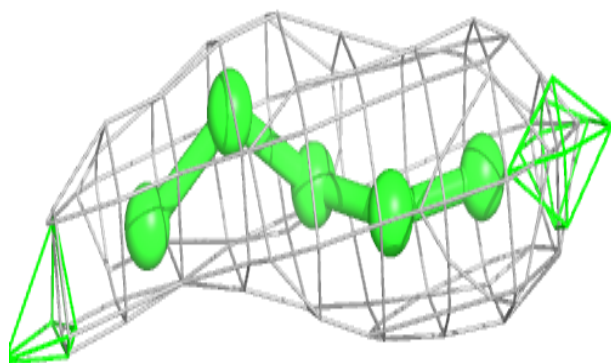
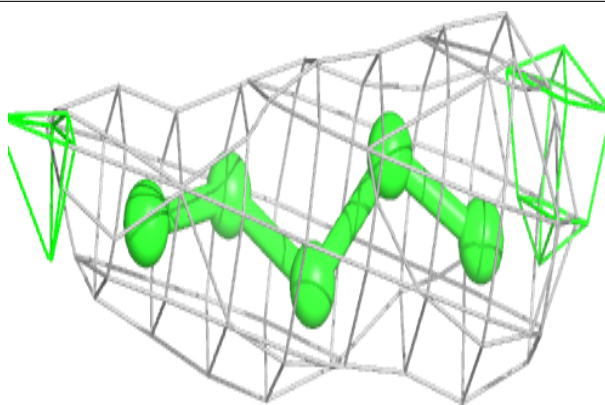
**Electron density around LFA D 301:**

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

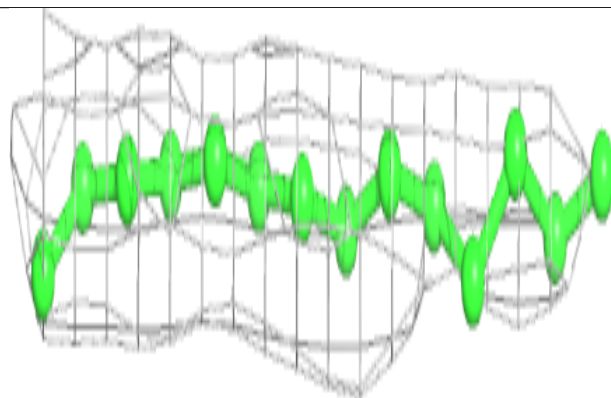
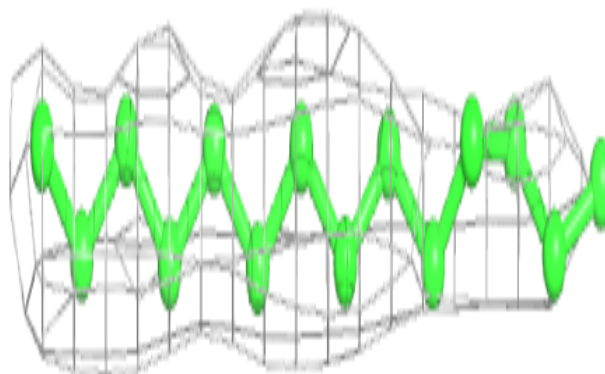


**Electron density around LFA B 307:**

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

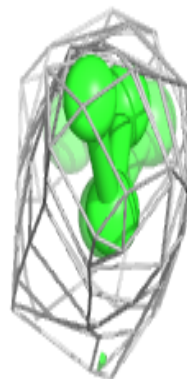
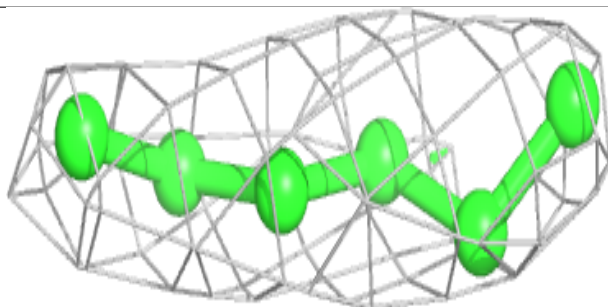
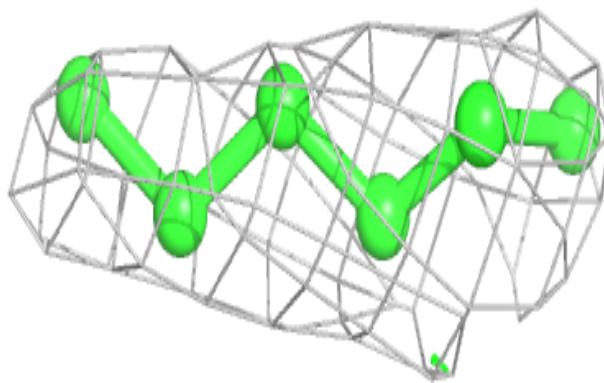
**Electron density around LFA E 314:**

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

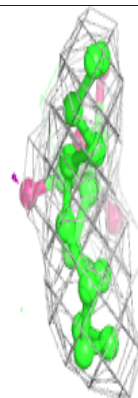
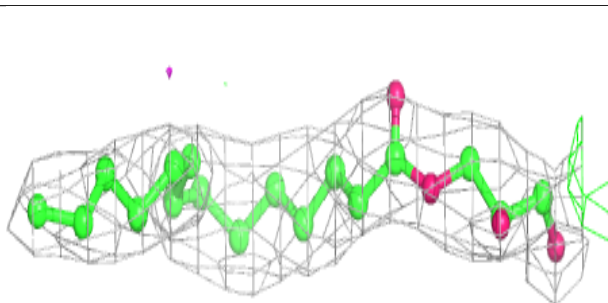
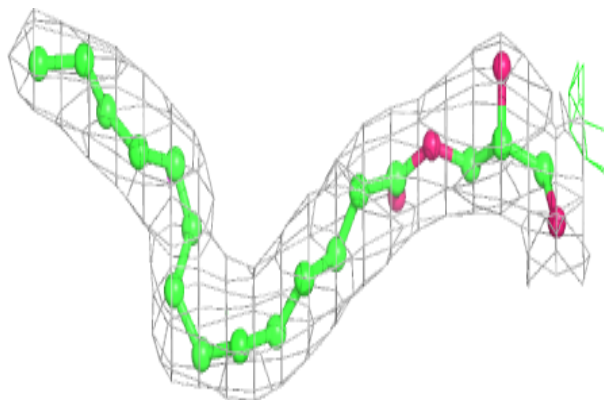


**Electron density around LFA B 310:**

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

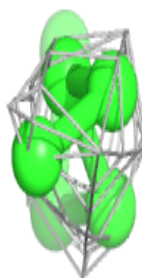
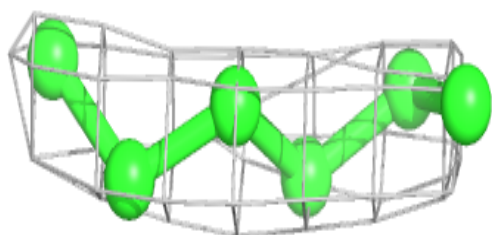
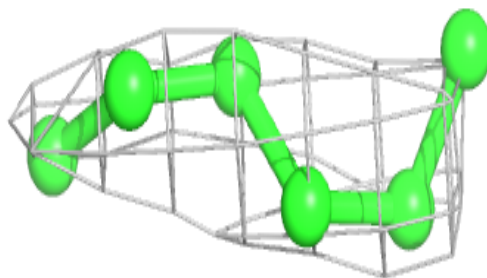
**Electron density around OLC C 301:**

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

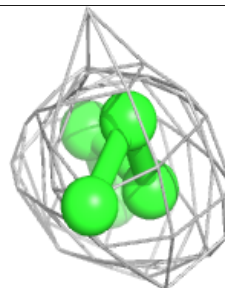
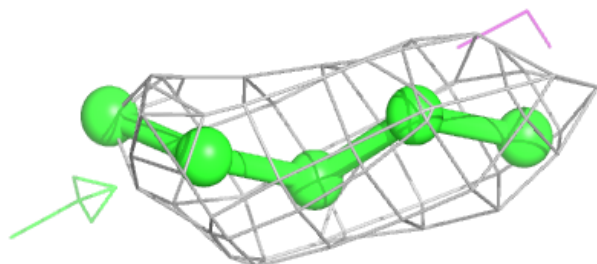
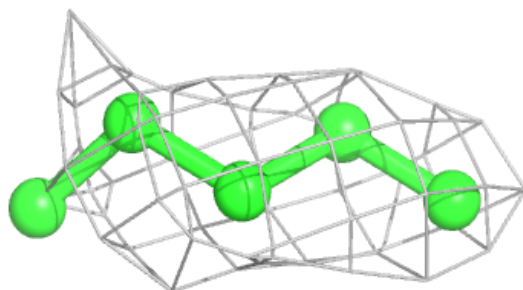


**Electron density around LFA E 306:**

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

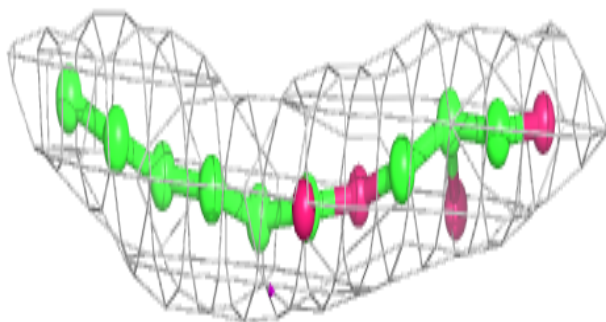
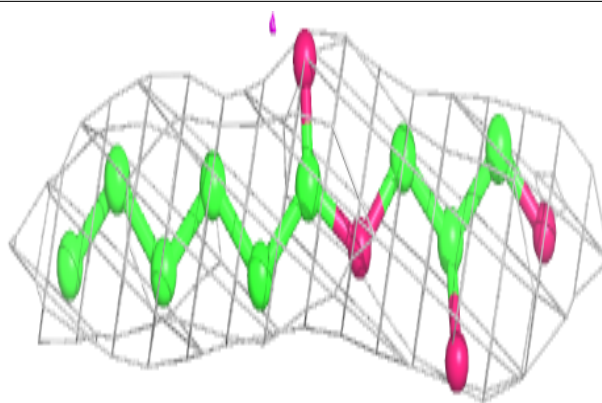
**Electron density around LFA A 305:**

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

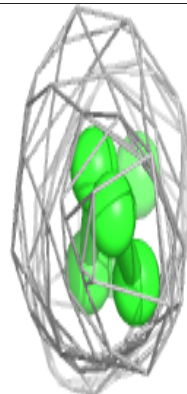
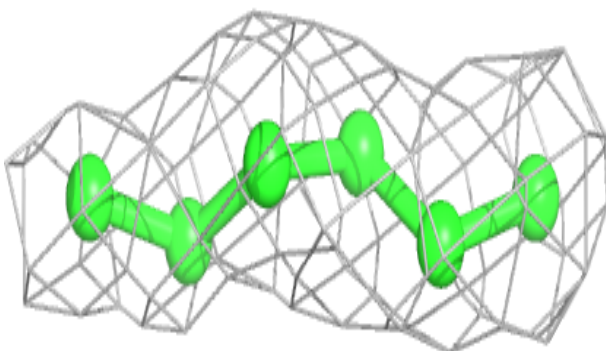
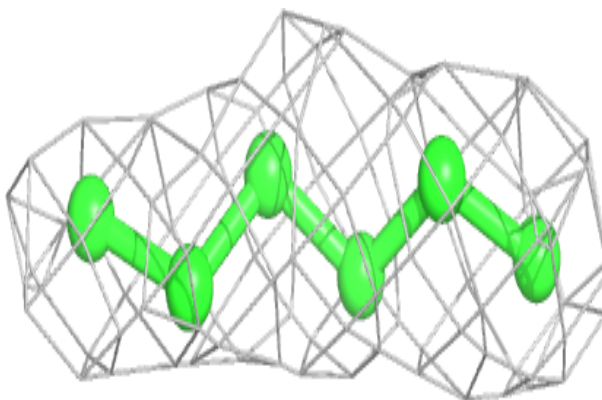


**Electron density around OLC A 302:**

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

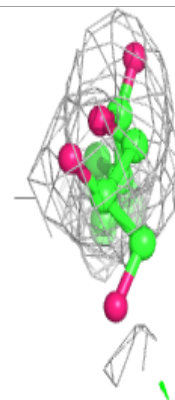
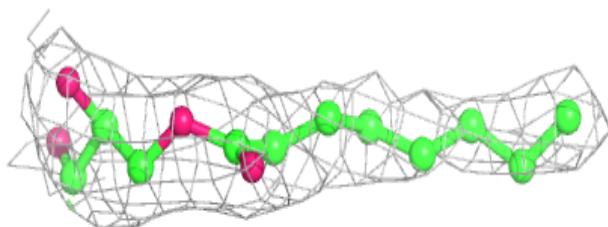
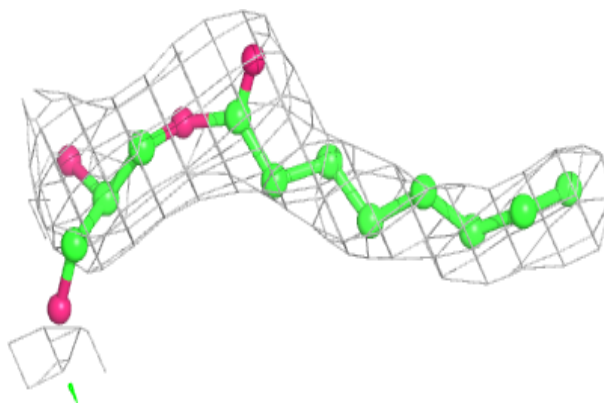
**Electron density around LFA D 311:**

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

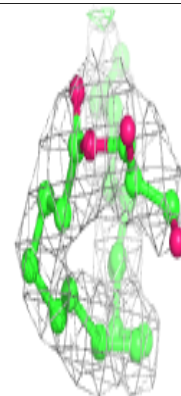
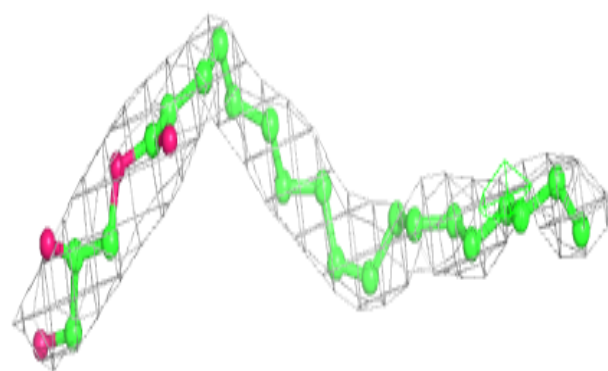
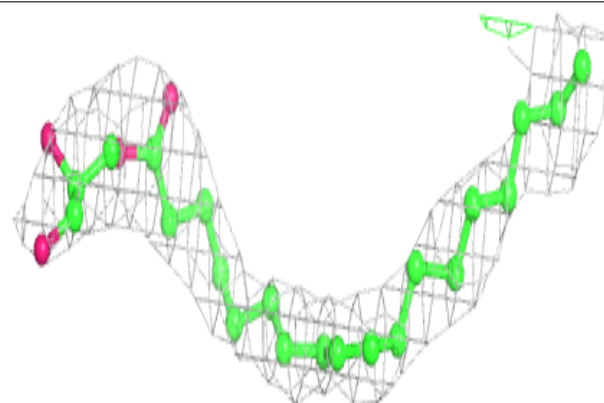


**Electron density around OLC A 303:**

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

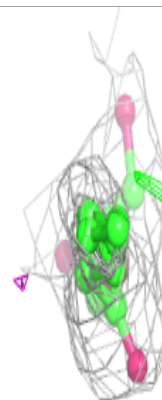
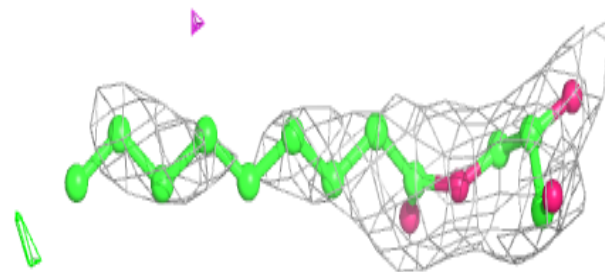
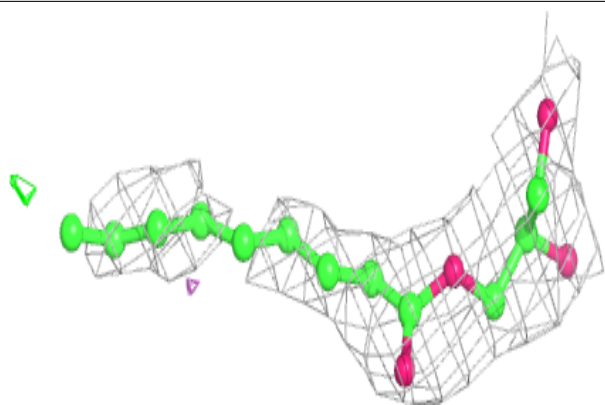
**Electron density around OLC B 301:**

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

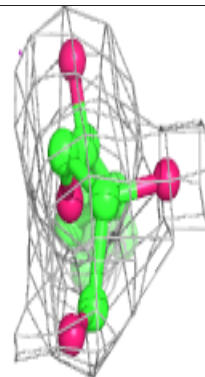
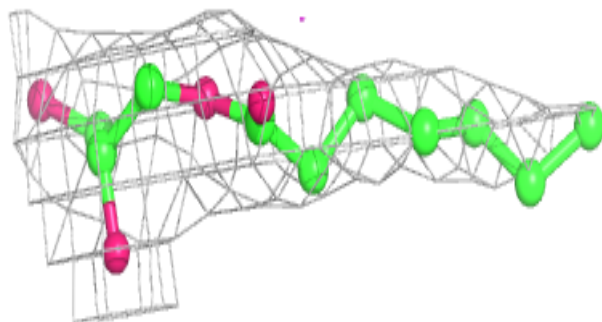
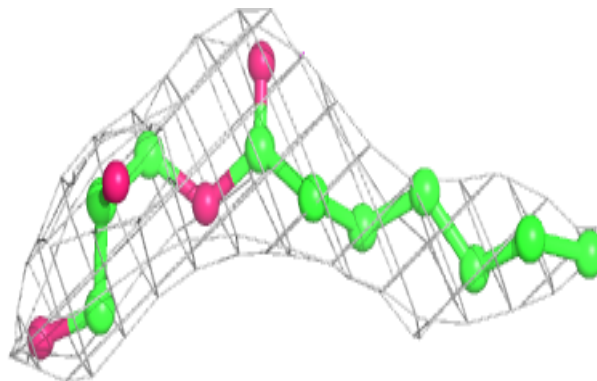


**Electron density around OLC B 304:**

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

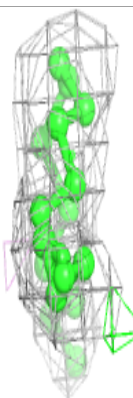
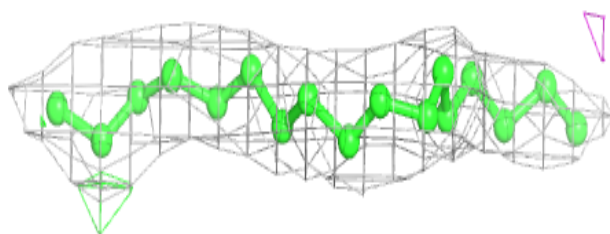
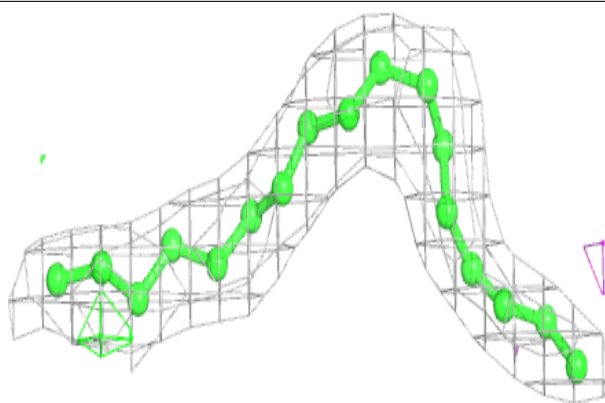
**Electron density around OLC D 304:**

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

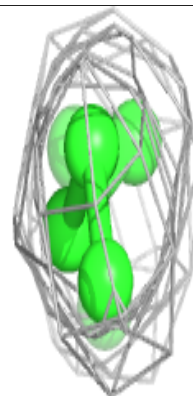
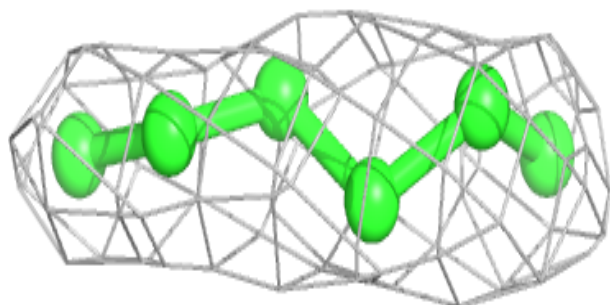
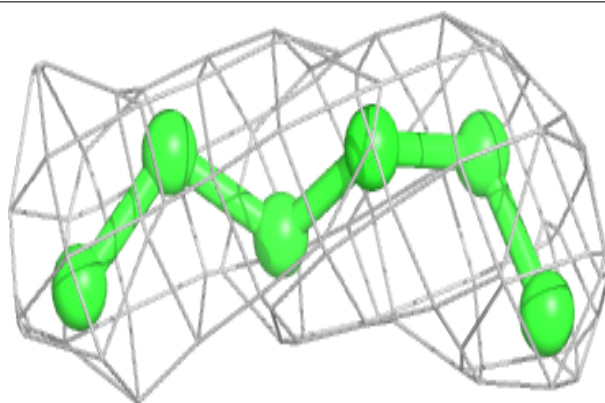


**Electron density around LFA D 309:**

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

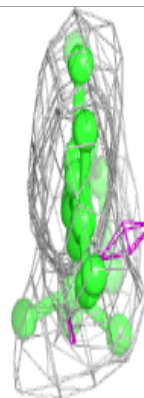
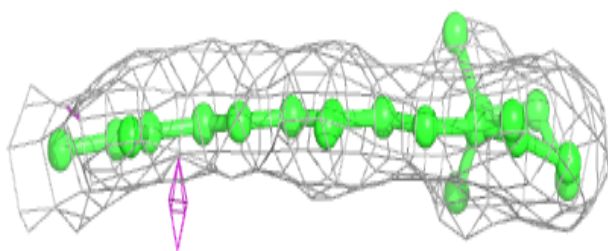
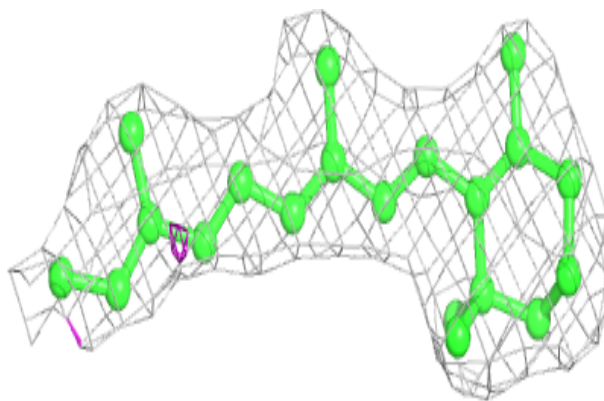
**Electron density around LFA C 315:**

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

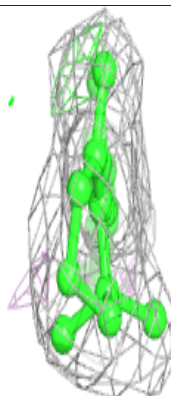
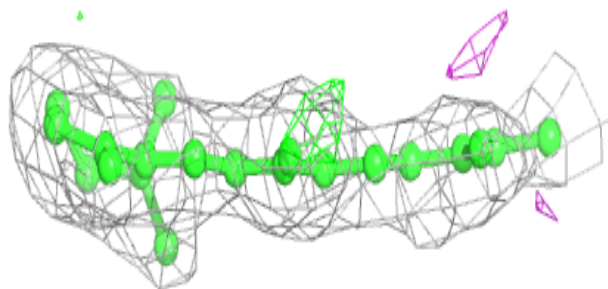
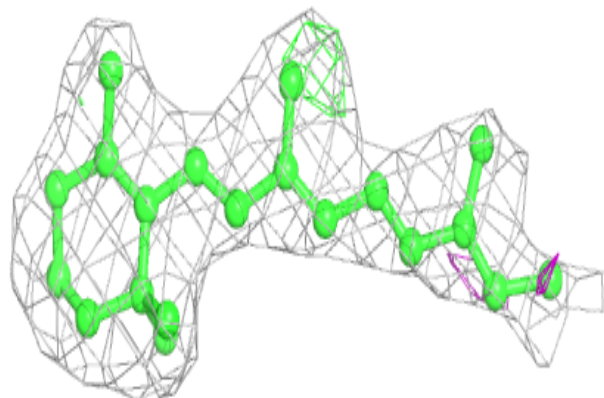


**Electron density around RET A 312:**

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

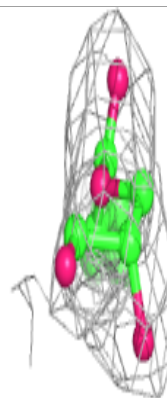
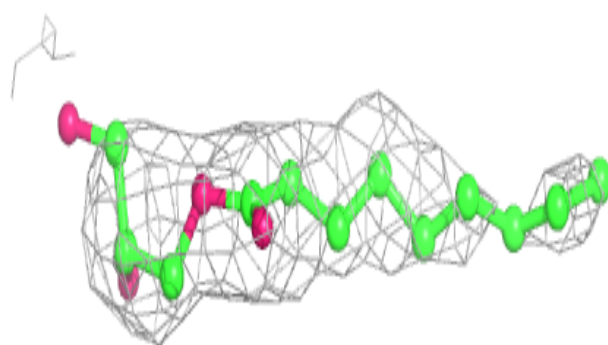
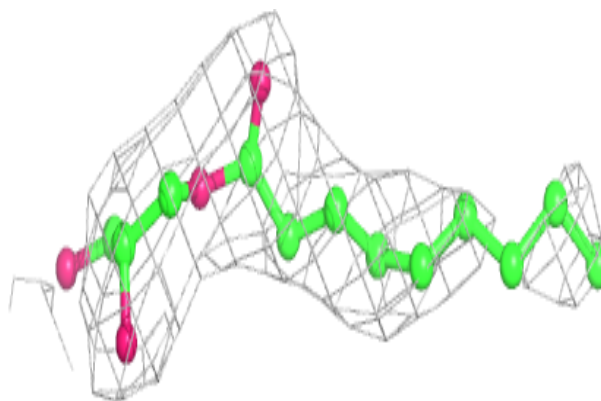
**Electron density around RET E 315:**

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

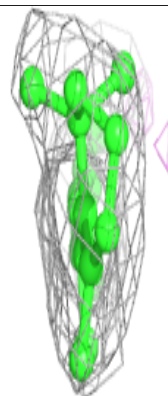
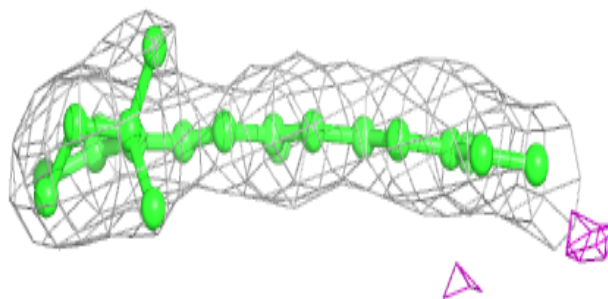
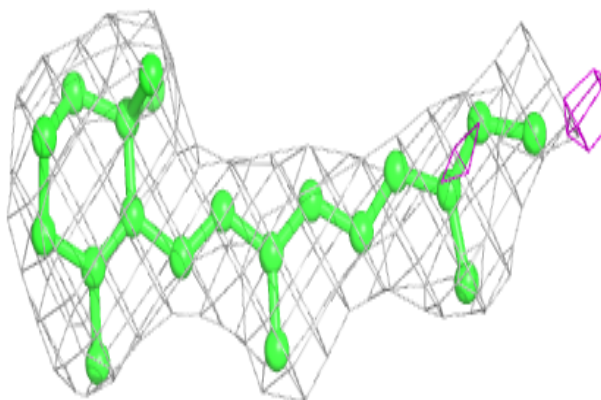


**Electron density around OLC C 308:**

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

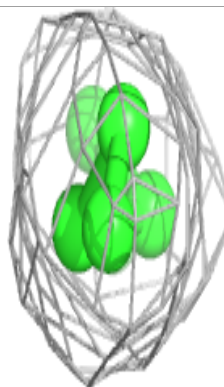
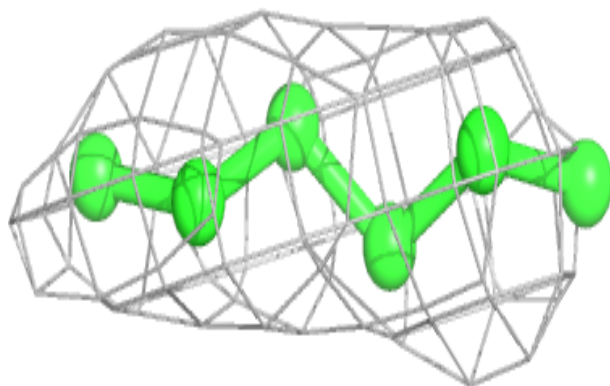
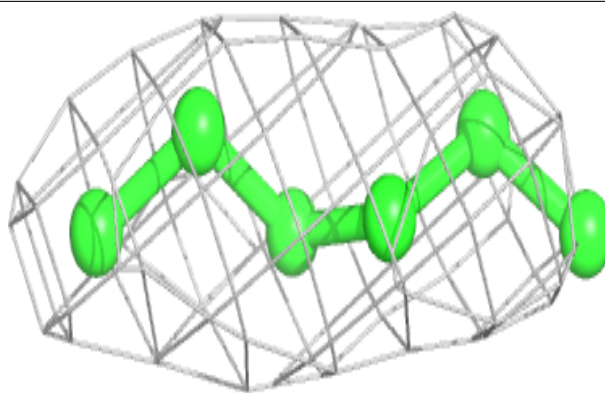
**Electron density around RET B 313:**

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

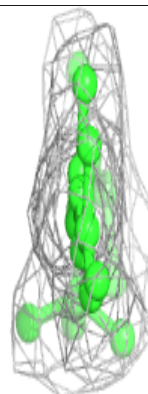
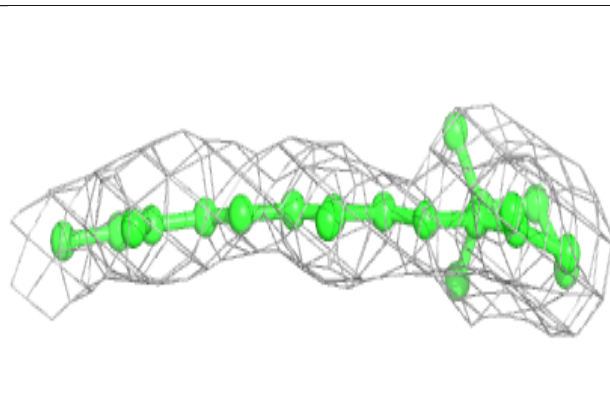
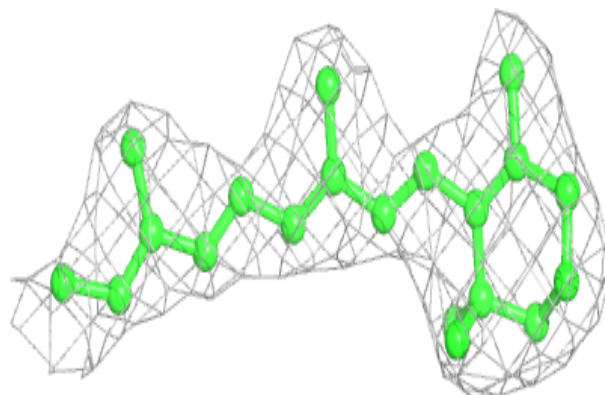


**Electron density around LFA A 308:**

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

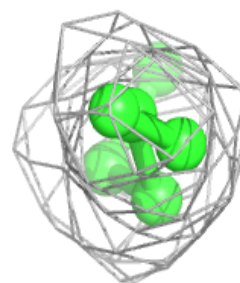
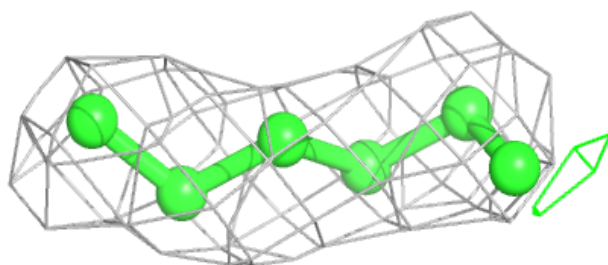
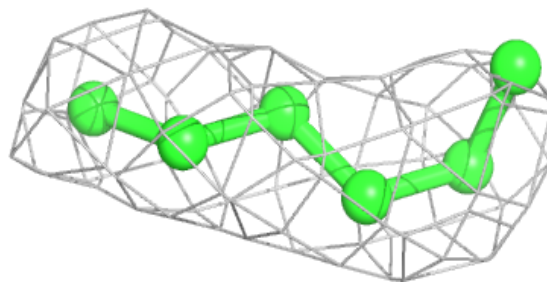
**Electron density around RET C 318:**

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

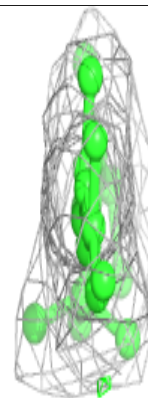
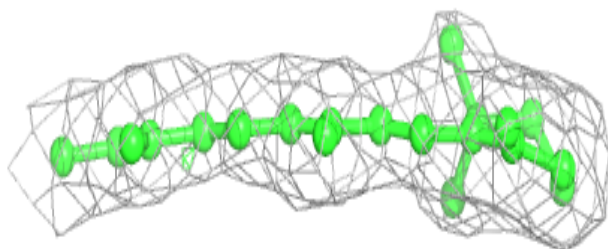
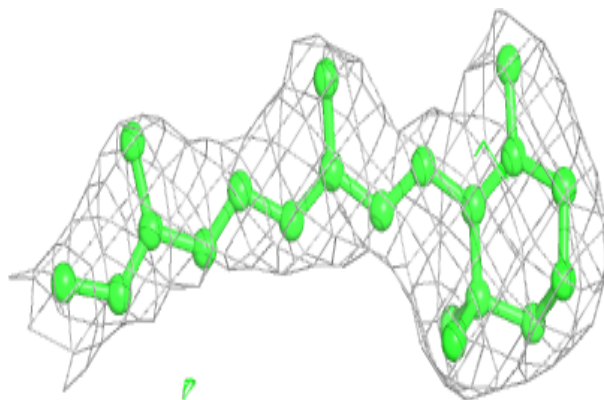


**Electron density around LFA E 310:**

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

**Electron density around RET D 315:**

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



## 6.5 Other polymers

There are no such residues in this entry.