



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:54 PM UTC

PDB ID : 6RF4 / pdb_00006rf4
Title : Crystal structure of the potassium-pumping S254A mutant of the light-driven sodium pump KR2 in the pentameric form, pH 8.0
Authors : Kovalev, K.; Polovinkin, V.; Gushchin, I.; Borshchevskiy, V.; Gordeliy, V.
Deposited on : 2019-04-12
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

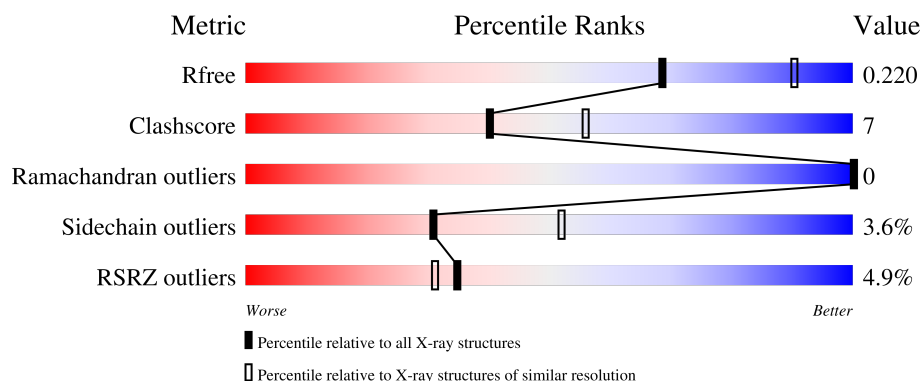
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	288	3% 82% 11% • 5%
1	B	288	6% 81% 14% 5%
1	C	288	4% 79% 14% • 5%
1	D	288	6% 83% 11% • 5%
1	E	288	4% 81% 12% • 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12194 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
			2178	1451	330	388	9			
1	B	273	Total	C	N	O	S	0	1	0
			2172	1446	331	386	9			
1	C	273	Total	C	N	O	S	0	1	0
			2177	1450	330	388	9			
1	D	273	Total	C	N	O	S	0	1	0
			2169	1445	330	385	9			
1	E	273	Total	C	N	O	S	0	1	0
			2171	1447	330	385	9			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	SER	engineered mutation	UNP N0DKS8
A	281	LEU	-	expression tag	UNP N0DKS8
A	282	GLU	-	expression tag	UNP N0DKS8
A	283	HIS	-	expression tag	UNP N0DKS8
A	284	HIS	-	expression tag	UNP N0DKS8
A	285	HIS	-	expression tag	UNP N0DKS8
A	286	HIS	-	expression tag	UNP N0DKS8
A	287	HIS	-	expression tag	UNP N0DKS8
A	288	HIS	-	expression tag	UNP N0DKS8
B	254	ALA	SER	engineered mutation	UNP N0DKS8
B	281	LEU	-	expression tag	UNP N0DKS8
B	282	GLU	-	expression tag	UNP N0DKS8
B	283	HIS	-	expression tag	UNP N0DKS8
B	284	HIS	-	expression tag	UNP N0DKS8
B	285	HIS	-	expression tag	UNP N0DKS8
B	286	HIS	-	expression tag	UNP N0DKS8
B	287	HIS	-	expression tag	UNP N0DKS8
B	288	HIS	-	expression tag	UNP N0DKS8
C	254	ALA	SER	engineered mutation	UNP N0DKS8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	281	LEU	-	expression tag	UNP N0DKS8
C	282	GLU	-	expression tag	UNP N0DKS8
C	283	HIS	-	expression tag	UNP N0DKS8
C	284	HIS	-	expression tag	UNP N0DKS8
C	285	HIS	-	expression tag	UNP N0DKS8
C	286	HIS	-	expression tag	UNP N0DKS8
C	287	HIS	-	expression tag	UNP N0DKS8
C	288	HIS	-	expression tag	UNP N0DKS8
D	254	ALA	SER	engineered mutation	UNP N0DKS8
D	281	LEU	-	expression tag	UNP N0DKS8
D	282	GLU	-	expression tag	UNP N0DKS8
D	283	HIS	-	expression tag	UNP N0DKS8
D	284	HIS	-	expression tag	UNP N0DKS8
D	285	HIS	-	expression tag	UNP N0DKS8
D	286	HIS	-	expression tag	UNP N0DKS8
D	287	HIS	-	expression tag	UNP N0DKS8
D	288	HIS	-	expression tag	UNP N0DKS8
E	254	ALA	SER	engineered mutation	UNP N0DKS8
E	281	LEU	-	expression tag	UNP N0DKS8
E	282	GLU	-	expression tag	UNP N0DKS8
E	283	HIS	-	expression tag	UNP N0DKS8
E	284	HIS	-	expression tag	UNP N0DKS8
E	285	HIS	-	expression tag	UNP N0DKS8
E	286	HIS	-	expression tag	UNP N0DKS8
E	287	HIS	-	expression tag	UNP N0DKS8
E	288	HIS	-	expression tag	UNP N0DKS8

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



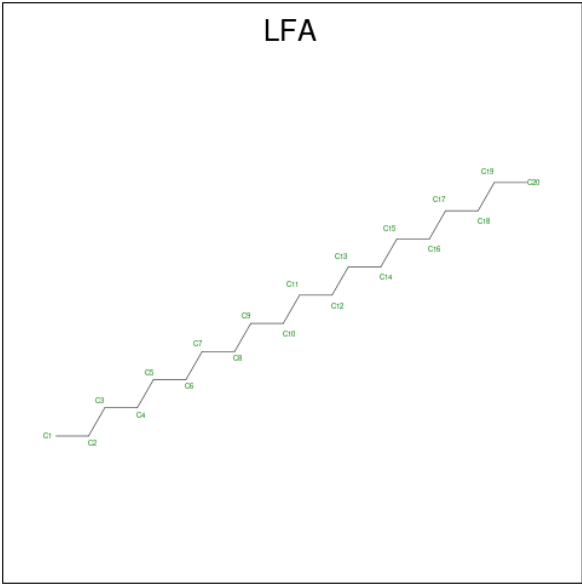
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C		0	0
			14	14			
2	A	1	Total	C	O	0	0
			13	9	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	A	1	Total	C		0	0
			14	14			
2	B	1	Total	C	O	0	0
			22	18	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			16	12	4		
2	C	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			14	10	4		
2	C	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			23	19	4		
2	C	1	Total	C	O	0	0
			25	21	4		
2	C	1	Total	C	O	0	0
			25	21	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 14 10 4	0	0
2	E	1	Total C 12 12	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 25 21 4	0	0

- Molecule 3 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 20 20	0	0
3	B	1	Total C 20 20	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 11 11	0	0
3	C	1	Total C 4 4	0	0
3	C	1	Total C 4 4	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

Continued on next page...

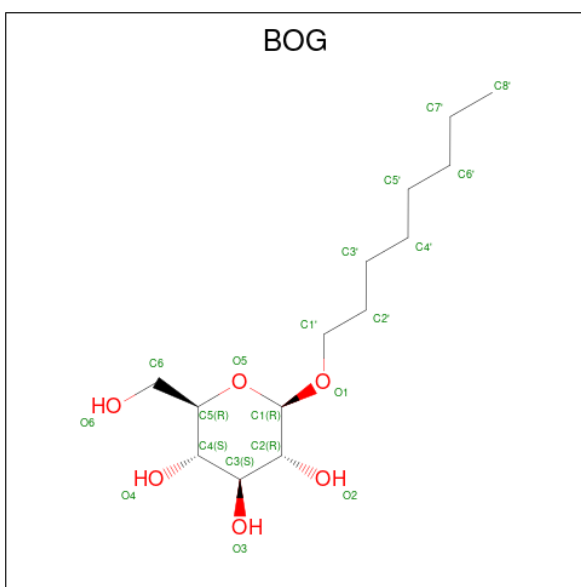
Continued from previous page...

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

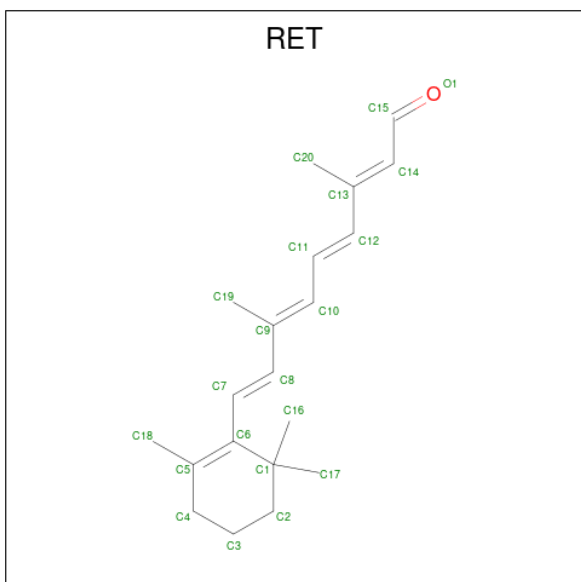
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

- Molecule 5 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



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

- Molecule 6 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$).



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

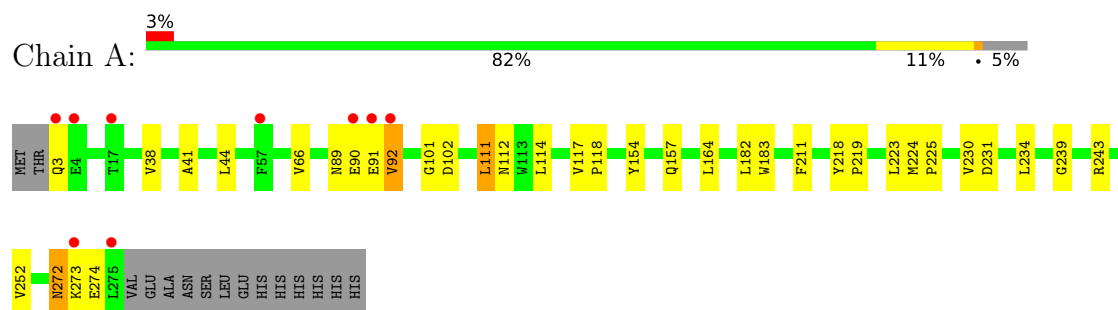
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	62	Total O 62 62	0	0
7	B	69	Total O 69 69	0	0
7	C	75	Total O 75 75	0	0
7	D	59	Total O 59 59	0	0
7	E	63	Total O 63 63	0	0

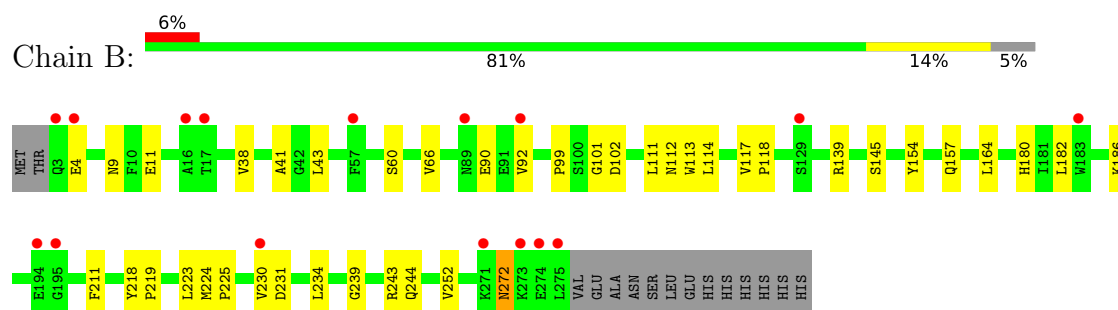
3 Residue-property plots [i](#)

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

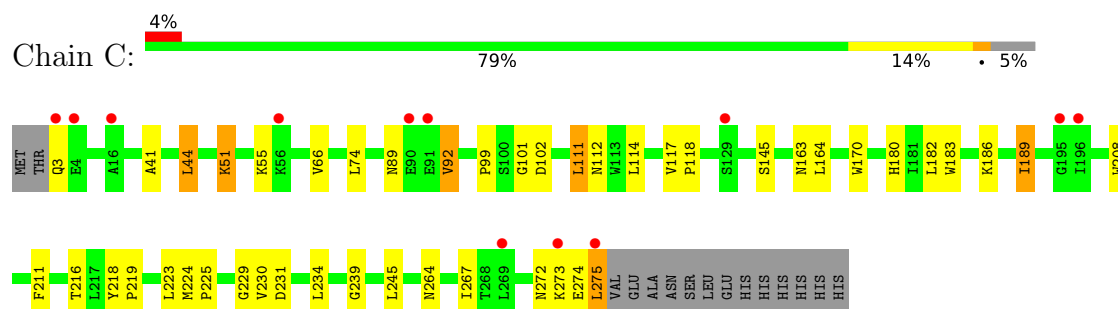
- Molecule 1: Sodium pumping rhodopsin



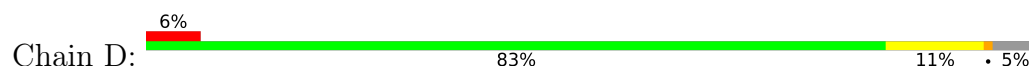
- Molecule 1: Sodium pumping rhodopsin

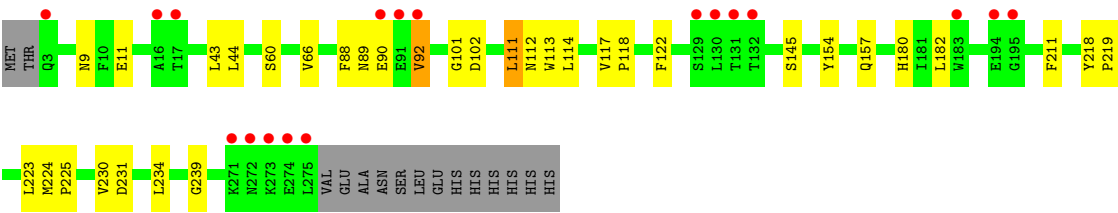


- Molecule 1: Sodium pumping rhodopsin

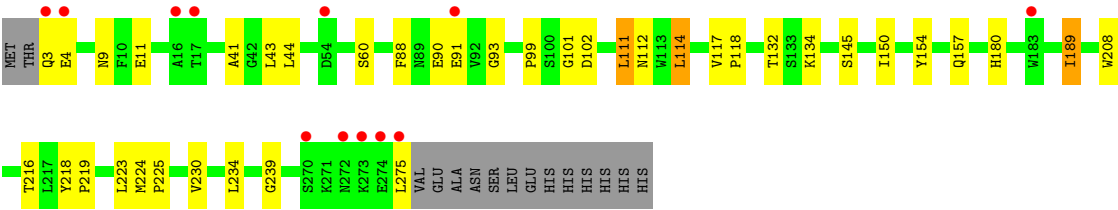
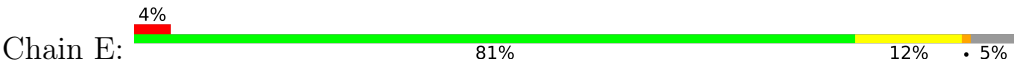


- Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.40Å 240.04Å 135.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.91 – 2.40 44.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.91-2.40) 99.8 (44.91-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.181 , 0.212 0.190 , 0.220	Depositor DCC
R_{free} test set	4223 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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	0.95	EDS
Total number of atoms	12194	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/2236	0.91	0/3040
1	B	0.47	0/2230	0.90	0/3033
1	C	0.47	0/2235	0.90	0/3039
1	D	0.46	0/2227	0.92	0/3028
1	E	0.47	0/2229	0.90	0/3031
All	All	0.47	0/11157	0.91	0/15171

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
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	B	243	ARG	Sidechain
1	C	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	2178	0	2154	25	0
1	B	2172	0	2149	33	0
1	C	2177	0	2152	35	0
1	D	2169	0	2142	25	0
1	E	2171	0	2149	24	0
2	A	56	0	78	0	0
2	B	58	0	79	4	0
2	C	260	0	370	9	0
2	D	32	0	40	0	0
2	E	53	0	84	1	0
3	A	61	0	119	1	0
3	B	37	0	74	1	0
3	C	74	0	147	5	0
3	D	98	0	198	0	0
3	E	65	0	127	2	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	3	0
5	D	20	0	28	2	0
5	E	20	0	28	0	0
6	A	20	0	27	6	0
6	B	20	0	27	5	0
6	C	20	0	27	5	0
6	D	20	0	27	6	0
6	E	20	0	27	5	0
7	A	62	0	0	0	0
7	B	69	0	0	2	0
7	C	75	0	0	2	0
7	D	59	0	0	2	0
7	E	63	0	0	1	0
All	All	12194	0	12337	159	0

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

All (159) 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:HD22	1:B:272:ASN:N	1.69	0.87
1:A:272:ASN:HD22	1:A:272:ASN:N	1.71	0.87
6:D:312:RET:H161	6:D:312:RET:H8	1.60	0.83
6:B:309:RET:H161	6:B:309:RET:H8	1.59	0.82
6:A:313:RET:H8	6:A:313:RET:H161	1.62	0.82
6:E:312:RET:H161	6:E:312:RET:H8	1.64	0.80
6:C:323:RET:H8	6:C:323:RET:H161	1.63	0.79
1:D:231:ASP:N	5:D:311:BOG:O6	2.21	0.70
1:E:60:SER:OG	7:E:401:HOH:O	2.10	0.69
1:A:164:LEU:HD21	5:A:310:BOG:H2'1	1.74	0.69
1:D:145:SER:OG	1:D:180:HIS:HD2	1.76	0.69
1:C:145:SER:OG	1:C:180:HIS:HD2	1.77	0.68
1:E:145:SER:OG	1:E:180:HIS:HD2	1.76	0.68
1:B:145:SER:OG	1:B:180:HIS:HD2	1.76	0.68
1:B:272:ASN:N	1:B:272:ASN:ND2	2.41	0.67
1:D:60:SER:OG	7:D:401:HOH:O	2.15	0.63
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.80	0.63
1:B:231:ASP:H	5:B:308:BOG:HO6	1.44	0.63
6:D:312:RET:H161	6:D:312:RET:C8	2.29	0.62
6:B:309:RET:H161	6:B:309:RET:C8	2.29	0.61
6:E:312:RET:H161	6:E:312:RET:C8	2.31	0.61
1:C:189:ILE:HD12	1:C:208:TRP:HB2	1.83	0.60
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.84	0.60
1:C:229:GLY:HA3	2:C:310:OLC:H22	1.83	0.59
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.83	0.59
1:A:234:LEU:O	1:A:239:GLY:HA3	2.03	0.59
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.85	0.59
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.85	0.59
1:D:234:LEU:O	1:D:239:GLY:HA3	2.03	0.59
1:A:224:MET:N	1:A:225:PRO:HD2	2.18	0.59
6:C:323:RET:H161	6:C:323:RET:C8	2.32	0.58
1:C:224:MET:N	1:C:225:PRO:HD2	2.18	0.58
1:E:234:LEU:O	1:E:239:GLY:HA3	2.03	0.58
1:E:189:ILE:HD12	1:E:208:TRP:HB2	1.86	0.57
1:C:234:LEU:O	1:C:239:GLY:HA3	2.04	0.57
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.85	0.57
1:E:224:MET:N	1:E:225:PRO:HD2	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:MET:N	1:D:225:PRO:HD2	2.19	0.57
1:B:234:LEU:O	1:B:239:GLY:HA3	2.04	0.56
1:B:224:MET:N	1:B:225:PRO:HD2	2.20	0.56
1:C:51:LYS:HD3	7:C:459:HOH:O	2.03	0.56
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.88	0.56
1:B:231:ASP:N	5:B:308:BOG:O6	2.22	0.56
3:E:306:LFA:H152	3:E:307:LFA:H201	1.86	0.55
1:C:164:LEU:HD21	5:C:321:BOG:H2'1	1.87	0.55
1:E:101:GLY:O	1:E:102:ASP:HB2	2.06	0.55
6:A:313:RET:H161	6:A:313:RET:C8	2.30	0.55
1:A:183:TRP:HE3	3:A:304:LFA:H162	1.72	0.54
1:C:231:ASP:N	5:C:321:BOG:O6	2.31	0.54
6:C:323:RET:H8	6:C:323:RET:H171	1.90	0.54
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.90	0.53
1:A:101:GLY:O	1:A:102:ASP:HB2	2.09	0.52
1:C:101:GLY:O	1:C:102:ASP:HB2	2.09	0.52
1:E:111:LEU:O	1:E:114:LEU:HB2	2.10	0.52
1:B:139:ARG:NH1	2:B:301:OLC:H24A	2.25	0.52
6:D:312:RET:H8	6:D:312:RET:H171	1.92	0.52
6:B:309:RET:H8	6:B:309:RET:H171	1.92	0.52
1:B:101:GLY:O	1:B:102:ASP:HB2	2.11	0.51
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.92	0.51
1:A:272:ASN:N	1:A:272:ASN:ND2	2.43	0.51
6:E:312:RET:H8	6:E:312:RET:H171	1.91	0.51
6:A:313:RET:H8	6:A:313:RET:H171	1.93	0.51
1:C:223:LEU:C	1:C:225:PRO:HD2	2.35	0.51
1:C:183:TRP:CE3	3:C:315:LFA:H41	2.45	0.51
1:A:223:LEU:C	1:A:225:PRO:HD2	2.35	0.51
1:B:223:LEU:C	1:B:225:PRO:HD2	2.36	0.51
1:A:3:GLN:NE2	1:E:90:GLU:OE1	2.44	0.50
1:E:223:LEU:C	1:E:225:PRO:HD2	2.36	0.50
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.93	0.50
1:D:223:LEU:C	1:D:225:PRO:HD2	2.37	0.50
1:D:231:ASP:H	5:D:311:BOG:HO6	1.55	0.49
1:B:139:ARG:HH11	2:B:301:OLC:H24A	1.77	0.49
1:D:101:GLY:O	1:D:102:ASP:HB2	2.14	0.48
1:A:44:LEU:HD21	1:B:43:LEU:HD11	1.95	0.48
2:C:313:OLC:O23	2:C:313:OLC:H2	2.14	0.47
1:B:186:LYS:HG2	3:B:305:LFA:H192	1.96	0.47
1:D:60:SER:CB	7:D:401:HOH:O	2.63	0.47
6:C:323:RET:C8	6:C:323:RET:H171	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:SER:HB3	7:B:409:HOH:O	2.14	0.46
1:C:231:ASP:H	5:C:321:BOG:HO6	1.60	0.46
1:C:180:HIS:CD2	2:C:307:OLC:H7A	2.51	0.46
6:D:312:RET:C8	6:D:312:RET:H171	2.46	0.46
3:E:306:LFA:H141	3:E:307:LFA:C20	2.46	0.46
1:D:44:LEU:HD21	1:E:43:LEU:HD11	1.97	0.45
1:C:216:THR:HG22	3:C:319:LFA:H201	1.98	0.45
6:B:309:RET:C8	6:B:309:RET:H171	2.46	0.45
1:C:163:ASN:HD22	2:C:312:OLC:C24	2.30	0.45
6:A:313:RET:C8	6:A:313:RET:H171	2.46	0.45
6:E:312:RET:C8	6:E:312:RET:H171	2.45	0.45
1:C:170:TRP:CH2	2:C:308:OLC:H9	2.52	0.45
1:D:90:GLU:OE2	1:E:3:GLN:NE2	2.50	0.45
1:C:55:LYS:NZ	7:C:408:HOH:O	2.49	0.43
1:B:38:VAL:HG11	1:B:252:VAL:HG22	2.00	0.43
2:C:304:OLC:H24	3:C:316:LFA:C13	2.49	0.43
1:C:216:THR:HG22	3:C:319:LFA:C20	2.49	0.43
1:B:145:SER:OG	1:B:180:HIS:CD2	2.65	0.43
1:B:139:ARG:HH11	2:B:301:OLC:C24	2.32	0.43
2:C:305:OLC:H3A	2:C:305:OLC:H6	1.79	0.43
1:A:90:GLU:HG2	1:B:99:PRO:HG3	2.01	0.43
1:B:154:TYR:O	1:B:157:GLN:HG3	2.18	0.43
1:D:114:LEU:O	1:D:118:PRO:HG2	2.19	0.43
1:B:114:LEU:O	1:B:118:PRO:HG2	2.19	0.43
1:C:114:LEU:O	1:C:118:PRO:HG2	2.19	0.43
1:D:154:TYR:O	1:D:157:GLN:HG3	2.19	0.42
1:A:114:LEU:O	1:A:118:PRO:HG2	2.19	0.42
1:C:186:LYS:HG2	3:C:315:LFA:H51	2.00	0.42
1:B:139:ARG:NH1	2:B:301:OLC:C24	2.83	0.42
1:D:88:PHE:CD2	1:E:99:PRO:HB3	2.55	0.42
1:A:224:MET:N	1:A:225:PRO:CD	2.83	0.42
1:E:224:MET:N	1:E:225:PRO:CD	2.83	0.42
6:E:312:RET:H7	6:E:312:RET:H181	1.72	0.42
1:E:101:GLY:O	1:E:102:ASP:CB	2.67	0.42
1:E:114:LEU:O	1:E:118:PRO:HG2	2.19	0.42
1:A:182:LEU:HD23	1:A:211:PHE:HE2	1.84	0.42
1:C:267:ILE:HG21	1:C:275:LEU:HB3	2.02	0.42
6:A:313:RET:H11	6:A:313:RET:H191	1.95	0.42
1:A:38:VAL:HG11	1:A:252:VAL:HG22	2.02	0.41
1:A:154:TYR:O	1:A:157:GLN:HG3	2.19	0.41
1:B:113:TRP:CD1	6:B:309:RET:H14	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HD23	1:B:211:PHE:HE2	1.84	0.41
1:B:90:GLU:HG2	1:C:99:PRO:HG3	2.03	0.41
1:C:89:ASN:OD1	1:C:92:VAL:HG13	2.20	0.41
1:C:245:LEU:HD11	2:C:314:OLC:H5A	2.02	0.41
6:C:323:RET:H7	6:C:323:RET:H181	1.72	0.41
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.20	0.41
1:E:114:LEU:HD12	1:E:114:LEU:HA	1.81	0.41
1:C:264:ASN:HD22	2:C:305:OLC:H24	1.85	0.41
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.55	0.41
1:A:101:GLY:O	1:A:102:ASP:CB	2.68	0.41
1:C:224:MET:N	1:C:225:PRO:CD	2.82	0.41
1:D:182:LEU:HD23	1:D:211:PHE:HE2	1.85	0.41
1:D:118:PRO:O	1:D:122:PHE:HB2	2.21	0.41
1:E:154:TYR:O	1:E:157:GLN:HG3	2.21	0.41
1:A:218:TYR:N	1:A:219:PRO:HD2	2.36	0.41
6:A:313:RET:H7	6:A:313:RET:H181	1.71	0.41
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.20	0.41
1:B:218:TYR:N	1:B:219:PRO:HD2	2.35	0.41
1:C:182:LEU:HD23	1:C:211:PHE:HE2	1.85	0.41
1:D:111:LEU:O	1:D:114:LEU:HB2	2.21	0.41
6:D:312:RET:H11	6:D:312:RET:H191	1.92	0.41
1:E:218:TYR:N	1:E:219:PRO:HD2	2.36	0.41
1:D:218:TYR:N	1:D:219:PRO:HD2	2.35	0.41
1:B:224:MET:N	1:B:225:PRO:CD	2.84	0.40
1:C:111:LEU:O	1:C:114:LEU:HB2	2.21	0.40
1:D:224:MET:N	1:D:225:PRO:CD	2.84	0.40
1:A:89:ASN:OD1	1:A:92:VAL:HG13	2.21	0.40
1:A:90:GLU:CG	1:B:99:PRO:HG3	2.51	0.40
1:C:44:LEU:HD11	1:D:43:LEU:HD11	2.04	0.40
1:C:218:TYR:N	1:C:219:PRO:HD2	2.36	0.40
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.21	0.40
1:A:231:ASP:H	5:A:310:BOG:HO6	1.64	0.40
1:B:90:GLU:CG	1:C:99:PRO:HG3	2.51	0.40
1:C:74:LEU:HD22	1:C:74:LEU:HA	1.95	0.40
1:D:89:ASN:OD1	1:D:92:VAL:HG13	2.21	0.40
1:E:216:THR:O	1:E:219:PRO:HG2	2.22	0.40
1:A:111:LEU:O	1:A:114:LEU:HB2	2.21	0.40
1:B:244:GLN:HG2	7:B:405:HOH:O	2.21	0.40
1:D:113:TRP:CD1	6:D:312:RET:H14	2.57	0.40
2:E:303:OLC:H11A	2:E:303:OLC:H8	1.66	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	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	B	272/288 (94%)	265 (97%)	7 (3%)	0	100	100
1	C	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	D	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
1	E	272/288 (94%)	266 (98%)	6 (2%)	0	100	100
All	All	1360/1440 (94%)	1329 (98%)	31 (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	230/247 (93%)	222 (96%)	8 (4%)	32	53
1	B	230/247 (93%)	223 (97%)	7 (3%)	36	58
1	C	230/247 (93%)	219 (95%)	11 (5%)	23	40
1	D	228/247 (92%)	224 (98%)	4 (2%)	51	73
1	E	229/247 (93%)	218 (95%)	11 (5%)	23	40
All	All	1147/1235 (93%)	1106 (96%)	41 (4%)	31	52

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLU
1	A	92	VAL
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	4	GLU
1	B	92	VAL
1	B	111	LEU
1	B	112	ASN
1	B	164	LEU
1	B	230	VAL
1	B	272	ASN
1	C	3	GLN
1	C	44	LEU
1	C	51	LYS
1	C	92	VAL
1	C	111	LEU
1	C	112	ASN
1	C	189	ILE
1	C	230	VAL
1	C	273	LYS
1	C	274	GLU
1	C	275	LEU
1	D	92	VAL
1	D	111	LEU
1	D	112	ASN
1	D	230	VAL
1	E	4	GLU
1	E	44	LEU
1	E	91	GLU
1	E	111	LEU
1	E	112	ASN
1	E	114	LEU
1	E	132	THR
1	E	134	LYS
1	E	189	ILE
1	E	230	VAL
1	E	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	272	ASN
1	B	180	HIS
1	B	272	ASN
1	C	3	GLN
1	C	141	GLN
1	C	180	HIS
1	D	141	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 5 are monoatomic - leaving 64 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	$\# Z > 2$
3	LFA	E	306	-	13,13,19	0.30	0	12,12,18	0.48	0
3	LFA	D	304	-	19,19,19	0.27	0	18,18,18	0.53	0
3	LFA	D	306	-	7,7,19	0.31	0	6,6,18	0.36	0
2	OLC	A	303	-	14,14,24	1.21	1 (7%)	15,15,25	1.15	2 (13%)
3	LFA	E	305	-	7,7,19	0.29	0	6,6,18	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BOG	E	310	-	20,20,20	0.54	0	25,25,25	0.57	0
2	OLC	E	301	-	11,11,24	0.28	0	10,10,25	0.52	0
2	OLC	C	314	-	15,15,24	1.22	1 (6%)	16,16,25	1.02	1 (6%)
3	LFA	B	302	-	19,19,19	0.36	0	18,18,18	0.39	0
2	OLC	C	304	-	13,13,24	1.29	1 (7%)	14,14,25	1.06	1 (7%)
2	OLC	D	301	-	17,17,24	1.12	1 (5%)	18,18,25	1.01	1 (5%)
2	OLC	B	301	-	21,21,24	1.00	1 (4%)	22,22,25	0.94	1 (4%)
3	LFA	D	308	-	6,6,19	0.31	0	5,5,18	0.40	0
2	OLC	C	301	-	20,20,24	1.02	1 (5%)	21,21,25	1.01	1 (4%)
2	OLC	C	310	-	15,15,24	1.22	1 (6%)	16,16,25	1.07	1 (6%)
6	RET	C	323	1	20,20,21	0.72	0	27,27,28	1.64	5 (18%)
2	OLC	C	307	-	24,24,24	0.97	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	C	312	-	15,15,24	1.19	1 (6%)	16,16,25	0.95	1 (6%)
2	OLC	E	304	-	24,24,24	0.91	1 (4%)	25,25,25	0.92	2 (8%)
2	OLC	B	304	-	15,15,24	1.11	1 (6%)	16,16,25	1.01	2 (12%)
3	LFA	C	303	-	19,19,19	0.39	0	18,18,18	0.32	0
3	LFA	D	309	-	5,5,19	0.31	0	4,4,18	0.29	0
2	OLC	A	302	-	12,12,24	1.32	1 (8%)	13,13,25	1.23	2 (15%)
3	LFA	A	304	-	6,6,19	0.30	0	5,5,18	0.39	0
2	OLC	B	303	-	19,19,24	1.06	1 (5%)	20,20,25	0.90	1 (5%)
3	LFA	D	307	-	16,16,19	0.30	0	15,15,18	0.48	0
6	RET	E	312	1	20,20,21	0.82	1 (5%)	27,27,28	1.57	5 (18%)
3	LFA	C	315	-	6,6,19	0.31	0	5,5,18	0.38	0
2	OLC	A	301	-	13,13,24	0.33	0	12,12,25	0.34	0
3	LFA	A	308	-	5,5,19	0.30	0	4,4,18	0.34	0
2	OLC	C	311	-	24,24,24	0.96	1 (4%)	25,25,25	0.84	1 (4%)
3	LFA	B	306	-	7,7,19	0.31	0	6,6,18	0.41	0
2	OLC	C	308	-	24,24,24	0.96	1 (4%)	25,25,25	0.86	1 (4%)
3	LFA	E	307	-	3,3,19	0.33	0	2,2,18	0.62	0
3	LFA	C	322	-	3,3,19	0.38	0	2,2,18	0.57	0
3	LFA	A	312	-	19,19,19	0.38	0	18,18,18	0.34	0
3	LFA	E	302	-	19,19,19	0.38	0	18,18,18	0.37	0
2	OLC	A	311	-	13,13,24	0.36	0	12,12,25	0.46	0
3	LFA	C	317	-	19,19,19	0.27	0	18,18,18	0.51	0
5	BOG	A	310	-	20,20,20	0.55	0	25,25,25	0.58	0
3	LFA	D	305	-	19,19,19	0.25	0	18,18,18	0.56	0
2	OLC	C	302	-	19,19,24	1.06	1 (5%)	20,20,25	0.93	2 (10%)
2	OLC	E	303	-	15,15,24	0.31	0	14,14,25	0.46	0
3	LFA	B	305	-	8,8,19	0.30	0	7,7,18	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	C	306	-	22,22,24	0.97	1 (4%)	23,23,25	0.89	2 (8%)
2	OLC	C	305	-	20,20,24	1.04	1 (5%)	21,21,25	0.88	1 (4%)
6	RET	B	309	1	20,20,21	0.69	0	27,27,28	1.61	6 (22%)
2	OLC	C	309	-	21,21,24	1.04	1 (4%)	22,22,25	0.91	1 (4%)
3	LFA	E	308	-	4,4,19	0.30	0	3,3,18	0.37	0
5	BOG	B	308	-	20,20,20	0.58	1 (5%)	25,25,25	0.54	0
3	LFA	A	306	-	7,7,19	0.30	0	6,6,18	0.43	0
3	LFA	D	302	-	19,19,19	0.37	0	18,18,18	0.37	0
3	LFA	C	319	-	3,3,19	0.34	0	2,2,18	0.63	0
5	BOG	D	311	-	20,20,20	0.53	0	25,25,25	0.64	0
2	OLC	D	303	-	13,13,24	1.22	1 (7%)	14,14,25	0.99	2 (14%)
6	RET	A	313	1	20,20,21	0.76	0	27,27,28	1.64	5 (18%)
5	BOG	C	321	-	20,20,20	0.56	0	25,25,25	0.71	0
3	LFA	A	307	-	11,11,19	0.31	0	10,10,18	0.40	0
6	RET	D	312	1	20,20,21	0.70	0	27,27,28	1.65	6 (22%)
3	LFA	E	311	-	13,13,19	0.27	0	12,12,18	0.51	0
3	LFA	C	316	-	7,7,19	0.29	0	6,6,18	0.38	0
3	LFA	C	318	-	10,10,19	0.29	0	9,9,18	0.49	0
3	LFA	A	305	-	7,7,19	0.31	0	6,6,18	0.43	0
2	OLC	C	313	-	15,15,24	1.22	1 (6%)	16,16,25	1.04	2 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	E	306	-	-	5/11/11/17	-
3	LFA	D	304	-	-	9/17/17/17	-
3	LFA	D	306	-	-	4/5/5/17	-
2	OLC	A	303	-	-	7/14/14/24	-
3	LFA	E	305	-	-	1/5/5/17	-
5	BOG	E	310	-	-	9/11/31/31	0/1/1/1
2	OLC	E	301	-	-	4/9/9/24	-
2	OLC	C	314	-	-	9/15/15/24	-
3	LFA	B	302	-	-	7/17/17/17	-
2	OLC	C	304	-	-	8/13/13/24	-
2	OLC	D	301	-	-	7/17/17/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	301	-	-	7/21/21/24	-
3	LFA	D	308	-	-	4/4/4/17	-
2	OLC	C	301	-	-	10/20/20/24	-
2	OLC	C	310	-	-	6/15/15/24	-
6	RET	C	323	1	-	0/13/30/31	0/1/1/1
2	OLC	C	307	-	-	13/24/24/24	-
2	OLC	C	312	-	-	7/15/15/24	-
2	OLC	E	304	-	-	15/24/24/24	-
2	OLC	B	304	-	-	2/15/15/24	-
3	LFA	C	303	-	-	11/17/17/17	-
3	LFA	D	309	-	-	0/3/3/17	-
2	OLC	A	302	-	-	1/12/12/24	-
3	LFA	A	304	-	-	1/4/4/17	-
2	OLC	B	303	-	-	7/19/19/24	-
3	LFA	D	307	-	-	7/14/14/17	-
6	RET	E	312	1	-	0/13/30/31	0/1/1/1
3	LFA	C	315	-	-	3/4/4/17	-
2	OLC	A	301	-	-	6/11/11/24	-
3	LFA	A	308	-	-	1/3/3/17	-
2	OLC	C	311	-	-	13/24/24/24	-
3	LFA	B	306	-	-	2/5/5/17	-
2	OLC	C	308	-	-	6/24/24/24	-
3	LFA	E	307	-	-	1/1/1/17	-
3	LFA	C	322	-	-	0/1/1/17	-
3	LFA	A	312	-	-	10/17/17/17	-
3	LFA	E	302	-	-	6/17/17/17	-
2	OLC	A	311	-	-	6/11/11/24	-
3	LFA	C	317	-	-	13/17/17/17	-
5	BOG	A	310	-	-	5/11/31/31	0/1/1/1
3	LFA	D	305	-	-	9/17/17/17	-
2	OLC	C	302	-	-	11/19/19/24	-
2	OLC	E	303	-	-	5/13/13/24	-
3	LFA	B	305	-	-	3/6/6/17	-
2	OLC	C	306	-	-	12/22/22/24	-
2	OLC	C	305	-	-	12/20/20/24	-
6	RET	B	309	1	-	0/13/30/31	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	309	-	-	13/21/21/24	-
3	LFA	E	308	-	-	1/2/2/17	-
5	BOG	B	308	-	-	6/11/31/31	0/1/1/1
3	LFA	A	306	-	-	3/5/5/17	-
3	LFA	D	302	-	-	7/17/17/17	-
3	LFA	C	319	-	-	1/1/1/17	-
5	BOG	D	311	-	-	2/11/31/31	0/1/1/1
2	OLC	D	303	-	-	4/13/13/24	-
6	RET	A	313	1	-	0/13/30/31	0/1/1/1
5	BOG	C	321	-	-	3/11/31/31	0/1/1/1
3	LFA	A	307	-	-	5/9/9/17	-
6	RET	D	312	1	-	0/13/30/31	0/1/1/1
3	LFA	E	311	-	-	3/11/11/17	-
3	LFA	C	316	-	-	4/5/5/17	-
3	LFA	C	318	-	-	4/8/8/17	-
3	LFA	A	305	-	-	3/5/5/17	-
2	OLC	C	313	-	-	10/15/15/24	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	310	OLC	O20-C1	4.51	1.46	1.33
2	C	313	OLC	O20-C1	4.49	1.46	1.33
2	C	314	OLC	O20-C1	4.48	1.46	1.33
2	C	307	OLC	O20-C1	4.46	1.46	1.33
2	C	309	OLC	O20-C1	4.45	1.46	1.33
2	C	304	OLC	O20-C1	4.43	1.46	1.33
2	C	311	OLC	O20-C1	4.41	1.46	1.33
2	C	305	OLC	O20-C1	4.39	1.46	1.33
2	C	312	OLC	O20-C1	4.38	1.46	1.33
2	C	308	OLC	O20-C1	4.38	1.46	1.33
2	D	301	OLC	O20-C1	4.36	1.46	1.33
2	A	302	OLC	O20-C1	4.35	1.46	1.33
2	B	303	OLC	O20-C1	4.35	1.46	1.33
2	C	301	OLC	O20-C1	4.33	1.46	1.33
2	C	302	OLC	O20-C1	4.32	1.45	1.33
2	B	301	OLC	O20-C1	4.30	1.45	1.33
2	A	303	OLC	O20-C1	4.29	1.45	1.33
2	C	306	OLC	O20-C1	4.26	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	303	OLC	O20-C1	4.16	1.45	1.33
2	B	304	OLC	O20-C1	4.07	1.45	1.33
2	E	304	OLC	O20-C1	4.07	1.45	1.33
6	E	312	RET	C14-C13	2.15	1.35	1.33
5	B	308	BOG	O1-C1	2.12	1.43	1.40

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	313	RET	C18-C5-C6	-4.37	119.72	124.48
6	C	323	RET	C18-C5-C6	-4.28	119.82	124.48
6	D	312	RET	C18-C5-C6	-4.15	119.96	124.48
6	E	312	RET	C18-C5-C6	-4.07	120.05	124.48
6	B	309	RET	C18-C5-C6	-3.96	120.17	124.48
6	D	312	RET	C7-C8-C9	-3.29	121.37	126.23
2	A	302	OLC	O20-C1-C2	3.23	121.67	111.83
2	A	303	OLC	O20-C1-C2	3.20	121.61	111.83
2	C	301	OLC	O20-C1-C2	3.20	121.59	111.83
6	C	323	RET	C7-C8-C9	-3.18	121.53	126.23
6	A	313	RET	C7-C8-C9	-3.15	121.58	126.23
6	B	309	RET	C7-C8-C9	-3.05	121.72	126.23
2	C	310	OLC	O20-C1-C2	3.01	121.00	111.83
2	E	304	OLC	O20-C1-C2	3.00	120.99	111.83
6	E	312	RET	C7-C8-C9	-2.97	121.84	126.23
2	B	301	OLC	O20-C1-C2	2.97	120.89	111.83
2	C	302	OLC	O20-C1-C2	2.90	120.68	111.83
2	C	307	OLC	O20-C1-C2	2.88	120.63	111.83
2	C	308	OLC	O20-C1-C2	2.88	120.61	111.83
2	C	309	OLC	O20-C1-C2	2.85	120.53	111.83
2	C	314	OLC	O20-C1-C2	2.83	120.48	111.83
2	C	313	OLC	O20-C1-C2	2.82	120.44	111.83
2	D	301	OLC	O20-C1-C2	2.81	120.42	111.83
2	C	304	OLC	O20-C1-C2	2.79	120.36	111.83
2	C	306	OLC	O20-C1-C2	2.78	120.31	111.83
6	D	312	RET	C11-C10-C9	-2.70	123.50	127.28
2	C	311	OLC	O20-C1-C2	2.69	120.04	111.83
6	B	309	RET	C11-C10-C9	-2.68	123.52	127.28
2	B	304	OLC	O20-C1-C2	2.67	119.99	111.83
2	C	305	OLC	O20-C1-C2	2.62	119.82	111.83
2	B	303	OLC	O20-C1-C2	2.60	119.77	111.83
2	D	303	OLC	O20-C1-C2	2.60	119.76	111.83
2	E	304	OLC	O20-C1-O19	-2.56	117.23	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	312	OLC	O20-C1-C2	2.56	119.63	111.83
2	A	302	OLC	O20-C1-O19	-2.51	117.35	123.63
6	D	312	RET	C20-C13-C12	2.50	121.91	118.09
6	A	313	RET	C10-C11-C12	-2.49	115.98	123.20
6	B	309	RET	C10-C11-C12	-2.49	115.99	123.20
6	C	323	RET	C11-C10-C9	-2.48	123.80	127.28
6	E	312	RET	C10-C11-C12	-2.43	116.15	123.20
6	D	312	RET	C10-C11-C12	-2.41	116.21	123.20
2	A	303	OLC	O20-C1-O19	-2.37	117.70	123.63
6	A	313	RET	C11-C10-C9	-2.28	124.09	127.28
2	C	302	OLC	O20-C1-O19	-2.27	117.95	123.63
6	C	323	RET	C10-C11-C12	-2.27	116.64	123.20
6	B	309	RET	C19-C9-C8	2.20	121.45	118.09
2	C	306	OLC	O20-C1-O19	-2.20	118.14	123.63
6	E	312	RET	C11-C10-C9	-2.18	124.22	127.28
6	B	309	RET	C20-C13-C12	2.14	121.36	118.09
6	A	313	RET	C20-C13-C12	2.13	121.35	118.09
6	E	312	RET	C19-C9-C8	2.06	121.23	118.09
2	B	304	OLC	O20-C1-O19	-2.05	118.49	123.63
6	C	323	RET	C19-C9-C8	2.04	121.20	118.09
2	C	313	OLC	O20-C1-O19	-2.02	118.56	123.63
6	D	312	RET	C19-C9-C8	2.01	121.16	118.09
2	D	303	OLC	O20-C1-O19	-2.01	118.60	123.63

There are no chirality outliers.

All (354) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	OLC	O20-C21-C22-C24
2	C	301	OLC	C21-C22-C24-O25
2	C	304	OLC	C21-C22-C24-O25
2	C	305	OLC	C21-C22-C24-O25
2	C	305	OLC	O20-C21-C22-O23
2	C	306	OLC	O20-C21-C22-C24
2	C	306	OLC	O20-C21-C22-O23
2	C	307	OLC	O20-C21-C22-C24
2	C	307	OLC	O20-C21-C22-O23
2	C	308	OLC	C21-C22-C24-O25
2	C	308	OLC	O23-C22-C24-O25
2	C	313	OLC	C21-C22-C24-O25
2	C	313	OLC	C2-C1-O20-C21
2	C	313	OLC	O19-C1-O20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	314	OLC	O20-C21-C22-O23
2	D	303	OLC	C21-C22-C24-O25
2	E	304	OLC	O20-C21-C22-C24
2	E	304	OLC	O20-C21-C22-O23
3	C	319	LFA	C17-C18-C19-C20
3	E	307	LFA	C17-C18-C19-C20
2	C	306	OLC	O19-C1-O20-C21
2	C	306	OLC	C2-C1-O20-C21
2	E	304	OLC	O19-C1-O20-C21
2	C	305	OLC	C2-C1-O20-C21
2	A	303	OLC	C2-C1-O20-C21
2	E	304	OLC	C2-C1-O20-C21
2	A	303	OLC	O19-C1-O20-C21
2	C	305	OLC	O19-C1-O20-C21
2	A	303	OLC	O20-C21-C22-O23
2	C	312	OLC	O20-C21-C22-O23
5	E	310	BOG	O5-C1-O1-C1'
2	B	301	OLC	C2-C1-O20-C21
2	B	303	OLC	C2-C1-O20-C21
2	B	304	OLC	C2-C1-O20-C21
2	C	304	OLC	C2-C1-O20-C21
2	C	310	OLC	C2-C1-O20-C21
2	C	312	OLC	C2-C1-O20-C21
2	D	301	OLC	C2-C1-O20-C21
2	B	304	OLC	O19-C1-O20-C21
2	C	302	OLC	O20-C21-C22-C24
2	C	305	OLC	O20-C21-C22-C24
2	C	312	OLC	O20-C21-C22-C24
5	E	310	BOG	C2-C1-O1-C1'
2	B	301	OLC	O19-C1-O20-C21
2	C	314	OLC	C2-C1-O20-C21
5	E	310	BOG	O5-C5-C6-O6
2	C	304	OLC	O23-C22-C24-O25
2	C	313	OLC	O23-C22-C24-O25
2	D	303	OLC	O23-C22-C24-O25
2	C	302	OLC	C1-C2-C3-C4
2	B	303	OLC	O19-C1-O20-C21
2	C	304	OLC	O19-C1-O20-C21
2	C	310	OLC	O19-C1-O20-C21
5	E	310	BOG	C4-C5-C6-O6
2	C	311	OLC	C1-C2-C3-C4
2	D	301	OLC	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	303	OLC	C1-C2-C3-C4
2	C	312	OLC	O19-C1-O20-C21
2	D	301	OLC	O19-C1-O20-C21
2	C	302	OLC	O20-C21-C22-O23
2	C	309	OLC	O20-C21-C22-O23
2	C	314	OLC	O19-C1-O20-C21
2	C	314	OLC	O20-C21-C22-C24
3	A	307	LFA	C7-C8-C9-C10
2	B	303	OLC	C10-C11-C12-C13
2	C	306	OLC	C21-C22-C24-O25
2	C	309	OLC	C21-C22-C24-O25
2	E	304	OLC	C21-C22-C24-O25
2	C	301	OLC	C5-C6-C7-C8
3	C	303	LFA	C7-C8-C9-C10
5	D	311	BOG	C1'-C2'-C3'-C4'
3	B	306	LFA	C3-C4-C5-C6
3	E	311	LFA	C2-C3-C4-C5
2	C	301	OLC	O23-C22-C24-O25
2	C	309	OLC	O23-C22-C24-O25
2	E	304	OLC	O23-C22-C24-O25
5	A	310	BOG	C2'-C1'-O1-C1
5	E	310	BOG	C2'-C1'-O1-C1
5	E	310	BOG	C2'-C3'-C4'-C5'
5	B	308	BOG	C1'-C2'-C3'-C4'
5	B	308	BOG	O5-C5-C6-O6
2	A	301	OLC	C3-C4-C5-C6
2	C	307	OLC	C12-C13-C14-C15
3	D	304	LFA	C6-C7-C8-C9
2	C	311	OLC	C5-C6-C7-C8
5	E	310	BOG	O1-C1'-C2'-C3'
3	C	316	LFA	C15-C16-C17-C18
5	B	308	BOG	C4-C5-C6-O6
2	A	311	OLC	C5-C6-C7-C8
3	A	307	LFA	C11-C10-C9-C8
3	E	306	LFA	C15-C16-C17-C18
3	B	305	LFA	C14-C15-C16-C17
3	D	302	LFA	C11-C10-C9-C8
2	C	313	OLC	O20-C21-C22-O23
2	D	301	OLC	O20-C21-C22-O23
2	C	307	OLC	C1-C2-C3-C4
2	C	306	OLC	C3-C4-C5-C6
2	C	313	OLC	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	307	LFA	C5-C6-C7-C8
2	E	303	OLC	C11-C12-C13-C14
3	D	305	LFA	C14-C15-C16-C17
2	E	301	OLC	C5-C6-C7-C8
2	C	306	OLC	C4-C5-C6-C7
3	C	316	LFA	C16-C17-C18-C19
3	D	306	LFA	C4-C5-C6-C7
2	A	301	OLC	C4-C5-C6-C7
2	C	307	OLC	C3-C4-C5-C6
2	C	302	OLC	C5-C6-C7-C8
2	C	302	OLC	C3-C4-C5-C6
3	E	306	LFA	C14-C15-C16-C17
3	B	305	LFA	C15-C16-C17-C18
2	C	311	OLC	C2-C3-C4-C5
3	C	317	LFA	C12-C13-C14-C15
3	E	306	LFA	C9-C10-C11-C12
2	D	301	OLC	O20-C21-C22-C24
3	D	306	LFA	C2-C3-C4-C5
3	B	302	LFA	C16-C17-C18-C19
2	C	301	OLC	C4-C5-C6-C7
3	B	305	LFA	C16-C17-C18-C19
3	D	302	LFA	C9-C10-C11-C12
3	D	302	LFA	C12-C13-C14-C15
3	A	306	LFA	C15-C16-C17-C18
2	B	301	OLC	C10-C11-C12-C13
2	C	311	OLC	C6-C7-C8-C9
2	E	301	OLC	C10-C11-C12-C13
3	D	308	LFA	C16-C17-C18-C19
2	A	311	OLC	C11-C12-C13-C14
5	C	321	BOG	C1'-C2'-C3'-C4'
5	E	310	BOG	C1'-C2'-C3'-C4'
2	C	307	OLC	C14-C15-C16-C17
3	E	311	LFA	C3-C4-C5-C6
2	A	301	OLC	C10-C11-C12-C13
2	A	301	OLC	C6-C7-C8-C9
2	C	305	OLC	C10-C11-C12-C13
2	C	311	OLC	C10-C11-C12-C13
3	A	312	LFA	C13-C14-C15-C16
2	C	313	OLC	C2-C3-C4-C5
3	C	318	LFA	C3-C4-C5-C6
2	C	309	OLC	C2-C3-C4-C5
2	C	312	OLC	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	304	OLC	C2-C3-C4-C5
2	C	307	OLC	C5-C6-C7-C8
3	C	317	LFA	C15-C16-C17-C18
3	B	302	LFA	C6-C7-C8-C9
3	C	317	LFA	C13-C14-C15-C16
5	B	308	BOG	C5'-C6'-C7'-C8'
3	C	303	LFA	C13-C14-C15-C16
3	D	304	LFA	C11-C12-C13-C14
3	C	303	LFA	C3-C4-C5-C6
3	A	306	LFA	C14-C15-C16-C17
2	B	303	OLC	C4-C5-C6-C7
2	C	301	OLC	C10-C11-C12-C13
3	D	306	LFA	C1-C2-C3-C4
5	E	310	BOG	C5'-C6'-C7'-C8'
3	D	307	LFA	C13-C14-C15-C16
2	C	313	OLC	C6-C7-C8-C9
3	D	305	LFA	C1-C2-C3-C4
2	C	313	OLC	O20-C21-C22-C24
3	E	306	LFA	C13-C14-C15-C16
2	E	304	OLC	C3-C4-C5-C6
3	A	312	LFA	C14-C15-C16-C17
2	C	311	OLC	O19-C1-O20-C21
2	C	311	OLC	C4-C5-C6-C7
3	B	302	LFA	C7-C8-C9-C10
3	D	304	LFA	C14-C15-C16-C17
3	C	316	LFA	C17-C18-C19-C20
3	D	306	LFA	C5-C6-C7-C8
3	A	307	LFA	C1-C2-C3-C4
5	C	321	BOG	C5'-C6'-C7'-C8'
2	C	304	OLC	C4-C5-C6-C7
2	B	301	OLC	C5-C6-C7-C8
3	E	306	LFA	C7-C8-C9-C10
2	C	307	OLC	C15-C16-C17-C18
2	C	304	OLC	C3-C4-C5-C6
2	C	309	OLC	C4-C5-C6-C7
2	E	304	OLC	C11-C12-C13-C14
2	C	310	OLC	C1-C2-C3-C4
2	E	301	OLC	C4-C5-C6-C7
2	C	311	OLC	C3-C4-C5-C6
3	C	317	LFA	C16-C17-C18-C19
3	A	306	LFA	C16-C17-C18-C19
3	A	312	LFA	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	314	OLC	C2-C3-C4-C5
5	A	310	BOG	C5'-C6'-C7'-C8'
3	C	318	LFA	C1-C2-C3-C4
2	C	306	OLC	O23-C22-C24-O25
2	C	311	OLC	O23-C22-C24-O25
2	C	314	OLC	O23-C22-C24-O25
3	A	305	LFA	C1-C2-C3-C4
5	A	310	BOG	C1'-C2'-C3'-C4'
2	C	314	OLC	C4-C5-C6-C7
5	A	310	BOG	O1-C1'-C2'-C3'
3	C	317	LFA	C9-C10-C11-C12
2	A	311	OLC	C10-C11-C12-C13
2	C	306	OLC	C10-C11-C12-C13
2	E	303	OLC	C10-C11-C12-C13
2	C	306	OLC	C12-C13-C14-C15
2	C	307	OLC	C4-C5-C6-C7
3	A	307	LFA	C9-C10-C11-C12
2	E	304	OLC	C12-C13-C14-C15
3	C	317	LFA	C3-C4-C5-C6
2	C	305	OLC	C4-C5-C6-C7
3	D	302	LFA	C4-C5-C6-C7
2	C	308	OLC	C5-C6-C7-C8
3	C	303	LFA	C4-C5-C6-C7
3	C	315	LFA	C2-C3-C4-C5
3	A	305	LFA	C5-C6-C7-C8
2	E	304	OLC	C10-C11-C12-C13
3	C	316	LFA	C13-C14-C15-C16
2	B	301	OLC	C12-C13-C14-C15
2	C	314	OLC	C6-C7-C8-C9
2	A	301	OLC	C2-C3-C4-C5
3	C	318	LFA	C2-C3-C4-C5
2	C	309	OLC	C11-C12-C13-C14
2	A	303	OLC	C3-C4-C5-C6
3	D	304	LFA	C7-C8-C9-C10
3	E	305	LFA	C16-C17-C18-C19
2	C	301	OLC	C11-C12-C13-C14
3	C	315	LFA	C4-C5-C6-C7
3	A	307	LFA	C2-C3-C4-C5
3	A	304	LFA	C16-C17-C18-C19
3	D	308	LFA	C15-C16-C17-C18
2	C	309	OLC	C12-C13-C14-C15
2	A	311	OLC	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	305	LFA	C16-C17-C18-C19
2	C	301	OLC	O19-C1-O20-C21
3	C	303	LFA	C1-C2-C3-C4
2	C	309	OLC	C3-C4-C5-C6
2	C	309	OLC	C7-C8-C9-C10
3	D	302	LFA	C3-C4-C5-C6
2	B	303	OLC	C7-C8-C9-C10
3	D	307	LFA	C3-C4-C5-C6
3	C	303	LFA	C12-C13-C14-C15
3	C	317	LFA	C11-C12-C13-C14
3	E	302	LFA	C5-C6-C7-C8
3	C	317	LFA	C4-C5-C6-C7
2	B	301	OLC	C7-C8-C9-C10
2	C	307	OLC	C7-C8-C9-C10
2	E	301	OLC	C7-C8-C9-C10
3	B	302	LFA	C11-C10-C9-C8
2	E	304	OLC	C9-C10-C11-C12
3	A	312	LFA	C9-C10-C11-C12
2	C	305	OLC	C3-C4-C5-C6
5	C	321	BOG	C3'-C4'-C5'-C6'
5	A	310	BOG	C4-C5-C6-O6
2	C	305	OLC	C7-C8-C9-C10
3	C	317	LFA	C7-C8-C9-C10
3	A	312	LFA	C17-C18-C19-C20
2	C	310	OLC	O20-C21-C22-C24
2	A	301	OLC	C9-C10-C11-C12
2	A	311	OLC	C9-C10-C11-C12
2	A	302	OLC	O20-C21-C22-O23
2	C	302	OLC	C7-C8-C9-C10
2	B	303	OLC	C5-C6-C7-C8
3	B	302	LFA	C10-C11-C12-C13
3	E	302	LFA	C15-C16-C17-C18
3	D	305	LFA	C2-C3-C4-C5
2	C	305	OLC	C11-C12-C13-C14
3	C	315	LFA	C1-C2-C3-C4
2	C	311	OLC	O20-C21-C22-C24
2	C	309	OLC	C5-C6-C7-C8
3	D	308	LFA	C17-C18-C19-C20
2	C	312	OLC	C6-C7-C8-C9
5	B	308	BOG	C4'-C5'-C6'-C7'
2	C	307	OLC	O23-C22-C24-O25
2	C	307	OLC	O19-C1-O20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	303	OLC	C3-C4-C5-C6
3	C	303	LFA	C17-C18-C19-C20
2	C	311	OLC	O20-C1-C2-C3
2	C	313	OLC	O20-C1-C2-C3

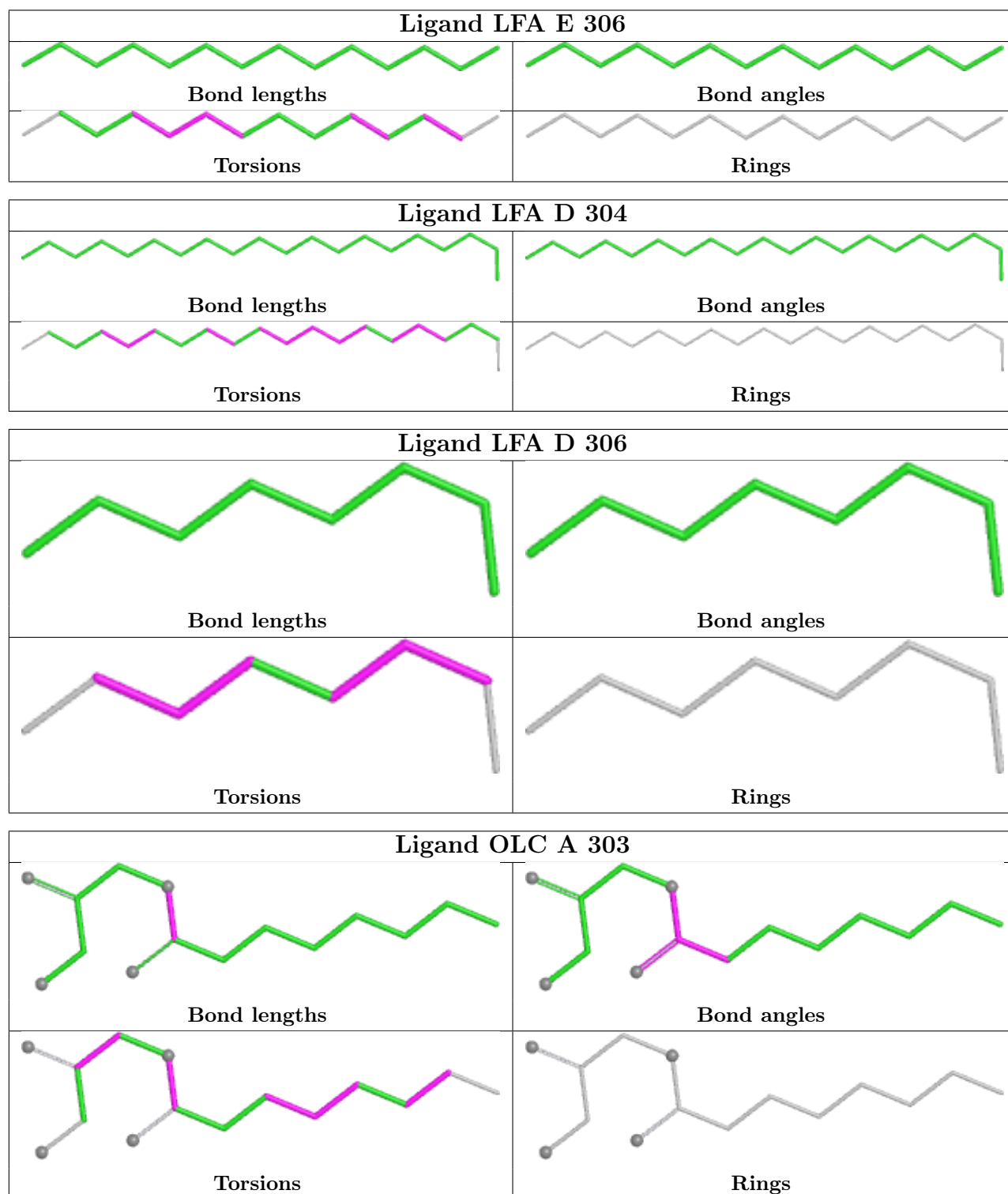
There are no ring outliers.

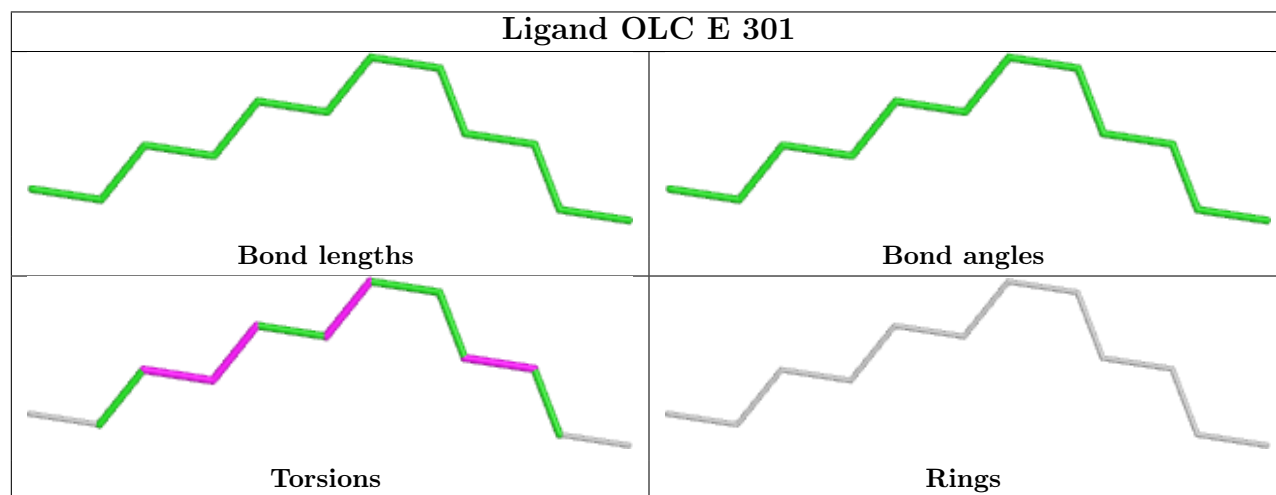
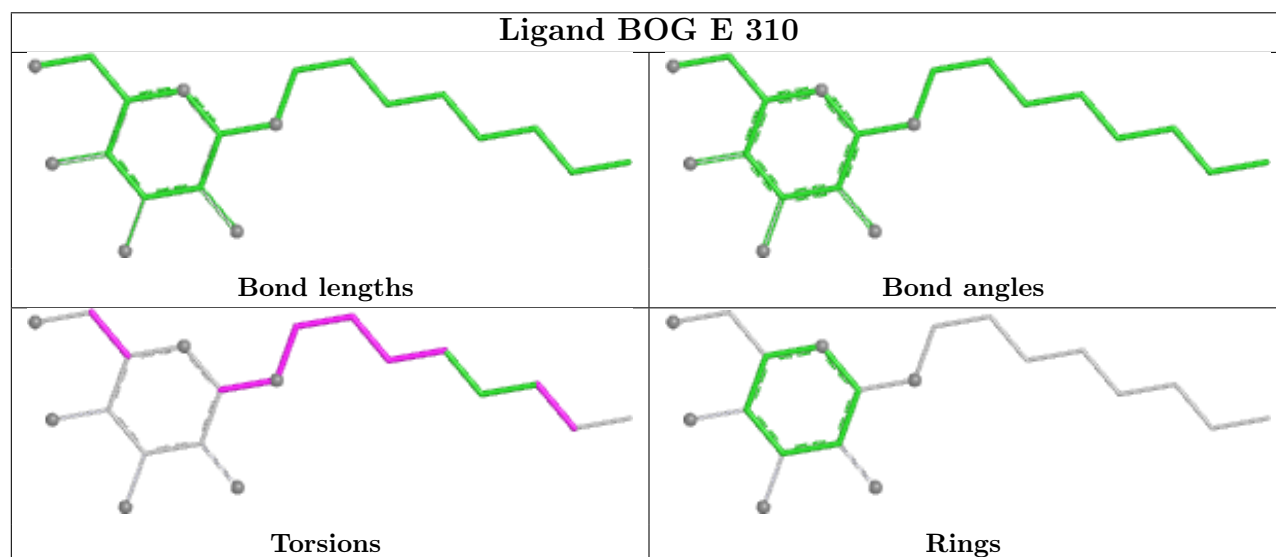
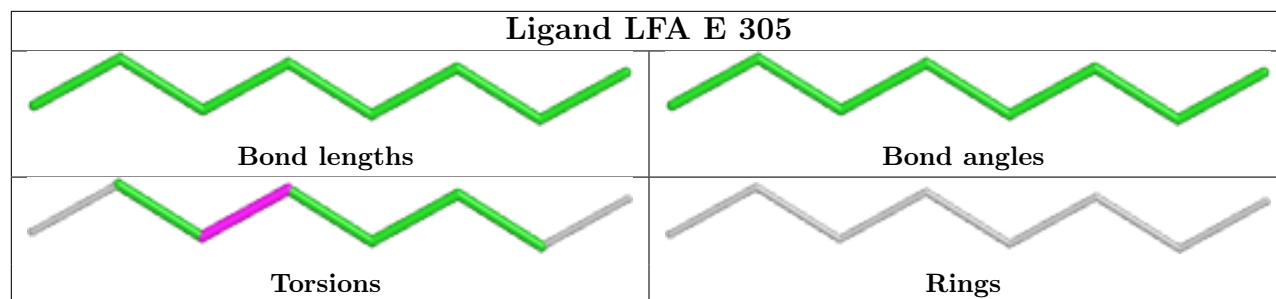
26 monomers are involved in 58 short contacts:

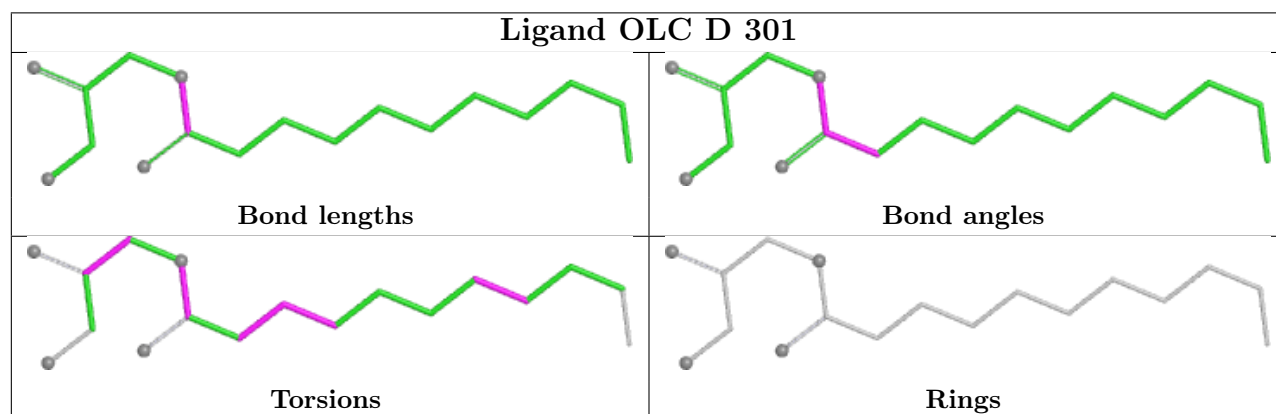
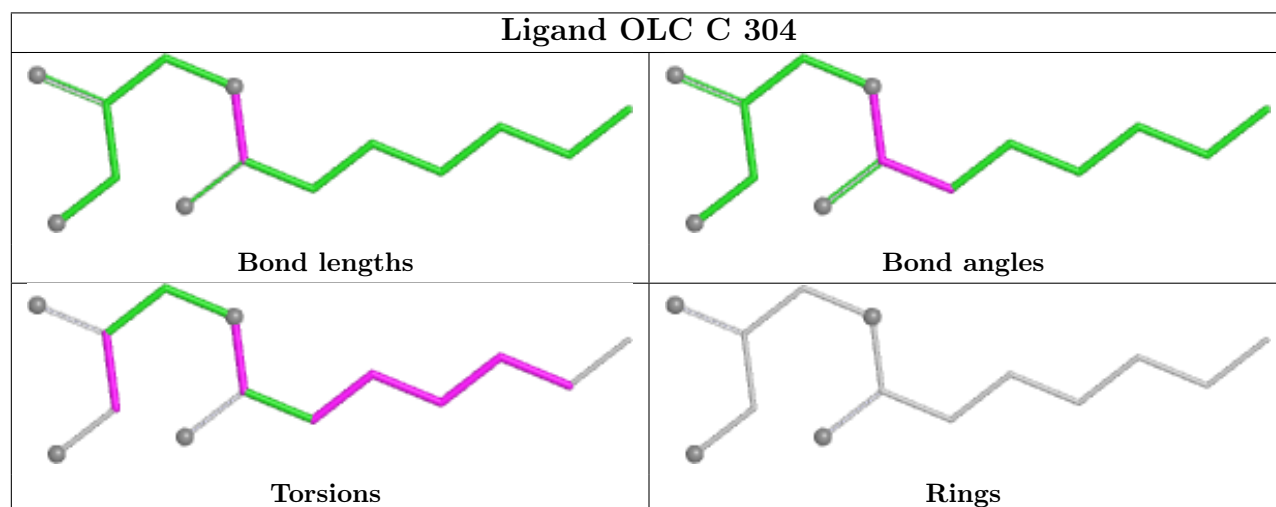
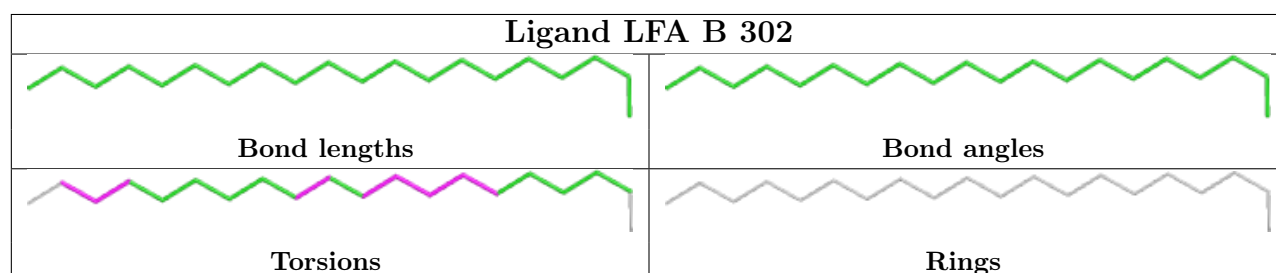
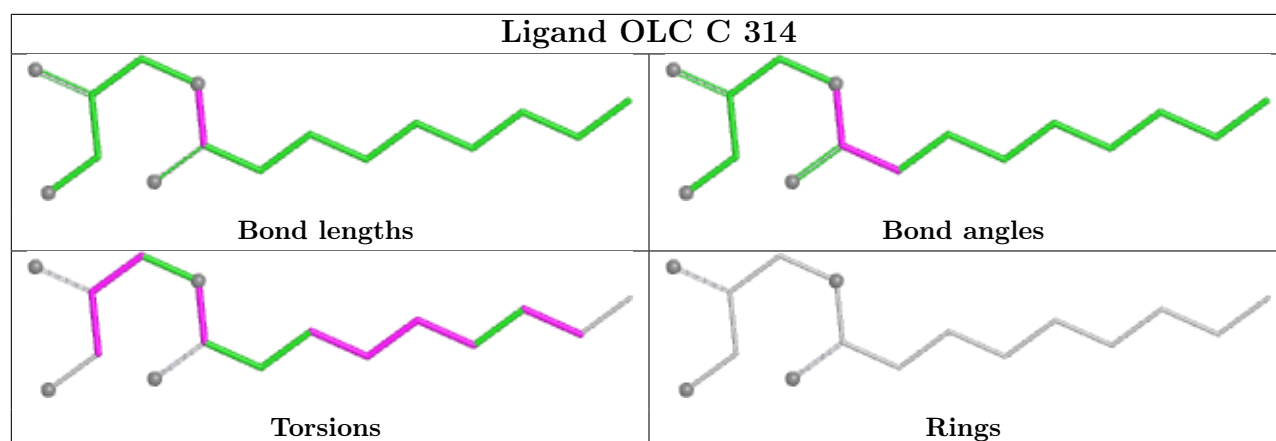
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	306	LFA	2	0
2	C	314	OLC	1	0
2	C	304	OLC	1	0
2	B	301	OLC	4	0
2	C	310	OLC	1	0
6	C	323	RET	5	0
2	C	307	OLC	1	0
2	C	312	OLC	1	0
3	A	304	LFA	1	0
6	E	312	RET	5	0
3	C	315	LFA	2	0
2	C	308	OLC	1	0
3	E	307	LFA	2	0
5	A	310	BOG	2	0
2	E	303	OLC	1	0
3	B	305	LFA	1	0
2	C	305	OLC	2	0
6	B	309	RET	5	0
5	B	308	BOG	2	0
3	C	319	LFA	2	0
5	D	311	BOG	2	0
6	A	313	RET	6	0
5	C	321	BOG	3	0
6	D	312	RET	6	0
3	C	316	LFA	1	0
2	C	313	OLC	1	0

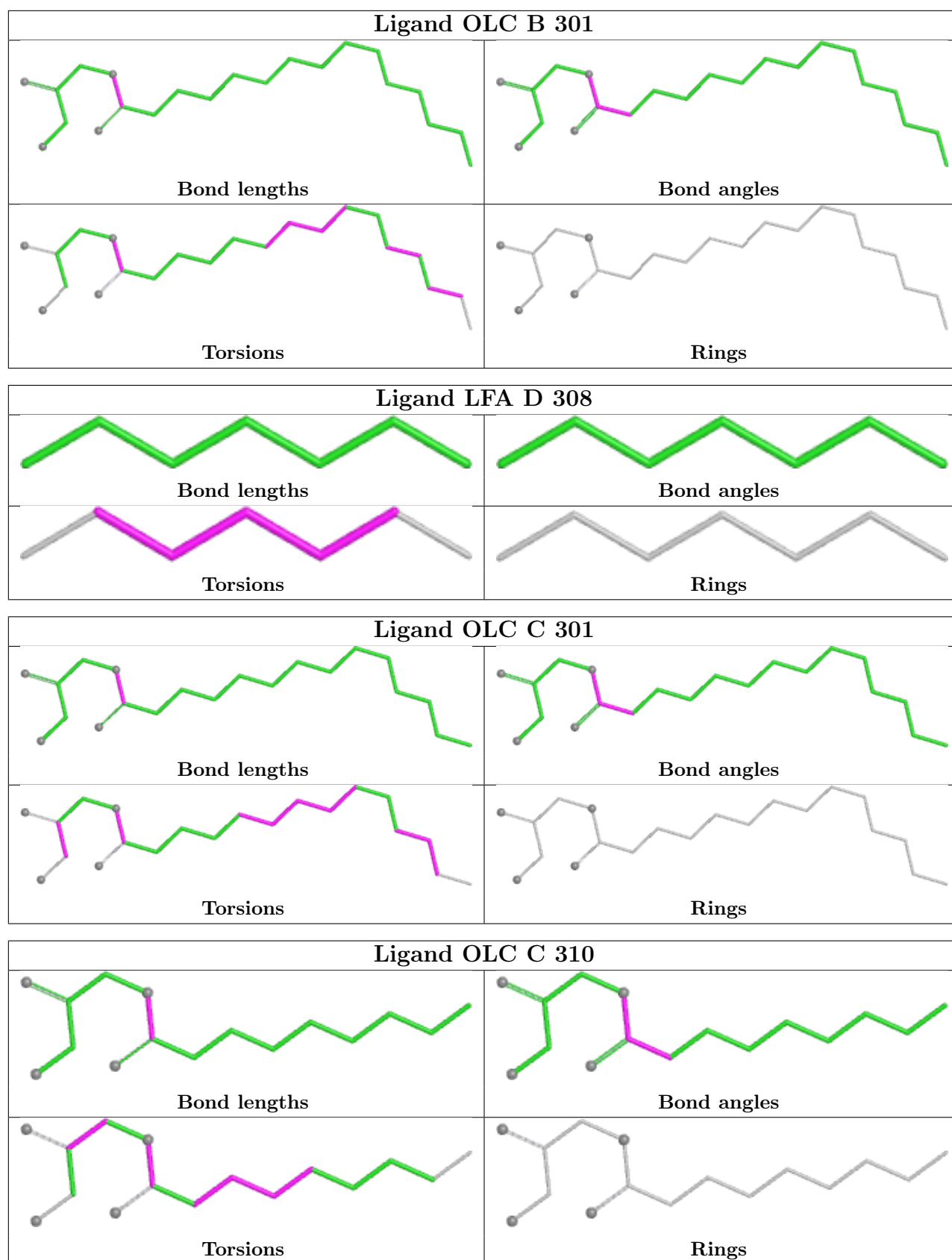
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

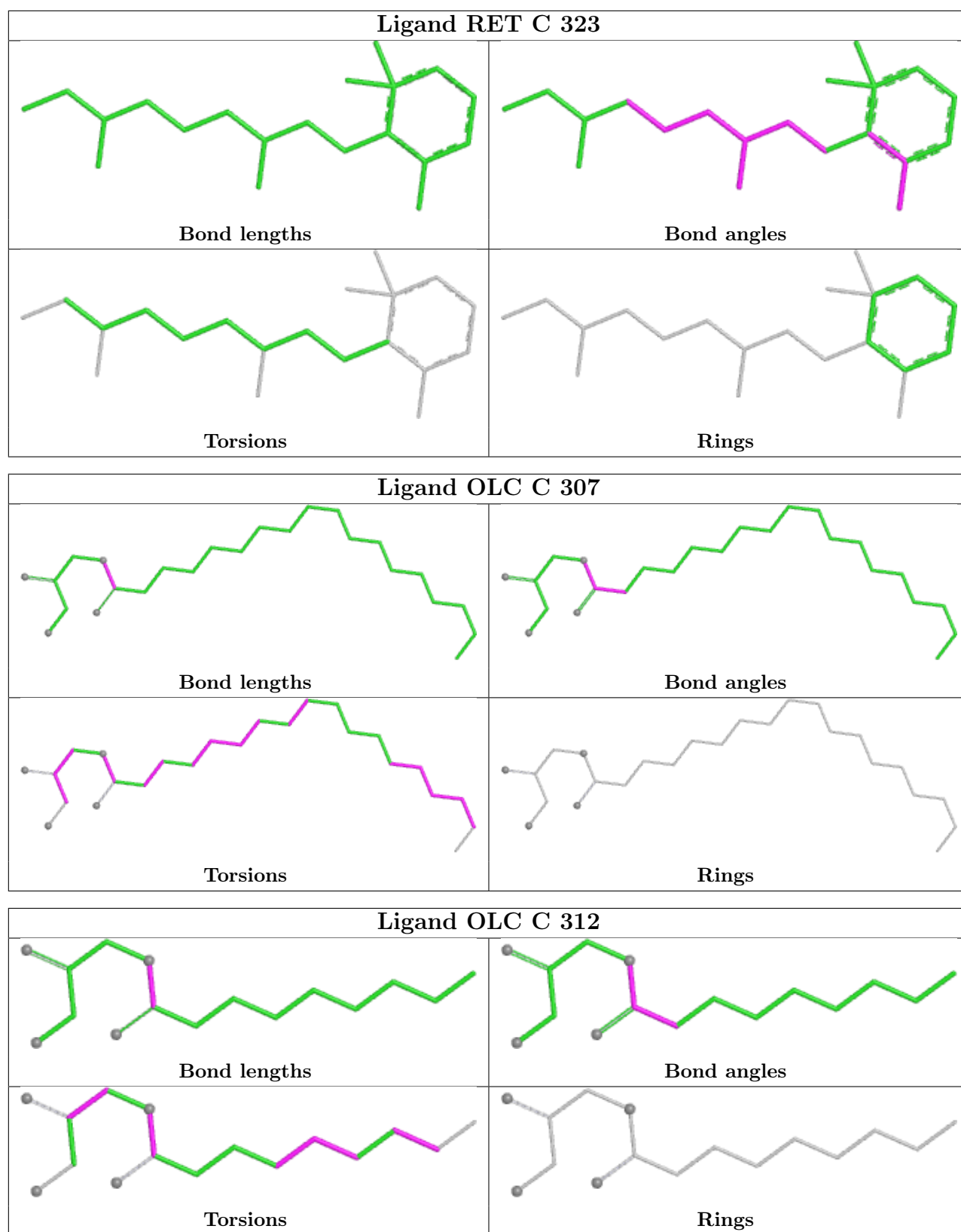
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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

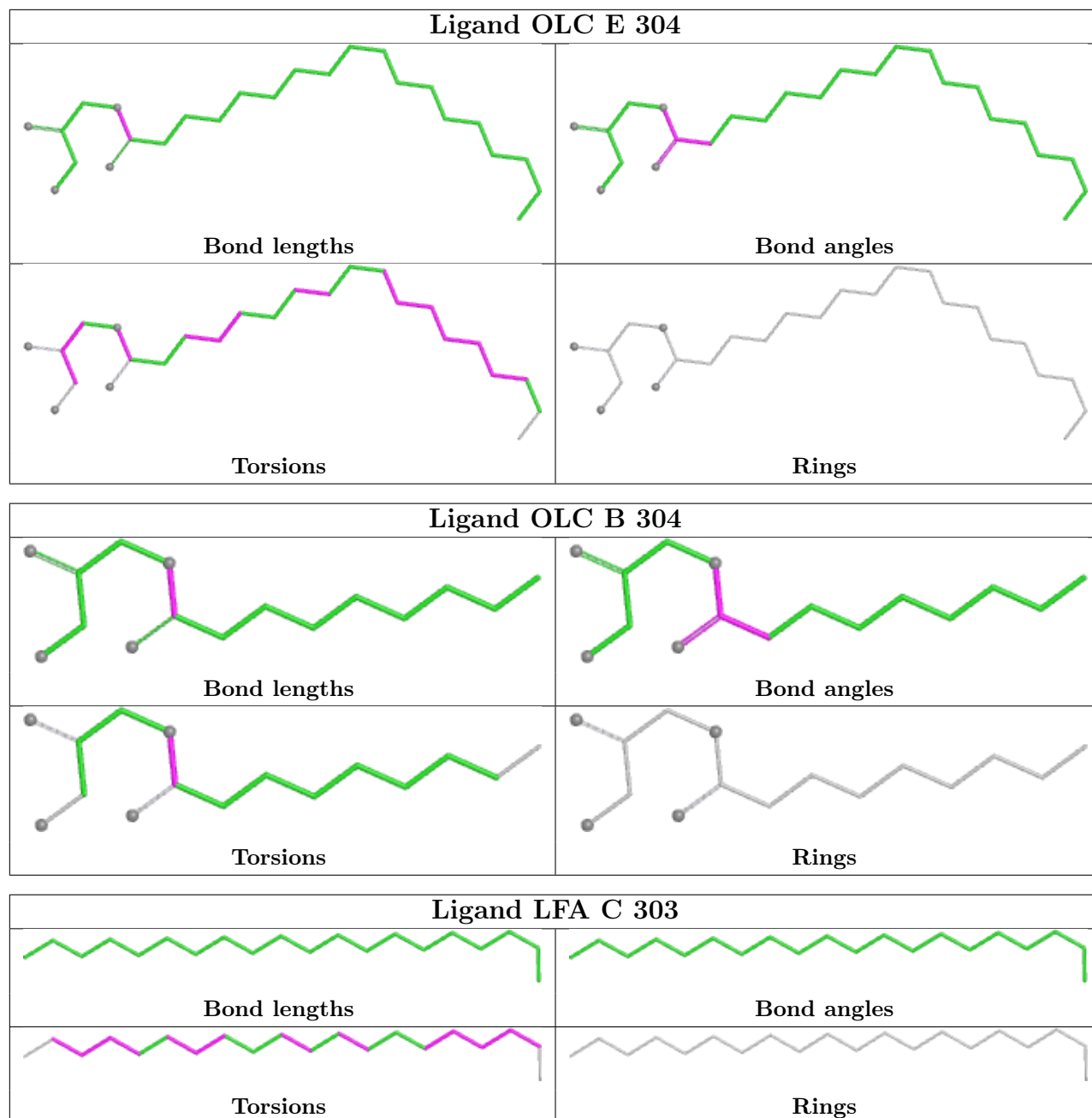


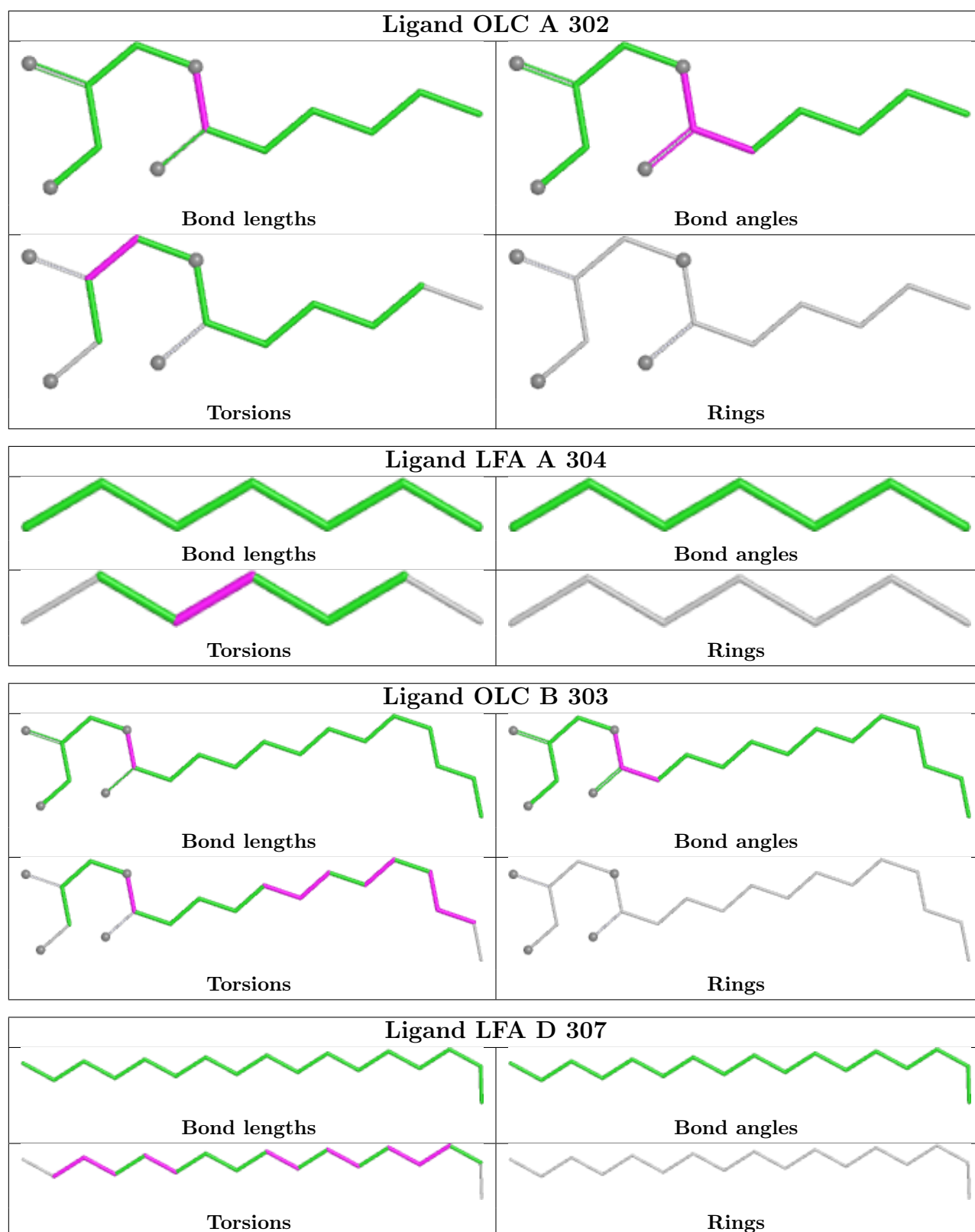


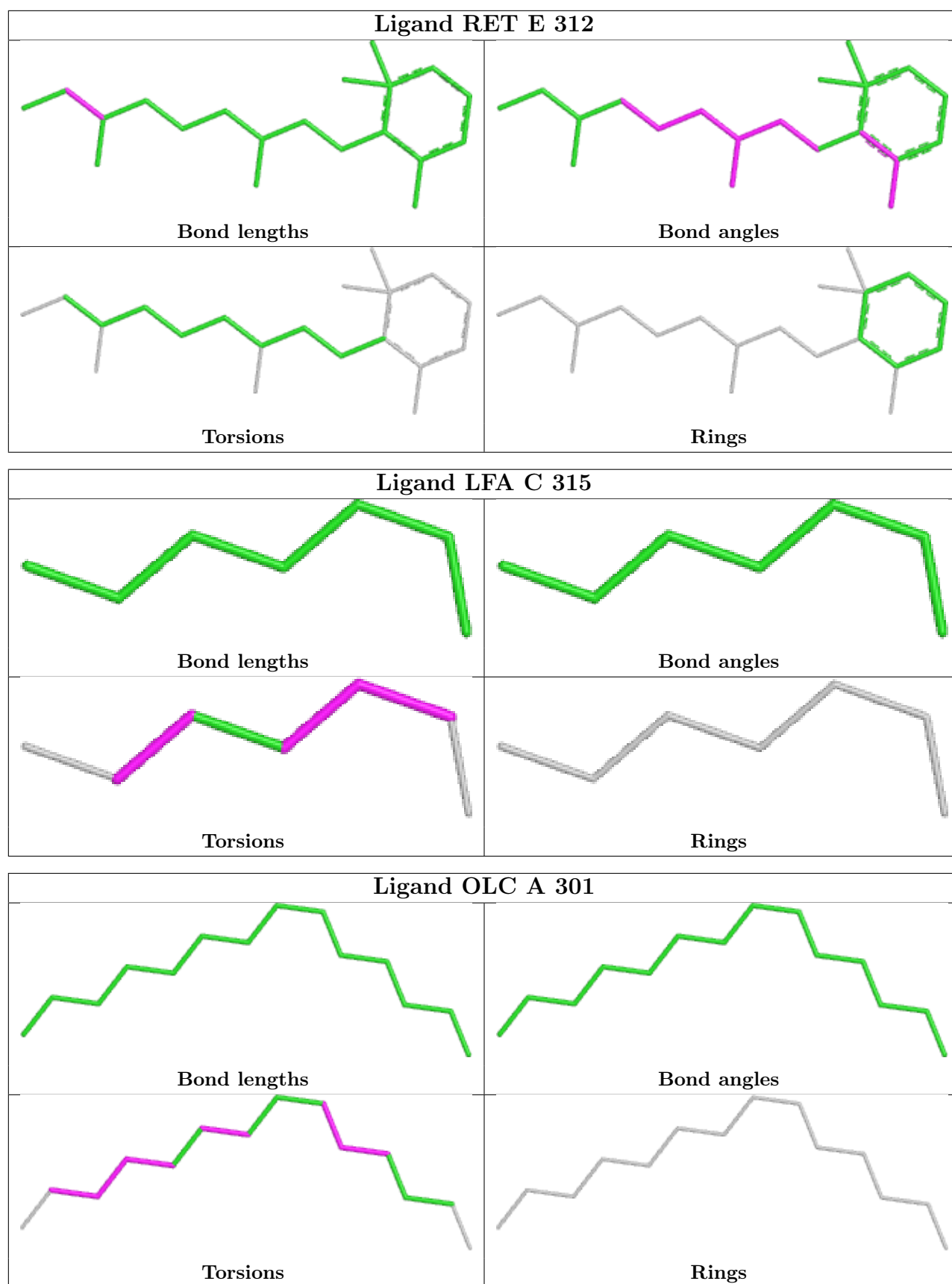


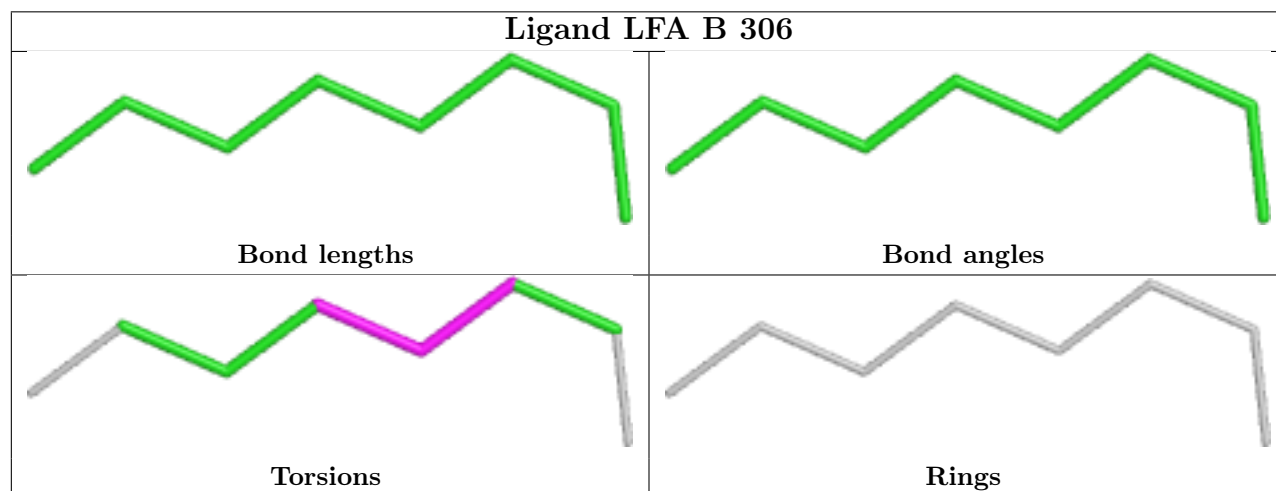
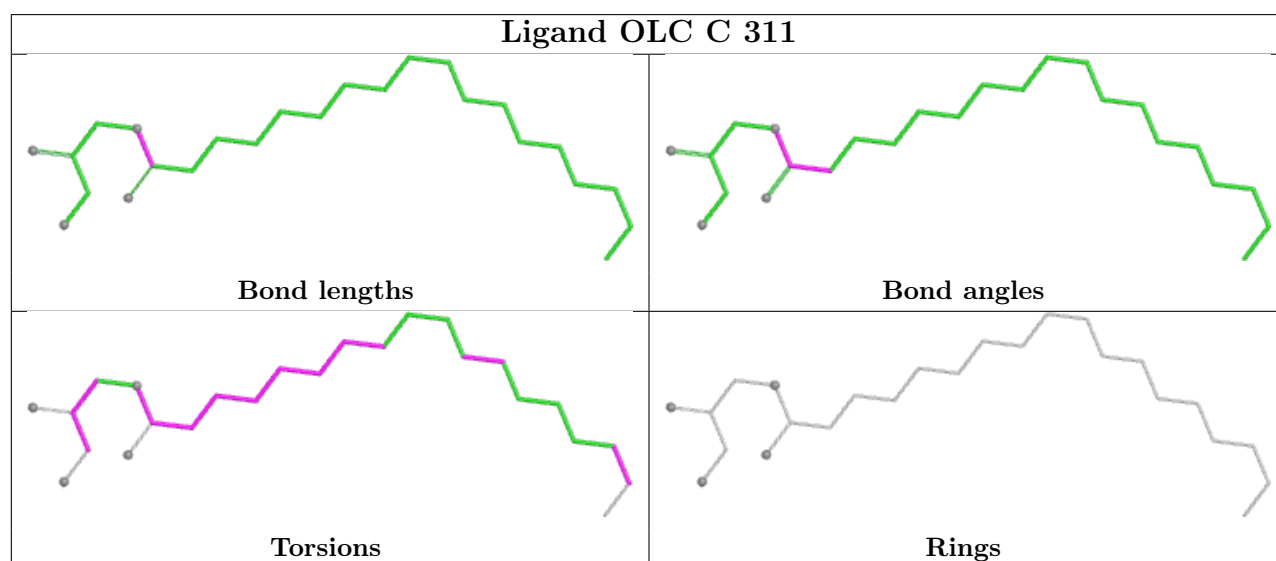
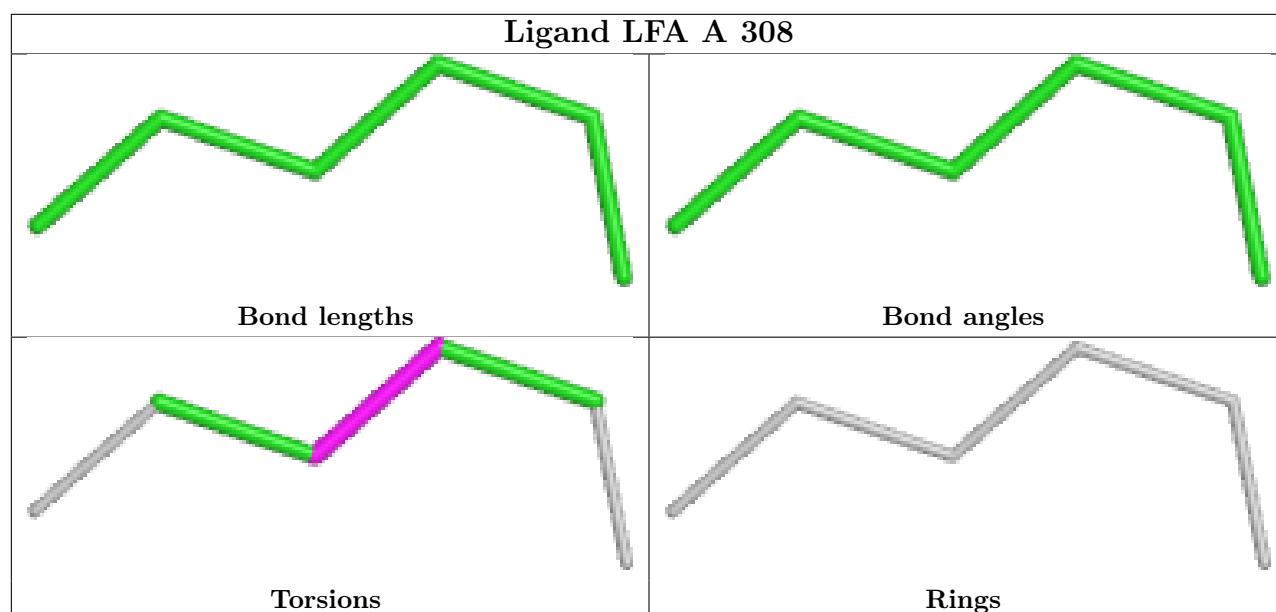


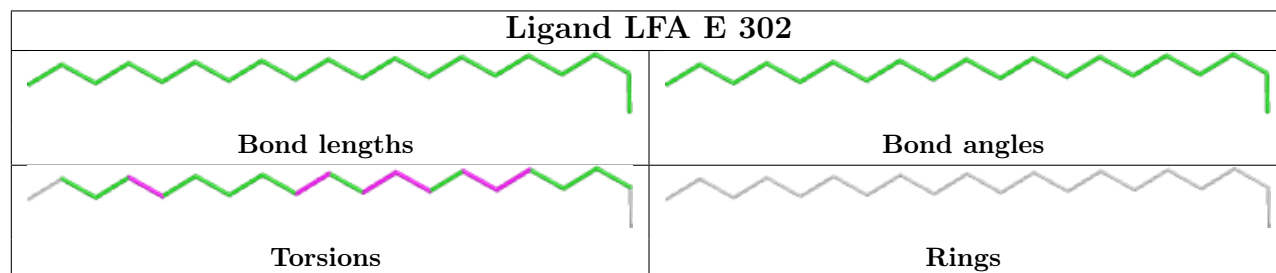
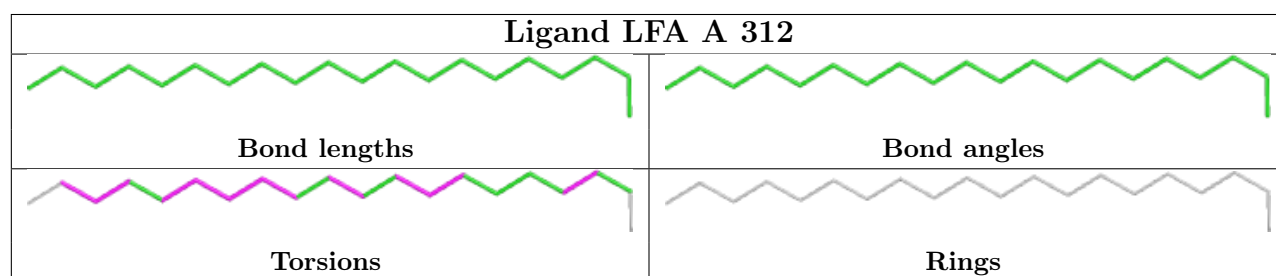
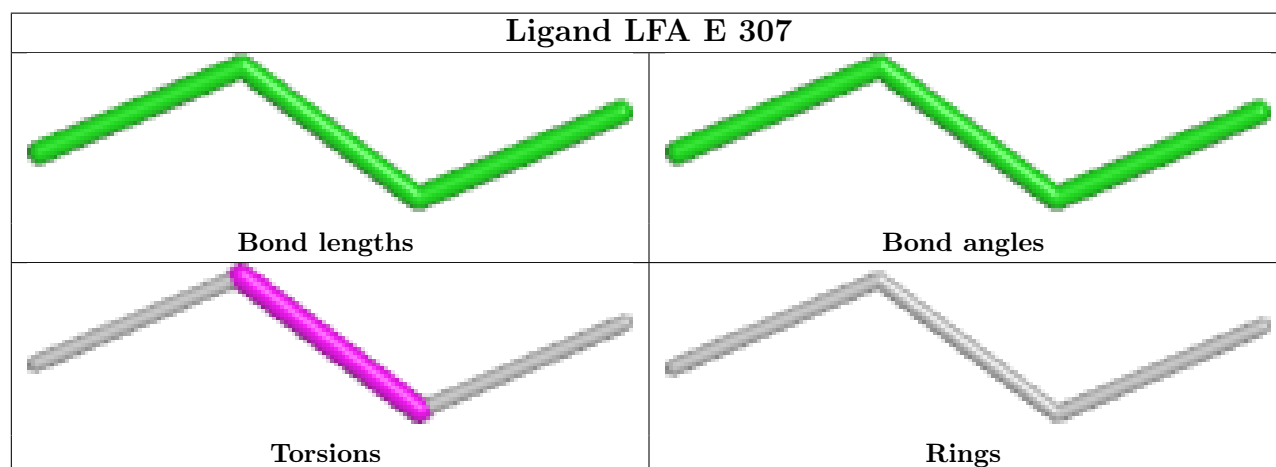
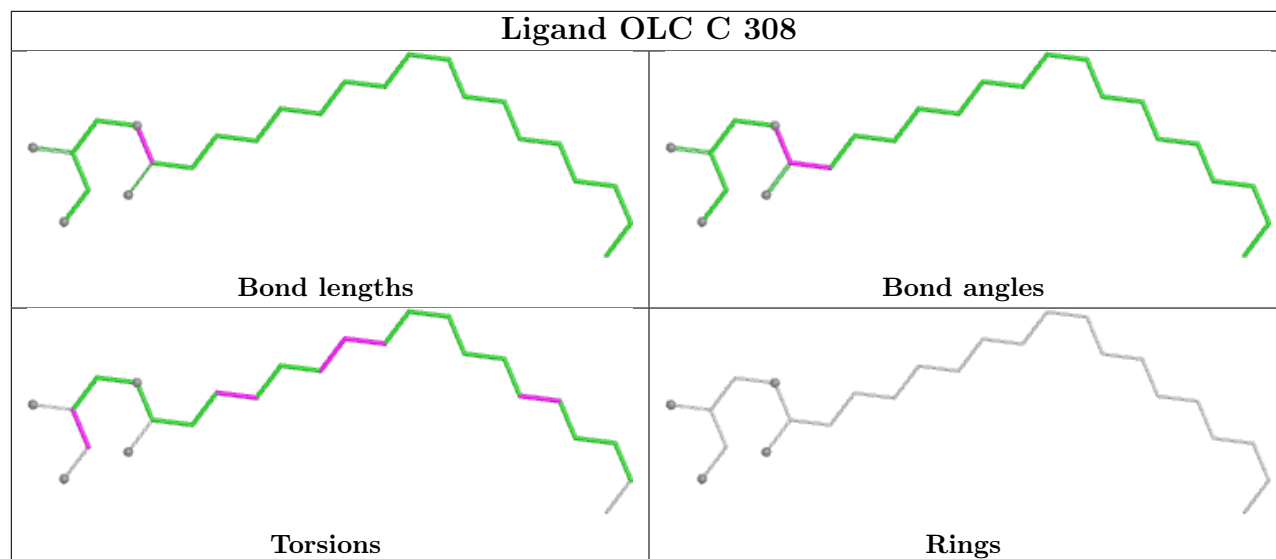


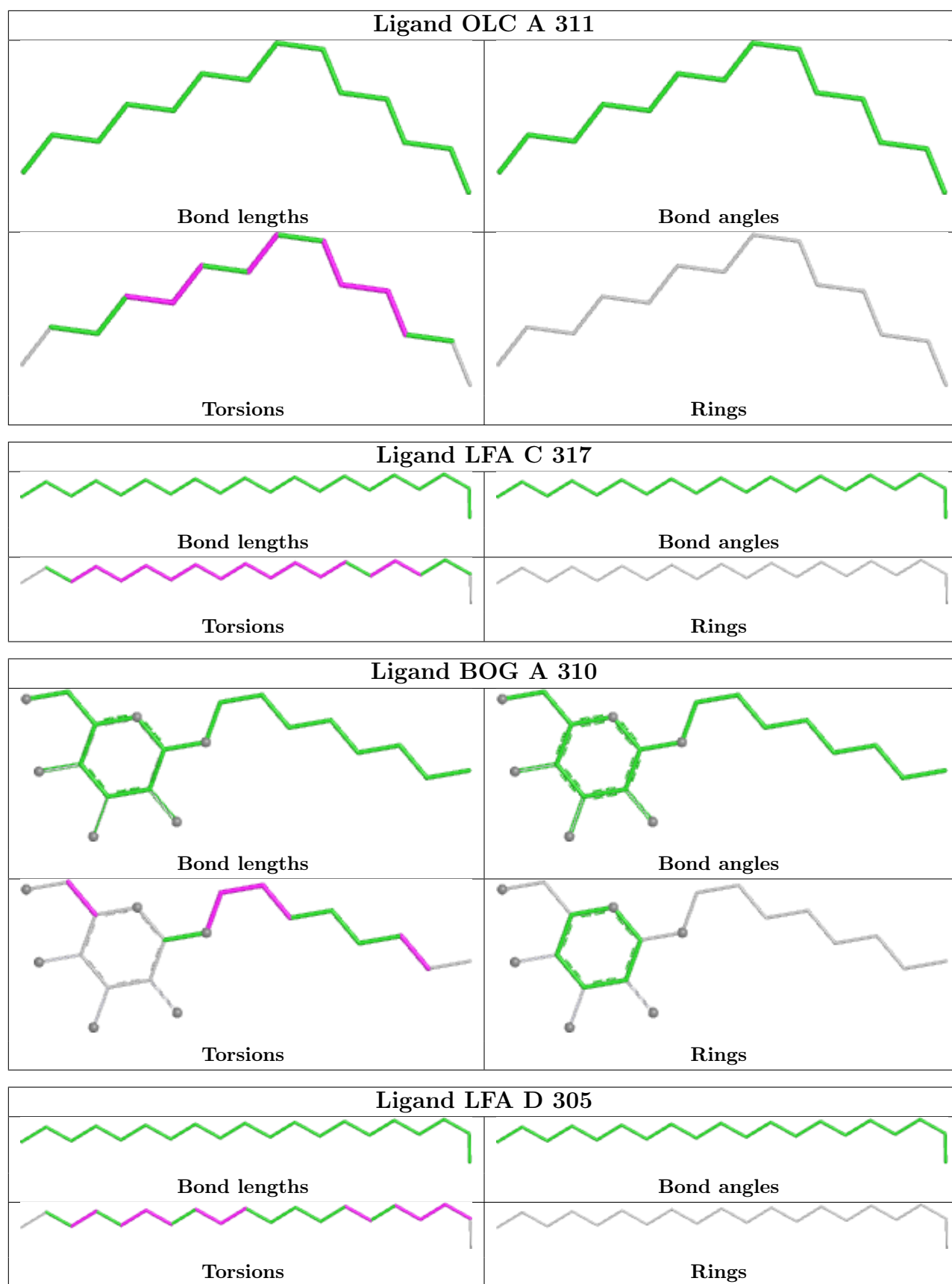


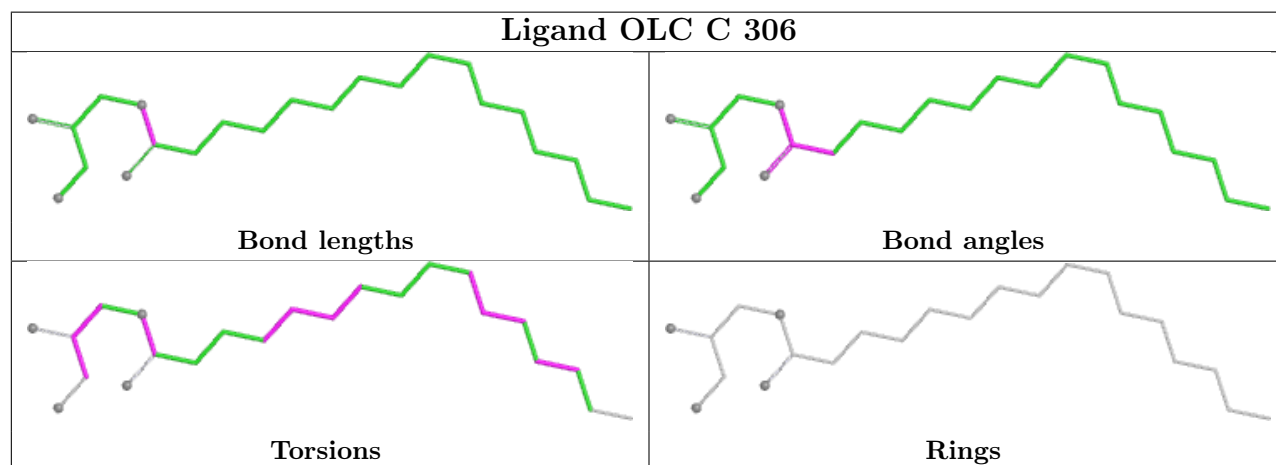
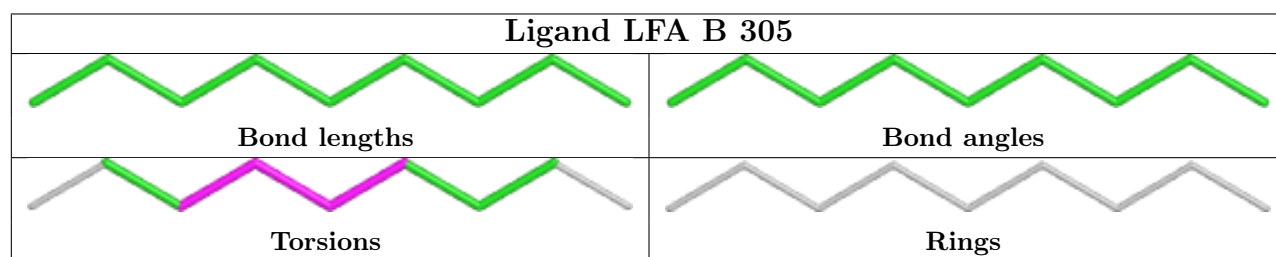
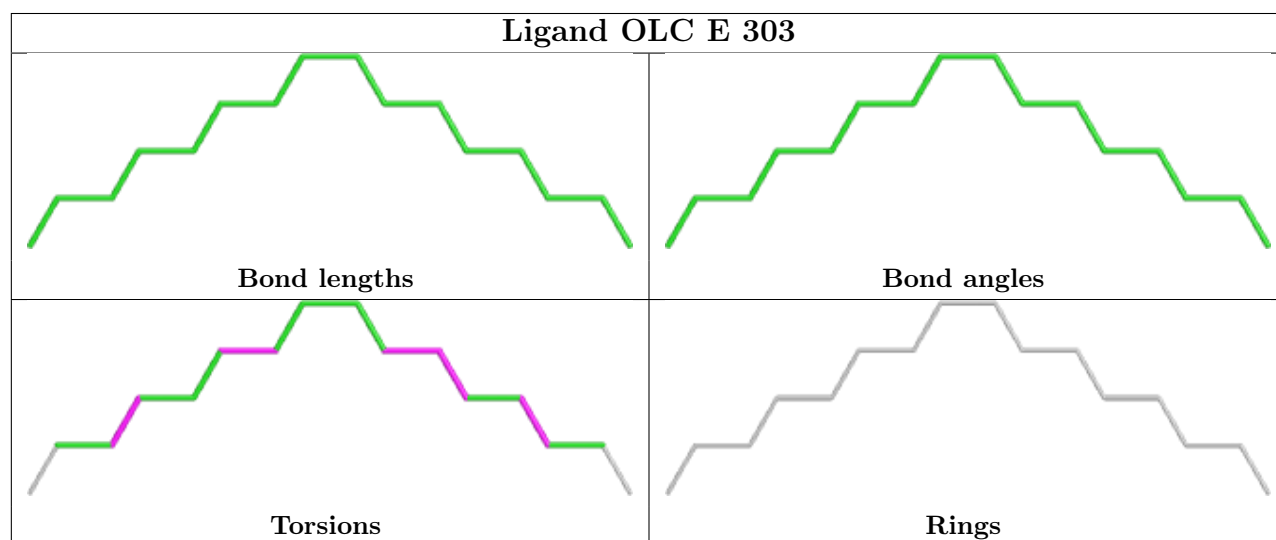
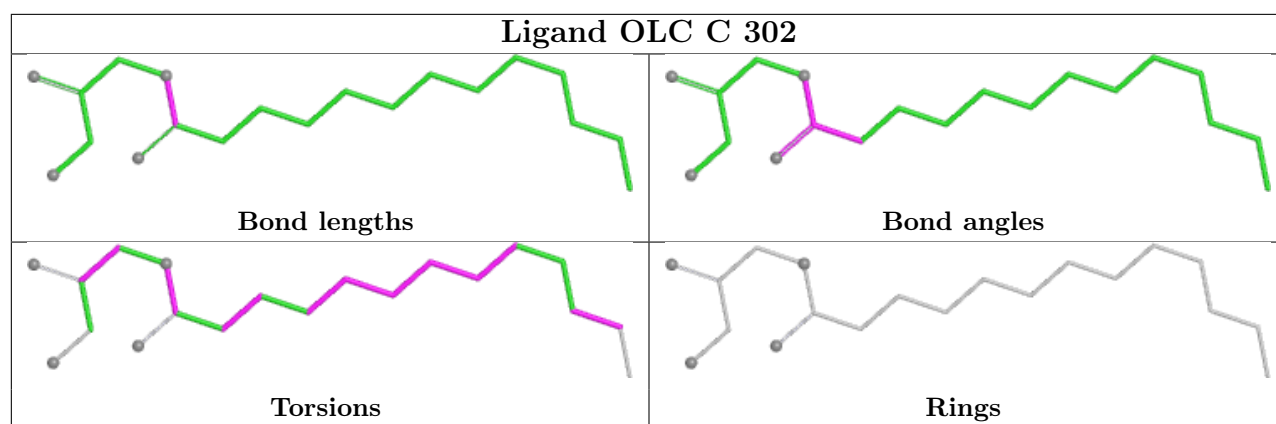


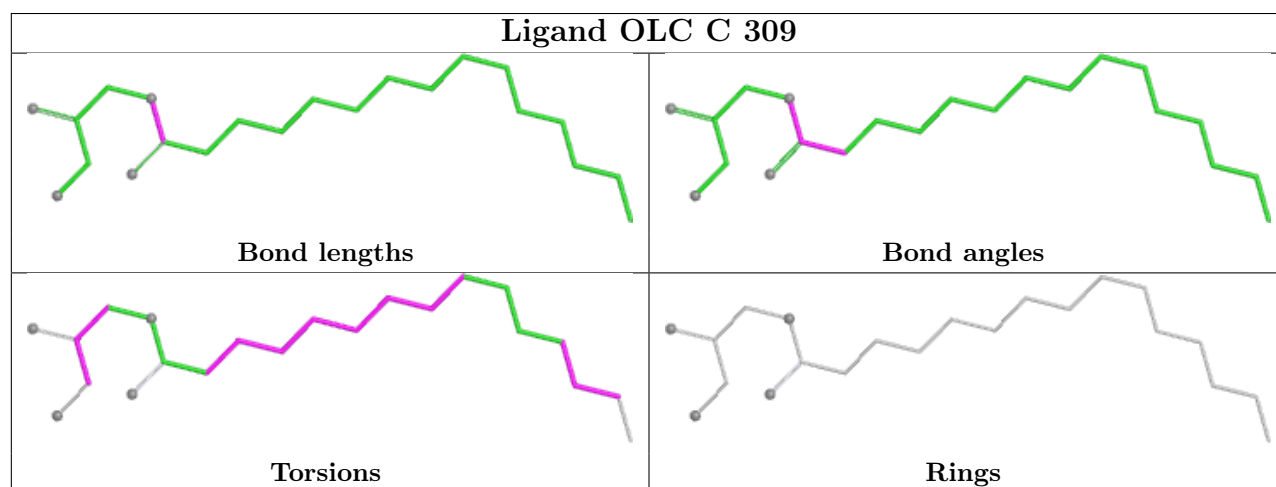
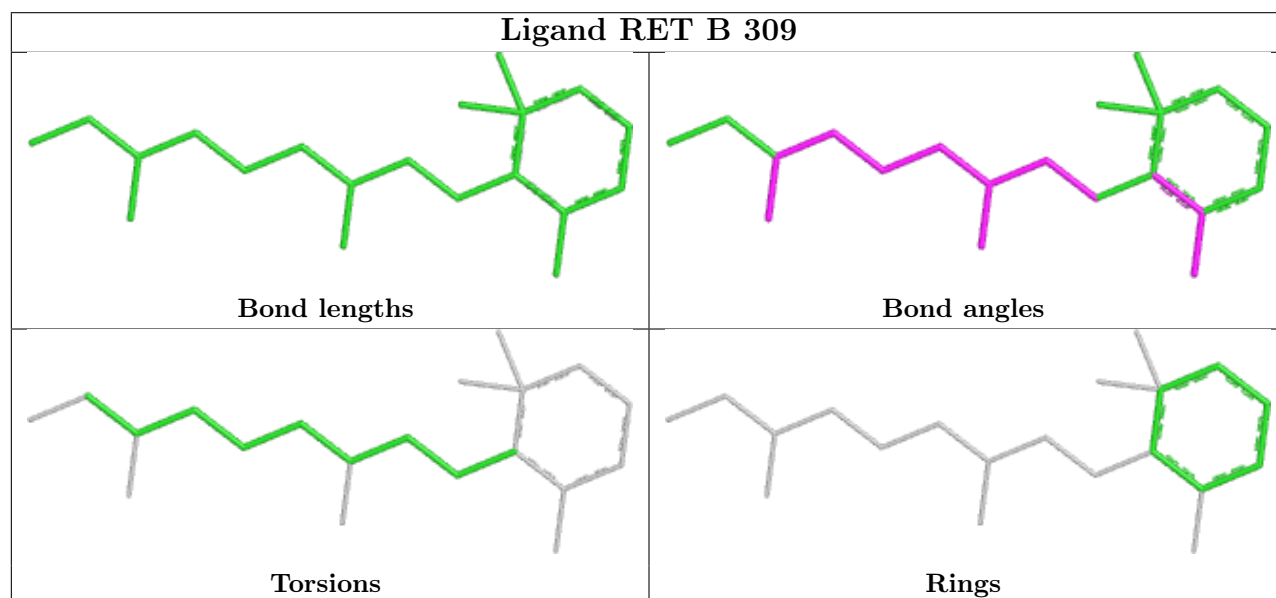
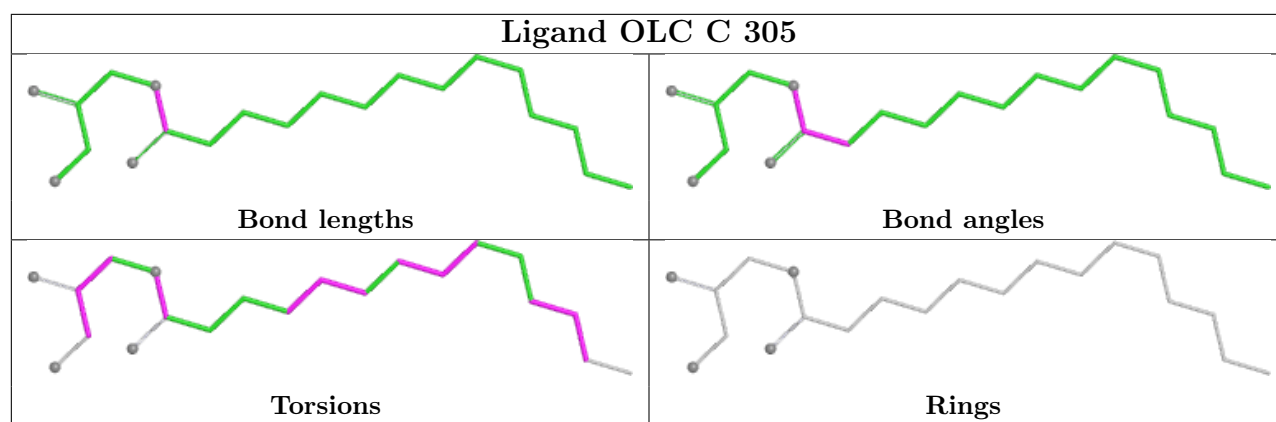


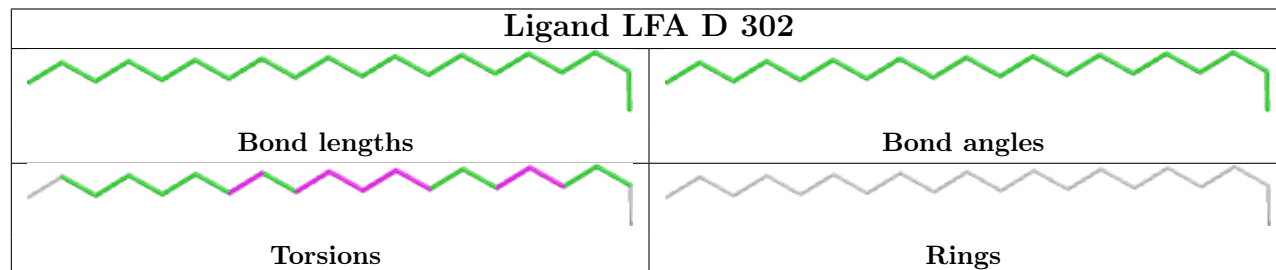
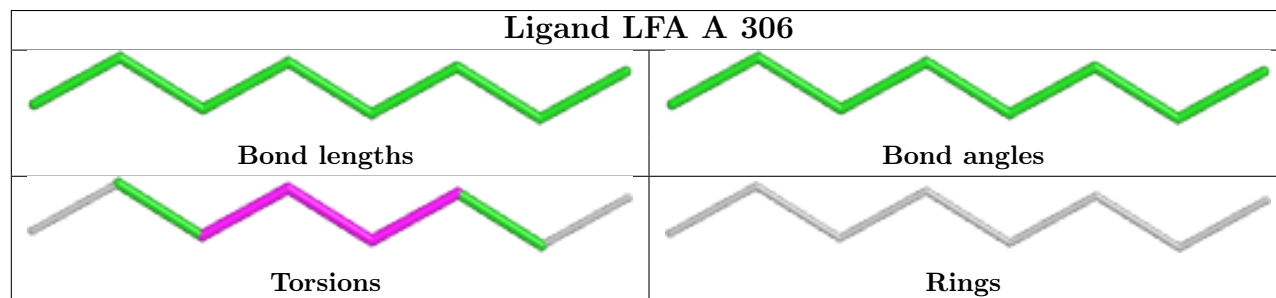
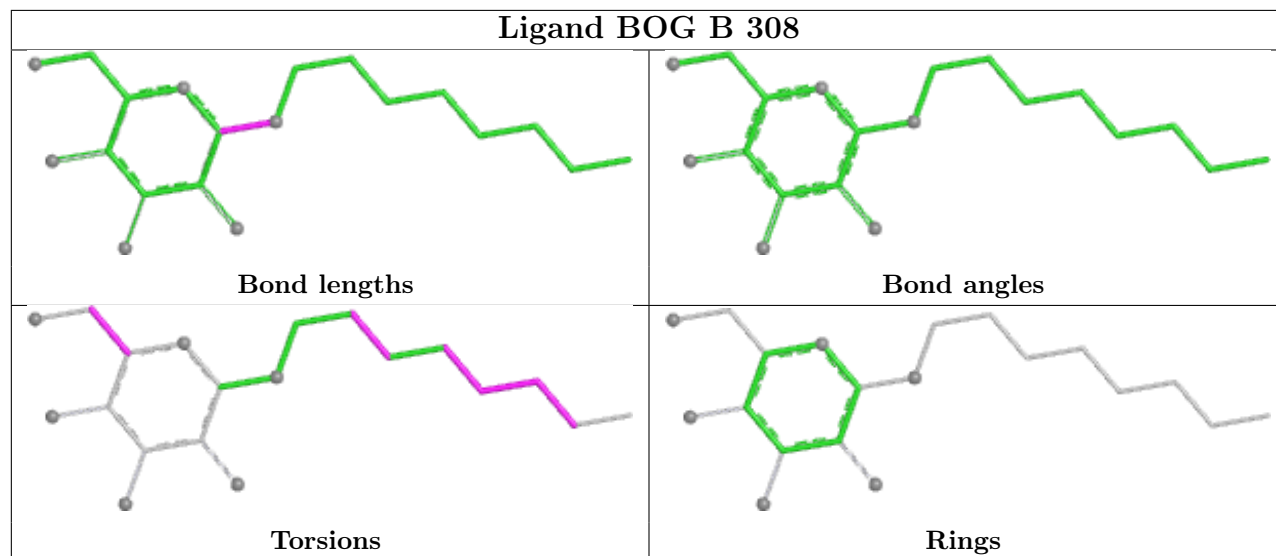
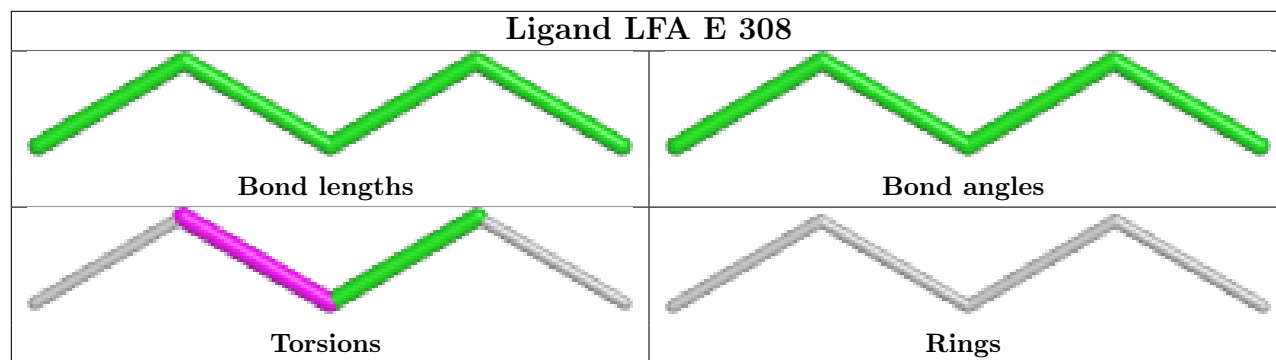


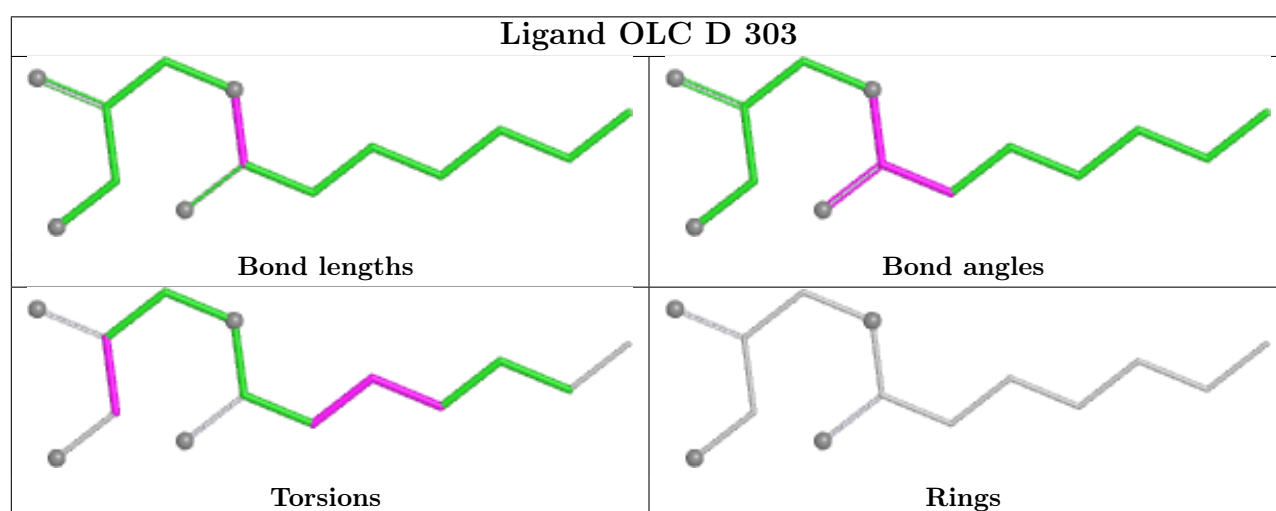
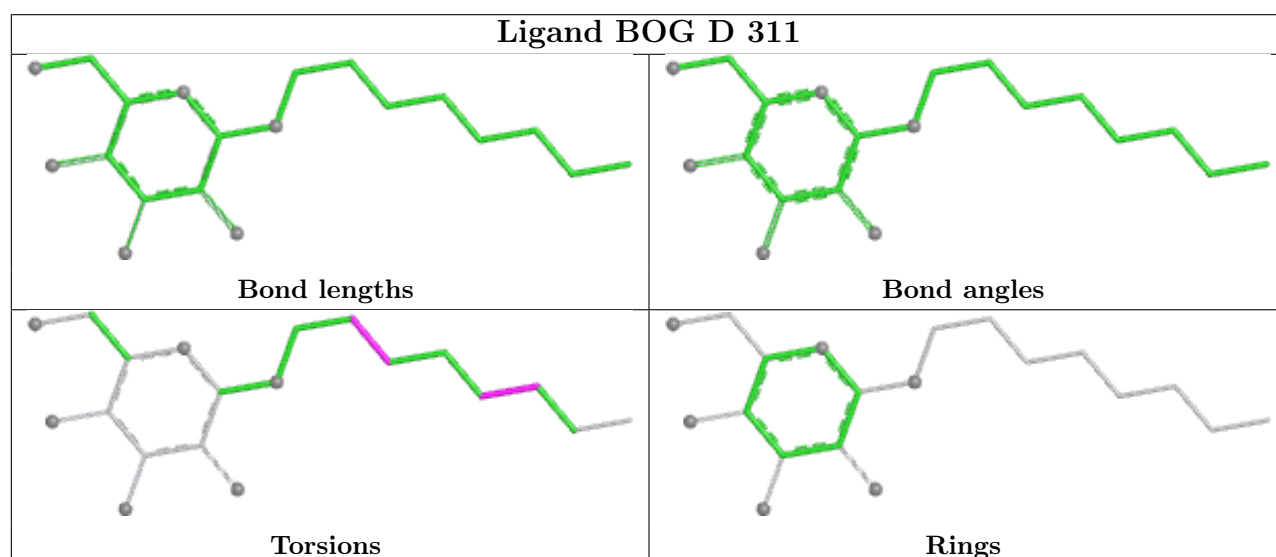
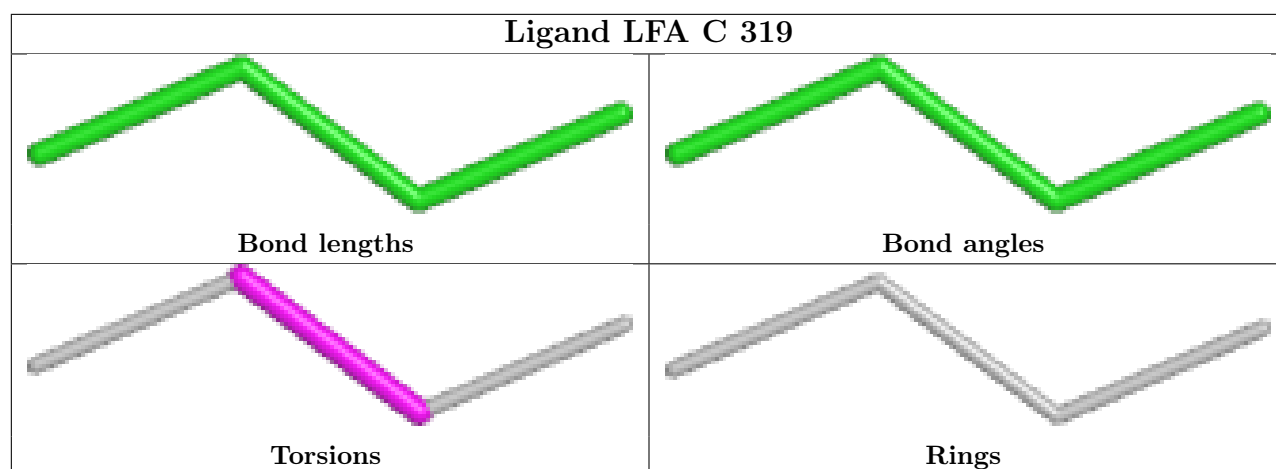


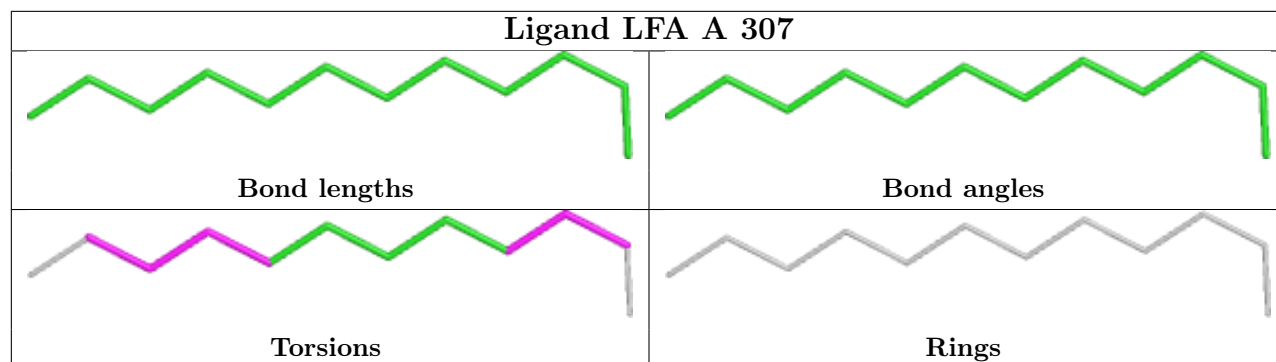
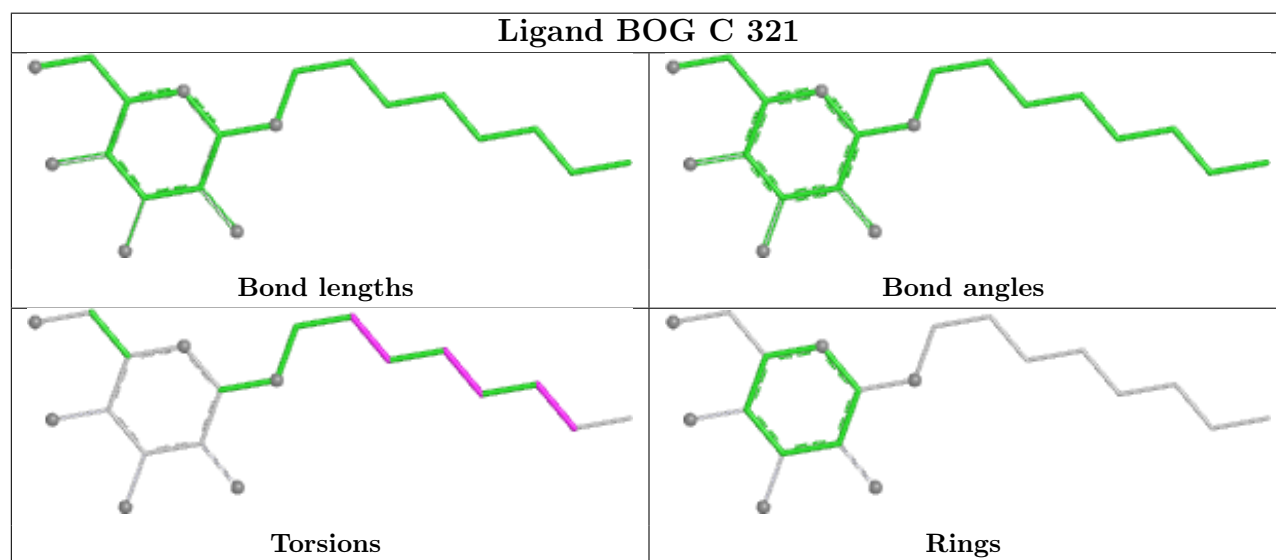
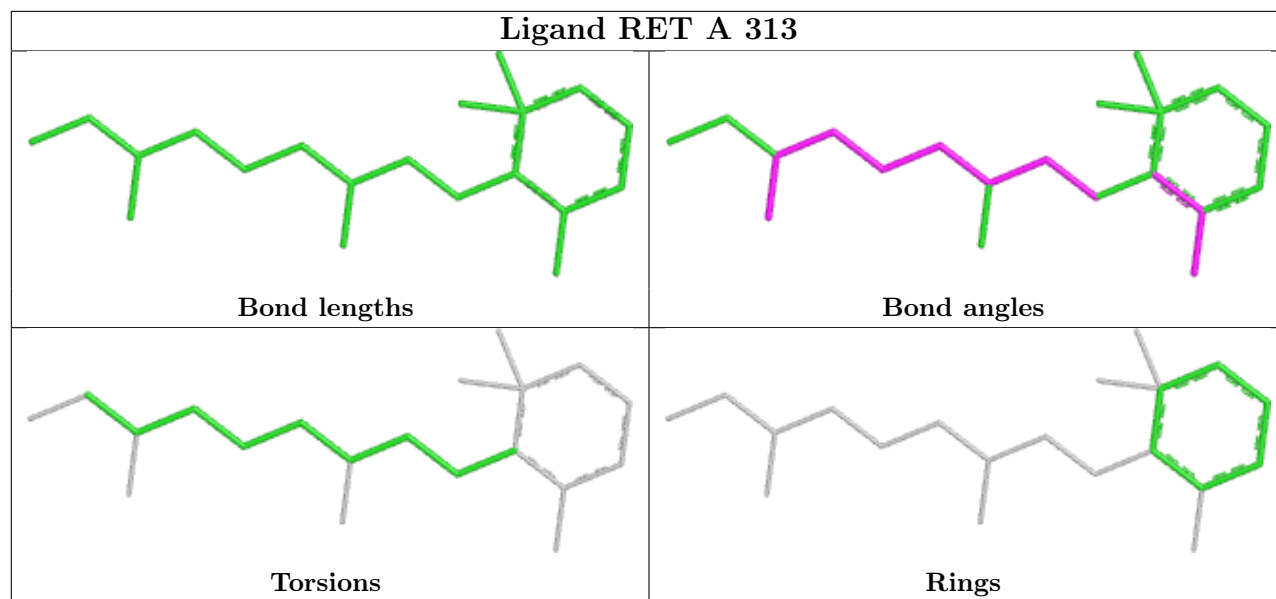


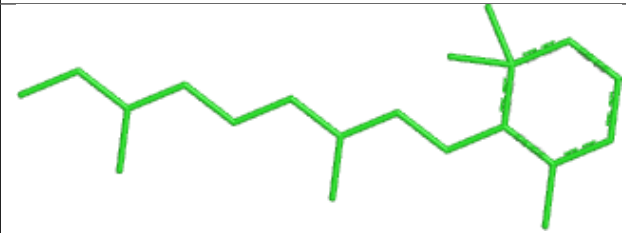
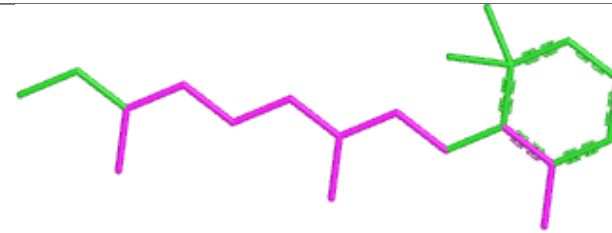
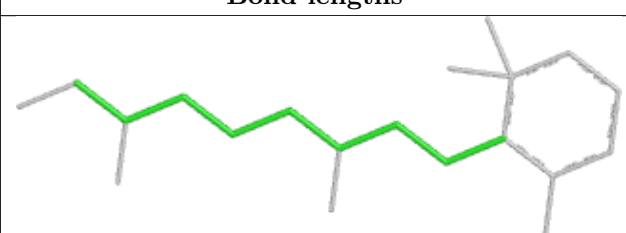
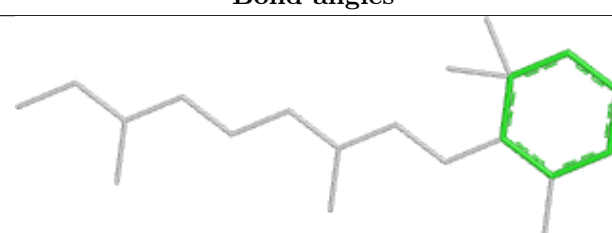


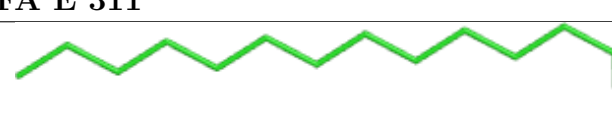
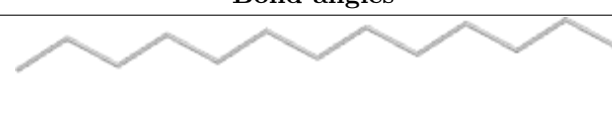


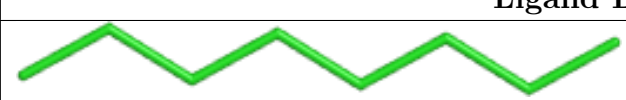
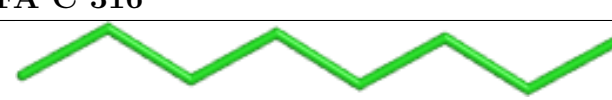


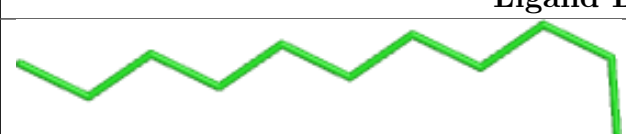
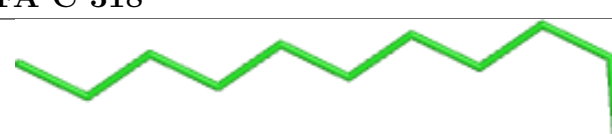
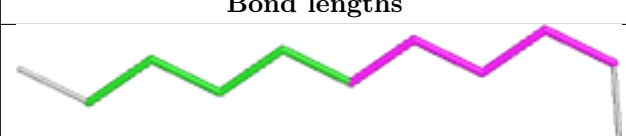
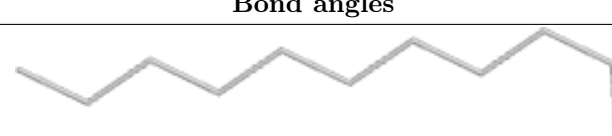


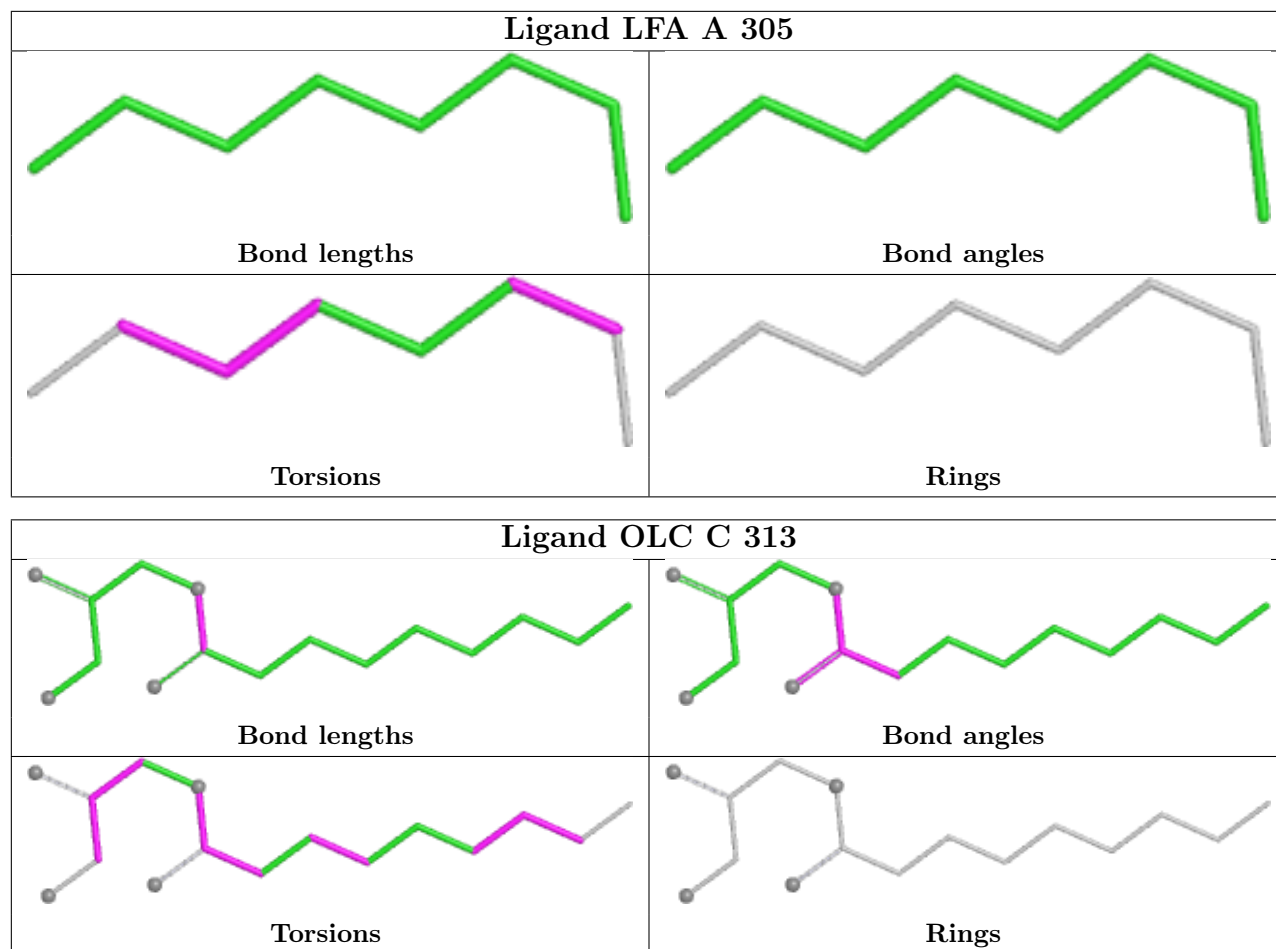


Ligand RET D 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LFA E 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LFA C 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LFA C 318	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	273/288 (94%)	0.06	9 (3%)	49	45	19, 48, 73, 154	1 (0%)
1	B	273/288 (94%)	0.16	16 (5%)	28	24	21, 48, 69, 139	1 (0%)
1	C	273/288 (94%)	0.05	12 (4%)	39	34	21, 48, 71, 152	1 (0%)
1	D	273/288 (94%)	0.11	18 (6%)	24	20	19, 50, 75, 164	1 (0%)
1	E	273/288 (94%)	0.06	12 (4%)	39	34	20, 48, 71, 169	1 (0%)
All	All	1365/1440 (94%)	0.09	67 (4%)	35	31	19, 48, 73, 169	5 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	GLN	5.8
1	C	91	GLU	4.8
1	E	275	LEU	4.7
1	E	274	GLU	4.7
1	E	3	GLN	4.6
1	A	275	LEU	4.6
1	C	275	LEU	4.5
1	D	195	GLY	4.5
1	E	4	GLU	4.4
1	B	273	LYS	4.2
1	B	275	LEU	4.1
1	A	90	GLU	3.9
1	A	3	GLN	3.6
1	E	273	LYS	3.5
1	C	3	GLN	3.4
1	D	91	GLU	3.3
1	B	16	ALA	3.3
1	C	16	ALA	3.1
1	B	194	GLU	3.1
1	B	89	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	195	GLY	3.1
1	A	91	GLU	3.0
1	E	91	GLU	3.0
1	D	130	LEU	2.9
1	D	3	GLN	2.9
1	A	57	PHE	2.9
1	C	269	LEU	2.8
1	E	183	TRP	2.8
1	A	92	VAL	2.8
1	D	275	LEU	2.8
1	E	17	THR	2.8
1	D	274	GLU	2.8
1	C	129	SER	2.7
1	D	92	VAL	2.7
1	B	17	THR	2.6
1	C	196	ILE	2.6
1	E	272	ASN	2.5
1	E	16	ALA	2.5
1	E	54	ASP	2.5
1	D	272	ASN	2.5
1	D	194	GLU	2.5
1	D	183	TRP	2.5
1	C	56	LYS	2.4
1	D	273	LYS	2.4
1	B	195	GLY	2.4
1	A	273	LYS	2.4
1	D	16	ALA	2.4
1	B	183	TRP	2.4
1	B	129	SER	2.3
1	C	4	GLU	2.3
1	D	131	THR	2.3
1	B	230	VAL	2.3
1	D	17	THR	2.3
1	C	273	LYS	2.3
1	D	132	THR	2.2
1	E	270	SER	2.2
1	B	274	GLU	2.2
1	D	90	GLU	2.2
1	D	129	SER	2.2
1	B	271	LYS	2.2
1	B	92	VAL	2.1
1	A	17	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	4	GLU	2.1
1	D	271	LYS	2.1
1	A	4	GLU	2.1
1	C	90	GLU	2.0
1	B	57	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LFA	D	309	6/20	0.68	0.32	80,90,93,94	0
5	BOG	B	308	20/20	0.70	0.23	80,101,109,114	0
2	OLC	C	310	16/25	0.72	0.23	91,111,137,138	0
3	LFA	B	305	9/20	0.73	0.36	82,90,110,112	0
3	LFA	C	322	4/20	0.73	0.29	72,76,78,80	0
3	LFA	C	315	7/20	0.74	0.30	75,94,106,109	0
2	OLC	C	304	14/25	0.74	0.23	95,118,144,157	0
3	LFA	E	302	20/20	0.76	0.27	61,81,101,101	0
3	LFA	C	303	20/20	0.76	0.26	59,77,86,88	0
3	LFA	A	307	12/20	0.77	0.30	89,102,110,113	0
3	LFA	B	302	20/20	0.77	0.24	60,77,100,103	0
3	LFA	D	302	20/20	0.77	0.22	54,69,89,89	0
3	LFA	A	312	20/20	0.78	0.25	64,80,91,95	0
5	BOG	A	310	20/20	0.79	0.18	81,101,112,115	0
5	BOG	E	310	20/20	0.79	0.16	71,98,112,112	0
3	LFA	A	305	8/20	0.80	0.32	77,87,92,94	0
2	OLC	C	307	25/25	0.80	0.21	74,104,118,129	0
3	LFA	E	311	14/20	0.81	0.32	102,117,127,133	0

Continued on next page...

Continued from previous page...

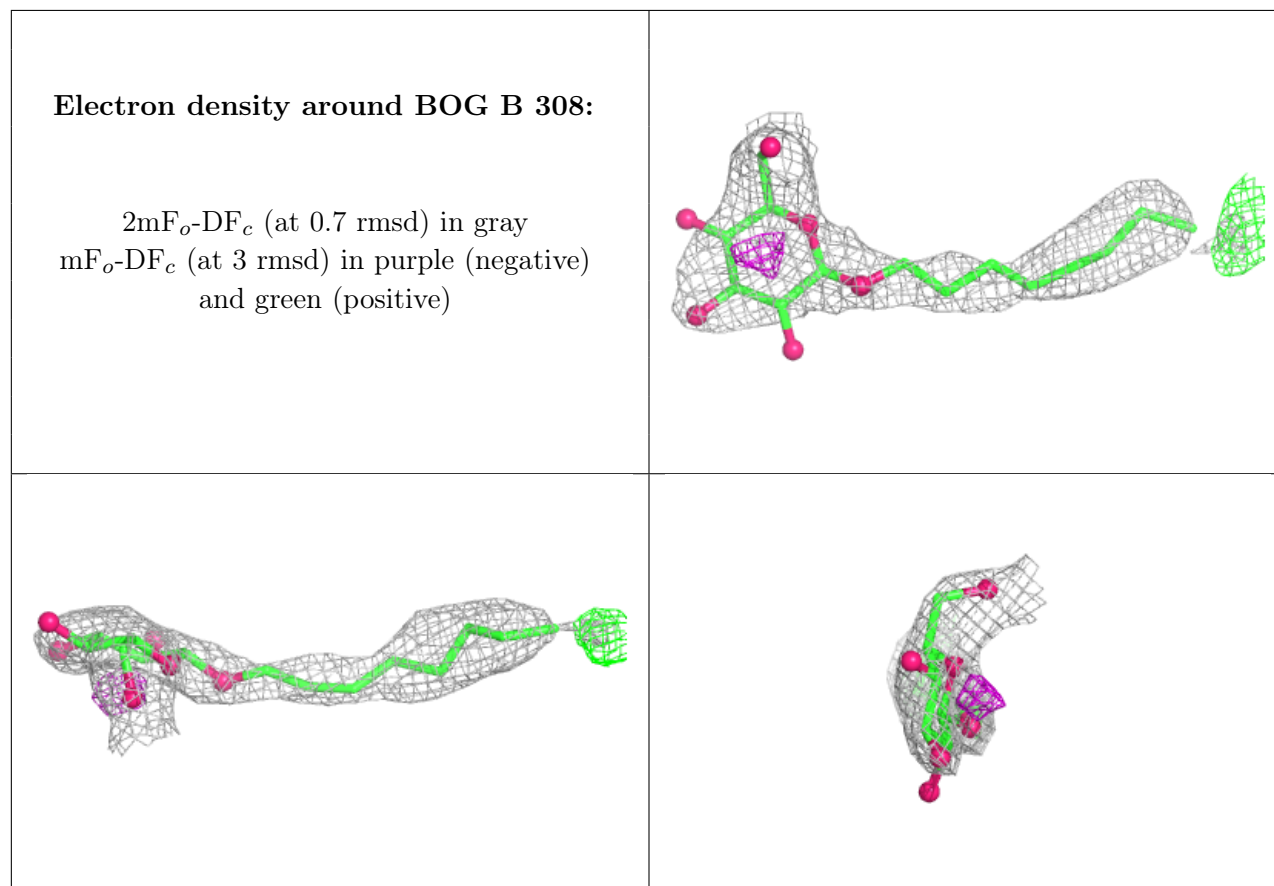
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LFA	D	308	7/20	0.81	0.26	74,89,98,102	0
2	OLC	C	311	25/25	0.81	0.23	87,111,133,135	0
2	OLC	C	308	25/25	0.81	0.22	67,101,124,139	0
3	LFA	D	304	20/20	0.82	0.28	81,102,113,115	0
3	LFA	A	304	7/20	0.83	0.29	79,84,94,99	0
3	LFA	C	319	4/20	0.83	0.24	78,78,78,87	0
2	OLC	B	303	20/25	0.84	0.17	69,87,106,107	0
3	LFA	E	307	4/20	0.84	0.28	67,72,78,78	0
3	LFA	C	318	11/20	0.84	0.32	65,99,118,118	0
3	LFA	C	316	8/20	0.85	0.26	76,89,94,97	0
3	LFA	E	306	14/20	0.85	0.27	73,95,106,109	0
3	LFA	D	306	8/20	0.85	0.30	81,95,117,120	0
3	LFA	E	308	5/20	0.85	0.32	78,90,101,103	0
2	OLC	A	311	14/25	0.86	0.24	67,82,92,92	0
2	OLC	C	309	22/25	0.86	0.16	60,90,121,126	0
2	OLC	E	303	16/25	0.86	0.20	56,64,80,83	0
5	BOG	C	321	20/20	0.86	0.13	71,88,104,105	0
3	LFA	C	317	20/20	0.86	0.26	73,92,103,108	0
2	OLC	E	304	25/25	0.87	0.20	55,96,127,129	0
2	OLC	A	303	15/25	0.87	0.19	64,83,106,117	0
2	OLC	C	314	16/25	0.87	0.26	79,100,117,128	0
3	LFA	B	306	8/20	0.87	0.27	76,86,100,105	0
3	LFA	A	306	8/20	0.87	0.30	70,93,119,125	0
3	LFA	E	305	8/20	0.87	0.28	80,86,90,92	0
5	BOG	D	311	20/20	0.87	0.15	75,96,104,105	0
2	OLC	B	301	22/25	0.87	0.18	76,85,104,111	0
2	OLC	A	302	13/25	0.88	0.13	67,74,85,88	0
2	OLC	B	304	16/25	0.88	0.17	66,89,96,108	0
2	OLC	A	301	14/25	0.88	0.18	54,64,73,73	0
2	OLC	C	312	16/25	0.89	0.15	62,83,96,101	0
2	OLC	C	305	21/25	0.89	0.22	90,116,139,140	0
2	OLC	D	303	14/25	0.89	0.16	61,82,100,102	0
3	LFA	D	305	20/20	0.90	0.24	83,103,113,115	0
2	OLC	C	313	16/25	0.90	0.17	58,99,118,123	0
2	OLC	E	301	12/25	0.90	0.21	65,76,88,92	0
3	LFA	A	308	6/20	0.90	0.20	68,71,79,86	0
2	OLC	C	302	20/25	0.90	0.16	71,91,100,101	0
3	LFA	D	307	17/20	0.93	0.14	56,65,77,77	0
2	OLC	C	301	21/25	0.94	0.14	55,72,89,104	0
6	RET	B	309	20/21	0.94	0.09	40,45,50,52	0
6	RET	E	312	20/21	0.94	0.10	37,44,48,49	0
2	OLC	C	306	23/25	0.95	0.14	59,73,107,144	0

Continued on next page...

Continued from previous page...

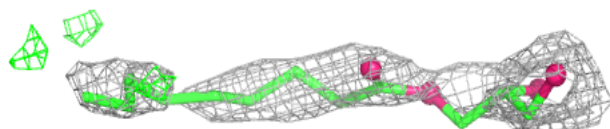
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	RET	D	312	20/21	0.95	0.09	44,52,59,64	0
2	OLC	D	301	18/25	0.95	0.13	79,91,107,119	0
6	RET	C	323	20/21	0.96	0.08	42,49,55,56	0
4	NA	D	310	1/1	0.97	0.05	46,46,46,46	0
6	RET	A	313	20/21	0.97	0.08	37,47,51,52	0
4	NA	A	309	1/1	0.98	0.04	47,47,47,47	0
4	NA	E	309	1/1	0.98	0.04	38,38,38,38	0
4	NA	B	307	1/1	0.99	0.04	41,41,41,41	0
4	NA	C	320	1/1	1.00	0.03	40,40,40,40	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.

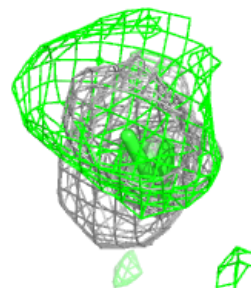
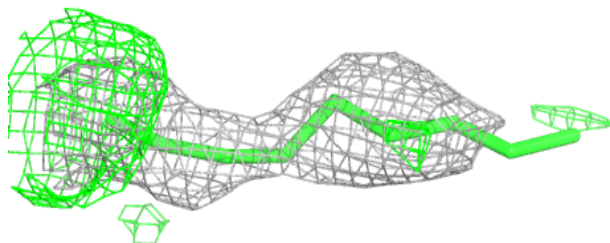
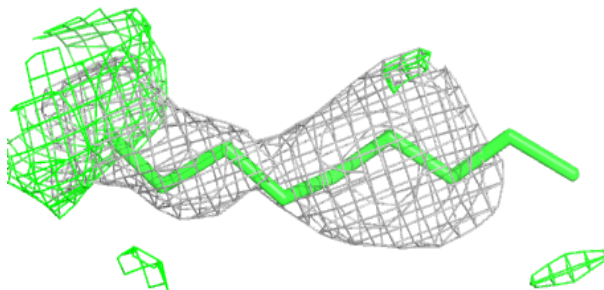


Electron density around OLC C 310:

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

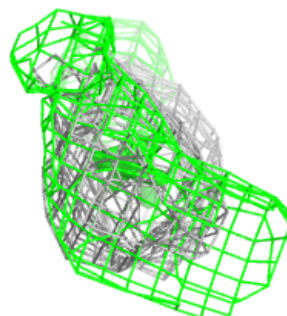
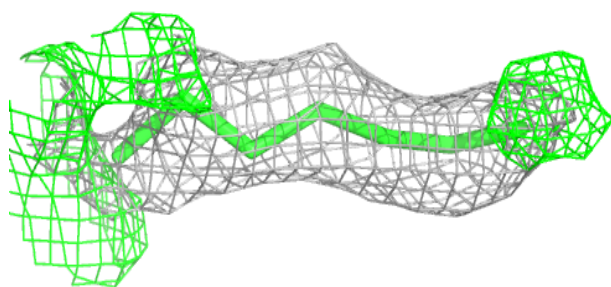
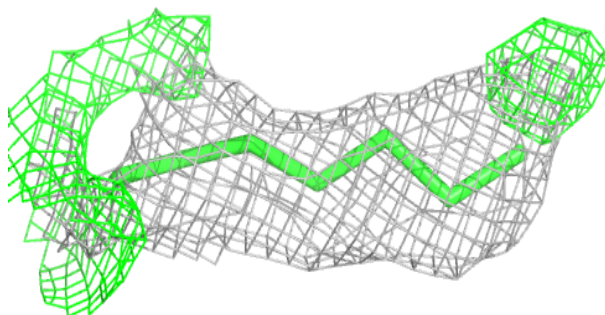
**Electron density around LFA B 305:**

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

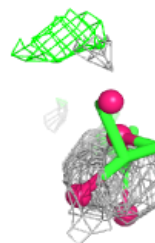
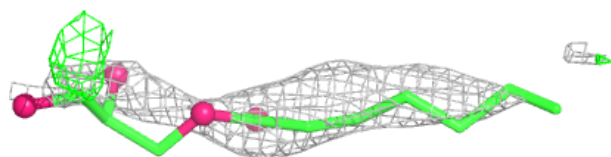
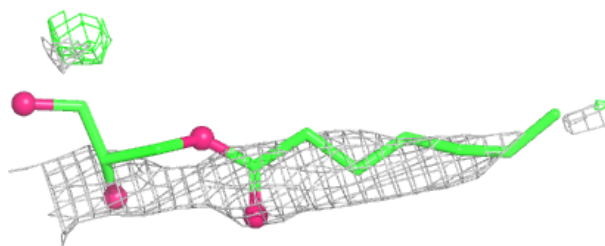


Electron density around LFA C 315:

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

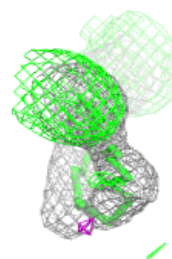
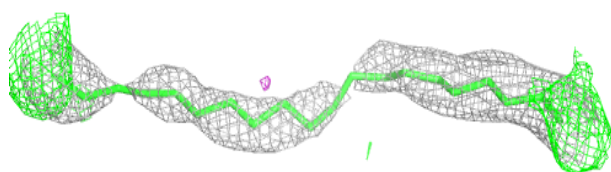
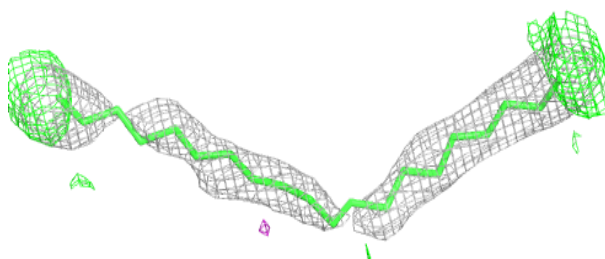
**Electron density around OLC C 304:**

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

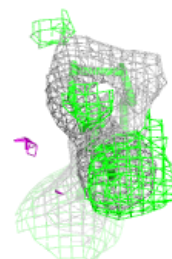
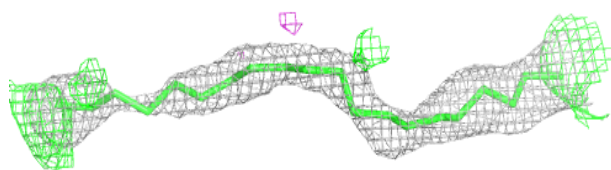
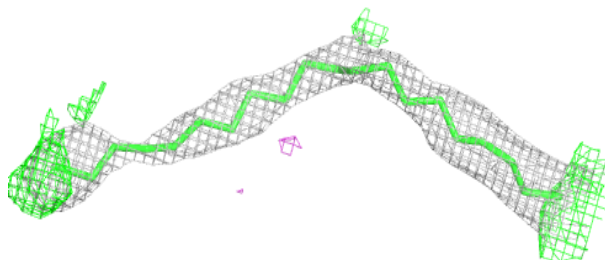


Electron density around LFA E 302:

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

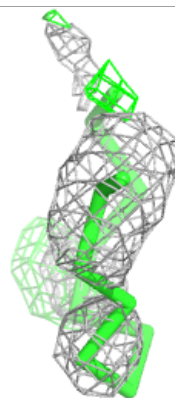
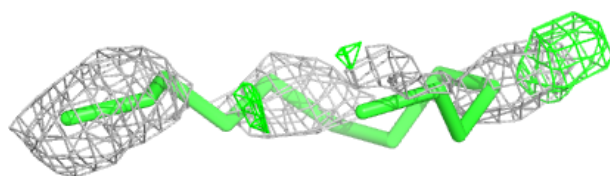
**Electron density around LFA C 303:**

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

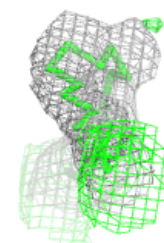
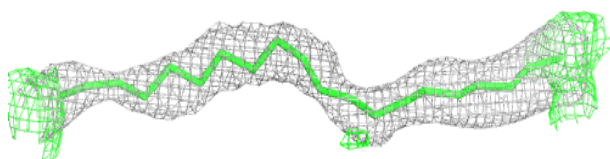
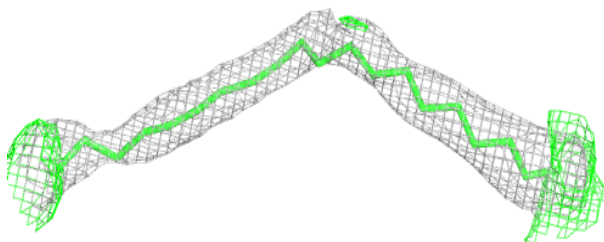


Electron density around LFA A 307:

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

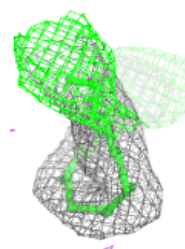
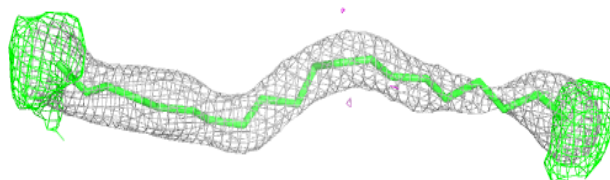
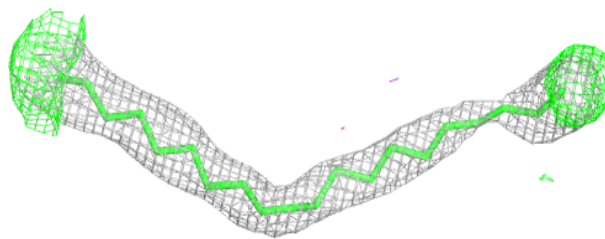
**Electron density around LFA B 302:**

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

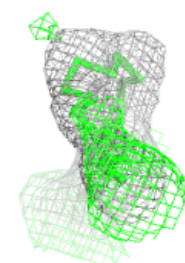
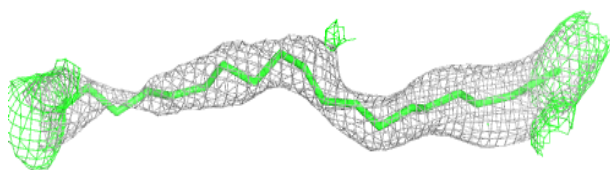
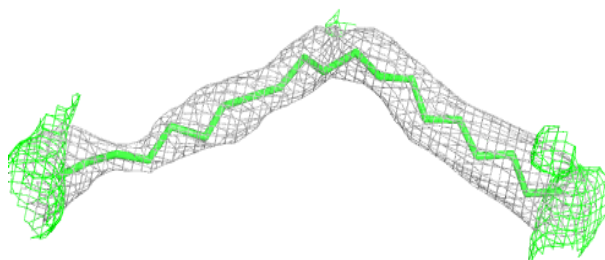


Electron density around LFA D 302:

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

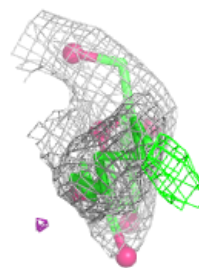
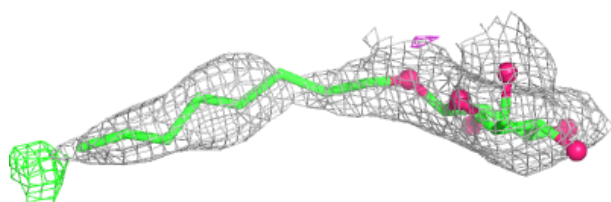
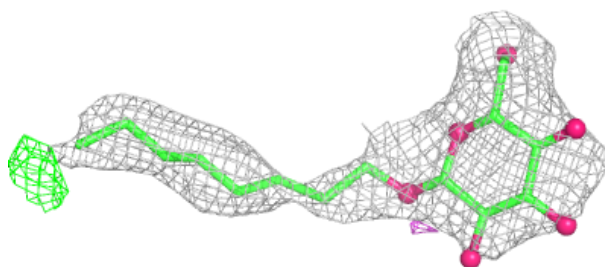
**Electron density around LFA A 312:**

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

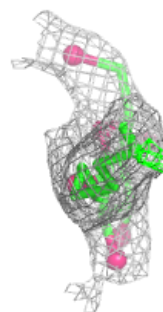
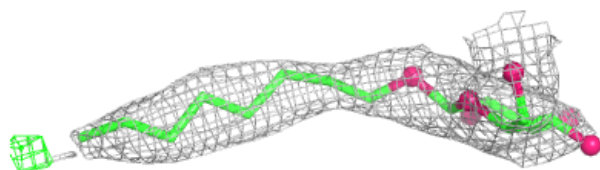
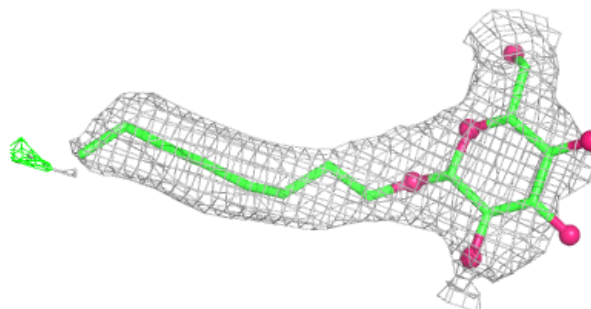


Electron density around BOG A 310:

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

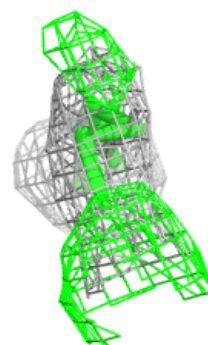
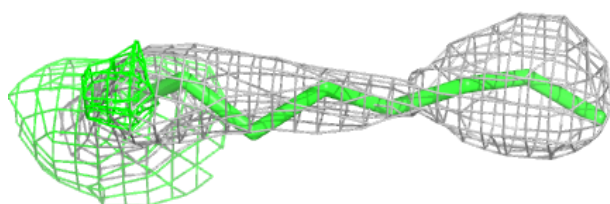
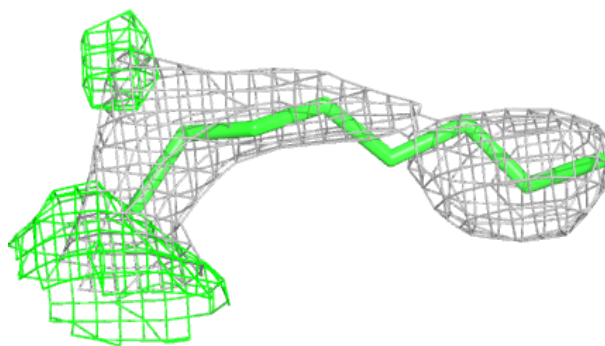
**Electron density around BOG E 310:**

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

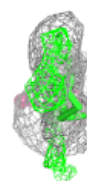
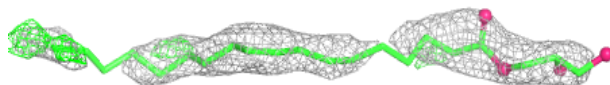
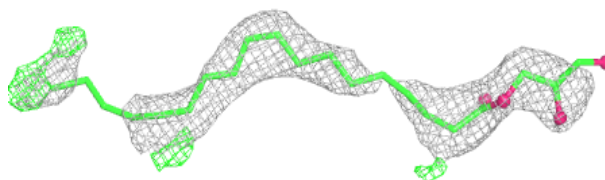


Electron density around LFA A 305:

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

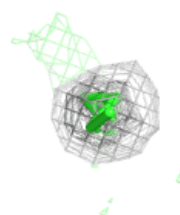
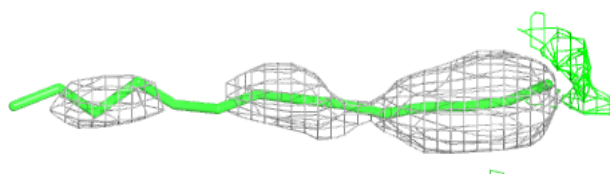
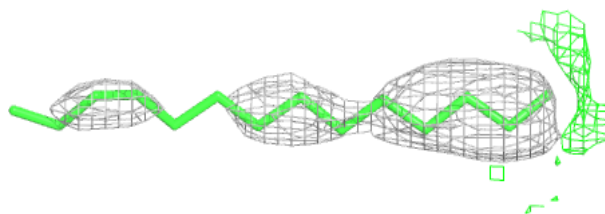
**Electron density around OLC C 307:**

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

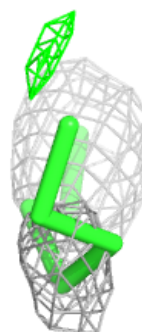
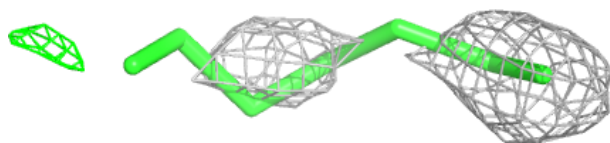
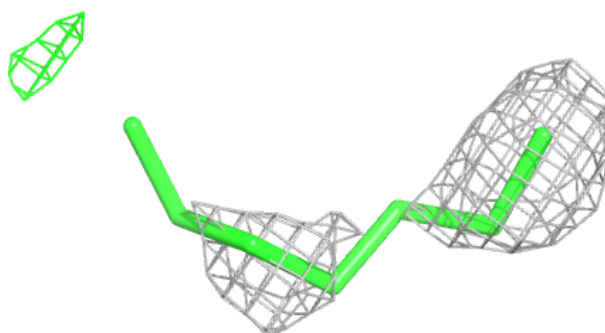


Electron density around LFA E 311:

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

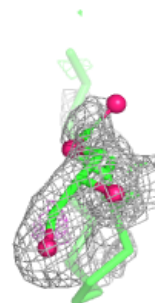
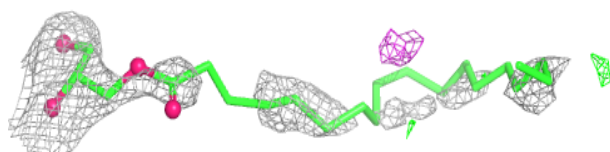
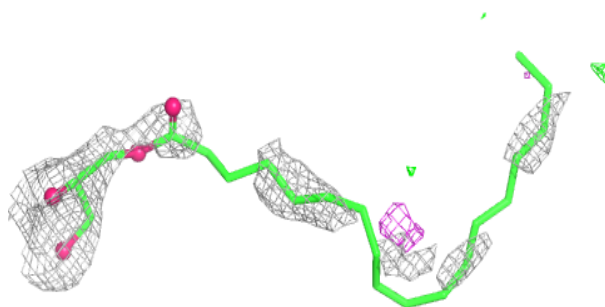
**Electron density around LFA D 308:**

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

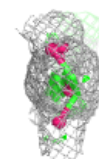
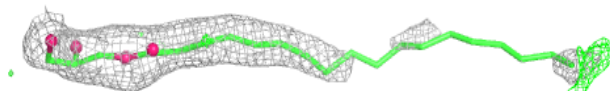
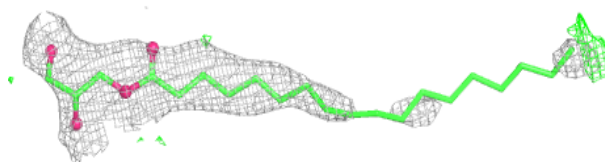


Electron density around OLC C 311:

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

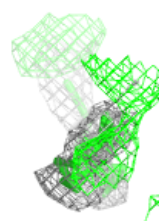
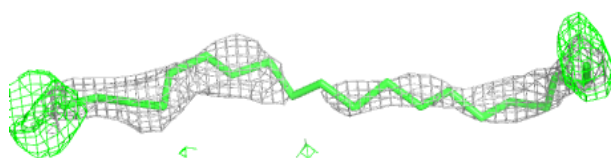
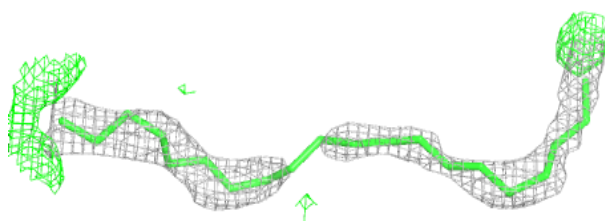
**Electron density around OLC C 308:**

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

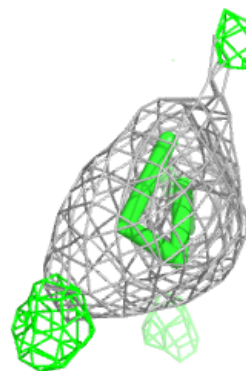
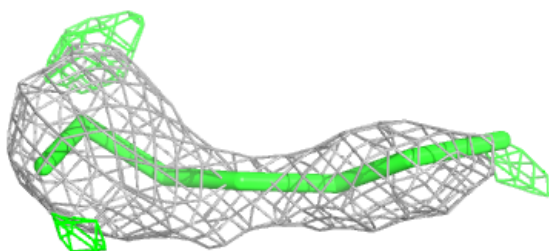
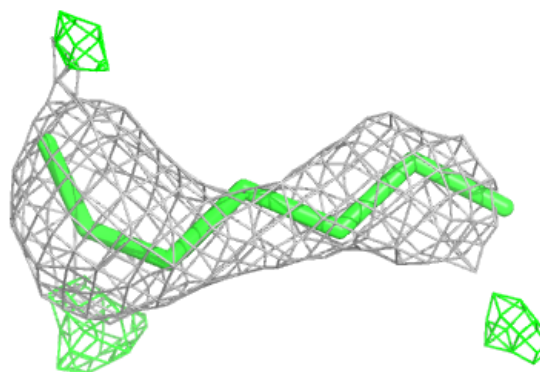


Electron density around LFA D 304:

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

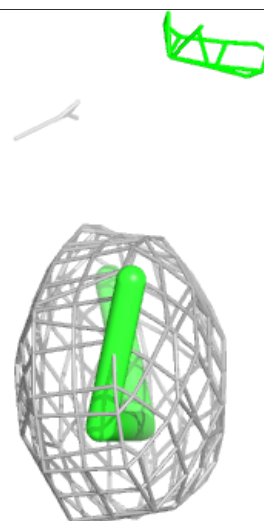
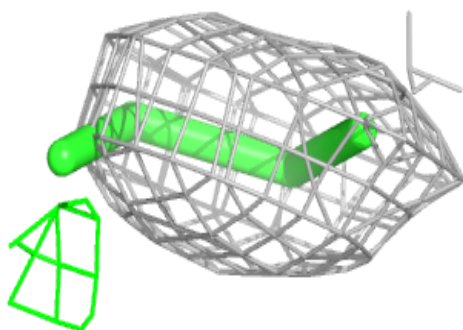
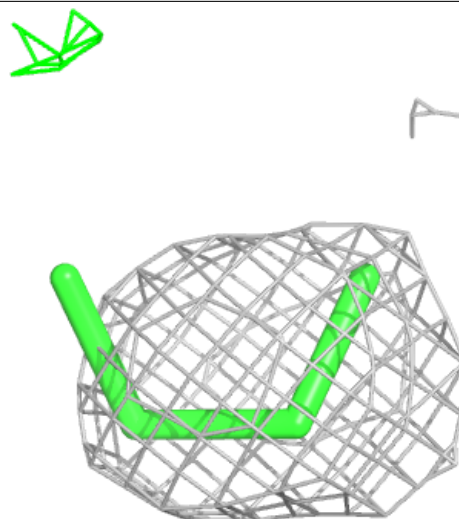
**Electron density around LFA A 304:**

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



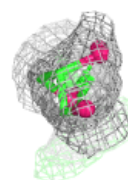
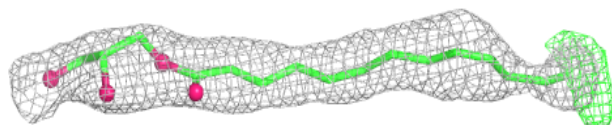
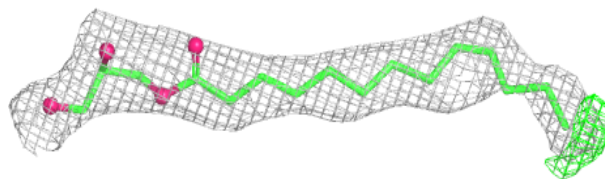
Electron density around LFA C 319:

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



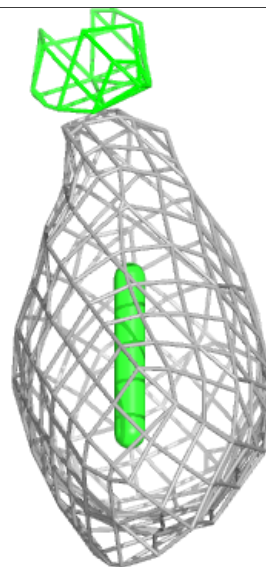
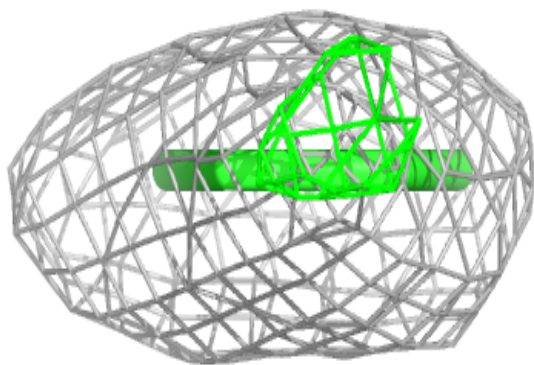
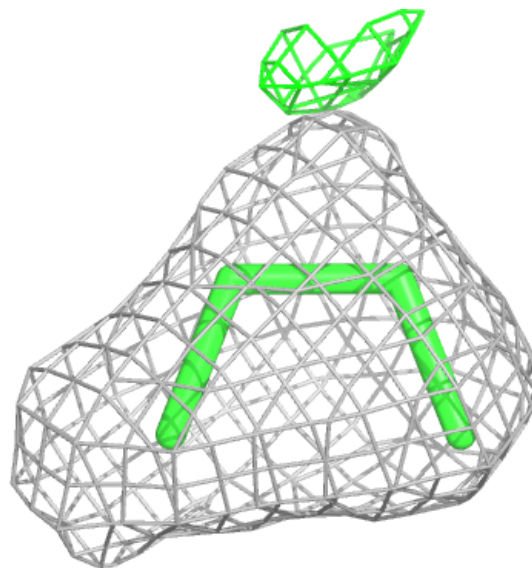
Electron density around OLC B 303:

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



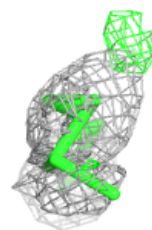
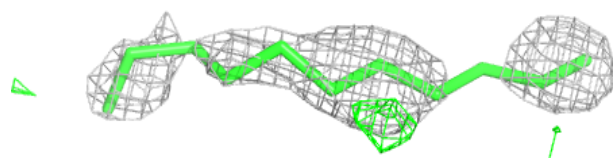
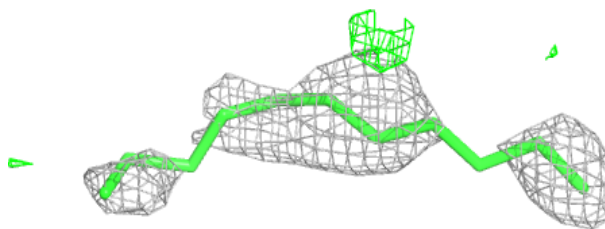
Electron density around LFA E 307:

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

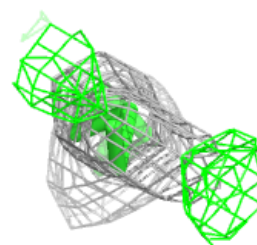
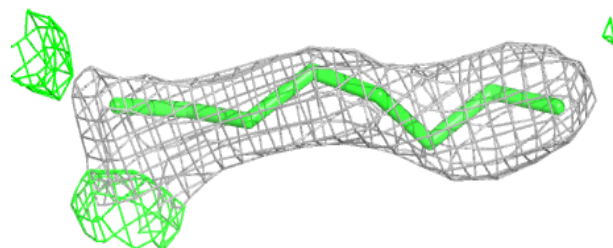
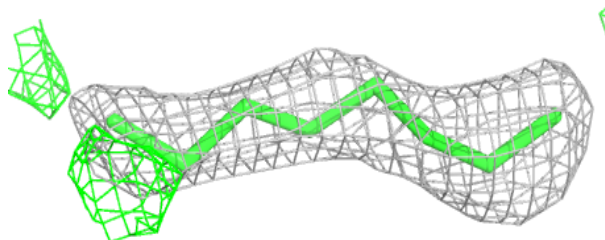


Electron density around LFA C 318:

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

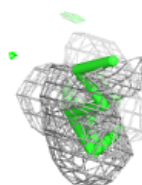
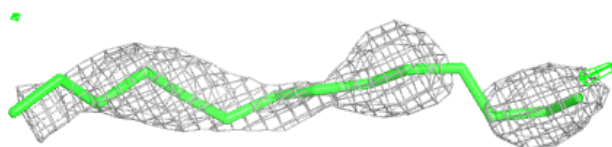
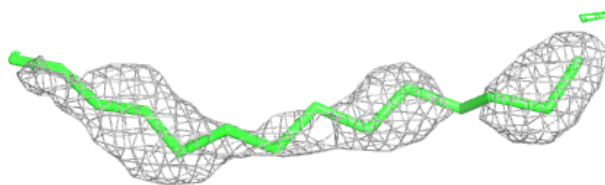
**Electron density around LFA C 316:**

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

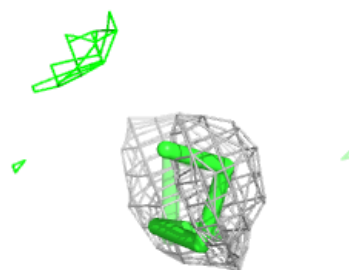
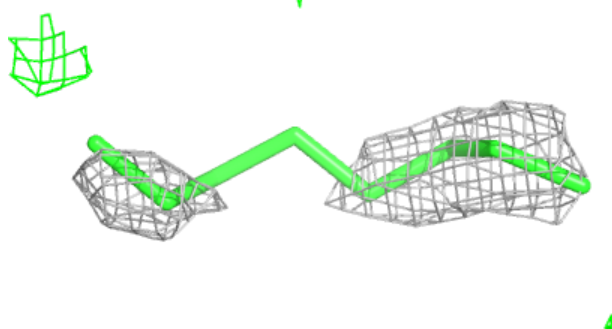
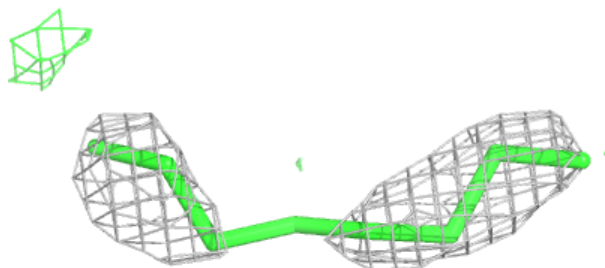


Electron density around LFA E 306:

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

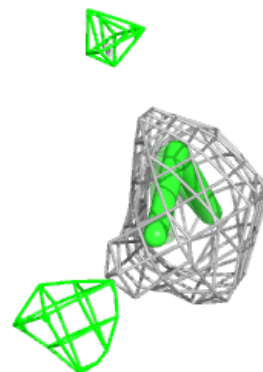
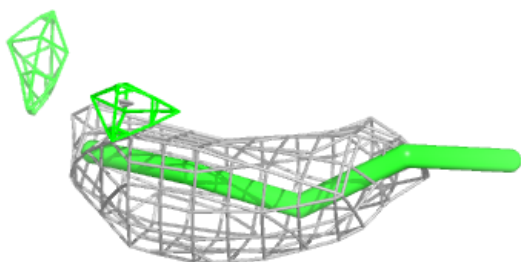
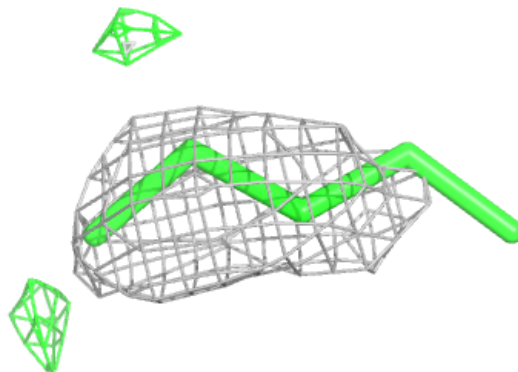
**Electron density around LFA D 306:**

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

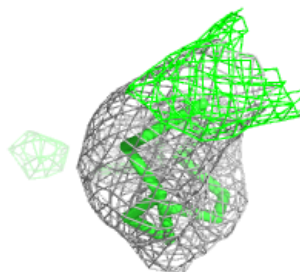
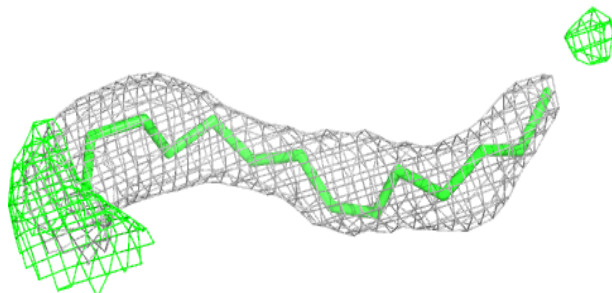
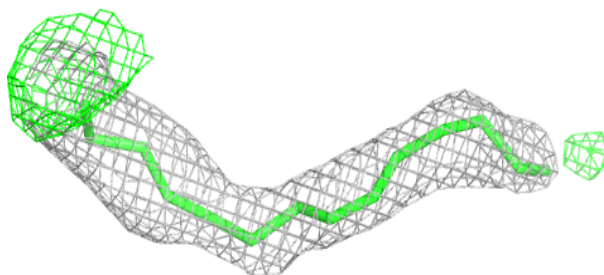


Electron density around LFA E 308:

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

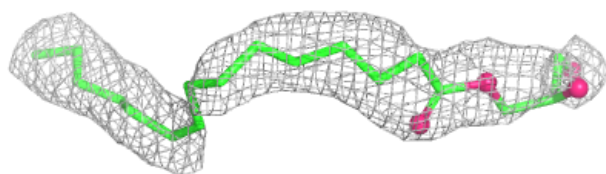
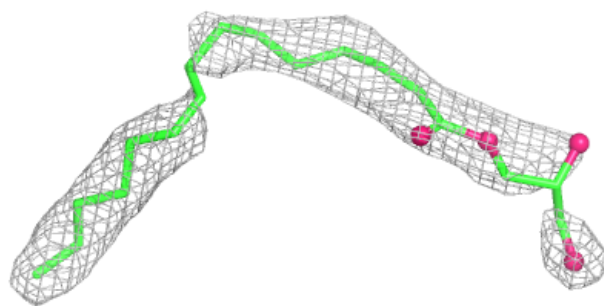
**Electron density around OLC A 311:**

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

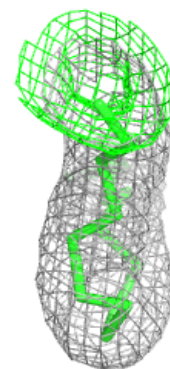
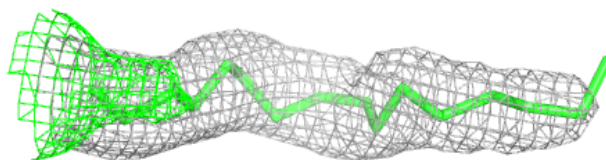
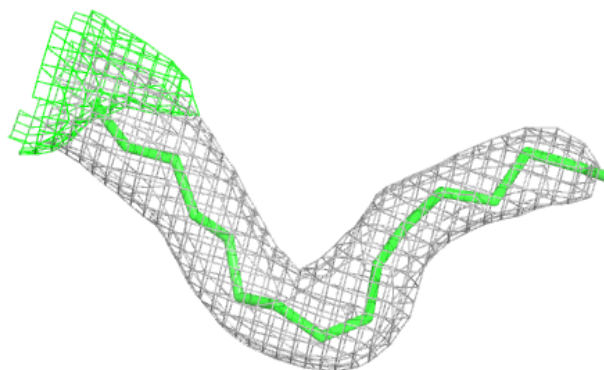


Electron density around OLC C 309:

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

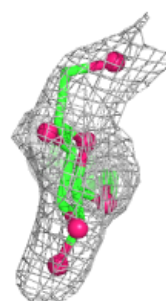
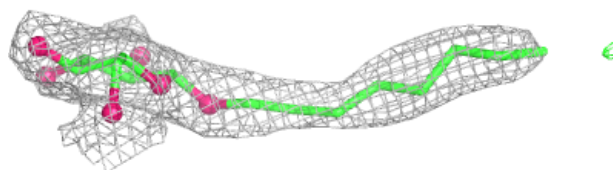
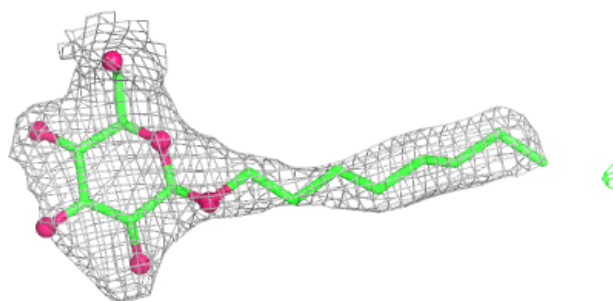
**Electron density around OLC E 303:**

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

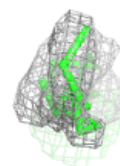
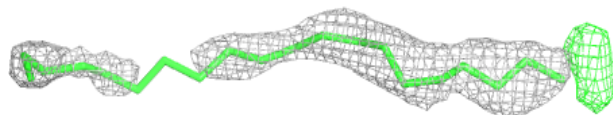
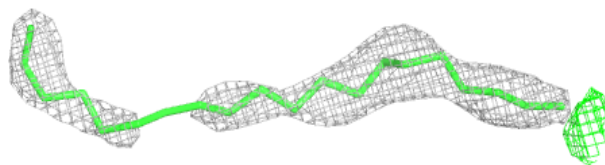


Electron density around BOG C 321:

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

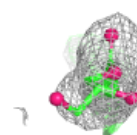
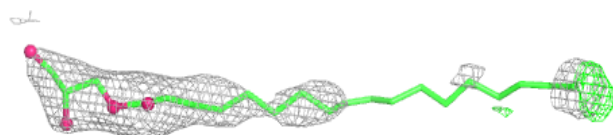
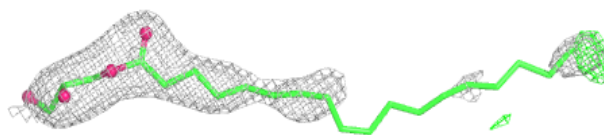
**Electron density around LFA C 317:**

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

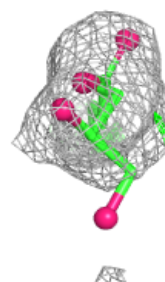
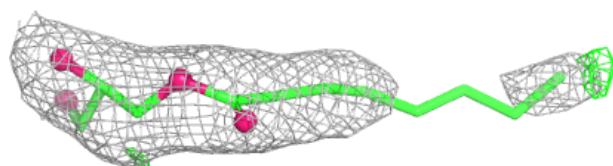
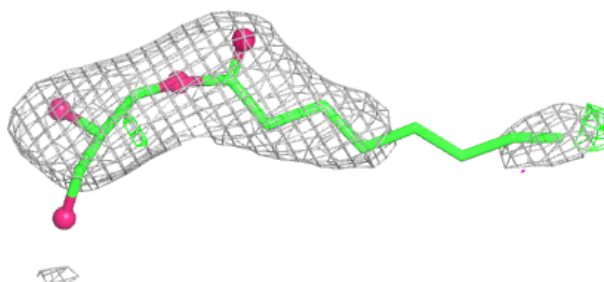


Electron density around OLC E 304:

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

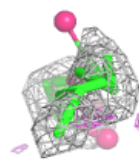
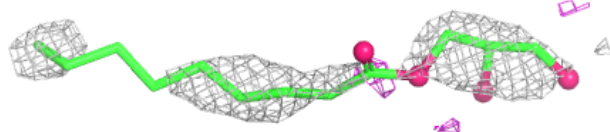
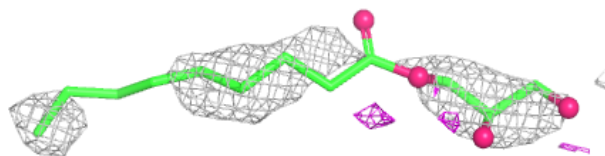
**Electron density around OLC A 303:**

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

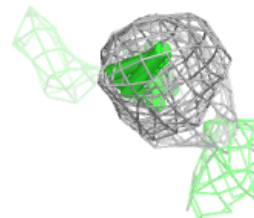
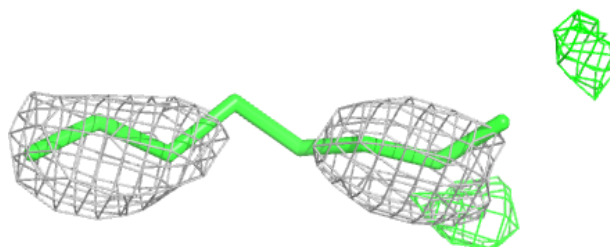
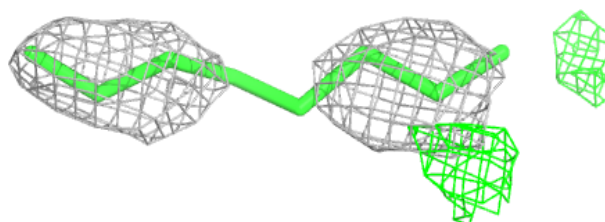


Electron density around OLC C 314:

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

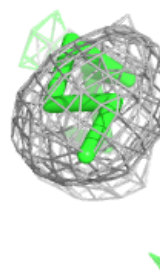
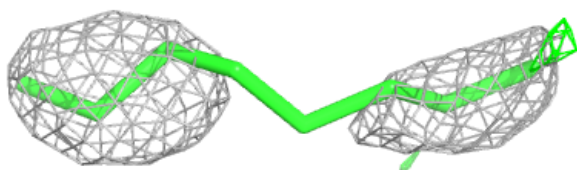
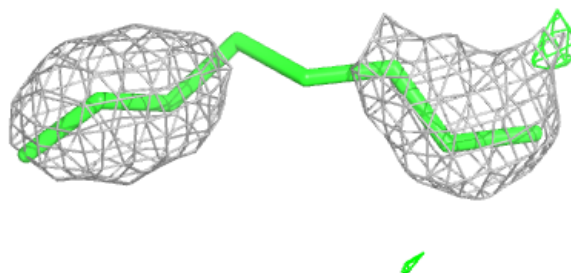
**Electron density around LFA B 306:**

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

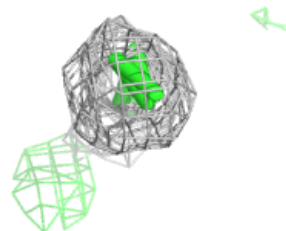
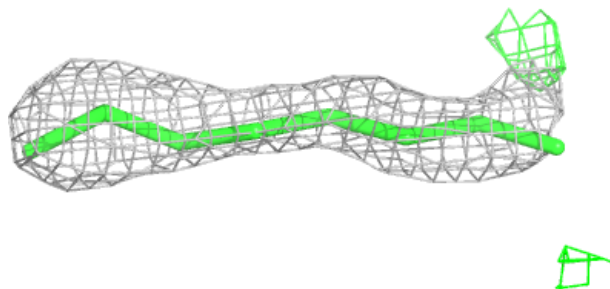
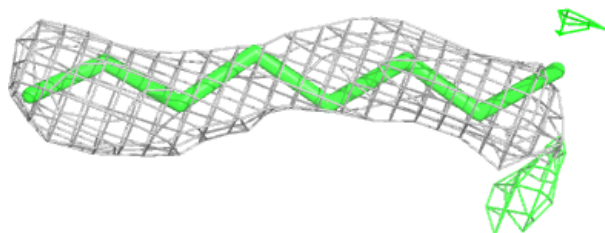


Electron density around LFA A 306:

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

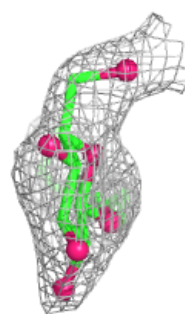
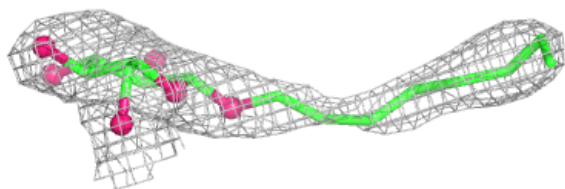
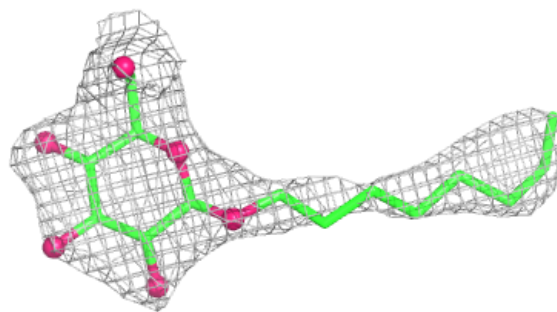
**Electron density around LFA E 305:**

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

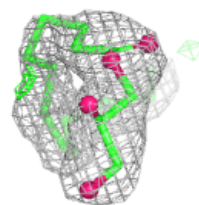
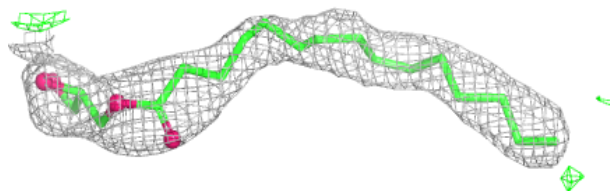
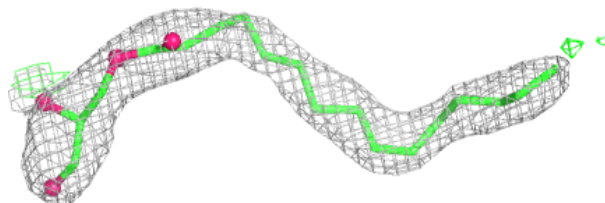


Electron density around BOG D 311:

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

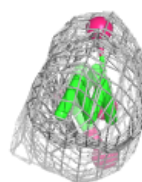
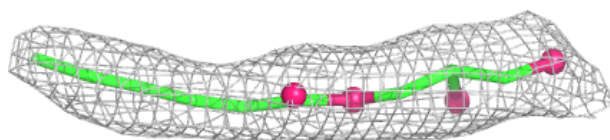
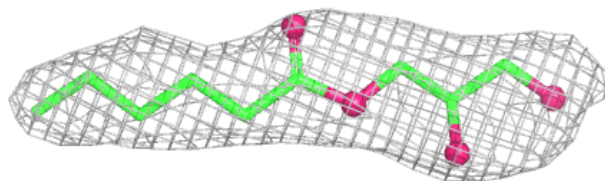
**Electron density around OLC B 301:**

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

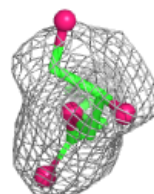
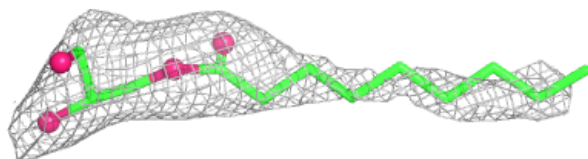
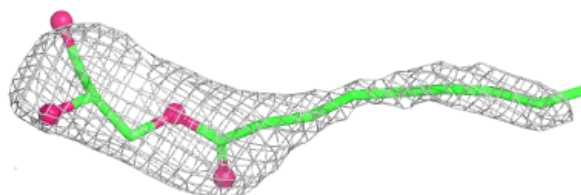


Electron density around OLC A 302:

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

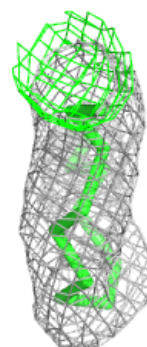
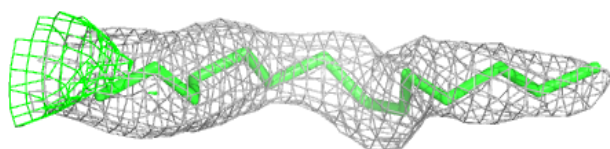
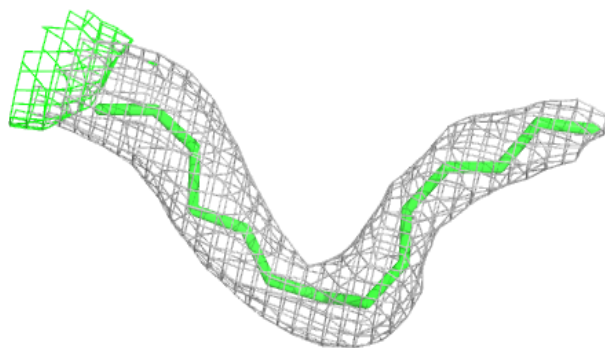
**Electron density around OLC B 304:**

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

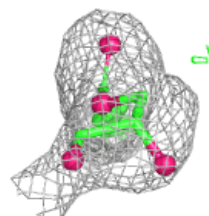
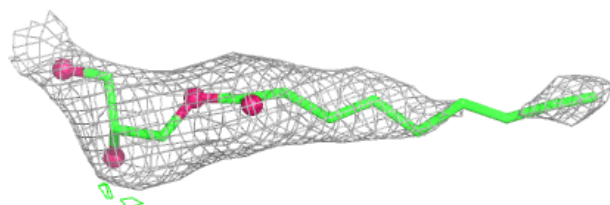
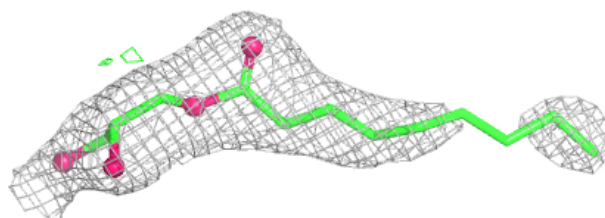


Electron density around OLC A 301:

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

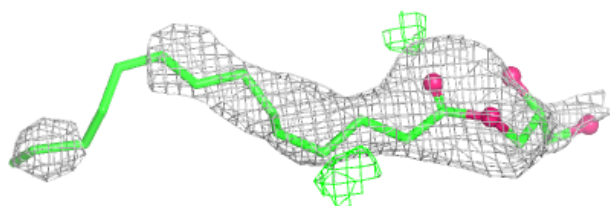
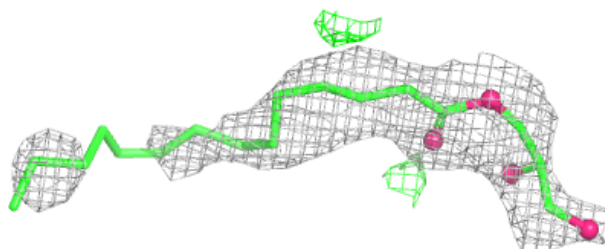
**Electron density around OLC C 312:**

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

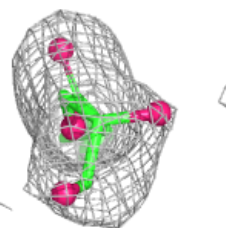
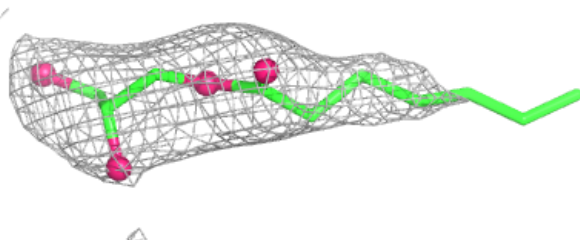
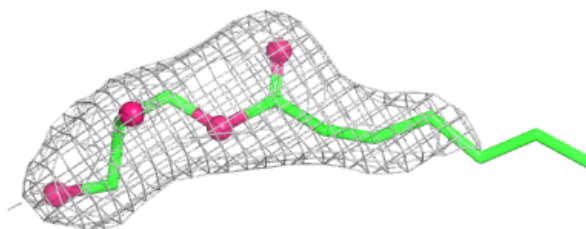


Electron density around OLC C 305:

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

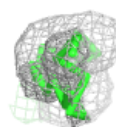
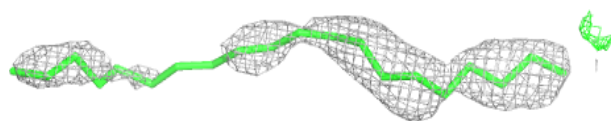
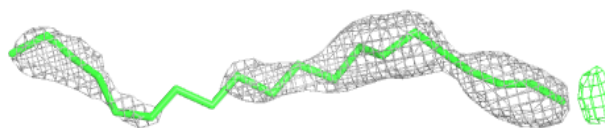
**Electron density around OLC D 303:**

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

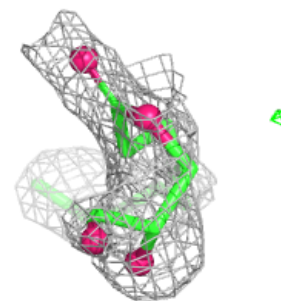
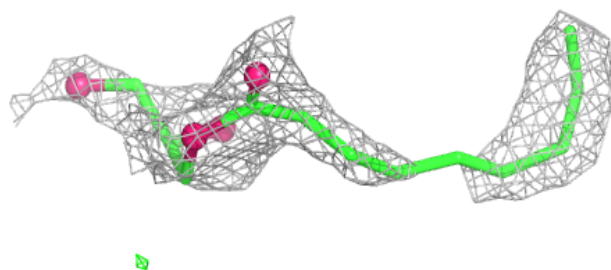
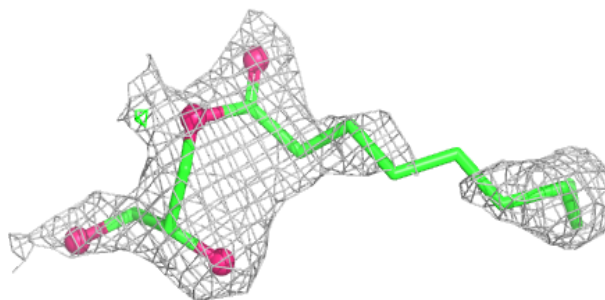


Electron density around LFA D 305:

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

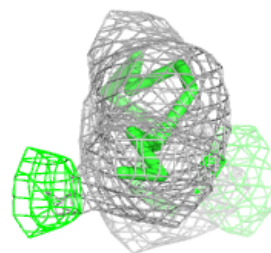
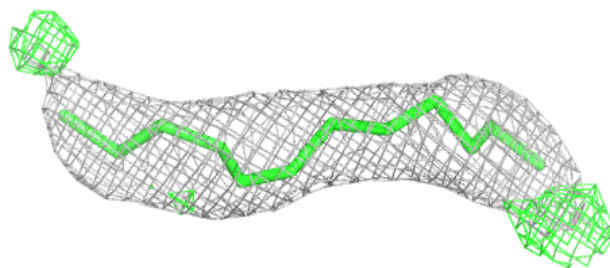
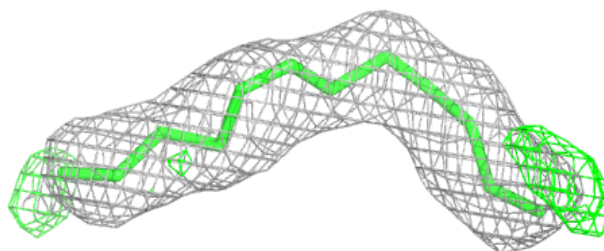
**Electron density around OLC C 313:**

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

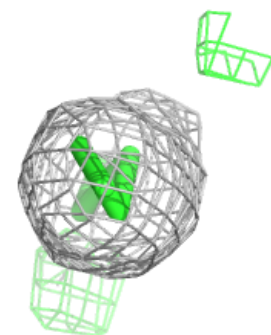
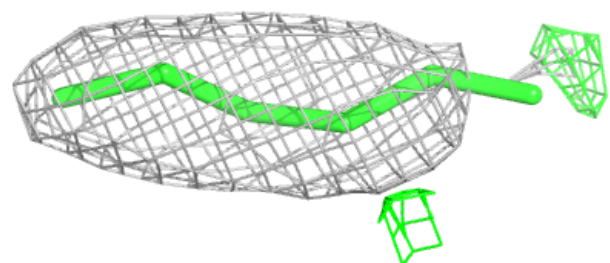
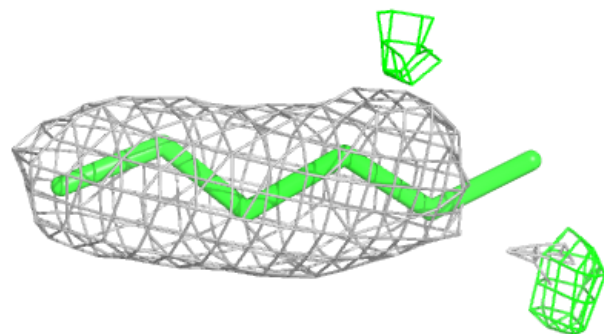


Electron density around OLC E 301:

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

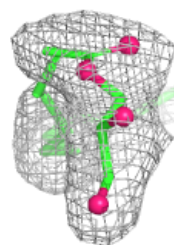
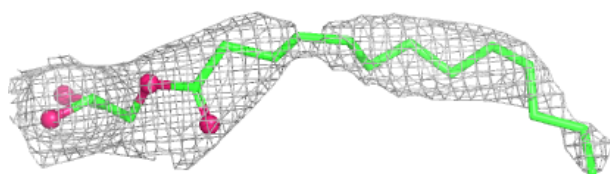
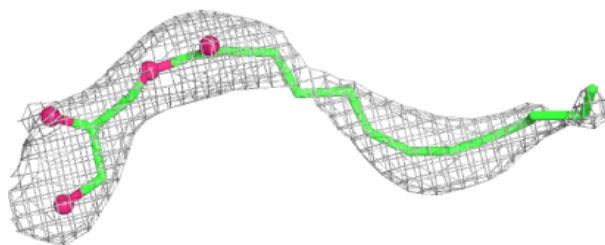
**Electron density around LFA A 308:**

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

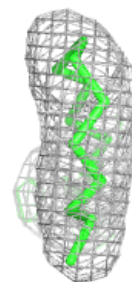
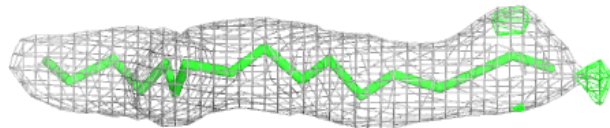
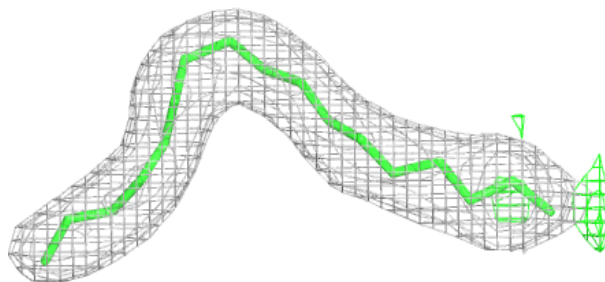


Electron density around OLC C 302:

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

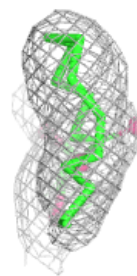
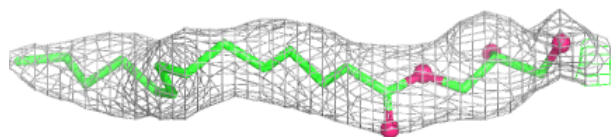
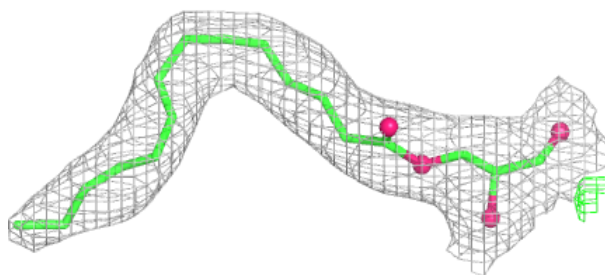
**Electron density around LFA D 307:**

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

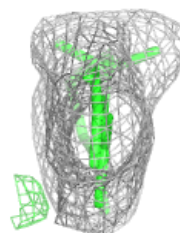
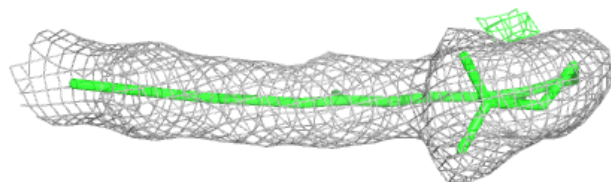
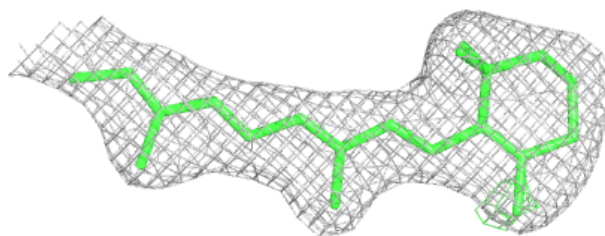


Electron density around OLC C 301:

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

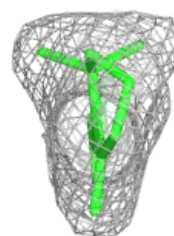
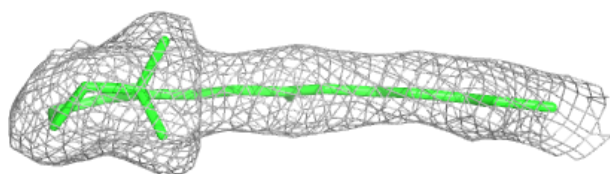
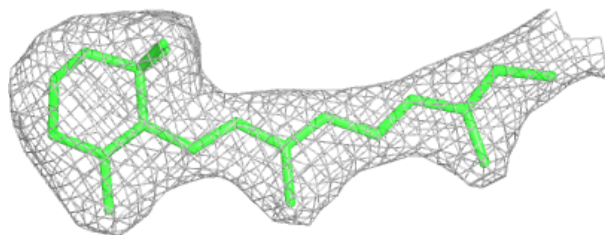
**Electron density around RET B 309:**

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

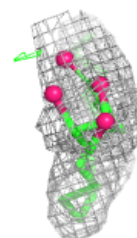
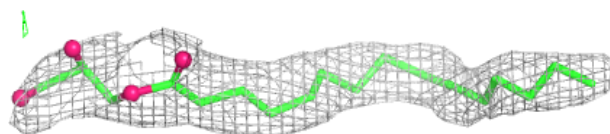
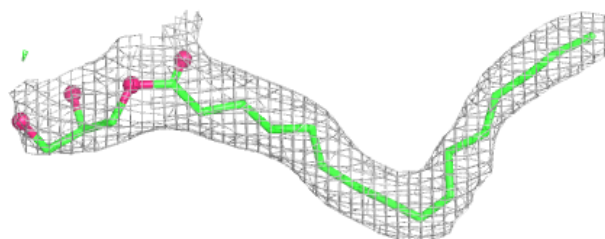


Electron density around RET E 312:

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

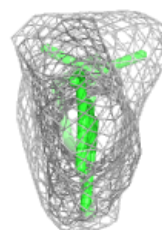
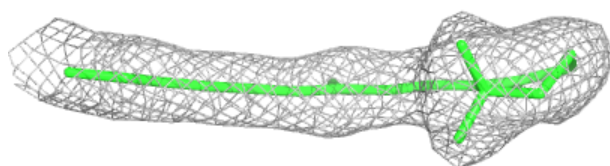
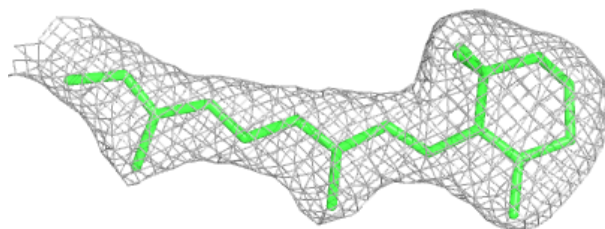
**Electron density around OLC C 306:**

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

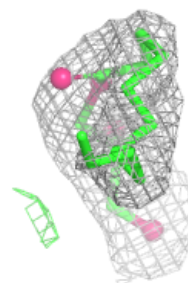
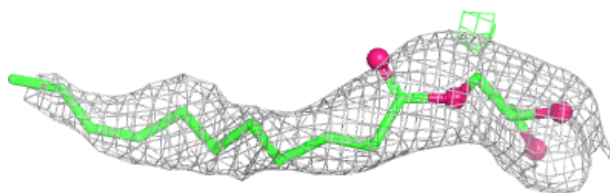
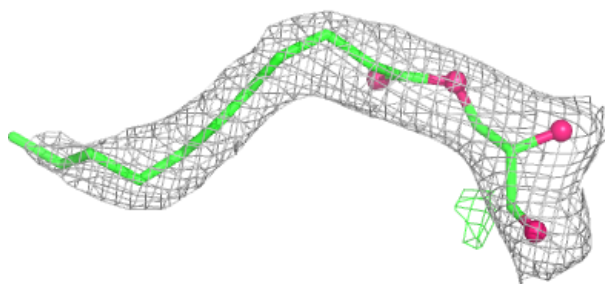


Electron density around RET D 312:

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

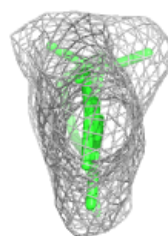
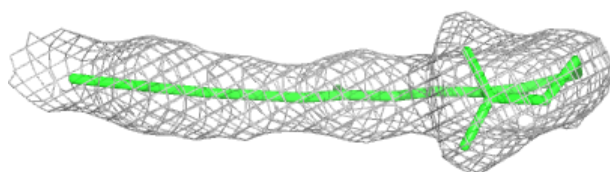
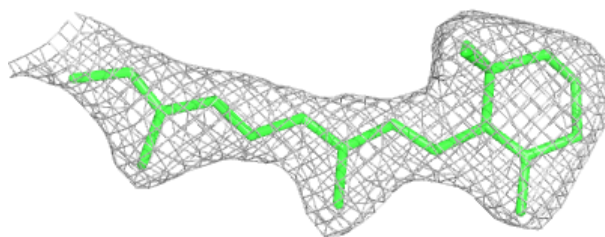
**Electron density around OLC D 301:**

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

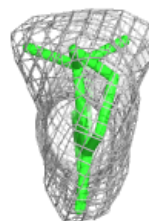
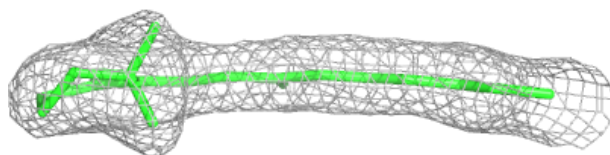
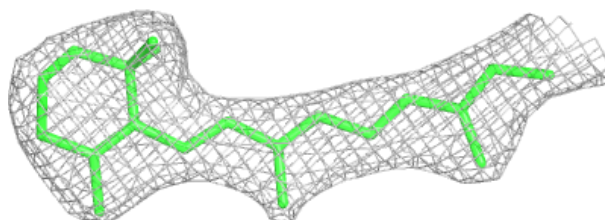


Electron density around RET C 323:

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

**Electron density around RET A 313:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.