



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 11:08 AM UTC

PDB ID : 6REX / pdb_00006rex
Title : Crystal structure of the light-driven sodium pump KR2 in the pentameric form, pH 6.0
Authors : Kovalev, K.; Polovinkin, V.; Gushchin, I.; Borshchevskiy, V.; Gordeliy, V.
Deposited on : 2019-04-12
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

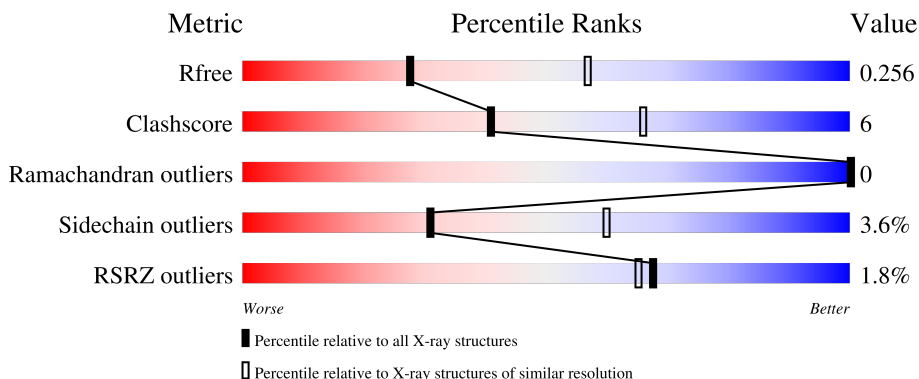
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	273	2% 90% 9%
1	B	273	% 86% 14%
1	C	273	2% 85% 13% .
1	D	273	2% 89% 11%
1	E	273	% 86% 13% .

2 Entry composition [i](#)

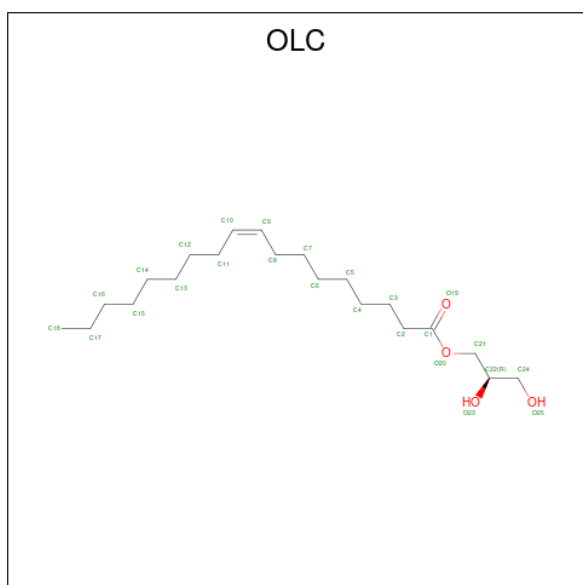
There are 7 unique types of molecules in this entry. The entry contains 12192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sodium pumping rhodopsin.

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

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



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

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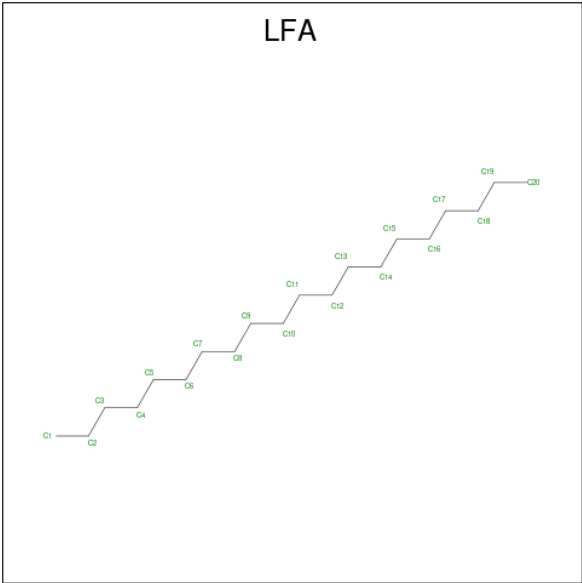
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	9	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			16	12	4		
2	B	1	Total	C	O	0	0
			17	13	4		
2	C	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			20	16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

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

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			5	5		
3	A	1	Total	C	0	0
			8	8		
3	A	1	Total	C	0	0
			4	4		
3	A	1	Total	C	0	0
			6	6		
3	A	1	Total	C	0	0
			20	20		
3	B	1	Total	C	0	0
			20	20		
3	B	1	Total	C	0	0
			9	9		
3	B	1	Total	C	0	0
			5	5		
3	B	1	Total	C	0	0
			10	10		

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

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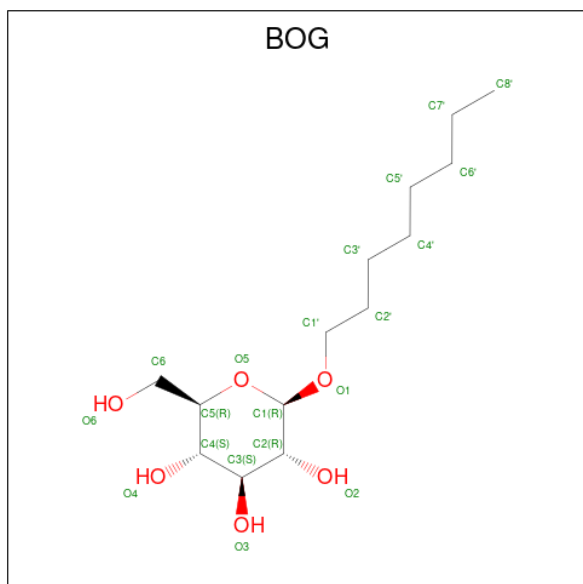
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 5 5	0	0
3	E	1	Total C 6 6	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 14 14	0	0

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

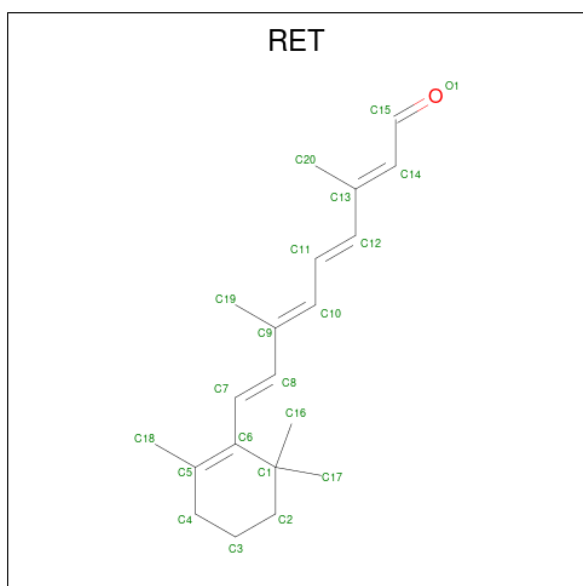
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

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



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

- Molecule 6 is RETINAL (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	64	Total 64	O 64	0	0
7	B	66	Total 66	O 66	0	0
7	C	76	Total 76	O 76	0	0
7	D	41	Total 41	O 41	0	0
7	E	69	Total 69	O 69	0	0

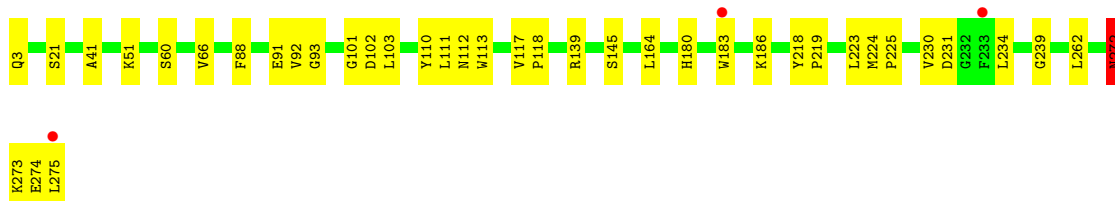
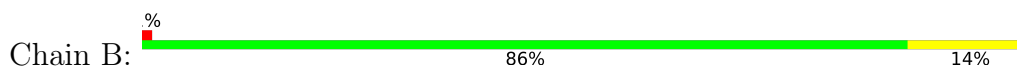
3 Residue-property plots [i](#)

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

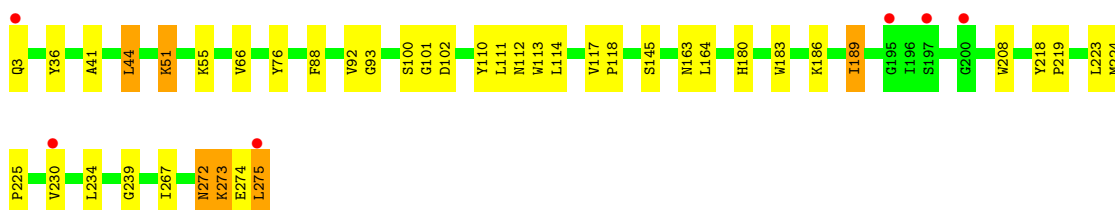
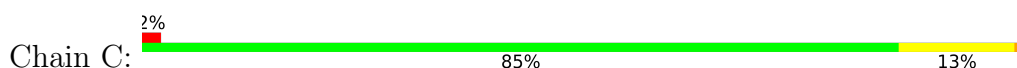
- Molecule 1: Sodium pumping rhodopsin



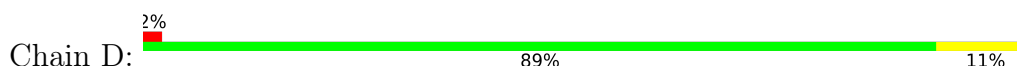
- Molecule 1: Sodium pumping rhodopsin



- Molecule 1: Sodium pumping rhodopsin

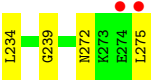
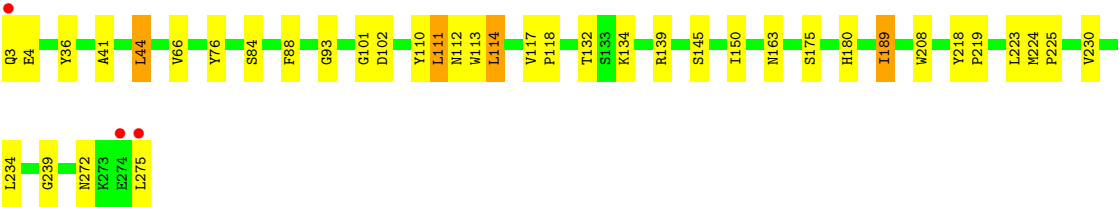
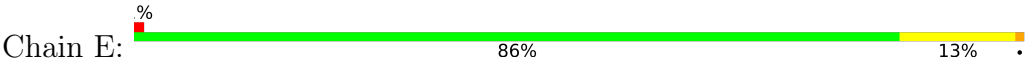


- Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.43Å 240.79Å 135.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.70 48.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.26-2.70) 96.5 (48.26-2.70)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.223 , 0.250 0.232 , 0.256	Depositor DCC
R_{free} test set	2803 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.9	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	0.92	EDS
Total number of atoms	12192	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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: RET, BOG, NA, LFA, OLC

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	0.44	0/2237	0.96	0/3041
1	B	0.44	0/2231	0.96	0/3034
1	C	0.44	0/2236	0.96	0/3040
1	D	0.44	0/2228	0.97	0/3029
1	E	0.44	0/2230	0.96	0/3032
All	All	0.44	0/11162	0.96	0/15176

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	E	272	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2179	0	2154	19	0
1	B	2173	0	2149	33	0
1	C	2178	0	2152	28	0
1	D	2170	0	2142	24	0
1	E	2172	0	2150	24	0
2	A	50	0	65	0	0
2	B	78	0	110	4	0
2	C	145	0	194	6	0
2	D	82	0	120	4	0
2	E	89	0	134	1	0
3	A	51	0	99	0	0
3	B	57	0	111	3	0
3	C	68	0	132	5	0
3	D	118	0	240	1	0
3	E	61	0	114	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	20	0	28	2	0
5	B	20	0	28	2	0
5	C	20	0	28	1	0
5	D	20	0	28	4	0
5	E	20	0	28	0	0
6	A	20	0	27	5	0
6	B	20	0	27	4	0
6	C	20	0	27	5	0
6	D	20	0	27	5	0
6	E	20	0	27	6	0
7	A	64	0	0	1	0
7	B	66	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	76	0	0	5	0
7	D	41	0	0	3	0
7	E	69	0	0	1	0
All	All	12192	0	12341	157	0

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

The worst 5 of 157 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:HD22	1:B:272:ASN:N	1.66	0.90
1:A:272:ASN:HD22	1:A:272:ASN:N	1.69	0.89
6:E:315:RET:H161	6:E:315:RET:H8	1.59	0.85
6:D:315:RET:H8	6:D:315:RET:H161	1.60	0.84
6:A:312:RET:H8	6:A:312:RET:H161	1.60	0.83

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/234 (99%)	222 (96%)	9 (4%)	28	57
1	B	231/234 (99%)	224 (97%)	7 (3%)	36	66
1	C	231/234 (99%)	220 (95%)	11 (5%)	23	50
1	D	229/234 (98%)	225 (98%)	4 (2%)	53	79
1	E	230/234 (98%)	220 (96%)	10 (4%)	26	54
All	All	1152/1170 (98%)	1111 (96%)	41 (4%)	31	60

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	111	LEU
1	E	114	LEU
1	D	112	ASN
1	E	44	LEU
1	E	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	201	GLN
1	E	180	HIS
1	B	272	ASN
1	C	3	GLN
1	C	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 73 ligands modelled in this entry, 5 are monoatomic - leaving 68 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OLC	C	305	-	22,22,24	0.97	1 (4%)	23,23,25	0.89	2 (8%)
3	LFA	E	314	-	13,13,19	0.29	0	12,12,18	0.49	0
2	OLC	E	301	-	23,23,24	0.96	1 (4%)	24,24,25	0.89	1 (4%)
2	OLC	C	308	-	15,15,24	1.19	1 (6%)	16,16,25	0.95	2 (12%)
3	LFA	A	308	-	5,5,19	0.29	0	4,4,18	0.34	0
3	LFA	B	307	-	4,4,19	0.36	0	3,3,18	0.29	0
2	OLC	A	303	-	14,14,24	1.19	1 (7%)	15,15,25	1.08	2 (13%)
5	BOG	B	312	-	20,20,20	0.55	0	25,25,25	0.64	0
3	LFA	D	306	-	19,19,19	0.27	0	18,18,18	0.56	0
3	LFA	D	308	-	7,7,19	0.32	0	6,6,18	0.34	0
3	LFA	E	306	-	5,5,19	0.46	0	4,4,18	0.34	0
2	OLC	C	301	-	20,20,24	1.01	1 (5%)	21,21,25	0.97	1 (4%)
3	LFA	C	311	-	7,7,19	0.33	0	6,6,18	0.32	0
3	LFA	D	301	-	19,19,19	0.37	0	18,18,18	0.38	0
6	RET	D	315	1	20,20,21	0.74	0	27,27,28	1.62	5 (18%)
5	BOG	C	317	-	20,20,20	0.57	1 (5%)	25,25,25	0.63	0
3	LFA	A	304	-	7,7,19	0.32	0	6,6,18	0.39	0
2	OLC	E	303	-	14,14,24	1.28	1 (7%)	15,15,25	1.08	1 (6%)
2	OLC	B	305	-	16,16,24	1.17	1 (6%)	17,17,25	0.98	1 (5%)
3	LFA	E	309	-	4,4,19	0.31	0	3,3,18	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	B	304	-	15,15,24	1.15	1 (6%)	16,16,25	1.07	2 (12%)
3	LFA	E	308	-	3,3,19	0.36	0	2,2,18	0.61	0
2	OLC	D	304	-	13,13,24	1.23	1 (7%)	14,14,25	1.05	2 (14%)
6	RET	B	313	1	20,20,21	0.80	1 (5%)	27,27,28	1.65	5 (18%)
2	OLC	B	301	-	24,24,24	0.94	1 (4%)	25,25,25	0.88	1 (4%)
3	LFA	B	309	-	6,6,19	0.27	0	5,5,18	0.44	0
5	BOG	A	310	-	20,20,20	0.59	1 (5%)	25,25,25	0.67	0
2	OLC	C	302	-	19,19,24	1.06	1 (5%)	20,20,25	0.95	2 (10%)
3	LFA	D	310	-	6,6,19	0.29	0	5,5,18	0.39	0
3	LFA	B	306	-	8,8,19	0.30	0	7,7,18	0.42	0
3	LFA	C	313	-	10,10,19	0.29	0	9,9,18	0.52	0
3	LFA	C	310	-	6,6,19	0.31	0	5,5,18	0.36	0
2	OLC	D	302	-	24,24,24	0.93	1 (4%)	25,25,25	0.88	1 (4%)
3	LFA	C	304	-	19,19,19	0.38	0	18,18,18	0.32	0
2	OLC	C	309	-	15,15,24	1.25	1 (6%)	16,16,25	1.06	1 (6%)
2	OLC	E	302	-	24,24,24	0.95	1 (4%)	25,25,25	0.91	1 (4%)
3	LFA	A	305	-	4,4,19	0.31	0	3,3,18	0.39	0
3	LFA	B	308	-	9,9,19	0.32	0	8,8,18	0.43	0
2	OLC	D	303	-	17,17,24	1.16	1 (5%)	18,18,25	1.05	1 (5%)
2	OLC	C	306	-	17,17,24	1.11	1 (5%)	18,18,25	1.00	1 (5%)
3	LFA	C	314	-	3,3,19	0.35	0	2,2,18	0.60	0
3	LFA	E	310	-	5,5,19	0.32	0	4,4,18	0.37	0
3	LFA	A	306	-	7,7,19	0.29	0	6,6,18	0.41	0
2	OLC	C	307	-	14,14,24	1.24	1 (7%)	15,15,25	1.03	1 (6%)
3	LFA	A	307	-	3,3,19	0.37	0	2,2,18	0.60	0
2	OLC	C	303	-	15,15,24	1.24	1 (6%)	16,16,25	1.05	1 (6%)
3	LFA	D	307	-	19,19,19	0.27	0	18,18,18	0.54	0
3	LFA	C	315	-	5,5,19	0.32	0	4,4,18	0.31	0
2	OLC	A	301	-	21,21,24	0.98	1 (4%)	22,22,25	0.89	2 (9%)
3	LFA	D	309	-	16,16,19	0.30	0	15,15,18	0.48	0
5	BOG	D	314	-	20,20,20	0.53	0	25,25,25	0.68	0
3	LFA	E	305	-	7,7,19	0.30	0	6,6,18	0.40	0
5	BOG	E	312	-	20,20,20	0.58	1 (5%)	25,25,25	0.56	0
2	OLC	E	304	-	24,24,24	0.95	1 (4%)	25,25,25	0.84	2 (8%)
3	LFA	E	313	-	3,3,19	0.38	0	2,2,18	0.58	0
3	LFA	E	307	-	13,13,19	0.27	0	12,12,18	0.54	0
2	OLC	A	302	-	12,12,24	1.33	1 (8%)	13,13,25	1.26	2 (15%)
3	LFA	D	312	-	19,19,19	0.40	0	18,18,18	0.35	0
3	LFA	B	310	-	5,5,19	0.28	0	4,4,18	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LFA	C	312	-	11,11,19	0.32	0	10,10,18	0.43	0
6	RET	A	312	1	20,20,21	0.75	0	27,27,28	1.65	5 (18%)
2	OLC	B	303	-	19,19,24	1.07	1 (5%)	20,20,25	0.93	1 (5%)
6	RET	C	318	1	20,20,21	0.77	0	27,27,28	1.61	4 (14%)
3	LFA	B	302	-	19,19,19	0.37	0	18,18,18	0.39	0
6	RET	E	315	1	20,20,21	0.78	1 (5%)	27,27,28	1.59	4 (14%)
3	LFA	A	311	-	19,19,19	0.37	0	18,18,18	0.37	0
2	OLC	D	305	-	24,24,24	0.95	1 (4%)	25,25,25	0.83	1 (4%)
3	LFA	D	311	-	5,5,19	0.33	0	4,4,18	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	305	-	-	9/22/22/24	-
3	LFA	E	314	-	-	4/11/11/17	-
2	OLC	E	301	-	-	14/23/23/24	-
2	OLC	C	308	-	-	9/15/15/24	-
3	LFA	A	308	-	-	3/3/3/17	-
3	LFA	B	307	-	-	2/2/2/17	-
2	OLC	A	303	-	-	5/14/14/24	-
5	BOG	B	312	-	-	7/11/31/31	0/1/1/1
3	LFA	D	306	-	-	10/17/17/17	-
3	LFA	D	308	-	-	4/5/5/17	-
3	LFA	E	306	-	-	1/3/3/17	-
2	OLC	C	301	-	-	9/20/20/24	-
3	LFA	C	311	-	-	5/5/5/17	-
3	LFA	D	301	-	-	8/17/17/17	-
6	RET	D	315	1	-	0/13/30/31	0/1/1/1
5	BOG	C	317	-	-	3/11/31/31	0/1/1/1
3	LFA	A	304	-	-	2/5/5/17	-
2	OLC	E	303	-	-	5/14/14/24	-
2	OLC	B	305	-	-	9/16/16/24	-
3	LFA	E	309	-	-	1/2/2/17	-
2	OLC	B	304	-	-	4/15/15/24	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	D	312	-	-	5/17/17/17	-
3	LFA	B	310	-	-	1/3/3/17	-
3	LFA	C	312	-	-	7/9/9/17	-
6	RET	A	312	1	-	0/13/30/31	0/1/1/1
2	OLC	B	303	-	-	7/19/19/24	-
6	RET	C	318	1	-	0/13/30/31	0/1/1/1
3	LFA	B	302	-	-	6/17/17/17	-
6	RET	E	315	1	-	0/13/30/31	0/1/1/1
3	LFA	A	311	-	-	9/17/17/17	-
2	OLC	D	305	-	-	14/24/24/24	-
3	LFA	D	311	-	-	1/3/3/17	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	309	OLC	O20-C1	4.62	1.46	1.33
2	C	303	OLC	O20-C1	4.57	1.46	1.33
2	E	303	OLC	O20-C1	4.57	1.46	1.33
2	D	303	OLC	O20-C1	4.52	1.46	1.33
2	C	307	OLC	O20-C1	4.44	1.46	1.33

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	312	RET	C18-C5-C6	-4.73	119.32	124.48
6	B	313	RET	C18-C5-C6	-4.53	119.54	124.48
6	D	315	RET	C18-C5-C6	-4.49	119.58	124.48
6	C	318	RET	C18-C5-C6	-4.44	119.64	124.48
6	E	315	RET	C18-C5-C6	-4.43	119.65	124.48

There are no chirality outliers.

5 of 343 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	OLC	C21-C22-C24-O25
2	A	301	OLC	O23-C22-C24-O25
2	B	303	OLC	C10-C11-C12-C13
2	B	305	OLC	O20-C21-C22-C24
2	B	305	OLC	O20-C21-C22-O23

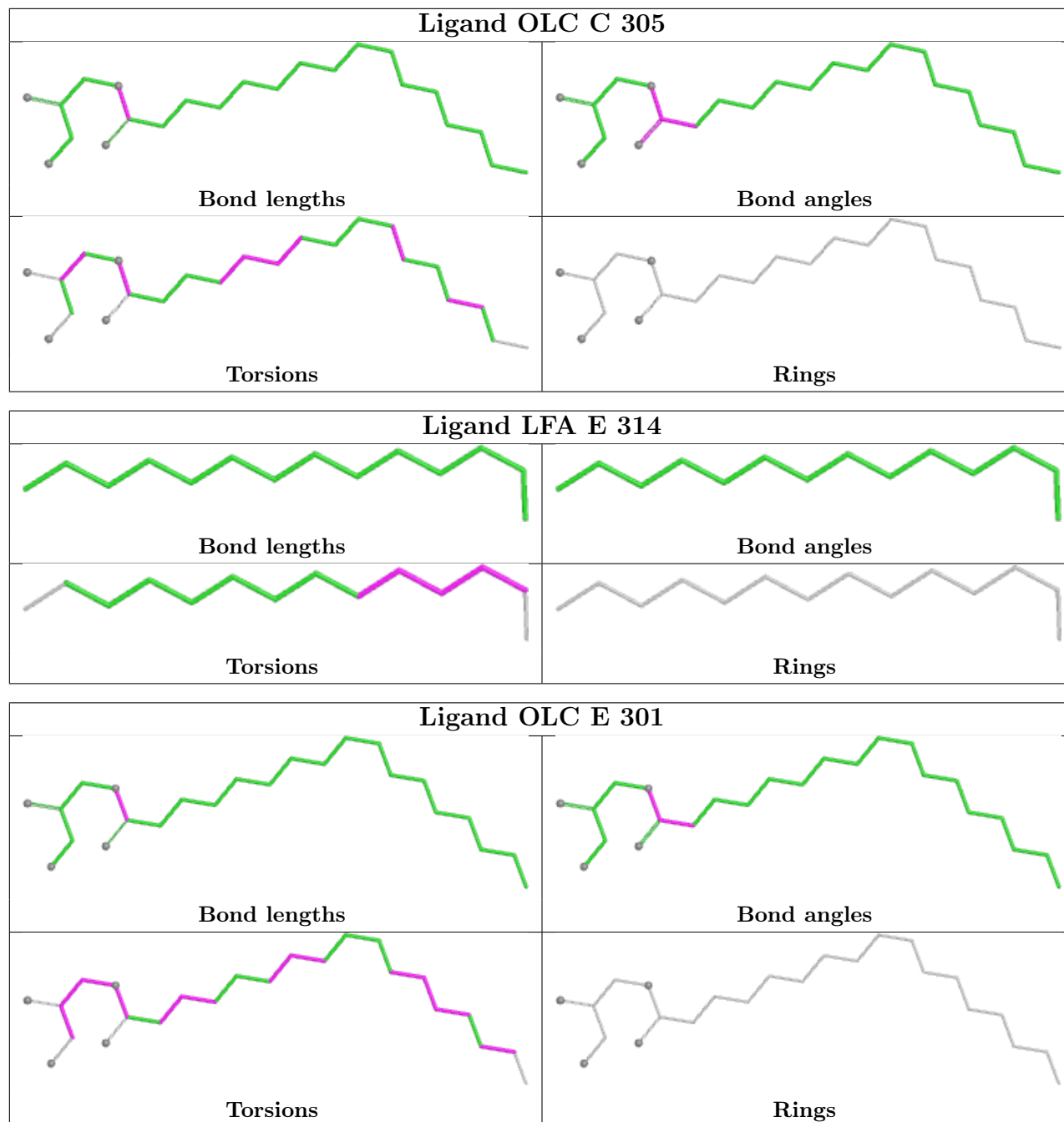
There are no ring outliers.

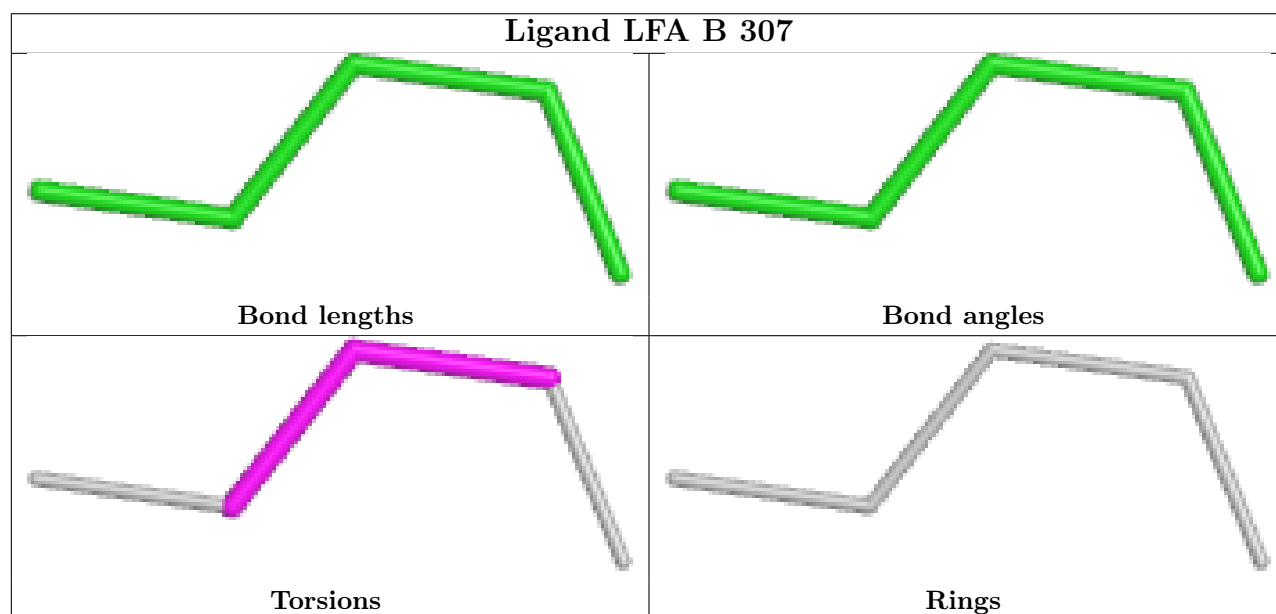
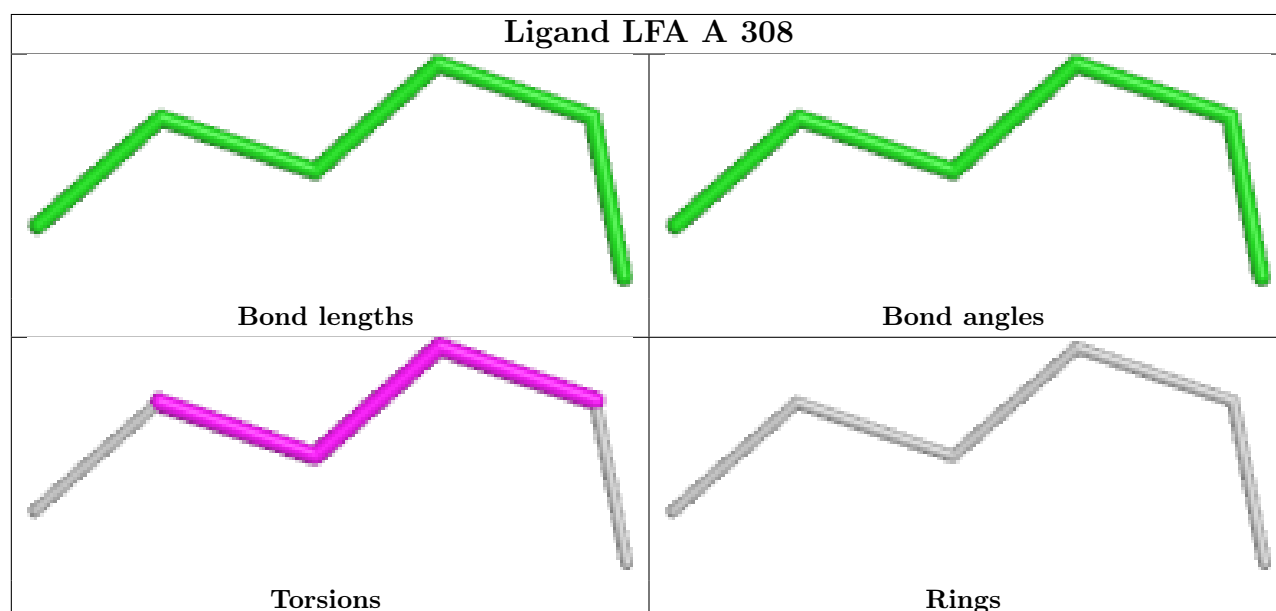
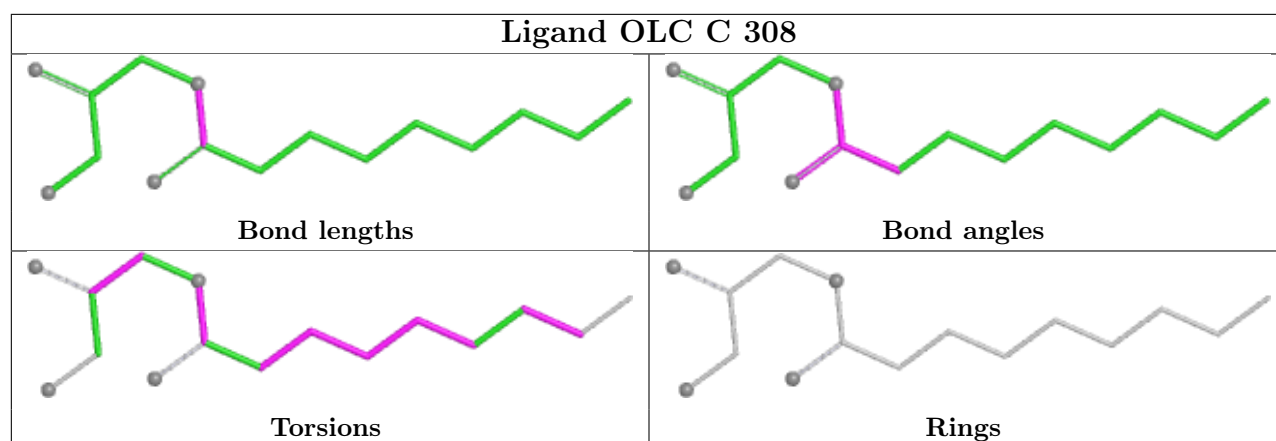
29 monomers are involved in 58 short contacts:

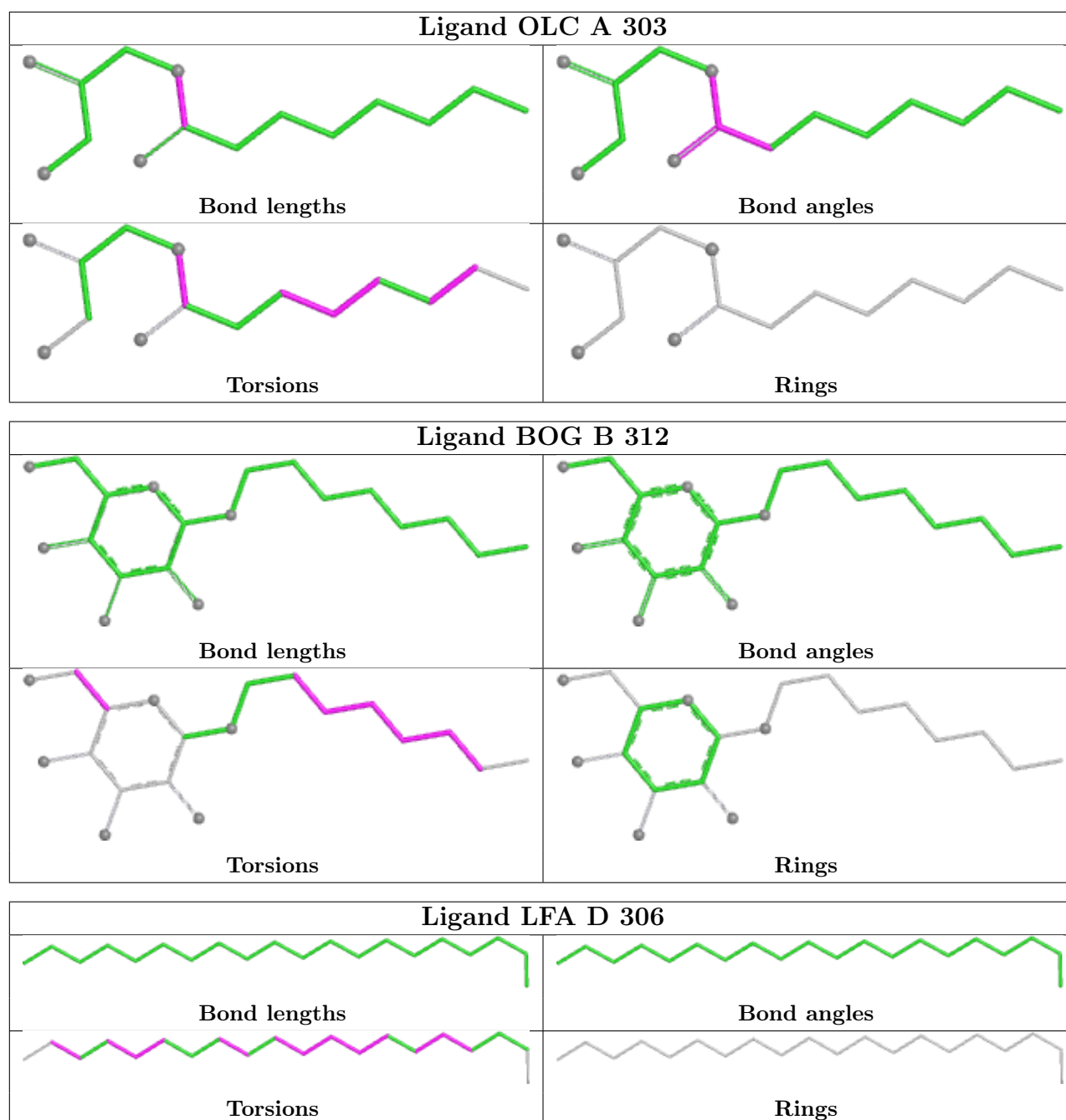
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	305	OLC	2	0
3	E	314	LFA	1	0
2	C	308	OLC	2	0
5	B	312	BOG	2	0
3	D	301	LFA	1	0
6	D	315	RET	5	0
5	C	317	BOG	1	0
2	B	305	OLC	3	0
3	E	308	LFA	1	0
6	B	313	RET	4	0
2	B	301	OLC	1	0
5	A	310	BOG	2	0
2	C	302	OLC	1	0
3	B	306	LFA	2	0
3	C	310	LFA	3	0
2	D	302	OLC	2	0
3	C	304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

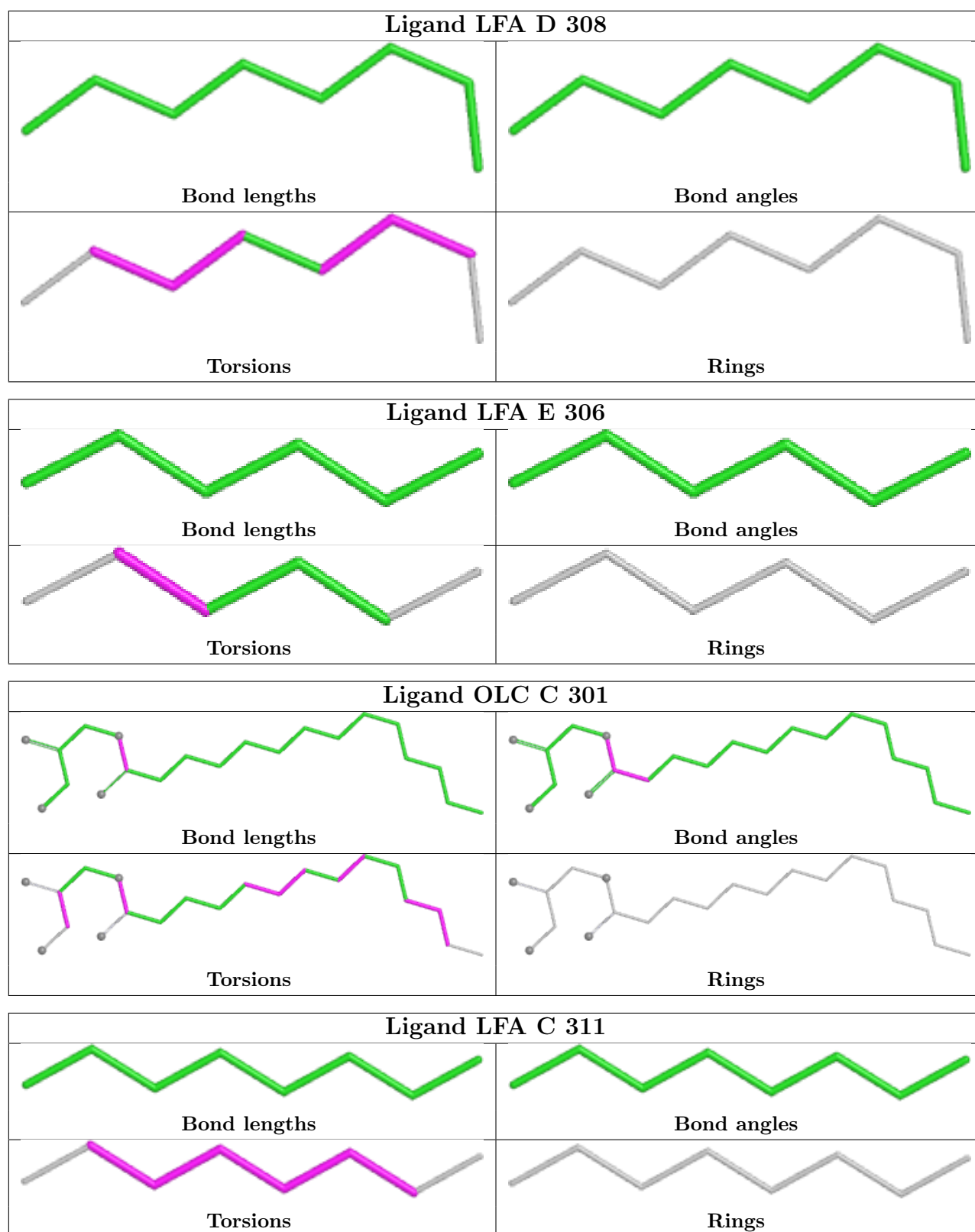
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

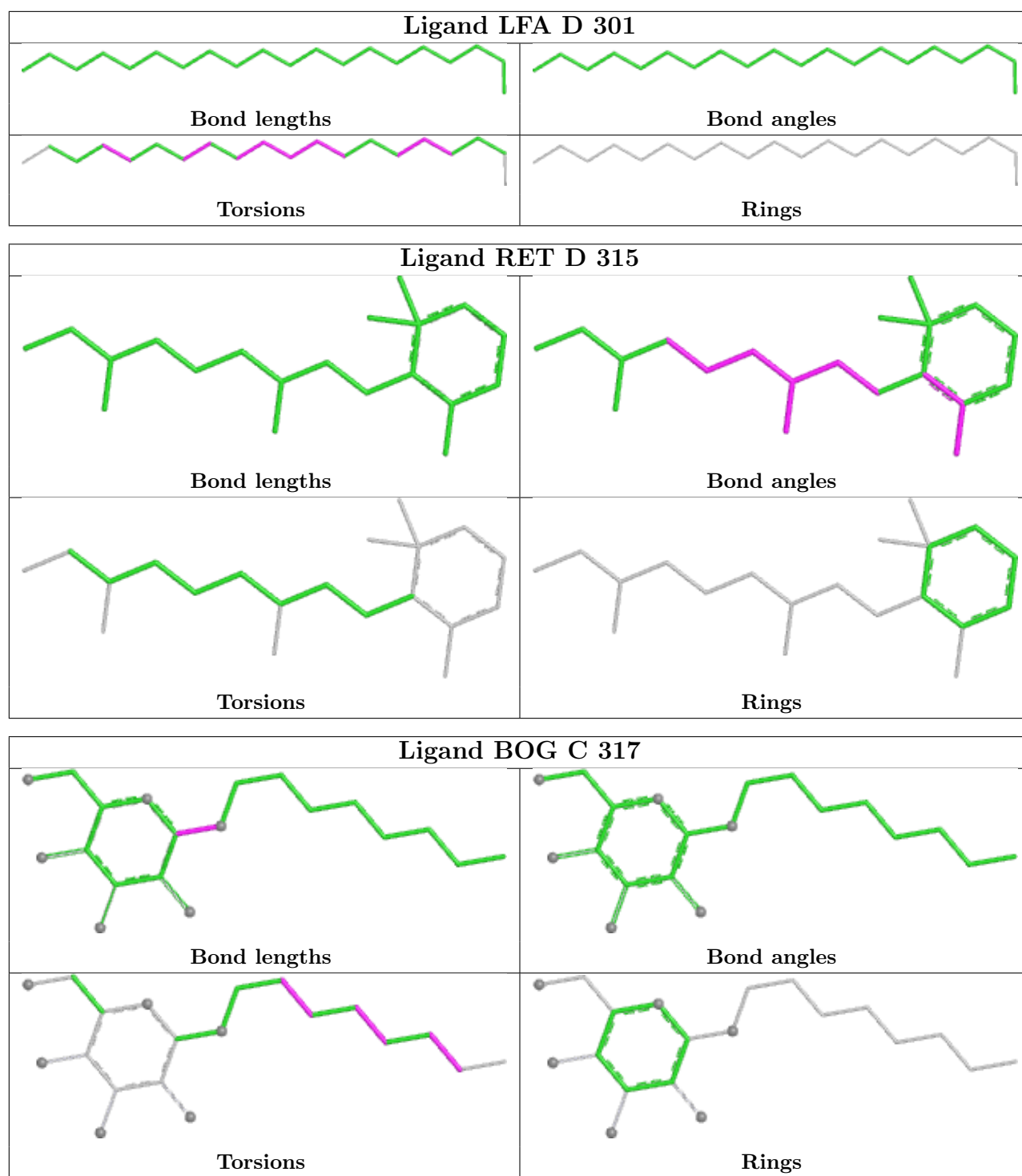
equivalents in the CSD to analyse the geometry.

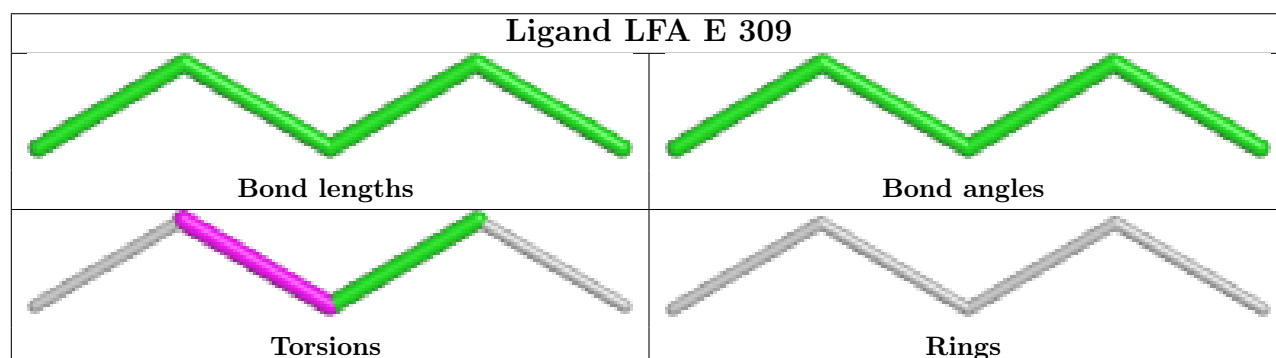
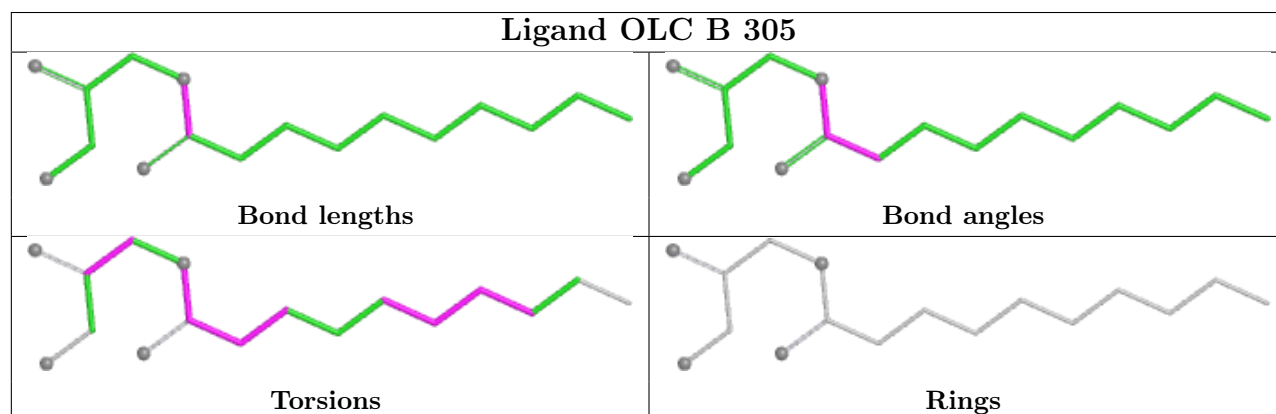
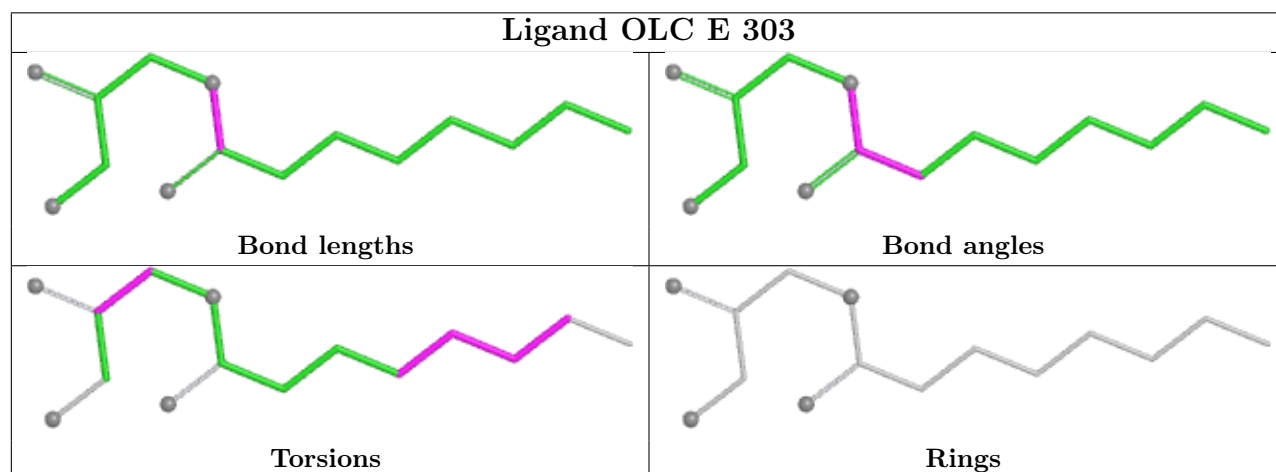
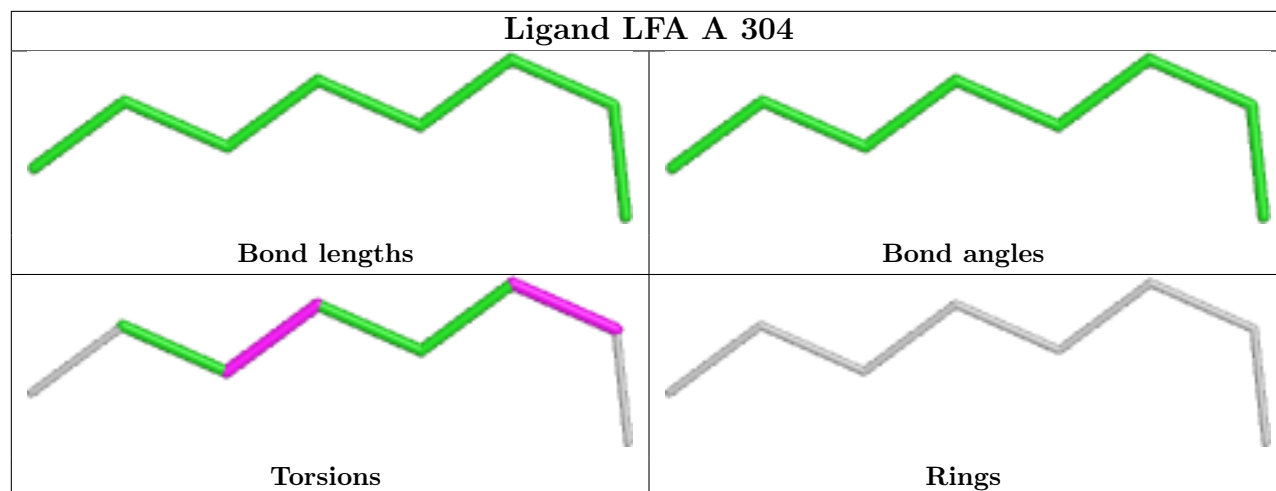


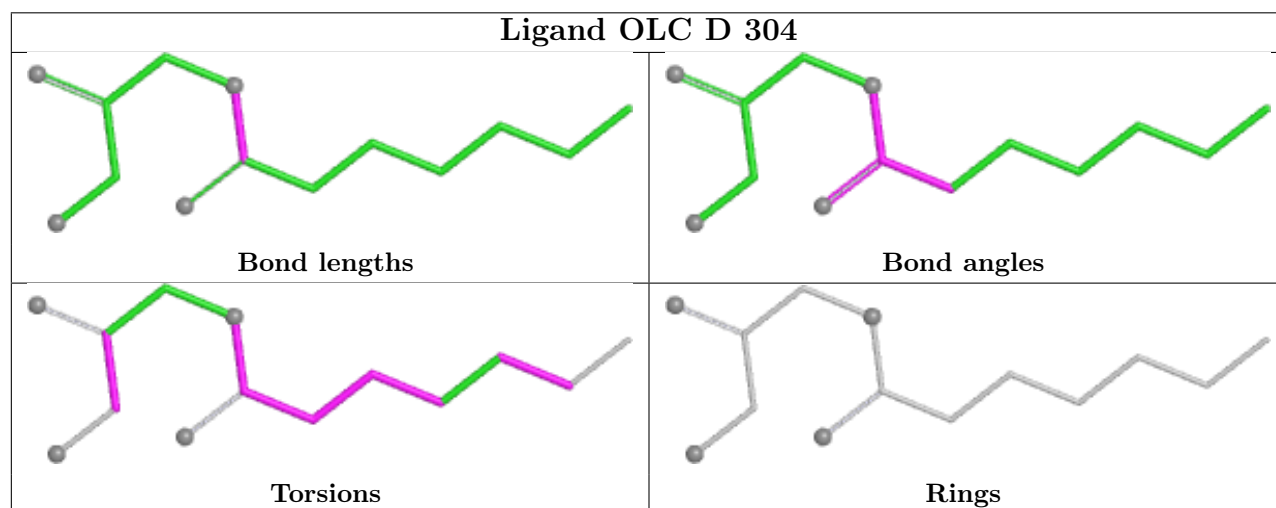
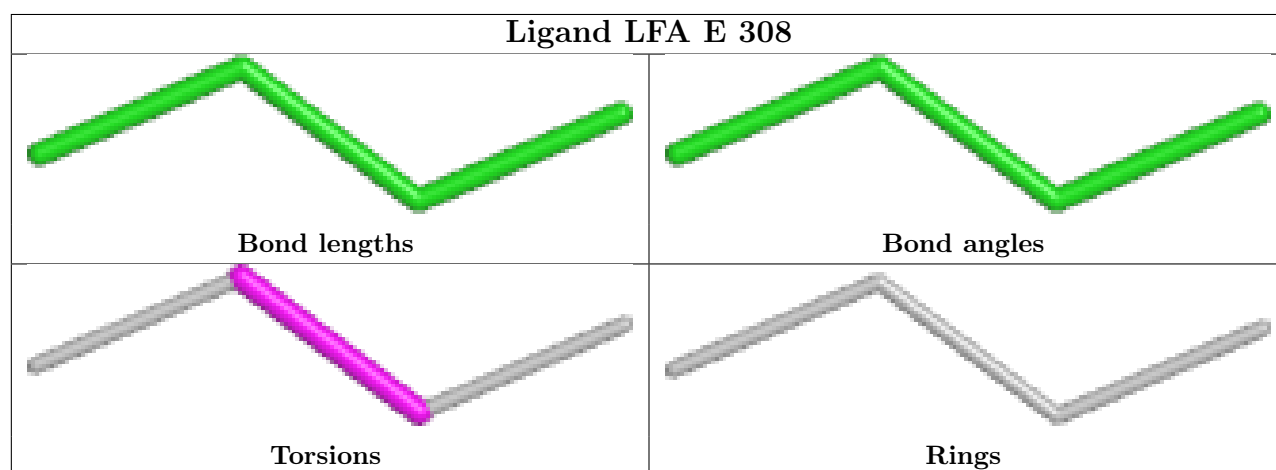
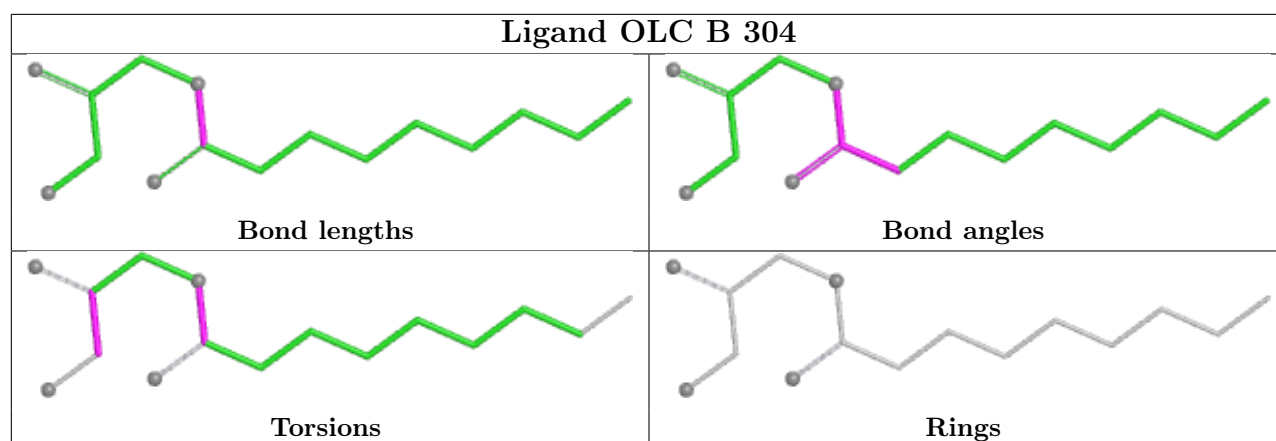


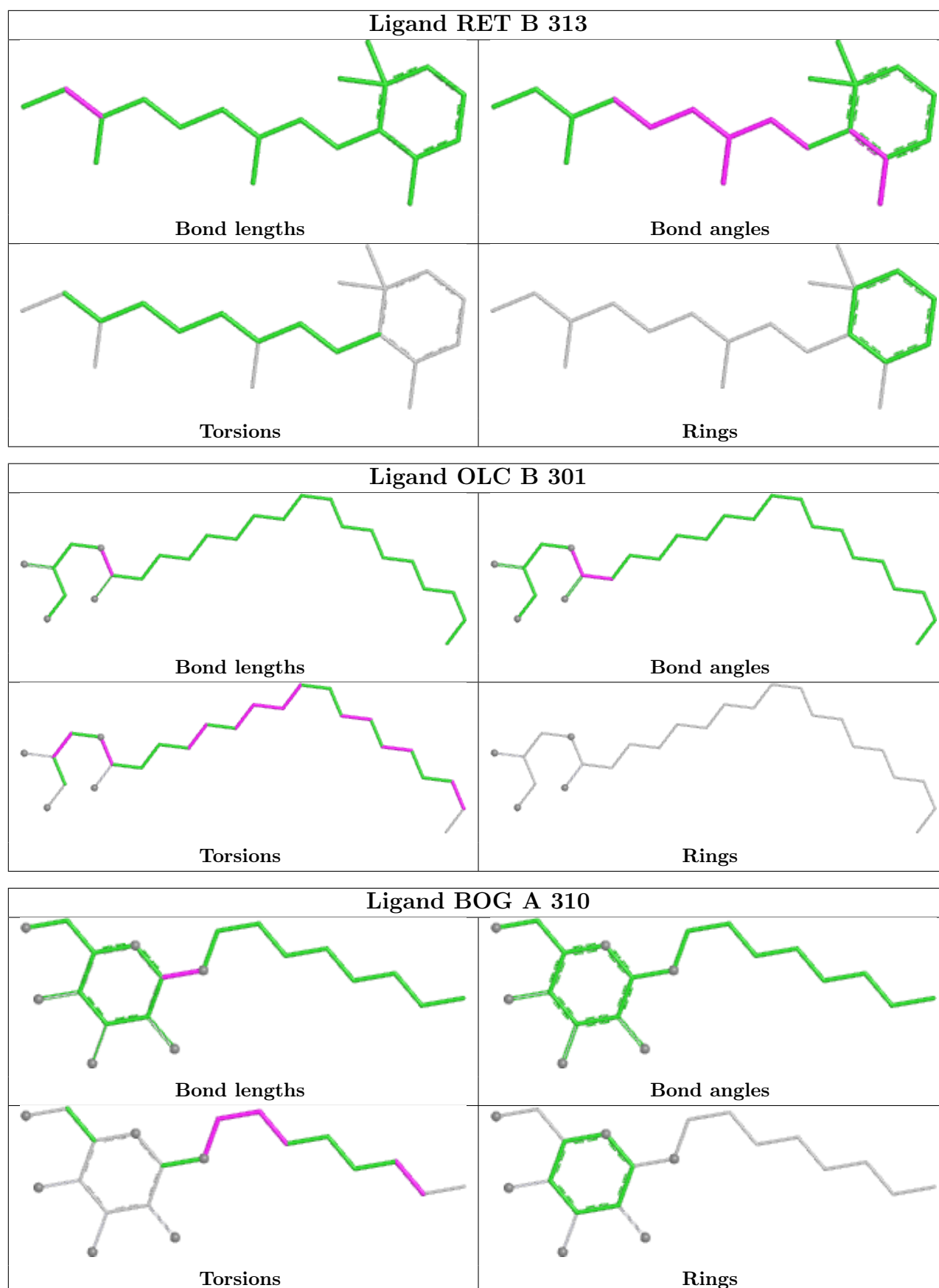


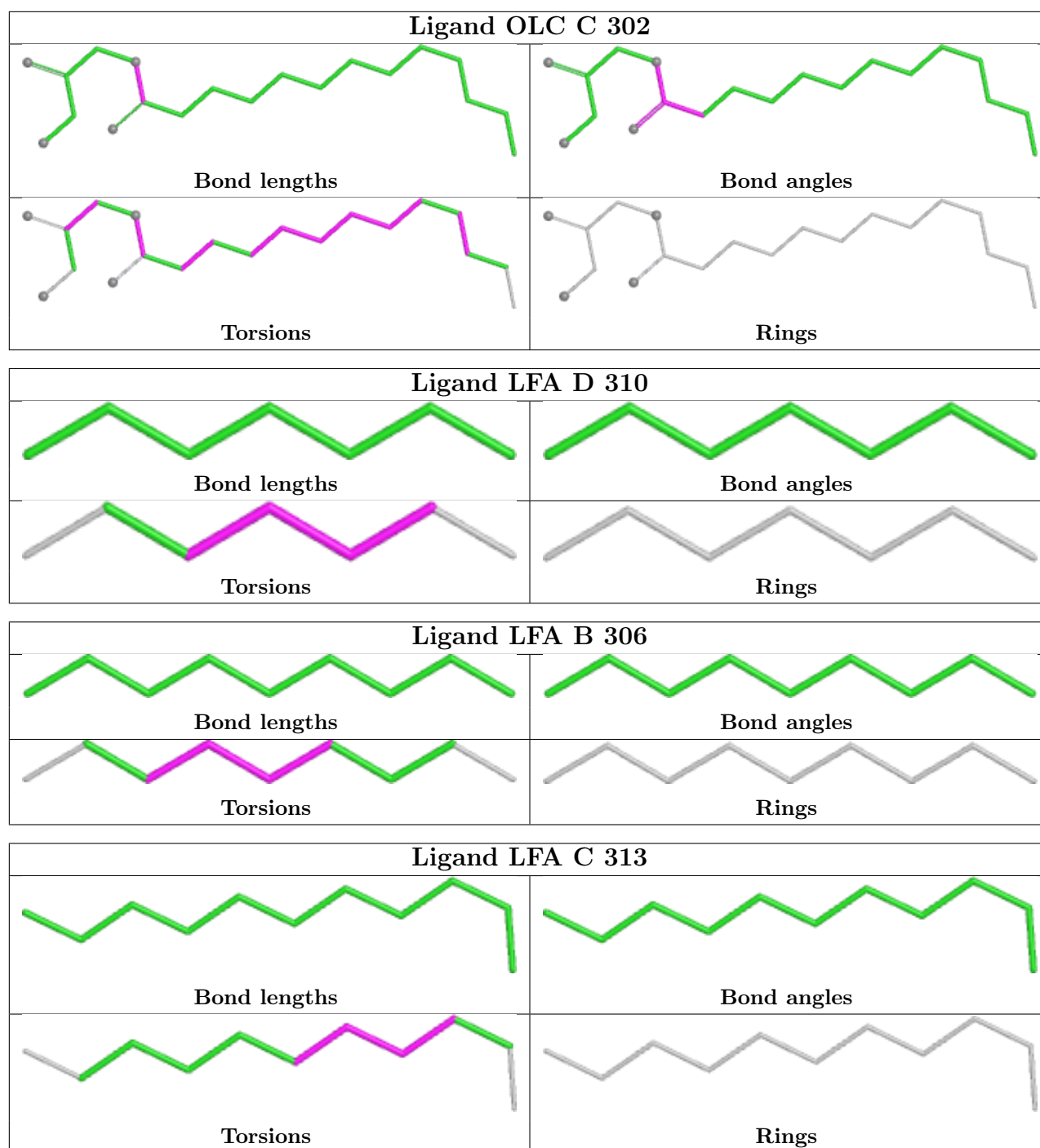


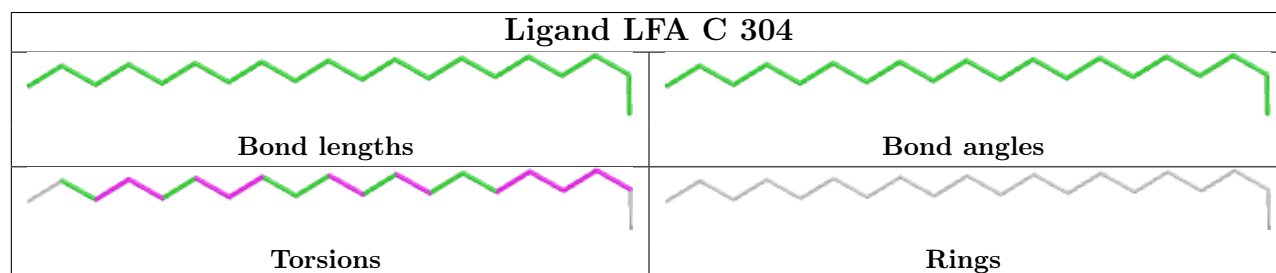
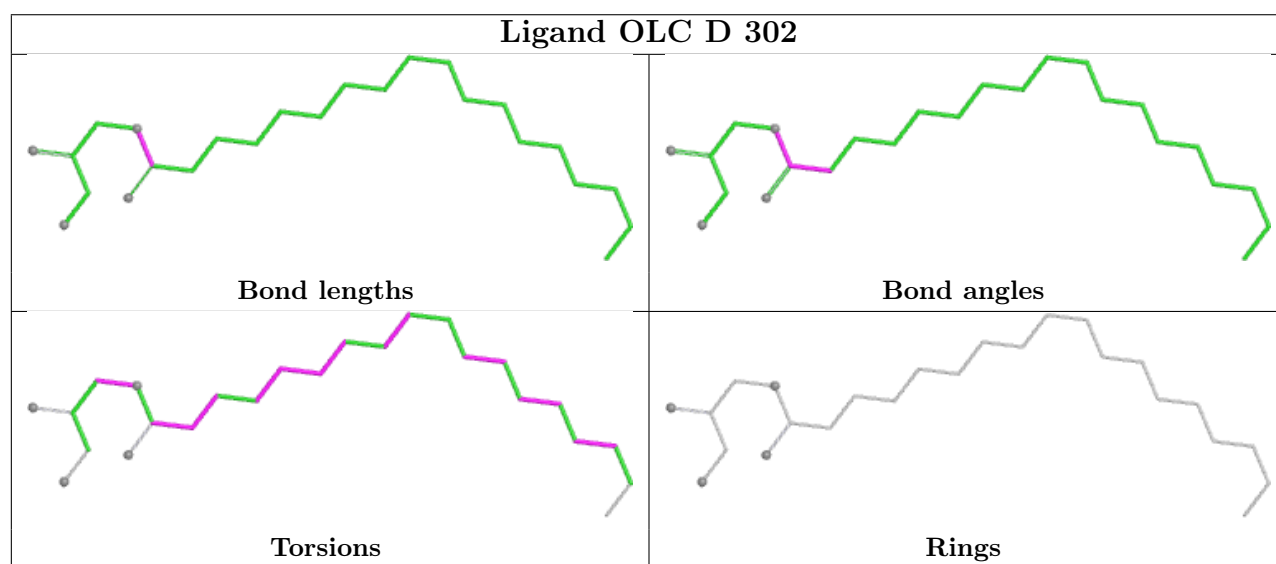
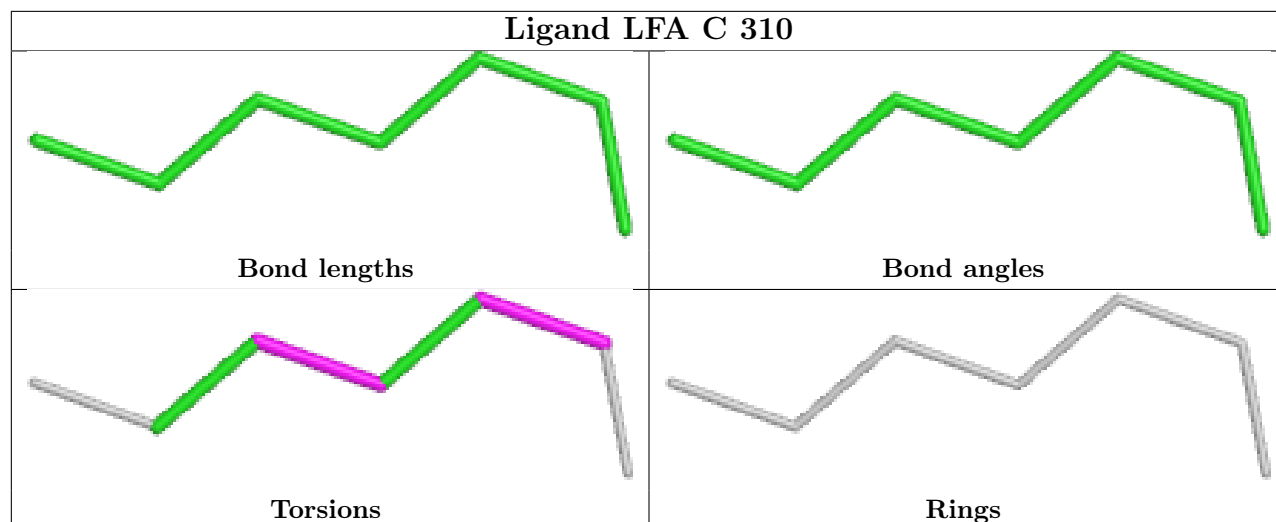


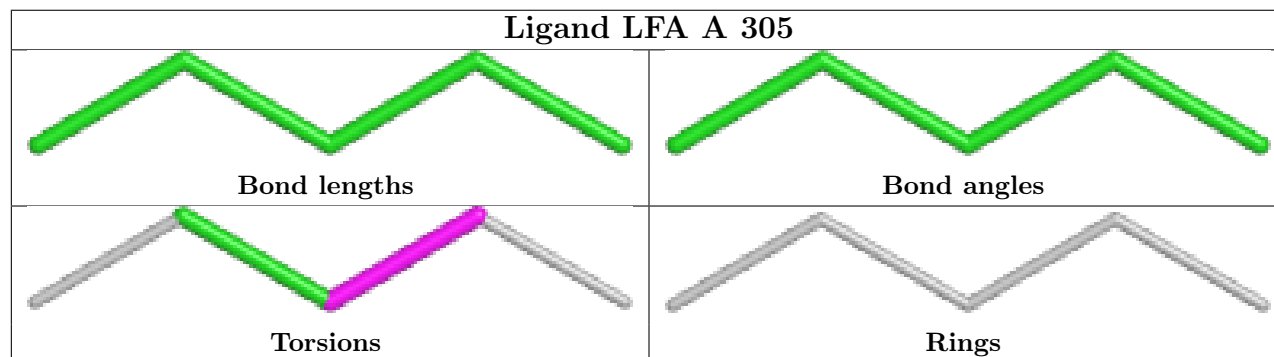
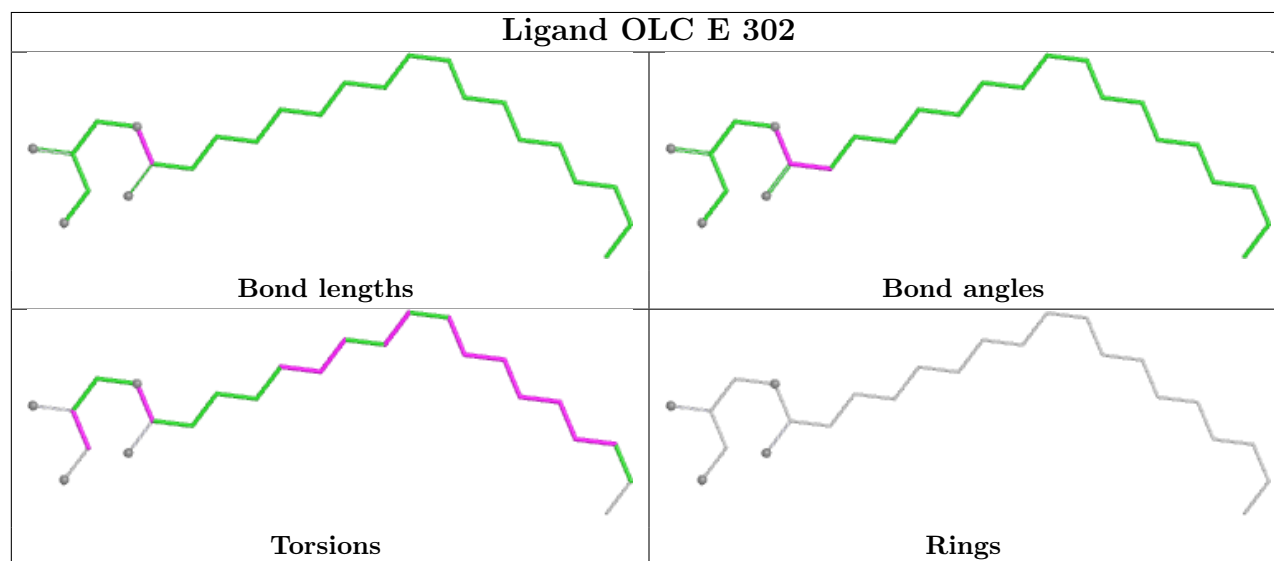
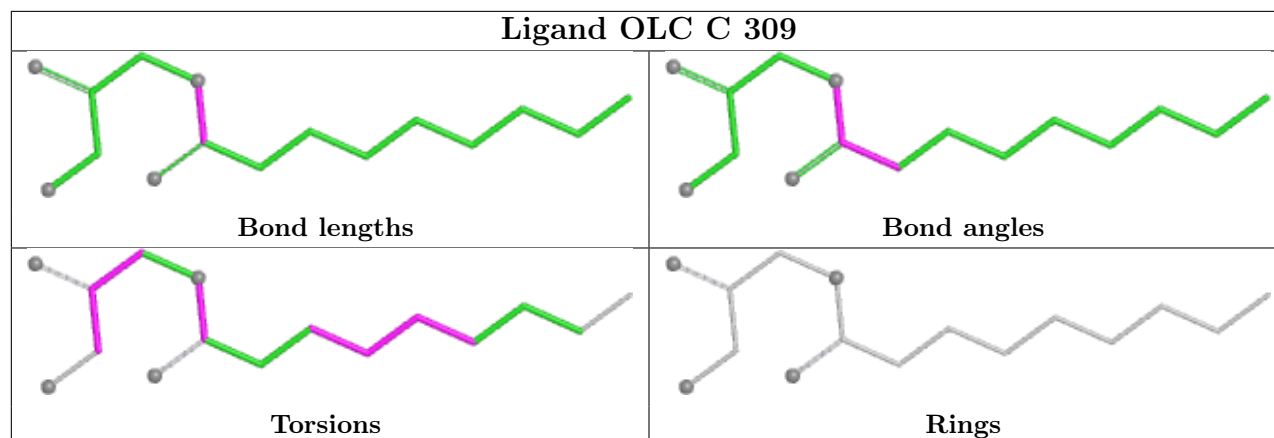


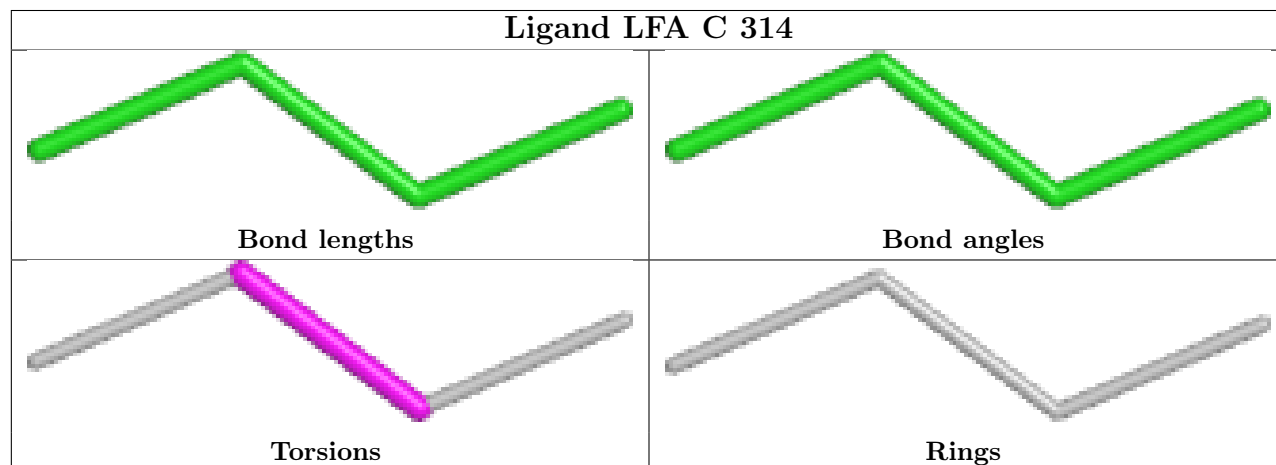
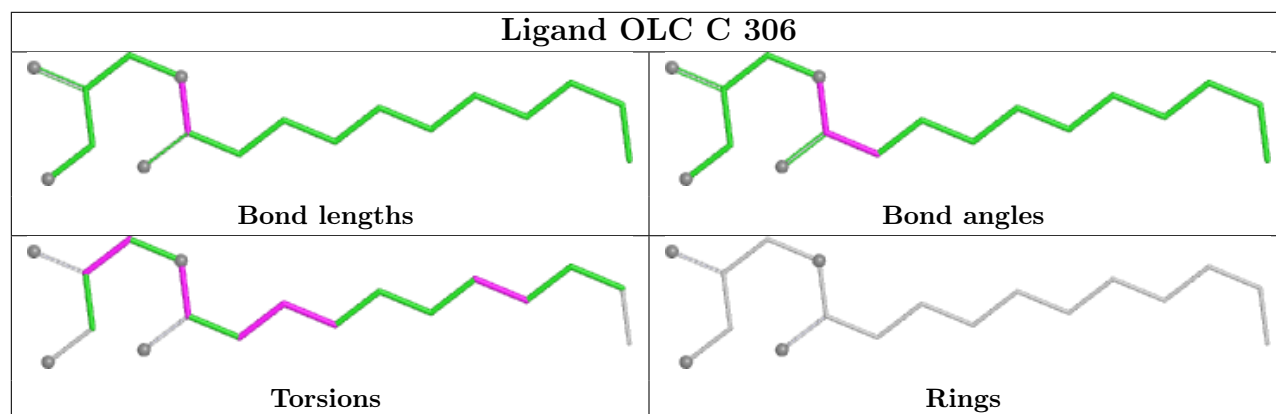
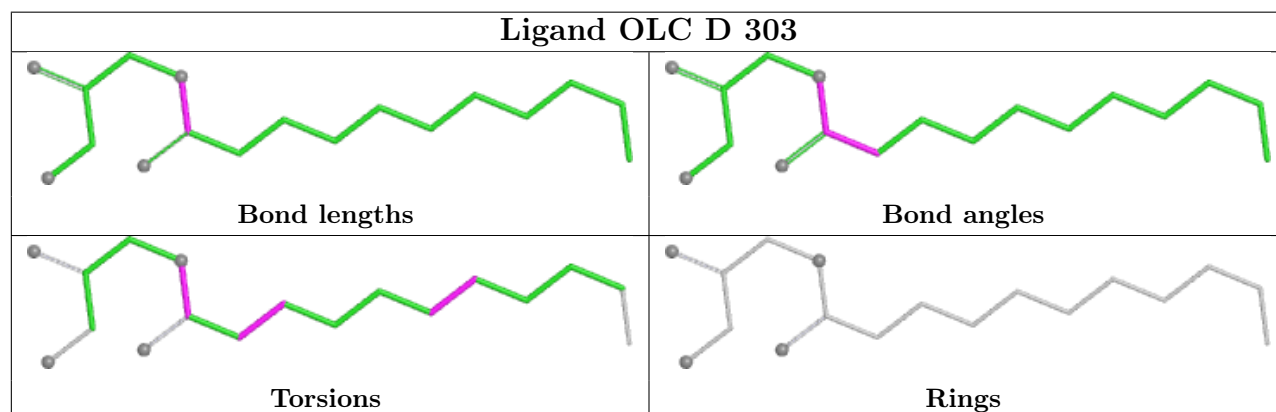
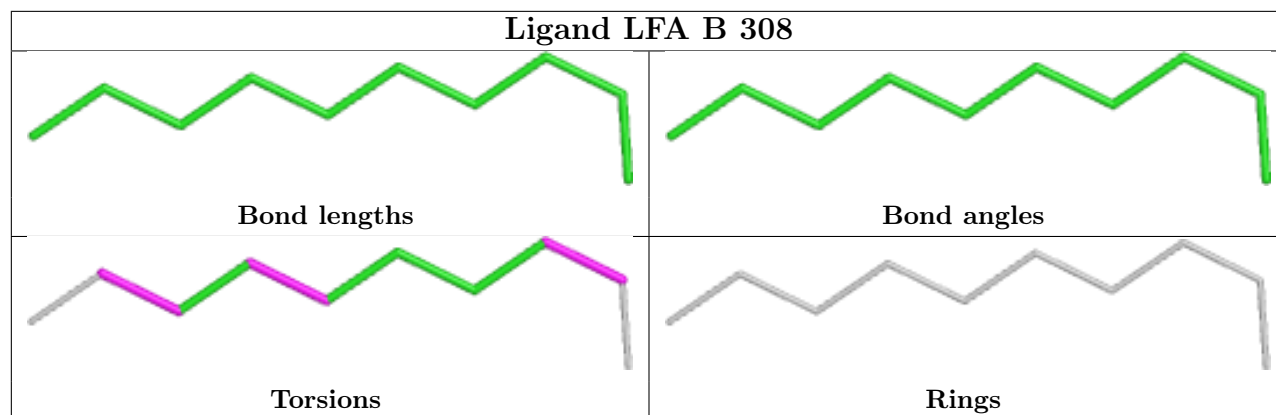


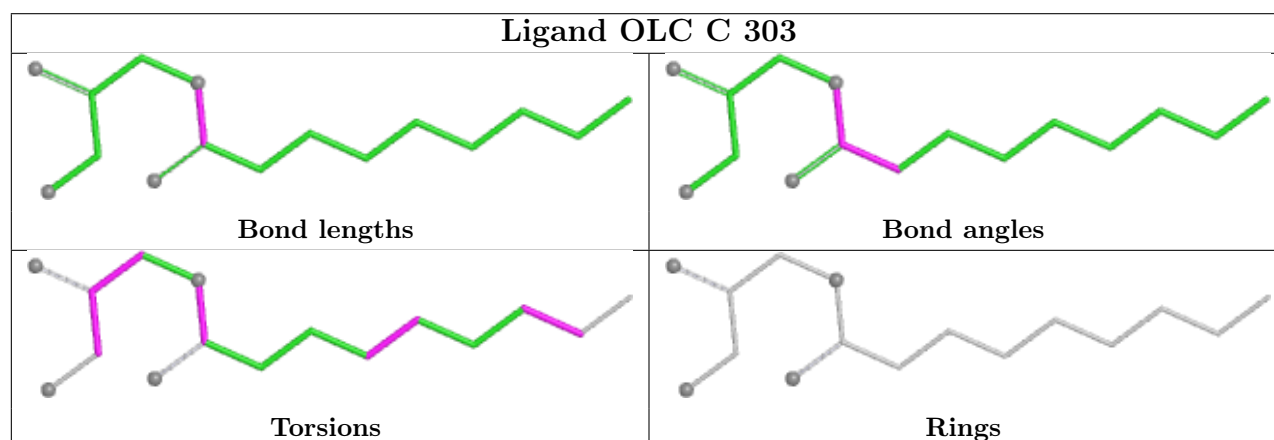
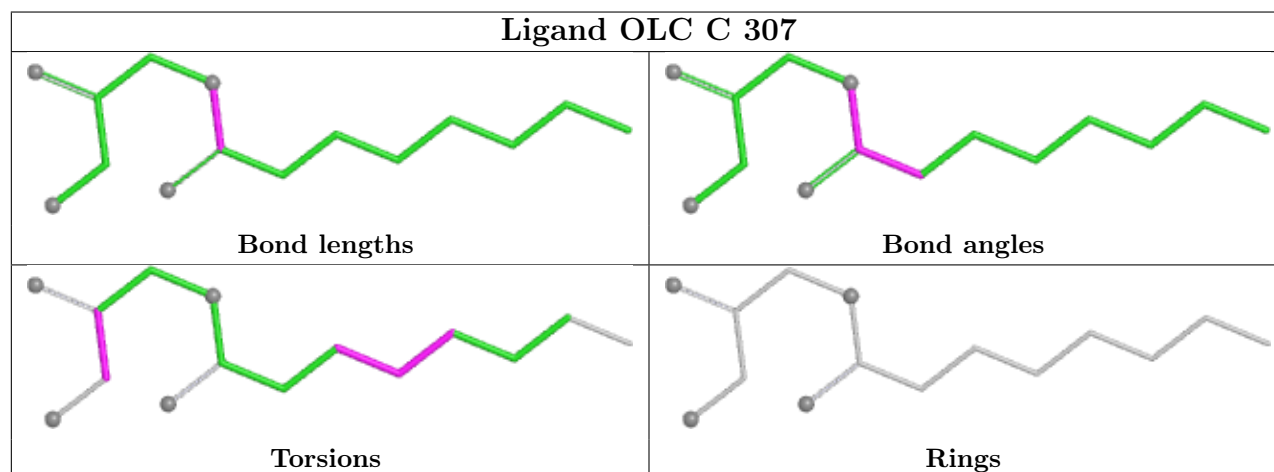
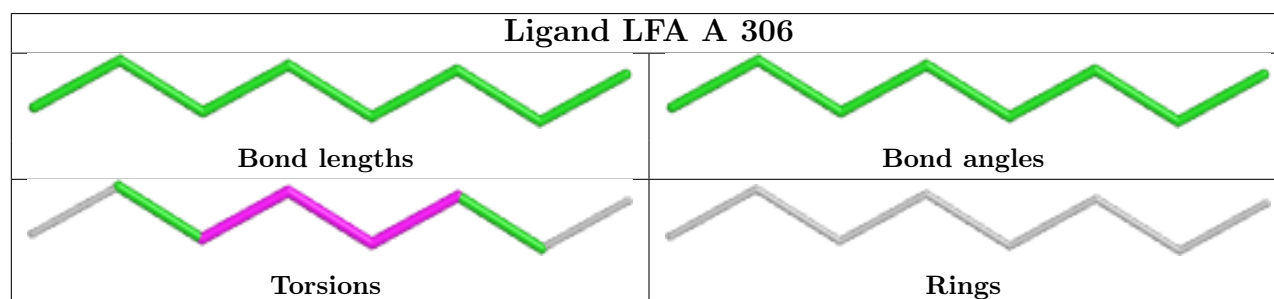
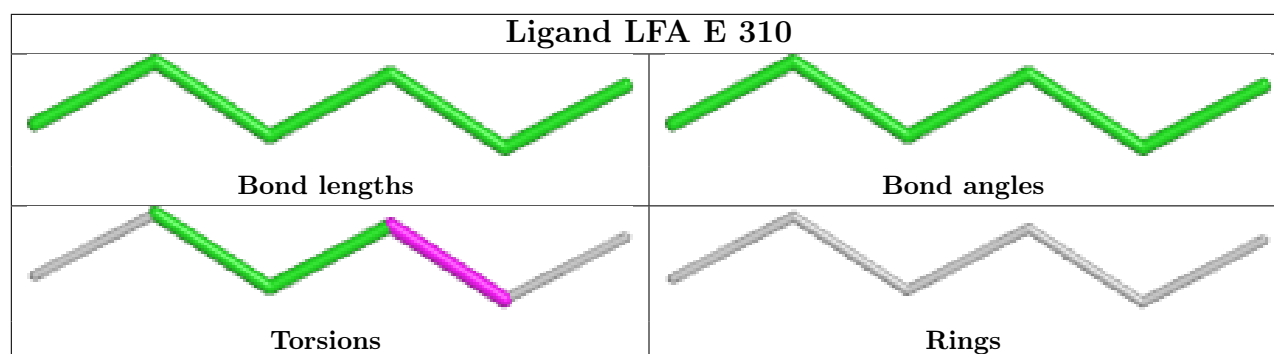


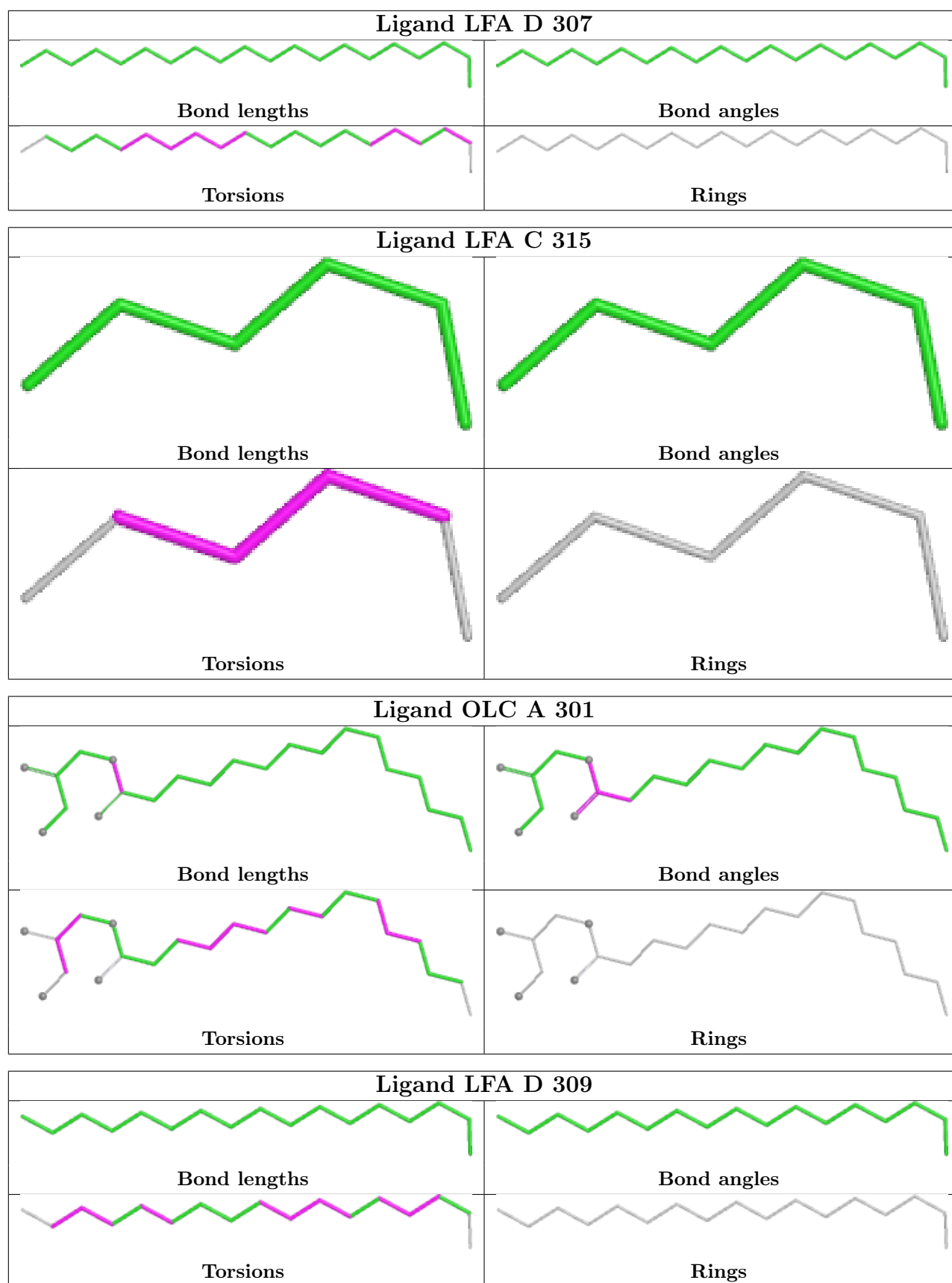


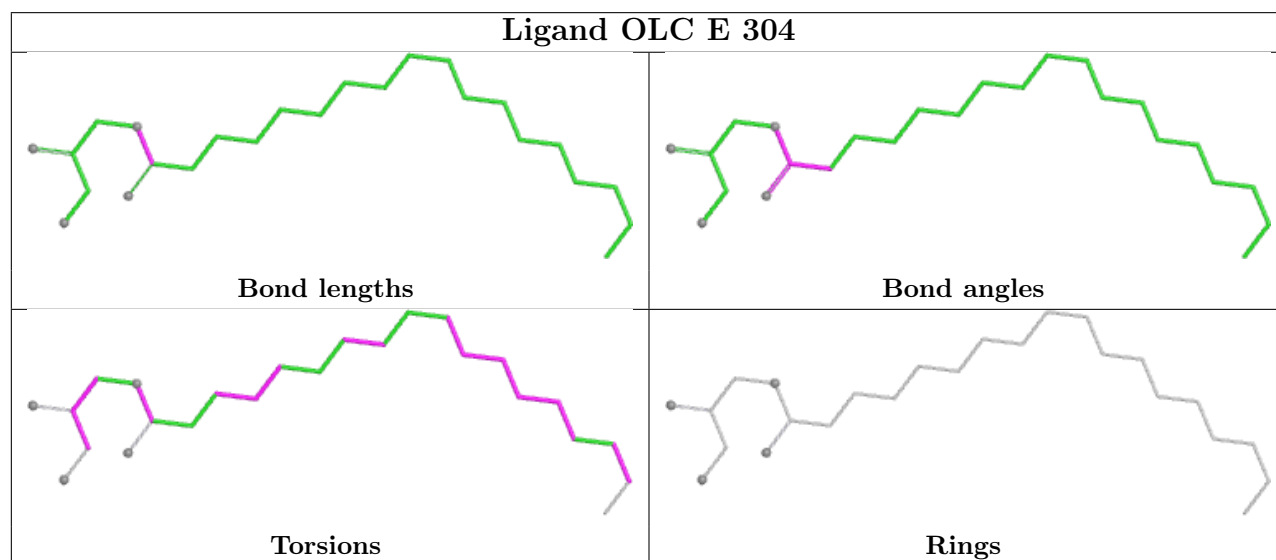
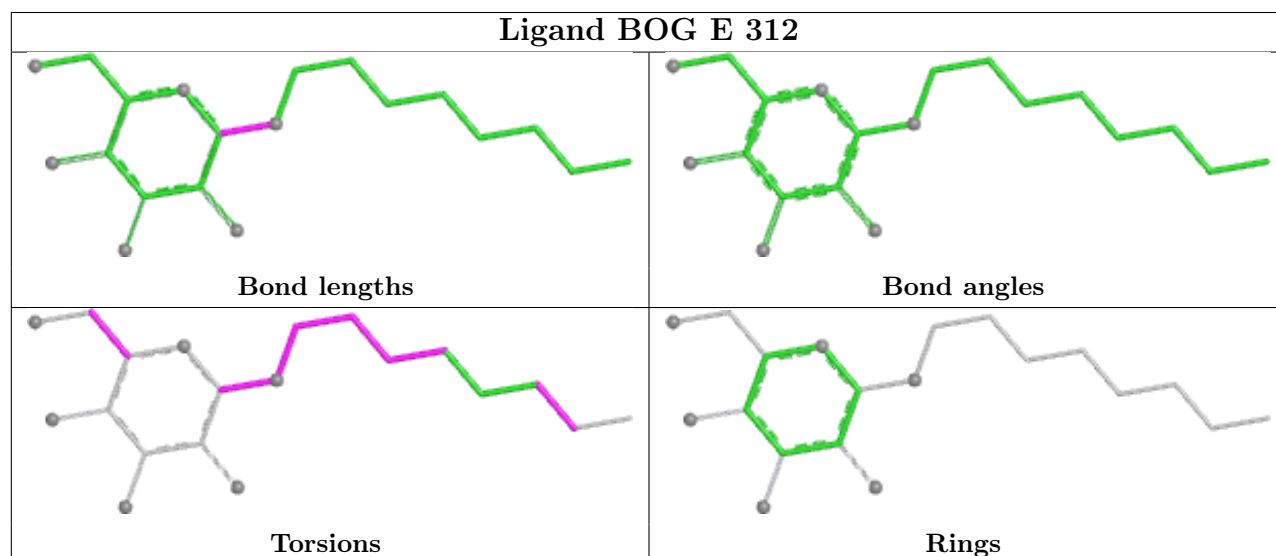
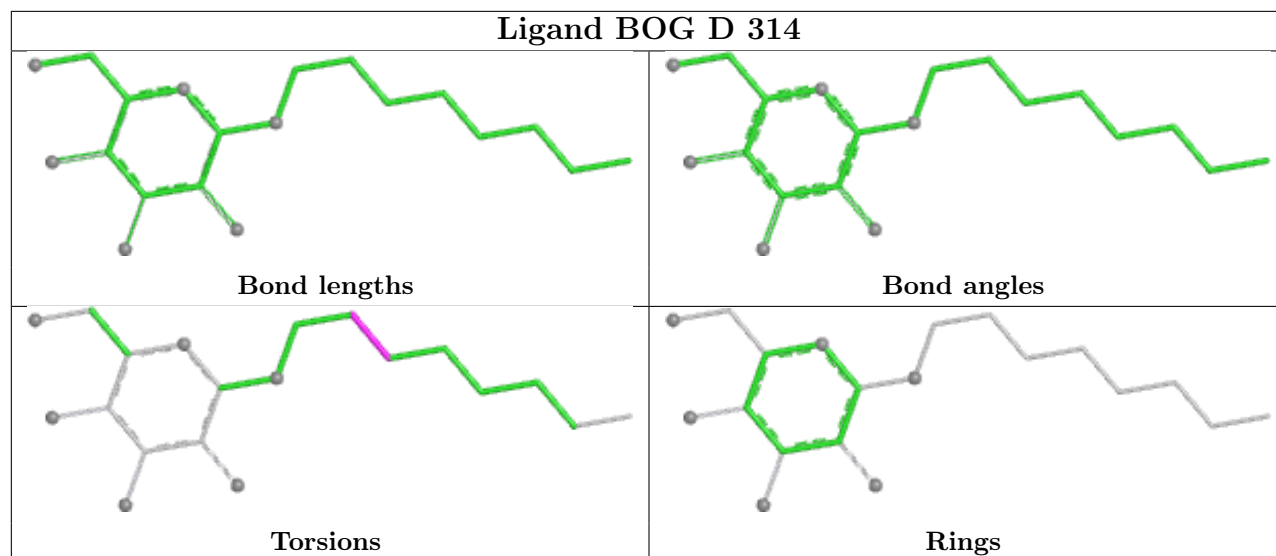


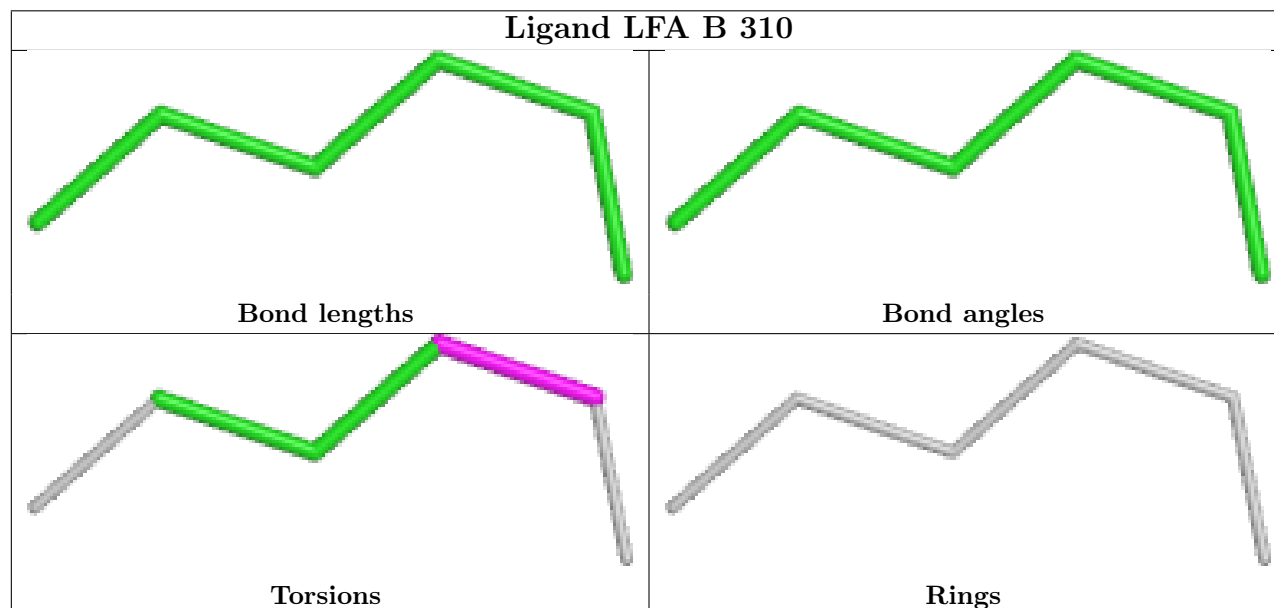
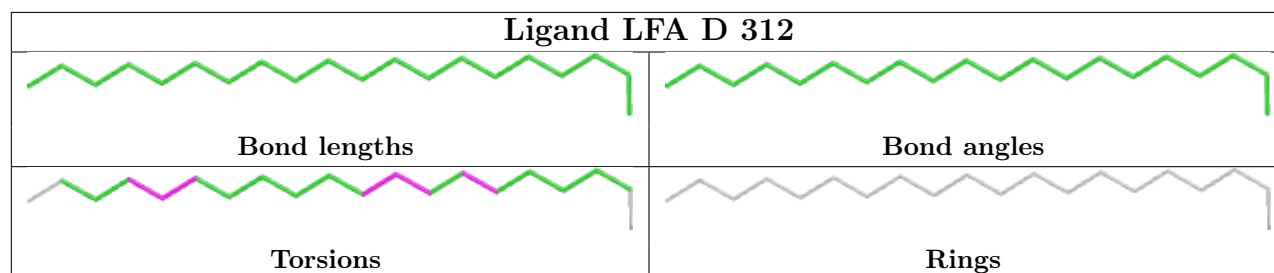
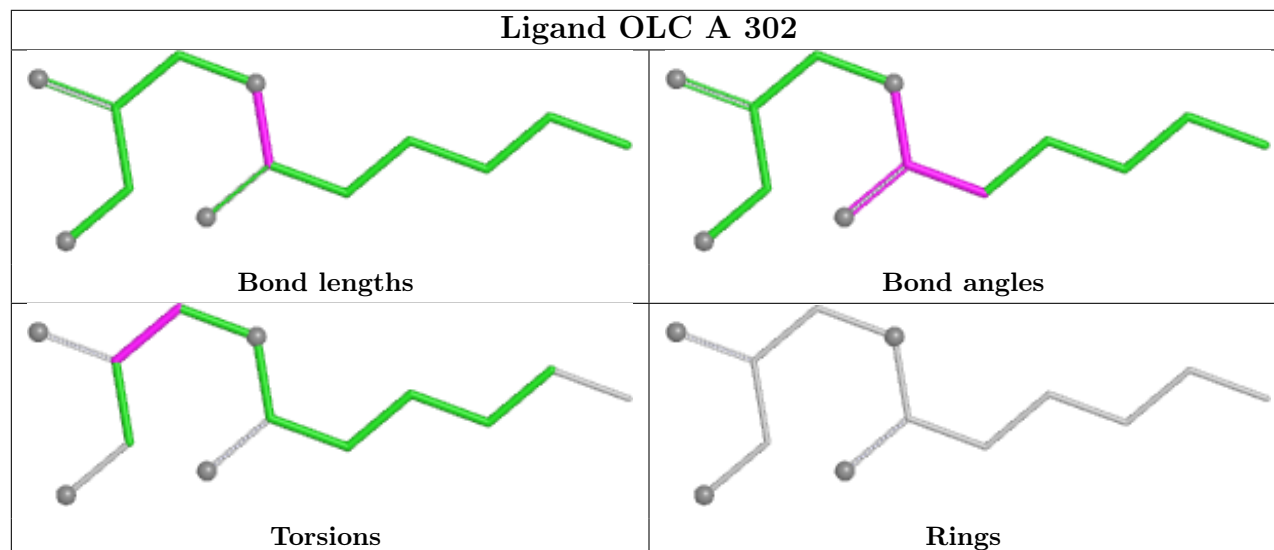
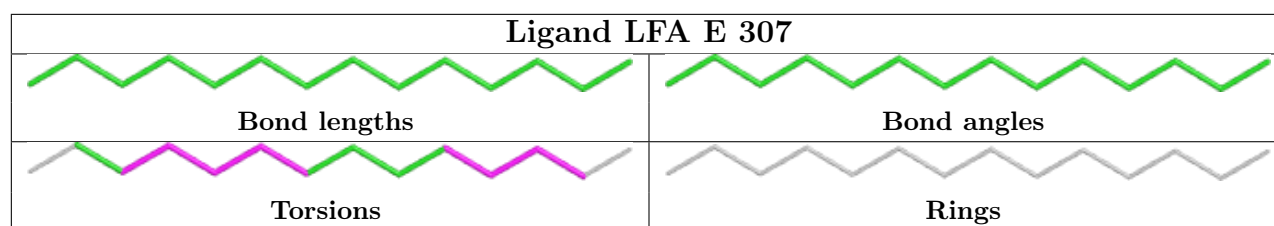


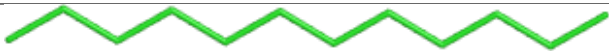
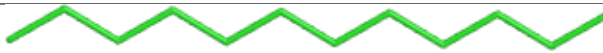


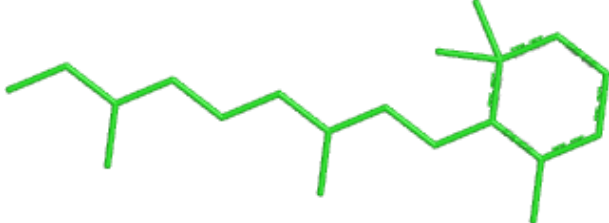
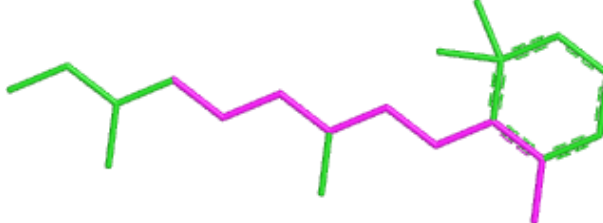
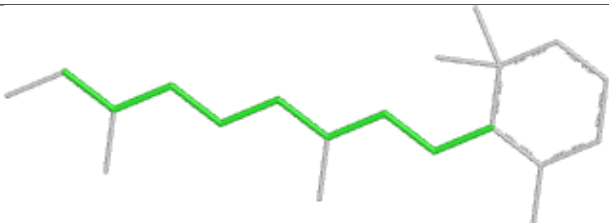
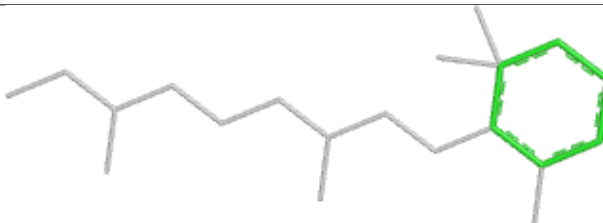


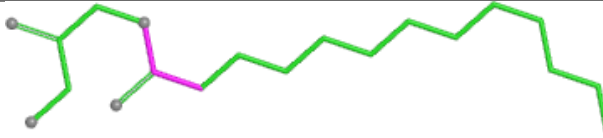
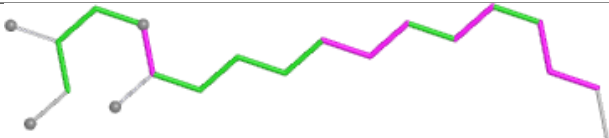
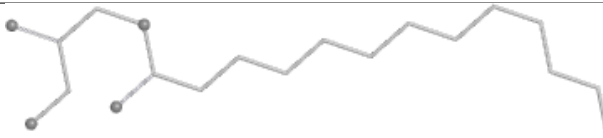


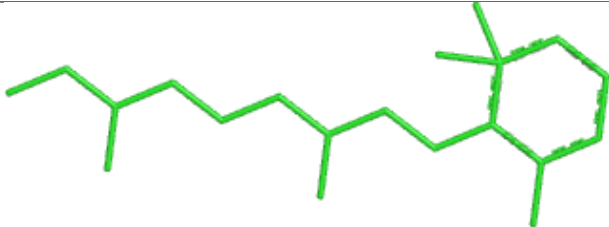
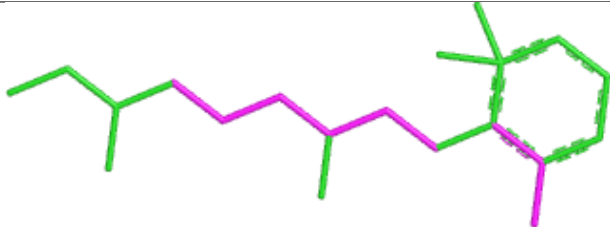
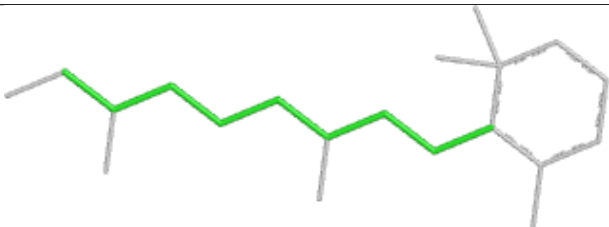
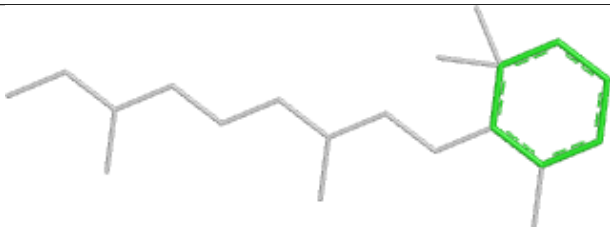


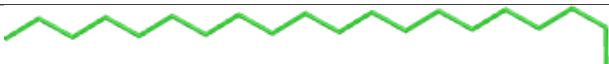
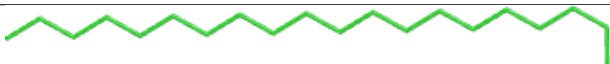
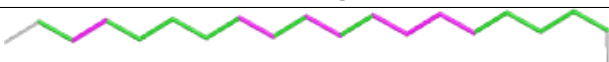
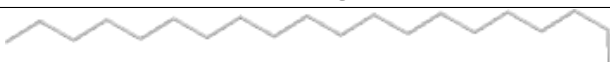


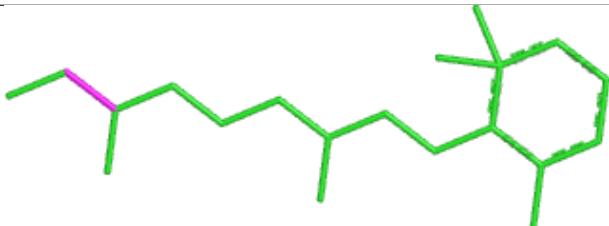
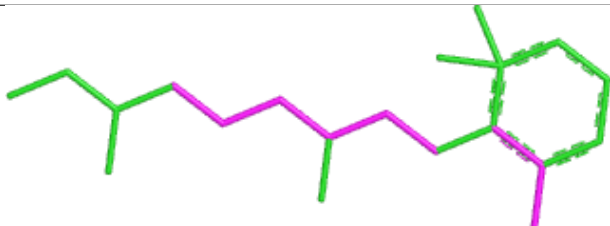
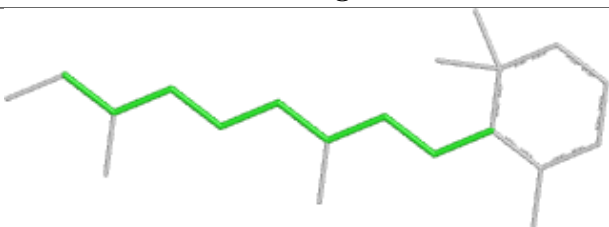
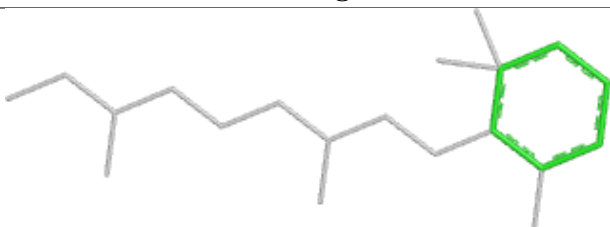
Ligand LFA C 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

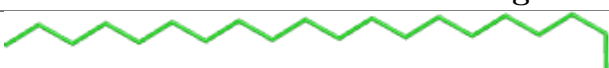
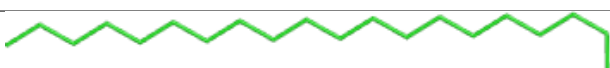
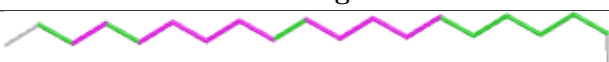
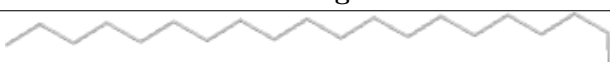
Ligand RET A 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

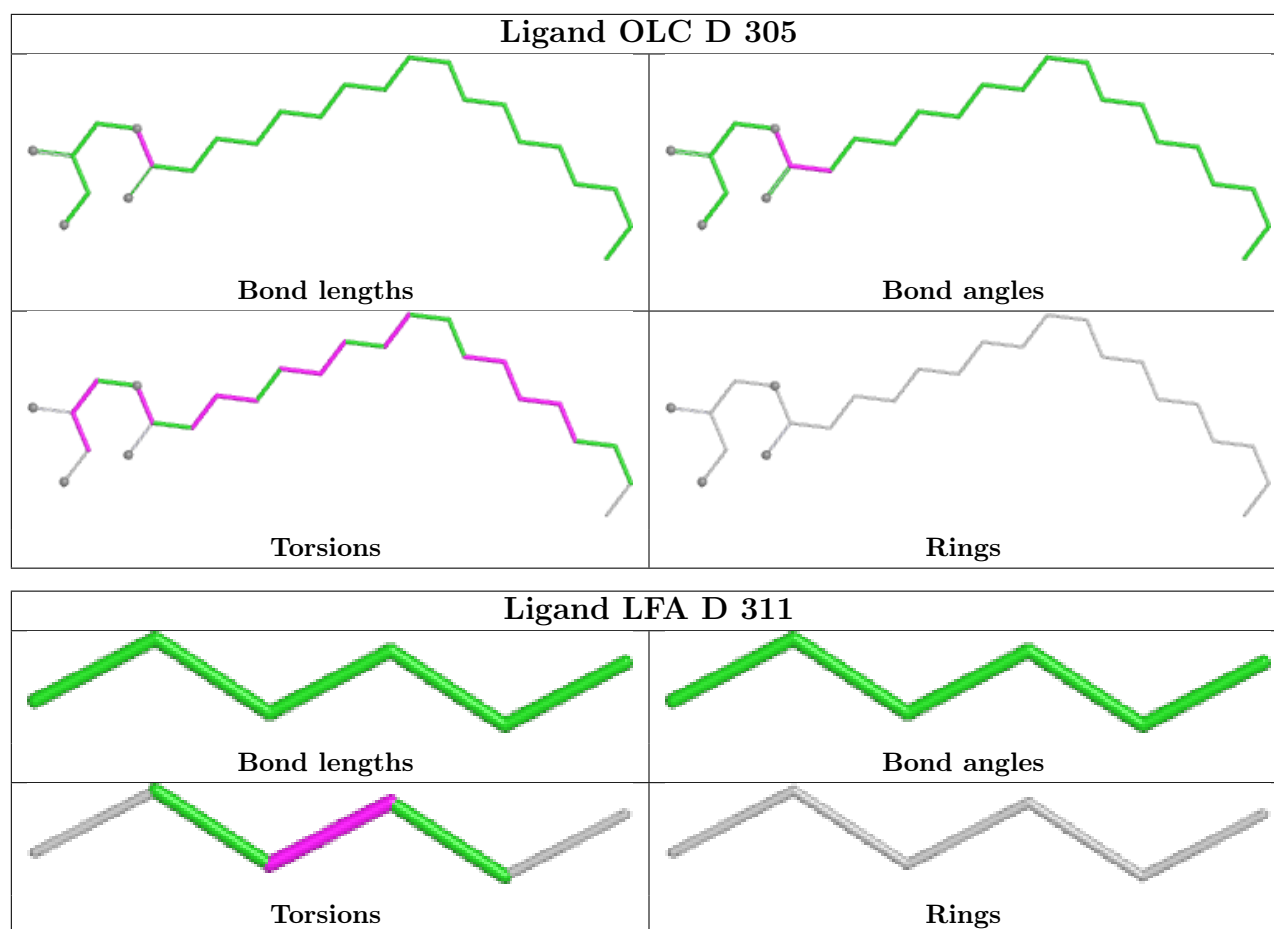
Ligand OLC B 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand RET C 318			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

Ligand LFA B 302			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

Ligand RET E 315			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

Ligand LFA A 311			
			
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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/273 (100%)	0.07	6 (2%) 62 59	14, 34, 59, 110	1 (0%)
1	B	273/273 (100%)	0.01	3 (1%) 78 76	15, 35, 59, 95	1 (0%)
1	C	273/273 (100%)	0.08	6 (2%) 62 59	16, 35, 58, 117	1 (0%)
1	D	273/273 (100%)	0.13	6 (2%) 62 59	13, 36, 60, 140	1 (0%)
1	E	273/273 (100%)	0.09	3 (1%) 78 76	14, 36, 59, 121	1 (0%)
All	All	1365/1365 (100%)	0.08	24 (1%) 67 65	13, 35, 59, 140	5 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	GLY	3.5
1	D	272	ASN	3.2
1	D	273	LYS	3.2
1	D	274	GLU	2.9
1	C	275	LEU	2.8

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	B	306	9/20	0.63	0.33	71,81,86,88	0
3	LFA	C	310	7/20	0.67	0.21	51,58,67,69	0
3	LFA	E	309	5/20	0.68	0.26	61,65,69,72	0
3	LFA	A	307	4/20	0.69	0.27	52,58,59,63	0
3	LFA	B	302	20/20	0.75	0.23	43,63,75,78	0
2	OLC	E	303	15/25	0.75	0.17	56,67,75,77	0
3	LFA	D	308	8/20	0.76	0.22	55,74,88,94	0
3	LFA	C	311	8/20	0.77	0.24	42,59,64,65	0
3	LFA	D	312	20/20	0.78	0.20	42,58,75,80	0
3	LFA	D	301	20/20	0.78	0.20	34,53,63,65	0
3	LFA	D	310	7/20	0.79	0.17	53,59,69,71	0
5	BOG	A	310	20/20	0.79	0.17	53,78,98,102	0
3	LFA	D	306	20/20	0.80	0.26	64,86,95,95	0
3	LFA	C	304	20/20	0.80	0.19	34,51,62,64	0
2	OLC	E	304	25/25	0.80	0.21	42,72,104,111	0
3	LFA	A	311	20/20	0.80	0.19	34,65,78,78	0
3	LFA	C	312	12/20	0.80	0.22	60,65,76,79	0
3	LFA	E	314	14/20	0.80	0.30	86,97,101,105	0
3	LFA	B	309	7/20	0.80	0.21	56,59,73,78	0
3	LFA	C	314	4/20	0.81	0.26	64,65,68,69	0
2	OLC	C	309	16/25	0.81	0.21	55,75,96,106	0
2	OLC	C	307	15/25	0.81	0.14	48,63,81,87	0
5	BOG	B	312	20/20	0.81	0.17	66,87,108,108	0
2	OLC	C	303	16/25	0.82	0.24	63,76,93,104	0
3	LFA	B	308	10/20	0.82	0.21	54,69,81,82	0
3	LFA	E	313	4/20	0.82	0.26	59,63,67,70	0
3	LFA	B	307	5/20	0.83	0.14	30,35,40,42	0
2	OLC	D	303	18/25	0.83	0.21	47,71,84,106	0
3	LFA	A	304	8/20	0.83	0.17	52,58,66,67	0
3	LFA	D	311	6/20	0.84	0.15	37,41,44,47	0
3	LFA	C	313	11/20	0.84	0.26	58,77,93,93	0
3	LFA	E	306	6/20	0.84	0.21	53,58,61,61	0
2	OLC	B	304	16/25	0.84	0.18	54,61,67,71	0
5	BOG	C	317	20/20	0.84	0.14	57,84,95,101	0
3	LFA	E	307	14/20	0.85	0.25	47,71,88,93	0
3	LFA	E	308	4/20	0.85	0.23	62,62,63,67	0
3	LFA	E	305	8/20	0.85	0.21	61,67,71,72	0
2	OLC	B	303	20/25	0.85	0.15	46,58,87,92	0
3	LFA	A	306	8/20	0.86	0.22	49,72,86,89	0
3	LFA	C	315	6/20	0.86	0.14	39,42,45,45	0
5	BOG	E	312	20/20	0.86	0.14	50,86,110,114	0

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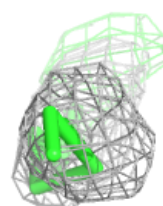
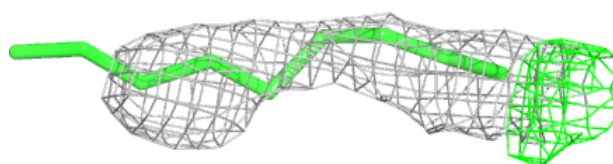
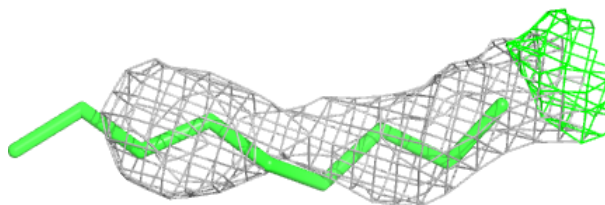
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LFA	A	305	5/20	0.87	0.19	50,51,56,57	0
2	OLC	D	305	25/25	0.87	0.20	63,78,95,109	0
3	LFA	D	307	20/20	0.87	0.20	56,70,85,90	0
2	OLC	B	301	25/25	0.88	0.18	60,77,94,100	0
2	OLC	D	304	14/25	0.88	0.17	46,68,75,77	0
2	OLC	A	302	13/25	0.88	0.13	47,59,65,79	0
2	OLC	A	303	15/25	0.88	0.16	50,56,78,81	0
2	OLC	C	302	20/25	0.89	0.16	55,68,73,81	0
2	OLC	C	306	18/25	0.89	0.17	57,71,86,90	0
2	OLC	D	302	25/25	0.89	0.17	55,76,110,116	0
2	OLC	E	302	25/25	0.89	0.18	62,78,114,119	0
3	LFA	B	310	6/20	0.89	0.13	49,51,53,54	0
2	OLC	A	301	22/25	0.90	0.14	38,51,92,94	0
2	OLC	B	305	17/25	0.90	0.18	49,79,102,104	0
3	LFA	A	308	6/20	0.90	0.12	43,44,45,47	0
2	OLC	E	301	24/25	0.90	0.17	41,52,91,94	0
5	BOG	D	314	20/20	0.90	0.13	66,84,88,90	0
2	OLC	C	308	16/25	0.90	0.12	41,58,71,77	0
2	OLC	C	305	23/25	0.91	0.13	34,45,95,121	0
3	LFA	E	310	6/20	0.92	0.15	46,50,51,55	0
6	RET	A	312	20/21	0.92	0.10	26,31,36,40	0
6	RET	E	315	20/21	0.92	0.11	24,28,38,38	0
2	OLC	C	301	21/25	0.93	0.13	39,46,63,83	0
4	NA	E	311	1/1	0.93	0.05	34,34,34,34	0
3	LFA	D	309	17/20	0.93	0.12	37,45,50,50	0
6	RET	C	318	20/21	0.94	0.09	27,31,38,38	0
6	RET	B	313	20/21	0.94	0.09	25,32,35,40	0
6	RET	D	315	20/21	0.95	0.09	29,34,40,41	0
4	NA	A	309	1/1	0.95	0.06	36,36,36,36	0
4	NA	B	311	1/1	0.97	0.05	33,33,33,33	0
4	NA	D	313	1/1	0.98	0.04	34,34,34,34	0
4	NA	C	316	1/1	0.99	0.02	25,25,25,25	0

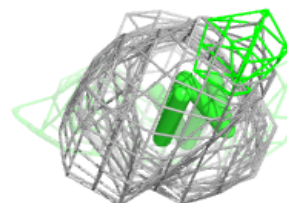
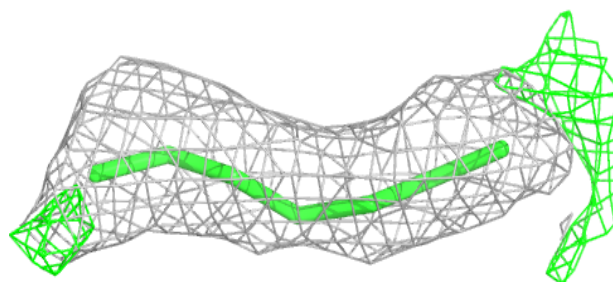
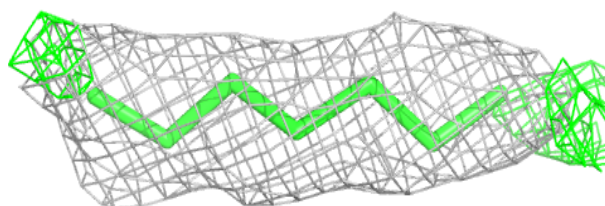
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA B 306:

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

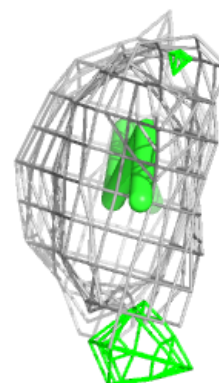
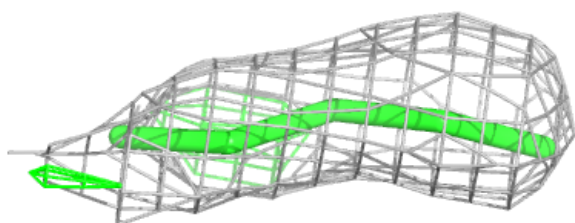
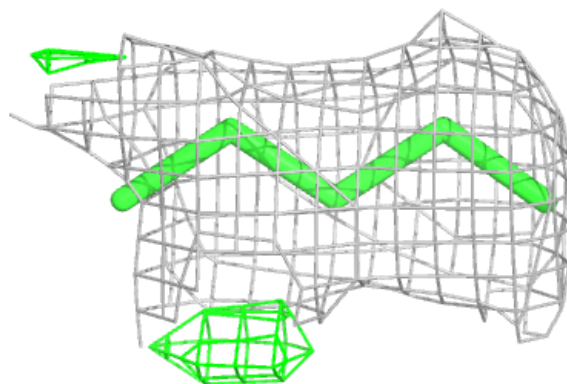
**Electron density around LFA C 310:**

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

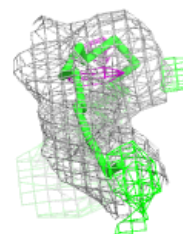
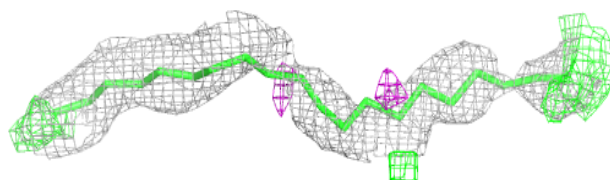
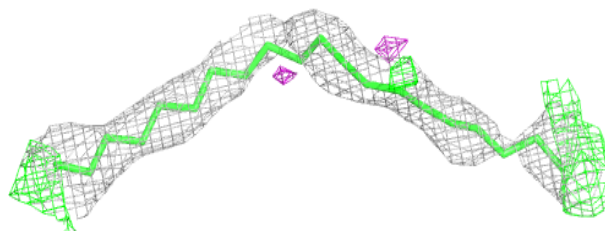


Electron density around LFA E 309:

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

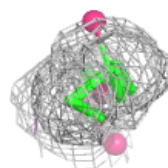
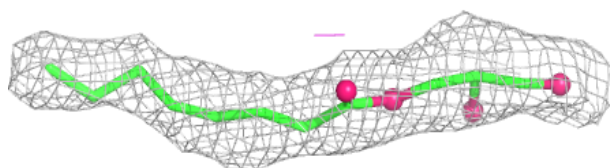
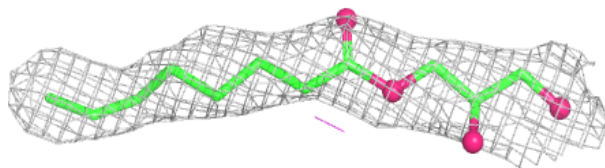
**Electron density around LFA B 302:**

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

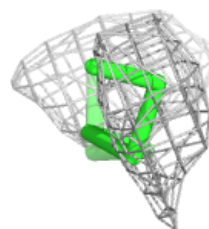
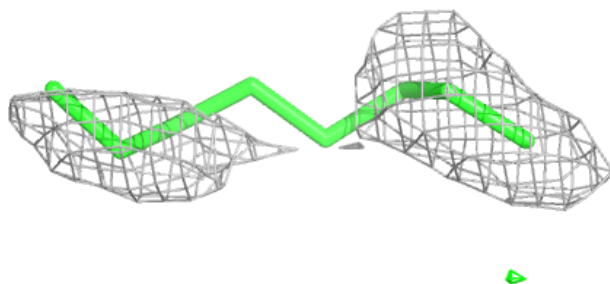
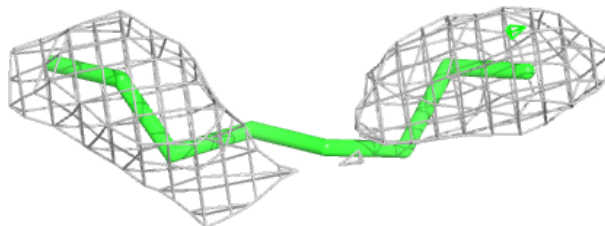


Electron density around OLC E 303:

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

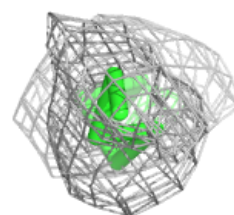
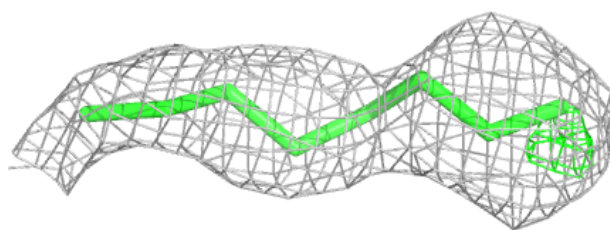
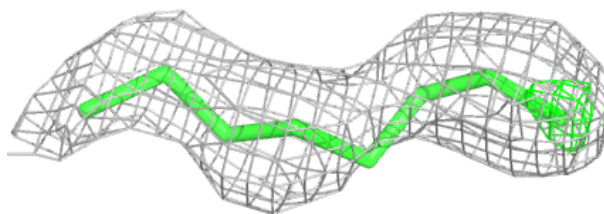
**Electron density around LFA D 308:**

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

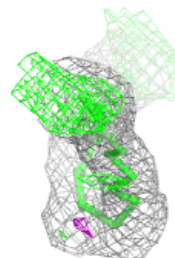
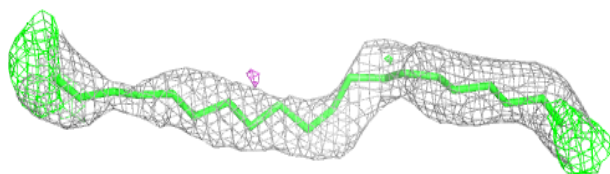
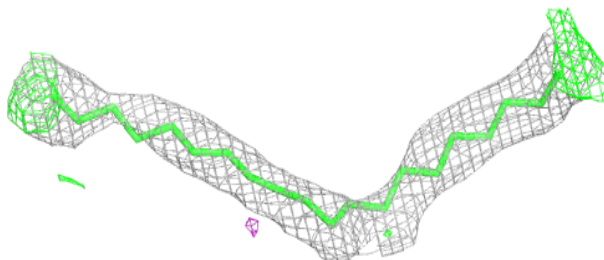


Electron density around LFA C 311:

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

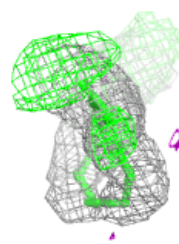
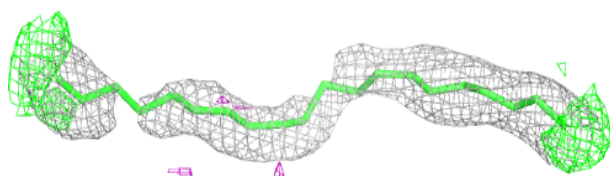
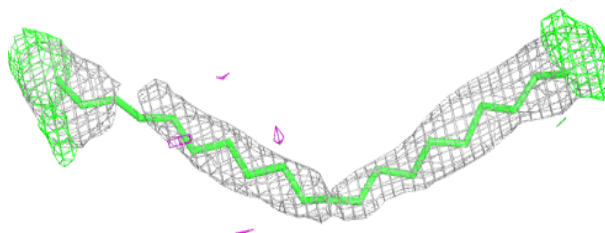
**Electron density around LFA D 312:**

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

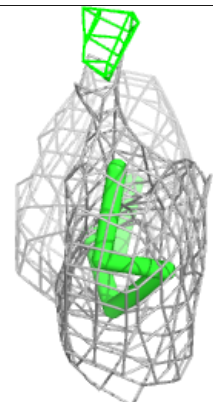
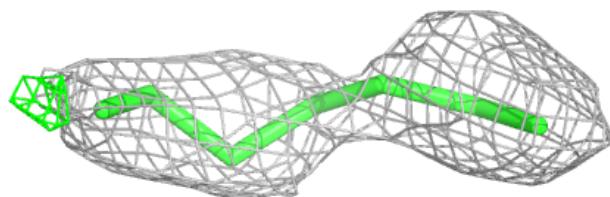
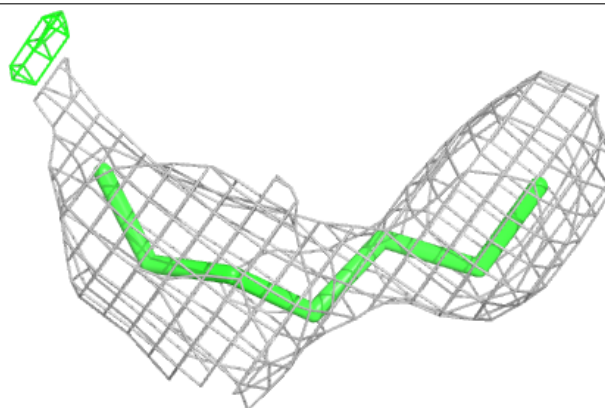


Electron density around LFA D 301:

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

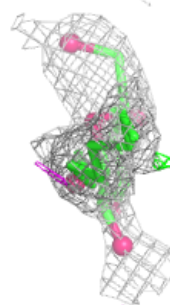
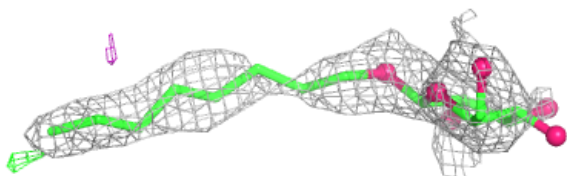
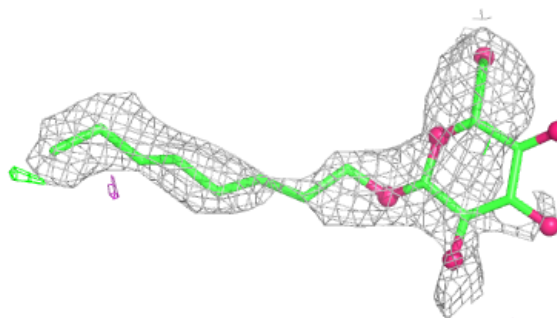
**Electron density around LFA D 310:**

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

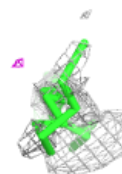
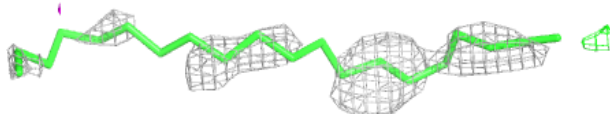
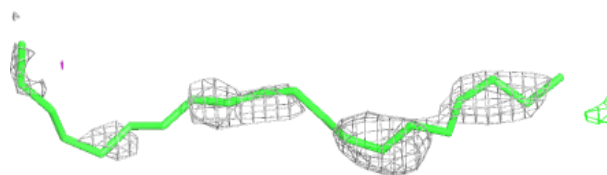


Electron density around BOG A 310:

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

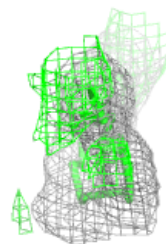
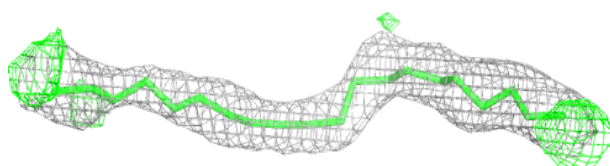
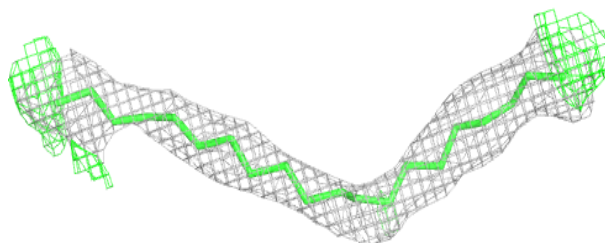
**Electron density around LFA D 306:**

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

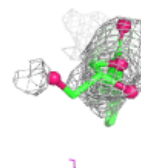
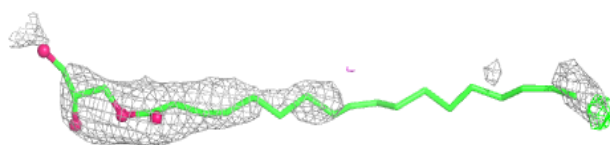
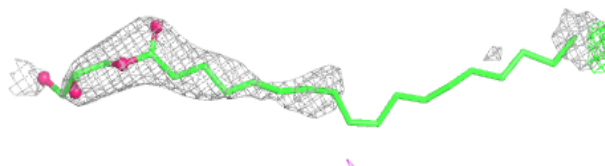


Electron density around LFA C 304:

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

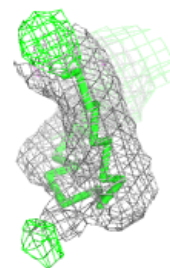
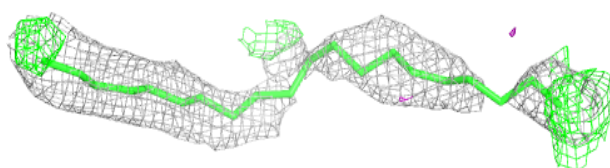
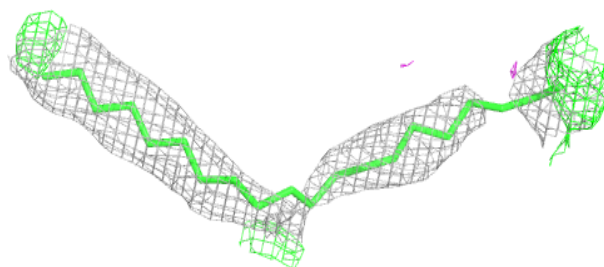
**Electron density around OLC E 304:**

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

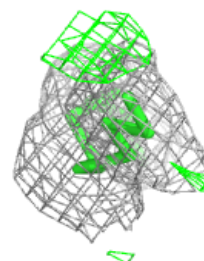
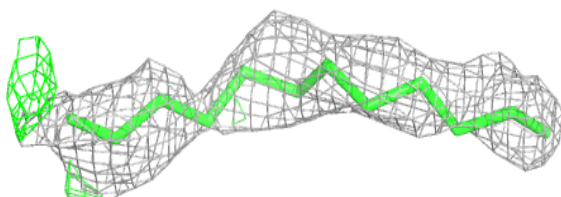
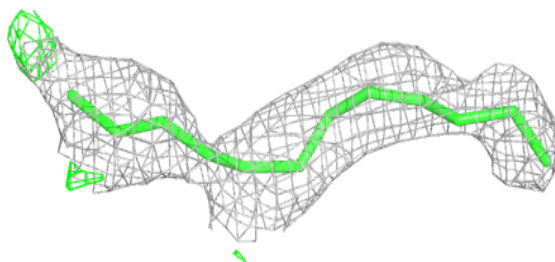


Electron density around LFA A 311:

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

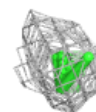
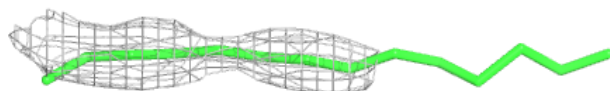
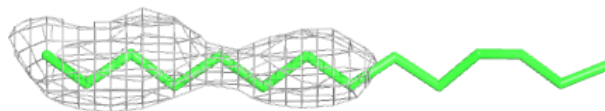
**Electron density around LFA C 312:**

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



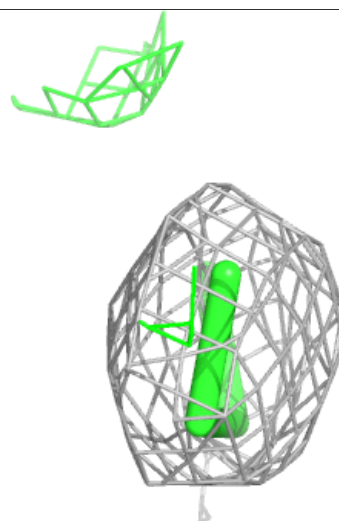
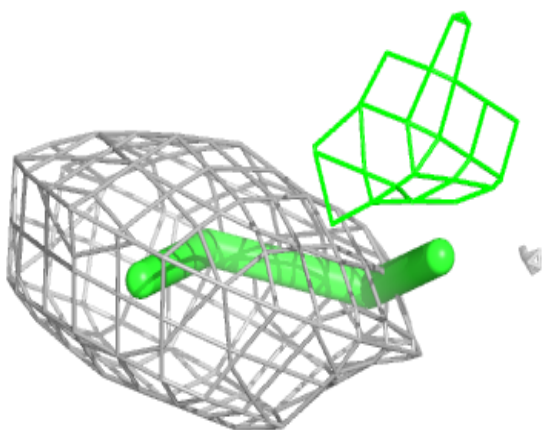
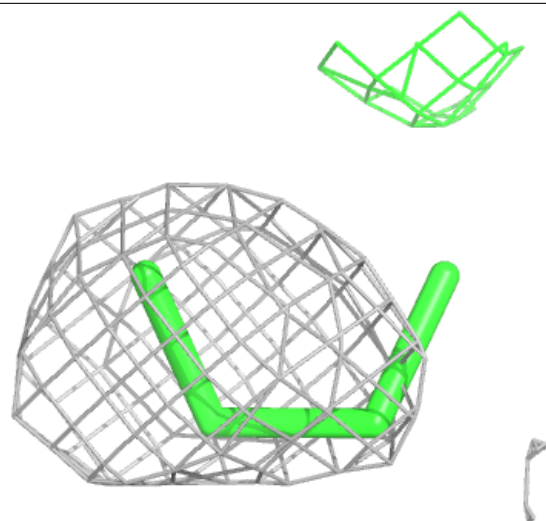
Electron density around LFA E 314:

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



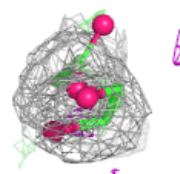
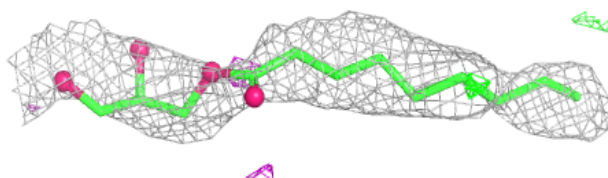
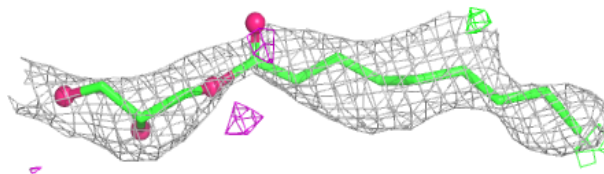
Electron density around LFA C 314:

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

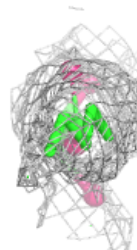
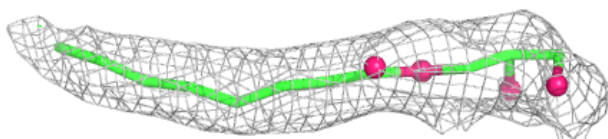
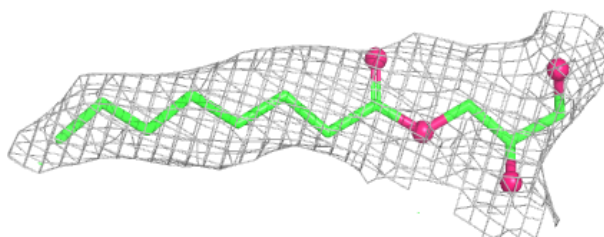


Electron density around OLC C 309:

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

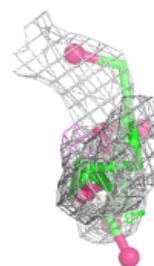
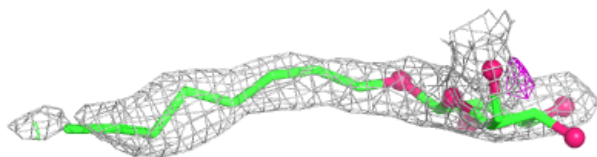
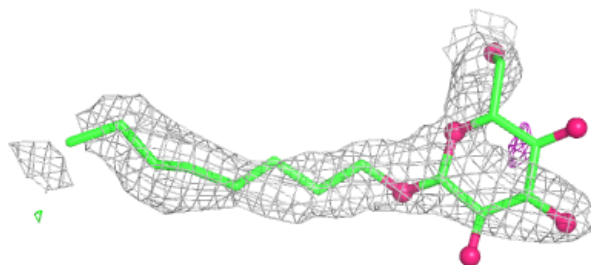
**Electron density around OLC C 307:**

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

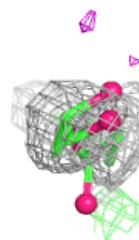
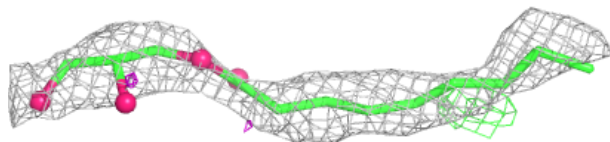
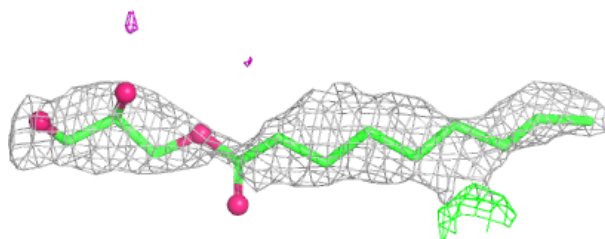


Electron density around BOG B 312:

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

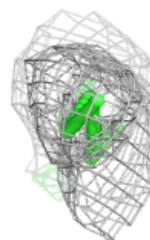
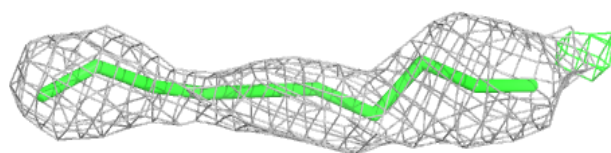
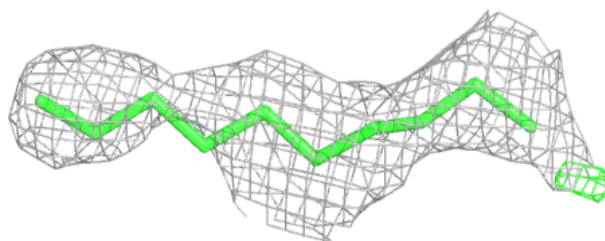
**Electron density around OLC C 303:**

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

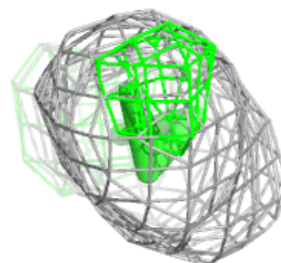
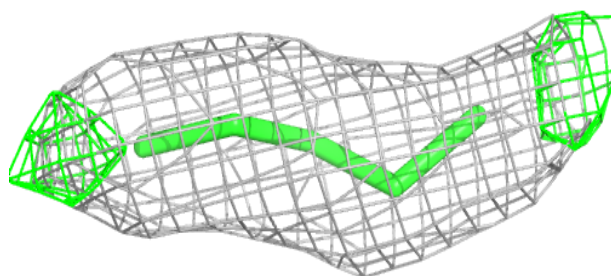
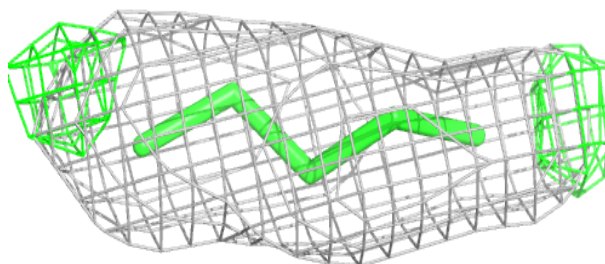


Electron density around LFA B 308:

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

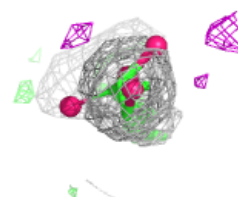
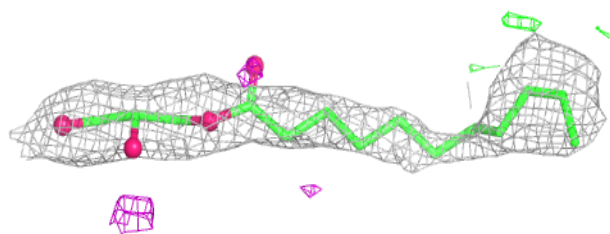
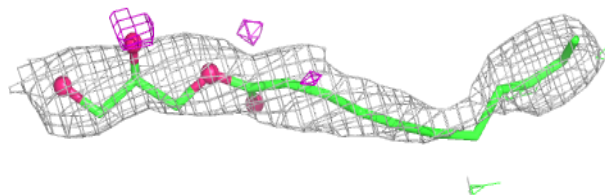
**Electron density around LFA B 307:**

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

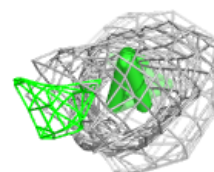
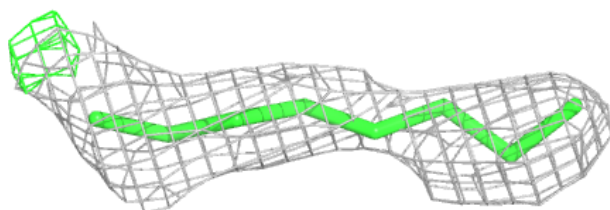
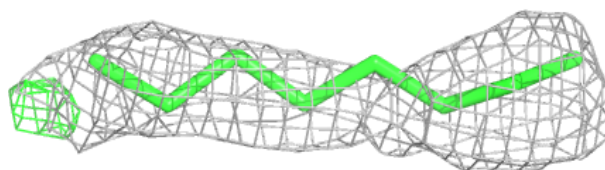


Electron density around OLC D 303:

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

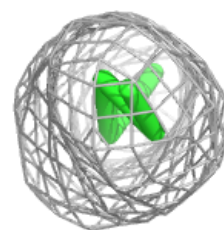
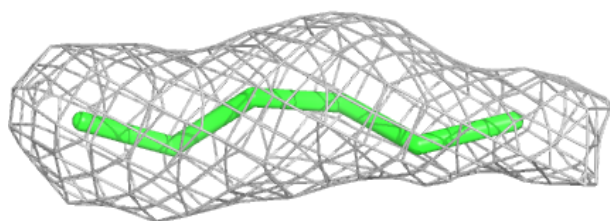
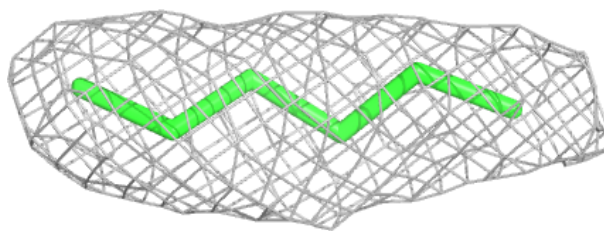
**Electron density around LFA A 304:**

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

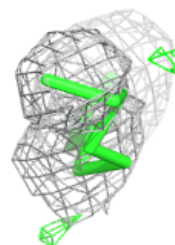
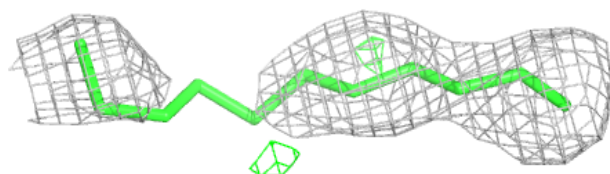
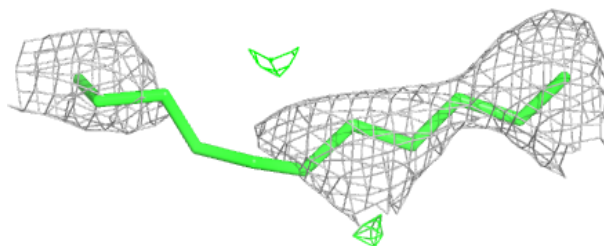


Electron density around LFA D 311:

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

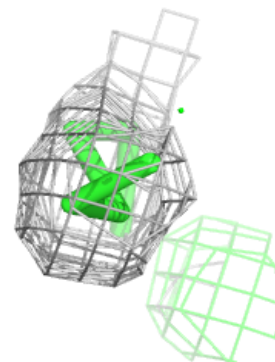
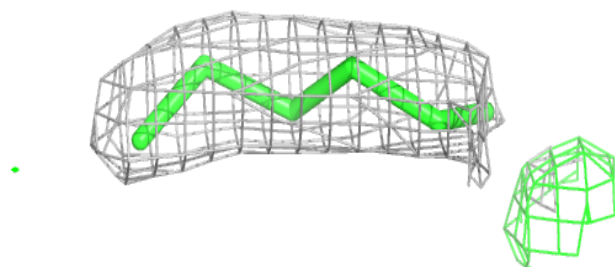
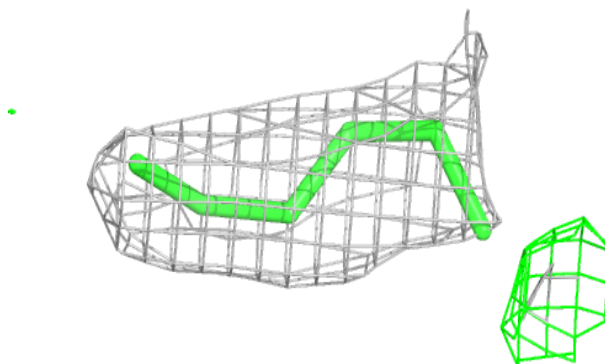
**Electron density around LFA C 313:**

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

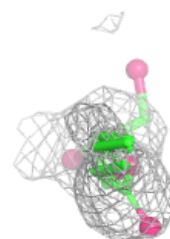
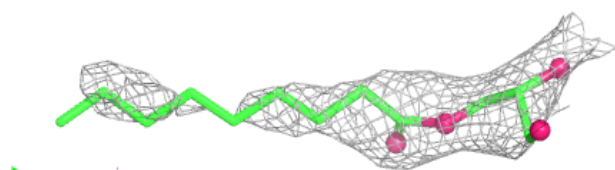
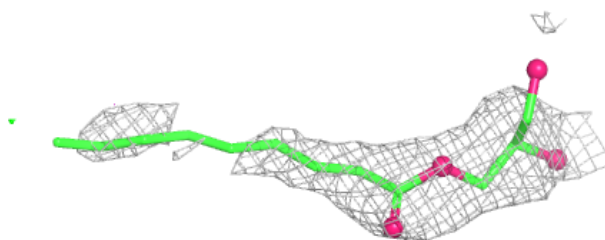


Electron density around LFA E 306:

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

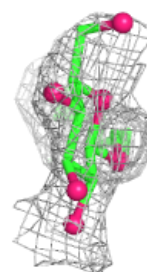
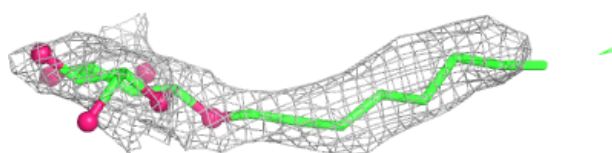
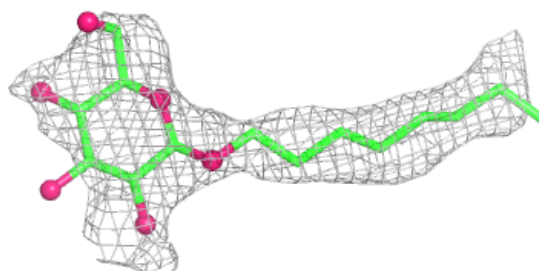
**Electron density around OLC B 304:**

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

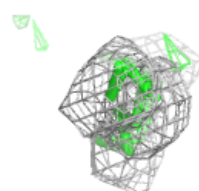
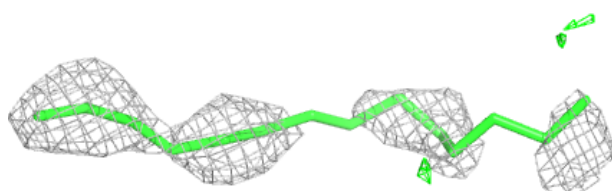
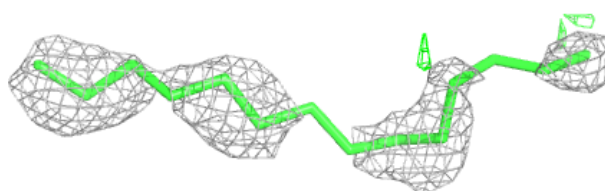


Electron density around BOG C 317:

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

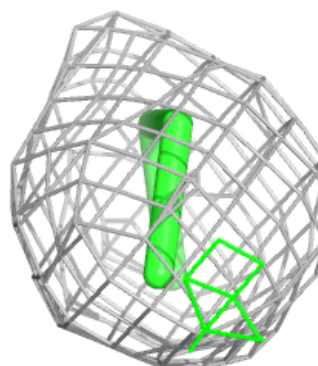
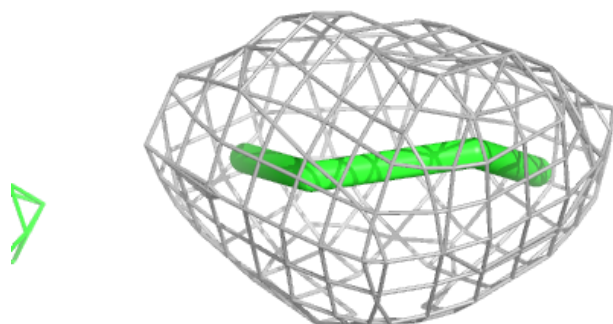
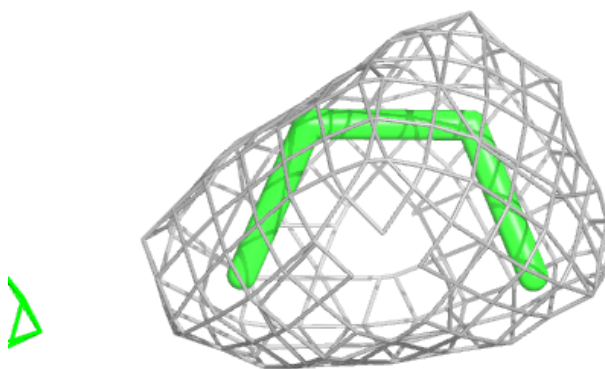
**Electron density around LFA E 307:**

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

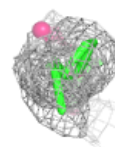
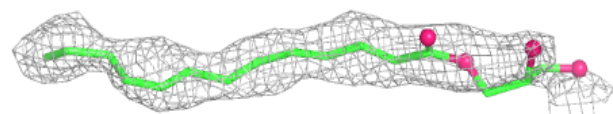
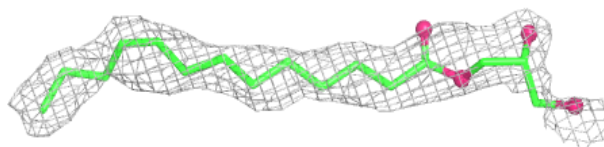


Electron density around LFA E 308:

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

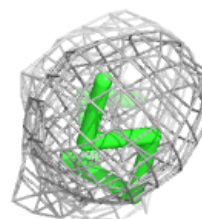
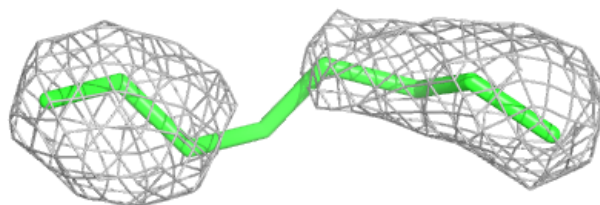
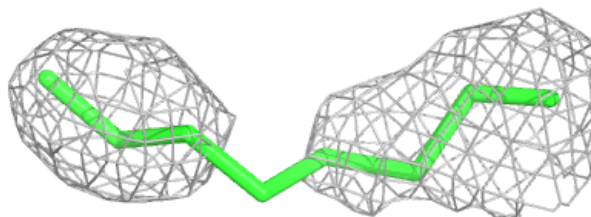
**Electron density around OLC B 303:**

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

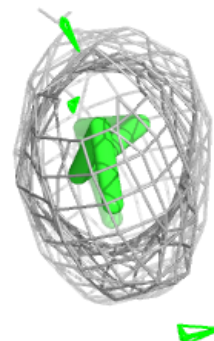
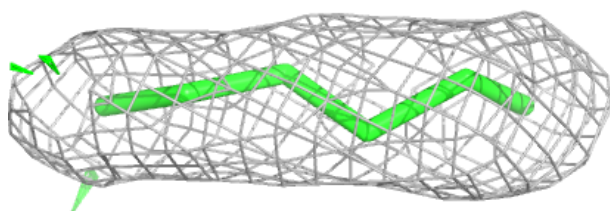
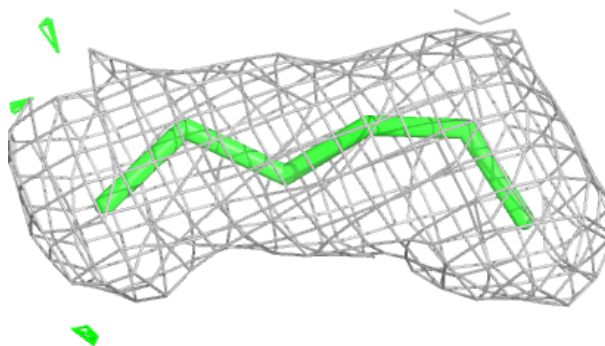


Electron density around LFA A 306:

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

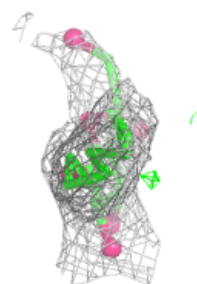
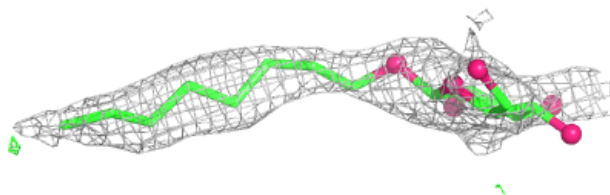
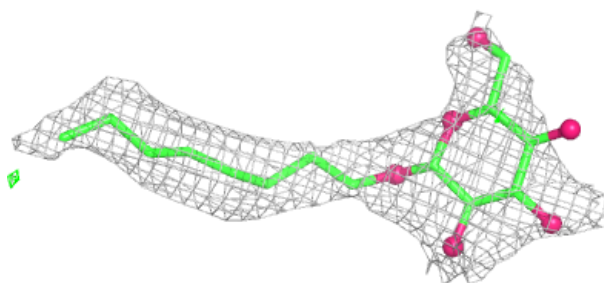
**Electron density around LFA C 315:**

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



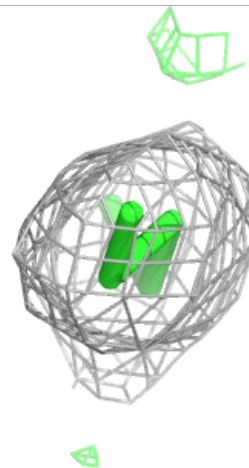
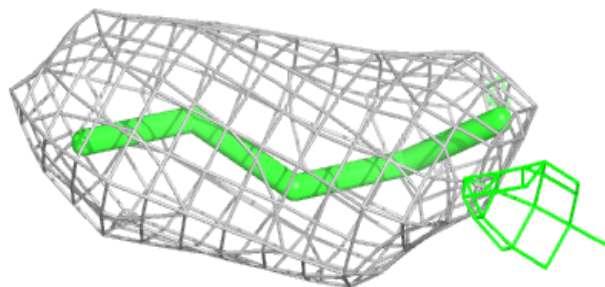
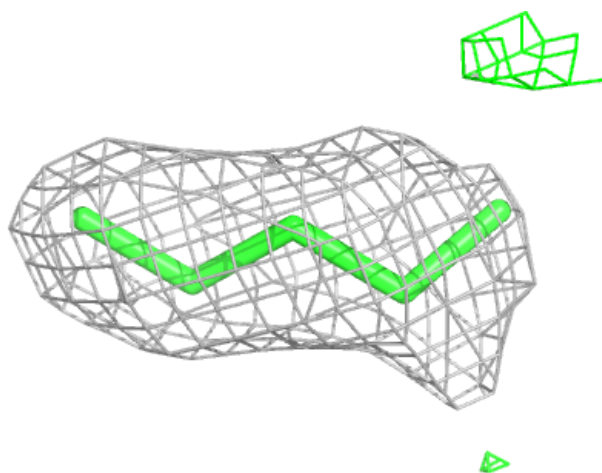
Electron density around BOG E 312:

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



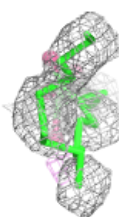
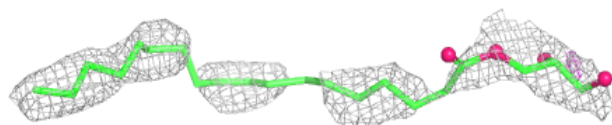
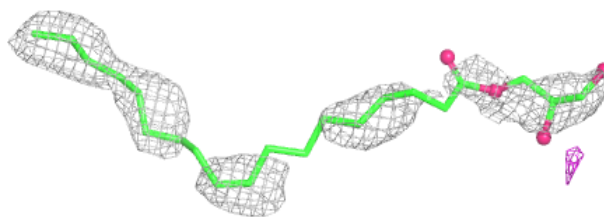
Electron density around LFA A 305:

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

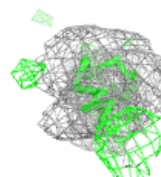
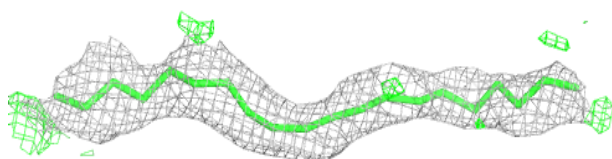
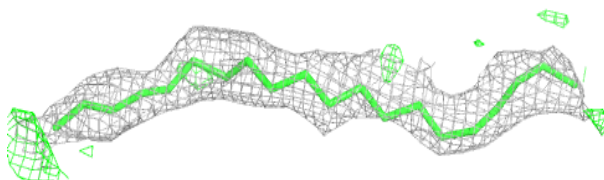


Electron density around OLC D 305:

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

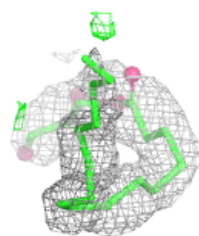
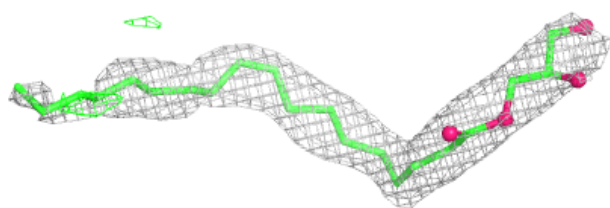
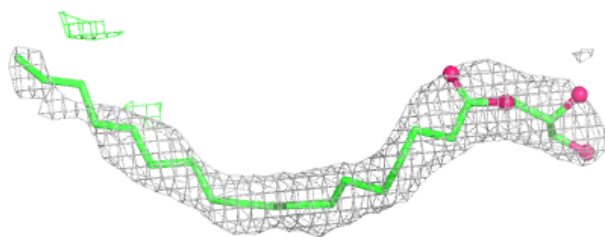
**Electron density around LFA D 307:**

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

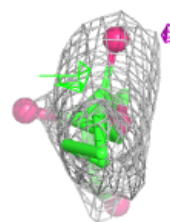
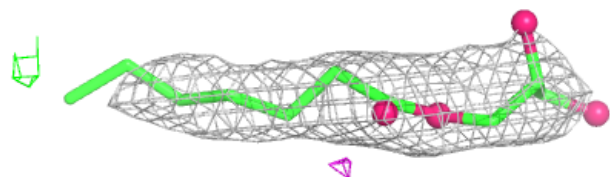
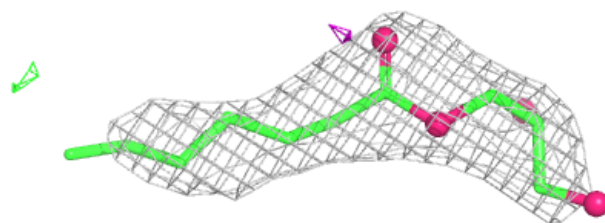


Electron density around OLC B 301:

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

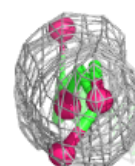
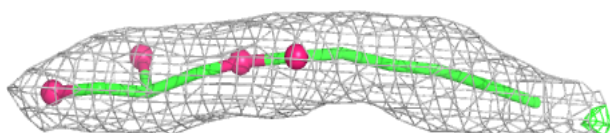
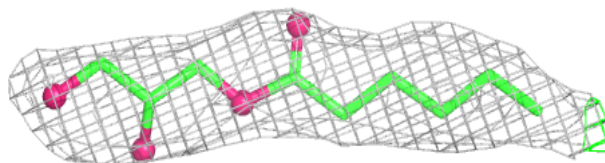
**Electron density around OLC D 304:**

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

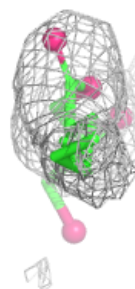
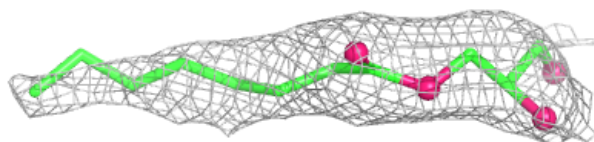
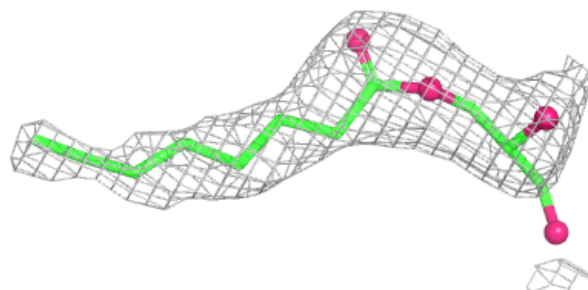


Electron density around OLC A 302:

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

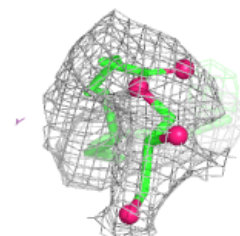
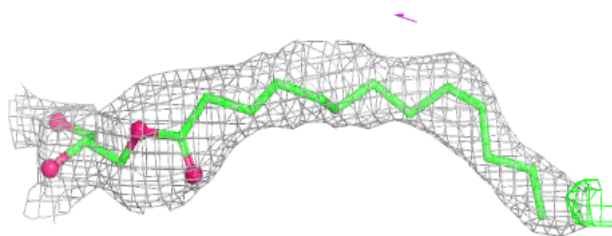
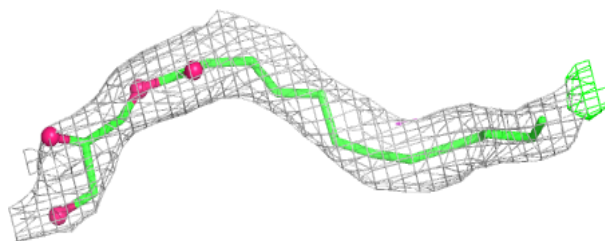
**Electron density around OLC A 303:**

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

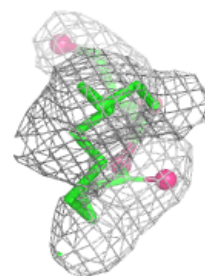
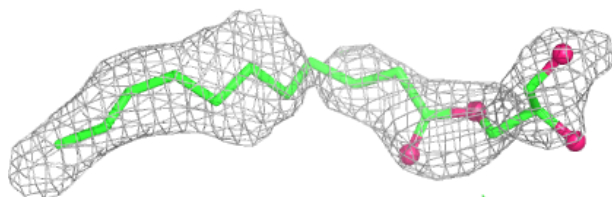
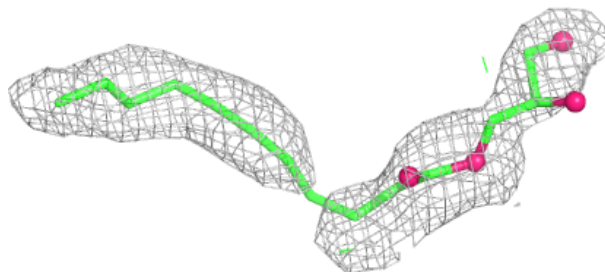


Electron density around OLC C 302:

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

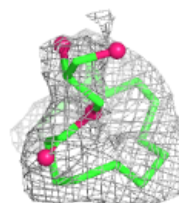
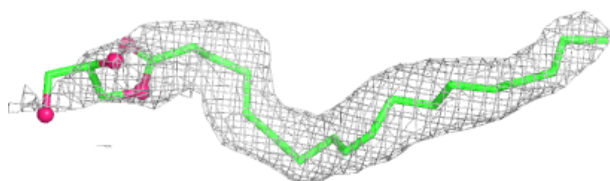
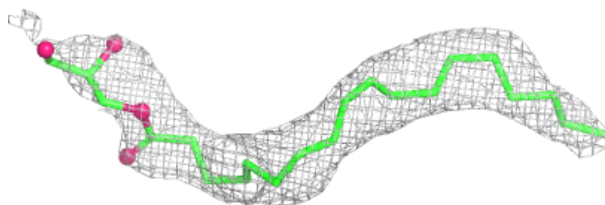
**Electron density around OLC C 306:**

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

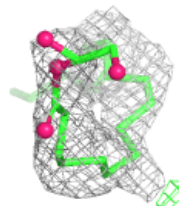
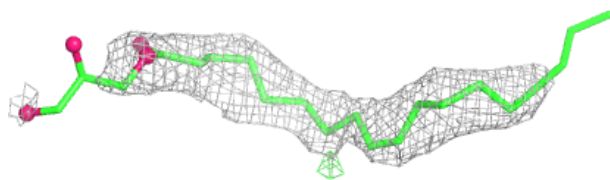
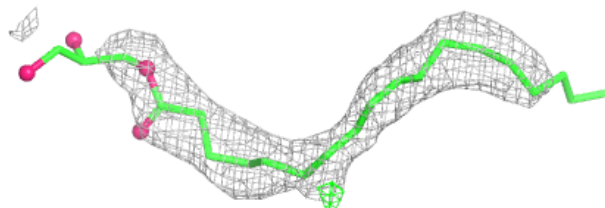


Electron density around OLC D 302:

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

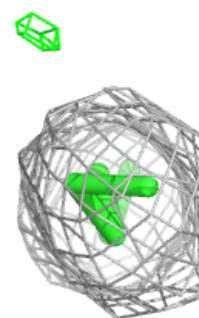
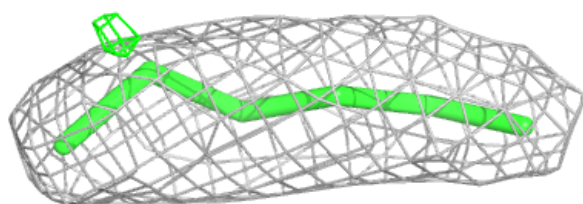
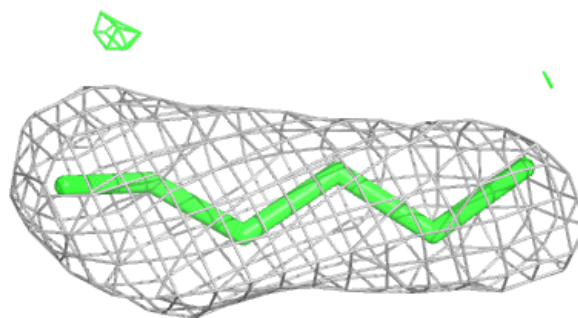
**Electron density around OLC E 302:**

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

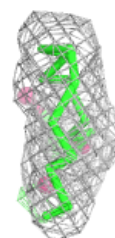
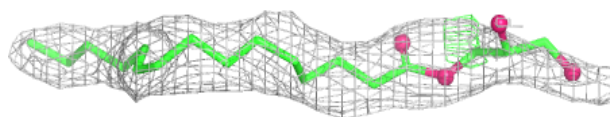
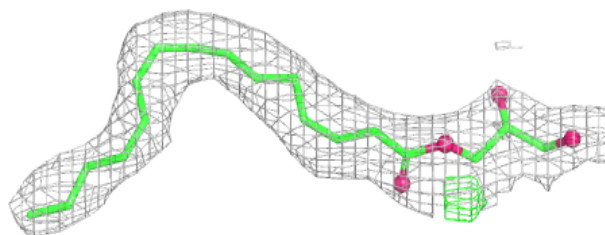


Electron density around LFA B 310:

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

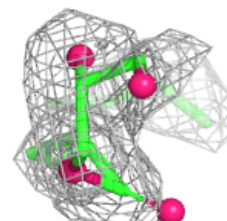
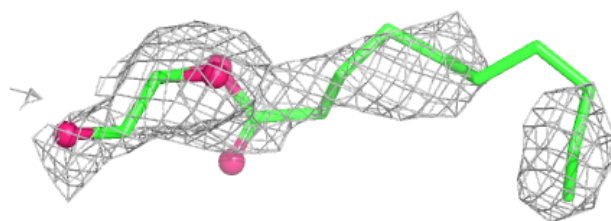
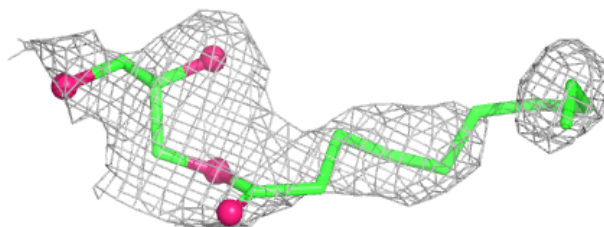
**Electron density around OLC A 301:**

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

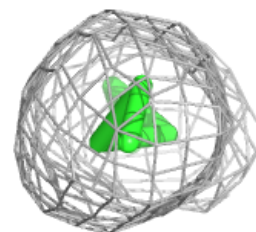
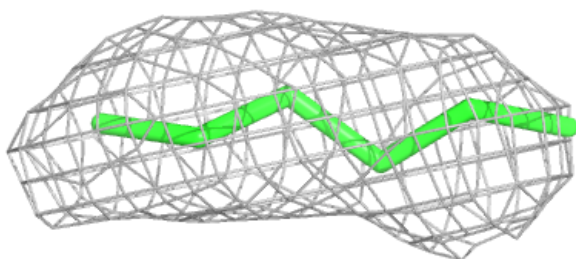
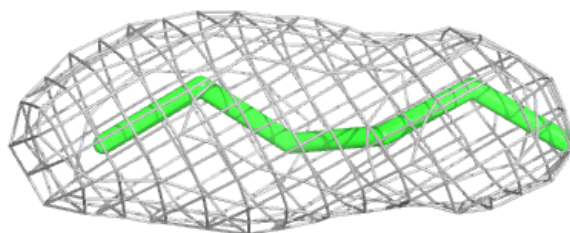


Electron density around OLC B 305:

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

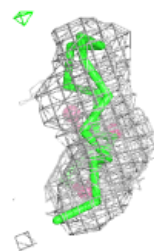
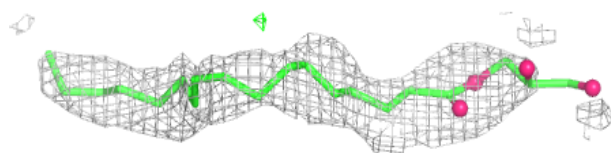
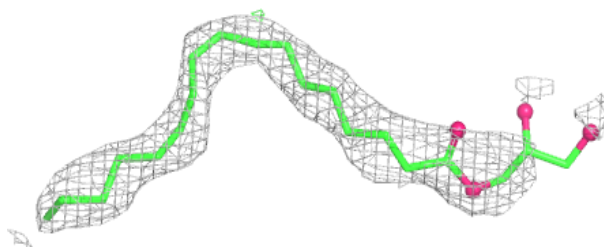
**Electron density around LFA A 308:**

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

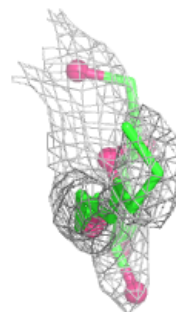
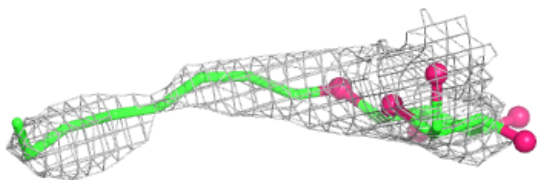
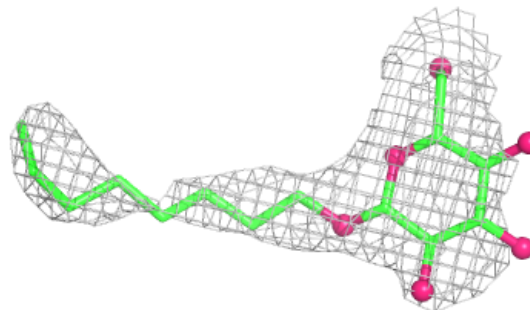


Electron density around OLC E 301:

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

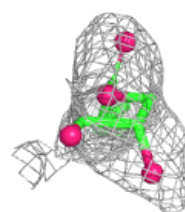
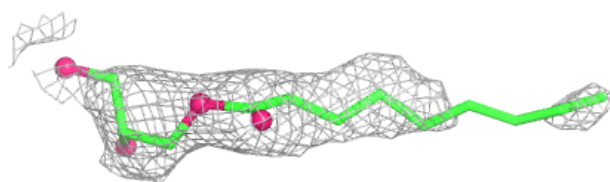
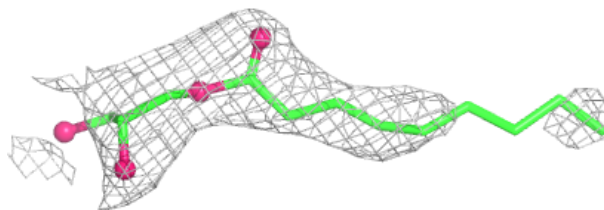
**Electron density around BOG D 314:**

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

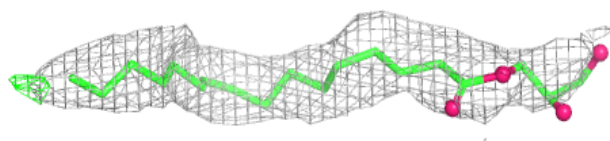
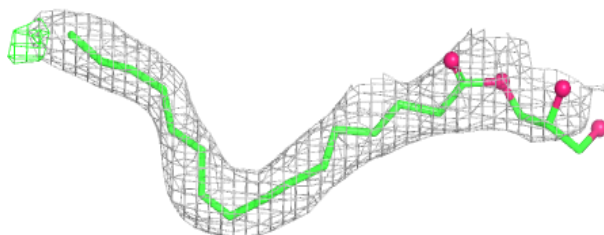


Electron density around OLC C 308:

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

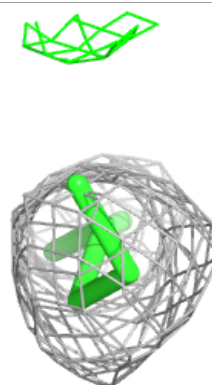
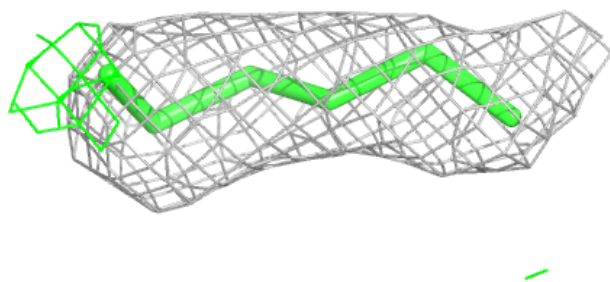
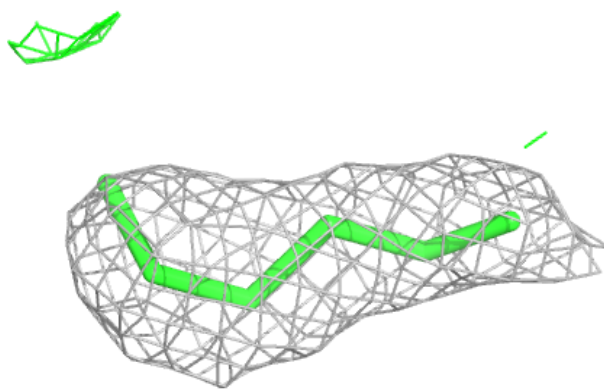
**Electron density around OLC C 305:**

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

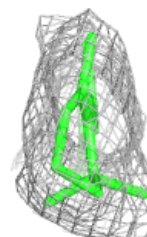
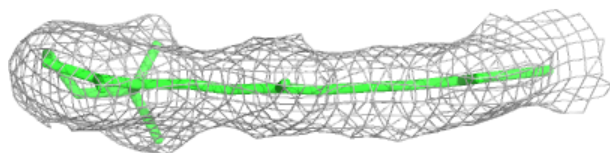
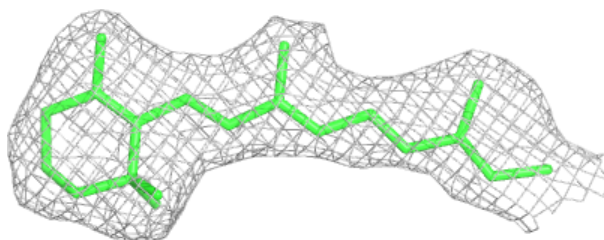


Electron density around LFA E 310:

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

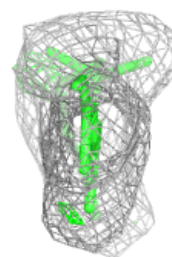
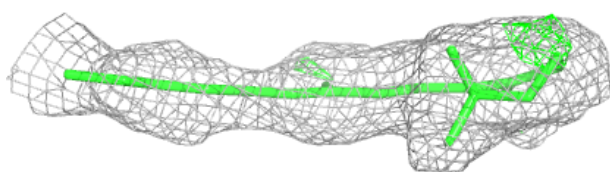
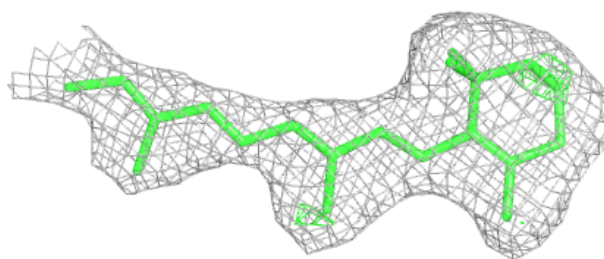
**Electron density around RET A 312:**

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

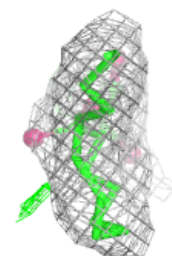
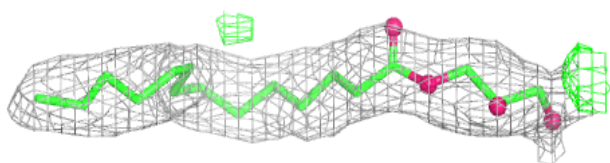
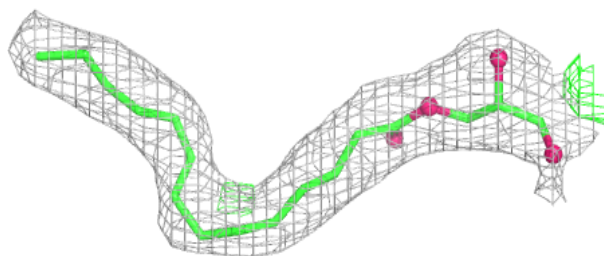


Electron density around RET E 315:

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

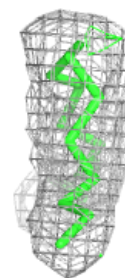
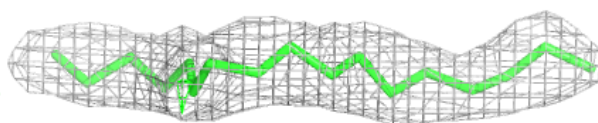
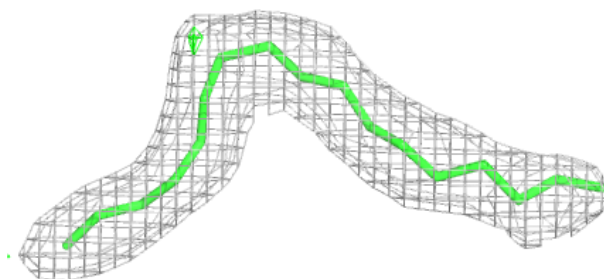
**Electron density around OLC C 301:**

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

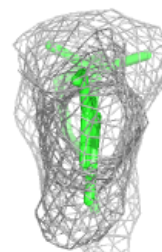
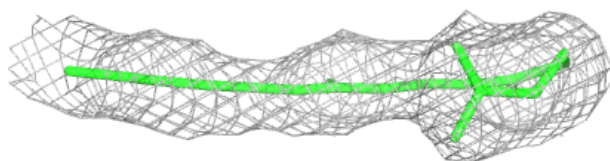
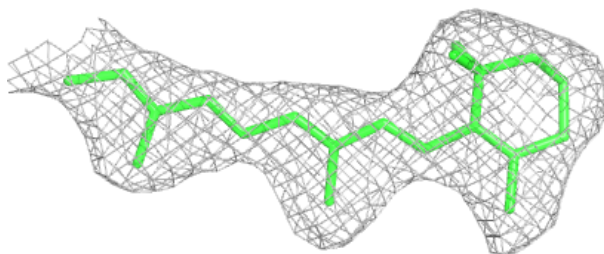


Electron density around LFA D 309:

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

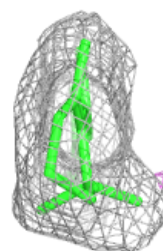
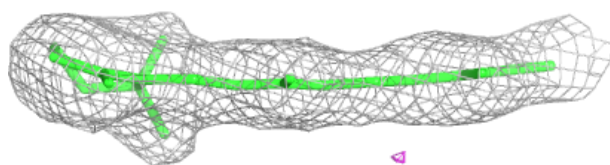
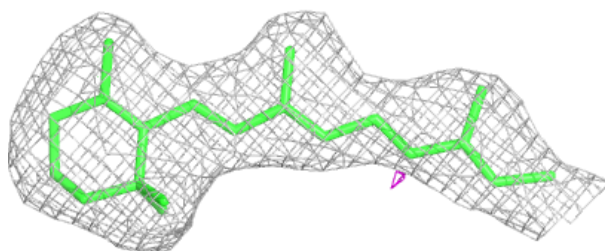
**Electron density around RET C 318:**

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

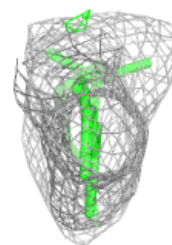
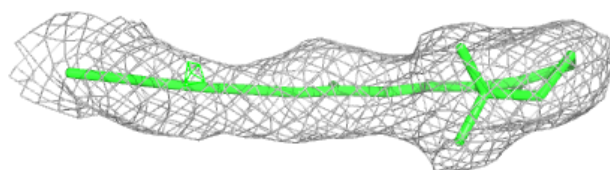
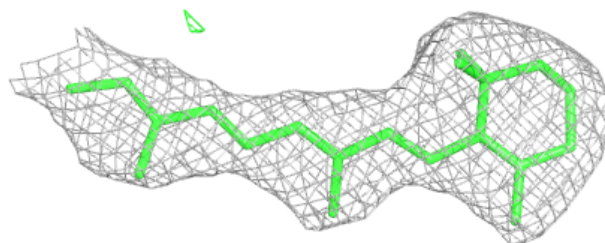


Electron density around RET B 313:

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

**Electron density around RET D 315:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.