



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 7, 2025 – 01:12 pm BST

PDB ID : 9I6H / pdb_00009i6h
Title : Room temperature structure of KR2 rhodopsin in pentameric form at 95% relative humidity
Authors : Zabelskii, D.; Round, E.; Han, H.; von Stetten, D.; Melo, D.; de Wijn, R.; Bean, R.; Round, A.
Deposited on : 2025-01-30
Resolution : 3.00 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

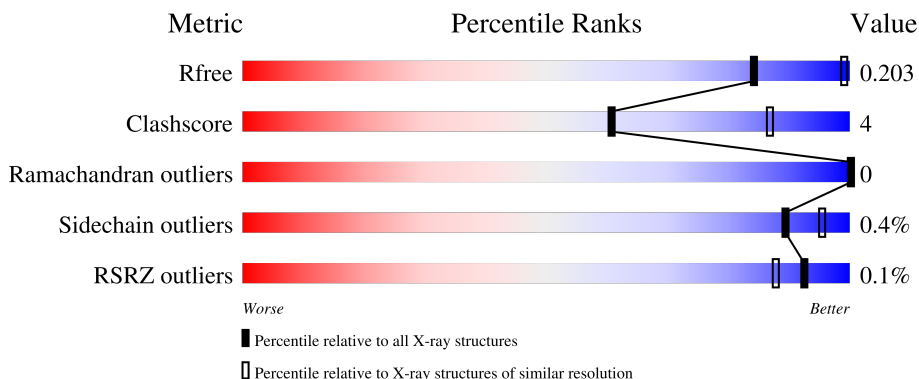
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	<div><div></div><div>90%</div><div>8%</div><div>.</div></div>
1	B	273	<div><div></div><div>91%</div><div>7%</div><div>.</div></div>
1	C	273	<div><div></div><div>89%</div><div>8%</div><div>.</div></div>
1	D	273	<div><div></div><div>89%</div><div>10%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	E	273	 A horizontal bar chart showing the quality of chain E. The bar is divided into three segments: a large green segment representing 86%, a smaller yellow segment representing 12%, and a very small grey segment at the end. A small black dot is visible at the far right end of the bar.

2 Entry composition [i](#)

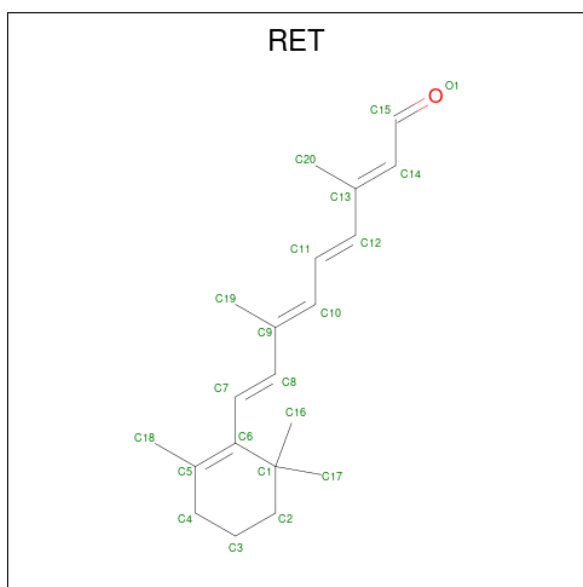
There are 6 unique types of molecules in this entry. The entry contains 11939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	269	Total	C	N	O	S	0	0	0
			2133	1424	322	378	9			
1	B	269	Total	C	N	O	S	0	0	0
			2130	1421	323	377	9			
1	C	268	Total	C	N	O	S	0	0	0
			2127	1420	321	377	9			
1	D	268	Total	C	N	O	S	0	0	0
			2120	1415	321	375	9			
1	E	268	Total	C	N	O	S	0	0	0
			2126	1419	322	376	9			

- Molecule 2 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

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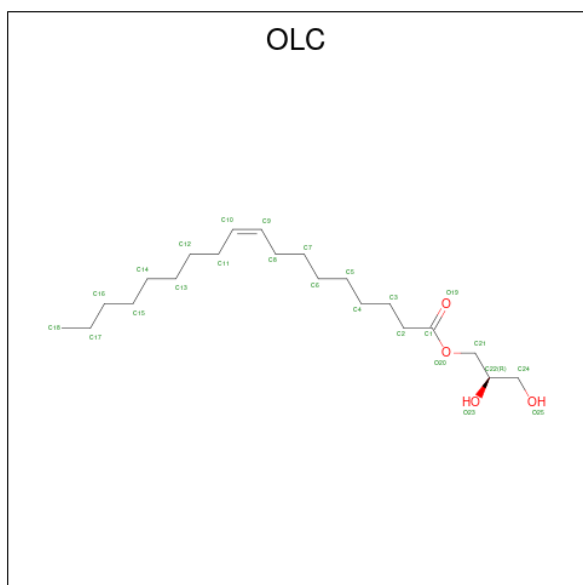
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 20 20	0	0
2	C	1	Total C 20 20	0	0
2	D	1	Total C 20 20	0	0
2	E	1	Total C 20 20	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



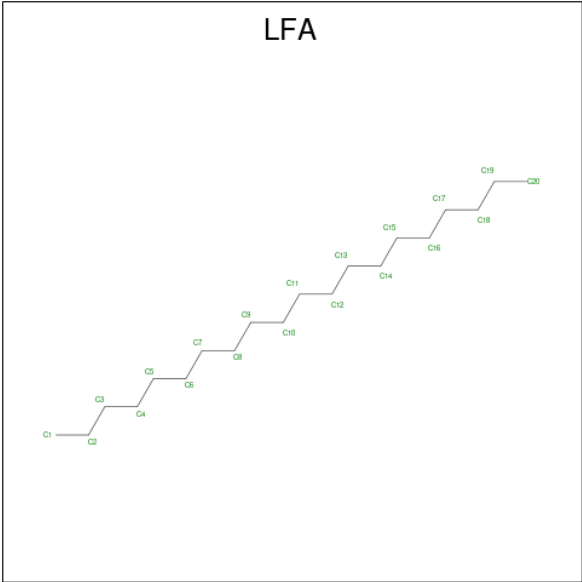
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C O 23 21 2	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C O 19 18 1	0	0
4	A	1	Total C O 23 21 2	0	0
4	A	1	Total C O 12 9 3	0	0
4	A	1	Total C O 20 19 1	0	0
4	A	1	Total C O 14 11 3	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C O 15 12 3	0	0
4	A	1	Total C O 19 18 1	0	0
4	A	1	Total C O 22 20 2	0	0
4	B	1	Total C O 20 17 3	0	0
4	B	1	Total C 13 13	0	0
4	B	1	Total C 14 14	0	0
4	B	1	Total C O 13 11 2	0	0
4	B	1	Total C O 20 17 3	0	0
4	B	1	Total C O 19 16 3	0	0
4	B	1	Total C O 17 15 2	0	0
4	C	1	Total C O 22 20 2	0	0
4	C	1	Total C O 22 19 3	0	0
4	C	1	Total C O 21 18 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 16 13 3	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C O 16 14 2	0	0
4	C	1	Total C O 15 12 3	0	0
4	C	1	Total C O 23 21 2	0	0
4	D	1	Total C O 17 14 3	0	0
4	D	1	Total C 18 18	0	0
4	D	1	Total C O 16 14 2	0	0
4	D	1	Total C O 13 10 3	0	0
4	D	1	Total C 7 7	0	0
4	D	1	Total C O 24 21 3	0	0
4	E	1	Total C 18 18	0	0
4	E	1	Total C 8 8	0	0
4	E	1	Total C 16 16	0	0
4	E	1	Total C O 19 16 3	0	0
4	E	1	Total C O 14 11 3	0	0
4	E	1	Total C 6 6	0	0
4	E	1	Total C O 19 17 2	0	0
4	E	1	Total C O 22 20 2	0	0
4	E	1	Total C O 18 17 1	0	0

- Molecule 5 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 7 7	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 4 4	0	0
5	A	1	Total C 6 6	0	0
5	A	1	Total C 16 16	0	0
5	A	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 8 8	0	0
5	B	1	Total C 10 10	0	0
5	B	1	Total C 7 7	0	0
5	B	1	Total C 11 11	0	0
5	B	1	Total C 11 11	0	0
5	C	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C 20 20	0	0
5	C	1	Total C 5 5	0	0
5	C	1	Total C 4 4	0	0
5	C	1	Total C 6 6	0	0
5	C	1	Total C 5 5	0	0
5	D	1	Total C 20 20	0	0
5	D	1	Total C 20 20	0	0
5	D	1	Total C 17 17	0	0
5	D	1	Total C 7 7	0	0
5	D	1	Total C 6 6	0	0
5	D	1	Total C 7 7	0	0
5	E	1	Total C 10 10	0	0
5	E	1	Total C 8 8	0	0
5	E	1	Total C 14 14	0	0
5	E	1	Total C 4 4	0	0
5	E	1	Total C 5 5	0	0
5	E	1	Total C 7 7	0	0
5	E	1	Total C 6 6	0	0
5	E	1	Total C 10 10	0	0


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total 34	O 34	0	0
6	B	45	Total 45	O 45	0	0
6	C	40	Total 40	O 40	0	0
6	D	43	Total 43	O 43	0	0
6	E	42	Total 42	O 42	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

Chain A:  90% 8% .




- Molecule 1: Sodium pumping rhodopsin

Chain B:  91% 7% .




- Molecule 1: Sodium pumping rhodopsin

Chain C:  89% 8% .



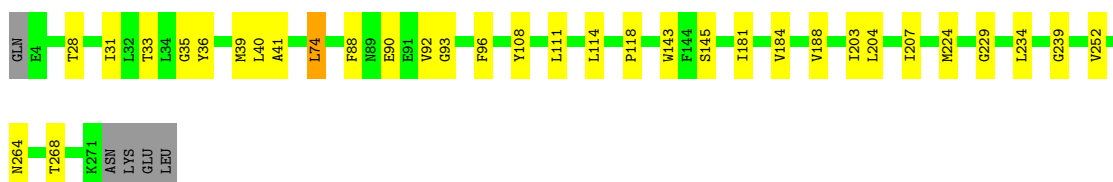
- Molecule 1: Sodium pumping rhodopsin

Chain D:  89% 10% .



- Molecule 1: Sodium pumping rhodopsin

Chain E:  86% 12% .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	136.10Å 240.90Å 138.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.25 – 3.00 69.25 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (69.25-3.00) 99.9 (69.25-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.171 , 0.203 0.171 , 0.203	Depositor DCC
R_{free} test set	2305 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.006 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	11939	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LFA, RET, NA, 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	0.18	0/2191	0.34	0/2981
1	B	0.19	0/2188	0.35	0/2977
1	C	0.20	0/2185	0.38	0/2973
1	D	0.19	0/2178	0.36	0/2965
1	E	0.23	0/2184	0.39	0/2971
All	All	0.20	0/10926	0.36	0/14867

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2133	0	2104	15	0
1	B	2130	0	2106	14	0
1	C	2127	0	2100	18	0
1	D	2120	0	2090	17	0
1	E	2126	0	2105	23	0
2	A	20	0	27	0	0
2	B	20	0	27	1	0
2	C	20	0	27	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	20	0	27	1	0
2	E	20	0	27	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	199	0	299	6	0
4	B	116	0	166	5	0
4	C	141	0	207	9	0
4	D	95	0	144	5	0
4	E	140	0	213	8	0
5	A	58	0	109	0	0
5	B	56	0	103	1	0
5	C	48	0	87	0	0
5	D	77	0	151	1	0
5	E	64	0	117	2	0
6	A	34	0	0	0	0
6	B	45	0	0	1	0
6	C	40	0	0	0	0
6	D	43	0	0	0	0
6	E	42	0	0	0	0
All	All	11939	0	12236	98	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 4.

The worst 5 of 98 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:C:74:LEU:HD21	1:C:108:TYR:HB3	1.63	0.79
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.80	0.64
4:C:303:OLC:H16A	4:E:318:OLC:H14	1.87	0.55
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.89	0.55
1:B:88:PHE:CZ	1:B:93:GLY:HA2	2.42	0.54

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	267/273 (98%)	260 (97%)	7 (3%)	0	100	100
1	B	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
1	C	266/273 (97%)	258 (97%)	8 (3%)	0	100	100
1	D	266/273 (97%)	259 (97%)	7 (3%)	0	100	100
1	E	266/273 (97%)	259 (97%)	7 (3%)	0	100	100
All	All	1332/1365 (98%)	1297 (97%)	35 (3%)	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	224/234 (96%)	222 (99%)	2 (1%)	75	89
1	B	225/234 (96%)	225 (100%)	0	100	100
1	C	224/234 (96%)	223 (100%)	1 (0%)	89	95
1	D	223/234 (95%)	223 (100%)	0	100	100
1	E	225/234 (96%)	223 (99%)	2 (1%)	75	89
All	All	1121/1170 (96%)	1116 (100%)	5 (0%)	89	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	91	GLU
1	C	74	LEU
1	E	74	LEU
1	E	90	GLU

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	E	112	ASN
1	E	141	GLN
1	C	123	GLN
1	C	141	GLN
1	D	123	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 5 are monoatomic - leaving 80 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
5	LFA	C	310	-	4,4,19	0.32	0	3,3,18	0.55	0
4	OLC	A	319	-	18,18,24	0.84	0	17,17,25	1.26	1 (5%)
4	OLC	D	307	-	6,6,24	0.81	0	5,5,25	0.65	0
5	LFA	E	312	-	13,13,19	0.30	0	12,12,18	0.82	0
4	OLC	C	307	-	5,5,24	0.83	0	4,4,25	0.54	0
4	OLC	C	312	-	15,15,24	0.87	0	14,14,25	1.30	2 (14%)
5	LFA	B	310	-	6,6,19	0.30	0	5,5,18	0.68	0
4	OLC	A	309	-	19,19,24	0.83	0	18,18,25	1.34	2 (11%)
4	OLC	D	305	-	15,15,24	0.88	0	14,14,25	1.26	1 (7%)
4	OLC	A	307	-	22,22,24	0.79	0	21,21,25	1.24	1 (4%)
4	OLC	C	316	-	22,22,24	0.79	0	21,21,25	1.26	1 (4%)
4	OLC	B	305	-	13,13,24	0.89	0	12,12,25	1.34	1 (8%)
4	OLC	B	306	-	12,12,24	0.77	0	11,11,25	0.94	0
5	LFA	E	311	-	7,7,19	0.31	0	6,6,18	0.73	0
4	OLC	A	304	-	22,22,24	0.79	0	21,21,25	1.25	2 (9%)
4	OLC	C	315	-	14,14,24	0.79	0	14,14,25	0.80	0
4	OLC	A	305	-	8,8,24	0.95	0	6,7,25	0.92	0
5	LFA	E	303	-	9,9,19	0.30	0	8,8,18	0.80	0
4	OLC	D	304	-	17,17,24	0.84	0	16,16,25	1.26	1 (6%)
5	LFA	B	307	-	8,8,19	0.31	0	7,7,18	0.73	0
4	OLC	A	306	-	18,18,24	0.82	0	17,17,25	1.27	1 (5%)
4	OLC	C	303	-	21,21,24	0.80	0	20,20,25	1.32	2 (10%)
4	OLC	E	309	-	5,5,24	0.81	0	4,4,25	0.54	0
5	LFA	A	314	-	7,7,19	0.31	0	6,6,18	0.73	0
4	OLC	A	311	-	6,6,24	0.84	0	5,5,25	0.62	0
5	LFA	C	308	-	7,7,19	0.31	0	6,6,18	0.72	0
5	LFA	C	309	-	19,19,19	0.29	0	18,18,18	0.88	0
5	LFA	A	316	-	3,3,19	0.41	0	2,2,18	0.74	0
5	LFA	B	313	-	10,10,19	0.30	0	9,9,18	0.77	0
2	RET	A	301	1	20,20,21	0.62	0	27,27,28	1.40	5 (18%)
5	LFA	D	313	-	5,5,19	0.31	0	4,4,18	0.59	0
4	OLC	A	303	-	15,15,24	0.87	0	14,14,25	1.33	2 (14%)
5	LFA	E	313	-	3,3,19	0.41	0	2,2,18	0.73	0
4	OLC	C	306	-	15,15,24	0.91	0	15,15,25	1.27	1 (6%)
4	OLC	D	308	-	23,23,24	0.82	0	23,23,25	1.14	1 (4%)
5	LFA	C	314	-	4,4,19	0.32	0	3,3,18	0.55	0
4	OLC	A	310	-	13,13,24	0.77	0	13,13,25	0.78	0
5	LFA	C	311	-	3,3,19	0.41	0	2,2,18	0.74	0
5	LFA	D	312	-	6,6,19	0.31	0	5,5,18	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LFA	D	314	-	6,6,19	0.31	0	5,5,18	0.65	0
5	LFA	D	310	-	19,19,19	0.29	0	18,18,18	0.92	0
4	OLC	E	319	-	17,17,24	0.85	0	16,16,25	1.30	1 (6%)
2	RET	C	301	1	20,20,21	0.64	0	27,27,28	1.38	5 (18%)
5	LFA	C	313	-	5,5,19	0.31	0	4,4,18	0.57	0
4	OLC	E	310	-	18,18,24	0.82	0	17,17,25	1.33	1 (5%)
5	LFA	D	311	-	16,16,19	0.29	0	15,15,18	0.88	0
4	OLC	B	303	-	19,19,24	0.85	0	19,19,25	1.20	1 (5%)
4	OLC	E	306	-	15,15,24	0.86	0	14,14,25	1.30	1 (7%)
4	OLC	E	308	-	13,13,24	0.77	0	13,13,25	0.77	0
4	OLC	D	303	-	16,16,24	0.89	0	16,16,25	1.14	1 (6%)
5	LFA	A	318	-	15,15,19	0.30	0	14,14,18	0.87	0
5	LFA	E	314	-	4,4,19	0.32	0	3,3,18	0.55	0
2	RET	D	301	1	20,20,21	0.64	0	27,27,28	1.36	5 (18%)
5	LFA	A	317	-	5,5,19	0.31	0	4,4,18	0.57	0
2	RET	E	301	-	20,20,21	0.64	0	27,27,28	1.46	5 (18%)
2	RET	B	301	1	20,20,21	0.65	0	27,27,28	1.38	5 (18%)
5	LFA	E	316	-	5,5,19	0.31	0	4,4,18	0.57	0
5	LFA	A	313	-	6,6,19	0.31	0	5,5,18	0.65	0
5	LFA	E	317	-	9,9,19	0.31	0	8,8,18	0.74	0
5	LFA	A	315	-	7,7,19	0.31	0	6,6,18	0.71	0
4	OLC	C	305	-	20,20,24	0.84	0	20,20,25	1.14	1 (5%)
5	LFA	B	314	-	10,10,19	0.30	0	9,9,18	0.81	0
4	OLC	E	318	-	21,21,24	0.79	0	20,20,25	1.24	1 (5%)
4	OLC	B	304	-	12,12,24	0.89	0	11,11,25	1.37	1 (9%)
4	OLC	D	306	-	12,12,24	0.75	0	12,12,25	0.77	0
4	OLC	A	308	-	11,11,24	0.74	0	11,11,25	0.74	0
5	LFA	E	315	-	6,6,19	0.31	0	5,5,18	0.67	0
4	OLC	E	307	-	18,18,24	0.83	0	18,18,25	1.19	1 (5%)
4	OLC	C	304	-	21,21,24	0.83	0	21,21,25	1.16	1 (4%)
4	OLC	B	315	-	16,16,24	0.85	0	14,15,25	1.39	2 (14%)
4	OLC	B	312	-	18,18,24	0.84	0	18,18,25	1.20	1 (5%)
5	LFA	D	309	-	19,19,19	0.28	0	18,18,18	0.91	0
4	OLC	E	305	-	7,7,24	0.83	0	6,6,25	0.70	0
5	LFA	B	308	-	7,7,19	0.31	0	6,6,18	0.72	0
4	OLC	A	321	-	21,21,24	0.80	0	20,20,25	1.27	2 (10%)
4	OLC	A	312	-	14,14,24	0.79	0	14,14,25	0.79	0
5	LFA	A	320	-	8,8,19	0.29	0	7,7,18	0.78	0
5	LFA	B	309	-	9,9,19	0.31	0	8,8,18	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLC	B	311	-	19,19,24	0.84	0	19,19,25	1.17	1 (5%)
4	OLC	E	304	-	17,17,24	0.85	0	16,16,25	1.23	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LFA	C	310	-	-	2/2/2/17	-
4	OLC	A	319	-	-	11/16/16/24	-
4	OLC	D	307	-	-	2/4/4/24	-
5	LFA	E	312	-	-	2/11/11/17	-
4	OLC	C	307	-	-	1/3/3/24	-
4	OLC	C	312	-	-	8/13/13/24	-
5	LFA	B	310	-	-	2/4/4/17	-
4	OLC	A	309	-	-	8/17/17/24	-
4	OLC	D	305	-	-	6/13/13/24	-
4	OLC	A	307	-	-	14/20/20/24	-
4	OLC	C	316	-	-	9/20/20/24	-
4	OLC	B	305	-	-	3/11/11/24	-
4	OLC	B	306	-	-	7/10/10/24	-
5	LFA	E	311	-	-	1/5/5/17	-
4	OLC	A	304	-	-	10/20/20/24	-
4	OLC	C	315	-	-	7/13/13/24	-
4	OLC	A	305	-	-	3/6/6/24	-
5	LFA	E	303	-	-	3/7/7/17	-
4	OLC	D	304	-	-	6/15/15/24	-
5	LFA	B	307	-	-	3/6/6/17	-
4	OLC	A	306	-	-	12/16/16/24	-
4	OLC	C	303	-	-	8/19/19/24	-
4	OLC	E	309	-	-	1/3/3/24	-
5	LFA	A	314	-	-	4/5/5/17	-
4	OLC	A	311	-	-	3/4/4/24	-
5	LFA	C	308	-	-	2/5/5/17	-
5	LFA	C	309	-	-	7/17/17/17	-
5	LFA	A	316	-	-	0/1/1/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LFA	B	313	-	-	6/8/8/17	-
2	RET	A	301	1	-	4/13/30/31	0/1/1/1
5	LFA	D	313	-	-	0/3/3/17	-
4	OLC	A	303	-	-	8/13/13/24	-
5	LFA	E	313	-	-	1/1/1/17	-
4	OLC	C	306	-	-	9/14/14/24	-
4	OLC	D	308	-	-	8/22/22/24	-
5	LFA	C	314	-	-	0/2/2/17	-
4	OLC	A	310	-	-	5/12/12/24	-
5	LFA	C	311	-	-	1/1/1/17	-
5	LFA	D	312	-	-	0/4/4/17	-
5	LFA	D	314	-	-	2/4/4/17	-
5	LFA	D	310	-	-	4/17/17/17	-
4	OLC	E	319	-	-	8/15/15/24	-
2	RET	C	301	1	-	4/13/30/31	0/1/1/1
5	LFA	C	313	-	-	0/3/3/17	-
4	OLC	E	310	-	-	7/16/16/24	-
5	LFA	D	311	-	-	7/14/14/17	-
4	OLC	B	303	-	-	13/18/18/24	-
4	OLC	E	306	-	-	6/13/13/24	-
4	OLC	E	308	-	-	9/12/12/24	-
4	OLC	D	303	-	-	4/15/15/24	-
5	LFA	A	318	-	-	4/13/13/17	-
5	LFA	E	314	-	-	0/2/2/17	-
2	RET	D	301	1	-	4/13/30/31	0/1/1/1
5	LFA	A	317	-	-	1/3/3/17	-
2	RET	E	301	-	-	1/13/30/31	0/1/1/1
2	RET	B	301	1	-	4/13/30/31	0/1/1/1
5	LFA	E	316	-	-	2/3/3/17	-
5	LFA	A	313	-	-	2/4/4/17	-
5	LFA	E	317	-	-	1/7/7/17	-
5	LFA	A	315	-	-	0/5/5/17	-
4	OLC	C	305	-	-	11/19/19/24	-
5	LFA	B	314	-	-	4/8/8/17	-
4	OLC	E	318	-	-	9/19/19/24	-
4	OLC	B	304	-	-	4/10/10/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLC	D	306	-	-	7/11/11/24	-
4	OLC	A	308	-	-	3/10/10/24	-
5	LFA	E	315	-	-	1/4/4/17	-
4	OLC	E	307	-	-	10/17/17/24	-
4	OLC	C	304	-	-	15/20/20/24	-
4	OLC	B	315	-	-	7/14/14/24	-
4	OLC	B	312	-	-	10/17/17/24	-
5	LFA	D	309	-	-	9/17/17/17	-
4	OLC	E	305	-	-	4/5/5/24	-
5	LFA	B	308	-	-	2/5/5/17	-
4	OLC	A	321	-	-	12/19/19/24	-
4	OLC	A	312	-	-	8/13/13/24	-
5	LFA	A	320	-	-	0/6/6/17	-
5	LFA	B	309	-	-	3/7/7/17	-
4	OLC	B	311	-	-	9/18/18/24	-
4	OLC	E	304	-	-	9/15/15/24	-

There are no bond length outliers.

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	306	OLC	C8-C9-C10	3.79	152.61	126.84
4	B	303	OLC	C8-C9-C10	3.77	153.65	124.73
4	A	319	OLC	C8-C9-C10	3.74	153.45	124.73
4	C	303	OLC	C8-C9-C10	3.69	153.01	124.73
4	E	319	OLC	C8-C9-C10	3.68	152.97	124.73

There are no chirality outliers.

5 of 407 torsion outliers are listed below:

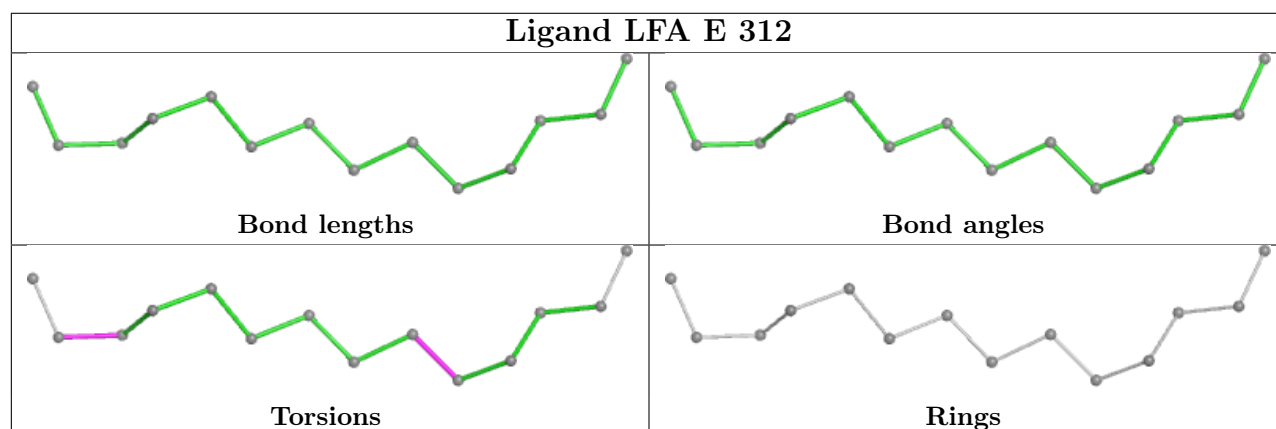
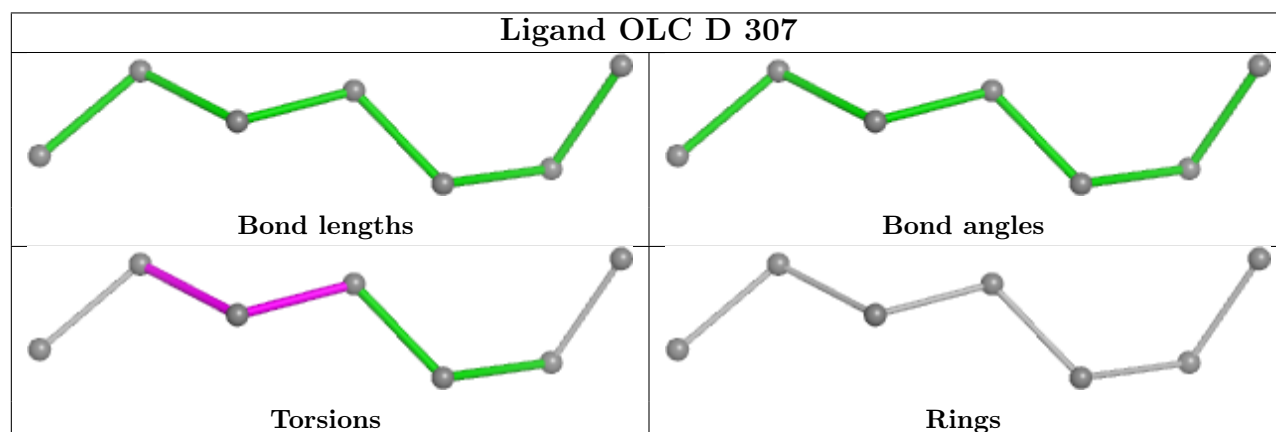
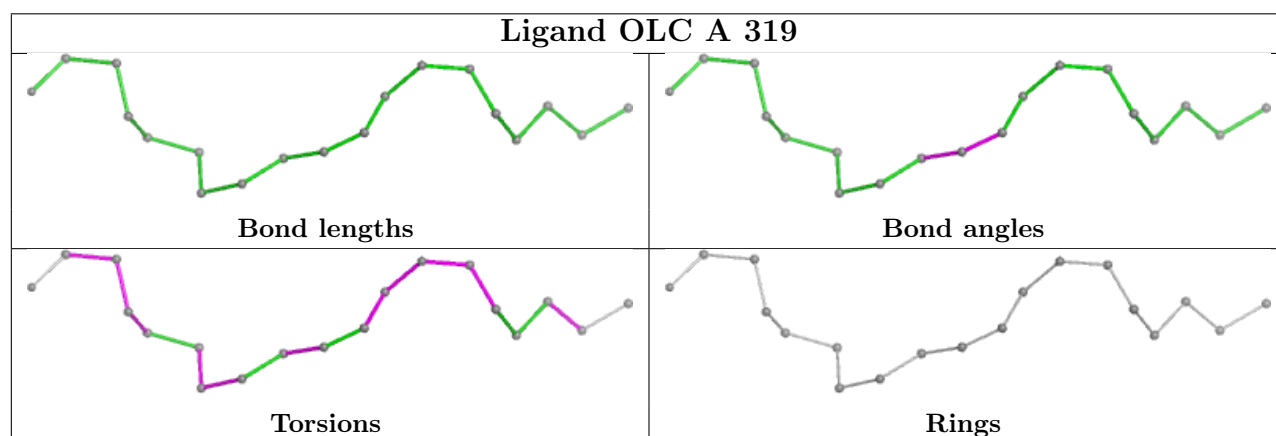
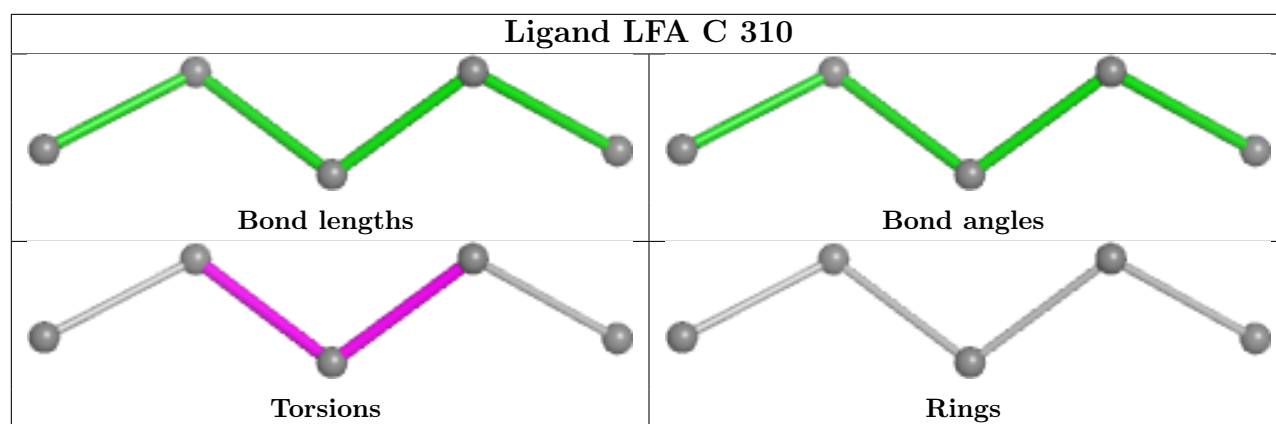
Mol	Chain	Res	Type	Atoms
4	A	303	OLC	C21-C22-C24-O25
4	A	304	OLC	C21-C22-C24-O25
4	A	309	OLC	C2-C1-O20-C21
4	A	312	OLC	C21-C22-C24-O25
4	B	312	OLC	O20-C21-C22-C24

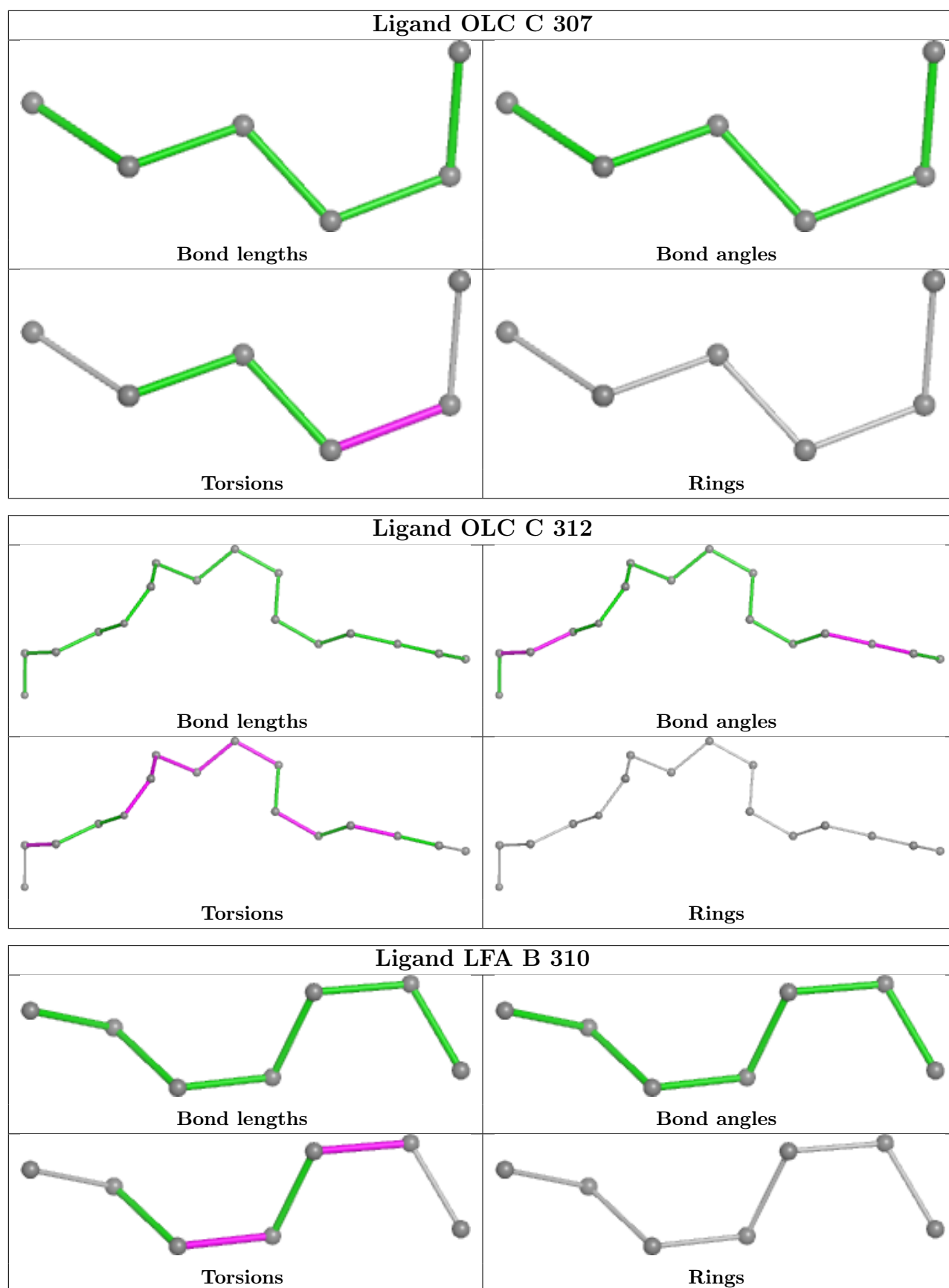
There are no ring outliers.

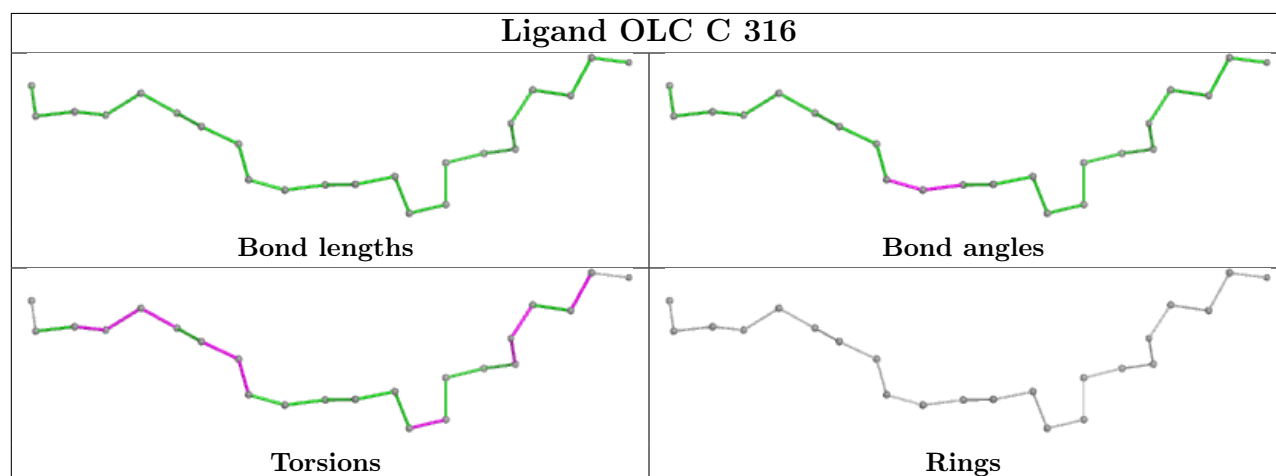
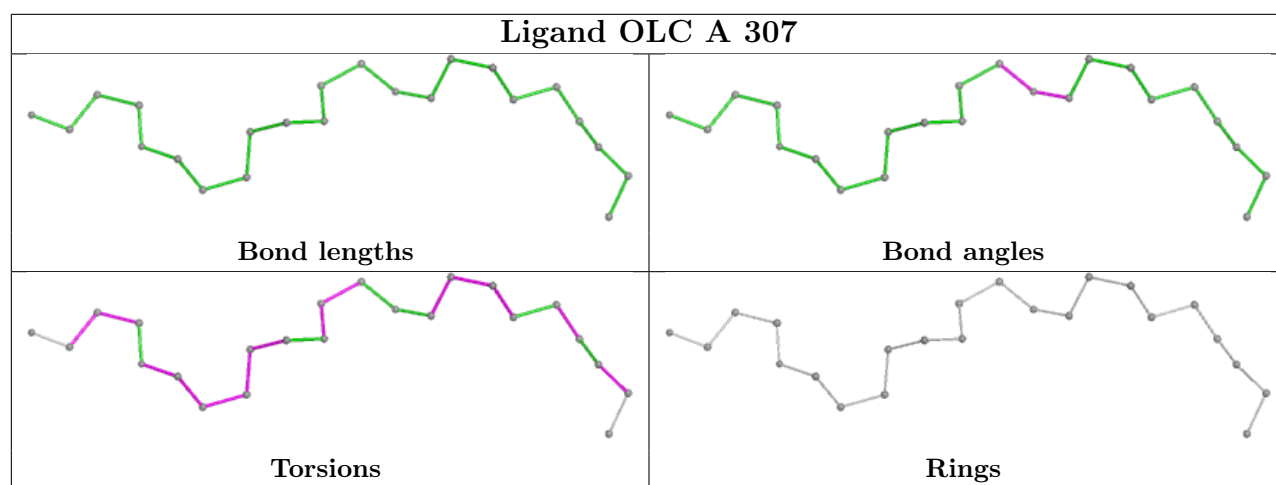
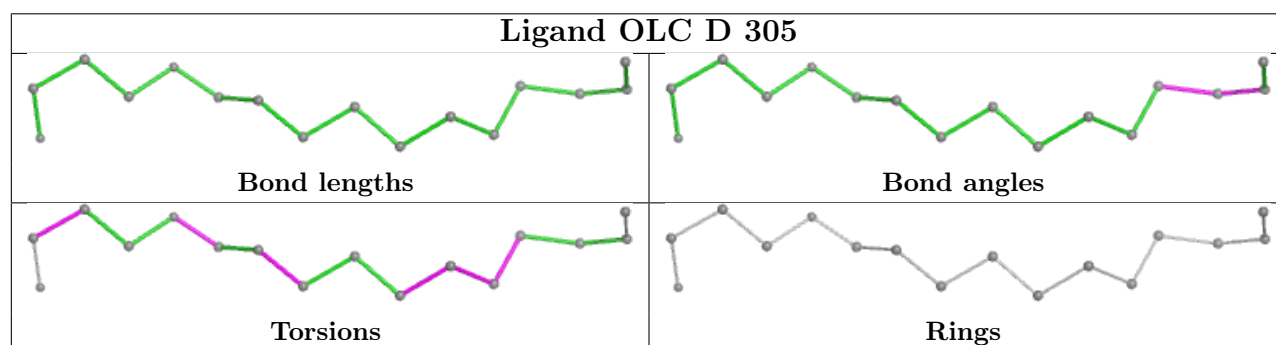
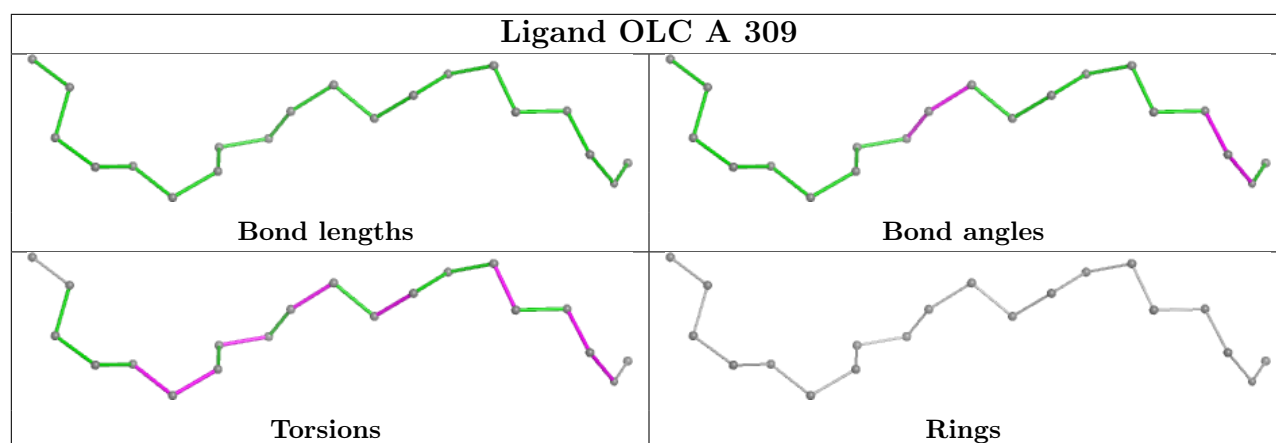
28 monomers are involved in 38 short contacts:

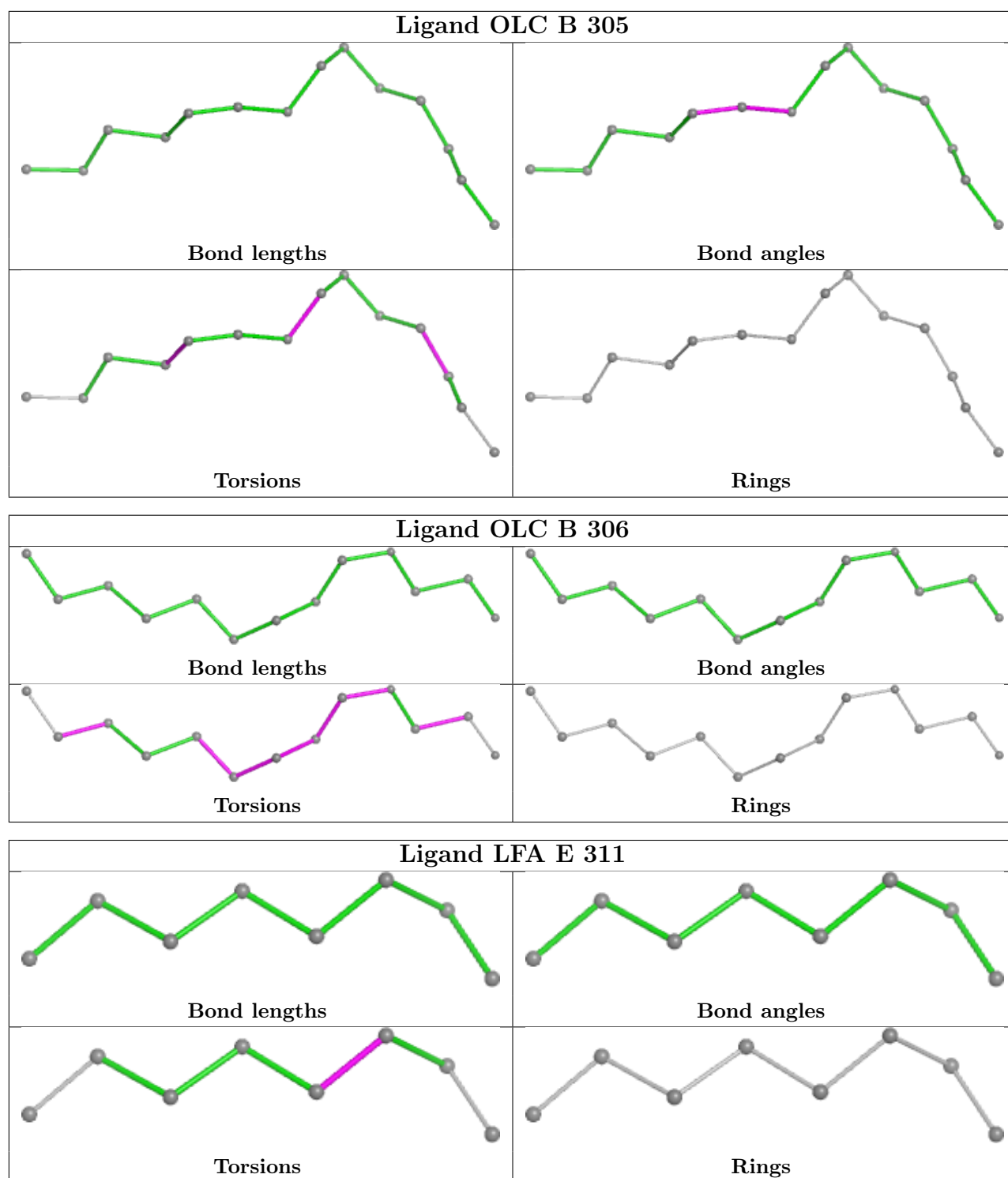
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	312	LFA	1	0
4	C	312	OLC	2	0
4	D	305	OLC	1	0
4	C	316	OLC	2	0
4	A	304	OLC	1	0
4	A	305	OLC	1	0
5	B	307	LFA	1	0
4	A	306	OLC	2	0
4	C	303	OLC	3	0
4	A	311	OLC	1	0
4	D	308	OLC	3	0
5	D	312	LFA	1	0
4	E	319	OLC	1	0
2	C	301	RET	2	0
4	B	303	OLC	1	0
2	D	301	RET	1	0
2	E	301	RET	1	0
2	B	301	RET	1	0
5	E	316	LFA	1	0
4	E	318	OLC	4	0
4	D	306	OLC	1	0
4	A	308	OLC	1	0
4	C	304	OLC	3	0
4	B	315	OLC	1	0
4	B	312	OLC	2	0
4	E	305	OLC	1	0
4	B	311	OLC	2	0
4	E	304	OLC	2	0

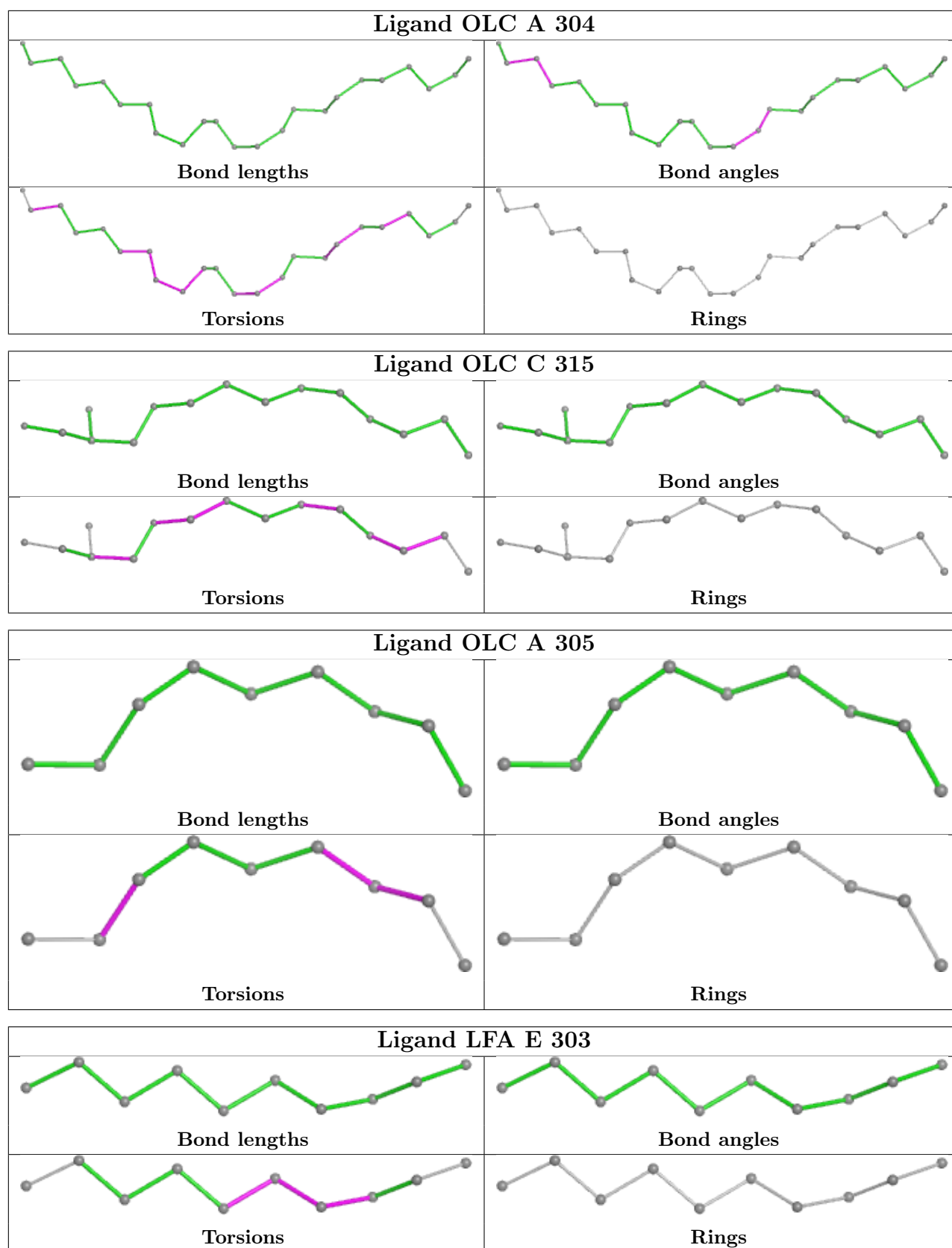
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

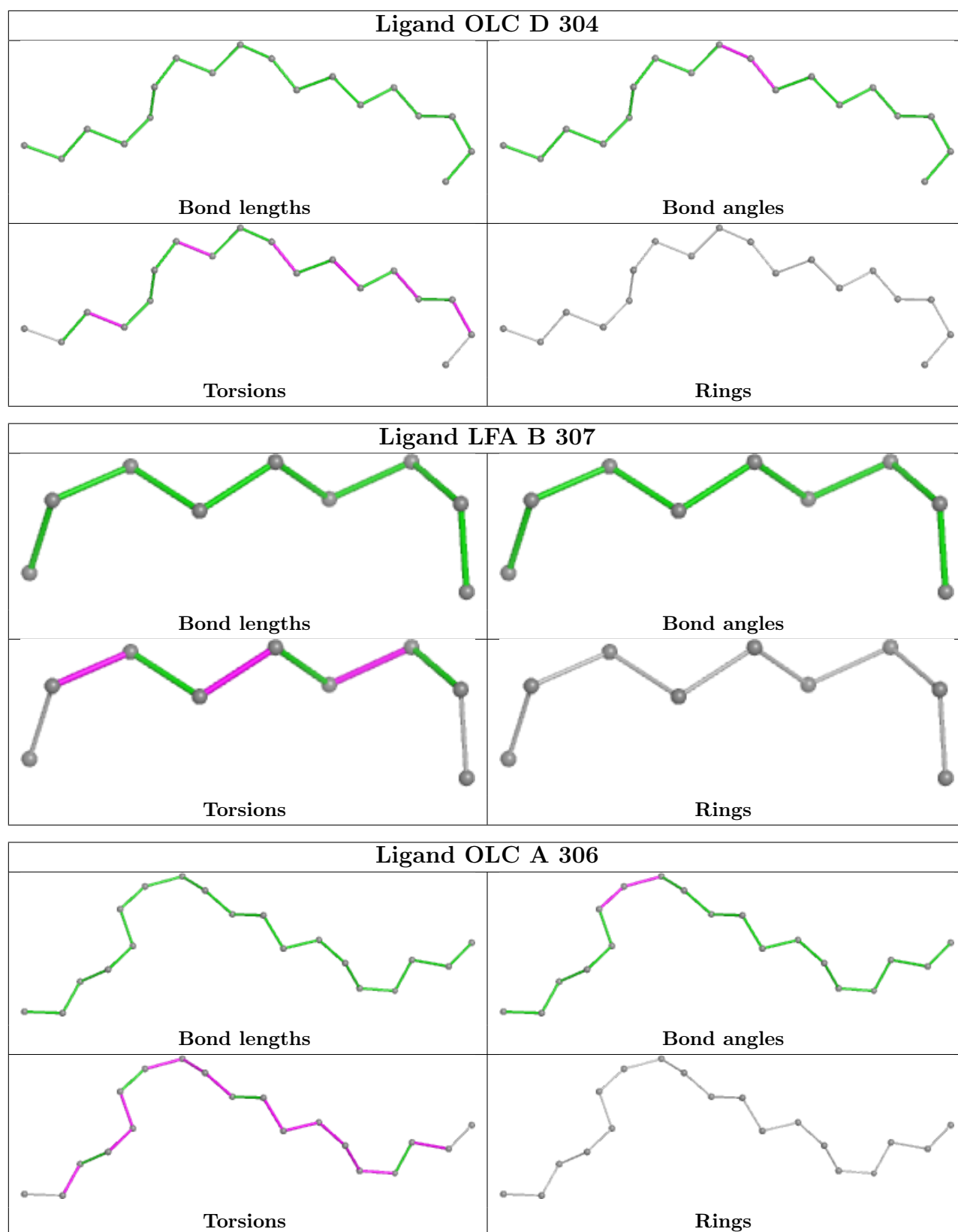


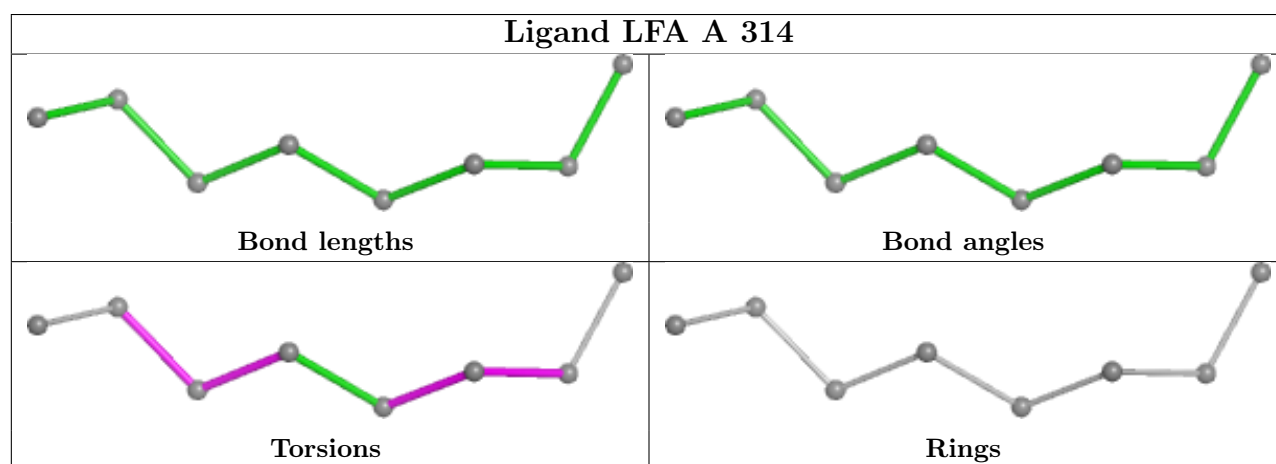
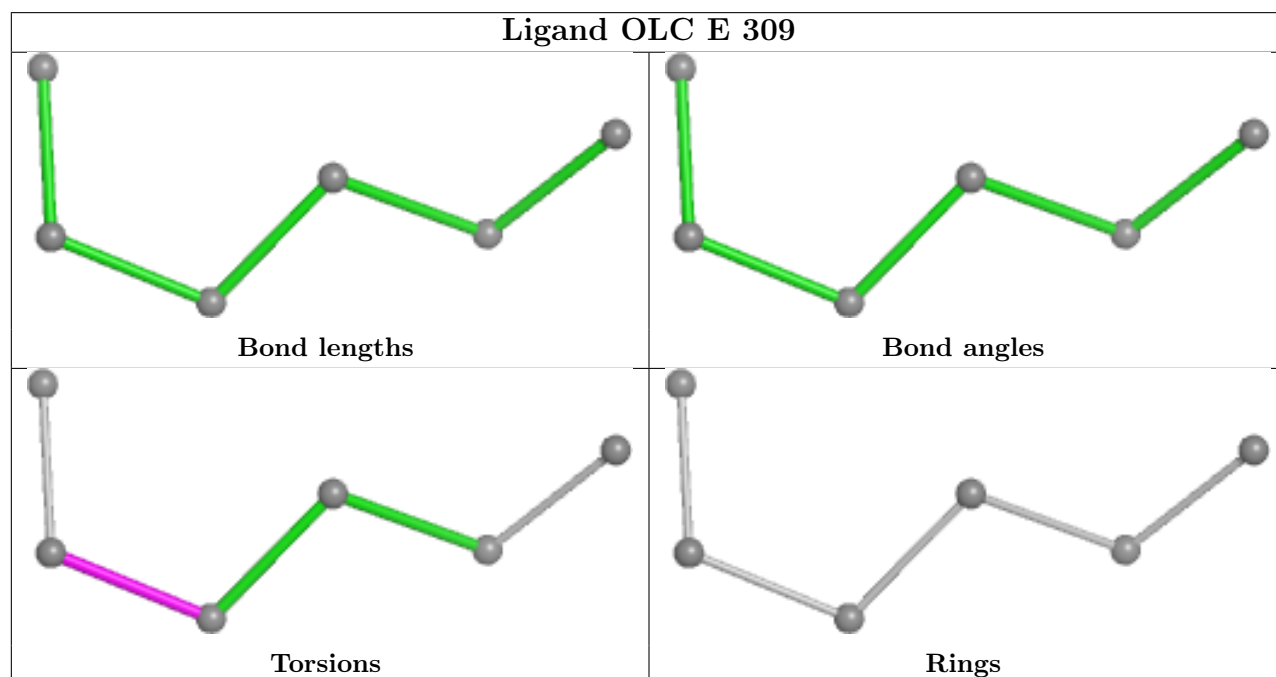
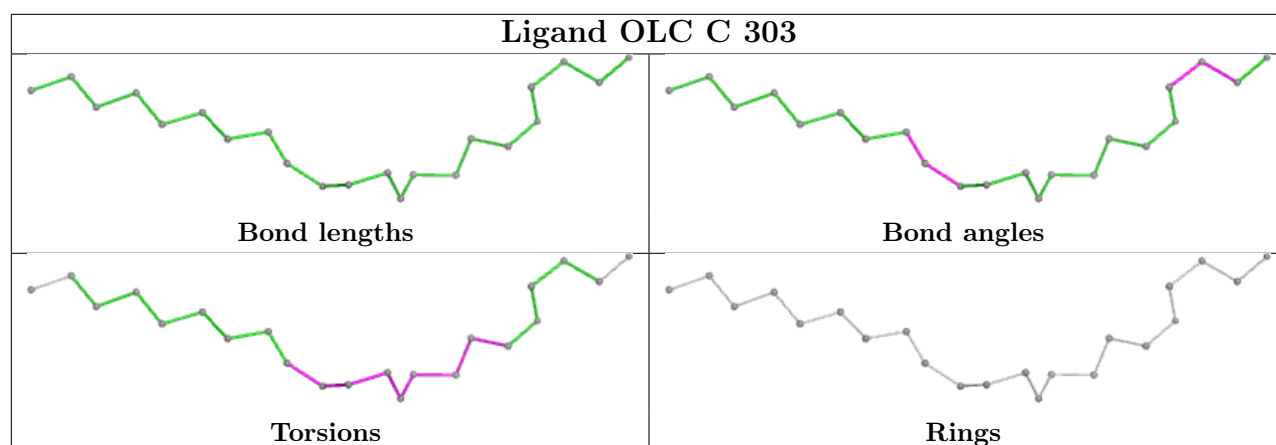


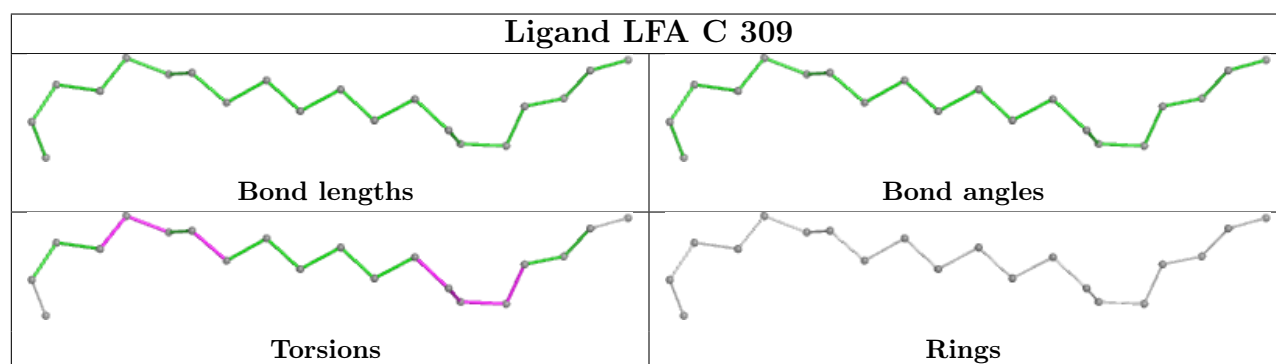
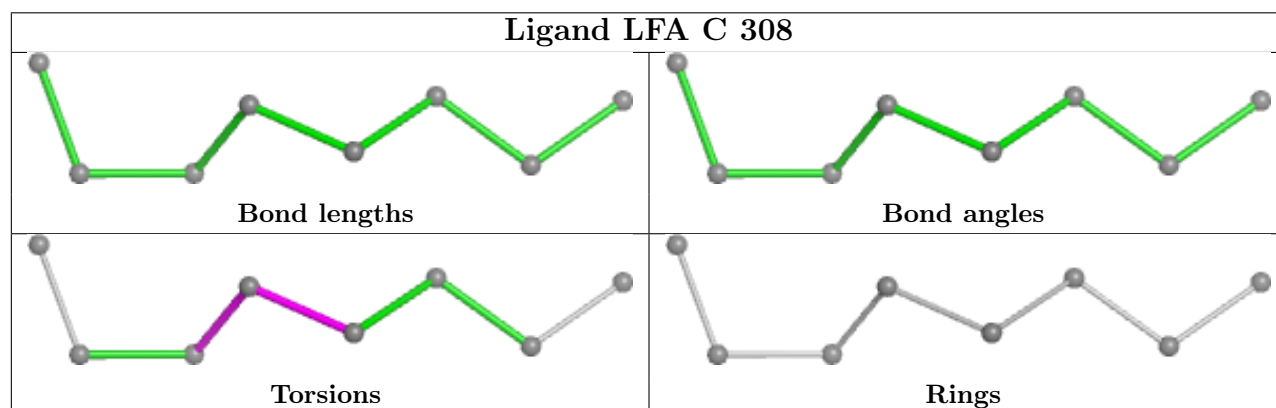
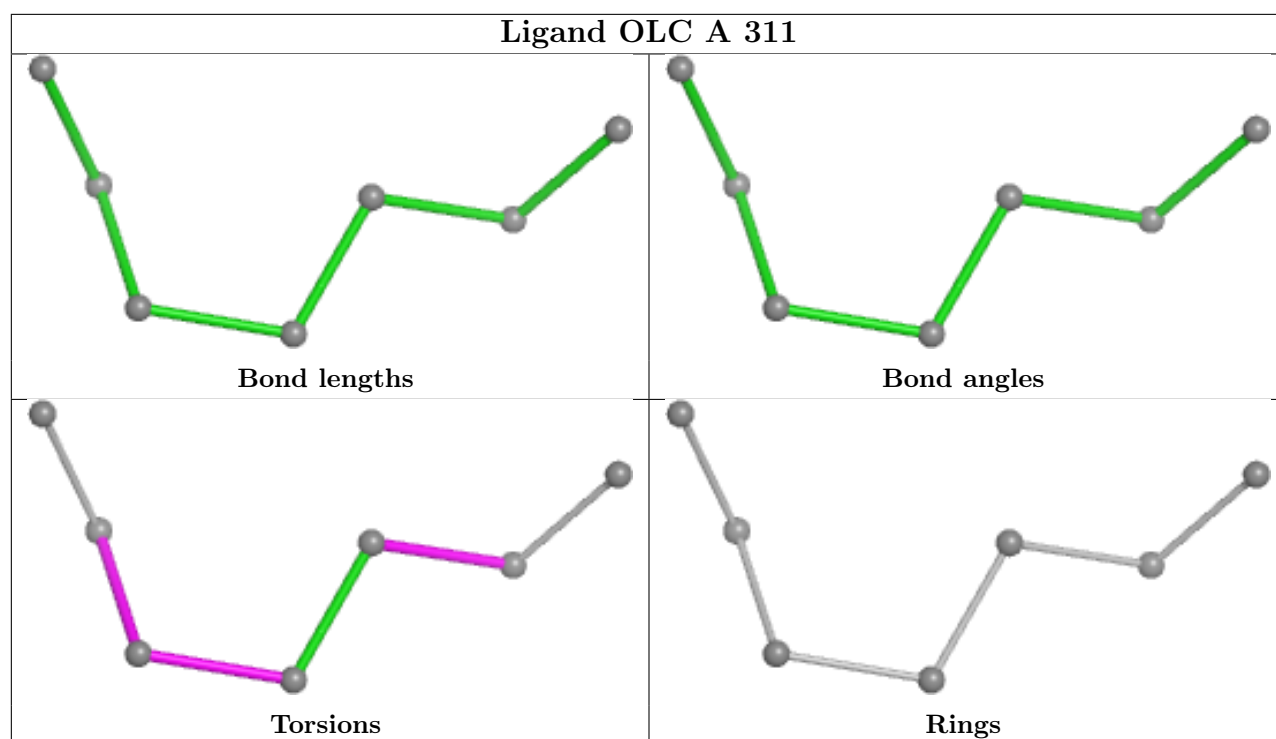


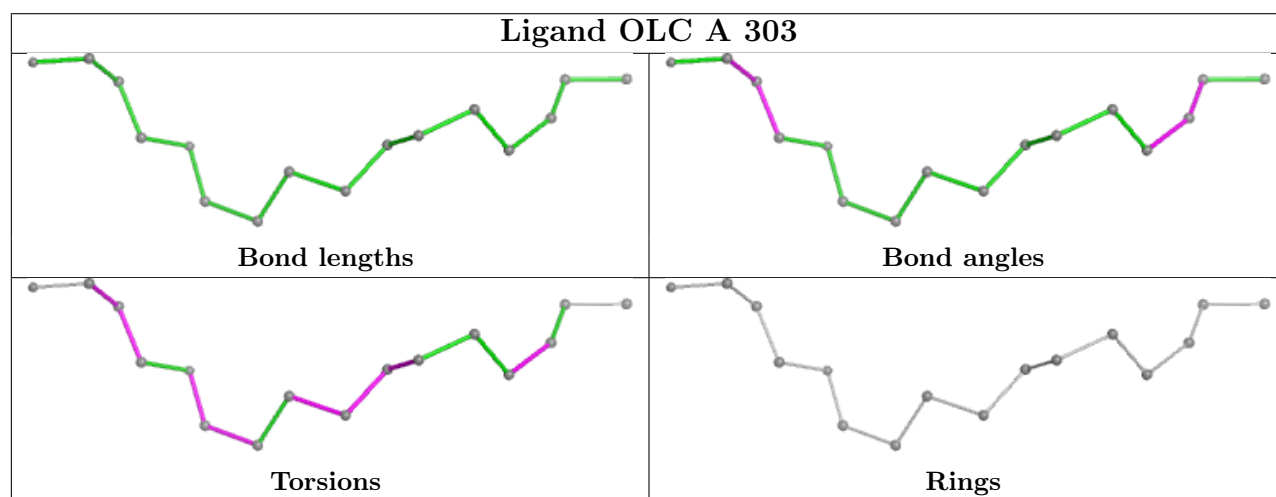
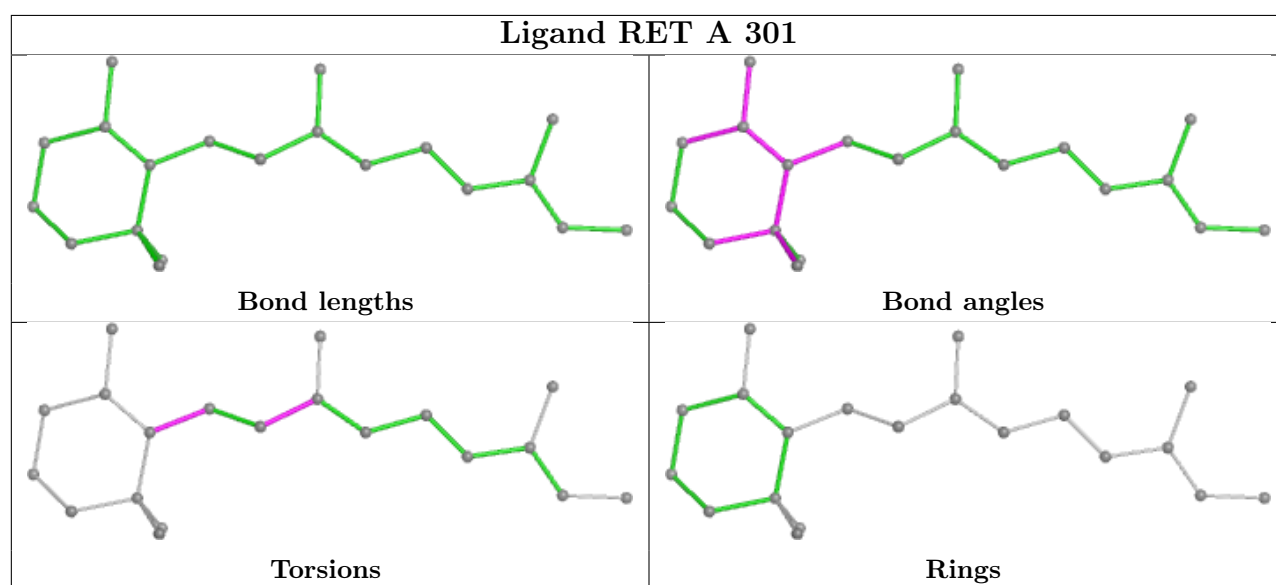
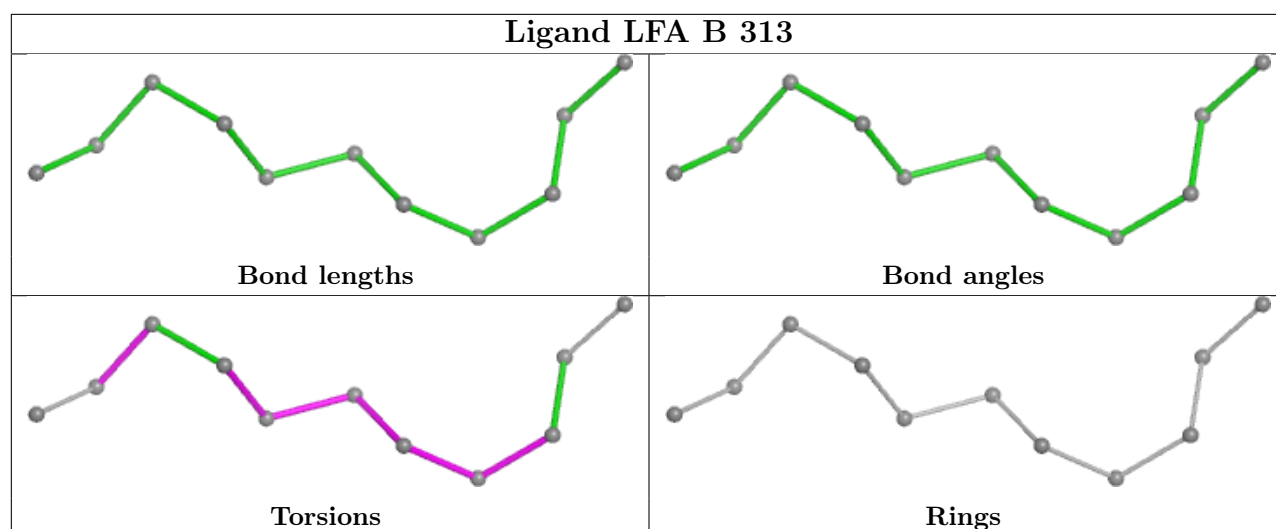


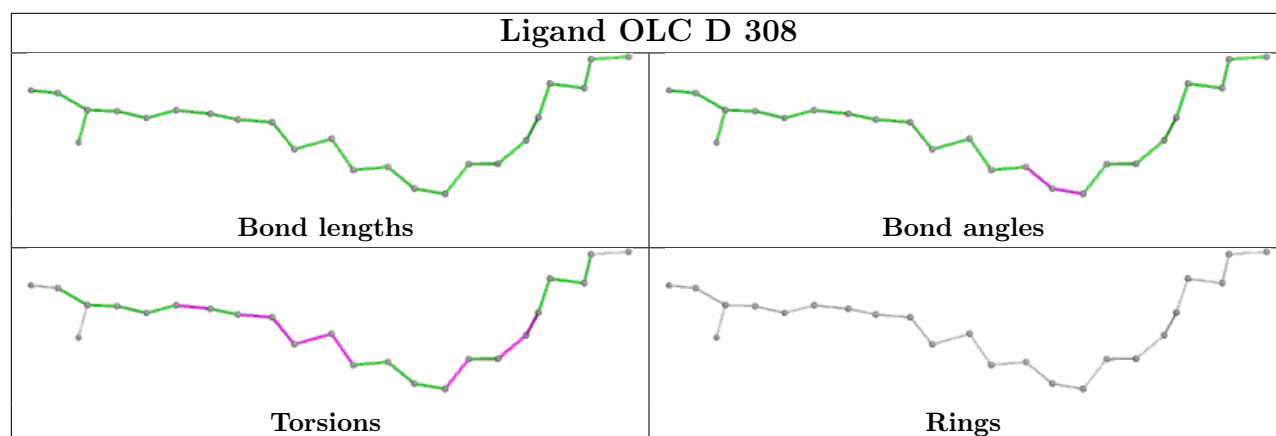
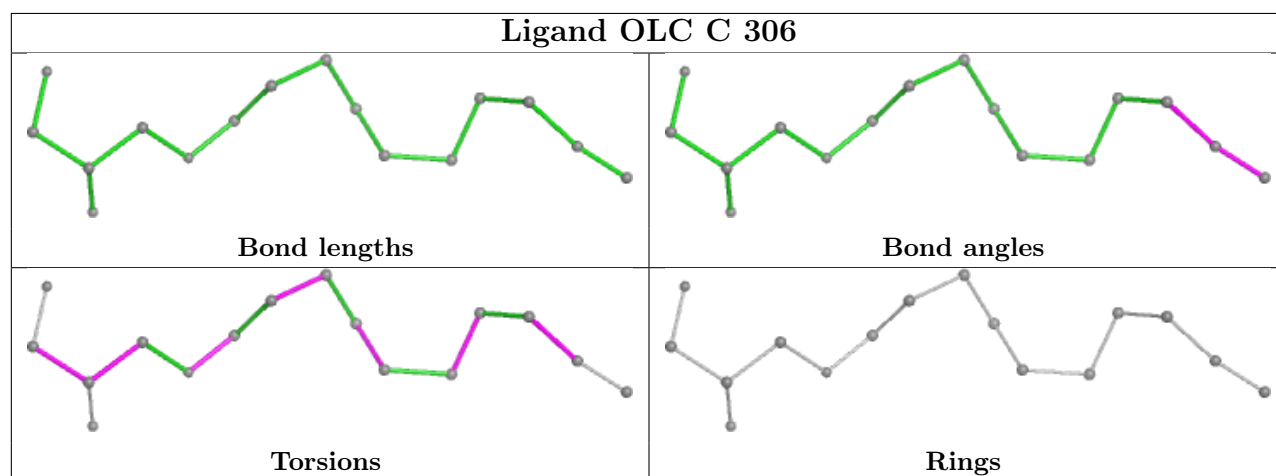
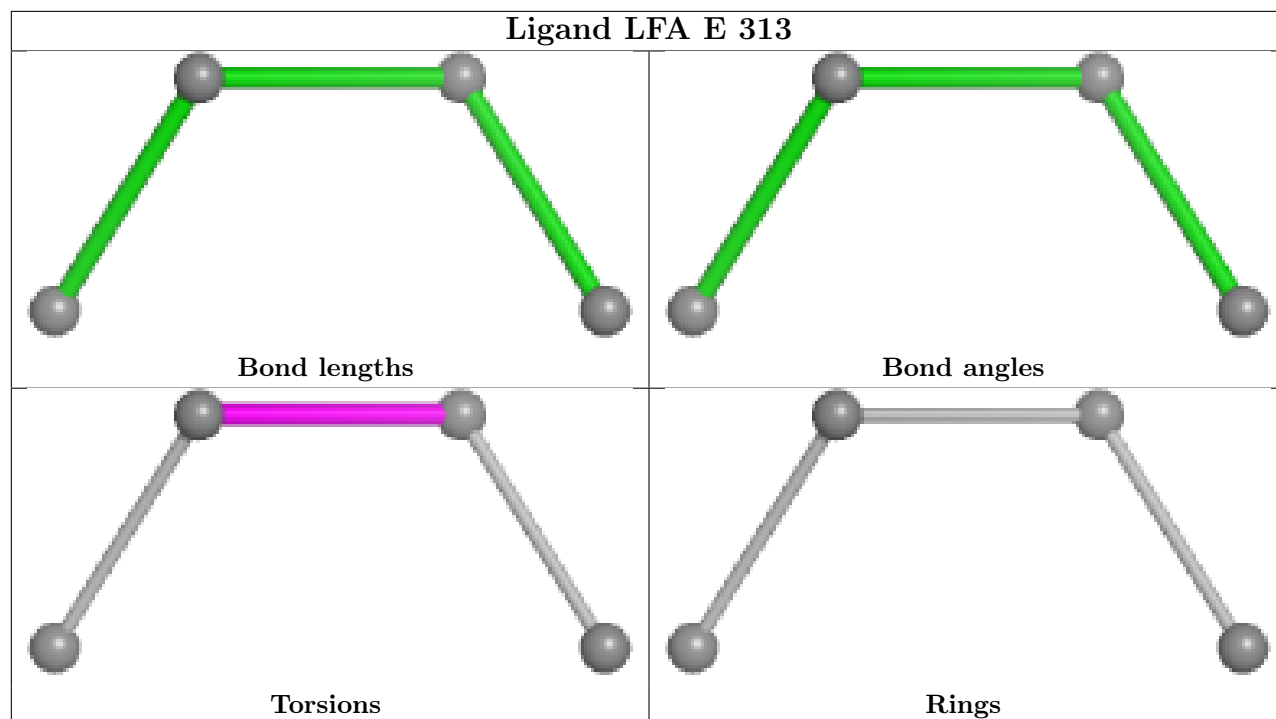


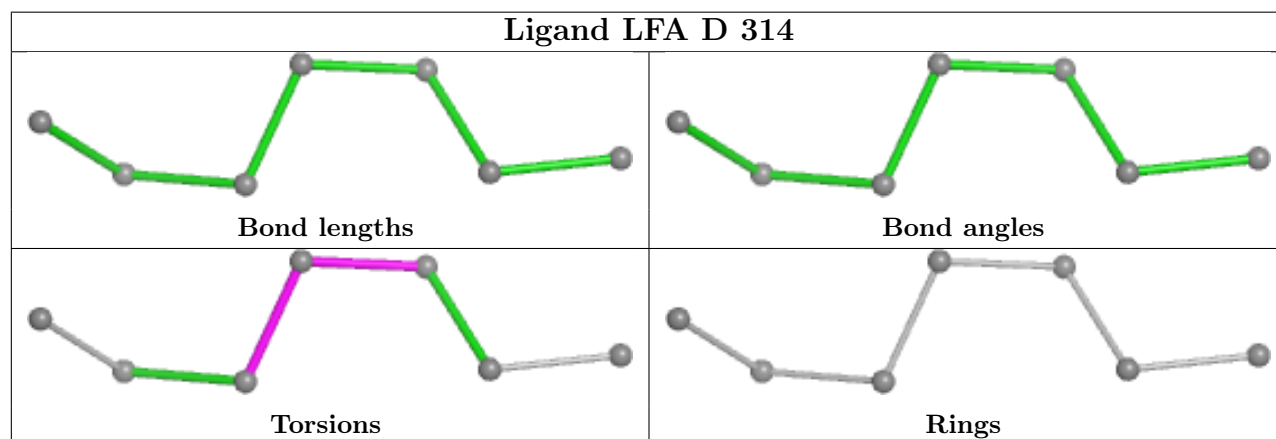
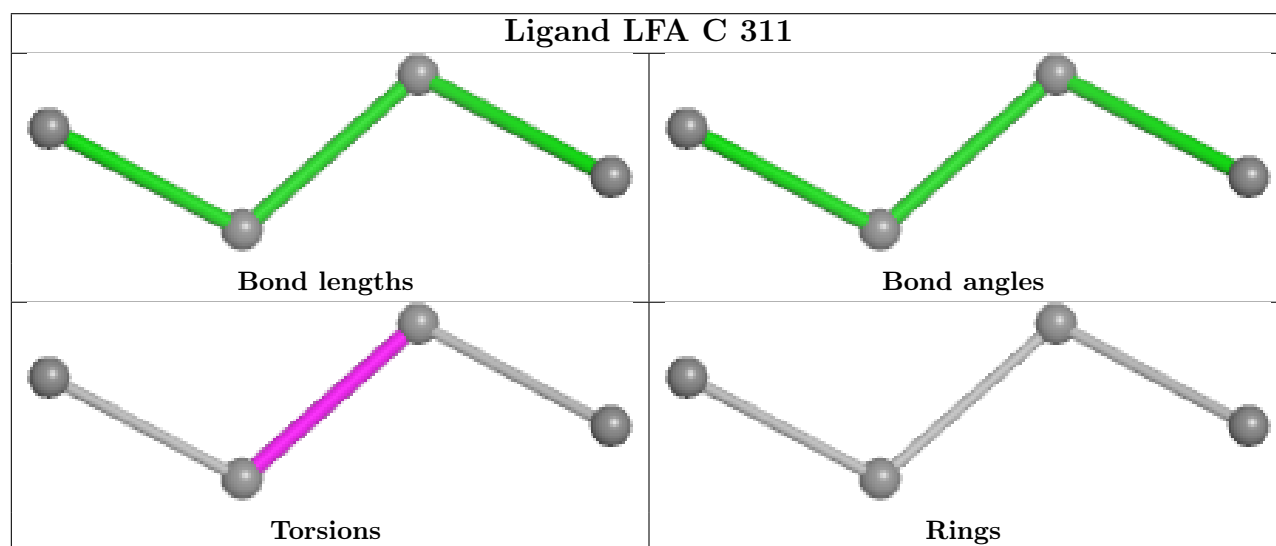
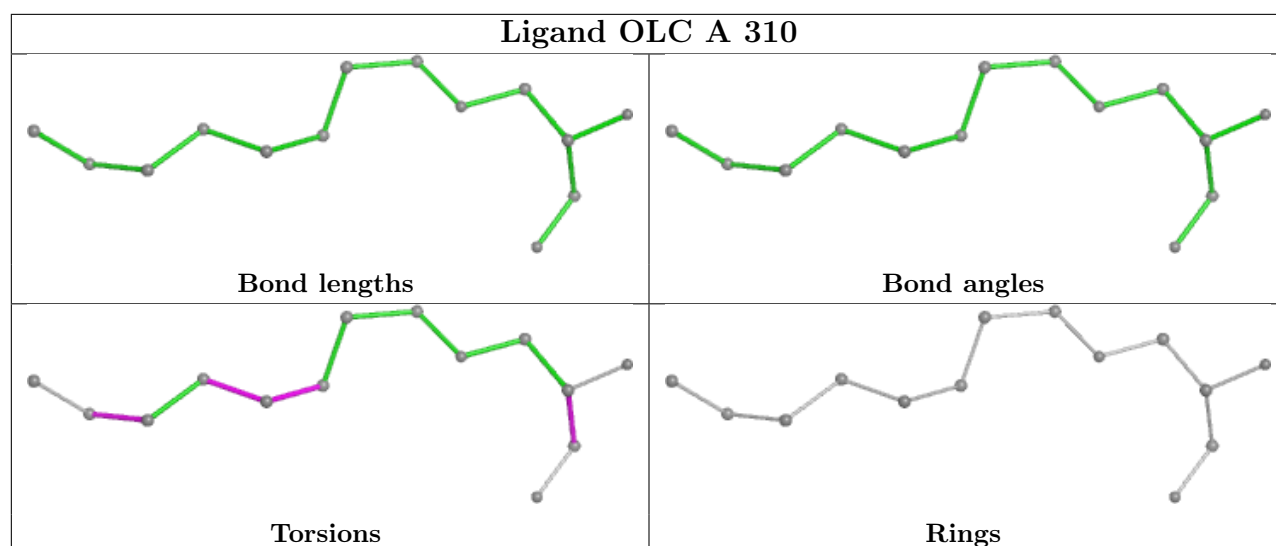


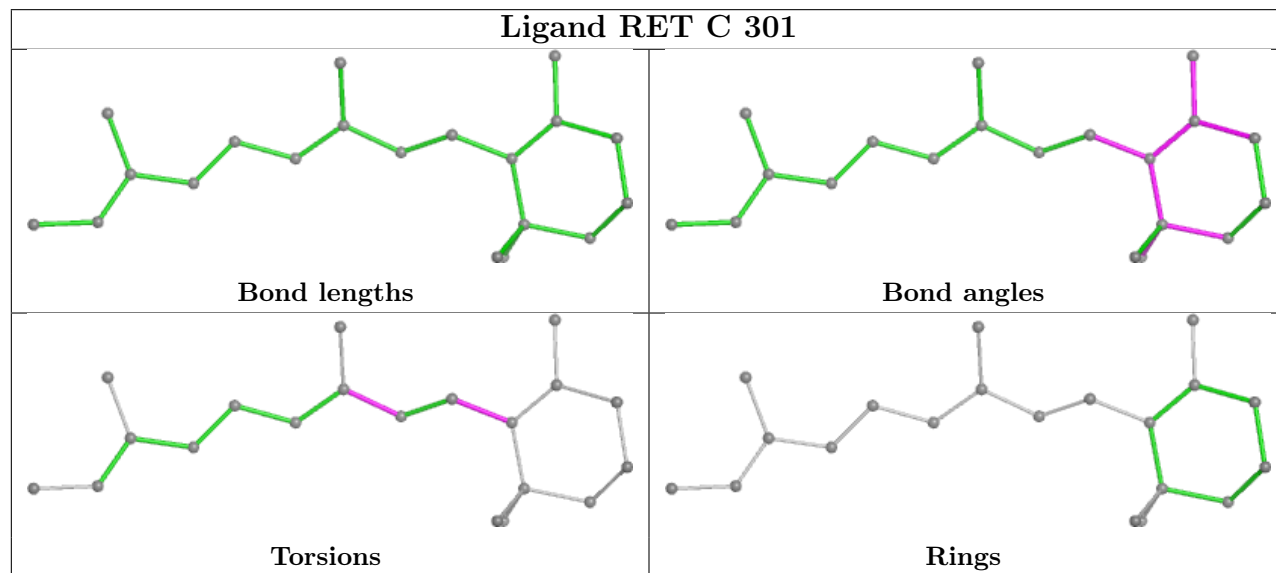
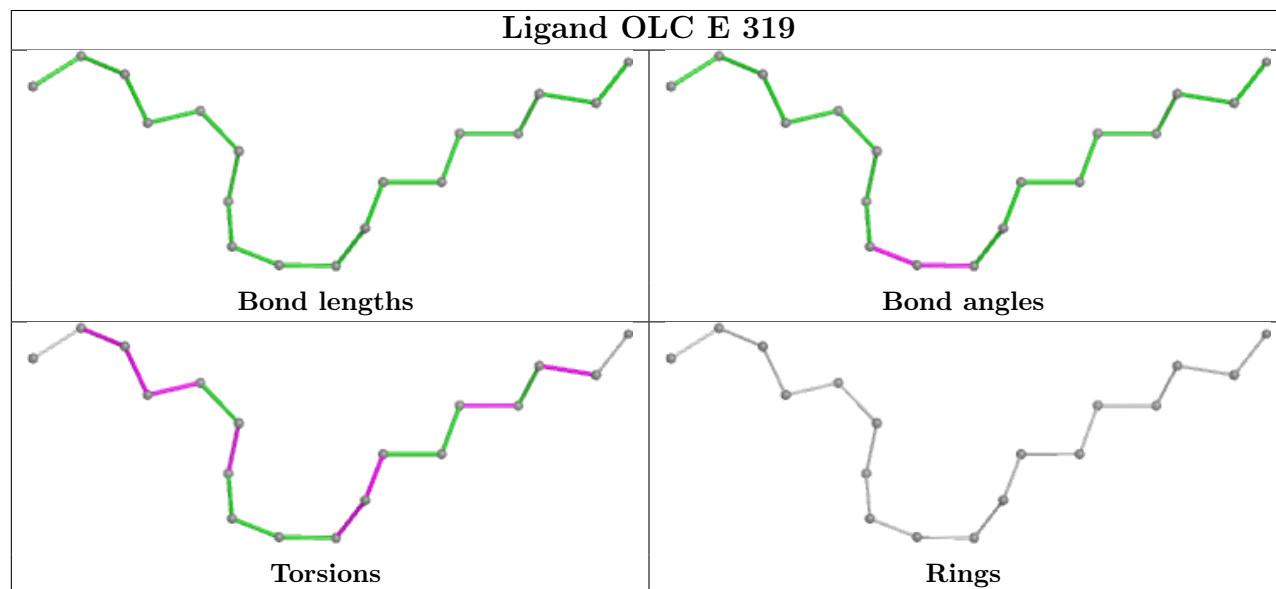
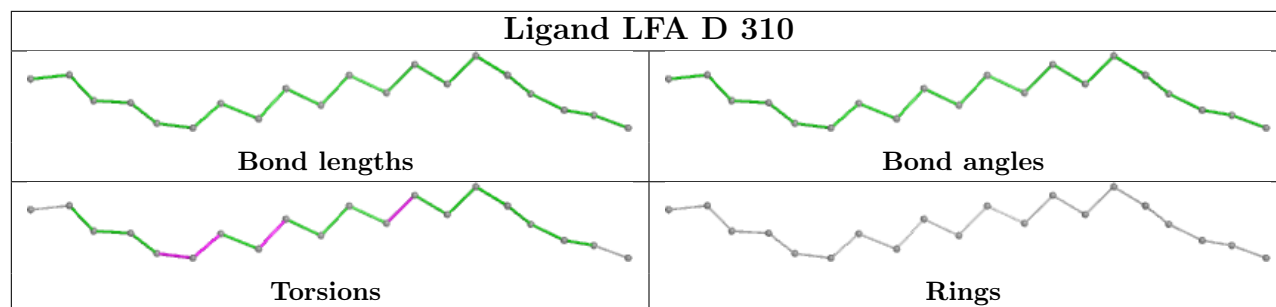


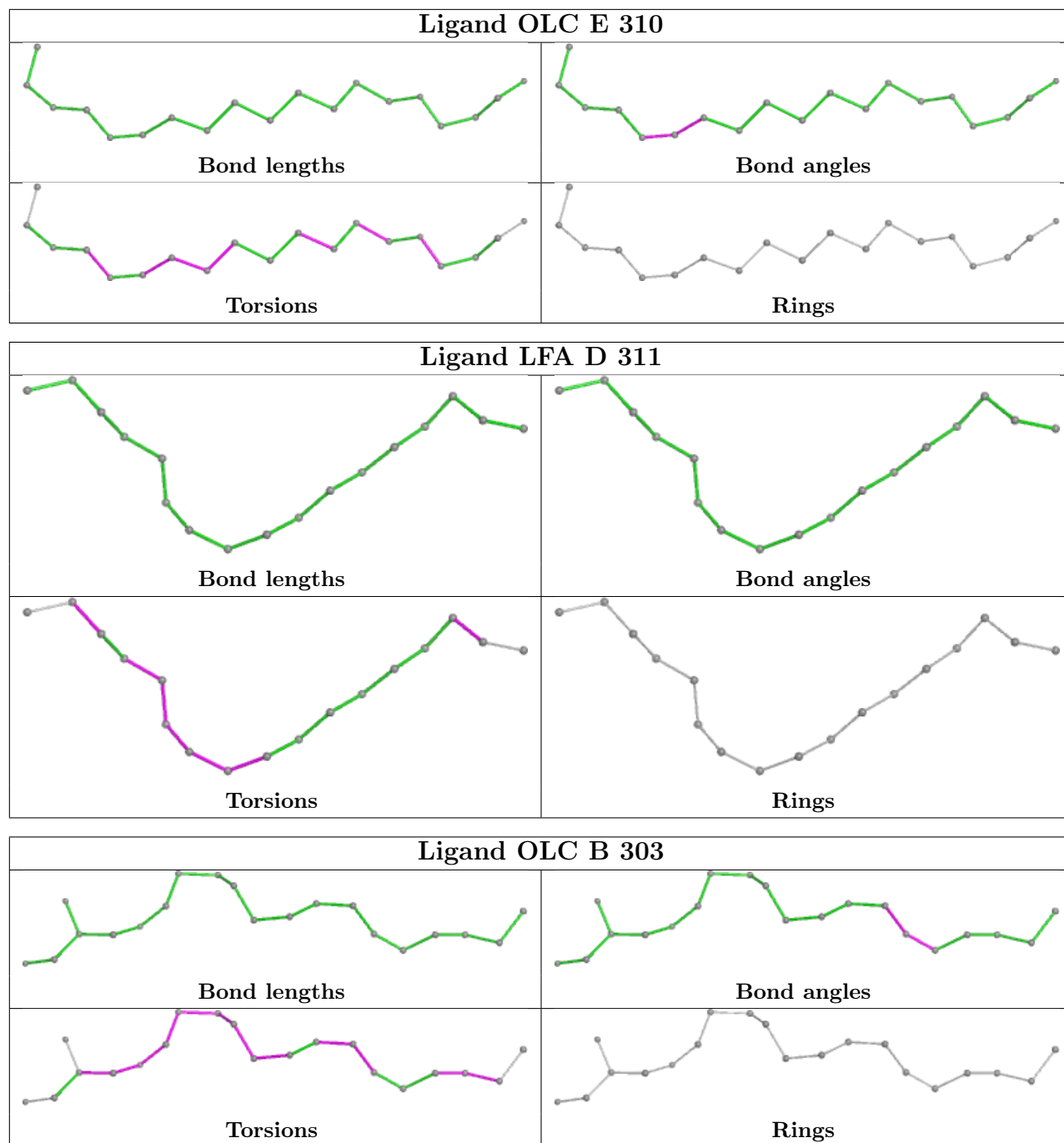


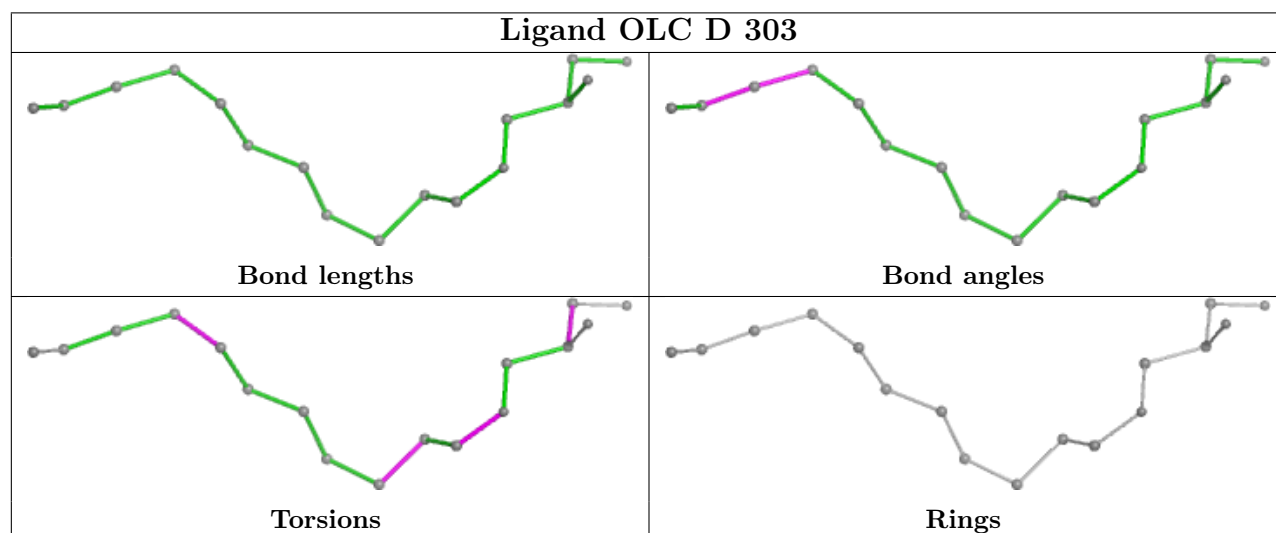
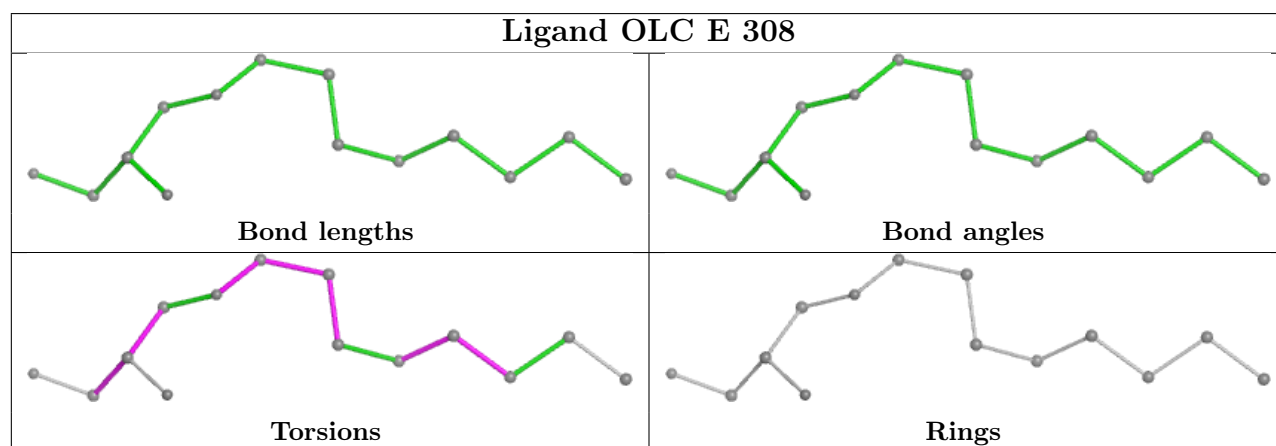
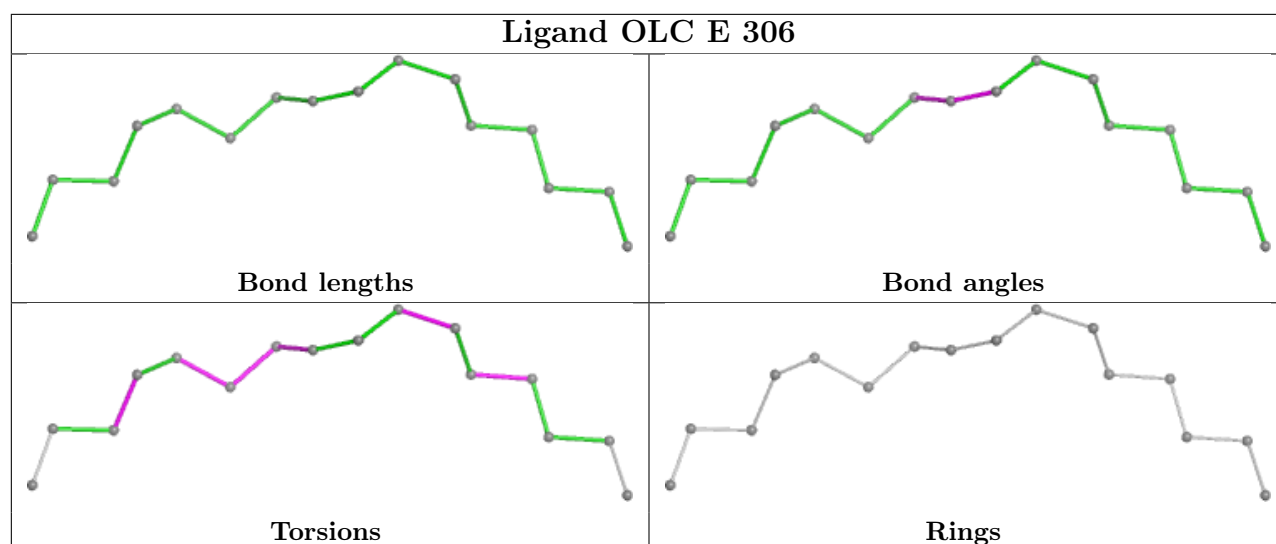


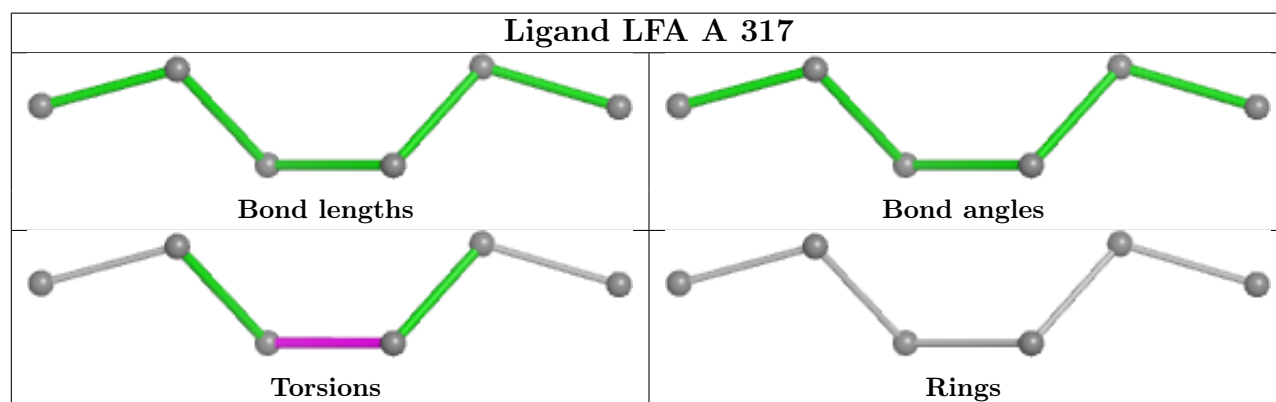
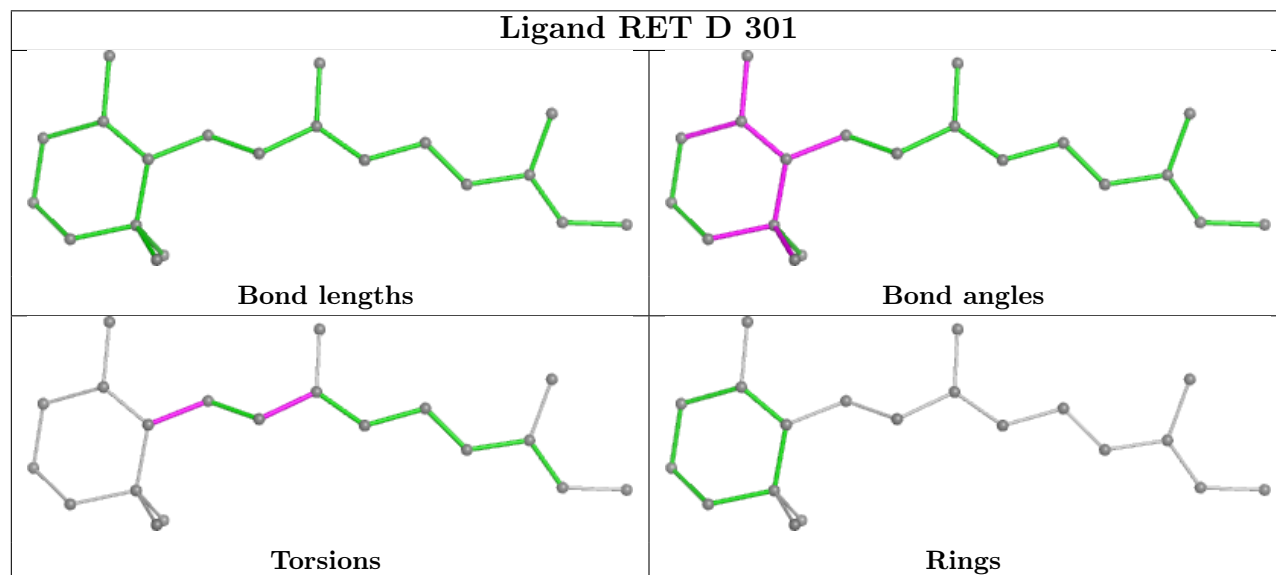
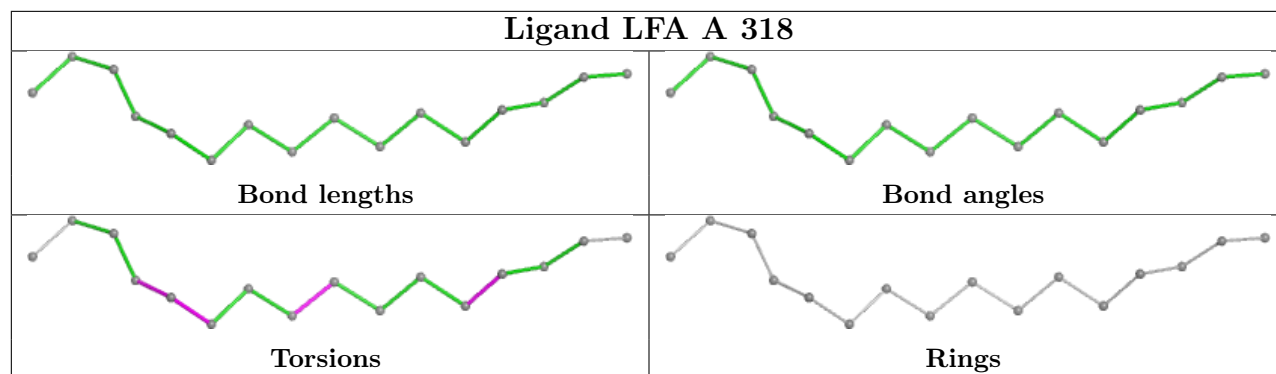




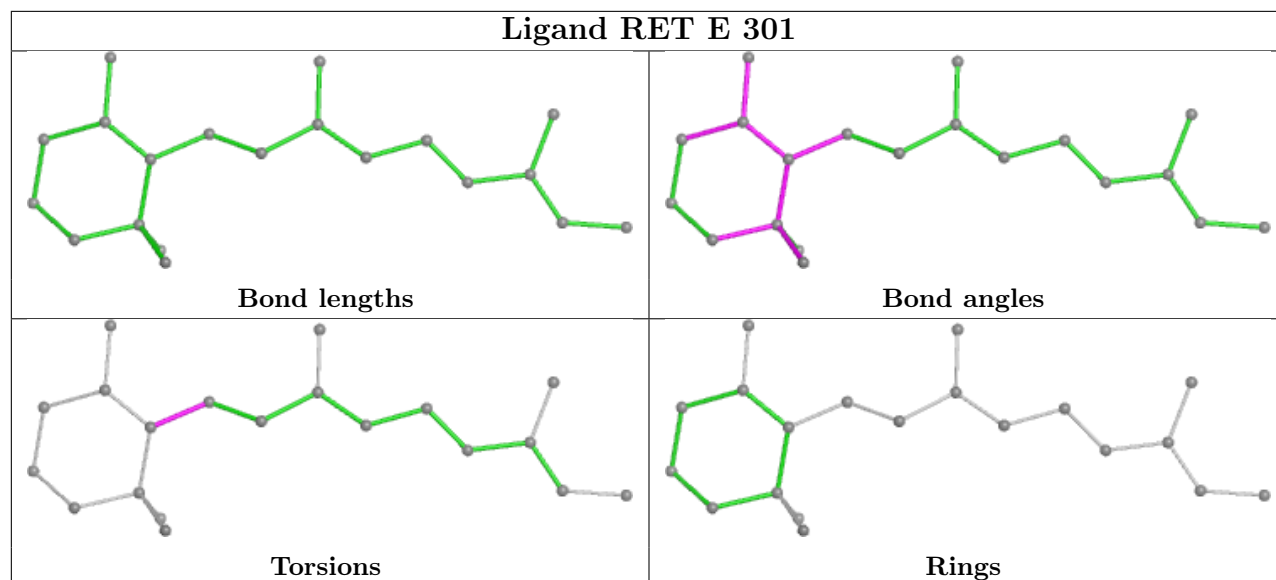




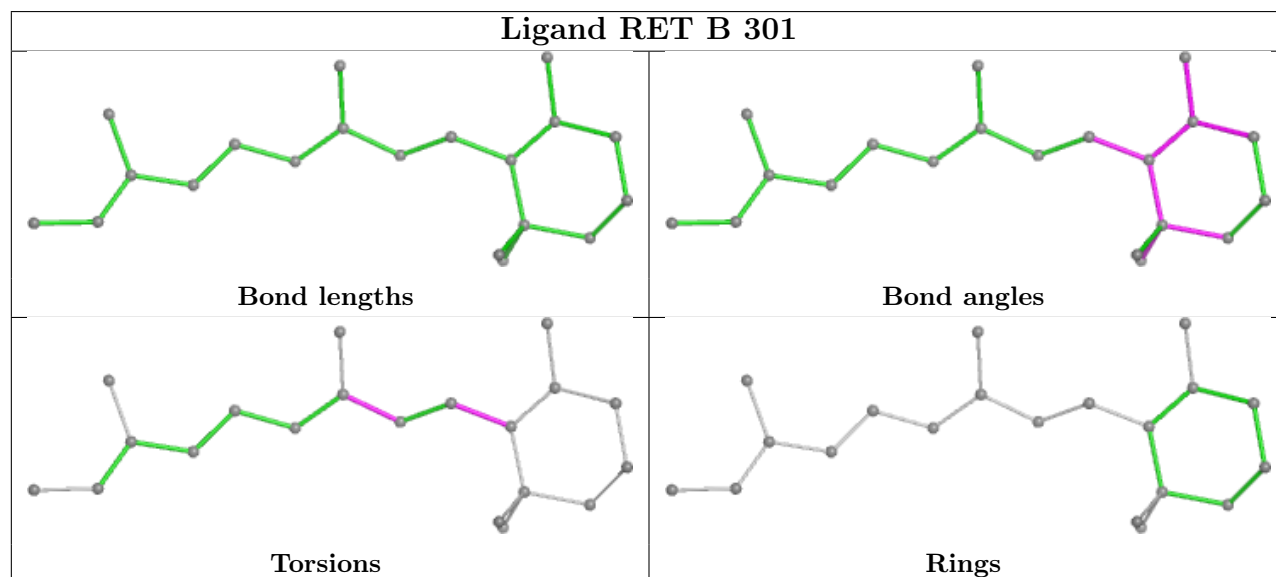




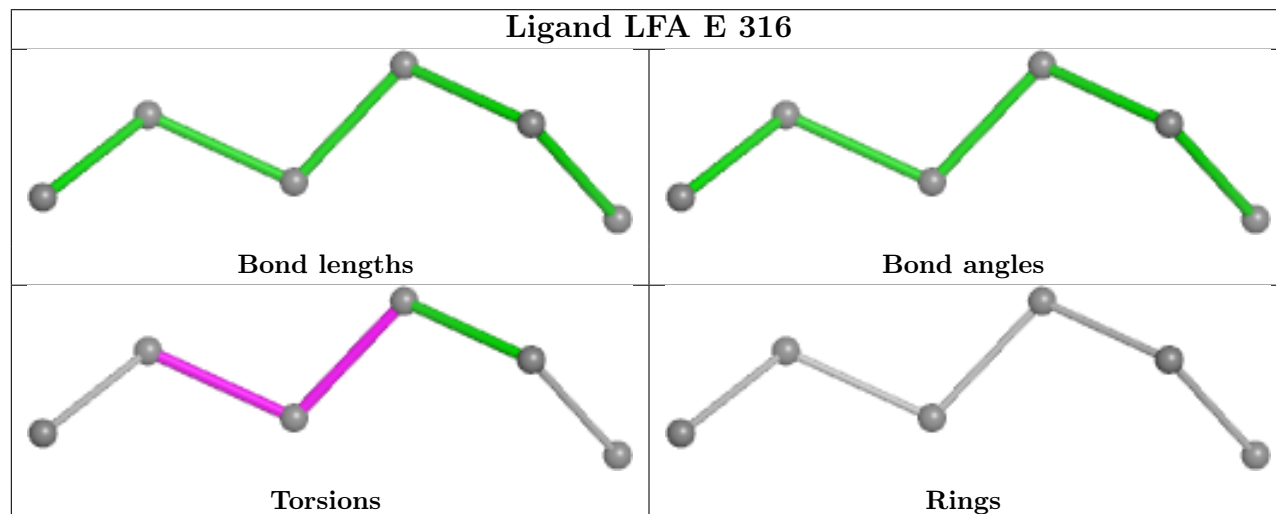
Ligand RET E 301

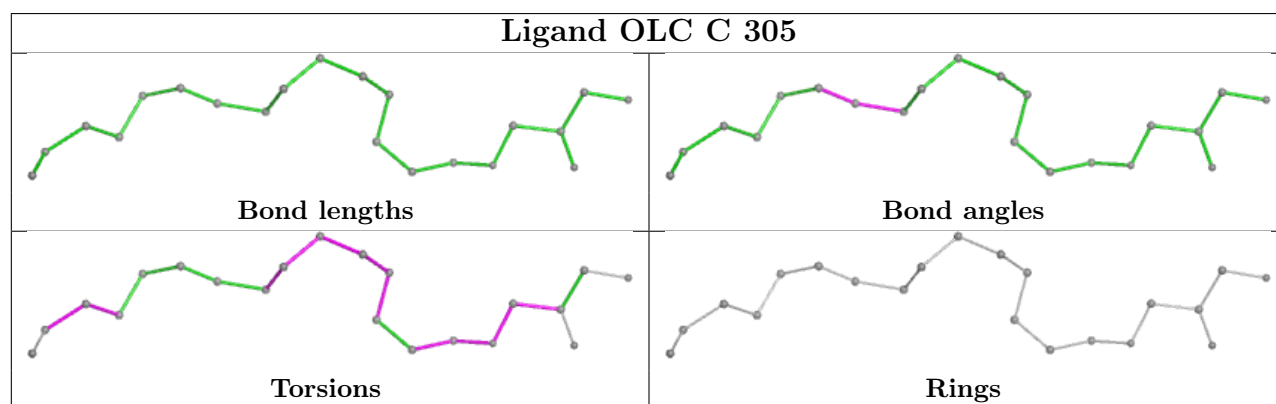
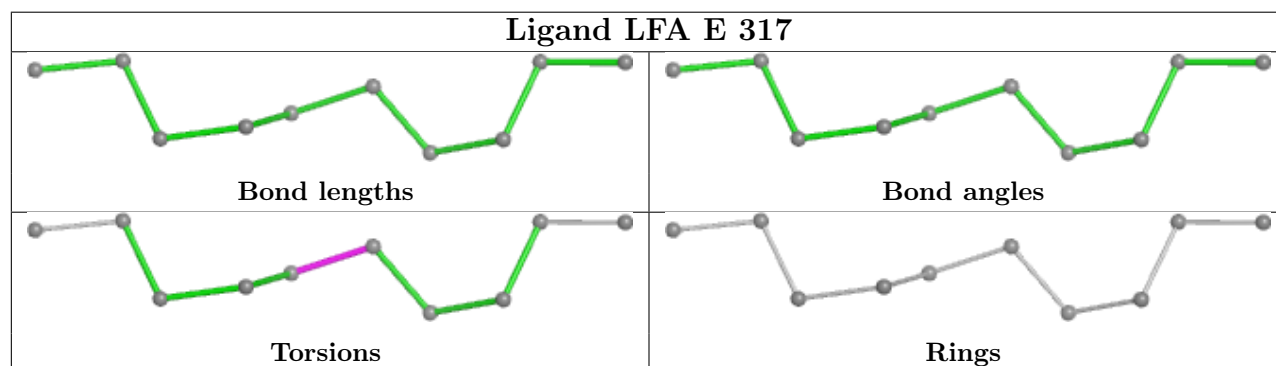
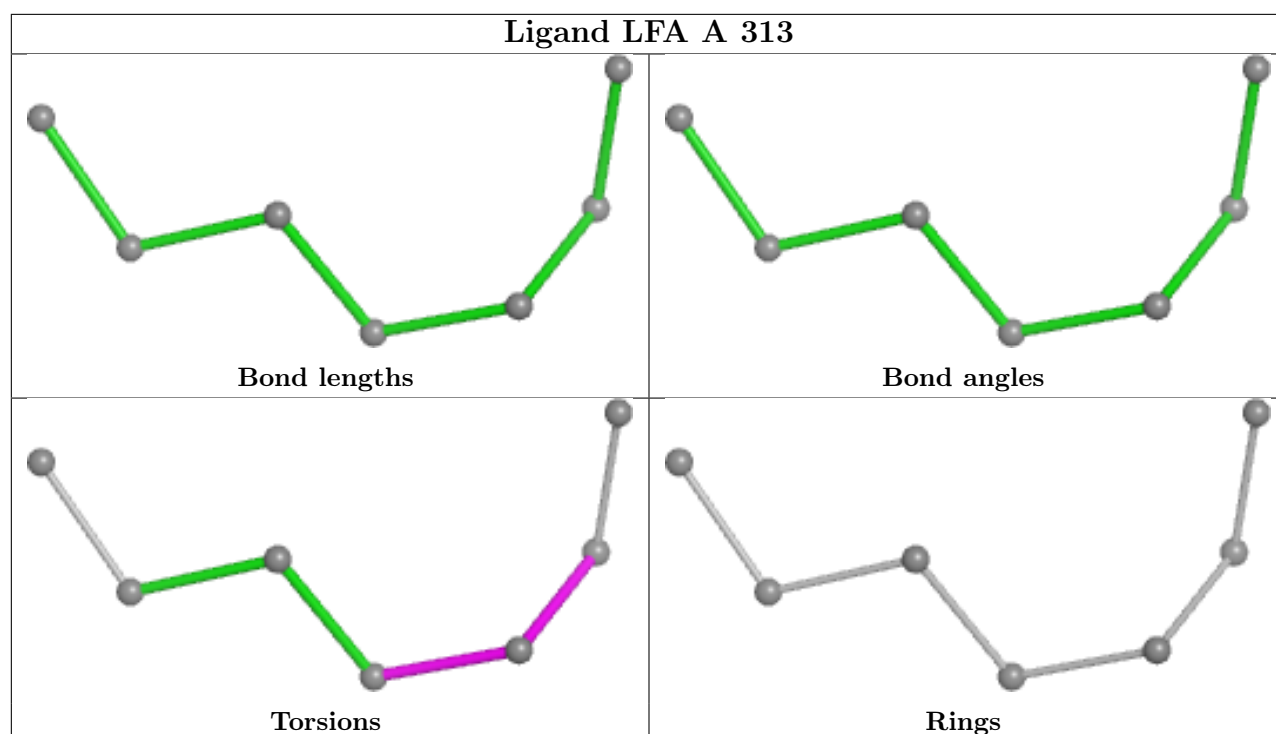


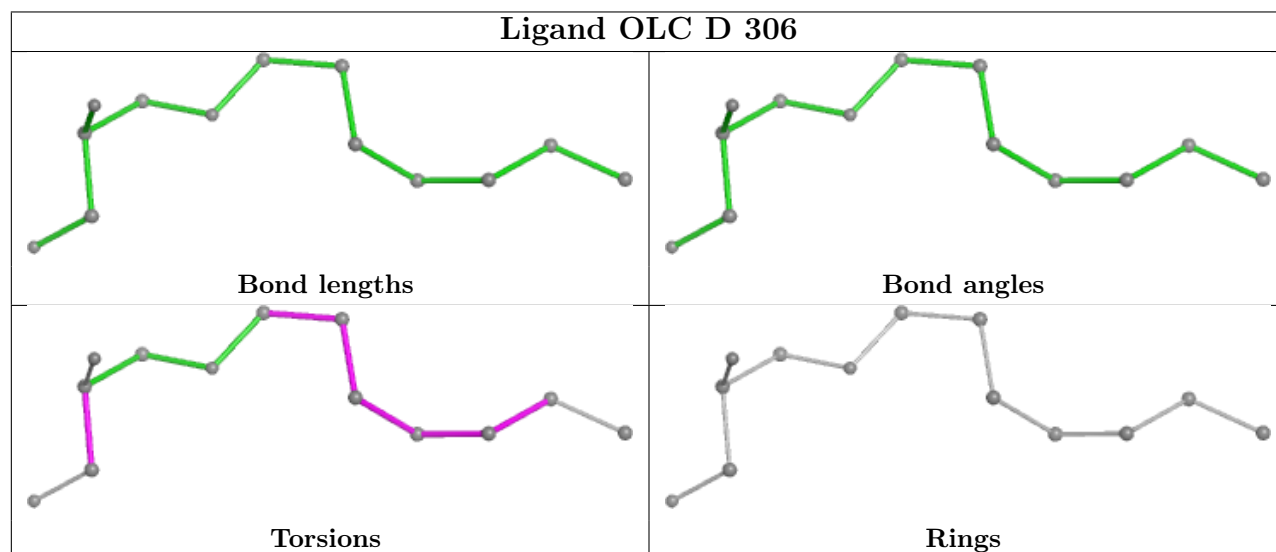
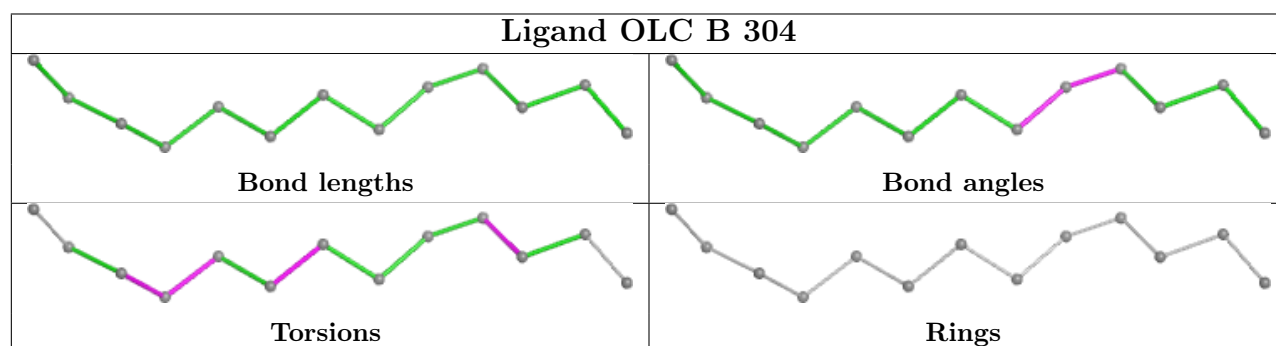
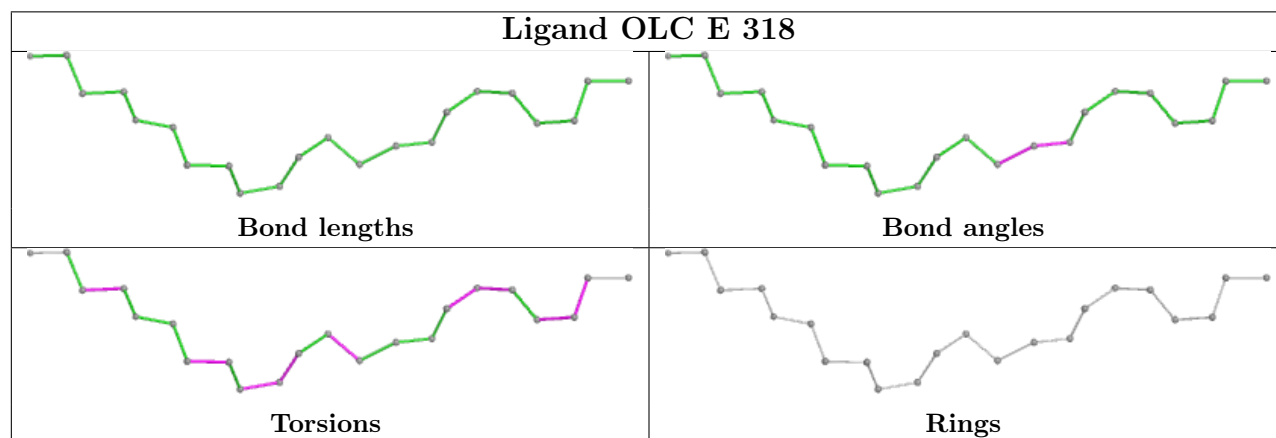
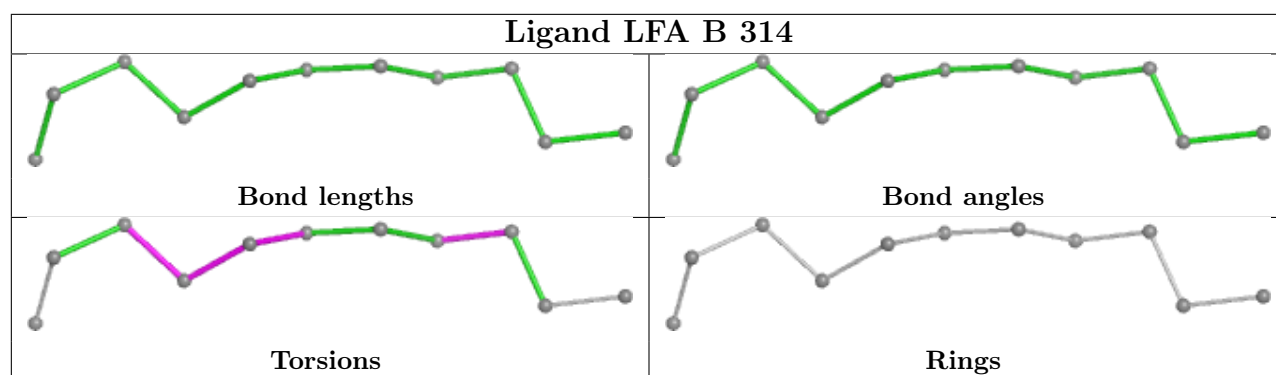
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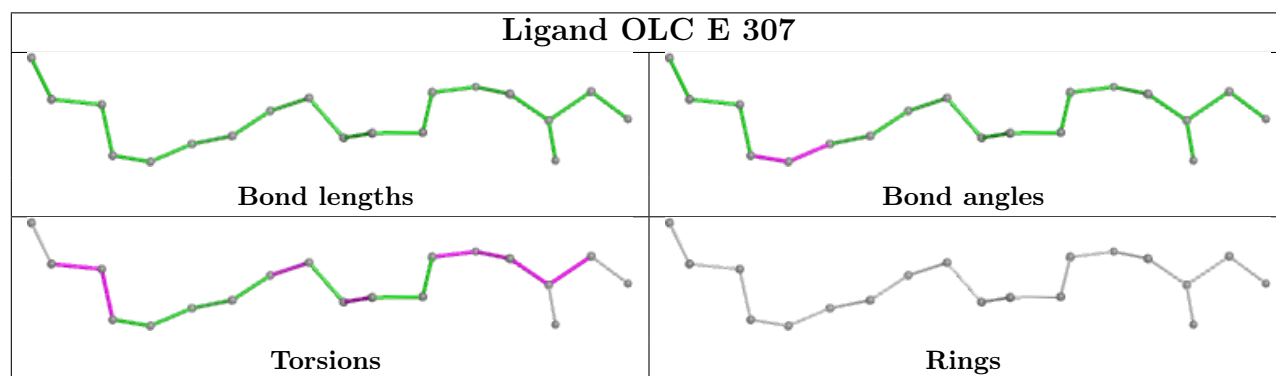
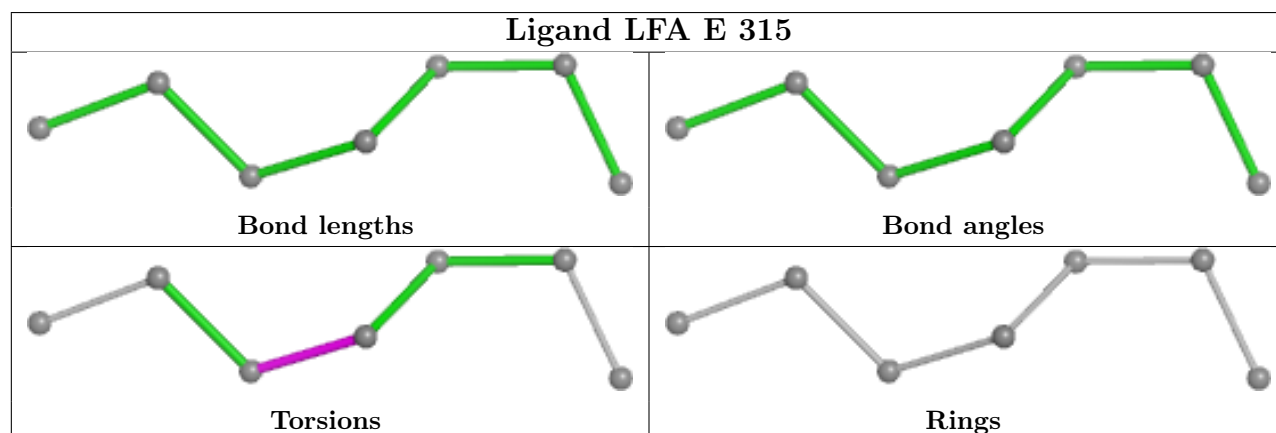
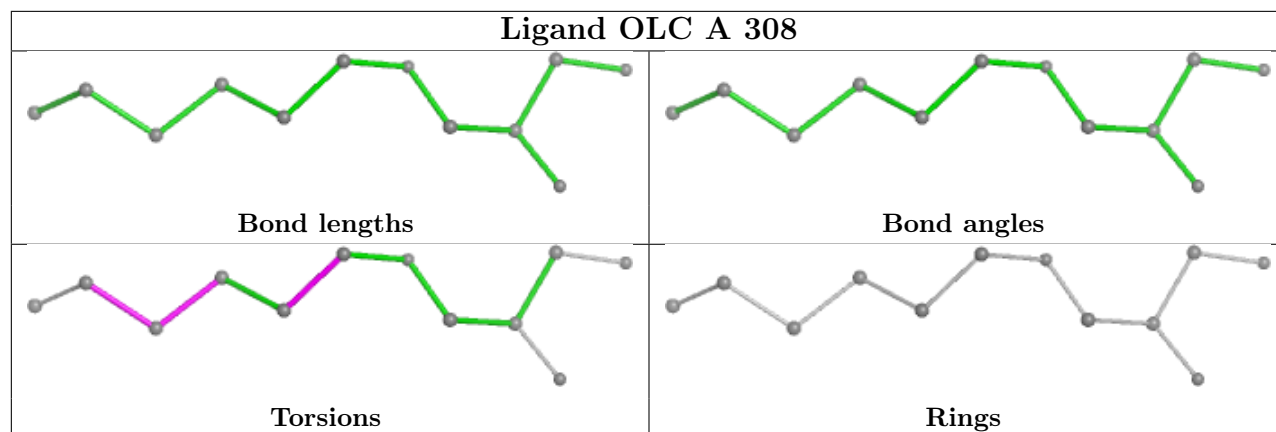


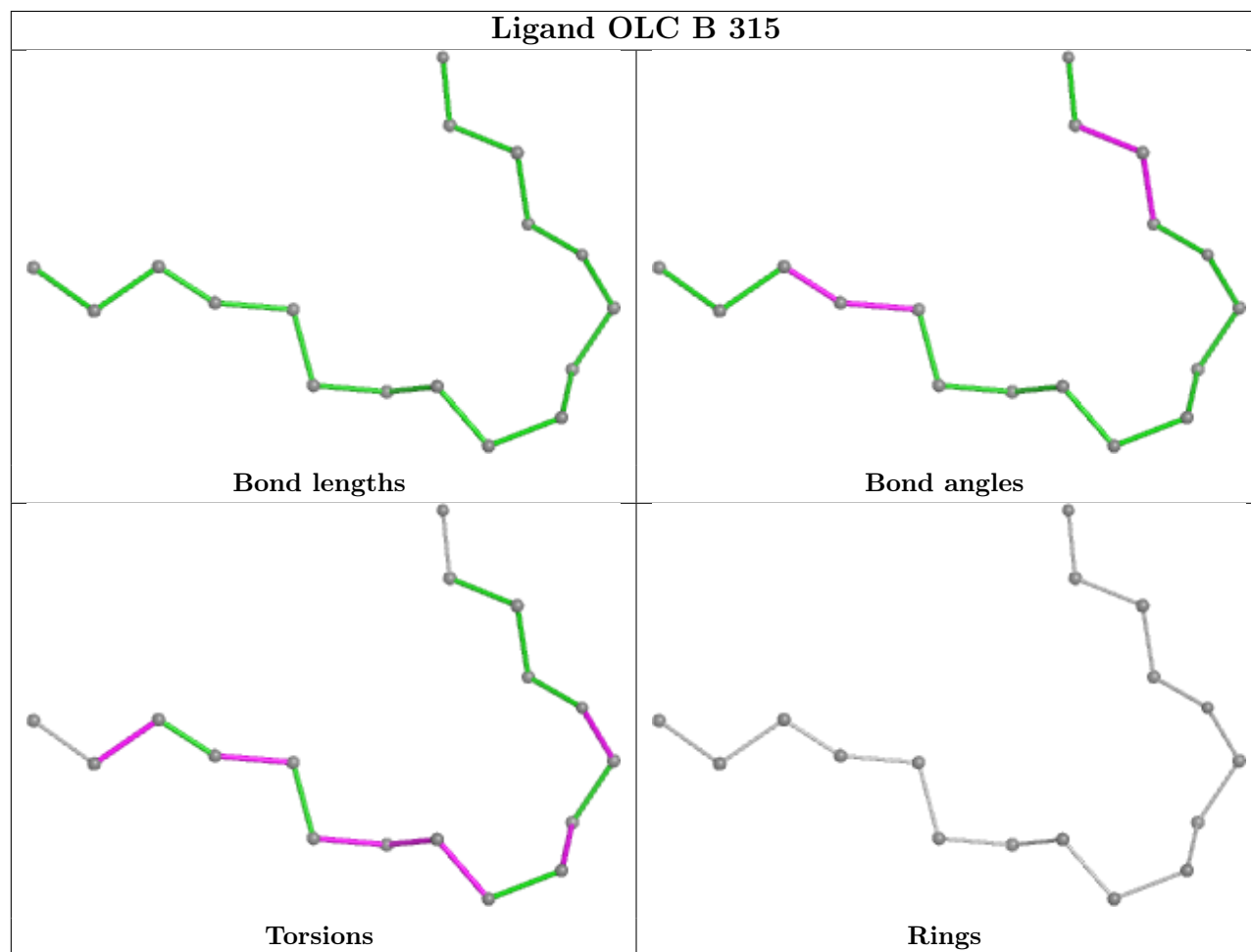
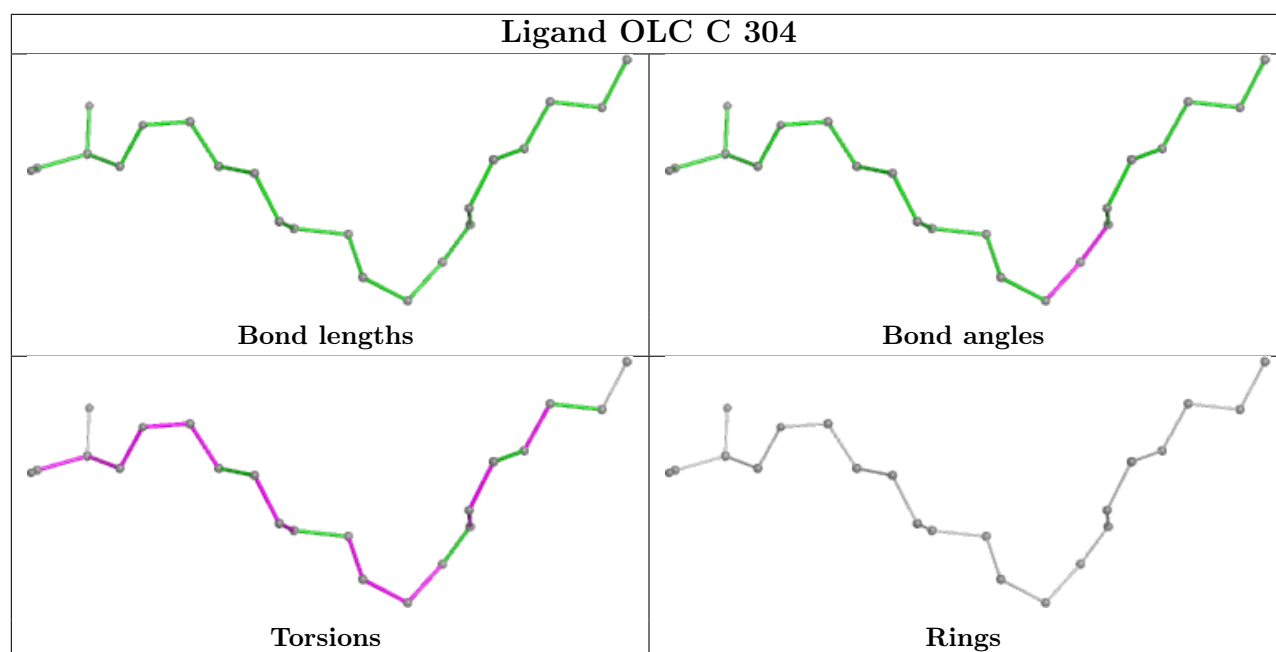
Ligand LFA E 316

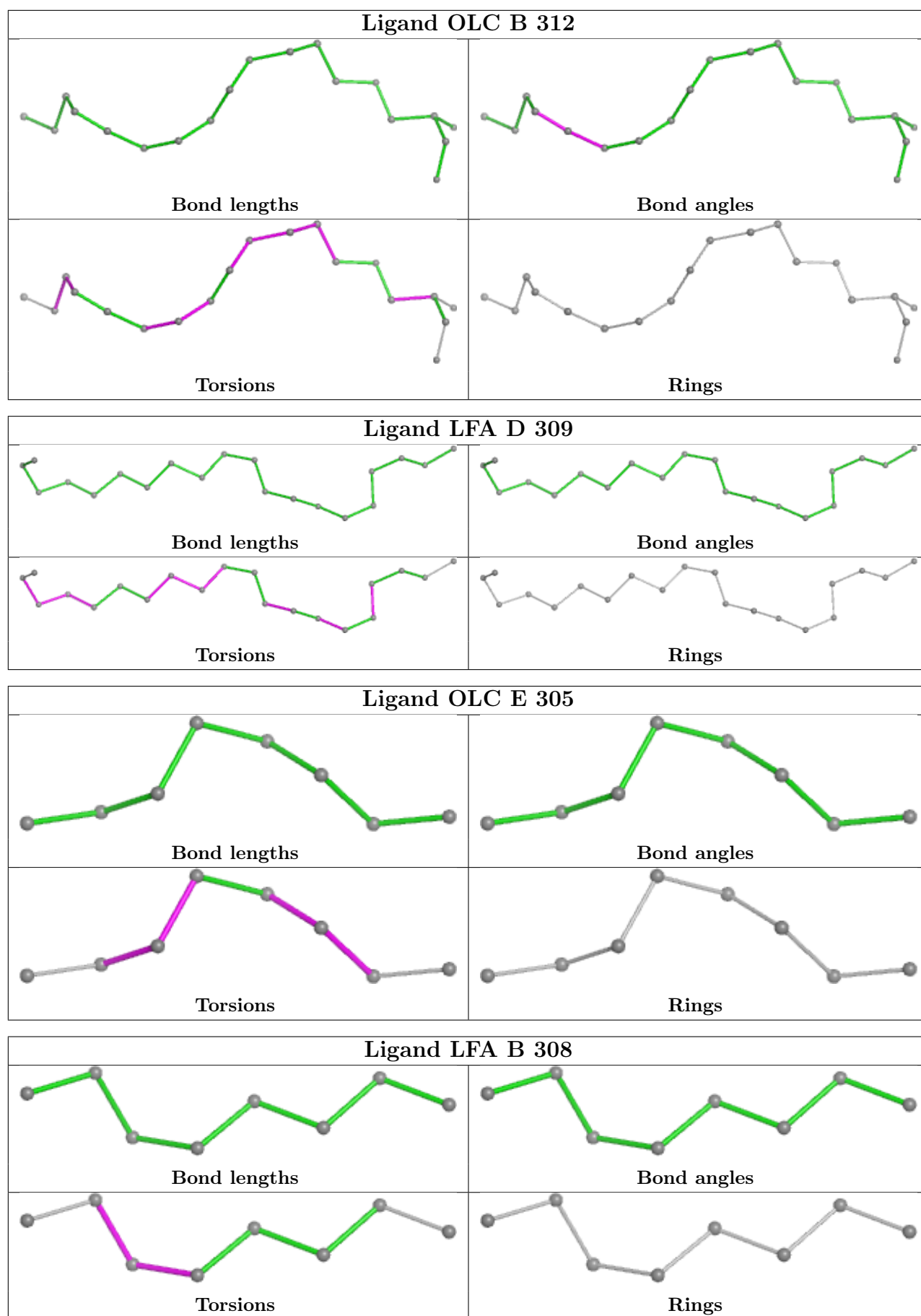


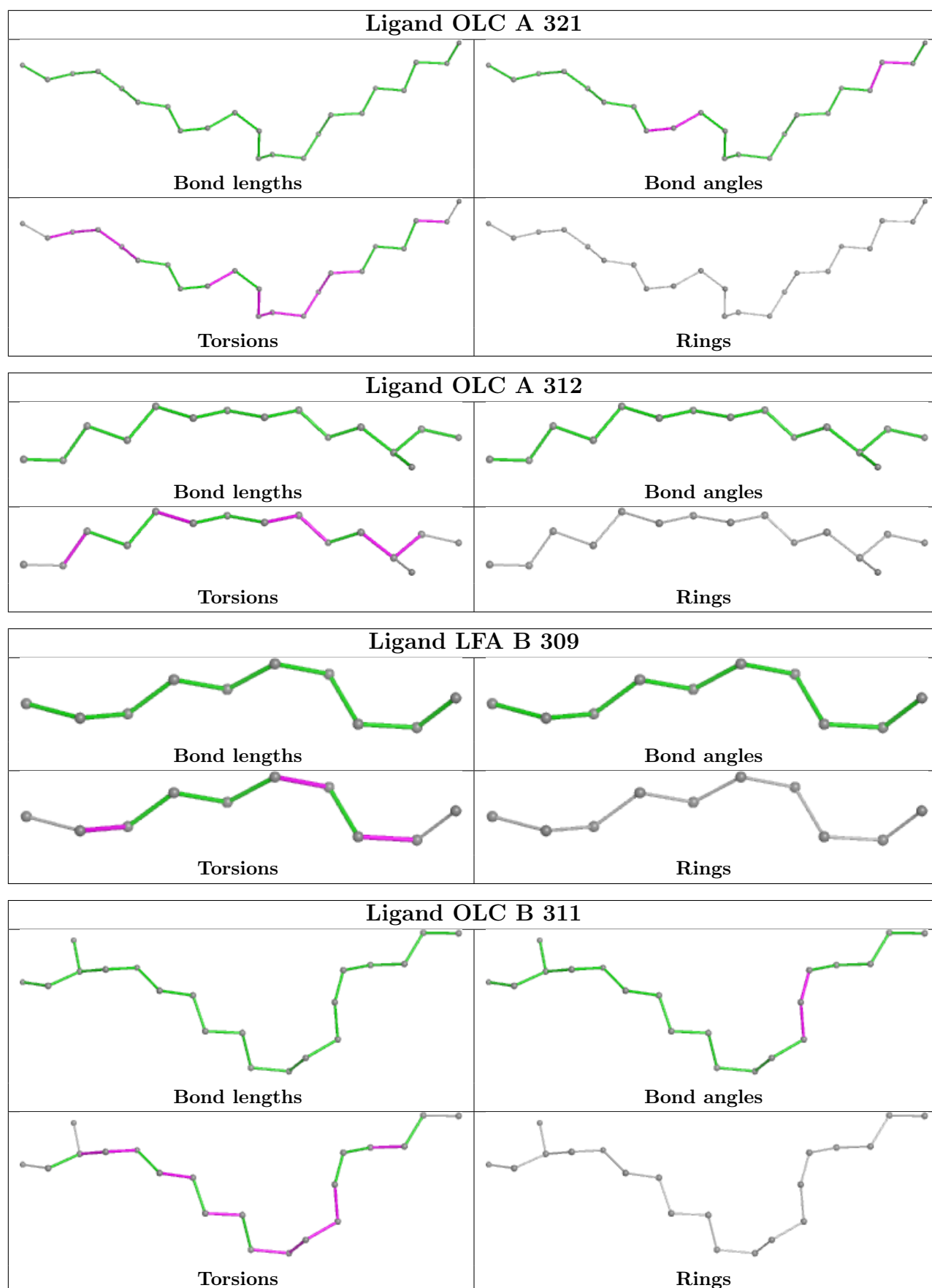


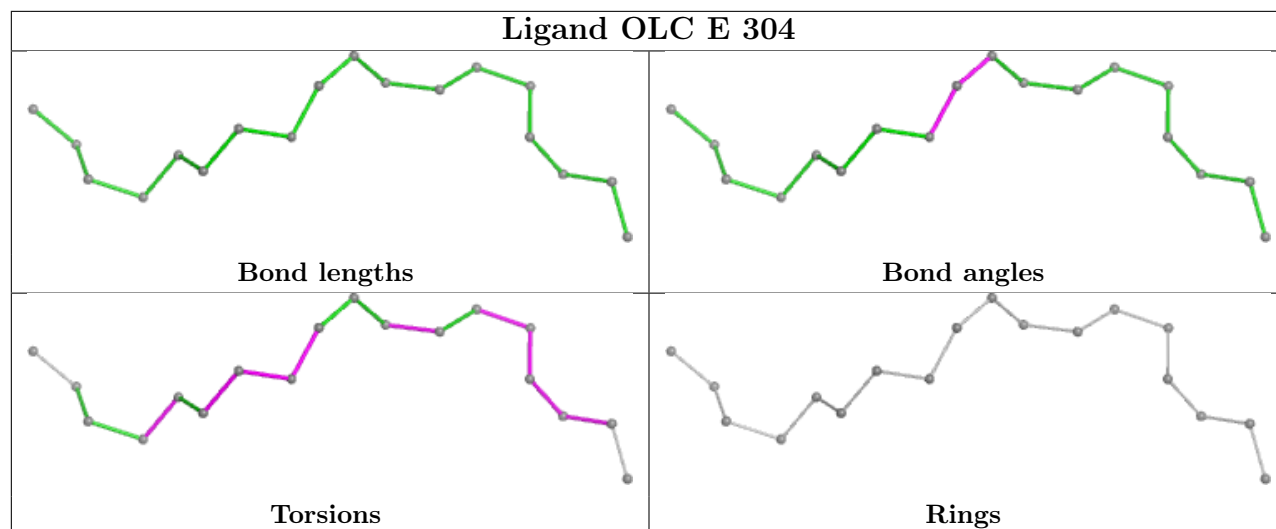












5.7 Other polymers [i](#)

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	269/273 (98%)	-0.66	0 100 100	38, 49, 71, 92	0
1	B	269/273 (98%)	-0.67	1 (0%) 89 77	39, 49, 67, 99	0
1	C	268/273 (98%)	-0.62	0 100 100	37, 50, 69, 111	0
1	D	268/273 (98%)	-0.63	0 100 100	38, 52, 74, 94	0
1	E	268/273 (98%)	-0.68	0 100 100	38, 51, 69, 100	0
All	All	1342/1365 (98%)	-0.65	1 (0%) 92 88	37, 50, 71, 111	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	GLN	2.9

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(\AA^2)	Q<0.9
5	LFA	E	316	6/20	0.59	0.34	75,83,84,88	0
5	LFA	A	316	4/20	0.70	0.27	62,67,69,69	0
5	LFA	C	314	5/20	0.78	0.27	69,74,85,91	0
4	OLC	E	309	6/25	0.79	0.27	61,68,85,86	0
5	LFA	B	307	9/20	0.79	0.23	69,82,93,94	0
5	LFA	A	318	16/20	0.81	0.22	69,77,82,85	0
5	LFA	A	315	8/20	0.81	0.28	67,87,94,95	0
5	LFA	E	317	10/20	0.81	0.22	65,82,91,95	0
5	LFA	B	314	11/20	0.82	0.23	70,80,90,97	0
4	OLC	E	307	19/25	0.84	0.17	71,84,91,93	0
5	LFA	A	313	7/20	0.85	0.24	66,73,77,79	0
5	LFA	B	313	11/20	0.85	0.19	72,74,81,82	0
4	OLC	C	312	16/25	0.85	0.18	67,73,100,100	0
4	OLC	E	305	8/25	0.86	0.19	63,67,73,75	0
4	OLC	A	308	12/25	0.86	0.13	57,76,82,100	0
4	OLC	A	309	20/25	0.86	0.17	66,77,85,86	0
5	LFA	A	320	9/20	0.86	0.19	77,82,91,92	0
4	OLC	A	307	23/25	0.86	0.17	66,77,83,91	0
5	LFA	C	311	4/20	0.87	0.21	70,71,72,73	0
5	LFA	B	310	7/20	0.87	0.21	60,65,70,72	0
5	LFA	D	312	7/20	0.87	0.22	74,78,82,85	0
5	LFA	D	314	7/20	0.87	0.19	64,69,75,79	0
4	OLC	B	305	14/25	0.87	0.20	59,82,87,93	0
4	OLC	C	305	21/25	0.87	0.16	55,81,90,93	0
4	OLC	D	306	13/25	0.88	0.16	67,76,85,91	0
4	OLC	D	307	7/25	0.88	0.18	57,66,70,75	0
5	LFA	D	310	20/20	0.88	0.18	73,82,90,90	0
5	LFA	B	309	10/20	0.88	0.20	74,81,88,90	0
4	OLC	A	312	15/25	0.88	0.18	63,73,86,92	0
4	OLC	B	315	17/25	0.88	0.16	59,73,83,91	0
4	OLC	E	308	14/25	0.88	0.13	60,75,88,95	0
5	LFA	A	314	8/20	0.89	0.15	54,59,66,68	0
4	OLC	C	307	6/25	0.89	0.18	65,69,71,72	0
4	OLC	B	303	20/25	0.89	0.15	65,78,91,95	0
5	LFA	E	303	10/20	0.89	0.26	79,83,89,90	0
5	LFA	E	312	14/20	0.89	0.18	59,81,92,94	0
5	LFA	C	313	6/20	0.89	0.17	70,73,74,74	0
4	OLC	C	306	16/25	0.89	0.15	65,76,96,102	0
4	OLC	C	303	22/25	0.90	0.20	54,75,82,85	0
4	OLC	B	304	13/25	0.90	0.16	64,72,89,90	0
4	OLC	E	306	16/25	0.90	0.16	64,77,88,91	0
5	LFA	D	309	20/20	0.90	0.16	73,79,85,88	0
4	OLC	A	310	14/25	0.90	0.13	74,80,88,92	0

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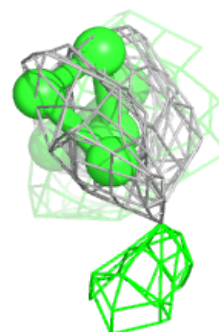
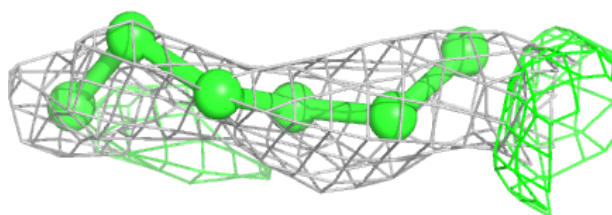
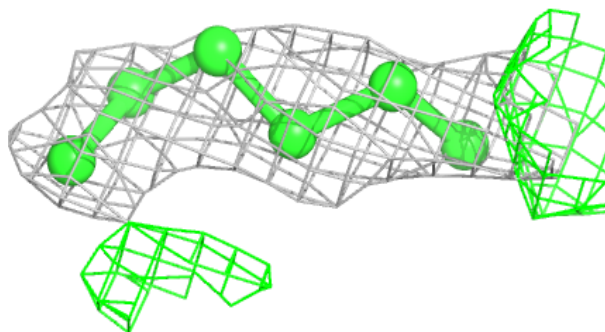
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	OLC	B	306	13/25	0.90	0.15	70,77,85,88	0
4	OLC	B	312	19/25	0.90	0.15	54,65,85,86	0
4	OLC	E	310	19/25	0.90	0.17	57,68,87,98	0
4	OLC	D	304	18/25	0.90	0.17	66,75,85,88	0
4	OLC	A	311	7/25	0.90	0.17	60,65,67,69	0
5	LFA	C	308	8/20	0.90	0.20	57,76,79,79	0
4	OLC	D	308	24/25	0.91	0.17	63,73,78,84	0
5	LFA	A	317	6/20	0.91	0.20	53,69,81,85	0
4	OLC	A	305	9/25	0.91	0.17	56,68,79,80	0
4	OLC	A	319	19/25	0.91	0.17	53,66,73,76	0
5	LFA	C	310	5/20	0.91	0.17	47,48,55,56	0
3	NA	D	302	1/1	0.91	0.09	42,42,42,42	0
5	LFA	E	314	5/20	0.91	0.20	63,63,73,75	0
5	LFA	B	308	8/20	0.91	0.19	60,70,73,83	0
4	OLC	A	303	16/25	0.91	0.17	63,70,79,80	0
4	OLC	E	304	18/25	0.92	0.17	60,69,82,83	0
5	LFA	E	311	8/20	0.92	0.15	49,69,75,75	0
4	OLC	E	318	22/25	0.92	0.16	52,69,80,81	0
5	LFA	E	313	4/20	0.92	0.20	67,68,68,75	0
4	OLC	C	316	23/25	0.92	0.17	56,76,83,89	0
5	LFA	D	313	6/20	0.92	0.18	51,64,69,70	0
4	OLC	D	303	17/25	0.92	0.15	63,69,90,90	0
4	OLC	A	321	22/25	0.93	0.14	51,70,79,83	0
4	OLC	D	305	16/25	0.93	0.13	62,70,79,82	0
5	LFA	E	315	7/20	0.93	0.16	49,65,68,75	0
4	OLC	C	315	15/25	0.93	0.14	60,70,75,81	0
5	LFA	C	309	20/20	0.93	0.14	59,68,84,85	0
5	LFA	D	311	17/20	0.94	0.13	45,55,60,61	0
4	OLC	C	304	22/25	0.94	0.13	47,58,84,87	0
4	OLC	A	306	19/25	0.94	0.13	39,53,79,80	0
4	OLC	A	304	23/25	0.94	0.15	60,70,82,84	0
2	RET	C	301	20/21	0.95	0.12	38,48,54,55	0
2	RET	D	301	20/21	0.95	0.11	45,49,55,56	0
2	RET	E	301	20/21	0.96	0.10	42,49,56,57	0
4	OLC	B	311	20/25	0.96	0.10	44,55,65,70	0
4	OLC	E	319	18/25	0.96	0.11	43,53,59,59	0
2	RET	A	301	20/21	0.97	0.10	39,45,52,54	0
2	RET	B	301	20/21	0.97	0.09	40,46,52,53	0
3	NA	E	302	1/1	0.97	0.04	39,39,39,39	0
3	NA	A	302	1/1	0.98	0.07	42,42,42,42	0
3	NA	C	302	1/1	0.99	0.03	41,41,41,41	0
3	NA	B	302	1/1	0.99	0.03	38,38,38,38	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.

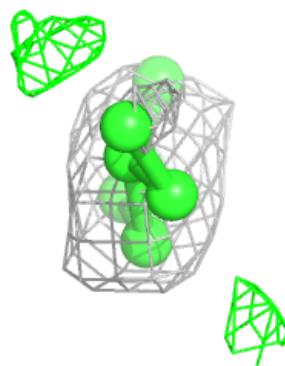
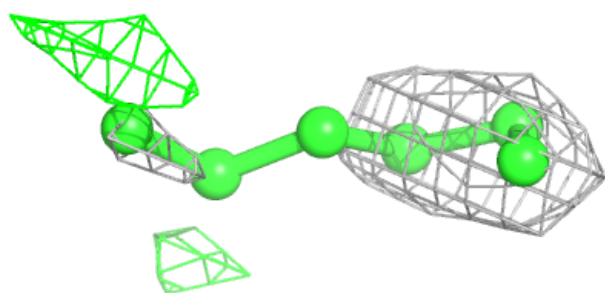
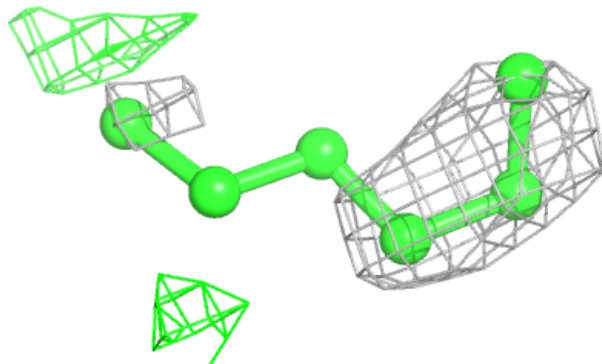
Electron density around LFA E 316:

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

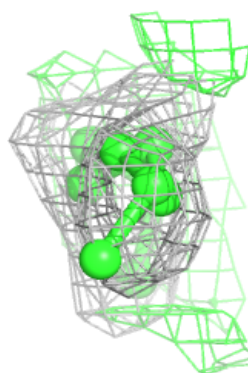
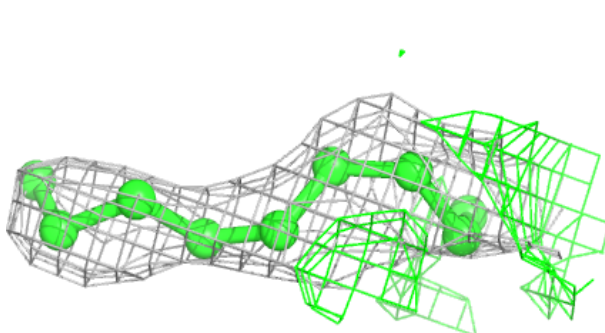
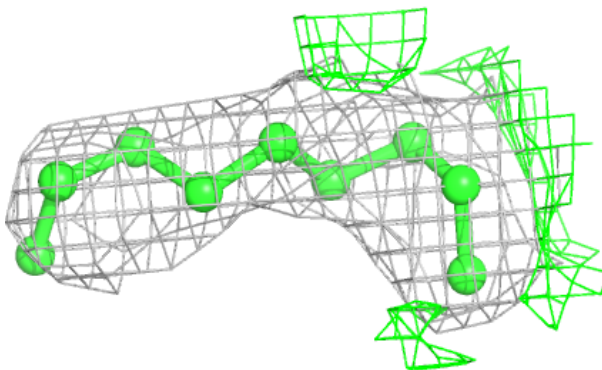


Electron density around OLC E 309:

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

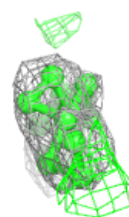
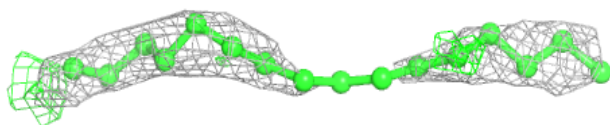
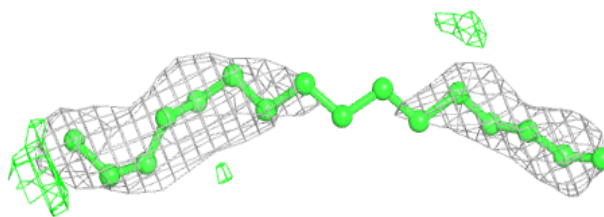
**Electron density around LFA B 307:**

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

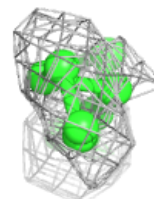
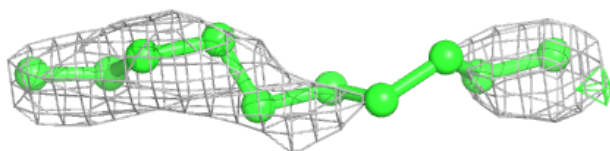
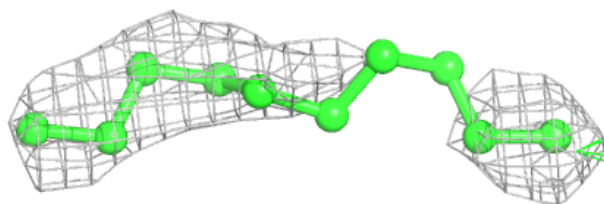


Electron density around LFA A 318:

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

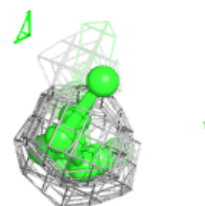
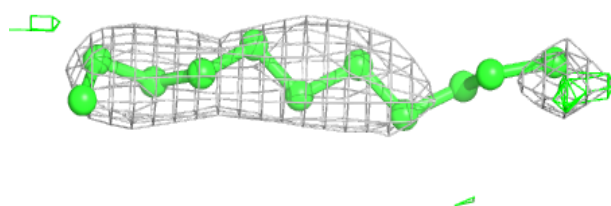
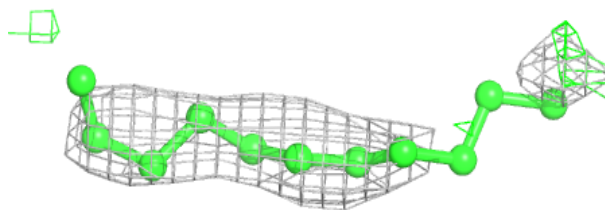
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

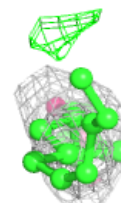
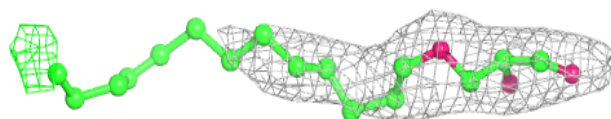
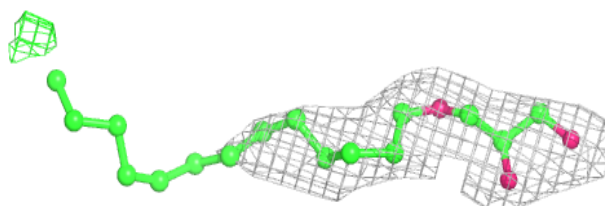


Electron density around LFA B 314:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

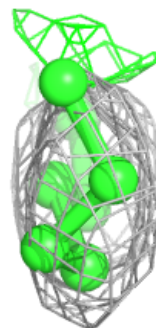
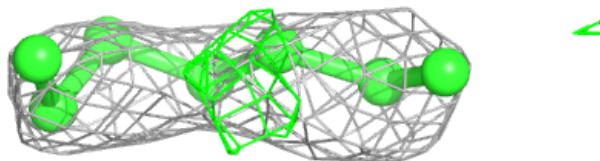
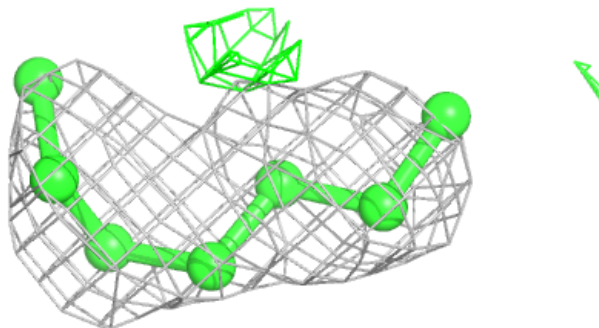
**Electron density around OLC E 307:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

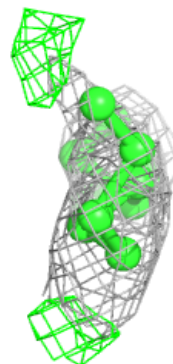
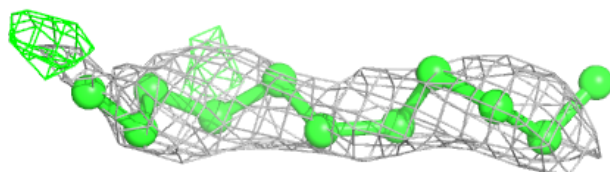
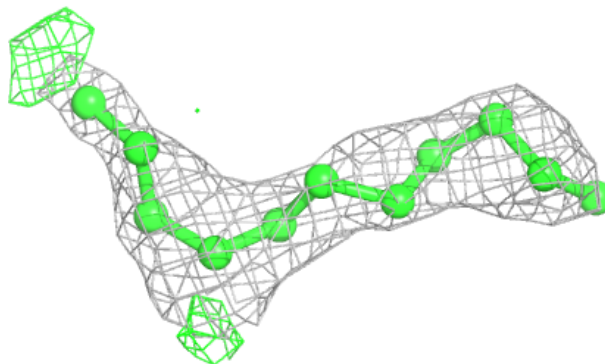


Electron density around LFA A 313:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

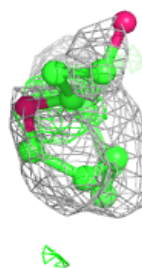
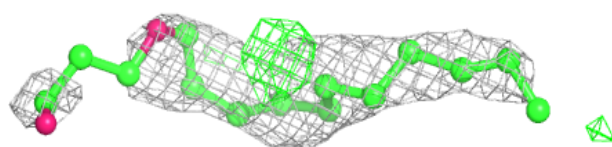
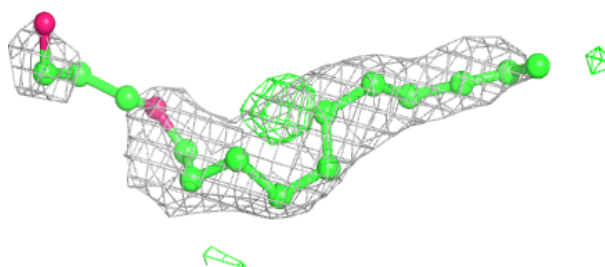
**Electron density around LFA B 313:**

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

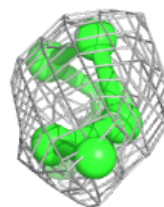
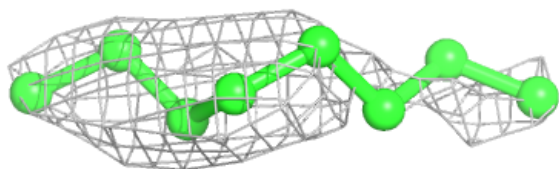
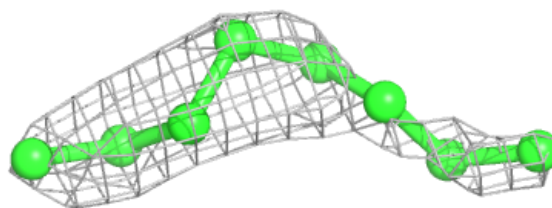


Electron density around OLC C 312:

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

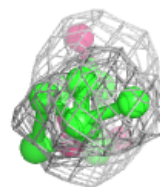
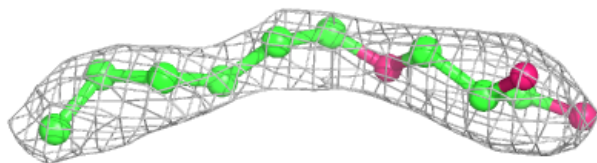
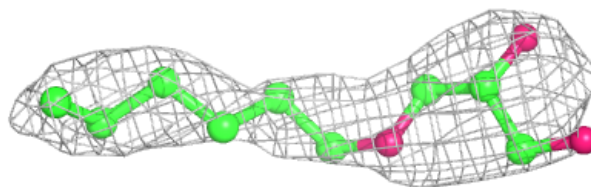
**Electron density around OLC E 305:**

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

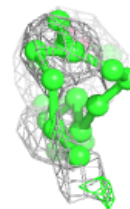
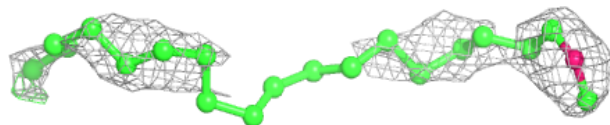
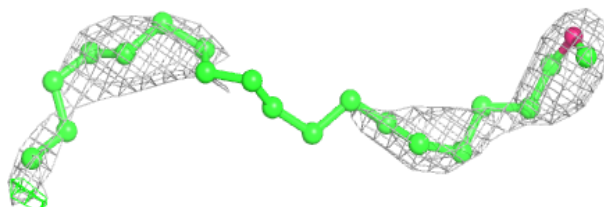


Electron density around OLC A 308:

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

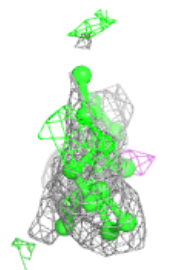
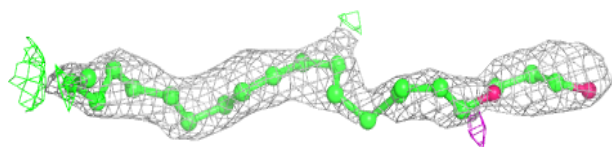
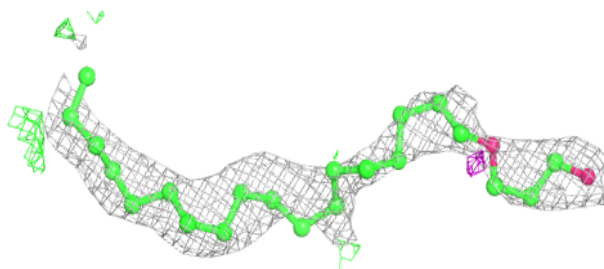
**Electron density around OLC A 309:**

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

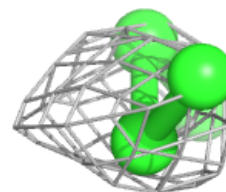
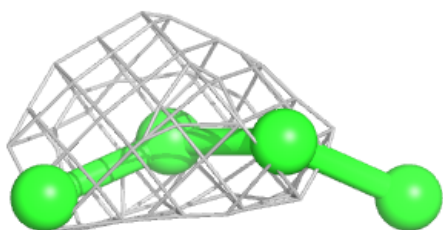
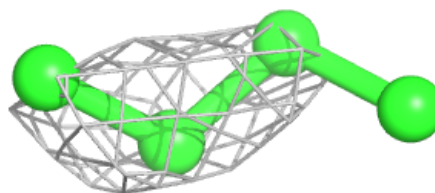


Electron density around OLC A 307:

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

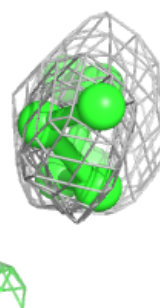
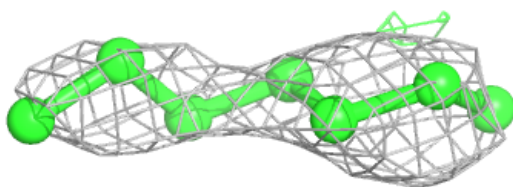
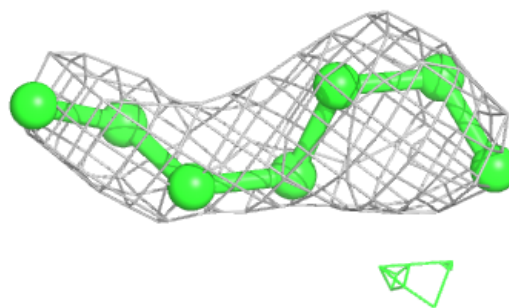
**Electron density around LFA C 311:**

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

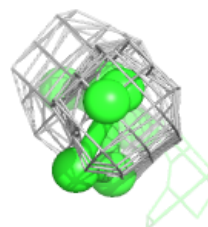
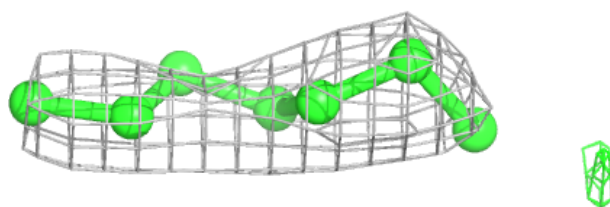
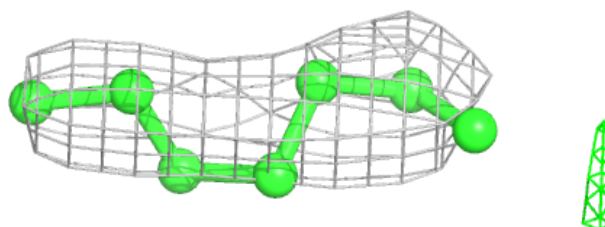


Electron density around LFA B 310:

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

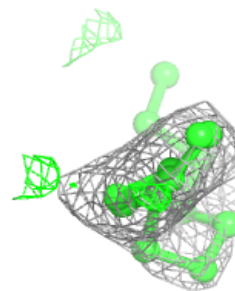
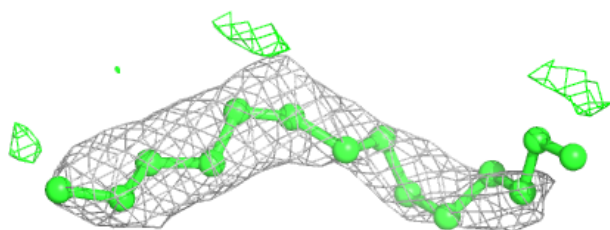
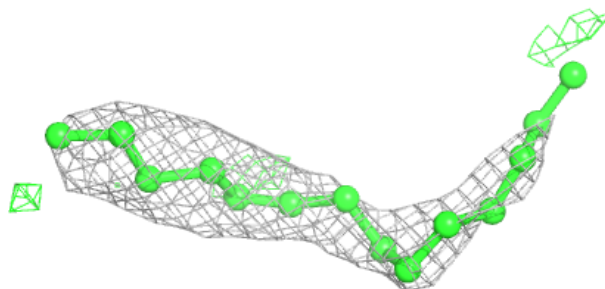
**Electron density around LFA D 314:**

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

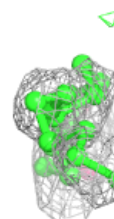
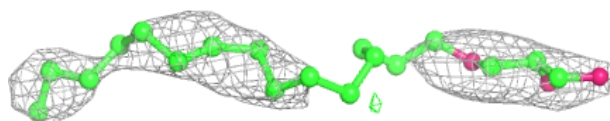
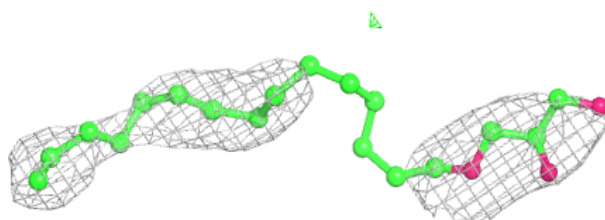


Electron density around OLC B 305:

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

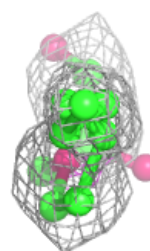
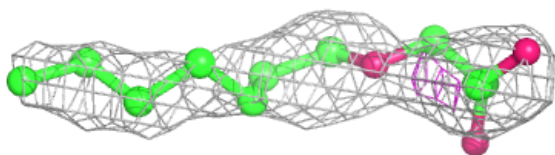
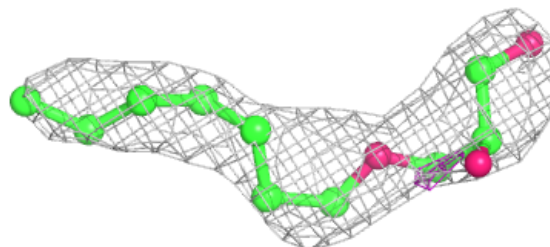
**Electron density around OLC C 305:**

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

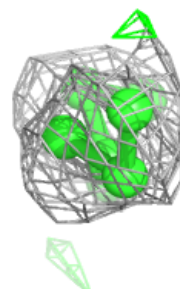
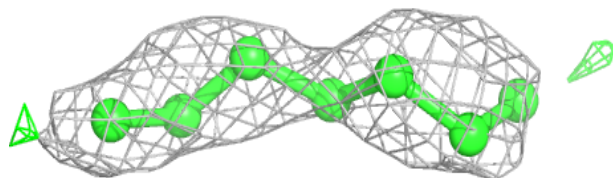
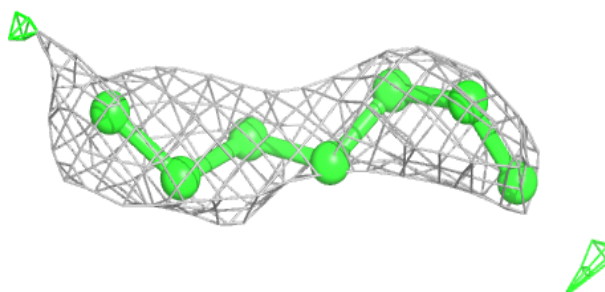


Electron density around OLC D 306:

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

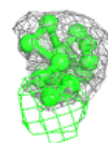
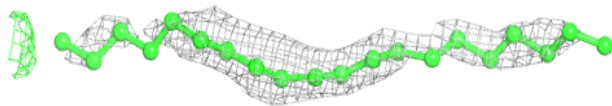
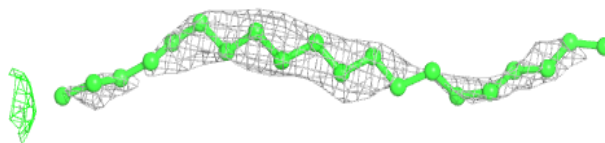
**Electron density around OLC D 307:**

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

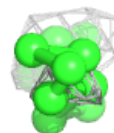
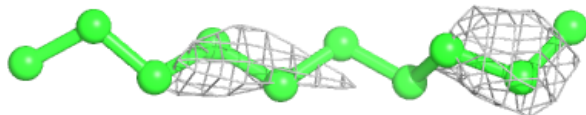
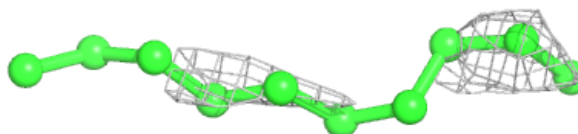


Electron density around LFA D 310:

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

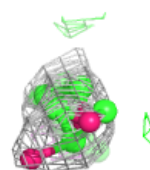
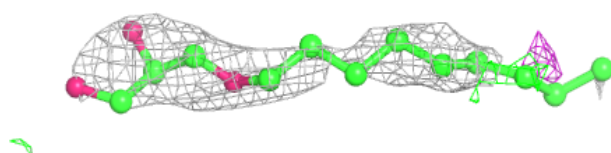
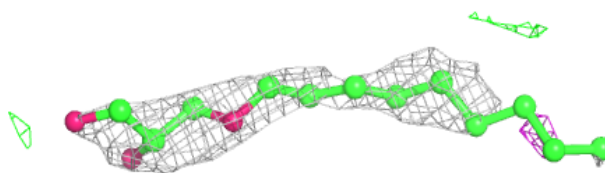
**Electron density around LFA B 309:**

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



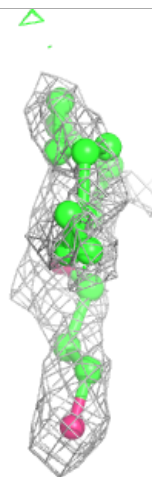
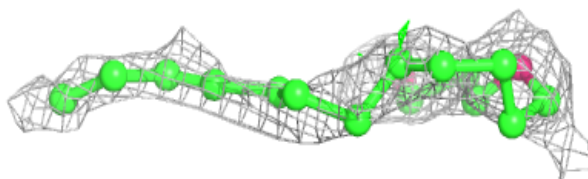
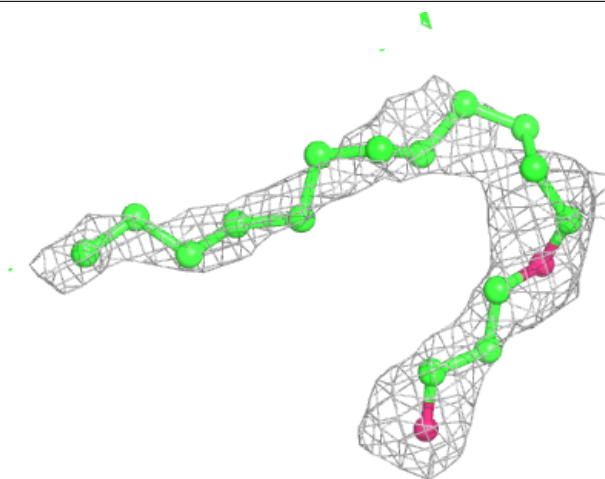
Electron density around OLC A 312:

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



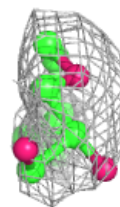
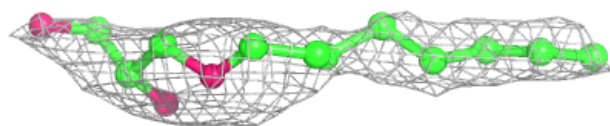
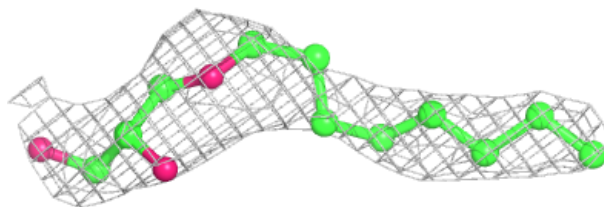
Electron density around OLC B 315:

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

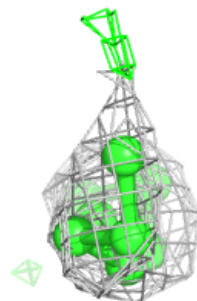
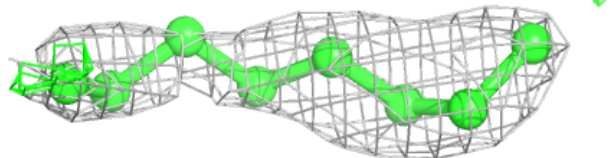
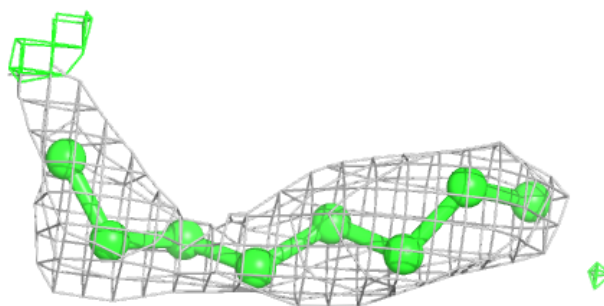


Electron density around OLC E 308:

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

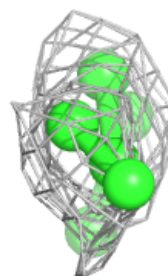
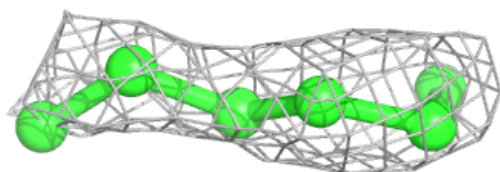
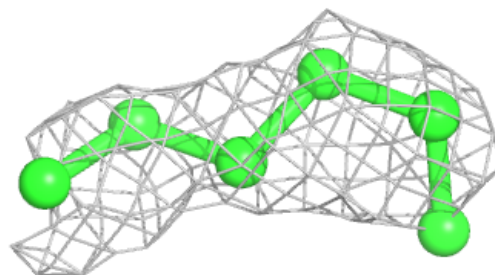
**Electron density around LFA A 314:**

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

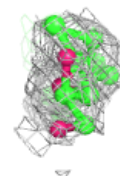
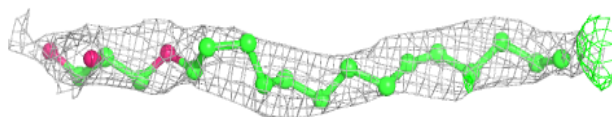
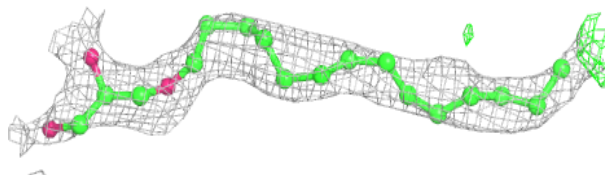


Electron density around OLC C 307:

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

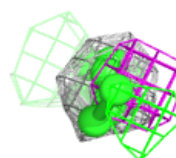
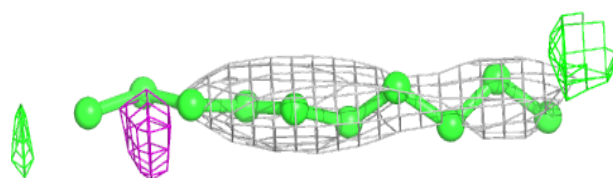
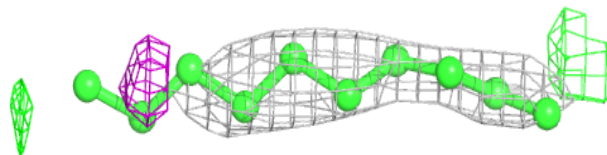
**Electron density around OLC B 303:**

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

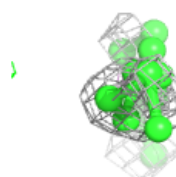
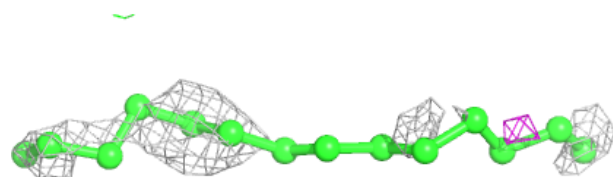
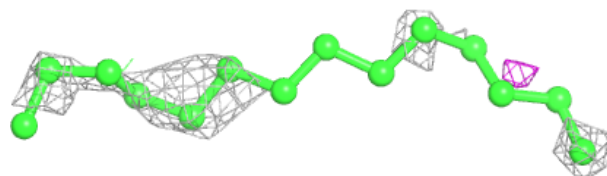


Electron density around LFA E 303:

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

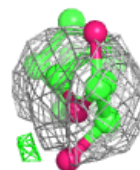
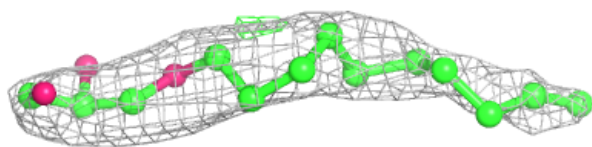
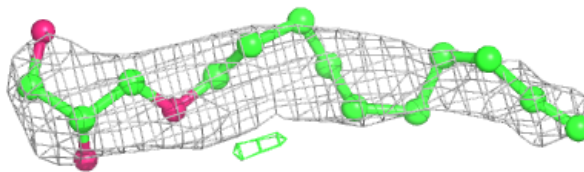
**Electron density around LFA E 312:**

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

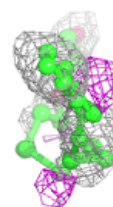
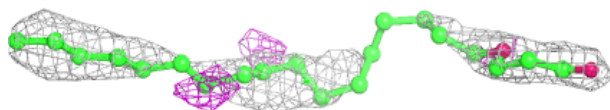
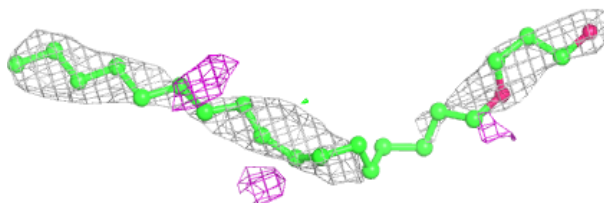


Electron density around OLC C 306:

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

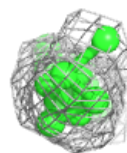
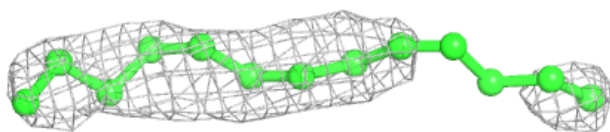
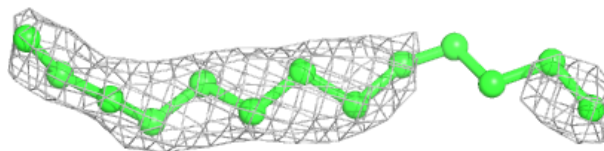
**Electron density around OLC C 303:**

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

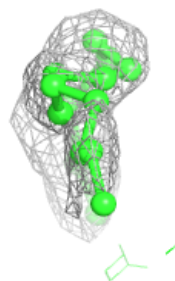
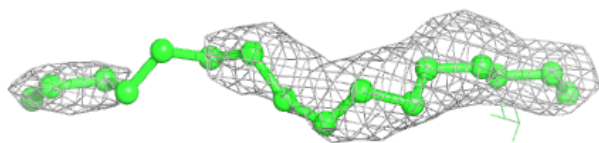
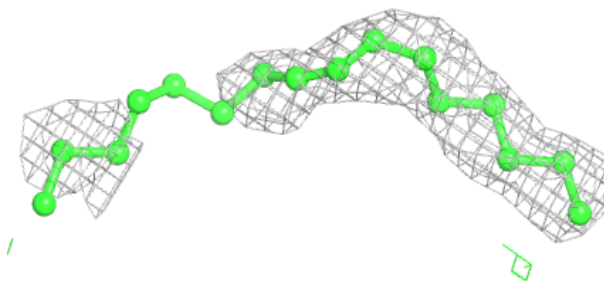


Electron density around OLC B 304:

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

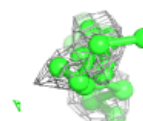
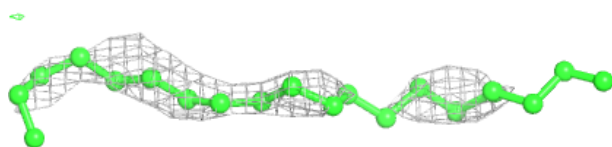
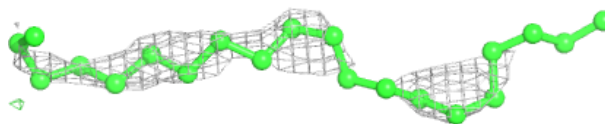
**Electron density around OLC E 306:**

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

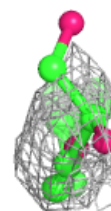
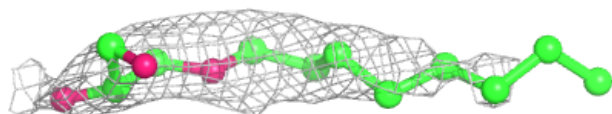
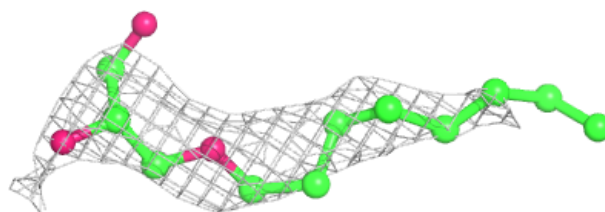


Electron density around LFA D 309:

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

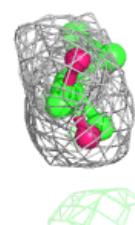
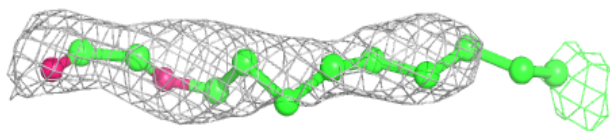
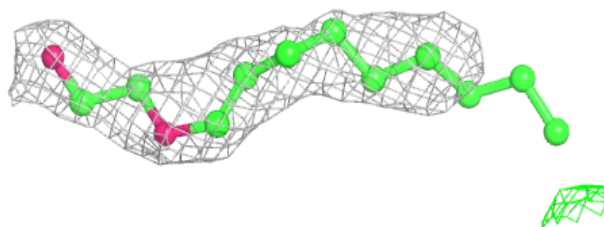
**Electron density around OLC A 310:**

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

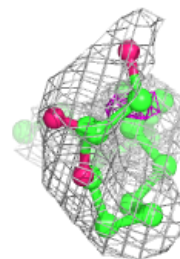
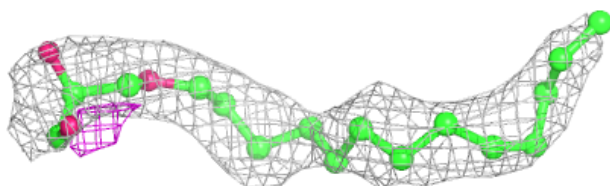
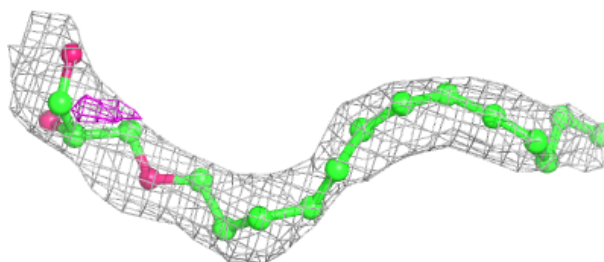


Electron density around OLC B 306:

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

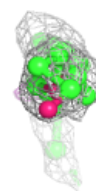
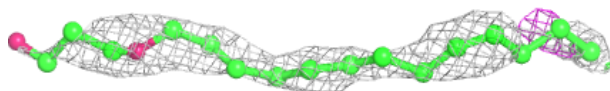
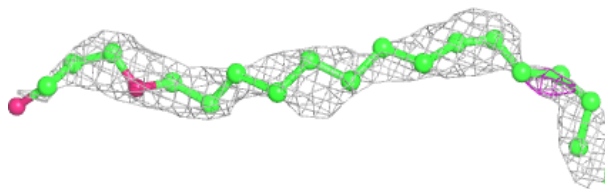
**Electron density around OLC B 312:**

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

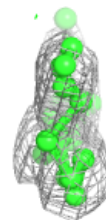
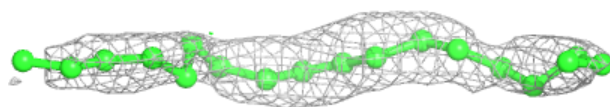
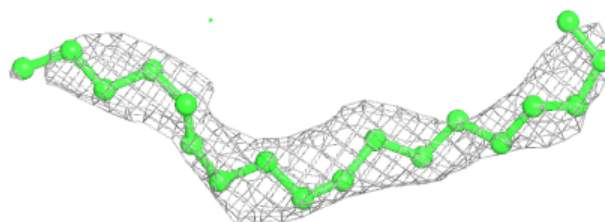


Electron density around OLC E 310:

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

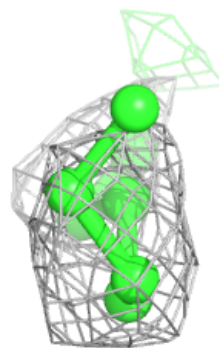
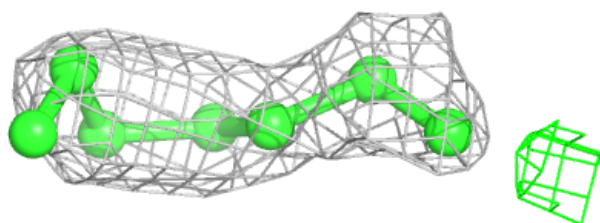
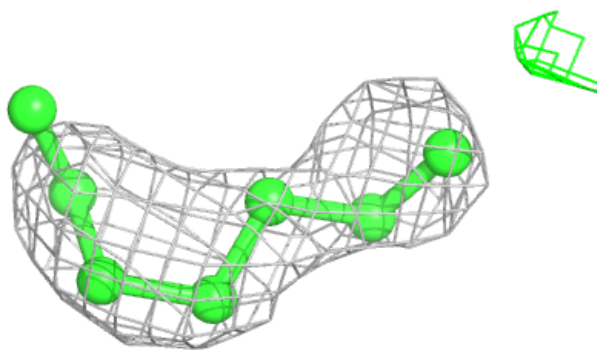
**Electron density around OLC D 304:**

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

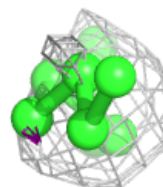
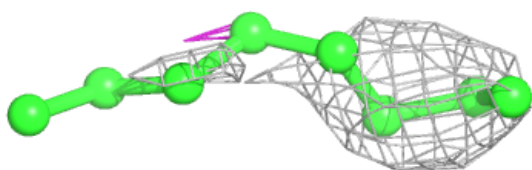
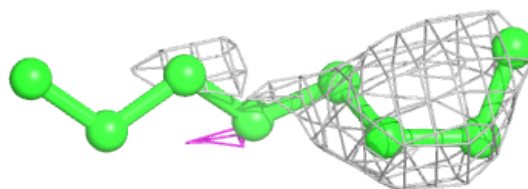


Electron density around OLC A 311:

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

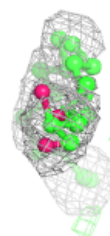
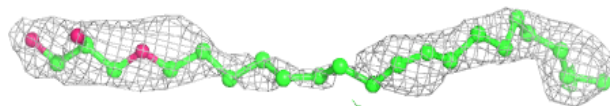
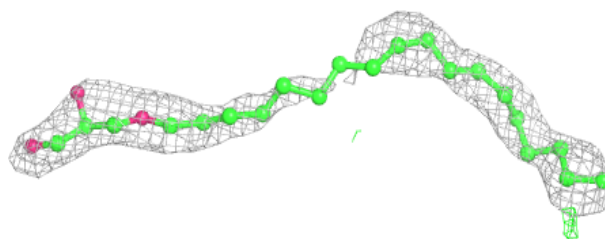
**Electron density around LFA C 308:**

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

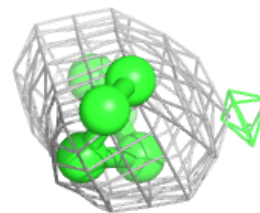
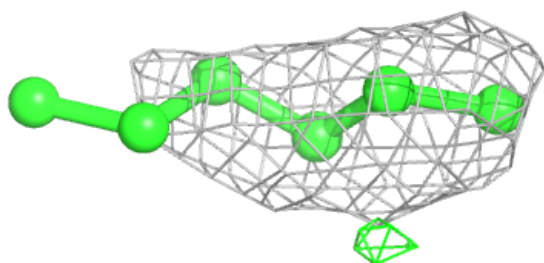
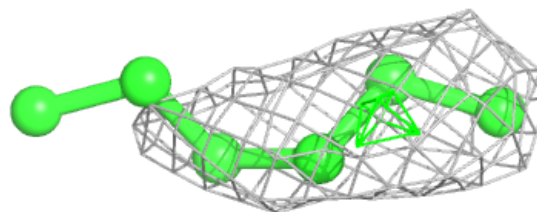


Electron density around OLC D 308:

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

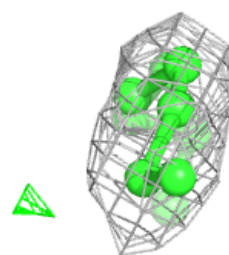
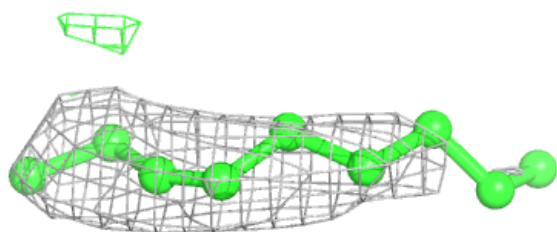
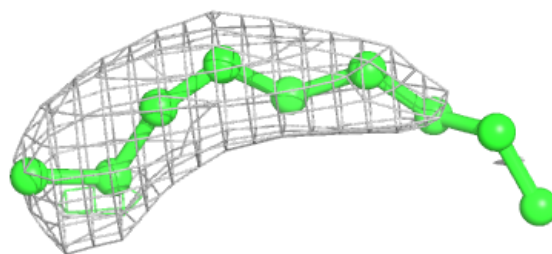
**Electron density around LFA A 317:**

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

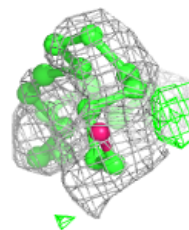
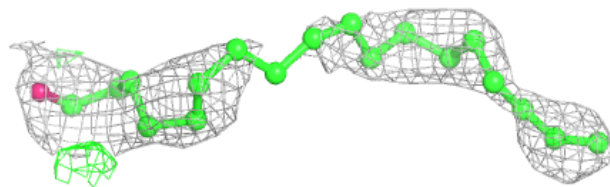
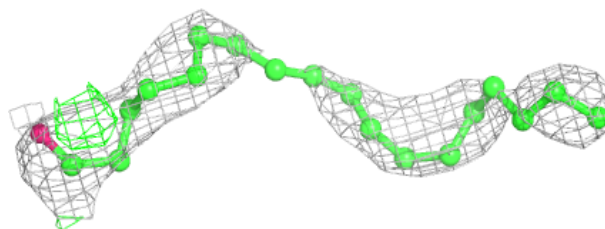


Electron density around OLC A 305:

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

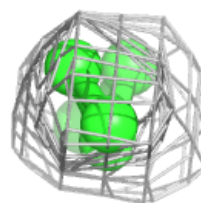
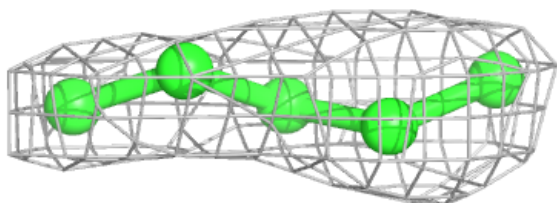
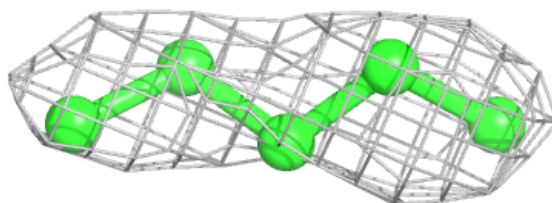
**Electron density around OLC A 319:**

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

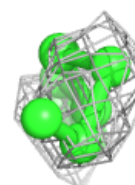
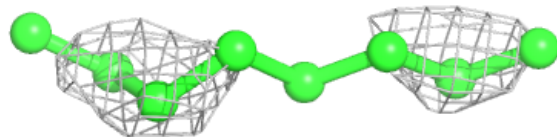
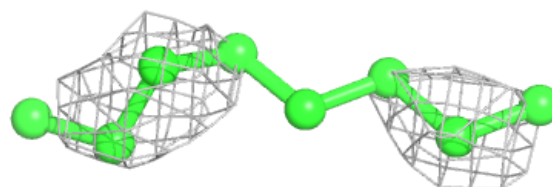


Electron density around LFA C 310:

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

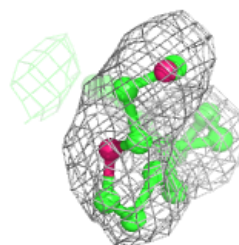
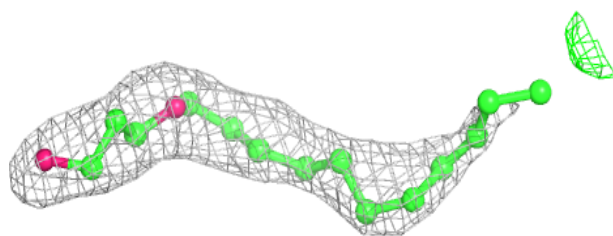
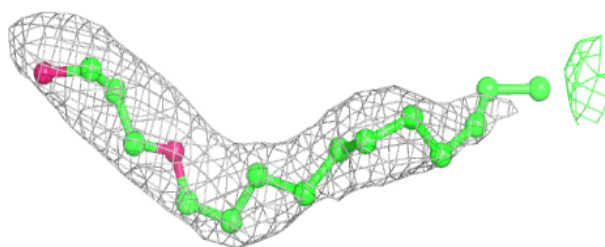
**Electron density around LFA B 308:**

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

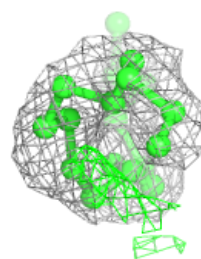
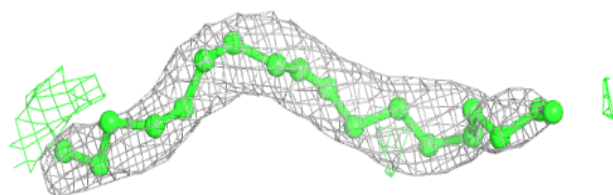
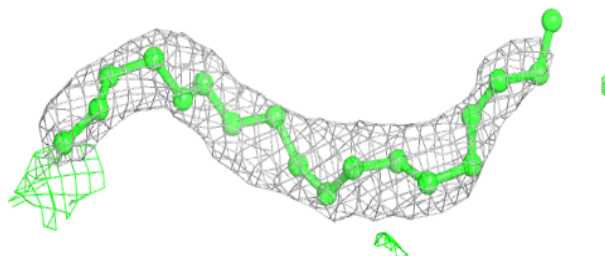


Electron density around OLC A 303:

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

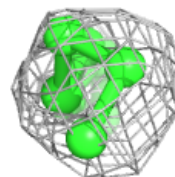
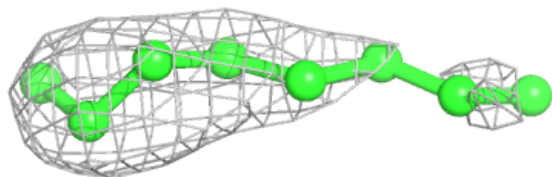
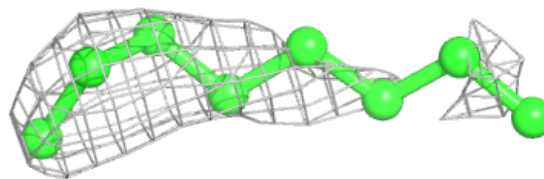
**Electron density around OLC E 304:**

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

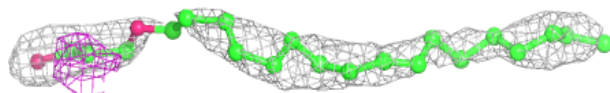
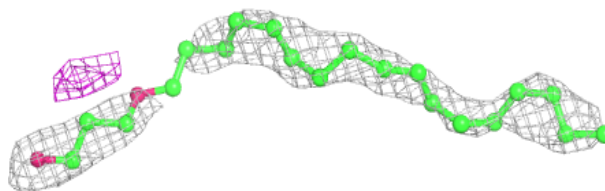


Electron density around LFA E 311:

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

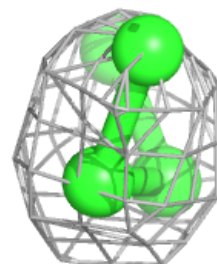
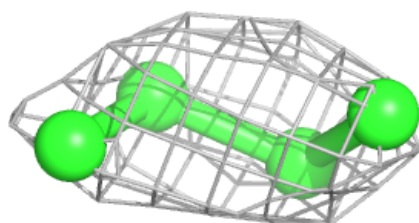
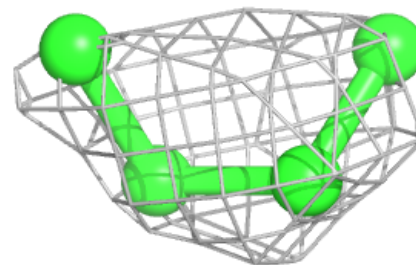
**Electron density around OLC E 318:**

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

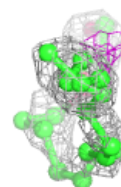
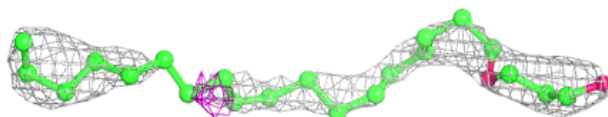
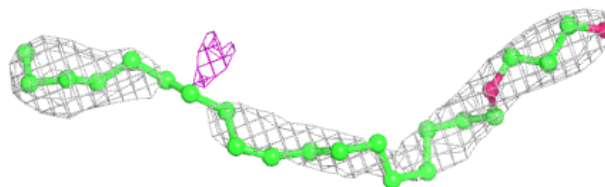


Electron density around LFA E 313:

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

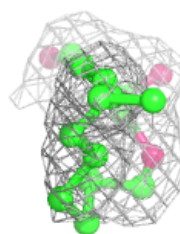
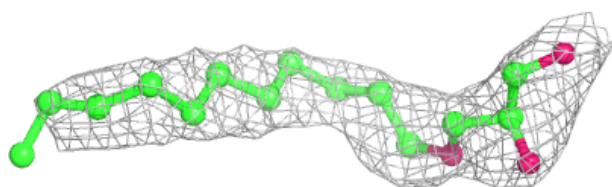
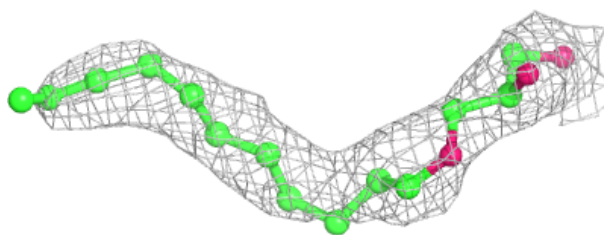
**Electron density around OLC C 316:**

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

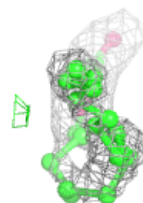
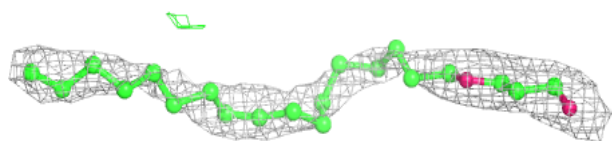
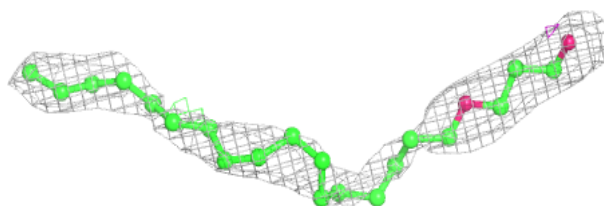


Electron density around OLC D 303:

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

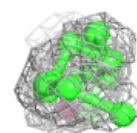
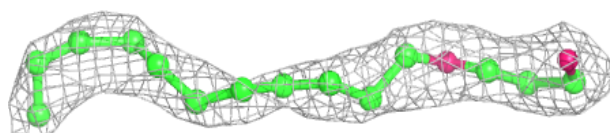
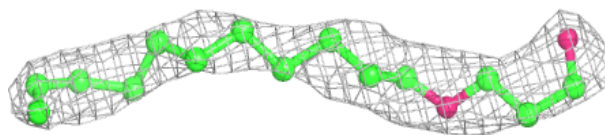
**Electron density around OLC A 321:**

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

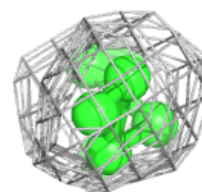
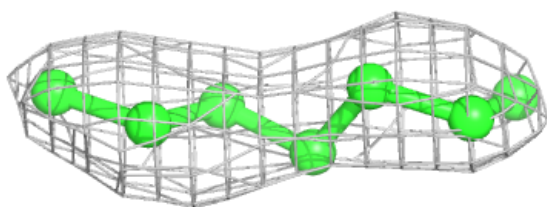
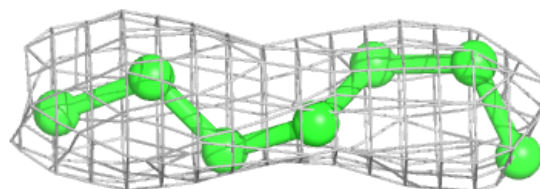


Electron density around OLC D 305:

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

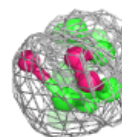
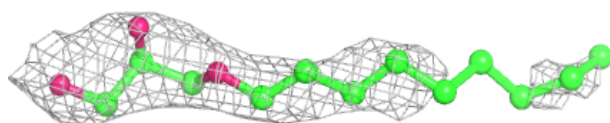
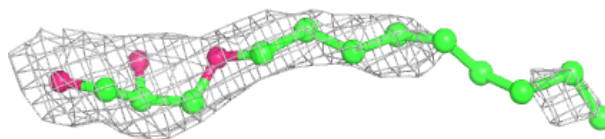
**Electron density around LFA E 315:**

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

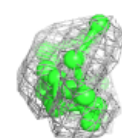
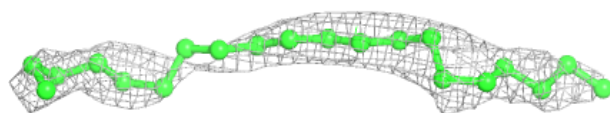
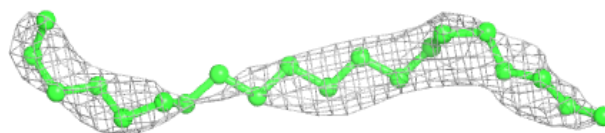


Electron density around OLC C 315:

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

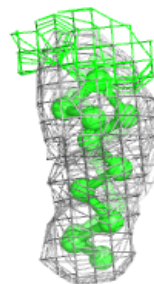
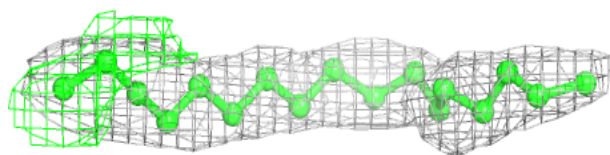
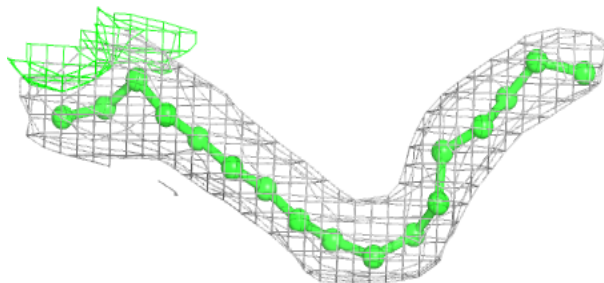
**Electron density around LFA C 309:**

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

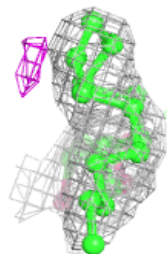
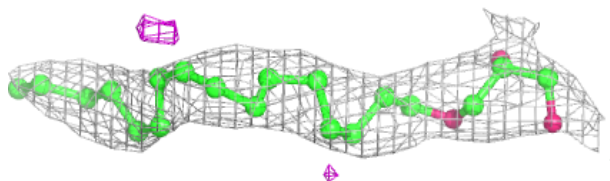
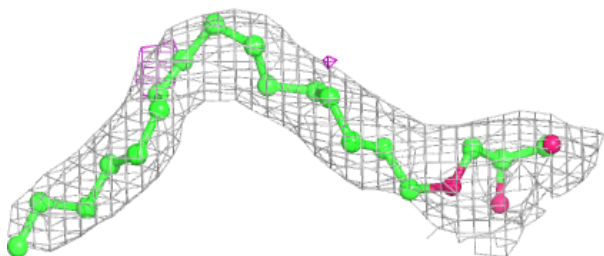


Electron density around LFA D 311:

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

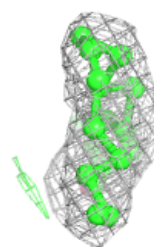
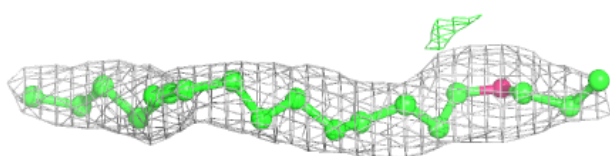
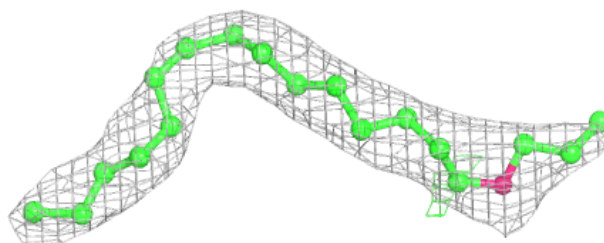
**Electron density around OLC C 304:**

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

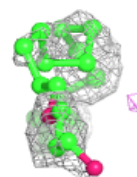
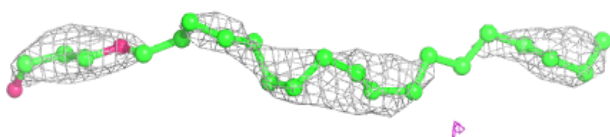
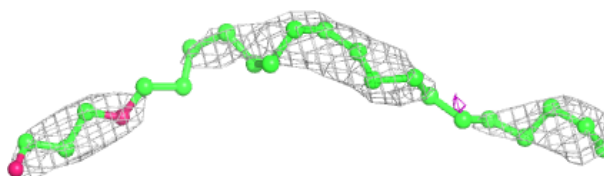


Electron density around OLC A 306:

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

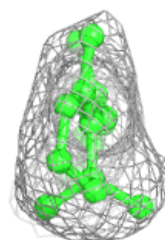
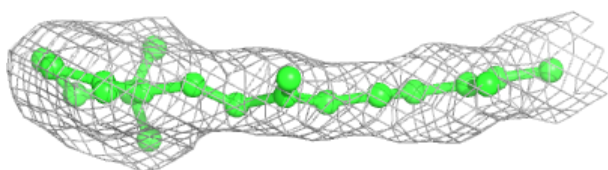
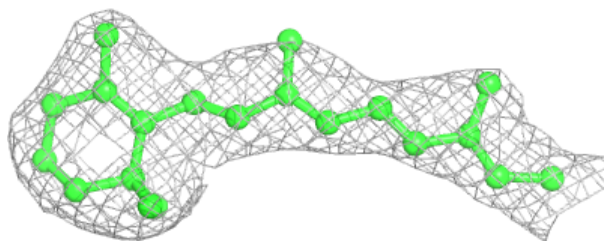
**Electron density around OLC A 304:**

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

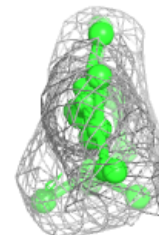
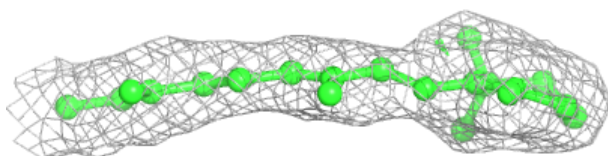
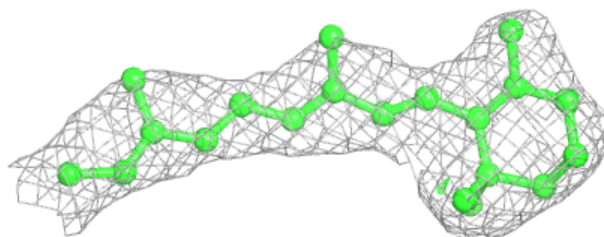


Electron density around RET C 301:

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

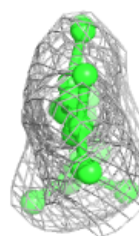
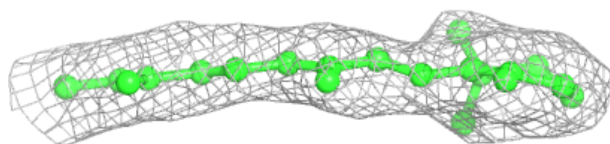
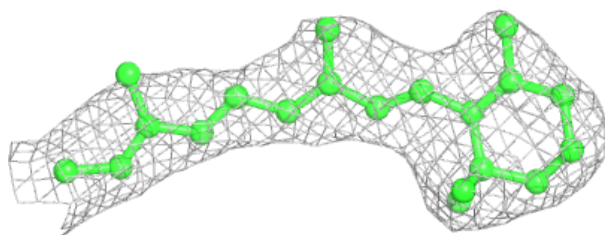
**Electron density around RET D 301:**

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

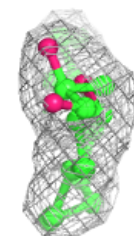
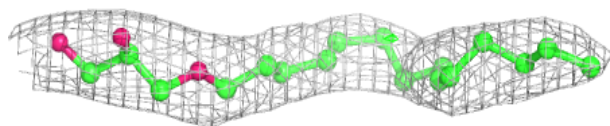
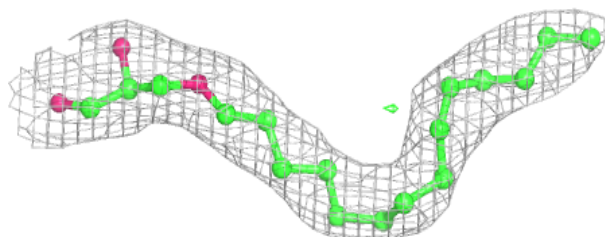


Electron density around RET E 301:

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

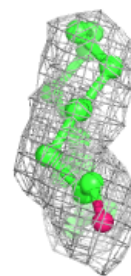
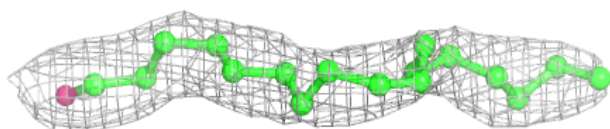
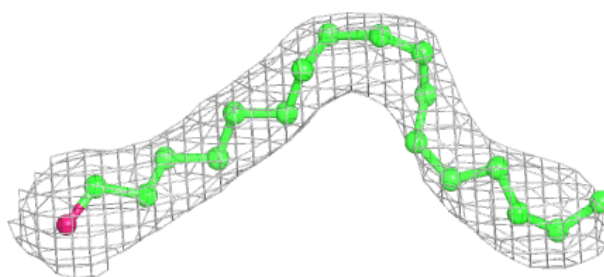
**Electron density around OLC B 311:**

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

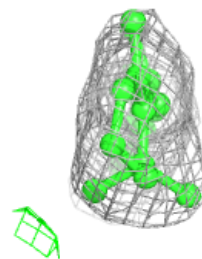
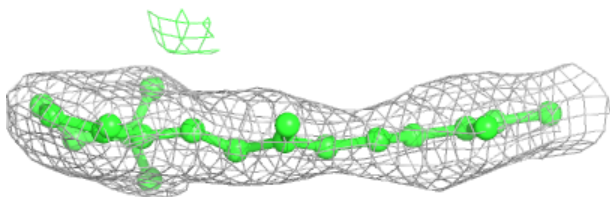
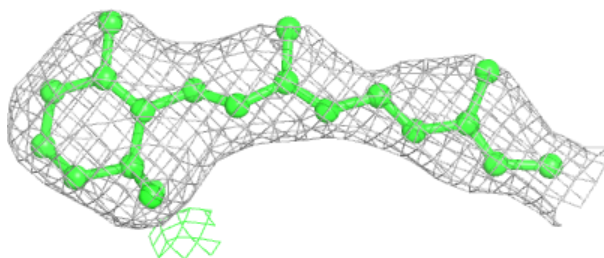


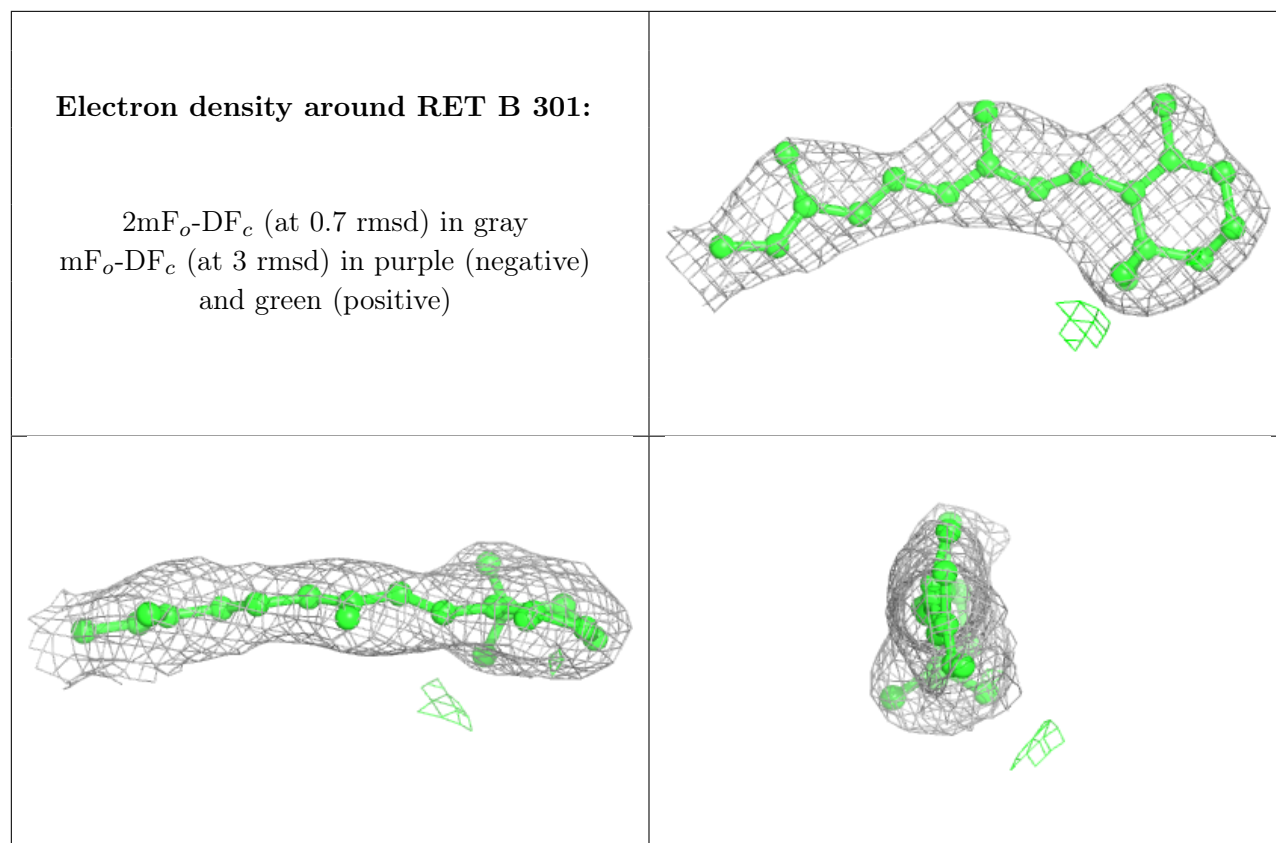
Electron density around OLC E 319:

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

**Electron density around RET 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.