



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 6YC1 / pdb_00006yc1
Title : Crystal structure of the H30A mutant of the light-driven sodium pump KR2 in the pentameric form, pH 8.0
Authors : Kovalev, K.; Gushchin, I.; Gordeliy, V.
Deposited on : 2020-03-18
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

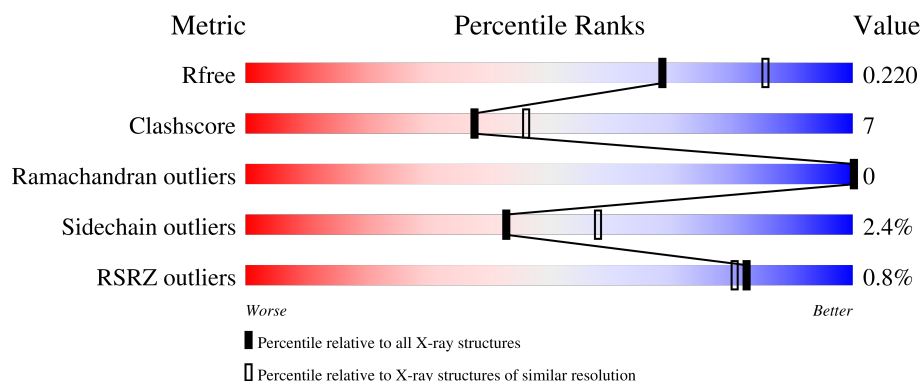
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	
1	B	273	
1	C	273	
1	D	273	
1	E	273	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

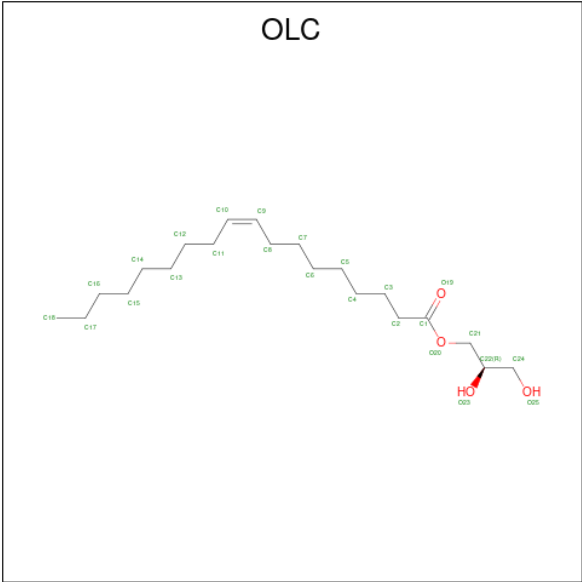
- Molecule 1 is a protein called Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	2	0
			2183	1456	328	390	9			
1	B	273	Total	C	N	O	S	0	2	0
			2180	1452	330	389	9			
1	C	273	Total	C	N	O	S	0	2	0
			2182	1455	328	390	9			
1	D	273	Total	C	N	O	S	0	2	0
			2177	1451	329	388	9			
1	E	273	Total	C	N	O	S	0	2	0
			2179	1453	329	388	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	HIS	conflict	UNP N0DKS8
B	30	ALA	HIS	conflict	UNP N0DKS8
C	30	ALA	HIS	conflict	UNP N0DKS8
D	30	ALA	HIS	conflict	UNP N0DKS8
E	30	ALA	HIS	conflict	UNP N0DKS8

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 9 9	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 13 9 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 15 11 4	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C O 19 17 2	0	0
2	A	1	Total C O 20 18 2	0	0
2	B	1	Total C O 22 18 4	0	0
2	B	1	Total C O 16 12 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 20 16 4	0	0
2	B	1	Total C O 21 17 4	0	0

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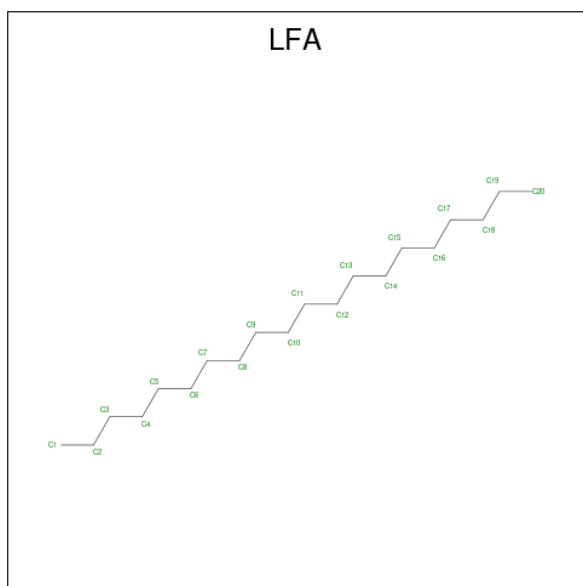
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 16 12 4	0	0
2	B	1	Total C 7 7	0	0
2	C	1	Total C O 21 17 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 12 8 4	0	0
2	C	1	Total C O 23 19 4	0	0
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C 7 7	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 16 12 4	0	0
2	D	1	Total C O 13 9 4	0	0
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 18 16 2	0	0
2	D	1	Total C O 14 10 4	0	0
2	D	1	Total C 7 7	0	0
2	D	1	Total C O 25 21 4	0	0
2	E	1	Total C O 25 21 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C 8 8	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 20 16 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C 6 6	0	0
2	E	1	Total C O 22 18 4	0	0
2	E	1	Total C O 20 16 4	0	0

- Molecule 3 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 20 20	0	0
3	A	1	Total C 9 9	0	0
3	B	1	Total C 20 20	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 4 4	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 4 4	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0

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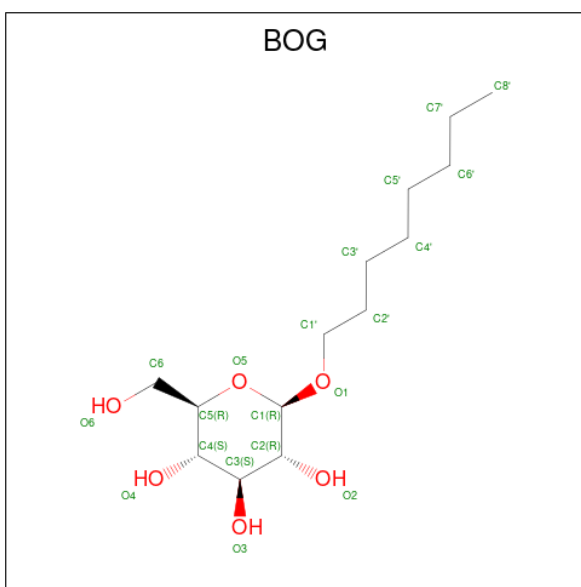
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 14 14	0	0
3	E	1	Total C 20 20	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

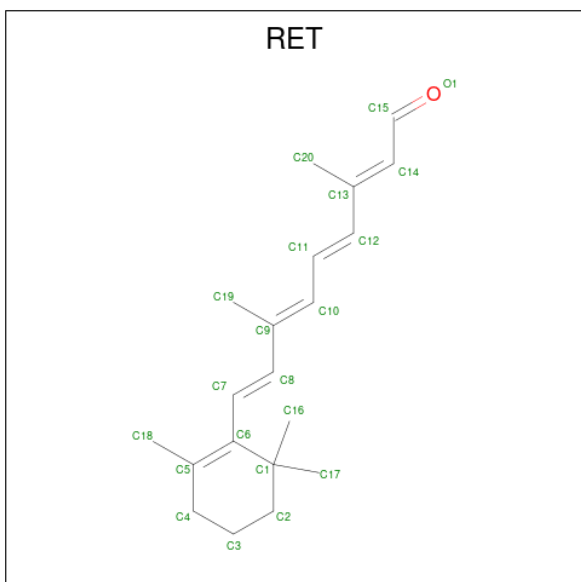
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0

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



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

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



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

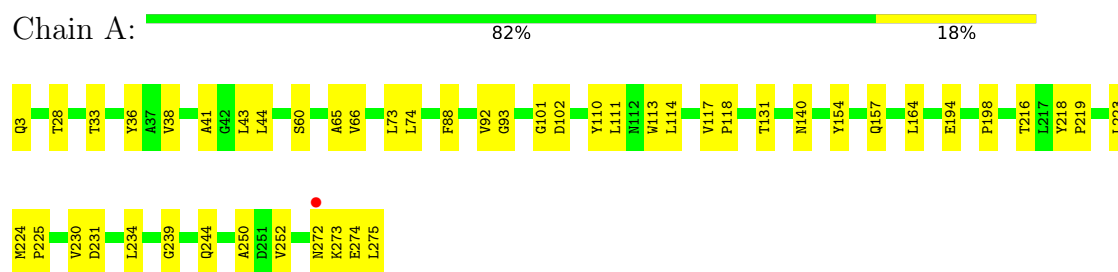
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	121	Total O 121 121	0	0
7	B	113	Total O 113 113	0	0
7	C	115	Total O 115 115	0	0
7	D	104	Total O 104 104	0	0
7	E	114	Total O 114 114	0	0

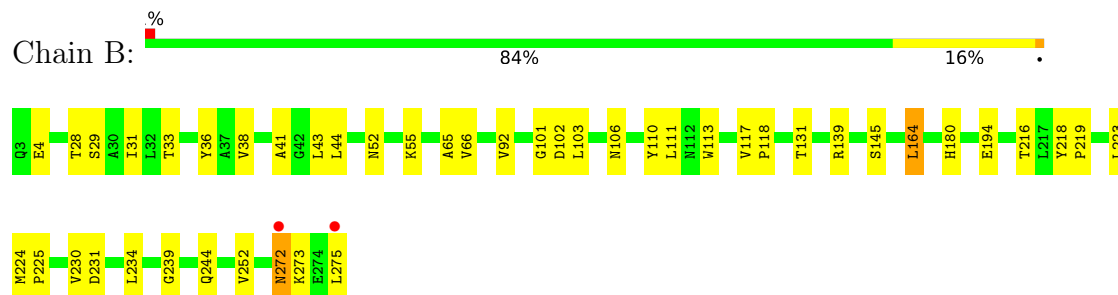
3 Residue-property plots

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

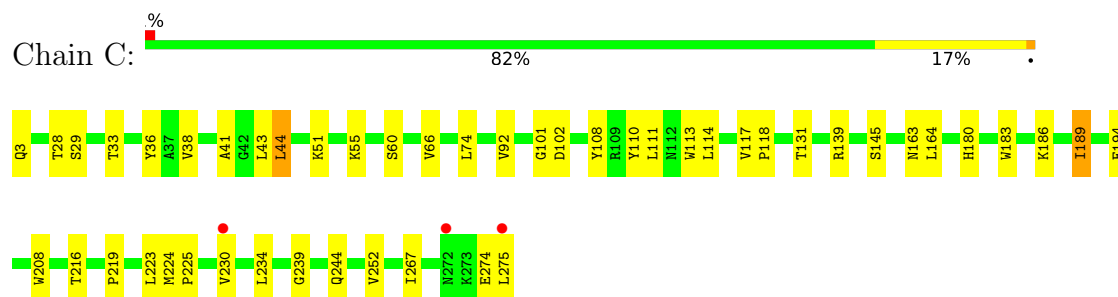
• Molecule 1: Sodium pumping rhodopsin



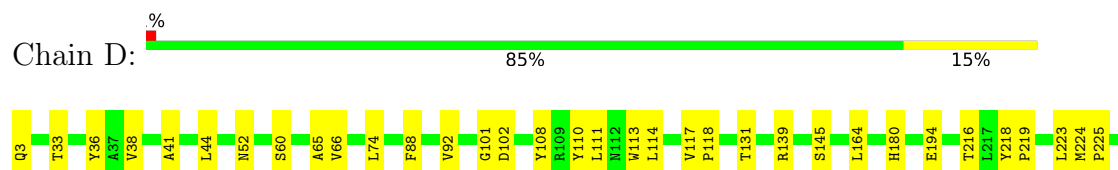
• Molecule 1: Sodium pumping rhodopsin

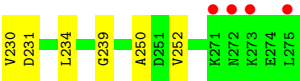


• Molecule 1: Sodium pumping rhodopsin

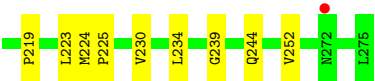
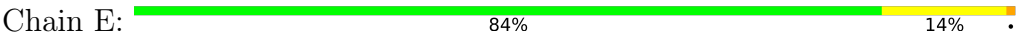


• Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.09Å 239.73Å 135.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.20) 98.6 (20.00-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.181 , 0.209 0.195 , 0.220	Depositor DCC
R_{free} test set	5272 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12783	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: NA, RET, OLC, LFA, BOG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.94	0/2241	1.48	0/3047
1	B	0.94	0/2238	1.47	0/3044
1	C	0.94	0/2240	1.48	0/3046
1	D	0.94	0/2235	1.49	0/3039
1	E	0.94	0/2237	1.48	0/3042
All	All	0.94	0/11191	1.48	0/15218

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	2183	0	2156	33	0
1	B	2180	0	2155	38	0
1	C	2182	0	2154	42	0
1	D	2177	0	2148	30	0
1	E	2179	0	2155	32	0
2	A	155	0	228	5	0
2	B	127	0	178	5	0
2	C	163	0	222	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	154	0	215	3	0
2	E	147	0	209	3	0
3	A	78	0	151	0	0
3	B	58	0	113	0	0
3	C	65	0	127	8	0
3	D	112	0	225	3	0
3	E	51	0	100	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	A	20	0	28	2	0
5	B	20	0	28	2	0
5	C	20	0	28	1	0
5	D	20	0	28	2	0
5	E	20	0	28	0	0
6	A	20	0	27	4	0
6	B	20	0	27	3	0
6	C	20	0	27	2	0
6	D	20	0	27	2	0
6	E	20	0	27	3	0
7	A	121	0	0	3	0
7	B	113	0	0	2	0
7	C	115	0	0	3	0
7	D	104	0	0	5	0
7	E	114	0	0	2	0
All	All	12783	0	12811	174	0

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

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:HD22	1:B:272:ASN:N	1.64	0.94
6:D:319:RET:H161	6:D:319:RET:H8	1.61	0.82
6:B:315:RET:H161	6:B:315:RET:H8	1.62	0.82
6:C:318:RET:H161	6:C:318:RET:H8	1.62	0.81
6:A:316:RET:H161	6:A:316:RET:H8	1.63	0.80
6:E:317:RET:H8	6:E:317:RET:H161	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:GLN:HG2	7:D:434:HOH:O	1.84	0.77
1:B:145:SER:OG	1:B:180:HIS:HD2	1.69	0.75
2:D:310:OLC:H11A	3:D:314:LFA:H12	1.68	0.75
1:A:3:GLN:HG2	7:E:412:HOH:O	1.87	0.74
1:B:272:ASN:N	1:B:272:ASN:ND2	2.35	0.73
1:E:145:SER:OG	1:E:180:HIS:HD2	1.73	0.71
1:C:145:SER:OG	1:C:180:HIS:HD2	1.72	0.70
1:D:231:ASP:N	5:D:318:BOG:O6	2.15	0.70
1:D:145:SER:OG	1:D:180:HIS:HD2	1.73	0.70
1:D:52:ASN:OD1	7:D:403:HOH:O	2.13	0.66
1:B:272:ASN:HD22	1:B:272:ASN:H	1.42	0.65
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.79	0.64
1:E:234:LEU:O	1:E:239:GLY:HA3	1.97	0.64
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.80	0.64
1:A:234:LEU:O	1:A:239:GLY:HA3	1.98	0.64
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.80	0.64
1:B:44:LEU:HD21	1:C:43:LEU:HD11	1.80	0.63
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.78	0.63
1:D:234:LEU:O	1:D:239:GLY:HA3	1.99	0.63
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.80	0.63
1:B:234:LEU:O	1:B:239:GLY:HA3	1.98	0.62
1:C:55:LYS:NZ	7:C:402:HOH:O	2.12	0.62
1:C:164:LEU:HD21	5:C:317:BOG:H2'1	1.81	0.62
1:B:272:ASN:ND2	1:B:272:ASN:H	1.95	0.62
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.81	0.62
1:A:44:LEU:HD21	1:B:43:LEU:HD11	1.81	0.61
1:C:234:LEU:O	1:C:239:GLY:HA3	2.01	0.61
1:E:141:GLN:HG2	2:E:304:OLC:H5A	1.82	0.60
6:D:319:RET:H161	6:D:319:RET:C8	2.32	0.60
1:A:231:ASP:H	5:A:315:BOG:HO6	1.44	0.59
1:C:186:LYS:HG2	3:C:311:LFA:C5	2.34	0.57
1:B:231:ASP:N	5:B:314:BOG:O6	2.24	0.57
2:C:305:OLC:H13	2:D:301:OLC:H4A	1.86	0.57
7:B:420:HOH:O	1:C:3:GLN:HB2	2.05	0.57
1:C:189:ILE:HD12	1:C:208:TRP:HB2	1.86	0.57
1:C:131:THR:HG21	1:C:194:GLU:OE1	2.06	0.56
1:A:272:ASN:CB	1:A:273:LYS:HE3	2.37	0.55
1:C:183:TRP:CE3	3:C:311:LFA:H41	2.41	0.55
1:E:141:GLN:HG2	2:E:304:OLC:C5	2.37	0.55
1:B:139:ARG:NH1	2:B:301:OLC:H24A	2.22	0.55
1:C:183:TRP:CZ3	3:C:311:LFA:H61	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:LYS:HG2	3:C:311:LFA:H51	1.90	0.54
1:E:18:GLU:OE1	7:E:403:HOH:O	2.19	0.53
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.90	0.53
6:A:316:RET:H161	6:A:316:RET:C8	2.33	0.53
1:C:139:ARG:NH2	3:C:313:LFA:H203	2.22	0.53
1:C:275:LEU:CD2	2:C:305:OLC:O23	2.56	0.53
1:B:131:THR:HG21	1:B:194:GLU:OE1	2.09	0.53
6:E:317:RET:H161	6:E:317:RET:C8	2.33	0.53
1:E:223:LEU:C	1:E:225:PRO:HD2	2.35	0.52
1:B:139:ARG:NH2	2:B:304:OLC:H21A	2.25	0.52
1:B:139:ARG:HH11	2:B:301:OLC:H24A	1.75	0.52
1:C:44:LEU:CD1	1:D:65:ALA:HB1	2.40	0.52
1:E:111:LEU:O	1:E:114:LEU:HB2	2.10	0.52
1:E:189:ILE:HD12	1:E:208:TRP:HB2	1.92	0.51
1:A:275:LEU:HD21	2:A:302:OLC:H24A	1.93	0.51
1:A:131:THR:HG21	1:A:194:GLU:OE1	2.11	0.51
1:A:110:TYR:O	1:A:113:TRP:HB2	2.11	0.51
1:A:275:LEU:CD2	2:A:302:OLC:H24A	2.41	0.51
1:A:223:LEU:C	1:A:225:PRO:HD2	2.34	0.51
6:B:315:RET:H161	6:B:315:RET:C8	2.32	0.51
1:C:223:LEU:C	1:C:225:PRO:HD2	2.35	0.51
1:B:223:LEU:C	1:B:225:PRO:HD2	2.37	0.50
1:D:131:THR:HG21	1:D:194:GLU:OE1	2.10	0.50
1:A:224:MET:N	1:A:225:PRO:HD2	2.26	0.50
1:B:139:ARG:HH11	2:B:301:OLC:C24	2.25	0.50
3:C:304:LFA:H172	3:D:303:LFA:H61	1.94	0.50
1:B:139:ARG:NH1	2:B:301:OLC:C24	2.74	0.49
1:D:223:LEU:C	1:D:225:PRO:HD2	2.37	0.49
1:B:224:MET:N	1:B:225:PRO:HD2	2.27	0.49
1:C:110:TYR:O	1:C:113:TRP:HB2	2.12	0.49
1:B:110:TYR:O	1:B:113:TRP:HB2	2.12	0.49
1:E:110:TYR:O	1:E:113:TRP:HB2	2.12	0.49
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.93	0.49
1:E:101:GLY:O	1:E:102:ASP:HB2	2.12	0.49
1:C:224:MET:N	1:C:225:PRO:HD2	2.27	0.49
1:B:44:LEU:CD2	1:C:43:LEU:HD11	2.43	0.48
1:D:224:MET:N	1:D:225:PRO:HD2	2.28	0.48
1:A:164:LEU:HD21	5:A:315:BOG:H2'1	1.95	0.48
1:E:131:THR:HG21	1:E:194:GLU:OE1	2.13	0.48
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.95	0.48
1:C:101:GLY:O	1:C:102:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:TYR:O	1:D:113:TRP:HB2	2.13	0.48
6:C:318:RET:H161	6:C:318:RET:C8	2.33	0.48
1:A:101:GLY:O	1:A:102:ASP:HB2	2.15	0.47
1:D:101:GLY:O	1:D:102:ASP:HB2	2.14	0.47
1:D:60:SER:CB	7:D:404:HOH:O	2.61	0.47
1:E:224:MET:N	1:E:225:PRO:HD2	2.28	0.47
1:B:101:GLY:O	1:B:102:ASP:HB2	2.15	0.47
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.96	0.47
1:D:38:VAL:HG11	1:D:252:VAL:HG22	1.97	0.47
1:B:216:THR:O	1:B:219:PRO:HG2	2.15	0.47
1:C:163:ASN:HD22	2:C:309:OLC:C24	2.28	0.47
1:C:114:LEU:HD22	2:C:302:OLC:H10	1.96	0.46
1:A:140:ASN:HB3	2:A:303:OLC:H2A	1.96	0.46
1:C:216:THR:O	1:C:219:PRO:HG2	2.15	0.46
1:D:44:LEU:HD21	1:E:43:LEU:HD11	1.97	0.46
1:E:216:THR:O	1:E:219:PRO:HG2	2.16	0.46
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.81	0.46
1:C:275:LEU:HD21	2:C:305:OLC:O23	2.16	0.46
1:C:38:VAL:HG11	1:C:252:VAL:HG22	1.97	0.45
1:D:41:ALA:HB1	1:E:66:VAL:HG13	1.97	0.45
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.81	0.45
1:A:216:THR:O	1:A:219:PRO:HG2	2.16	0.45
1:D:60:SER:HB3	7:D:404:HOH:O	2.14	0.45
1:C:33:THR:HG21	1:D:108[A]:TYR:CZ	2.52	0.45
1:C:44:LEU:HD11	1:D:65:ALA:HB1	1.97	0.45
1:A:198:PRO:HD2	7:A:488:HOH:O	2.16	0.45
1:C:186:LYS:HG2	3:C:311:LFA:H52	1.98	0.45
1:A:65:ALA:HB1	1:E:44:LEU:CD1	2.46	0.45
1:B:33:THR:HA	1:B:36:TYR:CE2	2.52	0.45
1:D:216:THR:O	1:D:219:PRO:HG2	2.15	0.45
1:B:52:ASN:O	1:B:273:LYS:HG3	2.17	0.45
1:A:33:THR:HA	1:A:36:TYR:CE2	2.52	0.45
1:B:29:SER:CB	1:C:108[B]:TYR:HH	2.21	0.44
1:C:51:LYS:HD3	7:C:470:HOH:O	2.17	0.44
1:D:88:PHE:CD2	1:E:99:PRO:HB3	2.52	0.44
1:B:38:VAL:HG11	1:B:252:VAL:HG22	1.98	0.44
2:A:317:OLC:H11A	2:A:317:OLC:H8	1.82	0.44
1:C:28:THR:HG23	1:C:244:GLN:HG3	1.98	0.44
1:D:33:THR:HA	1:D:36:TYR:CE2	2.52	0.44
1:A:38:VAL:HG11	1:A:252:VAL:HG22	1.99	0.43
1:B:164:LEU:HD23	1:B:164:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:CD2	1:B:43:LEU:HD11	2.46	0.43
6:B:315:RET:H7	6:B:315:RET:H181	1.81	0.43
1:D:139:ARG:NH1	2:D:301:OLC:H24	2.33	0.43
2:A:317:OLC:C17	2:E:309:OLC:C10	2.97	0.43
1:B:33:THR:HG21	1:C:108[A]:TYR:CZ	2.53	0.43
1:C:33:THR:HA	1:C:36:TYR:CE2	2.53	0.43
1:D:164:LEU:HD21	5:D:318:BOG:H2'1	2.01	0.43
1:E:33:THR:HA	1:E:36:TYR:CE2	2.53	0.43
1:A:44:LEU:HD21	1:B:65:ALA:HB1	2.02	0.42
1:B:28:THR:HG23	1:B:244:GLN:HG3	2.01	0.42
1:A:114:LEU:O	1:A:118:PRO:HG2	2.19	0.42
1:A:154:TYR:O	1:A:157:GLN:HG3	2.19	0.42
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.55	0.42
6:A:316:RET:H7	6:A:316:RET:H181	1.78	0.42
1:C:267:ILE:HG21	1:C:275:LEU:HG	2.02	0.42
1:D:114:LEU:O	1:D:118:PRO:HG2	2.20	0.42
1:E:74:LEU:HD22	1:E:74:LEU:HA	1.92	0.42
1:D:74:LEU:HD22	1:D:74:LEU:HA	1.91	0.41
1:C:114:LEU:O	1:C:118:PRO:HG2	2.20	0.41
1:D:44:LEU:HD21	1:E:65:ALA:HB1	2.02	0.41
1:A:73:LEU:CD1	1:E:37:ALA:HA	2.50	0.41
1:B:31:ILE:HD12	1:B:31:ILE:HA	1.90	0.41
1:C:74:LEU:HD22	1:C:74:LEU:HA	1.92	0.41
1:A:218:TYR:CE2	1:A:250:ALA:HB1	2.56	0.41
7:A:470:HOH:O	1:B:55:LYS:HE3	2.19	0.41
2:C:305:OLC:H7	2:C:305:OLC:H11	2.02	0.41
1:E:114:LEU:HD12	1:E:114:LEU:HA	1.84	0.41
1:A:43:LEU:HD11	1:E:44:LEU:HD11	2.03	0.41
1:C:60:SER:CB	7:C:403:HOH:O	2.69	0.41
1:A:60:SER:CB	7:A:402:HOH:O	2.68	0.41
1:B:231:ASP:H	5:B:314:BOG:HO6	1.60	0.41
1:C:29:SER:OG	1:D:108[B]:TYR:OH	2.07	0.41
3:C:304:LFA:H32	3:D:320:LFA:H102	2.03	0.41
7:D:403:HOH:O	1:E:55:LYS:CE	2.68	0.41
1:E:114:LEU:O	1:E:118:PRO:HG2	2.21	0.41
6:E:317:RET:H11	6:E:317:RET:H191	1.95	0.41
1:A:28:THR:HG23	1:A:244:GLN:HG3	2.03	0.40
1:E:28:THR:HG23	1:E:244:GLN:HG3	2.04	0.40
1:A:88:PHE:CZ	1:A:93:GLY:HA2	2.56	0.40
1:B:106:ASN:HB2	7:B:477:HOH:O	2.21	0.40
1:A:74:LEU:HD22	1:A:74:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TYR:N	1:B:219:PRO:HD2	2.36	0.40
6:A:316:RET:H11	6:A:316:RET:H191	1.96	0.40
1:D:218:TYR:CE2	1:D:250:ALA:HB1	2.57	0.40
1:E:38:VAL:HG11	1:E:252:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/273 (100%)	267 (98%)	6 (2%)	0	100	100
1	B	273/273 (100%)	267 (98%)	6 (2%)	0	100	100
1	C	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
1	D	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
1	E	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
All	All	1365/1365 (100%)	1338 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/233 (99%)	226 (98%)	4 (2%)	53	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	231/233 (99%)	223 (96%)	8 (4%)	32	43
1	C	230/233 (99%)	224 (97%)	6 (3%)	40	55
1	D	229/233 (98%)	226 (99%)	3 (1%)	61	76
1	E	230/233 (99%)	224 (97%)	6 (3%)	40	55
All	All	1150/1165 (99%)	1123 (98%)	27 (2%)	43	59

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	111	LEU
1	A	230	VAL
1	A	274	GLU
1	B	4	GLU
1	B	92	VAL
1	B	103	LEU
1	B	111	LEU
1	B	164	LEU
1	B	230	VAL
1	B	272	ASN
1	B	275	LEU
1	C	44	LEU
1	C	92	VAL
1	C	111	LEU
1	C	189	ILE
1	C	230	VAL
1	C	274	GLU
1	D	92	VAL
1	D	111	LEU
1	D	230	VAL
1	E	4	GLU
1	E	44	LEU
1	E	111	LEU
1	E	114	LEU
1	E	189	ILE
1	E	230	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	B	3	GLN
1	B	61	ASN
1	B	180	HIS
1	B	244	GLN
1	B	272	ASN
1	C	7	ASN
1	C	141	GLN
1	C	180	HIS
1	D	61	ASN
1	D	141	GLN
1	D	180	HIS
1	E	7	ASN
1	E	141	GLN
1	E	180	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 5 are monoatomic - leaving 86 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	D	306	-	17,17,24	1.13	1 (5%)	18,18,25	1.12	1 (5%)
3	LFA	E	312	-	13,13,19	0.07	0	12,12,18	0.06	0
6	RET	B	315	1	20,20,21	1.54	3 (15%)	27,27,28	1.07	2 (7%)
2	OLC	E	310	-	19,19,24	1.08	1 (5%)	20,20,25	0.97	1 (5%)
3	LFA	C	314	-	5,5,19	0.12	0	4,4,18	0.12	0
6	RET	E	317	1	20,20,21	1.63	3 (15%)	27,27,28	1.08	1 (3%)
2	OLC	E	304	-	15,15,24	0.28	0	14,14,25	0.49	0
2	OLC	D	307	-	17,17,24	1.14	1 (5%)	17,17,25	0.92	1 (5%)
2	OLC	C	307	-	19,19,24	1.06	1 (5%)	20,20,25	0.96	1 (5%)
3	LFA	E	302	-	19,19,19	0.13	0	18,18,18	0.12	0
2	OLC	A	306	-	14,14,24	1.21	1 (7%)	15,15,25	1.12	2 (13%)
2	OLC	A	307	-	6,6,24	0.28	0	5,5,25	0.45	0
3	LFA	B	311	-	9,9,19	0.08	0	8,8,18	0.07	0
2	OLC	D	302	-	15,15,24	1.22	1 (6%)	16,16,25	1.07	1 (6%)
2	OLC	C	302	-	19,19,24	1.05	1 (5%)	20,20,25	0.95	2 (10%)
3	LFA	D	320	-	13,13,19	0.07	0	12,12,18	0.07	0
2	OLC	A	303	-	24,24,24	0.96	1 (4%)	25,25,25	0.85	1 (4%)
3	LFA	A	311	-	3,3,19	0.23	0	2,2,18	0.44	0
3	LFA	D	314	-	16,16,19	0.06	0	15,15,18	0.09	0
2	OLC	A	305	-	24,24,24	0.99	1 (4%)	25,25,25	0.90	2 (8%)
5	BOG	D	318	-	20,20,20	0.52	0	25,25,25	0.58	0
3	LFA	D	303	-	19,19,19	0.11	0	18,18,18	0.11	0
3	LFA	D	312	-	19,19,19	0.07	0	18,18,18	0.06	0
2	OLC	E	306	-	14,14,24	1.23	1 (7%)	15,15,25	1.06	1 (6%)
2	OLC	A	317	-	18,18,24	1.11	1 (5%)	18,18,25	0.78	0
2	OLC	D	305	-	24,24,24	0.95	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	C	303	-	11,11,24	1.41	1 (9%)	12,12,25	1.09	1 (8%)
2	OLC	C	308	-	21,21,24	1.03	1 (4%)	22,22,25	0.94	1 (4%)
3	LFA	B	310	-	7,7,19	0.10	0	6,6,18	0.08	0
2	OLC	E	309	-	21,21,24	1.03	1 (4%)	22,22,25	0.86	1 (4%)
3	LFA	D	311	-	19,19,19	0.07	0	18,18,18	0.03	0
3	LFA	A	320	-	8,8,19	0.10	0	7,7,18	0.09	0
2	OLC	E	305	-	19,19,24	1.07	1 (5%)	20,20,25	1.00	1 (5%)
3	LFA	A	319	-	19,19,19	0.12	0	18,18,18	0.12	0
2	OLC	B	308	-	6,6,24	0.47	0	5,5,25	0.48	0
2	OLC	D	309	-	6,6,24	0.35	0	5,5,25	0.30	0
2	OLC	E	303	-	7,7,24	0.30	0	6,6,25	0.40	0
2	OLC	C	306	-	21,21,24	1.03	1 (4%)	22,22,25	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	B	301	-	21,21,24	0.98	1 (4%)	22,22,25	0.91	1 (4%)
5	BOG	C	317	-	20,20,20	0.56	1 (5%)	25,25,25	0.54	0
2	OLC	B	302	-	15,15,24	1.21	1 (6%)	16,16,25	0.99	1 (6%)
3	LFA	B	316	-	3,3,19	0.23	0	2,2,18	0.44	0
3	LFA	D	316	-	5,5,19	0.14	0	4,4,18	0.12	0
2	OLC	A	302	-	21,21,24	0.99	1 (4%)	22,22,25	0.95	2 (9%)
5	BOG	E	316	-	20,20,20	0.54	0	25,25,25	0.50	0
2	OLC	C	305	-	22,22,24	0.94	1 (4%)	23,23,25	0.83	2 (8%)
2	OLC	A	301	-	8,8,24	0.36	0	7,7,25	0.50	0
2	OLC	D	310	-	24,24,24	0.94	1 (4%)	25,25,25	0.79	1 (4%)
6	RET	A	316	1	20,20,21	1.62	3 (15%)	27,27,28	1.07	1 (3%)
3	LFA	B	309	-	8,8,19	0.10	0	7,7,18	0.09	0
3	LFA	A	312	-	5,5,19	0.13	0	4,4,18	0.11	0
2	OLC	C	309	-	15,15,24	1.19	1 (6%)	16,16,25	0.96	2 (12%)
2	OLC	B	307	-	15,15,24	1.15	1 (6%)	16,16,25	0.99	2 (12%)
2	OLC	D	304	-	12,12,24	1.36	1 (8%)	13,13,25	1.10	1 (7%)
3	LFA	C	313	-	19,19,19	0.07	0	18,18,18	0.05	0
5	BOG	A	315	-	20,20,20	0.55	0	25,25,25	0.67	0
2	OLC	D	301	-	17,17,24	1.11	1 (5%)	18,18,25	1.00	1 (5%)
3	LFA	D	313	-	7,7,19	0.09	0	6,6,18	0.07	0
2	OLC	B	304	-	24,24,24	0.95	1 (4%)	25,25,25	0.86	2 (8%)
6	RET	C	318	1	20,20,21	1.65	3 (15%)	27,27,28	1.04	1 (3%)
5	BOG	B	314	-	20,20,20	0.60	1 (5%)	25,25,25	0.60	0
3	LFA	A	310	-	7,7,19	0.08	0	6,6,18	0.07	0
3	LFA	C	311	-	6,6,19	0.11	0	5,5,18	0.09	0
2	OLC	A	304	-	12,12,24	1.31	1 (8%)	13,13,25	1.21	2 (15%)
3	LFA	C	312	-	7,7,19	0.10	0	6,6,18	0.08	0
2	OLC	C	310	-	6,6,24	0.31	0	5,5,25	0.38	0
2	OLC	E	308	-	5,5,24	0.34	0	4,4,25	0.30	0
3	LFA	A	313	-	15,15,19	0.07	0	14,14,18	0.06	0
2	OLC	A	318	-	19,19,24	1.09	1 (5%)	19,19,25	0.87	0
3	LFA	B	312	-	6,6,19	0.09	0	5,5,18	0.07	0
3	LFA	C	315	-	3,3,19	0.24	0	2,2,18	0.43	0
3	LFA	E	314	-	4,4,19	0.13	0	3,3,18	0.23	0
3	LFA	C	304	-	19,19,19	0.10	0	18,18,18	0.12	0
2	OLC	B	306	-	20,20,24	1.04	1 (5%)	21,21,25	0.95	1 (4%)
2	OLC	E	301	-	24,24,24	0.93	1 (4%)	25,25,25	0.88	1 (4%)
3	LFA	B	303	-	19,19,19	0.12	0	18,18,18	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	C	301	-	20,20,24	1.02	1 (5%)	21,21,25	1.00	2 (9%)
3	LFA	A	309	-	7,7,19	0.12	0	6,6,18	0.08	0
2	OLC	D	308	-	13,13,24	1.23	1 (7%)	14,14,25	1.01	2 (14%)
2	OLC	B	305	-	19,19,24	1.05	1 (5%)	20,20,25	0.98	2 (10%)
6	RET	D	319	1	20,20,21	1.54	3 (15%)	27,27,28	1.08	2 (7%)
3	LFA	D	315	-	6,6,19	0.10	0	5,5,18	0.08	0
3	LFA	E	311	-	7,7,19	0.09	0	6,6,18	0.08	0
2	OLC	E	307	-	14,14,24	1.19	1 (7%)	15,15,25	1.06	2 (13%)
3	LFA	A	308	-	6,6,19	0.11	0	5,5,18	0.08	0
3	LFA	E	313	-	3,3,19	0.21	0	2,2,18	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	D	306	-	-	3/17/17/24	-
3	LFA	E	312	-	-	5/11/11/17	-
6	RET	B	315	1	-	0/13/30/31	0/1/1/1
2	OLC	E	310	-	-	11/19/19/24	-
3	LFA	C	314	-	-	1/3/3/17	-
6	RET	E	317	1	-	0/13/30/31	0/1/1/1
2	OLC	E	304	-	-	7/13/13/24	-
2	OLC	D	307	-	-	4/15/15/24	-
2	OLC	C	307	-	-	5/19/19/24	-
3	LFA	E	302	-	-	8/17/17/17	-
2	OLC	A	306	-	-	6/14/14/24	-
2	OLC	A	307	-	-	3/4/4/24	-
3	LFA	B	311	-	-	4/7/7/17	-
2	OLC	D	302	-	-	7/15/15/24	-
2	OLC	C	302	-	-	8/19/19/24	-
3	LFA	D	320	-	-	5/11/11/17	-
2	OLC	A	303	-	-	12/24/24/24	-
3	LFA	A	311	-	-	0/1/1/17	-
3	LFA	D	314	-	-	9/14/14/17	-
2	OLC	A	305	-	-	13/24/24/24	-
5	BOG	D	318	-	-	3/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	D	303	-	-	7/17/17/17	-
3	LFA	D	312	-	-	9/17/17/17	-
2	OLC	E	306	-	-	9/14/14/24	-
2	OLC	A	317	-	-	9/16/16/24	-
2	OLC	D	305	-	-	12/24/24/24	-
2	OLC	C	303	-	-	3/11/11/24	-
2	OLC	C	308	-	-	9/21/21/24	-
3	LFA	B	310	-	-	4/5/5/17	-
2	OLC	E	309	-	-	7/21/21/24	-
3	LFA	D	311	-	-	8/17/17/17	-
3	LFA	A	320	-	-	3/6/6/17	-
2	OLC	E	305	-	-	6/19/19/24	-
3	LFA	A	319	-	-	7/17/17/17	-
2	OLC	B	308	-	-	3/4/4/24	-
2	OLC	D	309	-	-	3/4/4/24	-
2	OLC	E	303	-	-	1/5/5/24	-
2	OLC	C	306	-	-	8/21/21/24	-
2	OLC	B	301	-	-	7/21/21/24	-
5	BOG	C	317	-	-	3/11/31/31	0/1/1/1
2	OLC	B	302	-	-	5/15/15/24	-
3	LFA	B	316	-	-	0/1/1/17	-
3	LFA	D	316	-	-	0/3/3/17	-
2	OLC	A	302	-	-	12/21/21/24	-
5	BOG	E	316	-	-	9/11/31/31	0/1/1/1
2	OLC	C	305	-	-	11/22/22/24	-
2	OLC	A	301	-	-	3/6/6/24	-
2	OLC	D	310	-	-	15/24/24/24	-
6	RET	A	316	1	-	0/13/30/31	0/1/1/1
3	LFA	B	309	-	-	3/6/6/17	-
3	LFA	A	312	-	-	1/3/3/17	-
2	OLC	C	309	-	-	5/15/15/24	-
2	OLC	B	307	-	-	4/15/15/24	-
2	OLC	D	304	-	-	3/12/12/24	-
3	LFA	C	313	-	-	12/17/17/17	-
5	BOG	A	315	-	-	5/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	D	301	-	-	9/17/17/24	-
3	LFA	D	313	-	-	4/5/5/17	-
2	OLC	B	304	-	-	13/24/24/24	-
6	RET	C	318	1	-	0/13/30/31	0/1/1/1
5	BOG	B	314	-	-	5/11/31/31	0/1/1/1
3	LFA	A	310	-	-	3/5/5/17	-
3	LFA	C	311	-	-	2/4/4/17	-
2	OLC	A	304	-	-	2/12/12/24	-
3	LFA	C	312	-	-	5/5/5/17	-
2	OLC	C	310	-	-	2/4/4/24	-
2	OLC	E	308	-	-	0/3/3/24	-
3	LFA	A	313	-	-	8/13/13/17	-
2	OLC	A	318	-	-	9/17/17/24	-
3	LFA	B	312	-	-	2/4/4/17	-
3	LFA	C	315	-	-	1/1/1/17	-
3	LFA	E	314	-	-	1/2/2/17	-
3	LFA	C	304	-	-	12/17/17/17	-
2	OLC	B	306	-	-	12/20/20/24	-
2	OLC	E	301	-	-	10/24/24/24	-
3	LFA	B	303	-	-	8/17/17/17	-
2	OLC	C	301	-	-	9/20/20/24	-
3	LFA	A	309	-	-	3/5/5/17	-
2	OLC	D	308	-	-	5/13/13/24	-
2	OLC	B	305	-	-	5/19/19/24	-
6	RET	D	319	1	-	0/13/30/31	0/1/1/1
3	LFA	D	315	-	-	4/4/4/17	-
3	LFA	E	311	-	-	2/5/5/17	-
2	OLC	E	307	-	-	8/14/14/24	-
3	LFA	A	308	-	-	1/4/4/17	-
3	LFA	E	313	-	-	1/1/1/17	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	318	RET	C14-C13	5.06	1.37	1.33
6	E	317	RET	C14-C13	4.82	1.37	1.33
6	A	316	RET	C14-C13	4.79	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	318	OLC	O20-C1	4.64	1.46	1.30
2	A	317	OLC	O20-C1	4.58	1.46	1.30
2	D	307	OLC	O20-C1	4.58	1.46	1.30
2	A	305	OLC	O20-C1	4.53	1.46	1.33
2	D	304	OLC	O20-C1	4.52	1.46	1.33
2	D	302	OLC	O20-C1	4.51	1.46	1.33
2	C	303	OLC	O20-C1	4.51	1.46	1.33
2	C	308	OLC	O20-C1	4.47	1.46	1.33
2	C	306	OLC	O20-C1	4.46	1.46	1.33
2	E	305	OLC	O20-C1	4.45	1.46	1.33
2	B	302	OLC	O20-C1	4.44	1.46	1.33
2	E	309	OLC	O20-C1	4.44	1.46	1.33
2	A	303	OLC	O20-C1	4.44	1.46	1.33
2	D	306	OLC	O20-C1	4.42	1.46	1.33
2	E	310	OLC	O20-C1	4.42	1.46	1.33
2	E	306	OLC	O20-C1	4.40	1.46	1.33
2	B	306	OLC	O20-C1	4.37	1.46	1.33
2	C	309	OLC	O20-C1	4.37	1.46	1.33
2	A	304	OLC	O20-C1	4.36	1.46	1.33
2	C	301	OLC	O20-C1	4.36	1.46	1.33
2	C	307	OLC	O20-C1	4.35	1.46	1.33
2	D	305	OLC	O20-C1	4.34	1.46	1.33
2	B	304	OLC	O20-C1	4.33	1.46	1.33
2	E	301	OLC	O20-C1	4.33	1.46	1.33
2	B	305	OLC	O20-C1	4.32	1.45	1.33
6	D	319	RET	C14-C13	4.30	1.36	1.33
2	C	302	OLC	O20-C1	4.30	1.45	1.33
2	A	306	OLC	O20-C1	4.30	1.45	1.33
2	D	301	OLC	O20-C1	4.28	1.45	1.33
2	D	310	OLC	O20-C1	4.27	1.45	1.33
2	B	301	OLC	O20-C1	4.23	1.45	1.33
2	B	307	OLC	O20-C1	4.22	1.45	1.33
2	D	308	OLC	O20-C1	4.22	1.45	1.33
2	A	302	OLC	O20-C1	4.19	1.45	1.33
2	E	307	OLC	O20-C1	4.18	1.45	1.33
6	B	315	RET	C14-C13	4.17	1.36	1.33
2	C	305	OLC	O20-C1	4.11	1.45	1.33
6	B	315	RET	C8-C9	-2.71	1.40	1.46
6	E	317	RET	C8-C9	-2.58	1.40	1.46
6	A	316	RET	C8-C9	-2.57	1.40	1.46
6	C	318	RET	C8-C9	-2.55	1.40	1.46
6	D	319	RET	C8-C9	-2.53	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	318	RET	C10-C9	2.39	1.41	1.35
6	A	316	RET	C10-C9	2.38	1.41	1.35
6	B	315	RET	C10-C9	2.37	1.41	1.35
6	E	317	RET	C10-C9	2.37	1.41	1.35
6	D	319	RET	C10-C9	2.31	1.41	1.35
5	B	314	BOG	O1-C1	2.20	1.43	1.40
5	C	317	BOG	O1-C1	2.03	1.43	1.40

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	319	RET	C19-C9-C10	-3.45	117.22	122.82
6	B	315	RET	C19-C9-C10	-3.42	117.28	122.82
6	E	317	RET	C19-C9-C10	-3.34	117.40	122.82
6	A	316	RET	C19-C9-C10	-3.21	117.61	122.82
6	C	318	RET	C19-C9-C10	-3.18	117.66	122.82
2	A	304	OLC	O20-C1-C2	3.17	121.50	111.83
2	D	306	OLC	O20-C1-C2	3.16	121.48	111.83
2	C	301	OLC	O20-C1-C2	3.15	121.44	111.83
2	E	305	OLC	O20-C1-C2	3.13	121.38	111.83
2	A	302	OLC	O20-C1-C2	3.10	121.28	111.83
2	A	306	OLC	O20-C1-C2	3.06	121.16	111.83
2	D	302	OLC	O20-C1-C2	3.03	121.07	111.83
2	C	308	OLC	O20-C1-C2	3.03	121.06	111.83
2	A	305	OLC	O20-C1-C2	3.00	120.98	111.83
2	E	310	OLC	O20-C1-C2	2.96	120.86	111.83
2	C	307	OLC	O20-C1-C2	2.95	120.84	111.83
2	B	304	OLC	O20-C1-C2	2.95	120.83	111.83
2	B	305	OLC	O20-C1-C2	2.93	120.77	111.83
2	C	302	OLC	O20-C1-C2	2.90	120.68	111.83
2	E	306	OLC	O20-C1-C2	2.89	120.65	111.83
2	B	306	OLC	O20-C1-C2	2.88	120.60	111.83
2	D	304	OLC	O20-C1-C2	2.86	120.56	111.83
2	C	306	OLC	O20-C1-C2	2.82	120.42	111.83
2	B	301	OLC	O20-C1-C2	2.80	120.37	111.83
2	E	307	OLC	O20-C1-C2	2.80	120.36	111.83
2	A	303	OLC	O20-C1-C2	2.78	120.31	111.83
2	E	301	OLC	O20-C1-C2	2.74	120.17	111.83
2	B	302	OLC	O20-C1-C2	2.72	120.14	111.83
2	D	305	OLC	O20-C1-C2	2.71	120.11	111.83
2	B	307	OLC	O20-C1-C2	2.70	120.07	111.83
2	D	301	OLC	O20-C1-C2	2.69	120.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	OLC	O20-C1-C2	2.69	120.02	111.83
2	D	308	OLC	O20-C1-C2	2.68	120.01	111.83
2	E	309	OLC	O20-C1-C2	2.65	119.92	111.83
2	D	310	OLC	O20-C1-C2	2.58	119.69	111.83
2	C	309	OLC	O20-C1-C2	2.57	119.66	111.83
2	C	305	OLC	O20-C1-C2	2.55	119.60	111.83
2	E	307	OLC	O20-C1-O19	-2.42	117.58	123.63
2	A	302	OLC	O20-C1-O19	-2.34	117.77	123.63
2	A	306	OLC	O20-C1-O19	-2.32	117.83	123.63
2	A	304	OLC	O20-C1-O19	-2.30	117.89	123.63
2	C	305	OLC	O20-C1-O19	-2.25	117.99	123.63
6	D	319	RET	C8-C9-C10	2.24	122.53	119.01
6	B	315	RET	C8-C9-C10	2.17	122.43	119.01
2	D	307	OLC	O20-C1-C2	2.08	120.56	114.00
2	B	305	OLC	O20-C1-O19	-2.07	118.46	123.63
2	C	302	OLC	O20-C1-O19	-2.06	118.47	123.63
2	D	308	OLC	O20-C1-O19	-2.06	118.48	123.63
2	A	305	OLC	O20-C1-O19	-2.04	118.53	123.63
2	C	309	OLC	O20-C1-O19	-2.04	118.53	123.63
2	B	307	OLC	O20-C1-O19	-2.03	118.54	123.63
2	B	304	OLC	O20-C1-O19	-2.03	118.56	123.63
2	C	301	OLC	O20-C1-O19	-2.02	118.58	123.63

There are no chirality outliers.

All (466) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	OLC	C6-C7-C8-C9
2	A	305	OLC	O20-C21-C22-C24
2	A	305	OLC	O20-C21-C22-O23
2	A	305	OLC	O19-C1-O20-C21
2	A	306	OLC	O20-C21-C22-C24
2	B	302	OLC	C21-C22-C24-O25
2	B	305	OLC	C10-C11-C12-C13
2	B	306	OLC	C21-C22-C24-O25
2	B	306	OLC	O20-C21-C22-C24
2	B	307	OLC	C21-C22-C24-O25
2	B	307	OLC	O23-C22-C24-O25
2	C	301	OLC	C21-C22-C24-O25
2	C	303	OLC	C21-C22-C24-O25
2	C	306	OLC	O20-C21-C22-C24
2	C	306	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
2	C	307	OLC	C21-C22-C24-O25
2	C	307	OLC	O23-C22-C24-O25
2	C	308	OLC	C21-C22-C24-O25
2	C	308	OLC	O23-C22-C24-O25
2	D	302	OLC	O20-C21-C22-O23
2	D	305	OLC	C21-C22-C24-O25
2	D	308	OLC	C21-C22-C24-O25
2	D	308	OLC	O23-C22-C24-O25
2	D	310	OLC	C21-C22-C24-O25
2	D	310	OLC	O23-C22-C24-O25
2	D	310	OLC	O19-C1-O20-C21
2	E	301	OLC	C21-C22-C24-O25
2	E	301	OLC	O23-C22-C24-O25
2	E	306	OLC	C21-C22-C24-O25
2	E	306	OLC	O20-C21-C22-O23
2	E	307	OLC	O20-C21-C22-C24
2	E	307	OLC	O20-C21-C22-O23
3	C	315	LFA	C17-C18-C19-C20
3	E	313	LFA	C17-C18-C19-C20
2	A	305	OLC	C2-C1-O20-C21
2	A	306	OLC	O19-C1-O20-C21
2	C	305	OLC	O19-C1-O20-C21
2	D	305	OLC	O19-C1-O20-C21
2	C	305	OLC	C2-C1-O20-C21
2	D	305	OLC	C2-C1-O20-C21
2	D	310	OLC	C2-C1-O20-C21
2	A	306	OLC	C2-C1-O20-C21
2	D	301	OLC	C2-C1-O20-C21
2	E	307	OLC	O19-C1-O20-C21
2	E	307	OLC	C2-C1-O20-C21
5	E	316	BOG	O5-C5-C6-O6
2	A	304	OLC	O20-C21-C22-O23
2	A	306	OLC	O20-C21-C22-O23
2	B	306	OLC	O20-C21-C22-O23
2	D	301	OLC	O19-C1-O20-C21
5	E	316	BOG	O5-C1-O1-C1'
5	E	316	BOG	C4-C5-C6-O6
2	A	303	OLC	C2-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
2	B	305	OLC	C2-C1-O20-C21
2	D	302	OLC	C2-C1-O20-C21
2	D	306	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	B	304	OLC	O20-C21-C22-C24
5	E	316	BOG	C2-C1-O1-C1'
2	A	303	OLC	O19-C1-O20-C21
5	A	315	BOG	O5-C5-C6-O6
2	B	301	OLC	O19-C1-O20-C21
2	D	306	OLC	O19-C1-O20-C21
2	B	307	OLC	C2-C1-O20-C21
2	B	302	OLC	O23-C22-C24-O25
2	E	310	OLC	C1-C2-C3-C4
2	B	305	OLC	O19-C1-O20-C21
2	E	309	OLC	C1-C2-C3-C4
5	B	314	BOG	O5-C5-C6-O6
5	A	315	BOG	C4-C5-C6-O6
2	C	302	OLC	C1-C2-C3-C4
2	D	304	OLC	C1-C2-C3-C4
2	D	302	OLC	O19-C1-O20-C21
2	B	304	OLC	C1-C2-C3-C4
2	D	308	OLC	C1-C2-C3-C4
5	B	314	BOG	C4-C5-C6-O6
2	B	304	OLC	O20-C21-C22-O23
2	D	304	OLC	O20-C21-C22-O23
2	E	309	OLC	O20-C21-C22-O23
2	E	310	OLC	O20-C21-C22-O23
2	B	302	OLC	C1-C2-C3-C4
2	B	307	OLC	O19-C1-O20-C21
2	B	306	OLC	C2-C1-O20-C21
2	E	306	OLC	C2-C1-O20-C21
2	E	304	OLC	C4-C5-C6-C7
2	A	303	OLC	C1-C2-C3-C4
2	D	302	OLC	O20-C21-C22-C24
2	D	304	OLC	O20-C21-C22-C24
2	E	306	OLC	O20-C21-C22-C24
2	E	309	OLC	O20-C21-C22-C24
2	E	310	OLC	O20-C21-C22-C24
5	E	316	BOG	O1-C1'-C2'-C3'
2	E	305	OLC	C10-C11-C12-C13
2	D	301	OLC	O20-C21-C22-O23
2	E	305	OLC	O20-C21-C22-O23
2	A	302	OLC	C21-C22-C24-O25
2	B	304	OLC	C21-C22-C24-O25
2	C	305	OLC	C21-C22-C24-O25
2	E	307	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
2	C	309	OLC	C2-C1-O20-C21
2	A	305	OLC	C4-C5-C6-C7
2	D	310	OLC	C11-C12-C13-C14
3	D	314	LFA	C5-C6-C7-C8
5	E	316	BOG	C2'-C3'-C4'-C5'
2	A	318	OLC	C13-C14-C15-C16
2	C	310	OLC	C5-C6-C7-C8
5	B	314	BOG	C3'-C4'-C5'-C6'
2	A	305	OLC	C13-C14-C15-C16
2	B	306	OLC	C2-C3-C4-C5
2	E	309	OLC	C11-C12-C13-C14
3	A	310	LFA	C16-C17-C18-C19
3	C	312	LFA	C15-C16-C17-C18
3	C	312	LFA	C16-C17-C18-C19
3	D	320	LFA	C2-C3-C4-C5
2	C	301	OLC	O23-C22-C24-O25
2	D	305	OLC	O23-C22-C24-O25
2	E	307	OLC	O23-C22-C24-O25
5	E	316	BOG	C2'-C1'-O1-C1
3	D	313	LFA	C2-C3-C4-C5
2	C	306	OLC	C1-C2-C3-C4
2	C	302	OLC	C3-C4-C5-C6
2	C	301	OLC	C5-C6-C7-C8
5	A	315	BOG	C1'-C2'-C3'-C4'
2	A	318	OLC	C5-C6-C7-C8
3	D	312	LFA	C14-C15-C16-C17
5	D	318	BOG	C1'-C2'-C3'-C4'
2	B	306	OLC	O19-C1-O20-C21
2	E	306	OLC	O19-C1-O20-C21
2	A	307	OLC	C4-C5-C6-C7
2	E	305	OLC	C5-C6-C7-C8
5	C	317	BOG	C1'-C2'-C3'-C4'
2	C	305	OLC	C4-C5-C6-C7
3	E	312	LFA	C9-C10-C11-C12
3	E	312	LFA	C13-C14-C15-C16
2	A	302	OLC	C3-C4-C5-C6
2	C	306	OLC	C3-C4-C5-C6
3	A	312	LFA	C2-C3-C4-C5
3	B	310	LFA	C3-C4-C5-C6
2	C	305	OLC	C3-C4-C5-C6
2	D	310	OLC	C4-C5-C6-C7
3	B	310	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	D	303	LFA	C11-C10-C9-C8
3	D	311	LFA	C6-C7-C8-C9
2	E	305	OLC	C3-C4-C5-C6
3	A	309	LFA	C4-C5-C6-C7
3	A	313	LFA	C10-C11-C12-C13
5	B	314	BOG	C1'-C2'-C3'-C4'
2	C	309	OLC	O19-C1-O20-C21
2	A	305	OLC	C10-C11-C12-C13
2	D	301	OLC	C6-C7-C8-C9
2	D	307	OLC	C10-C11-C12-C13
2	C	302	OLC	C5-C6-C7-C8
2	A	318	OLC	C12-C13-C14-C15
2	D	307	OLC	C2-C3-C4-C5
3	B	303	LFA	C16-C17-C18-C19
2	C	309	OLC	C3-C4-C5-C6
3	A	313	LFA	C3-C4-C5-C6
3	A	313	LFA	C4-C5-C6-C7
3	E	312	LFA	C14-C15-C16-C17
2	D	301	OLC	O20-C21-C22-C24
2	E	306	OLC	C4-C5-C6-C7
3	D	315	LFA	C15-C16-C17-C18
3	D	303	LFA	C12-C13-C14-C15
3	D	314	LFA	C11-C12-C13-C14
3	B	309	LFA	C14-C15-C16-C17
3	D	311	LFA	C9-C10-C11-C12
3	D	312	LFA	C11-C12-C13-C14
3	D	303	LFA	C9-C10-C11-C12
3	D	320	LFA	C3-C4-C5-C6
2	D	310	OLC	C13-C14-C15-C16
3	D	314	LFA	C7-C8-C9-C10
2	A	305	OLC	C2-C3-C4-C5
2	B	306	OLC	C5-C6-C7-C8
3	D	312	LFA	C4-C5-C6-C7
2	E	301	OLC	C10-C11-C12-C13
2	D	305	OLC	C4-C5-C6-C7
2	A	305	OLC	C3-C4-C5-C6
2	C	301	OLC	C4-C5-C6-C7
3	E	312	LFA	C15-C16-C17-C18
3	C	304	LFA	C7-C8-C9-C10
2	A	302	OLC	C4-C5-C6-C7
2	C	308	OLC	C5-C6-C7-C8
2	C	308	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	303	OLC	C13-C14-C15-C16
2	D	301	OLC	C1-C2-C3-C4
3	D	311	LFA	C3-C4-C5-C6
2	A	318	OLC	C11-C12-C13-C14
2	E	301	OLC	C1-C2-C3-C4
3	C	313	LFA	C13-C14-C15-C16
2	A	301	OLC	C10-C11-C12-C13
2	B	304	OLC	C3-C4-C5-C6
3	D	312	LFA	C13-C14-C15-C16
3	C	313	LFA	C4-C5-C6-C7
3	D	314	LFA	C13-C14-C15-C16
3	E	302	LFA	C7-C8-C9-C10
2	D	310	OLC	C12-C13-C14-C15
3	A	319	LFA	C16-C17-C18-C19
2	E	305	OLC	C4-C5-C6-C7
2	E	310	OLC	C4-C5-C6-C7
3	B	309	LFA	C16-C17-C18-C19
3	B	311	LFA	C5-C6-C7-C8
2	A	302	OLC	O23-C22-C24-O25
2	B	306	OLC	O23-C22-C24-O25
2	C	303	OLC	O23-C22-C24-O25
2	E	306	OLC	O23-C22-C24-O25
2	E	310	OLC	C3-C4-C5-C6
3	C	304	LFA	C2-C3-C4-C5
3	C	311	LFA	C2-C3-C4-C5
2	A	305	OLC	C6-C7-C8-C9
2	A	317	OLC	C6-C7-C8-C9
2	B	304	OLC	C10-C11-C12-C13
2	B	306	OLC	C10-C11-C12-C13
2	E	310	OLC	C6-C7-C8-C9
3	D	311	LFA	C11-C10-C9-C8
2	B	304	OLC	C14-C15-C16-C17
3	C	304	LFA	C16-C17-C18-C19
3	D	311	LFA	C4-C5-C6-C7
3	E	302	LFA	C11-C10-C9-C8
2	A	302	OLC	C6-C7-C8-C9
2	A	305	OLC	C12-C13-C14-C15
2	C	305	OLC	C12-C13-C14-C15
2	C	306	OLC	C2-C1-O20-C21
2	C	308	OLC	C1-C2-C3-C4
2	B	304	OLC	C4-C5-C6-C7
3	A	319	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	A	315	BOG	C3'-C4'-C5'-C6'
5	E	316	BOG	C1'-C2'-C3'-C4'
3	A	319	LFA	C13-C14-C15-C16
3	C	304	LFA	C15-C16-C17-C18
3	C	313	LFA	C12-C13-C14-C15
3	D	303	LFA	C7-C8-C9-C10
3	D	313	LFA	C4-C5-C6-C7
3	D	320	LFA	C4-C5-C6-C7
3	A	313	LFA	C7-C8-C9-C10
2	E	310	OLC	C2-C1-O20-C21
2	A	302	OLC	C10-C11-C12-C13
2	C	307	OLC	C6-C7-C8-C9
2	E	304	OLC	C5-C6-C7-C8
2	D	306	OLC	C5-C6-C7-C8
3	A	313	LFA	C11-C12-C13-C14
3	D	315	LFA	C16-C17-C18-C19
3	A	309	LFA	C5-C6-C7-C8
5	A	315	BOG	C5'-C6'-C7'-C8'
2	D	308	OLC	C2-C3-C4-C5
3	D	311	LFA	C14-C15-C16-C17
5	B	314	BOG	C5'-C6'-C7'-C8'
3	A	320	LFA	C4-C5-C6-C7
2	B	308	OLC	C4-C5-C6-C7
2	C	302	OLC	C4-C5-C6-C7
2	D	307	OLC	C5-C6-C7-C8
3	C	304	LFA	C13-C14-C15-C16
2	A	303	OLC	C14-C15-C16-C17
3	B	303	LFA	C11-C10-C9-C8
3	B	312	LFA	C15-C16-C17-C18
5	C	317	BOG	C5'-C6'-C7'-C8'
2	A	317	OLC	C13-C14-C15-C16
2	A	307	OLC	C6-C7-C8-C9
2	C	308	OLC	C6-C7-C8-C9
2	D	305	OLC	C6-C7-C8-C9
2	D	310	OLC	C10-C11-C12-C13
3	D	312	LFA	C1-C2-C3-C4
2	C	306	OLC	C5-C6-C7-C8
2	C	310	OLC	C6-C7-C8-C9
3	D	314	LFA	C14-C15-C16-C17
3	D	312	LFA	C3-C4-C5-C6
3	B	311	LFA	C7-C8-C9-C10
2	E	301	OLC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
2	B	304	OLC	C5-C6-C7-C8
3	A	313	LFA	C5-C6-C7-C8
2	A	317	OLC	C14-C15-C16-C17
3	D	314	LFA	C3-C4-C5-C6
2	D	310	OLC	C2-C3-C4-C5
2	E	301	OLC	C4-C5-C6-C7
3	C	304	LFA	C4-C5-C6-C7
2	A	302	OLC	O20-C21-C22-C24
2	A	305	OLC	C11-C12-C13-C14
3	D	311	LFA	C11-C12-C13-C14
3	D	313	LFA	C5-C6-C7-C8
2	A	317	OLC	C11-C12-C13-C14
2	C	309	OLC	C4-C5-C6-C7
2	D	309	OLC	C2-C3-C4-C5
3	A	313	LFA	C13-C14-C15-C16
2	C	306	OLC	O19-C1-O20-C21
3	B	303	LFA	C6-C7-C8-C9
3	E	311	LFA	C16-C17-C18-C19
2	E	310	OLC	O19-C1-O20-C21
3	A	319	LFA	C6-C7-C8-C9
2	D	309	OLC	C4-C5-C6-C7
2	E	309	OLC	C4-C5-C6-C7
3	C	313	LFA	C15-C16-C17-C18
2	D	310	OLC	C5-C6-C7-C8
2	E	303	OLC	C4-C5-C6-C7
2	E	306	OLC	C3-C4-C5-C6
2	C	305	OLC	C10-C11-C12-C13
2	C	305	OLC	C5-C6-C7-C8
2	E	306	OLC	C5-C6-C7-C8
3	B	303	LFA	C10-C11-C12-C13
3	C	312	LFA	C17-C18-C19-C20
3	C	313	LFA	C10-C11-C12-C13
5	D	318	BOG	C3'-C4'-C5'-C6'
3	C	313	LFA	C9-C10-C11-C12
2	B	308	OLC	C6-C7-C8-C9
2	A	302	OLC	O20-C21-C22-O23
2	A	317	OLC	C3-C4-C5-C6
3	D	303	LFA	C10-C11-C12-C13
2	D	309	OLC	C5-C6-C7-C8
2	D	301	OLC	C7-C8-C9-C10
2	B	304	OLC	O23-C22-C24-O25
2	D	305	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	D	302	OLC	C4-C5-C6-C7
3	A	309	LFA	C1-C2-C3-C4
3	A	313	LFA	C11-C10-C9-C8
3	A	320	LFA	C3-C4-C5-C6
2	C	302	OLC	C10-C11-C12-C13
3	D	315	LFA	C14-C15-C16-C17
2	B	302	OLC	C2-C1-O20-C21
2	E	307	OLC	C2-C3-C4-C5
5	E	316	BOG	C5'-C6'-C7'-C8'
2	E	304	OLC	C11-C12-C13-C14
3	C	304	LFA	C3-C4-C5-C6
3	C	311	LFA	C4-C5-C6-C7
2	B	301	OLC	C10-C11-C12-C13
2	B	308	OLC	C7-C8-C9-C10
3	C	313	LFA	C11-C12-C13-C14
3	A	310	LFA	C15-C16-C17-C18
2	E	310	OLC	C2-C3-C4-C5
2	D	301	OLC	C2-C3-C4-C5
3	D	320	LFA	C11-C12-C13-C14
2	C	308	OLC	C10-C11-C12-C13
2	E	304	OLC	C13-C14-C15-C16
2	B	302	OLC	O19-C1-O20-C21
3	A	308	LFA	C17-C18-C19-C20
3	D	313	LFA	C1-C2-C3-C4
2	C	303	OLC	O20-C21-C22-O23
3	D	312	LFA	C10-C11-C12-C13
2	A	302	OLC	C2-C3-C4-C5
2	A	317	OLC	C5-C6-C7-C8
2	D	302	OLC	C5-C6-C7-C8
3	B	311	LFA	C1-C2-C3-C4
2	A	317	OLC	C12-C13-C14-C15
3	D	312	LFA	C5-C6-C7-C8
2	A	317	OLC	C2-C3-C4-C5
3	C	313	LFA	C14-C15-C16-C17
2	D	302	OLC	C6-C7-C8-C9
3	C	304	LFA	C14-C15-C16-C17
3	C	304	LFA	C9-C10-C11-C12
3	C	304	LFA	C1-C2-C3-C4
3	B	303	LFA	C9-C10-C11-C12
2	A	318	OLC	C15-C16-C17-C18
2	E	307	OLC	C4-C5-C6-C7
3	D	312	LFA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
3	C	312	LFA	C13-C14-C15-C16
3	C	313	LFA	C16-C17-C18-C19
2	A	318	OLC	C7-C8-C9-C10
2	D	305	OLC	C9-C10-C11-C12
2	E	304	OLC	C7-C8-C9-C10
2	B	305	OLC	C4-C5-C6-C7
3	E	302	LFA	C12-C13-C14-C15
3	E	312	LFA	C7-C8-C9-C10
2	A	318	OLC	C6-C7-C8-C9
3	B	310	LFA	C5-C6-C7-C8
3	D	314	LFA	C11-C10-C9-C8
3	E	302	LFA	C15-C16-C17-C18
3	D	311	LFA	C7-C8-C9-C10
2	C	308	OLC	C7-C8-C9-C10
2	D	310	OLC	C1-C2-C3-C4
2	C	301	OLC	C10-C11-C12-C13
2	B	306	OLC	C4-C5-C6-C7
3	C	304	LFA	C12-C13-C14-C15
2	A	306	OLC	C3-C4-C5-C6
2	C	305	OLC	O23-C22-C24-O25
2	B	301	OLC	O20-C21-C22-C24
3	E	311	LFA	C17-C18-C19-C20
2	E	310	OLC	C5-C6-C7-C8
2	A	303	OLC	C9-C10-C11-C12
2	B	301	OLC	C7-C8-C9-C10
2	E	301	OLC	C3-C4-C5-C6
2	E	301	OLC	C5-C6-C7-C8
3	C	312	LFA	C14-C15-C16-C17
3	D	303	LFA	C4-C5-C6-C7
2	C	308	OLC	C4-C5-C6-C7
2	E	309	OLC	C7-C8-C9-C10
2	E	301	OLC	C22-C21-O20-C1
2	C	307	OLC	C2-C3-C4-C5
3	E	314	LFA	C17-C18-C19-C20
3	B	310	LFA	C1-C2-C3-C4
3	E	302	LFA	C17-C18-C19-C20
2	C	301	OLC	C11-C12-C13-C14
2	D	305	OLC	C1-C2-C3-C4
2	B	305	OLC	C9-C10-C11-C12
2	E	301	OLC	C7-C8-C9-C10
2	C	307	OLC	C5-C6-C7-C8
2	B	304	OLC	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	B	306	OLC	C3-C4-C5-C6
2	B	301	OLC	C5-C6-C7-C8
2	A	307	OLC	C5-C6-C7-C8
2	A	304	OLC	O20-C21-C22-C24
2	C	302	OLC	O20-C21-C22-C24
2	C	302	OLC	O20-C21-C22-O23
3	C	313	LFA	C6-C7-C8-C9
5	C	317	BOG	C4-C5-C6-O6
2	A	318	OLC	C14-C15-C16-C17
3	D	303	LFA	C17-C18-C19-C20
3	E	302	LFA	C5-C6-C7-C8
2	C	309	OLC	C6-C7-C8-C9
3	C	313	LFA	C11-C10-C9-C8
2	A	305	OLC	C9-C10-C11-C12
2	D	310	OLC	C7-C8-C9-C10
2	E	305	OLC	C9-C10-C11-C12
2	E	310	OLC	C9-C10-C11-C12
3	E	302	LFA	C4-C5-C6-C7
2	A	303	OLC	C15-C16-C17-C18
2	D	310	OLC	C15-C16-C17-C18
2	D	305	OLC	C12-C13-C14-C15
2	D	310	OLC	C3-C4-C5-C6
2	C	306	OLC	C9-C10-C11-C12
2	D	307	OLC	C7-C8-C9-C10
2	A	317	OLC	C10-C11-C12-C13
2	A	301	OLC	C9-C10-C11-C12
3	A	320	LFA	C1-C2-C3-C4
2	B	304	OLC	C7-C8-C9-C10
2	B	306	OLC	C7-C8-C9-C10
2	C	301	OLC	C7-C8-C9-C10
2	E	304	OLC	C9-C10-C11-C12
3	C	314	LFA	C6-C7-C8-C9
3	B	309	LFA	C15-C16-C17-C18
3	E	302	LFA	C11-C12-C13-C14
3	A	319	LFA	C12-C13-C14-C15
2	C	305	OLC	C9-C10-C11-C12
3	D	314	LFA	C6-C7-C8-C9
2	A	303	OLC	C7-C8-C9-C10
2	A	318	OLC	C9-C10-C11-C12
2	C	302	OLC	C9-C10-C11-C12
2	A	301	OLC	C11-C12-C13-C14
3	B	312	LFA	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
3	B	311	LFA	C2-C3-C4-C5
3	D	314	LFA	C2-C3-C4-C5
2	D	305	OLC	O20-C21-C22-C24
2	B	304	OLC	C9-C10-C11-C12
3	B	303	LFA	C17-C18-C19-C20
2	E	304	OLC	C3-C4-C5-C6
2	A	302	OLC	C9-C10-C11-C12
2	E	309	OLC	C9-C10-C11-C12
3	A	319	LFA	C14-C15-C16-C17
2	A	306	OLC	C5-C6-C7-C8
3	A	319	LFA	C2-C3-C4-C5
2	D	305	OLC	C14-C15-C16-C17
3	B	303	LFA	C7-C8-C9-C10
2	C	305	OLC	C7-C8-C9-C10
2	A	303	OLC	O20-C1-C2-C3
2	B	301	OLC	C3-C4-C5-C6
3	A	310	LFA	C14-C15-C16-C17
3	D	315	LFA	C17-C18-C19-C20
3	B	303	LFA	C5-C6-C7-C8
2	A	302	OLC	O19-C1-O20-C21
2	C	301	OLC	O19-C1-O20-C21
2	A	302	OLC	C2-C1-O20-C21
2	D	308	OLC	C2-C1-O20-C21
3	C	313	LFA	C7-C8-C9-C10
2	D	301	OLC	C4-C5-C6-C7
3	D	320	LFA	C1-C2-C3-C4
3	C	304	LFA	C17-C18-C19-C20
2	A	303	OLC	O19-C1-C2-C3
2	C	301	OLC	C2-C1-O20-C21
2	A	303	OLC	C12-C13-C14-C15
5	D	318	BOG	C2'-C3'-C4'-C5'

There are no ring outliers.

27 monomers are involved in 49 short contacts:

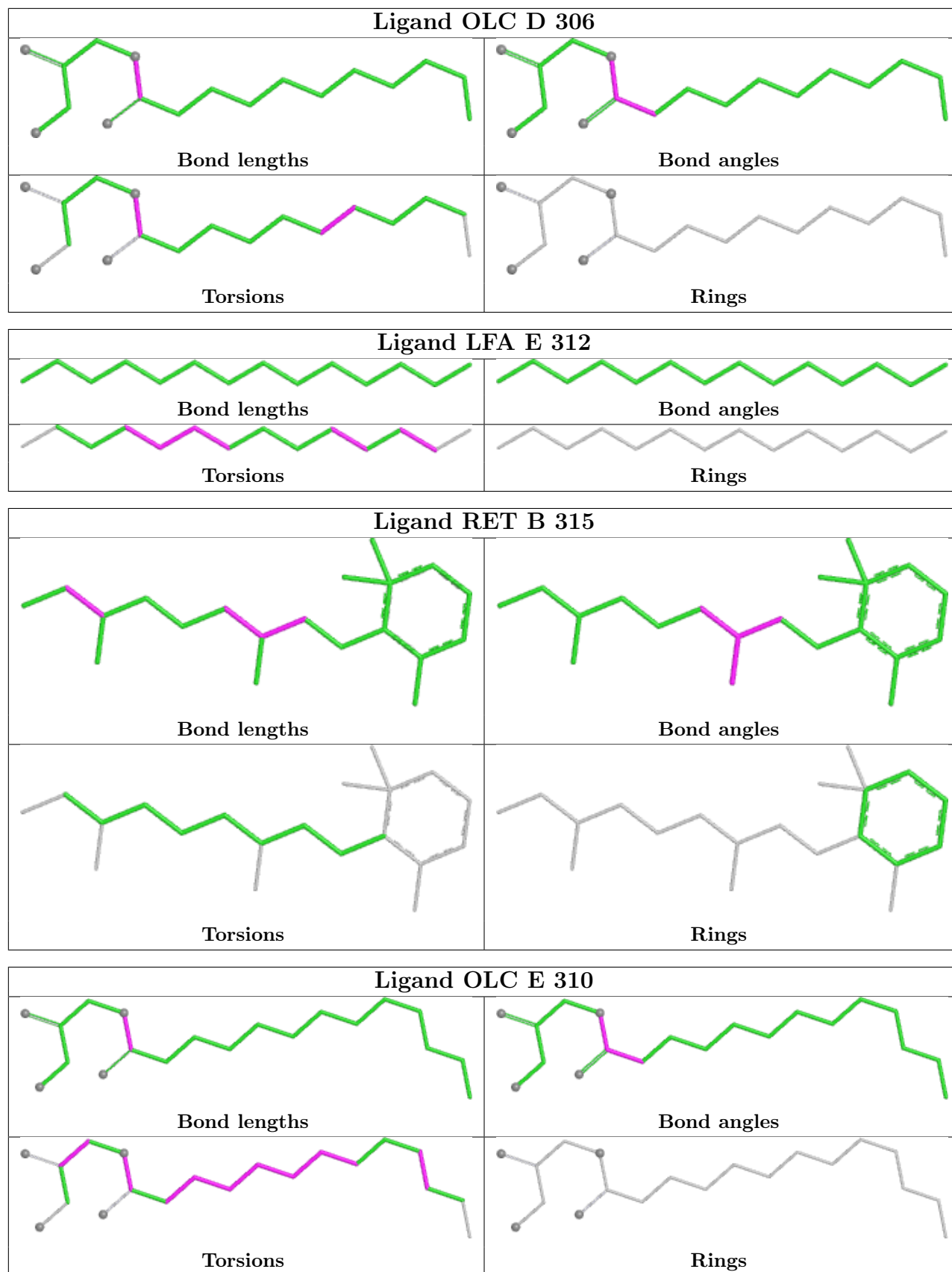
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	315	RET	3	0
6	E	317	RET	3	0
2	E	304	OLC	2	0
2	C	302	OLC	1	0
3	D	320	LFA	1	0
2	A	303	OLC	1	0

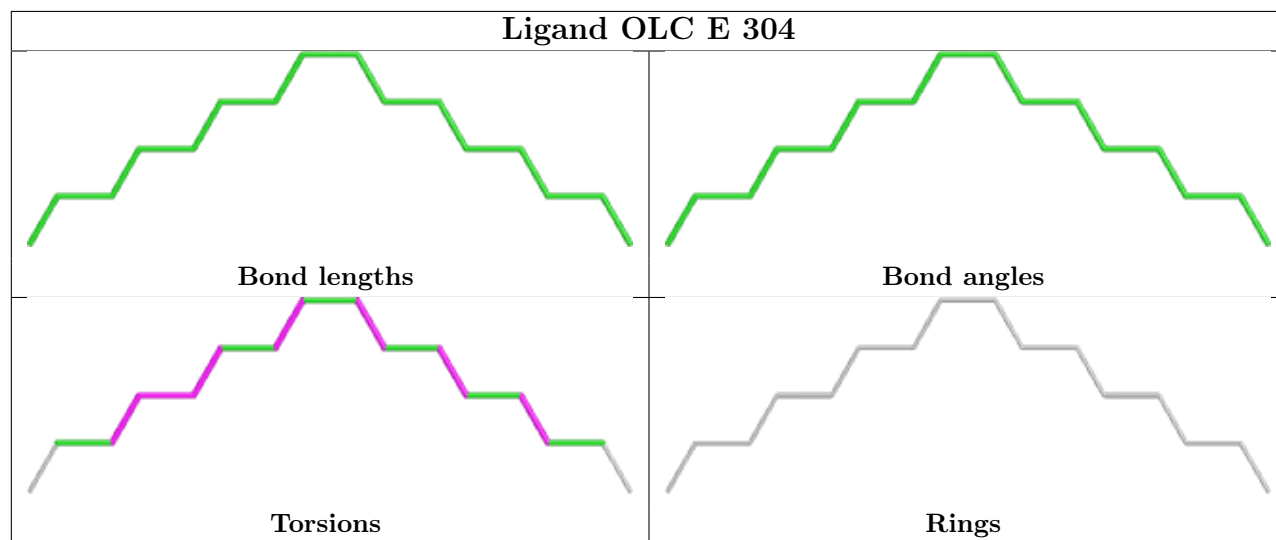
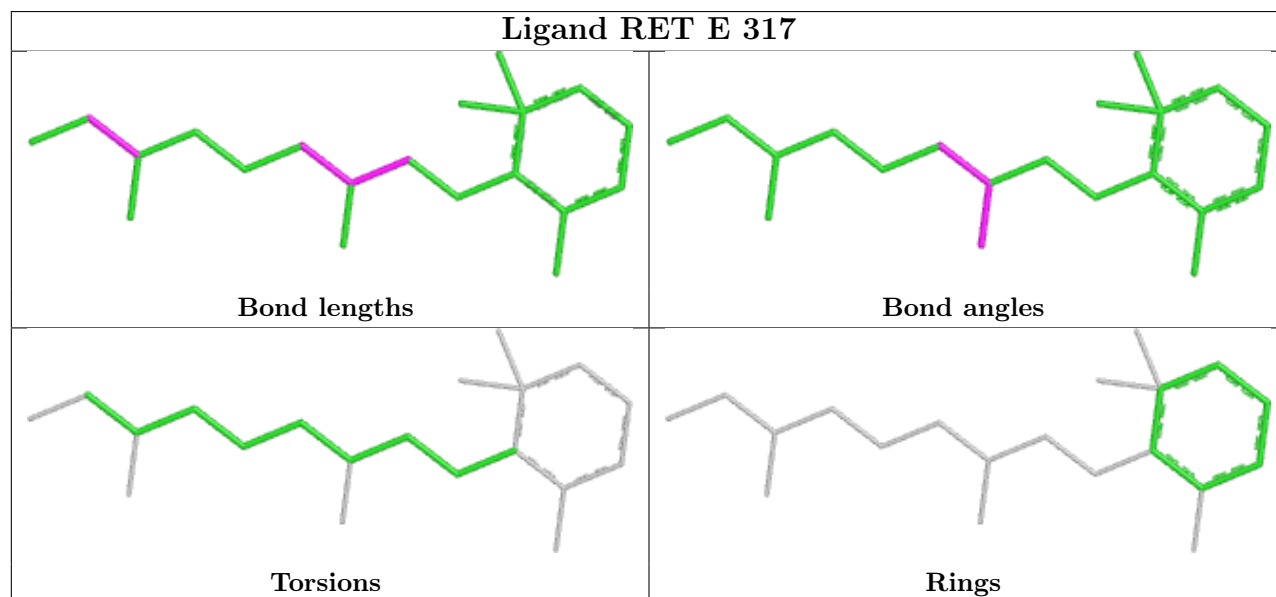
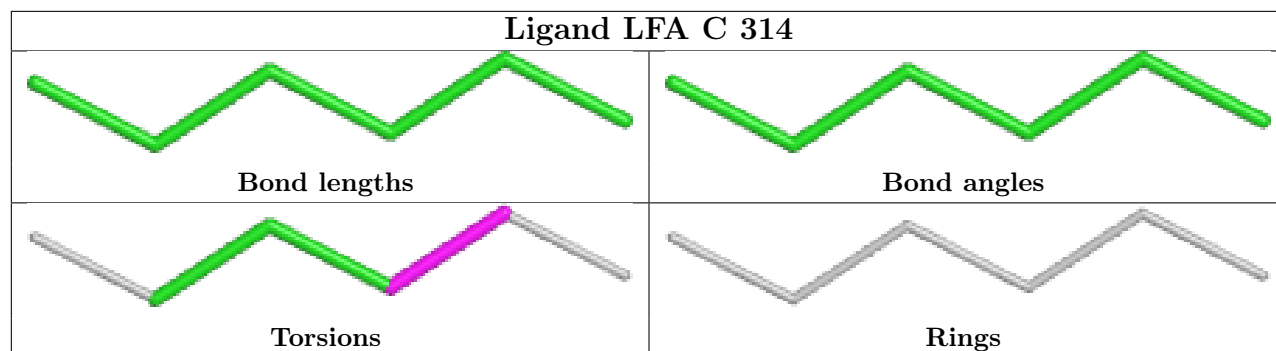
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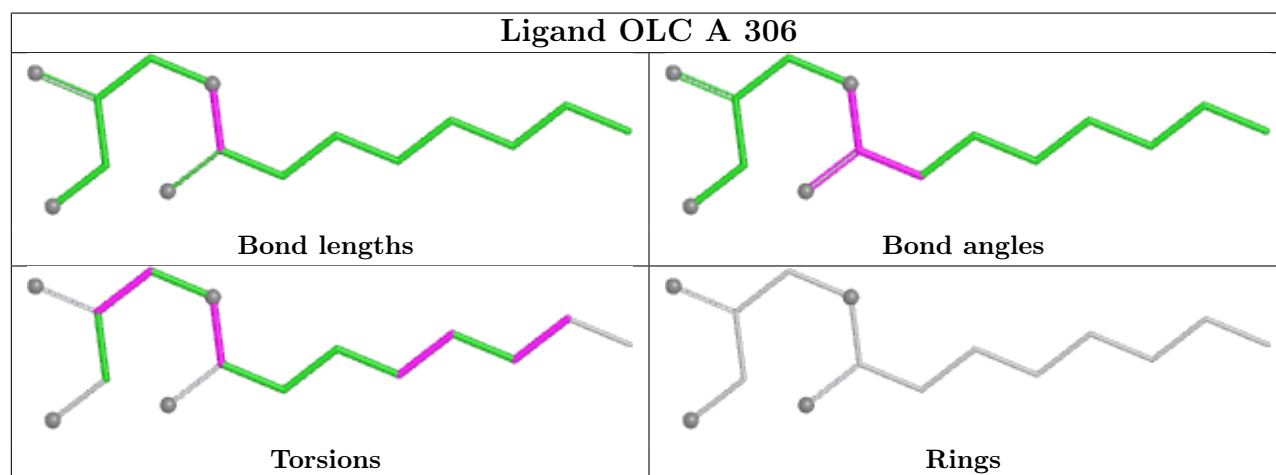
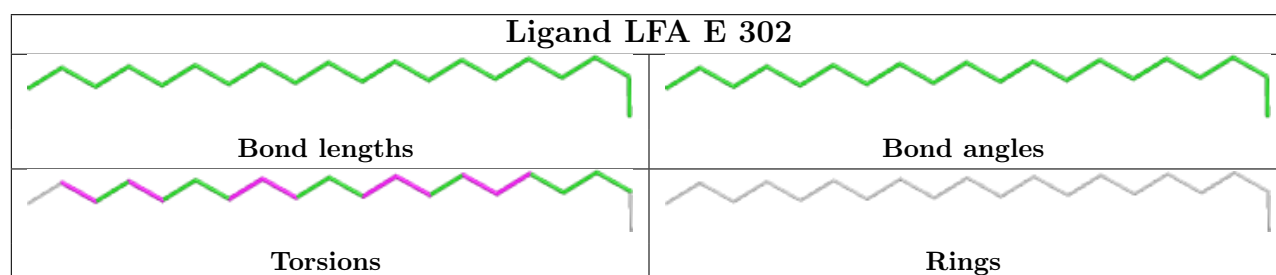
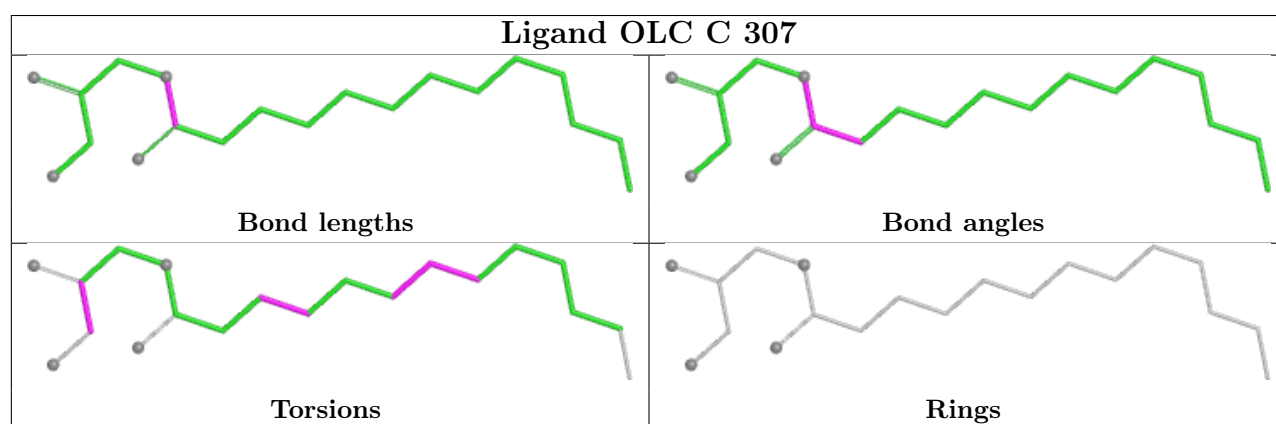
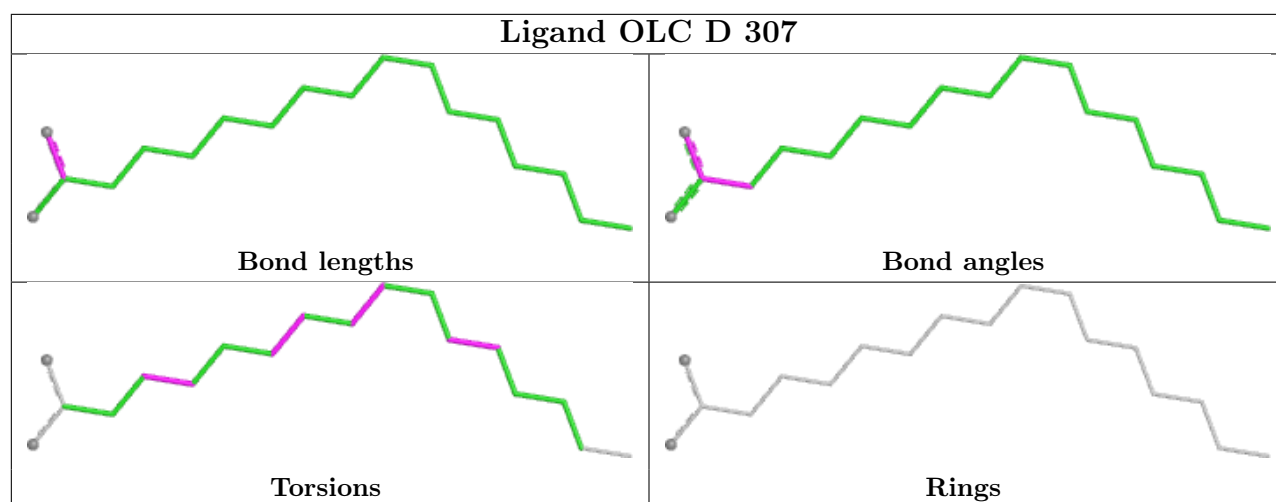
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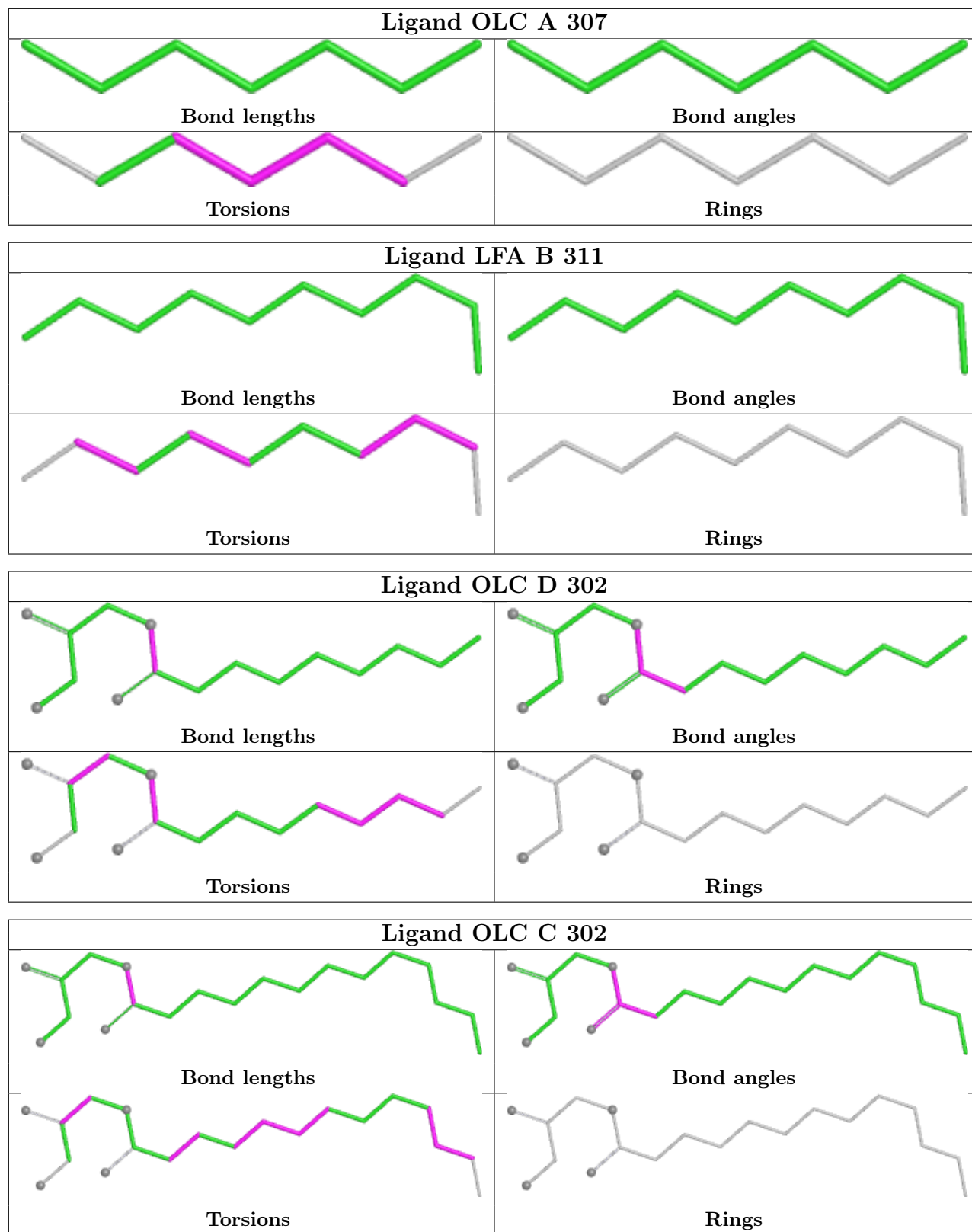
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	314	LFA	1	0
5	D	318	BOG	2	0
3	D	303	LFA	1	0
2	A	317	OLC	2	0
2	E	309	OLC	1	0
2	B	301	OLC	4	0
5	C	317	BOG	1	0
2	A	302	OLC	2	0
2	C	305	OLC	4	0
2	D	310	OLC	1	0
6	A	316	RET	4	0
2	C	309	OLC	1	0
3	C	313	LFA	1	0
5	A	315	BOG	2	0
2	D	301	OLC	2	0
2	B	304	OLC	1	0
6	C	318	RET	2	0
5	B	314	BOG	2	0
3	C	311	LFA	5	0
3	C	304	LFA	2	0
6	D	319	RET	2	0

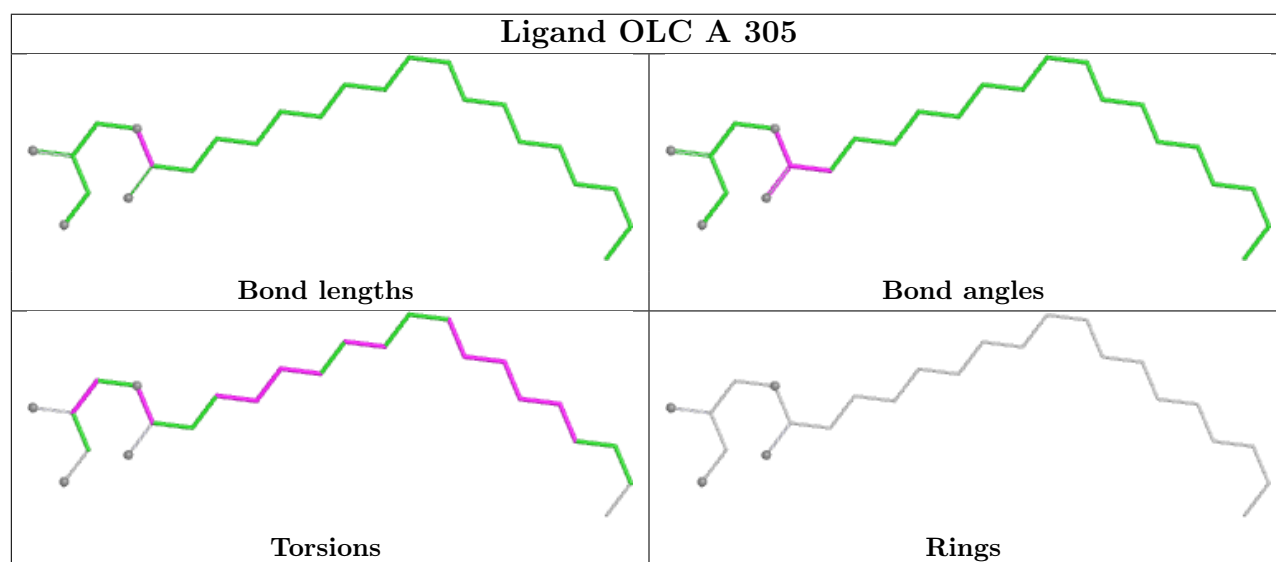
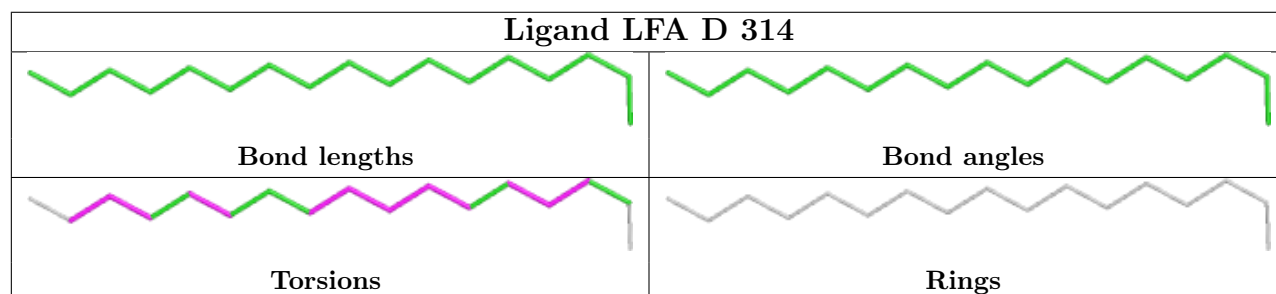
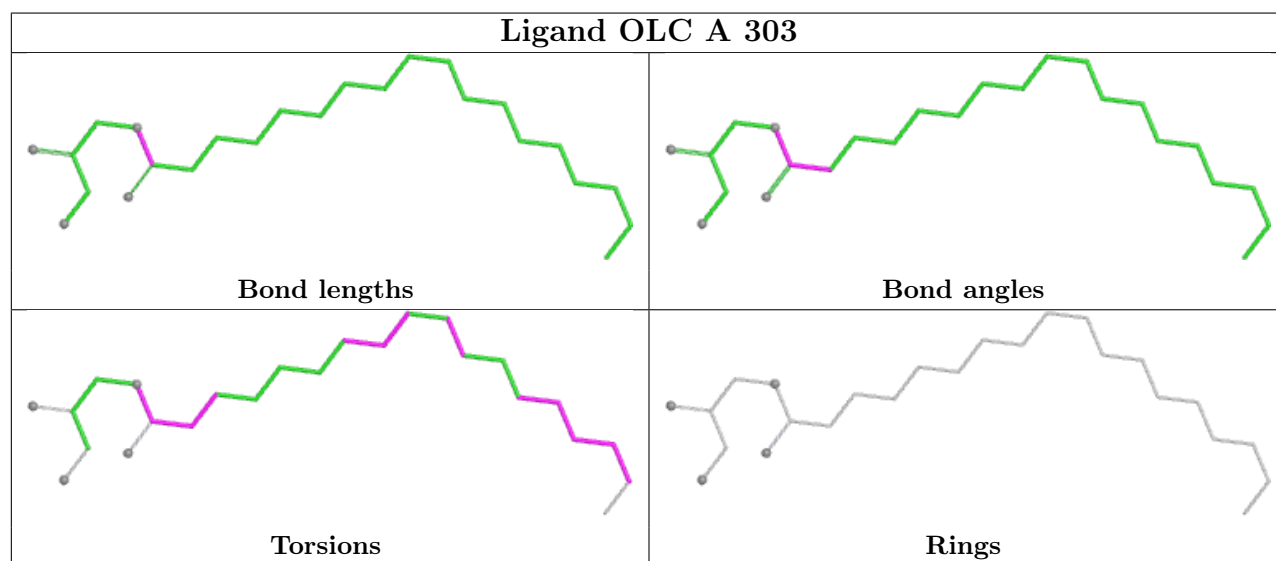
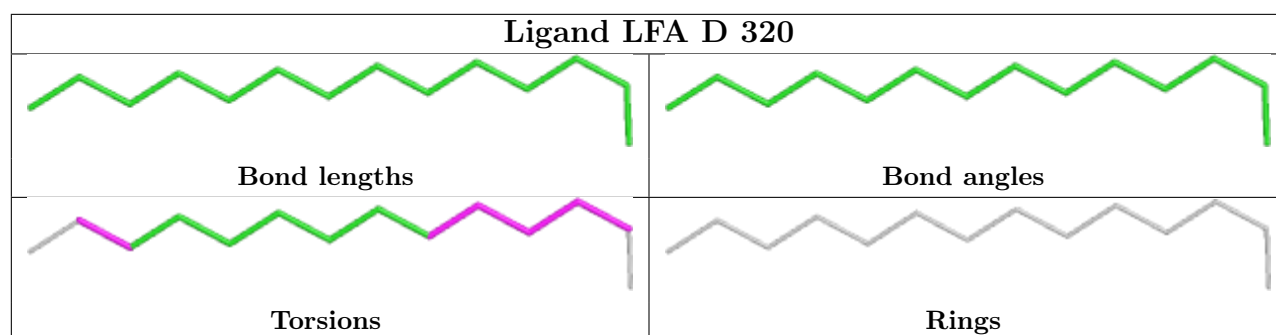
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

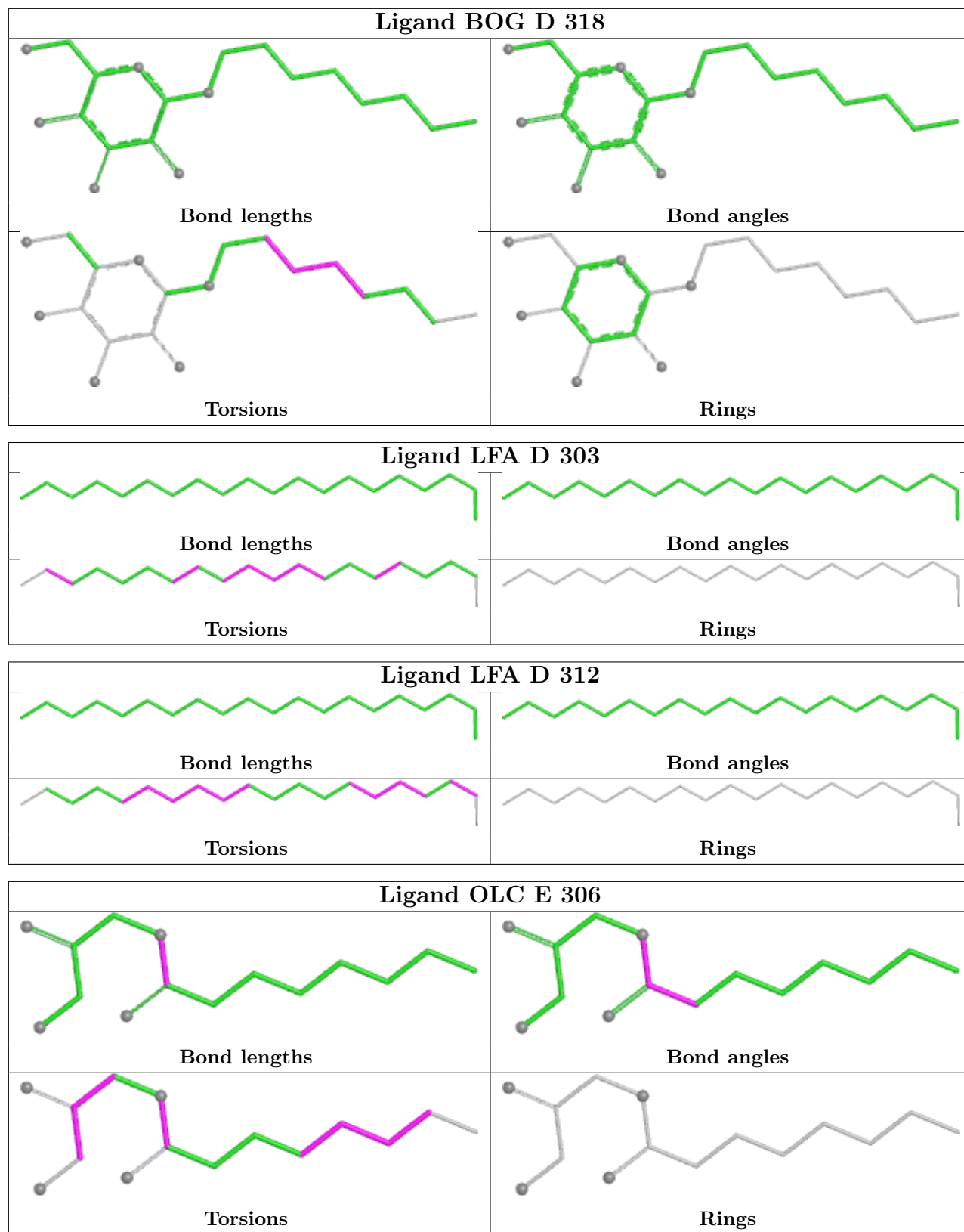


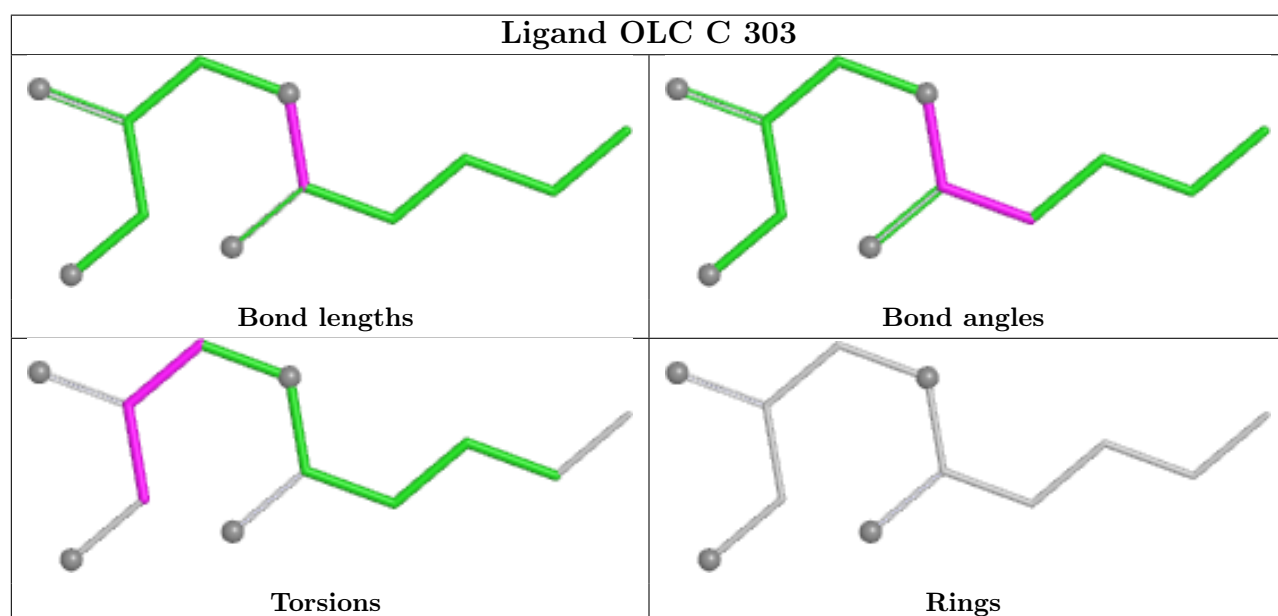
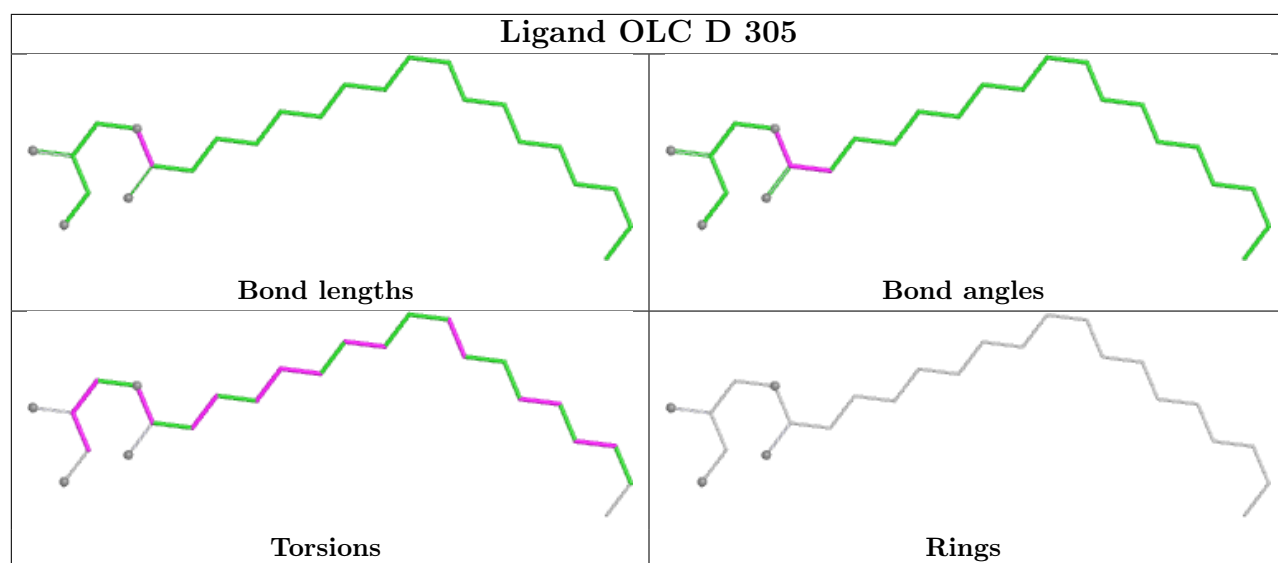
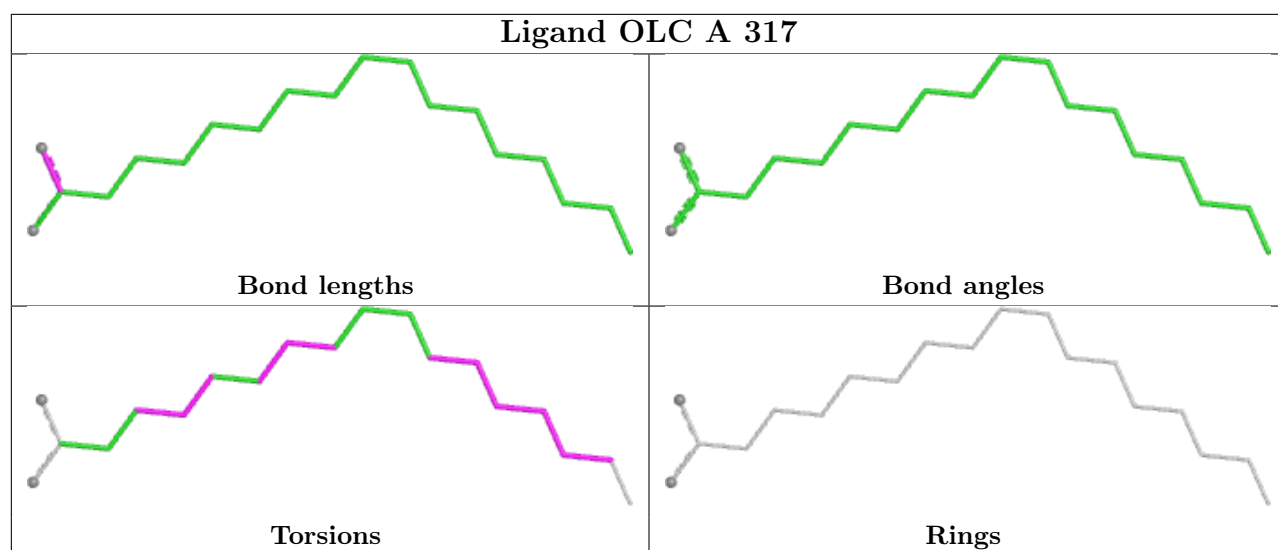


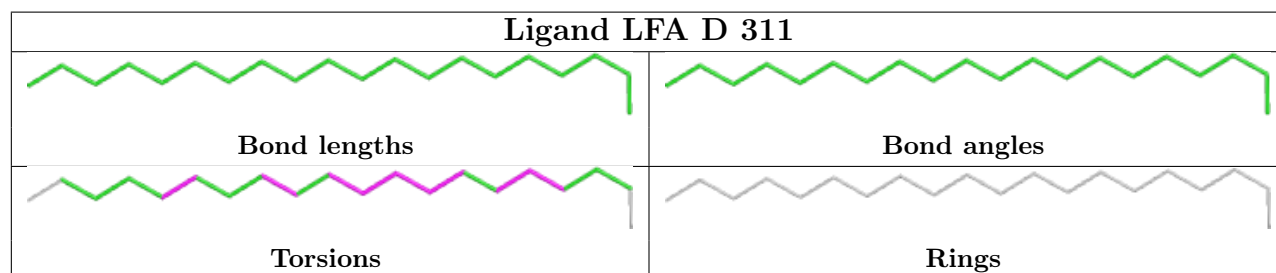
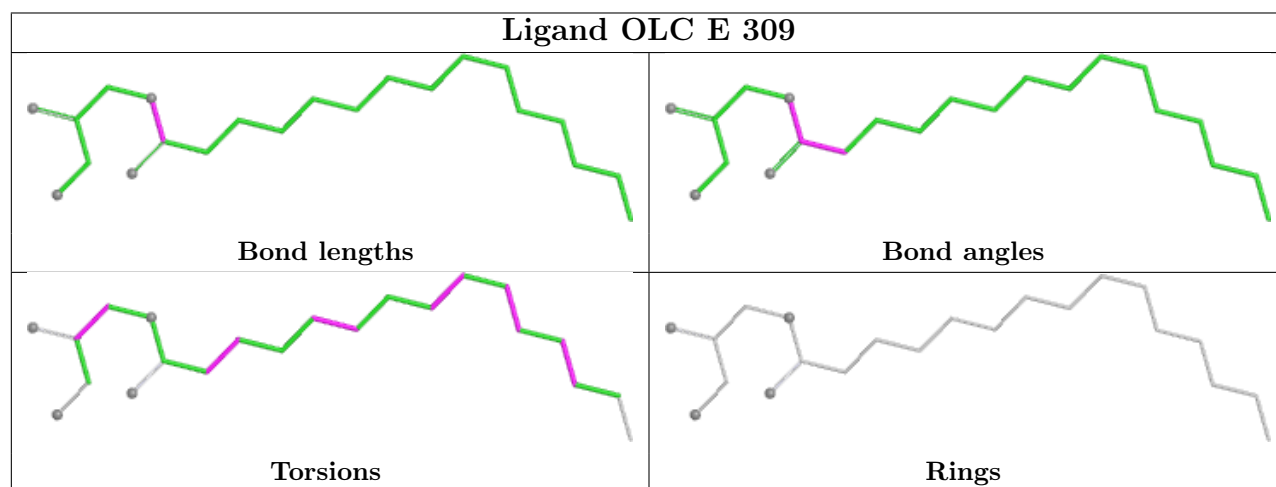
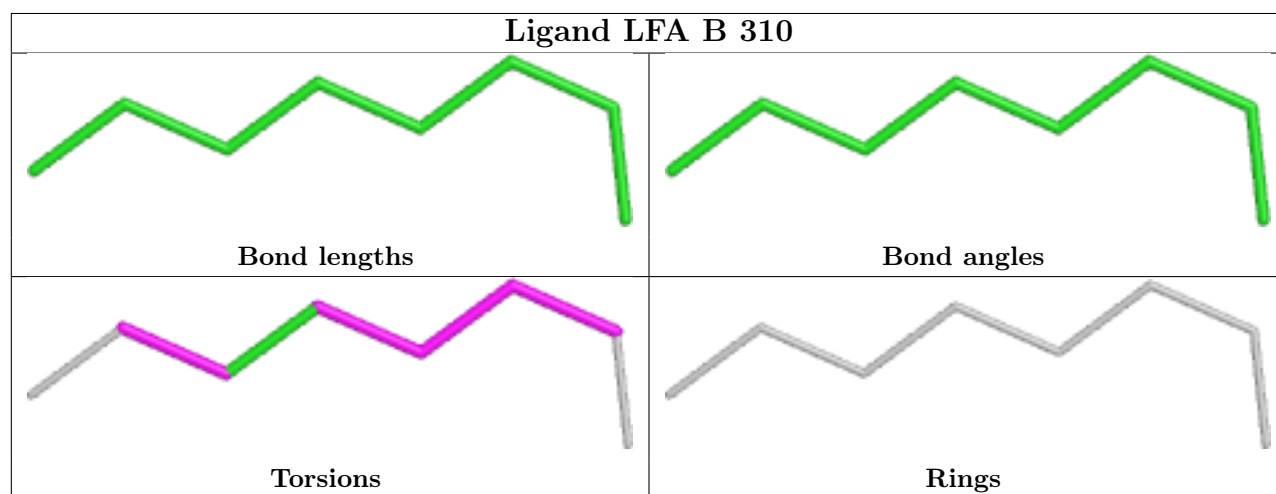
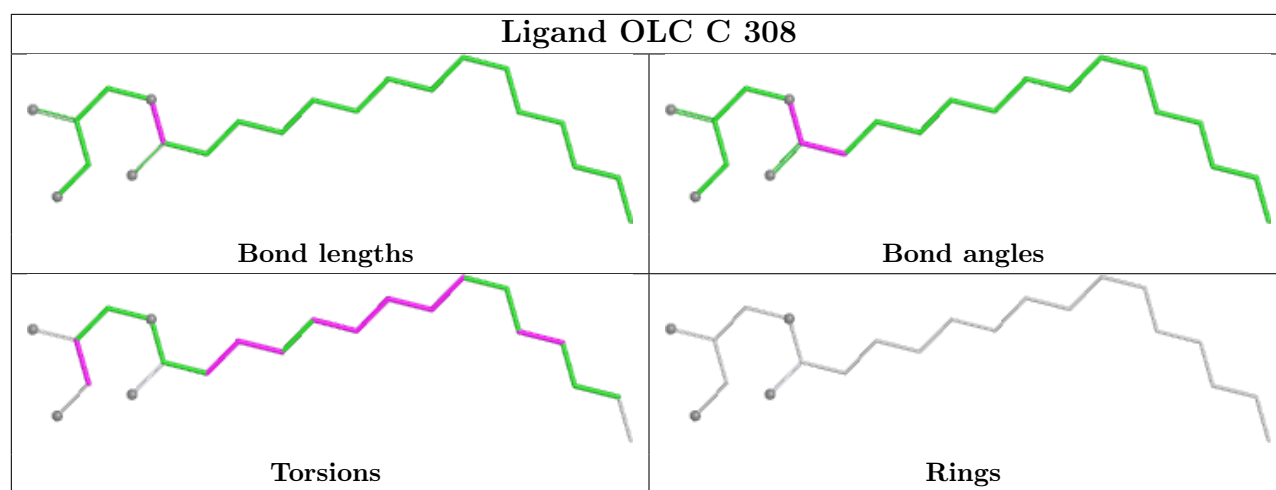


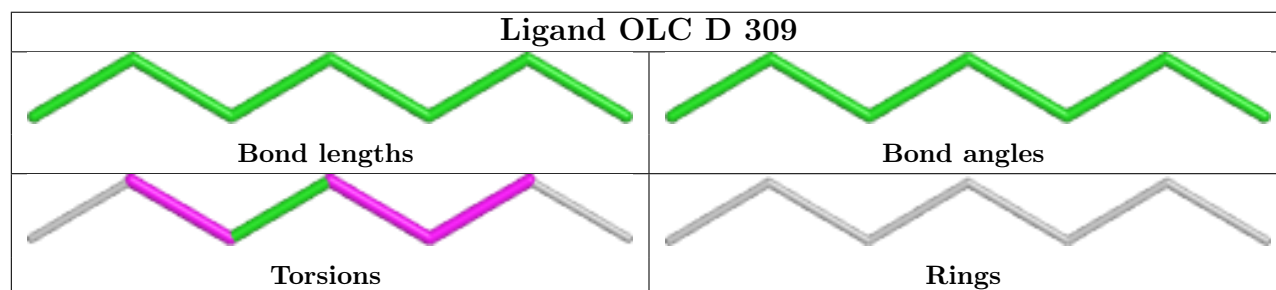
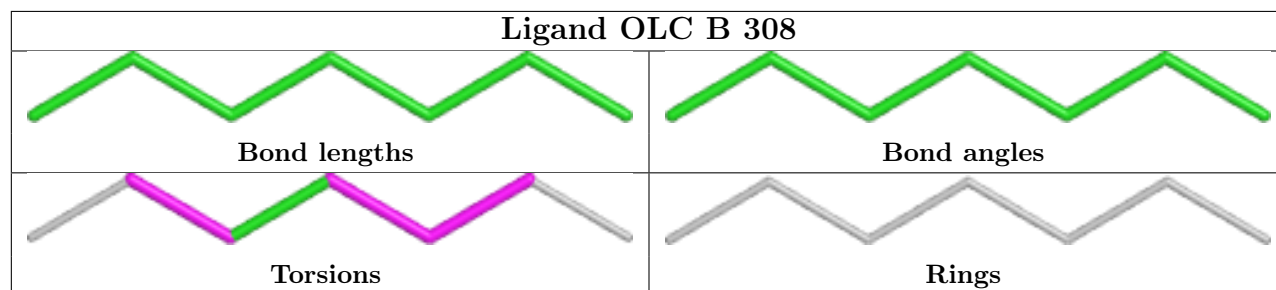
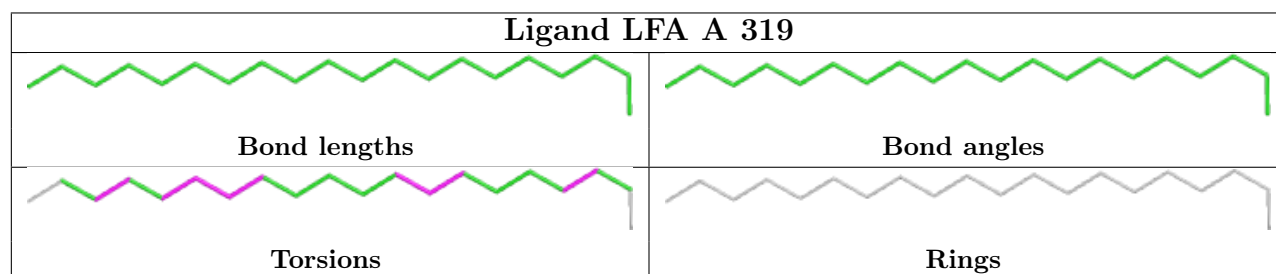
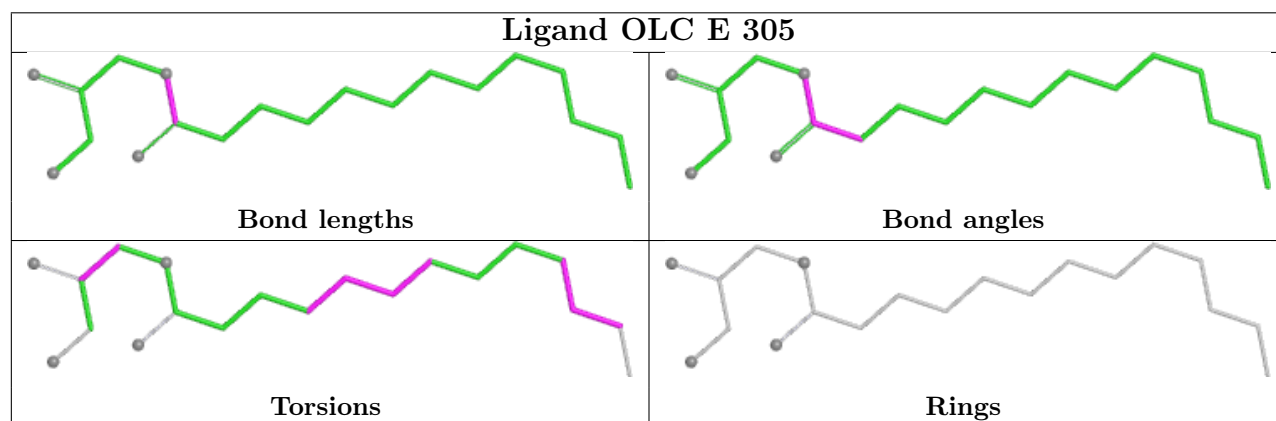
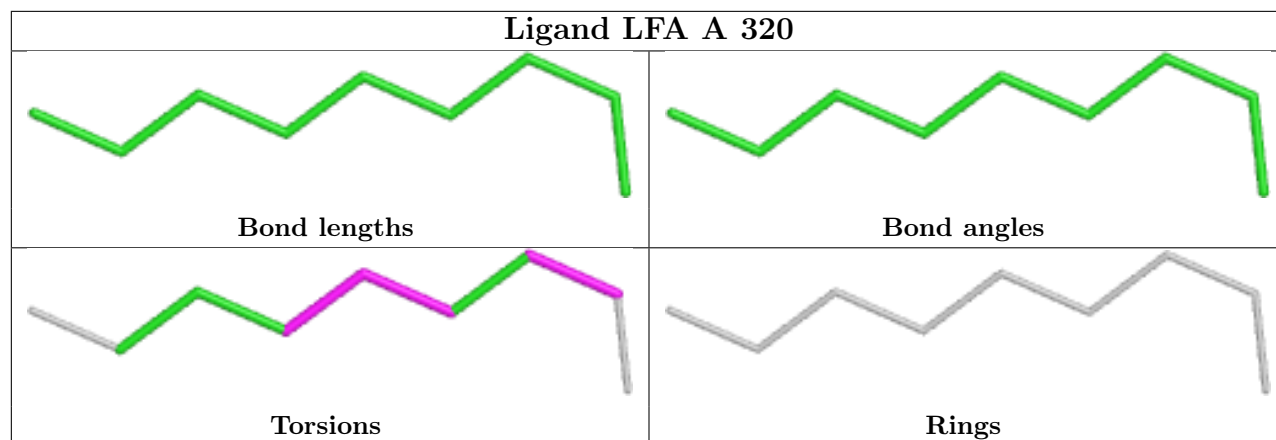


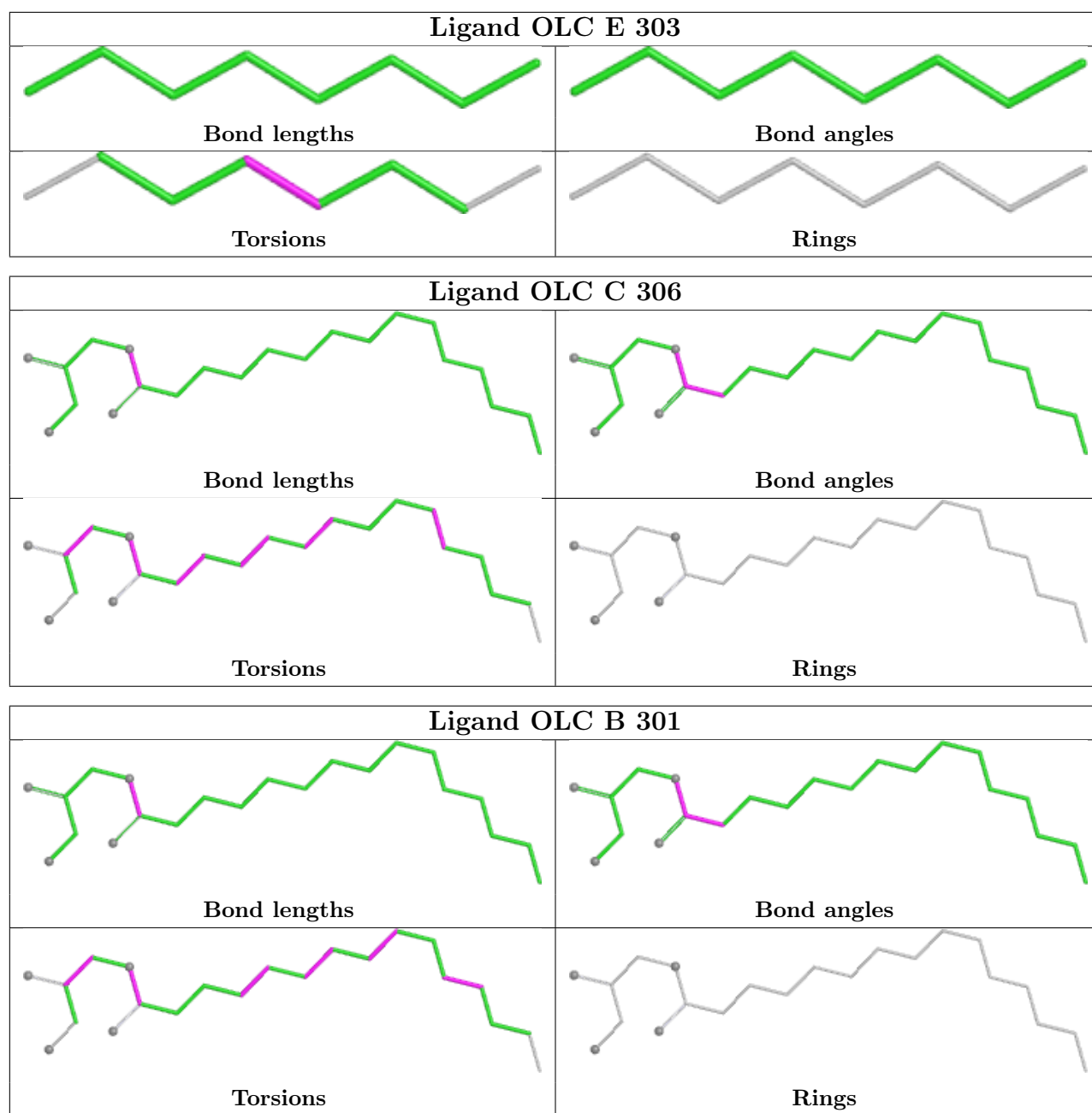


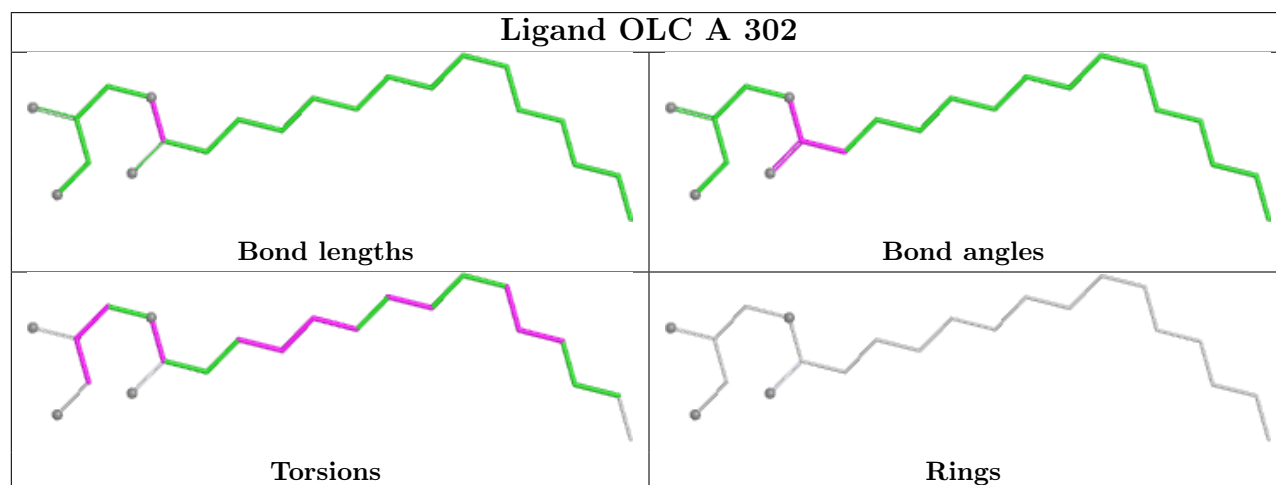
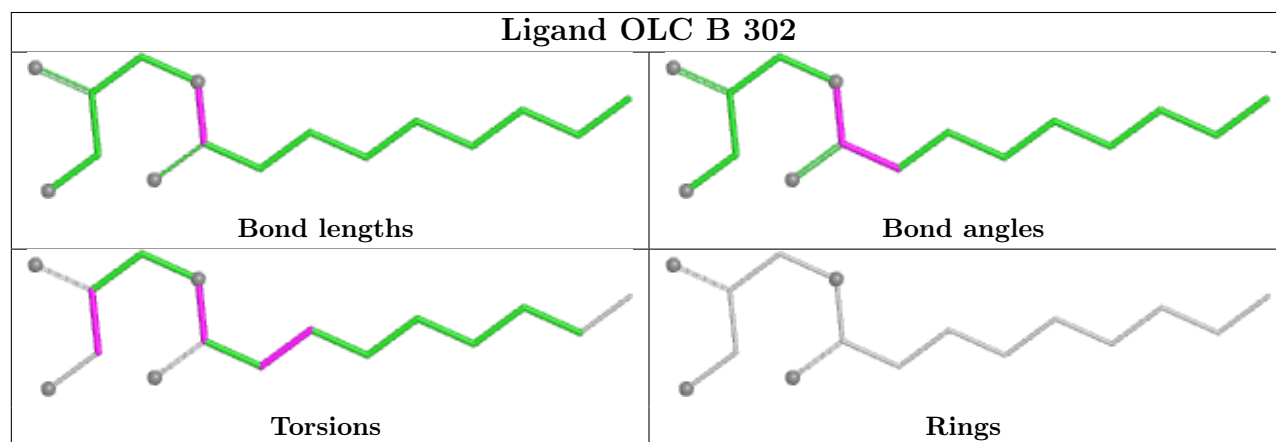
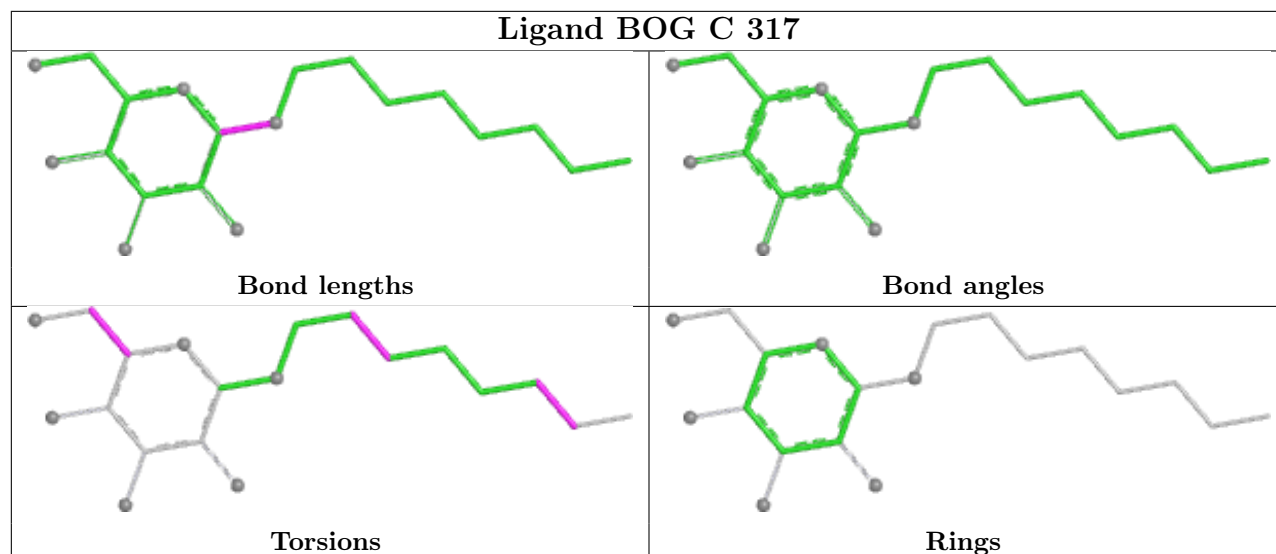


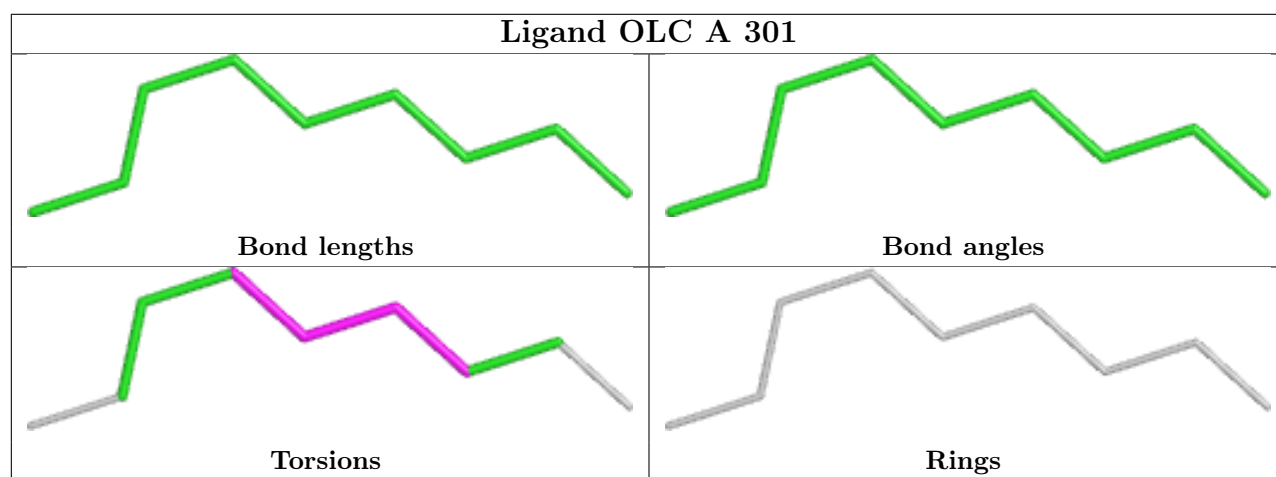
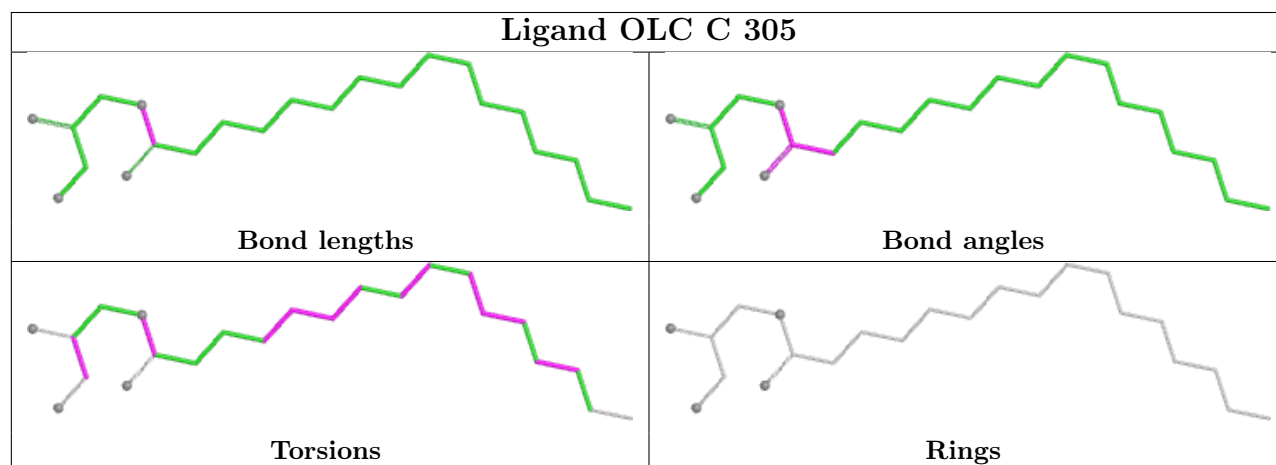
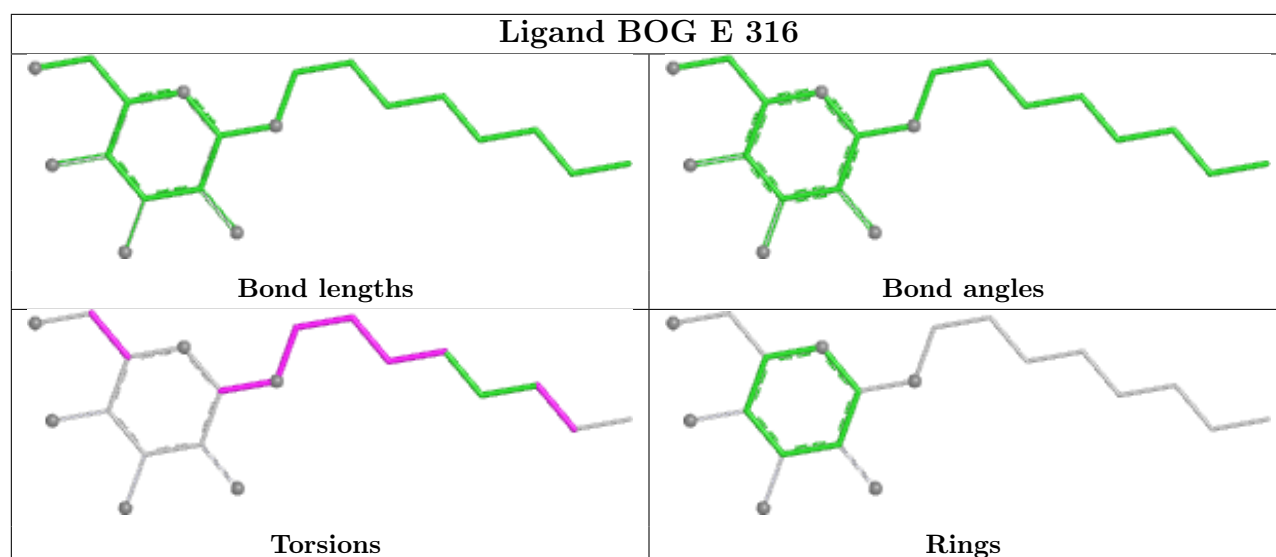


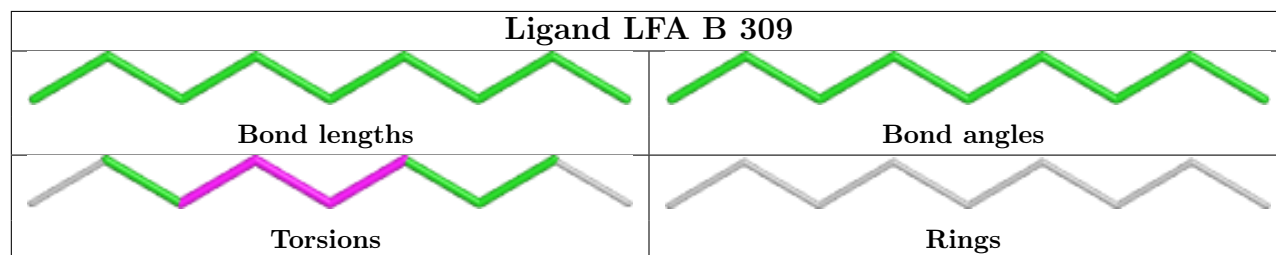
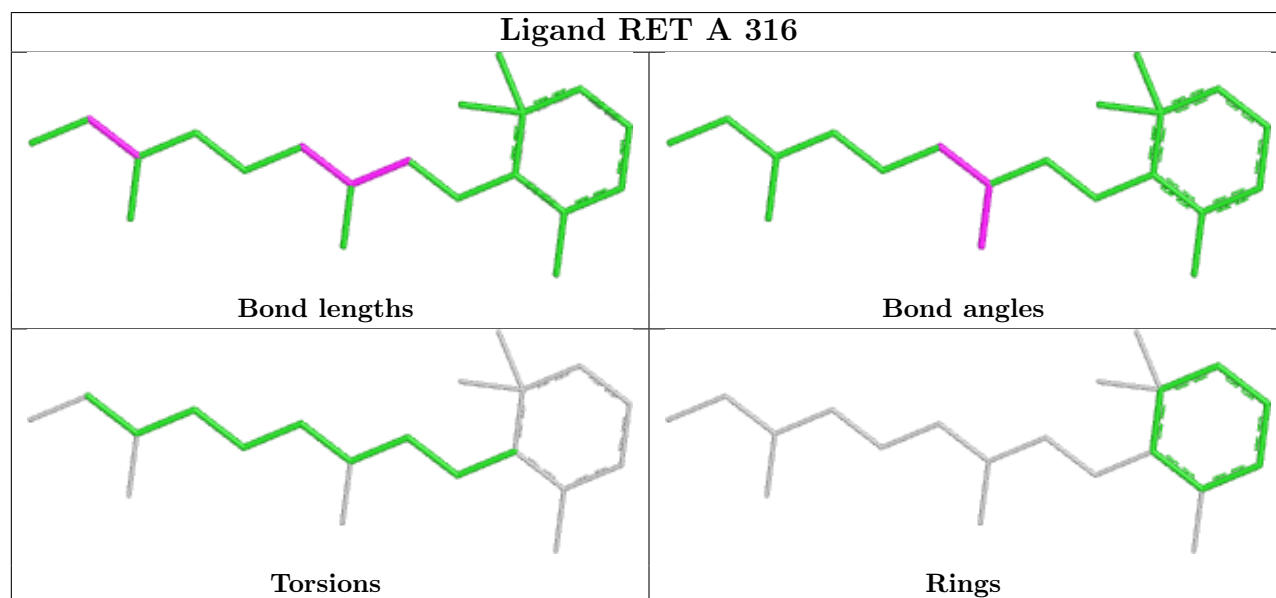
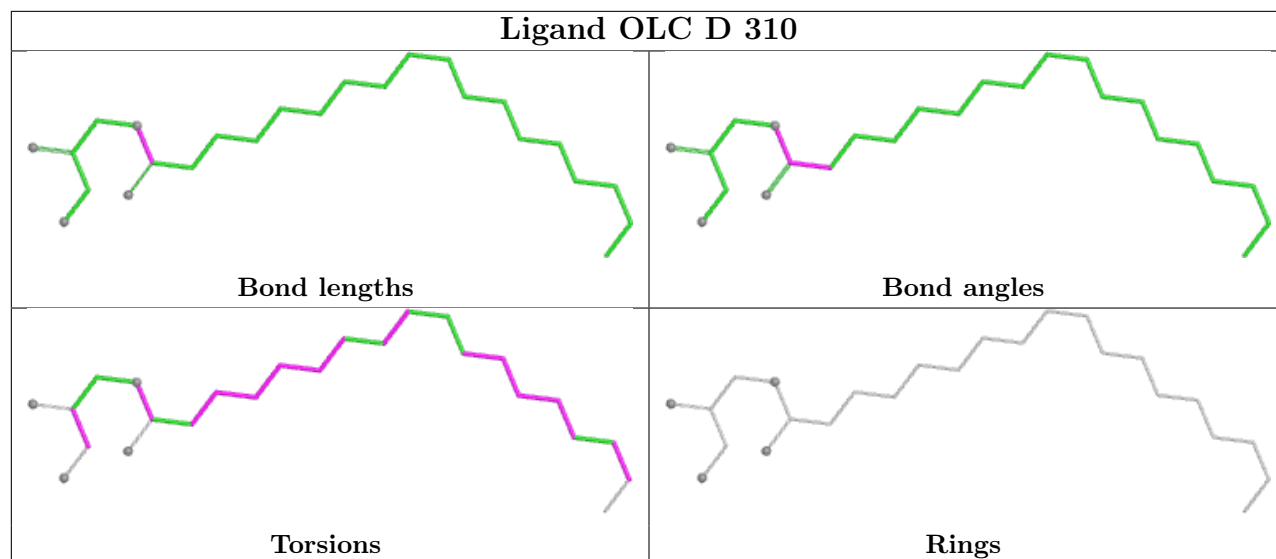


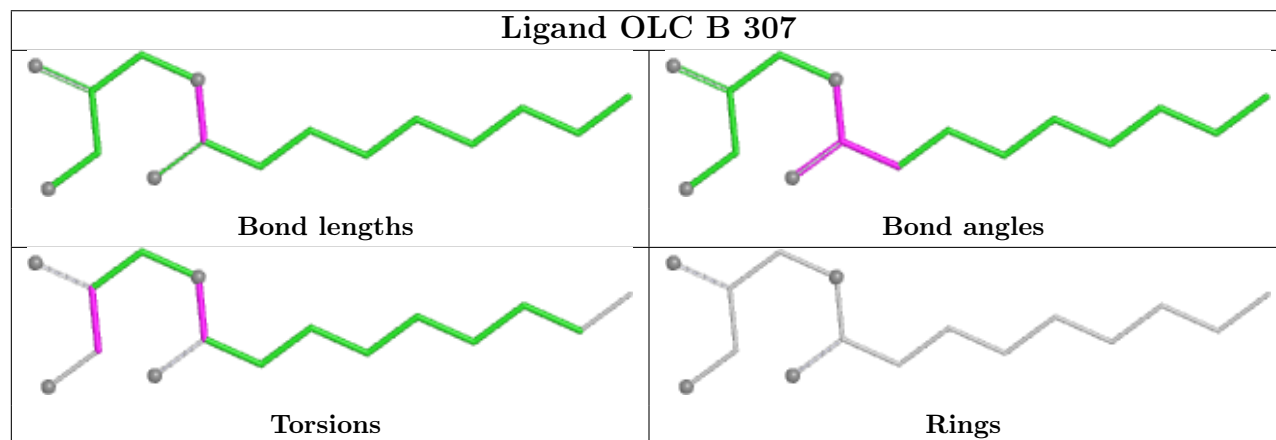
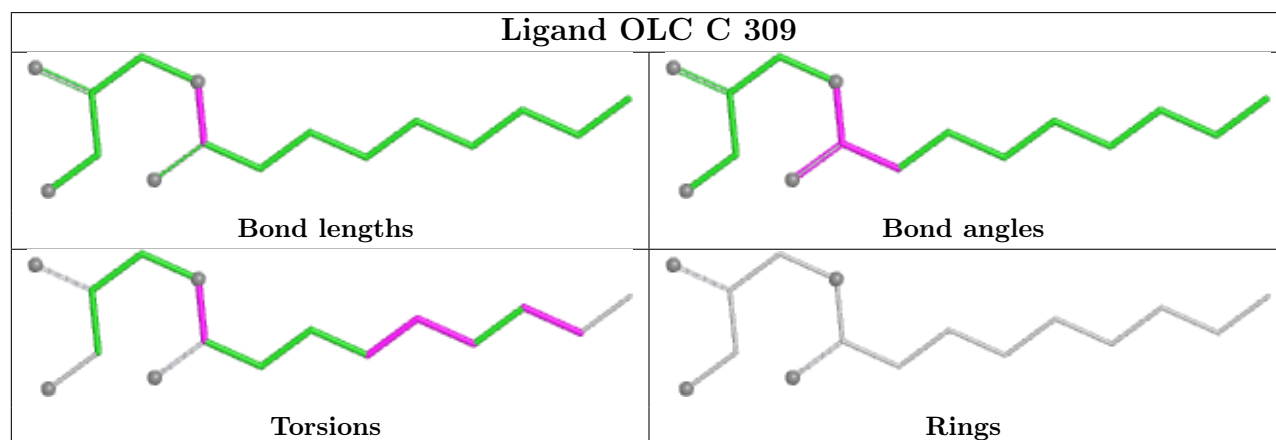
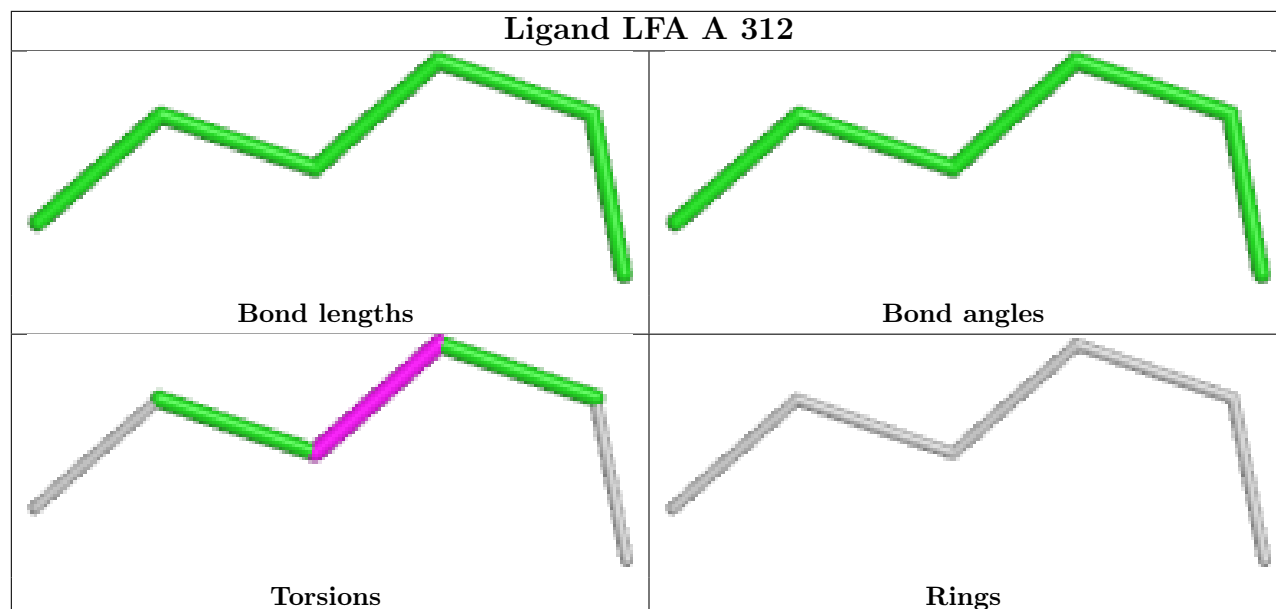


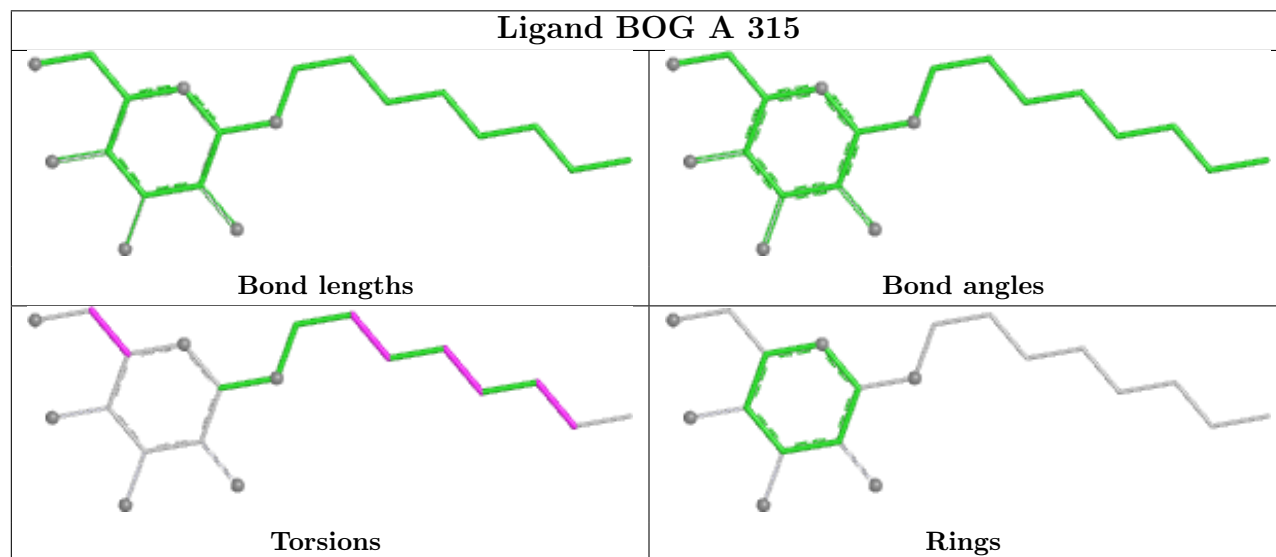
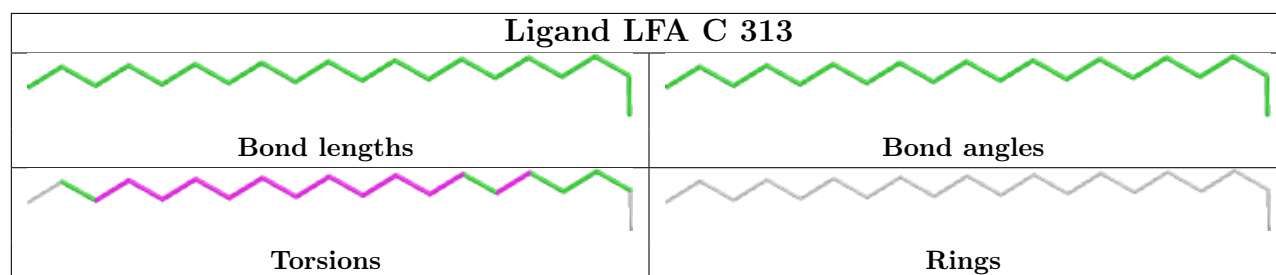
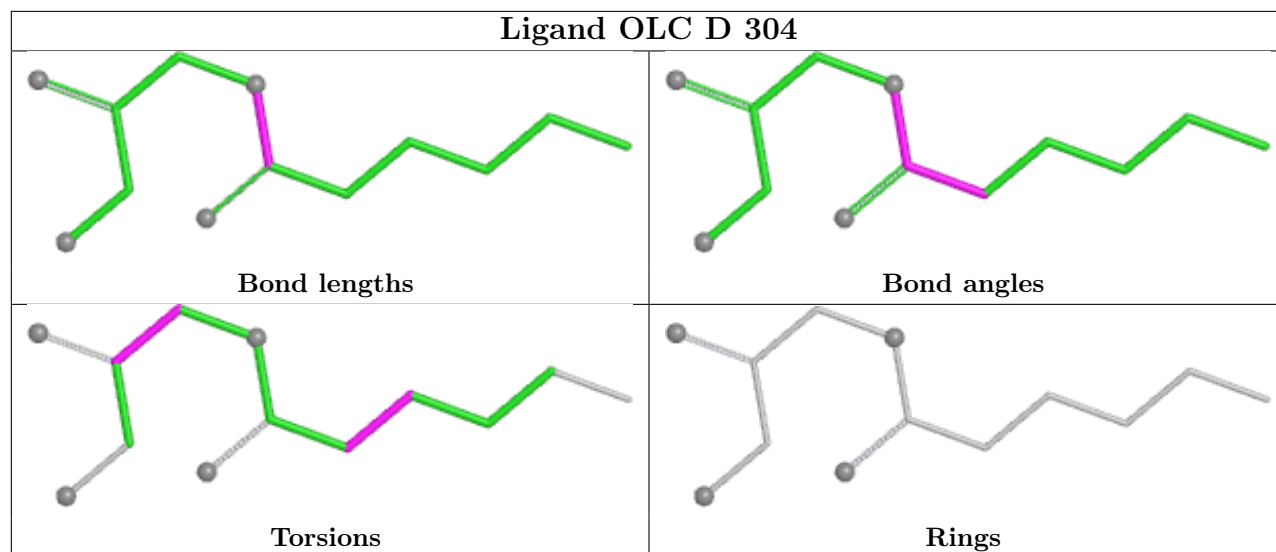


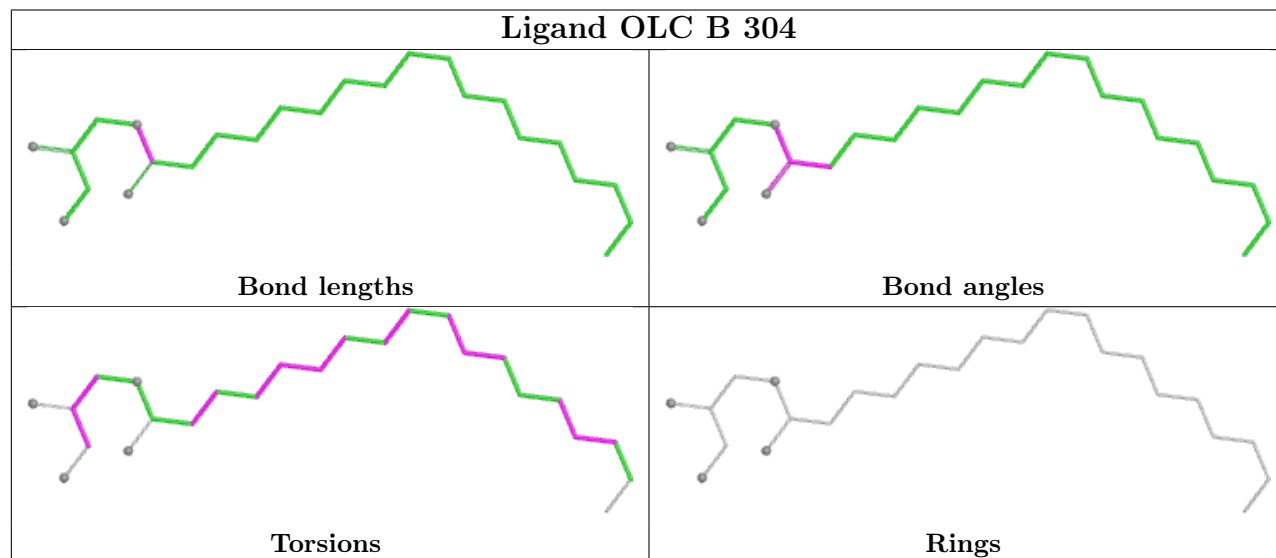
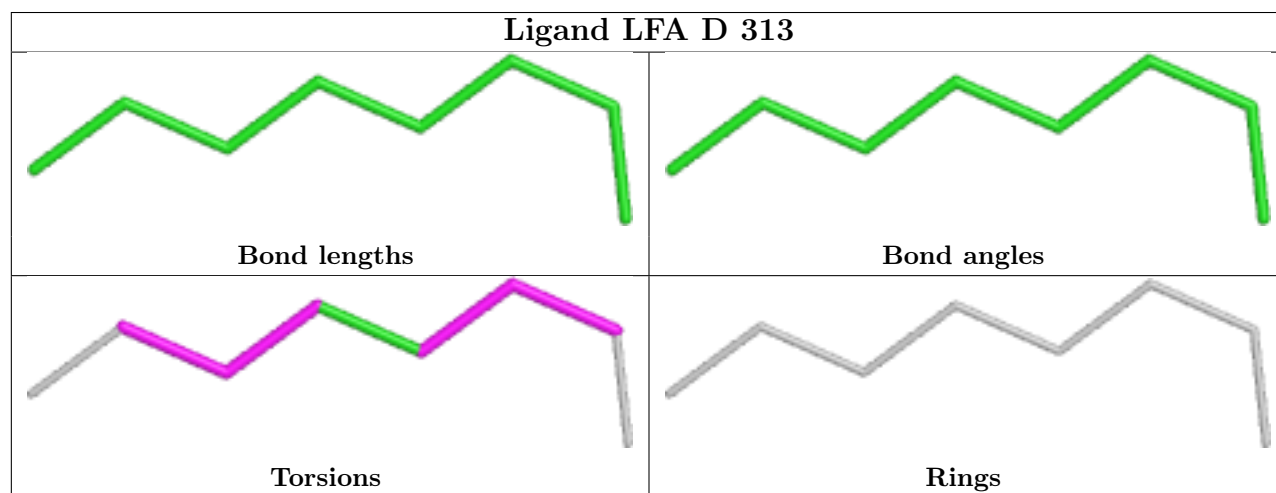
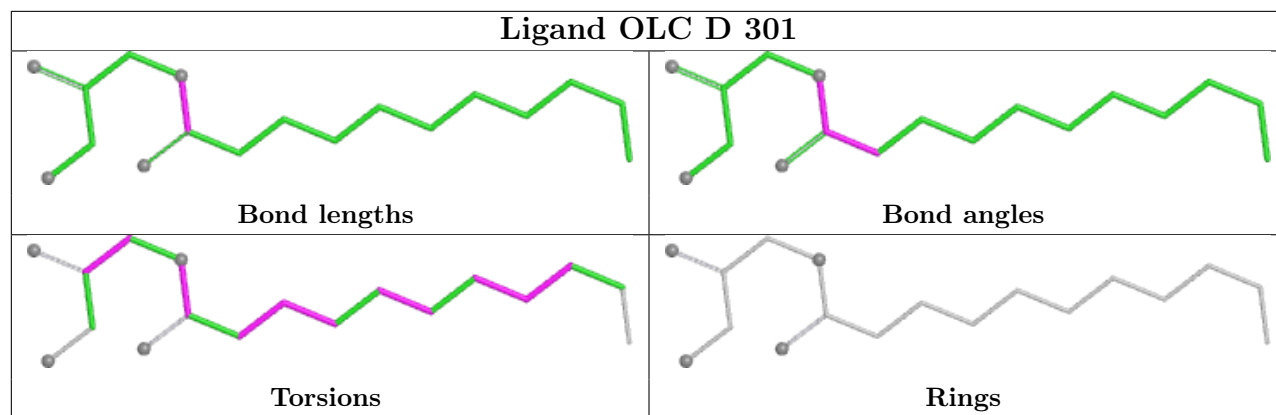


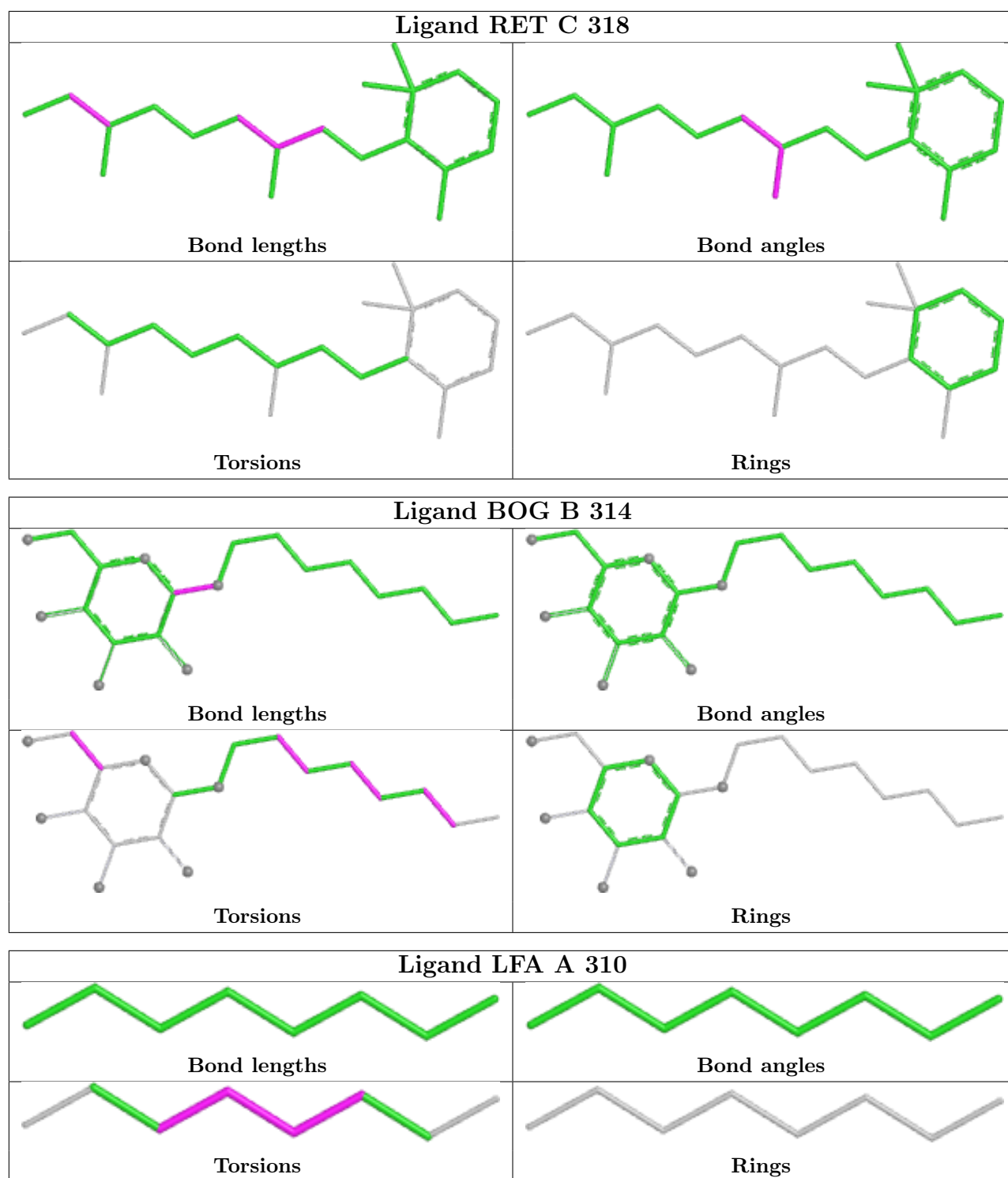


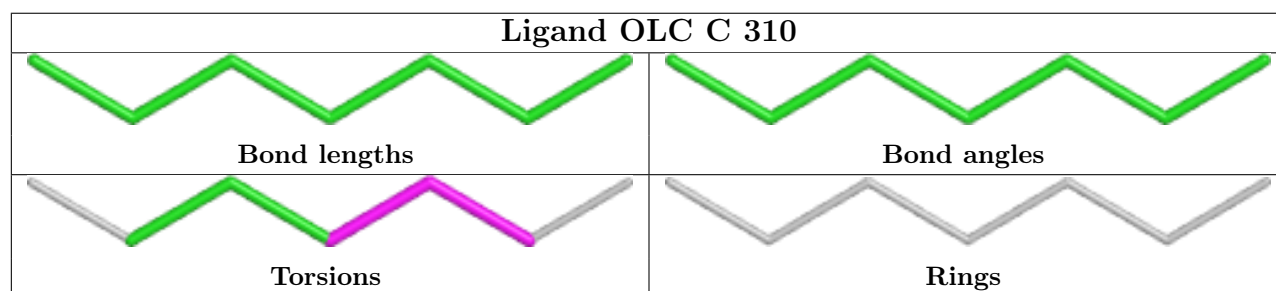
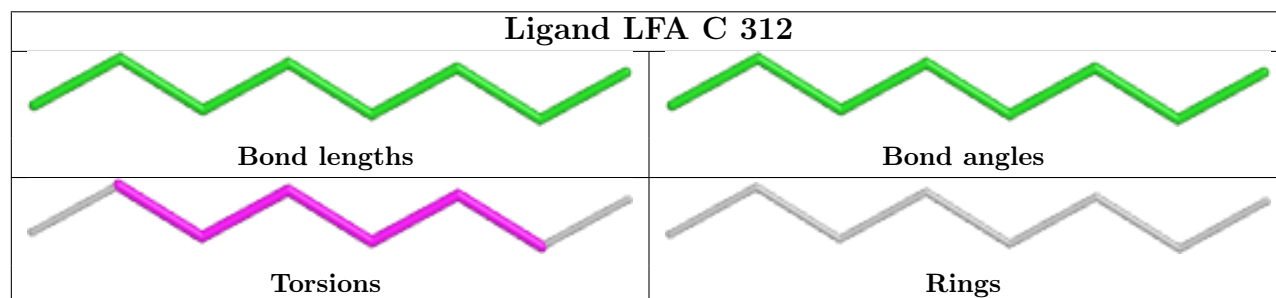
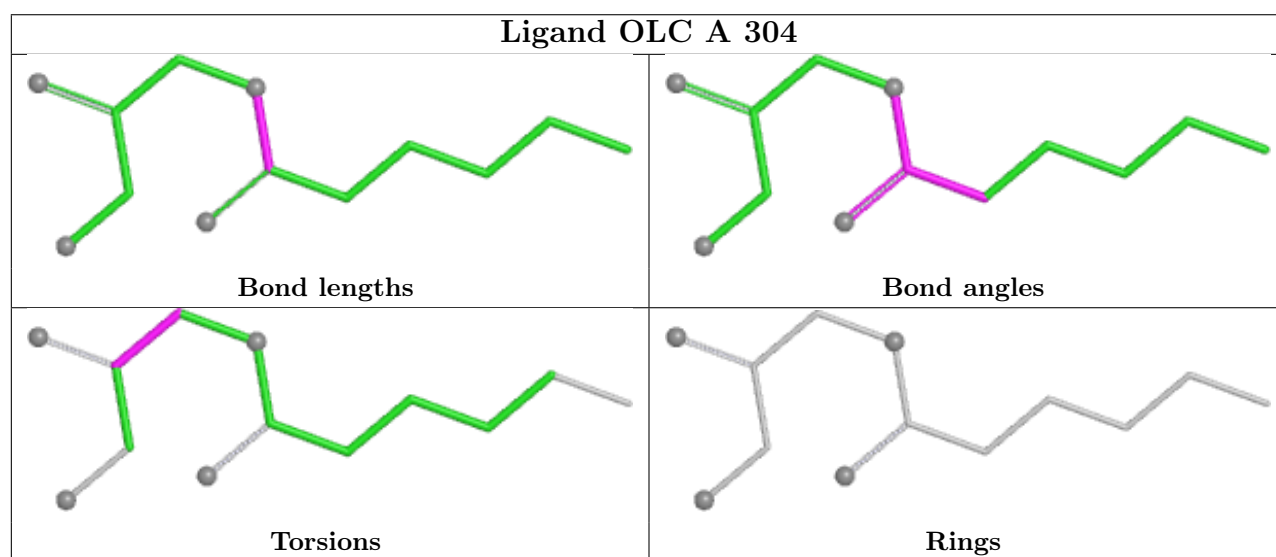
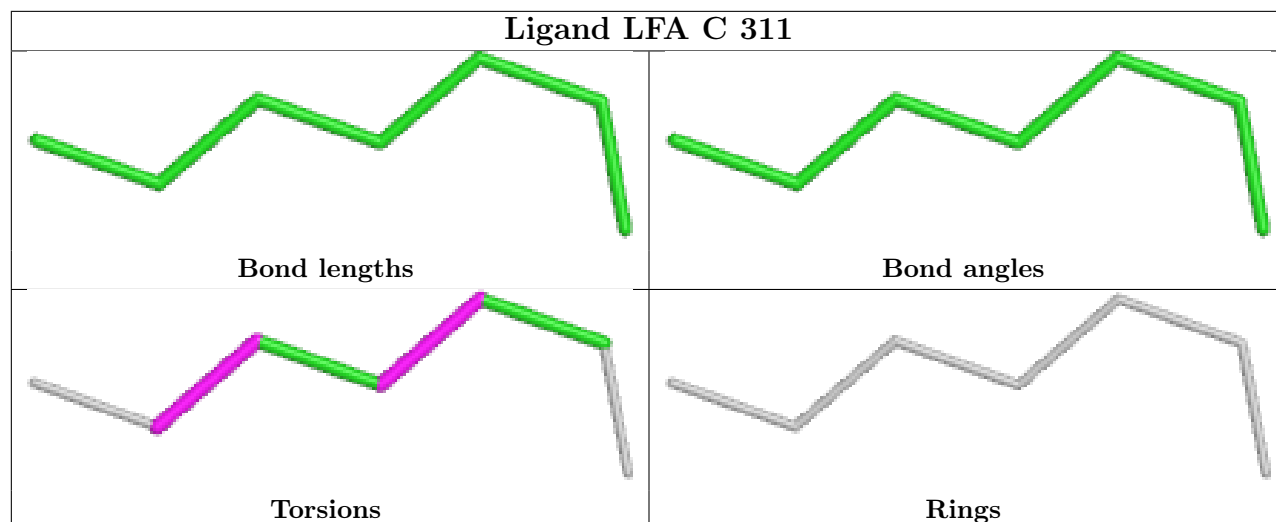


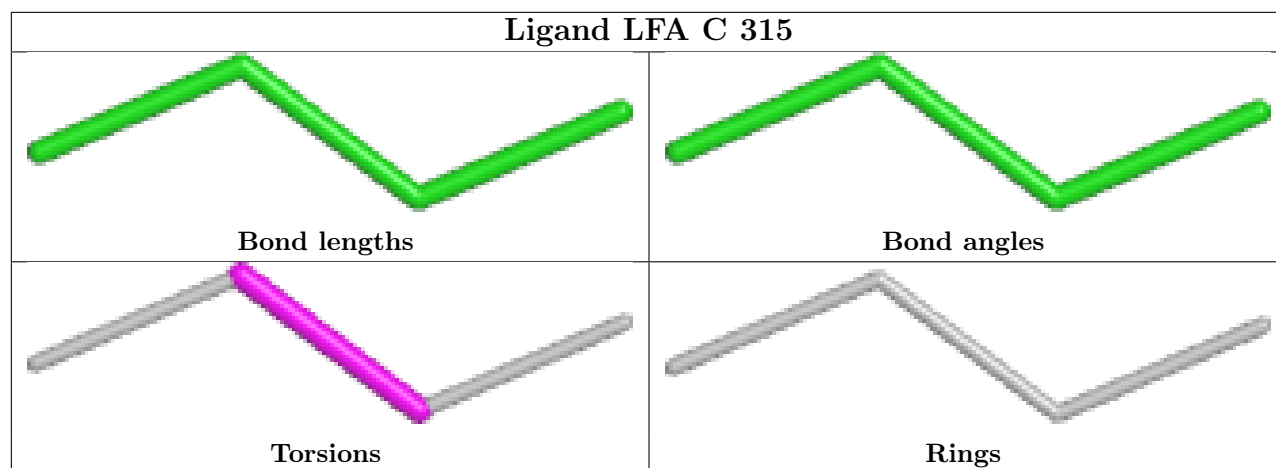
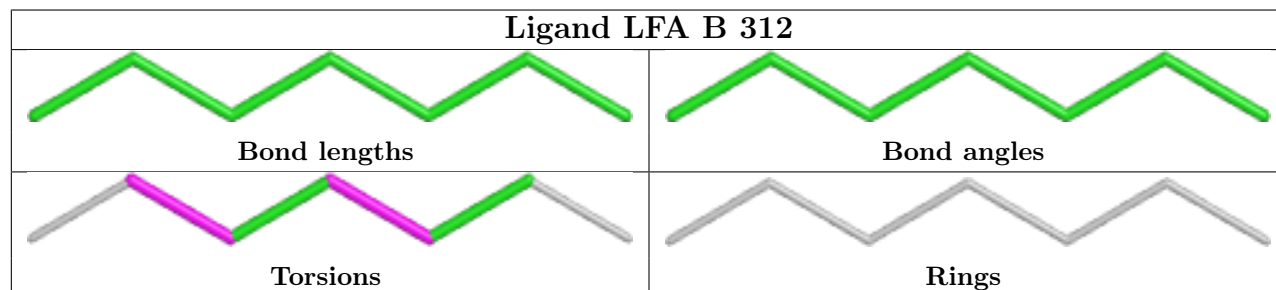
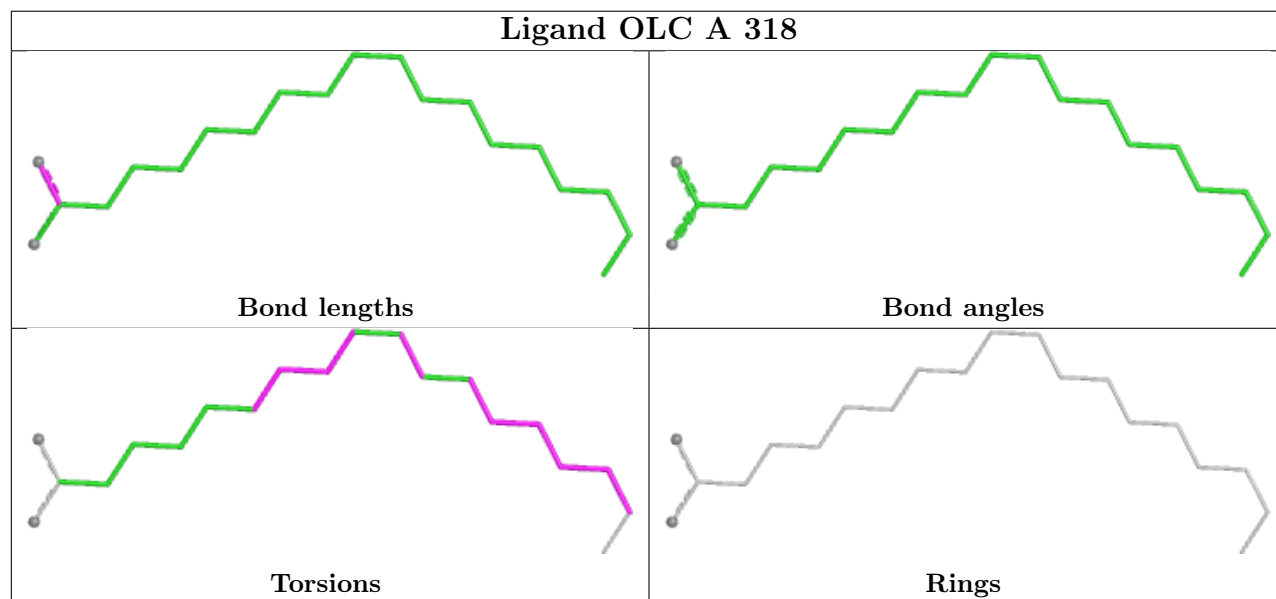
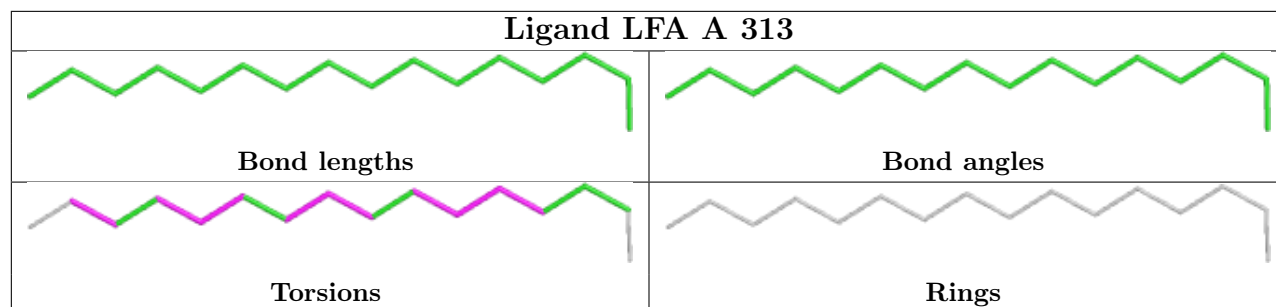


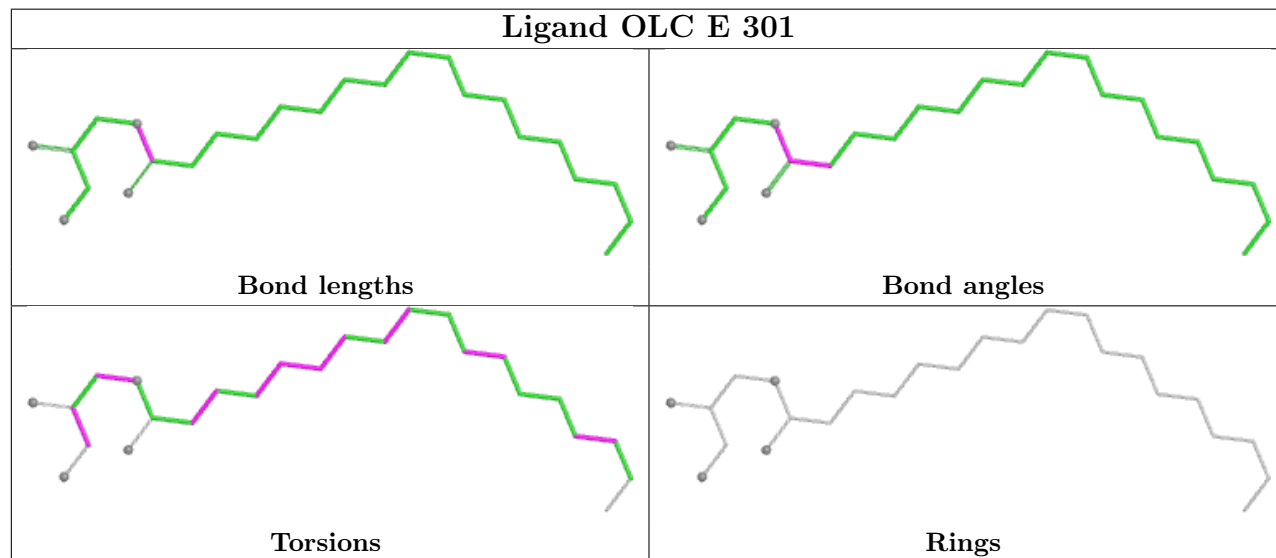
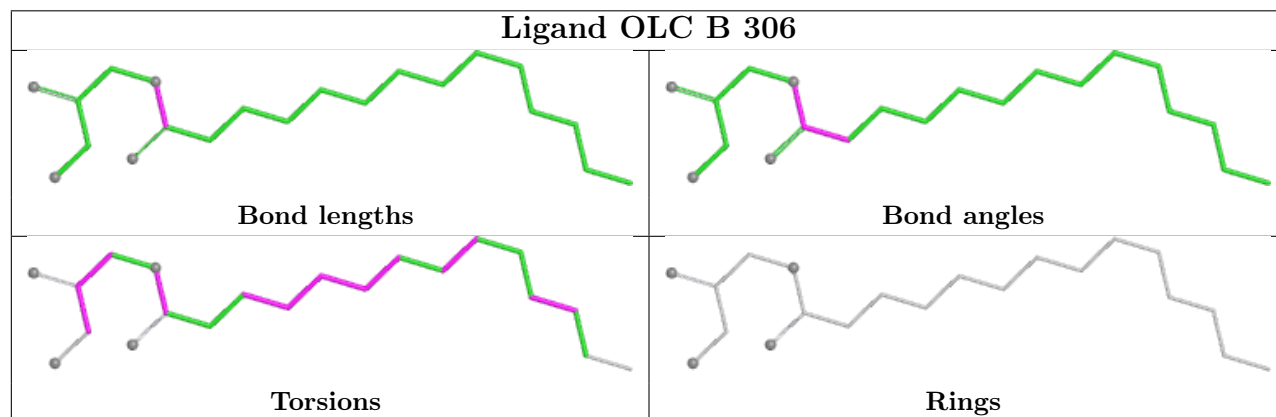
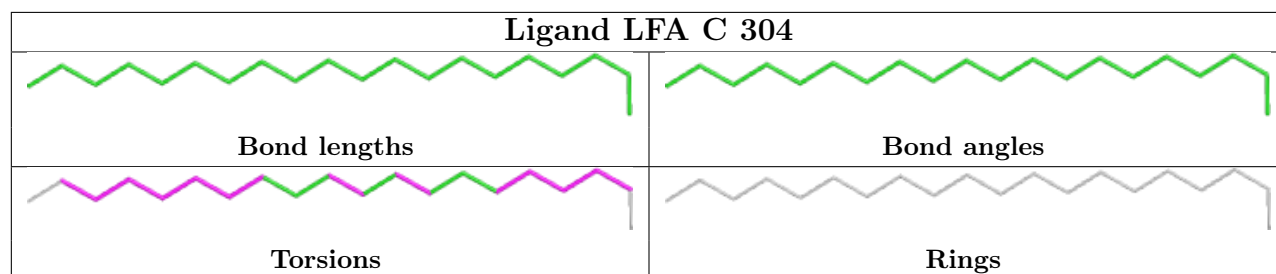
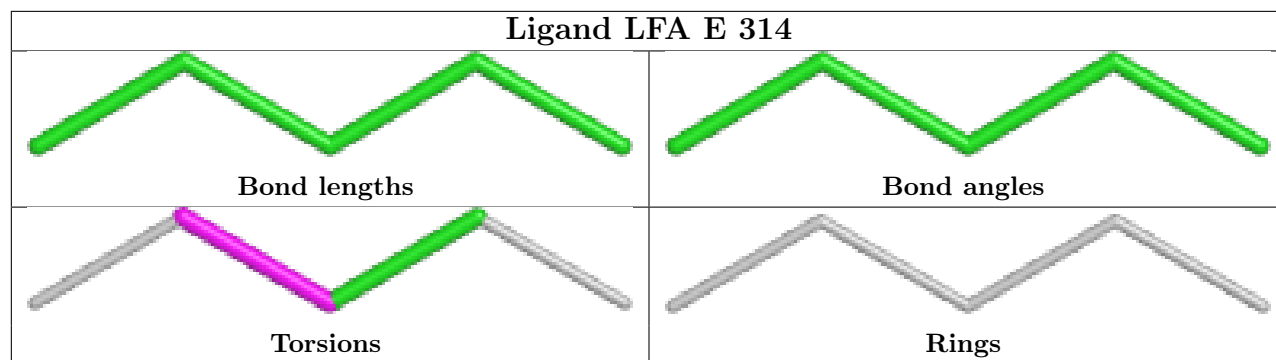


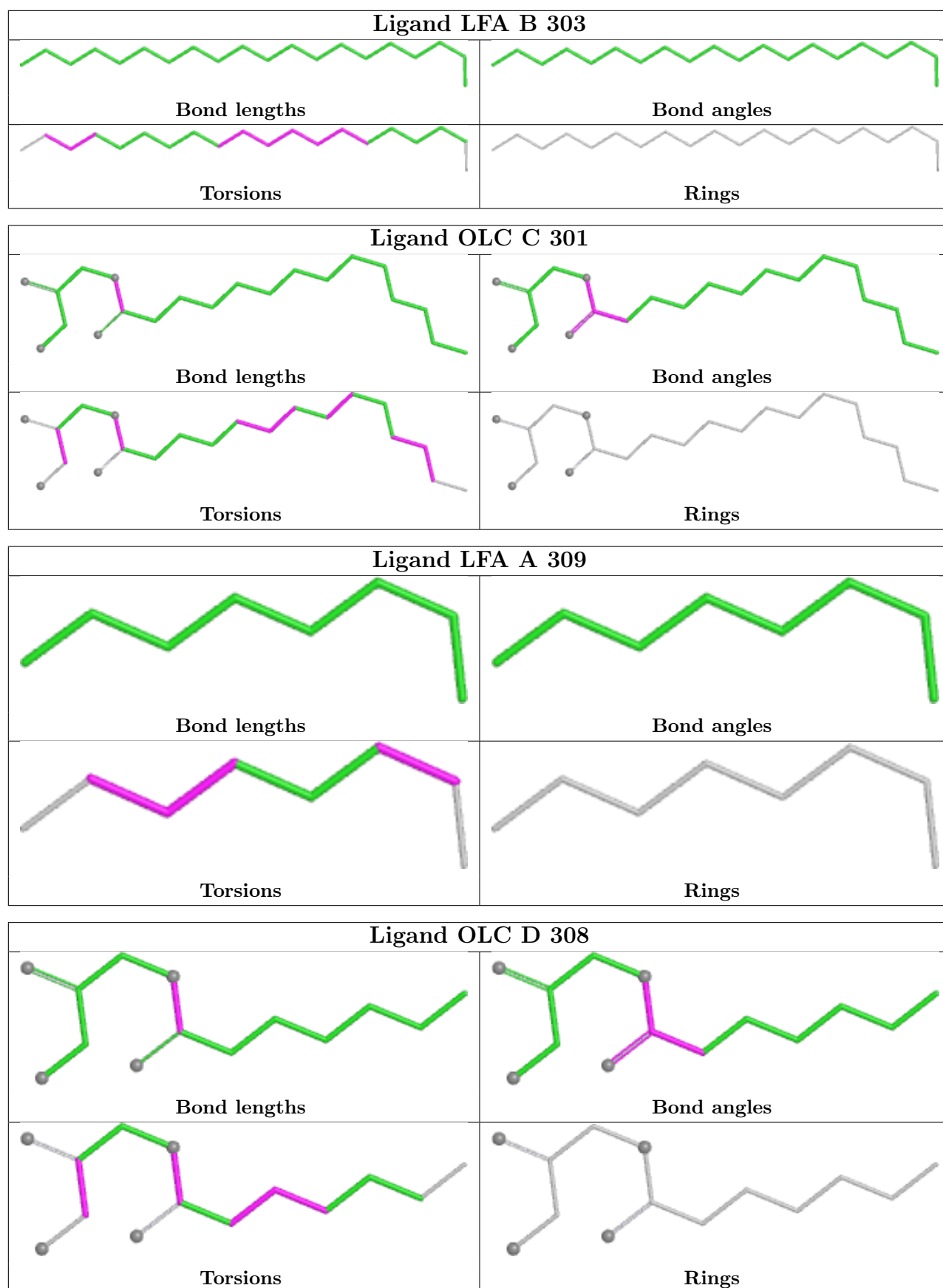


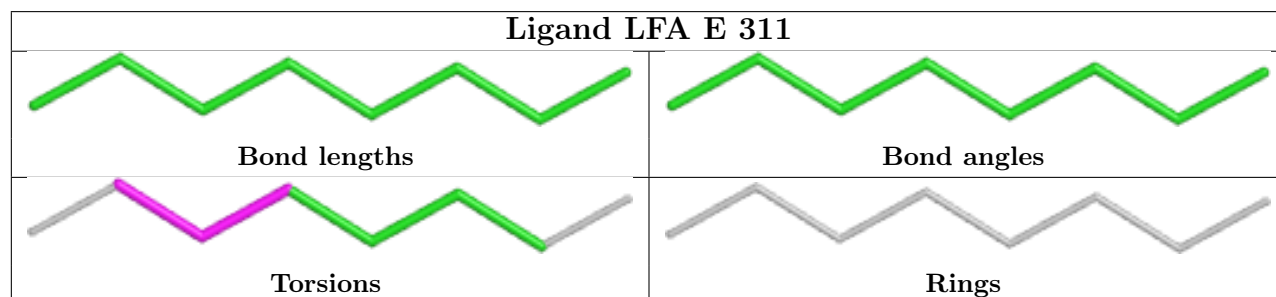
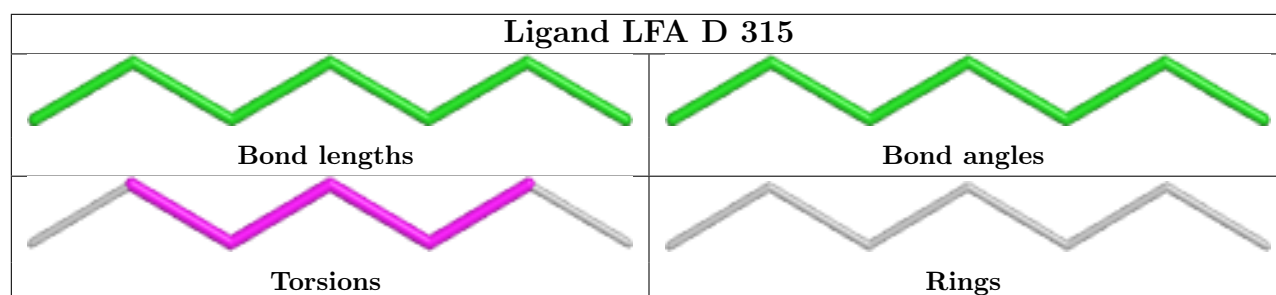
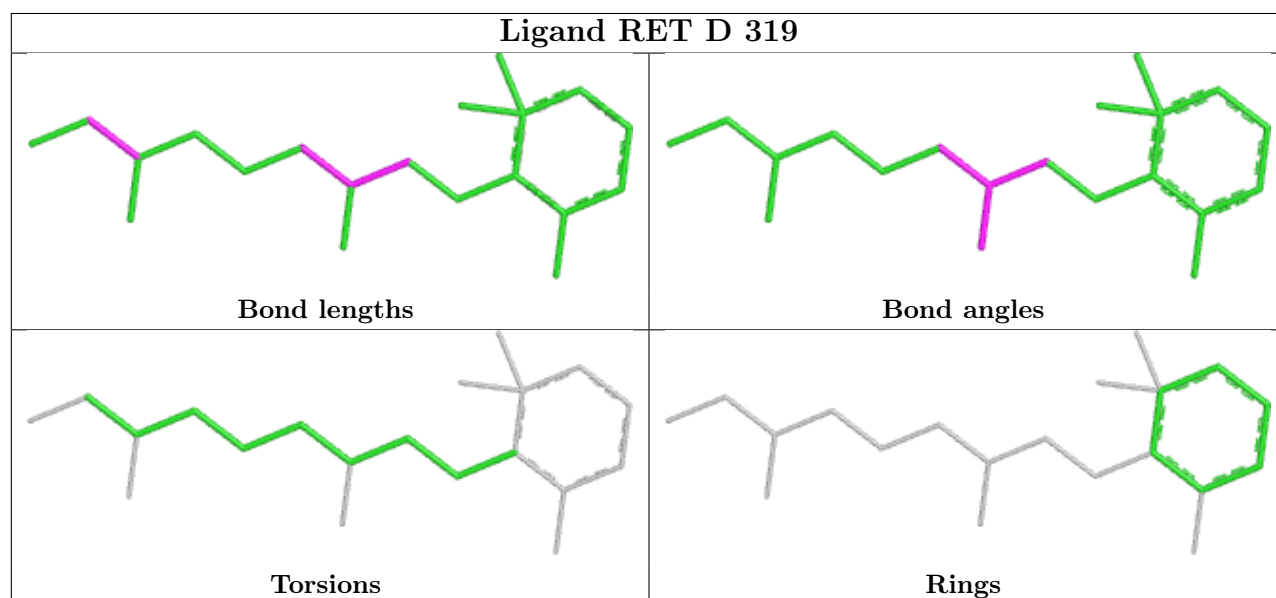
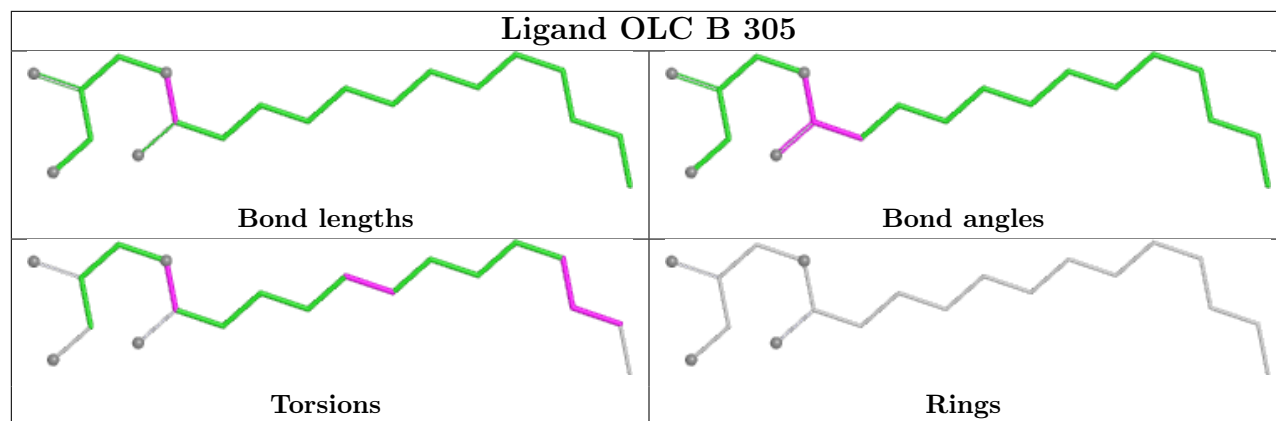


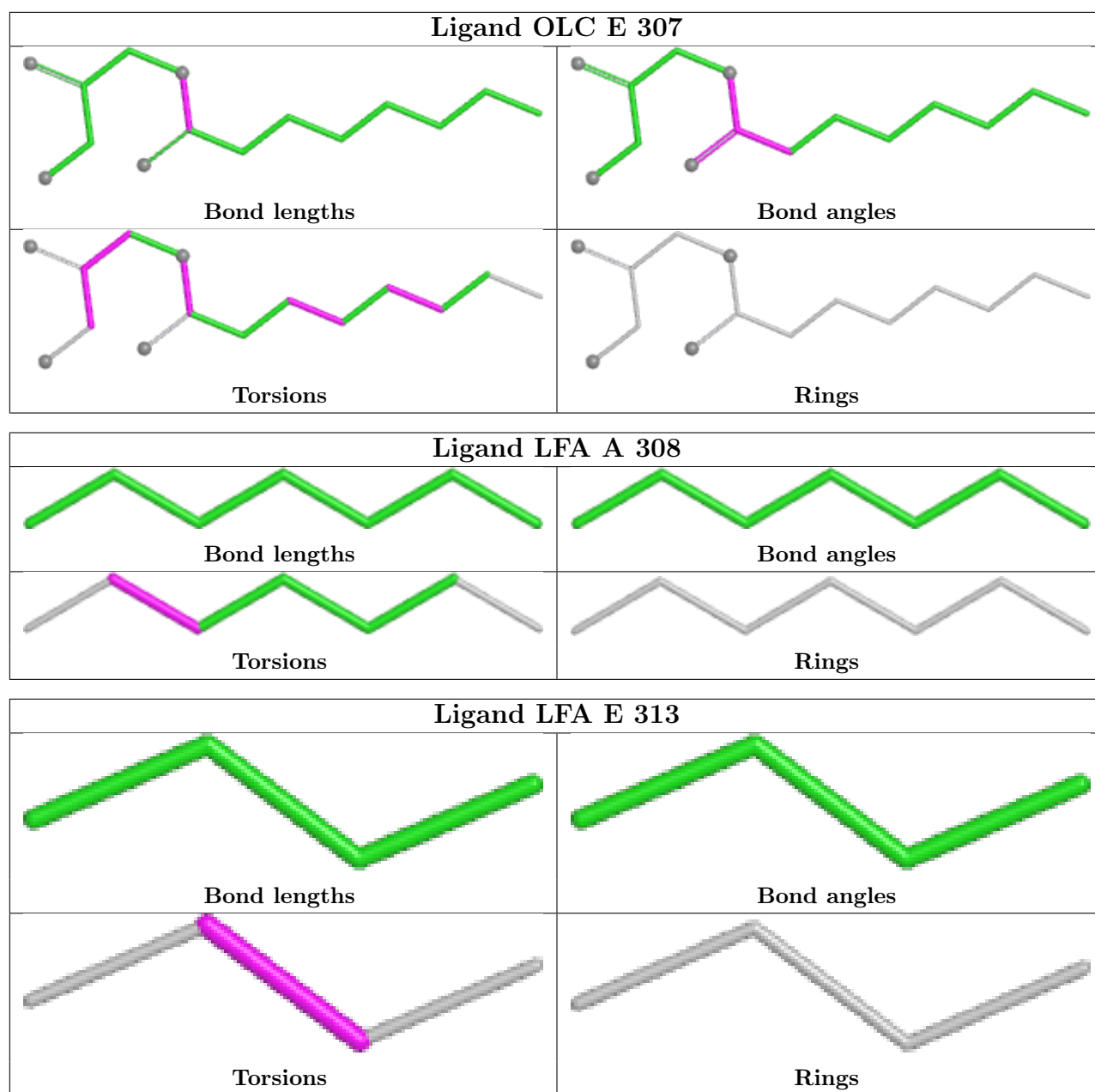












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/273 (100%)	-0.32	1 (0%) 88 87	19, 43, 66, 123	2 (0%)
1	B	273/273 (100%)	-0.27	2 (0%) 84 82	19, 45, 69, 124	2 (0%)
1	C	273/273 (100%)	-0.28	3 (1%) 78 76	19, 44, 66, 129	2 (0%)
1	D	273/273 (100%)	-0.18	4 (1%) 72 69	19, 46, 73, 138	2 (0%)
1	E	273/273 (100%)	-0.26	1 (0%) 88 87	20, 45, 67, 120	2 (0%)
All	All	1365/1365 (100%)	-0.26	11 (0%) 82 80	19, 44, 70, 138	10 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	272	ASN	4.8
1	A	272	ASN	4.2
1	D	272	ASN	3.7
1	C	272	ASN	3.6
1	B	275	LEU	3.3
1	C	275	LEU	3.0
1	C	230	VAL	2.6
1	D	273	LYS	2.3
1	D	275	LEU	2.2
1	B	272	ASN	2.1
1	D	271	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	D	304	13/25	0.55	0.17	100,119,160,162	0
3	LFA	C	315	4/20	0.57	0.29	78,80,88,89	0
3	LFA	D	316	6/20	0.57	0.23	85,101,111,117	0
3	LFA	A	319	20/20	0.64	0.14	59,71,83,86	0
3	LFA	D	303	20/20	0.66	0.16	55,73,91,91	0
3	LFA	E	302	20/20	0.67	0.15	59,71,84,92	0
2	OLC	E	306	15/25	0.68	0.19	85,104,129,131	0
3	LFA	A	311	4/20	0.69	0.26	77,78,78,84	0
3	LFA	D	320	14/20	0.69	0.11	78,93,109,110	0
3	LFA	A	320	9/20	0.69	0.22	72,78,96,99	0
3	LFA	B	303	20/20	0.70	0.17	61,76,90,100	0
2	OLC	E	308	6/25	0.70	0.23	65,78,83,84	0
2	OLC	B	304	25/25	0.71	0.15	66,94,105,112	0
2	OLC	C	310	7/25	0.71	0.21	65,79,91,98	0
3	LFA	C	304	20/20	0.72	0.13	53,67,80,82	0
2	OLC	A	305	25/25	0.72	0.16	74,97,112,116	0
3	LFA	B	309	9/20	0.74	0.23	75,88,108,117	0
3	LFA	B	311	10/20	0.74	0.22	76,91,95,97	0
2	OLC	D	309	7/25	0.74	0.20	74,76,81,85	0
3	LFA	A	308	7/20	0.74	0.23	80,85,92,93	0
3	LFA	D	311	20/20	0.75	0.18	83,91,106,109	0
3	LFA	E	314	5/20	0.75	0.27	75,78,80,88	0
5	BOG	B	314	20/20	0.75	0.17	73,94,108,109	0
3	LFA	A	309	8/20	0.76	0.20	70,75,79,80	0
2	OLC	A	303	25/25	0.76	0.20	76,101,116,141	0
2	OLC	E	310	20/25	0.76	0.16	58,106,126,127	0
5	BOG	A	315	20/20	0.76	0.14	72,96,118,132	0
2	OLC	B	308	7/25	0.76	0.19	67,74,84,85	0
3	LFA	C	314	6/20	0.77	0.22	64,70,78,84	0
2	OLC	D	306	18/25	0.77	0.18	69,88,116,126	0
3	LFA	A	313	16/20	0.78	0.21	77,98,114,116	0
3	LFA	E	311	8/20	0.78	0.19	67,91,98,99	0
3	LFA	C	311	7/20	0.78	0.20	77,92,106,109	0
2	OLC	D	305	25/25	0.78	0.20	71,101,116,120	0
3	LFA	B	316	4/20	0.78	0.11	72,74,78,81	0
2	OLC	E	303	8/25	0.79	0.18	66,70,90,96	0
2	OLC	C	303	12/25	0.79	0.14	74,86,123,131	0

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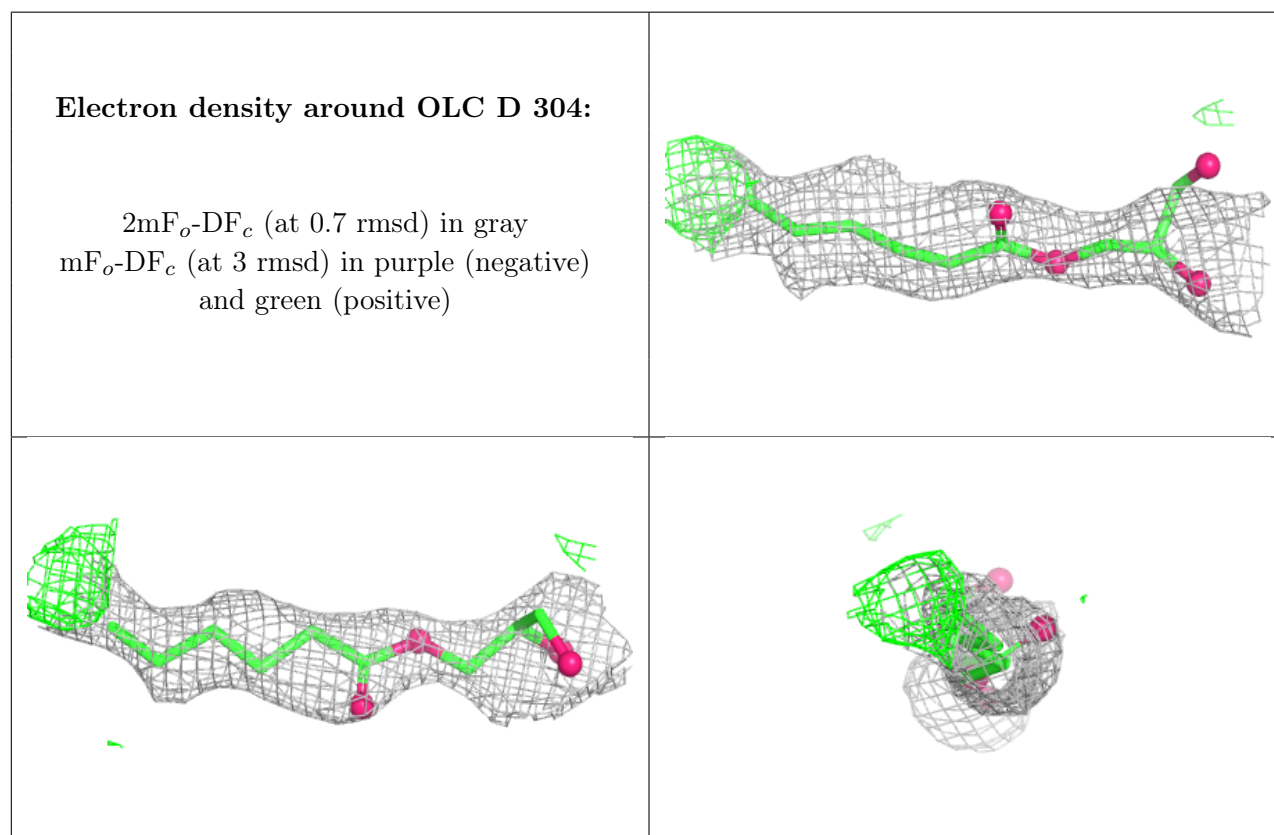
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LFA	E	312	14/20	0.79	0.21	77,86,98,98	0
2	OLC	A	301	9/25	0.80	0.14	63,71,81,87	0
3	LFA	D	315	7/20	0.80	0.19	72,74,97,101	0
2	OLC	E	304	16/25	0.80	0.22	73,88,101,106	0
2	OLC	D	302	16/25	0.80	0.16	70,90,108,120	0
2	OLC	C	306	22/25	0.80	0.18	69,95,112,117	0
5	BOG	E	316	20/20	0.80	0.14	69,102,118,125	0
2	OLC	E	309	22/25	0.81	0.16	77,92,116,119	0
3	LFA	D	312	20/20	0.81	0.16	76,89,100,101	0
2	OLC	C	307	20/25	0.82	0.17	65,93,123,125	0
2	OLC	D	310	25/25	0.82	0.15	69,90,112,138	0
3	LFA	A	310	8/20	0.82	0.21	69,93,107,114	0
3	LFA	B	310	8/20	0.82	0.18	69,84,85,94	0
5	BOG	C	317	20/20	0.82	0.13	65,88,109,110	0
3	LFA	C	312	8/20	0.82	0.17	69,81,87,91	0
2	OLC	A	304	13/25	0.83	0.13	60,71,80,82	0
2	OLC	C	309	16/25	0.83	0.12	57,76,83,84	0
2	OLC	A	307	7/25	0.83	0.16	72,76,87,89	0
3	LFA	C	313	20/20	0.83	0.17	65,84,115,119	0
3	LFA	B	312	7/20	0.84	0.21	72,79,90,101	0
2	OLC	B	307	16/25	0.84	0.12	60,80,97,101	0
2	OLC	C	308	22/25	0.84	0.14	51,89,123,128	0
3	LFA	D	313	8/20	0.84	0.17	69,83,101,103	0
2	OLC	B	302	16/25	0.84	0.14	68,85,125,142	0
2	OLC	B	306	21/25	0.85	0.12	58,81,114,116	0
2	OLC	A	306	15/25	0.85	0.12	60,72,102,112	0
2	OLC	E	305	20/25	0.85	0.13	76,86,95,98	0
2	OLC	B	305	20/25	0.85	0.15	61,83,97,106	0
2	OLC	E	307	15/25	0.85	0.13	62,73,90,97	0
2	OLC	E	301	25/25	0.85	0.12	62,89,127,140	0
2	OLC	D	307	18/25	0.86	0.14	55,93,113,117	0
2	OLC	C	302	20/25	0.86	0.12	65,82,96,104	0
3	LFA	E	313	4/20	0.87	0.23	68,70,71,76	0
2	OLC	B	301	22/25	0.87	0.10	65,82,92,98	0
5	BOG	D	318	20/20	0.88	0.13	84,99,116,125	0
2	OLC	D	308	14/25	0.89	0.12	58,83,93,110	0
2	OLC	A	318	20/25	0.89	0.11	65,76,96,100	0
2	OLC	A	302	22/25	0.90	0.11	43,64,96,102	0
2	OLC	C	301	21/25	0.90	0.11	49,55,82,91	0
3	LFA	A	312	6/20	0.91	0.16	56,59,72,82	0
2	OLC	D	301	18/25	0.91	0.09	62,77,93,102	0
3	LFA	D	314	17/20	0.91	0.10	51,60,79,79	0

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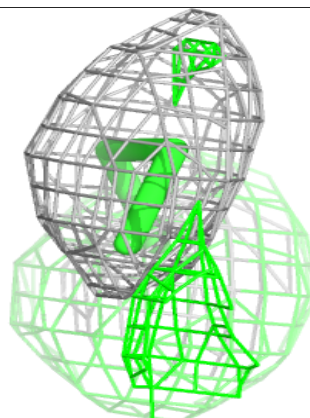
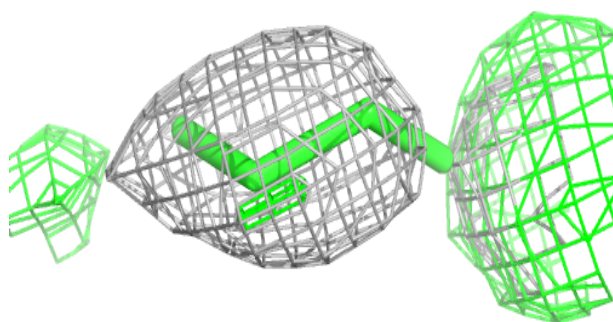
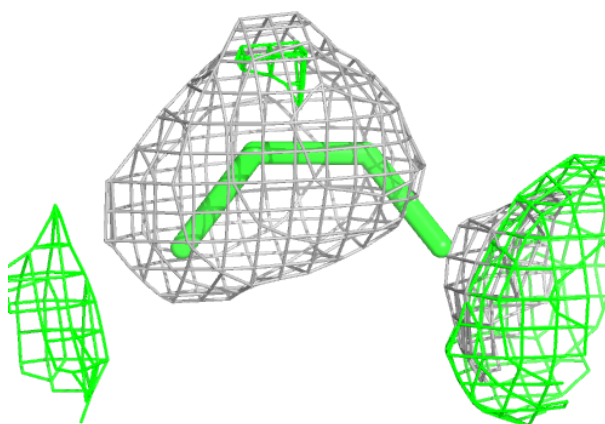
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	C	305	23/25	0.91	0.11	46,70,115,119	0
2	OLC	A	317	19/25	0.94	0.09	55,60,71,74	0
6	RET	A	316	20/21	0.94	0.09	35,42,47,48	0
6	RET	B	315	20/21	0.95	0.08	36,41,46,53	0
6	RET	D	319	20/21	0.95	0.08	39,43,50,55	0
6	RET	E	317	20/21	0.95	0.08	36,41,45,46	0
6	RET	C	318	20/21	0.96	0.07	38,43,48,50	0
4	NA	A	314	1/1	0.97	0.08	41,41,41,41	0
4	NA	D	317	1/1	0.98	0.09	39,39,39,39	0
4	NA	B	313	1/1	0.99	0.08	35,35,35,35	0
4	NA	E	315	1/1	0.99	0.06	36,36,36,36	0
4	NA	C	316	1/1	0.99	0.06	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.

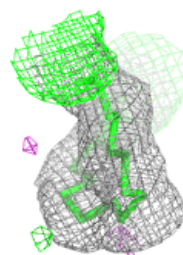
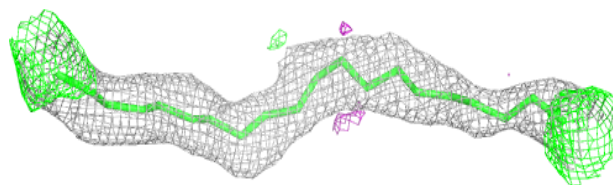
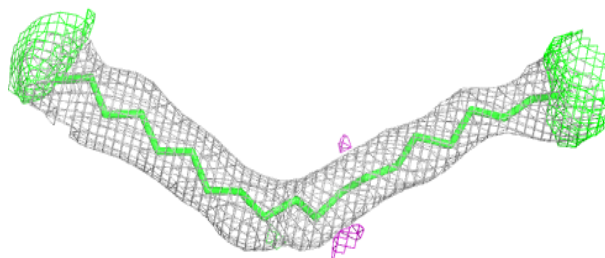


Electron density around LFA C 315:

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

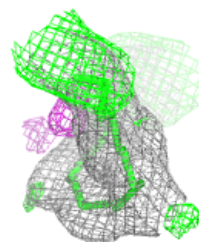
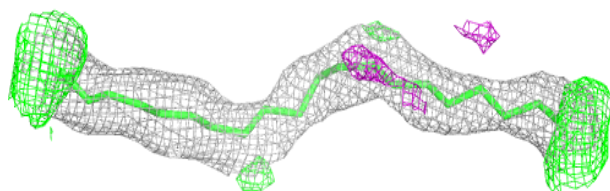
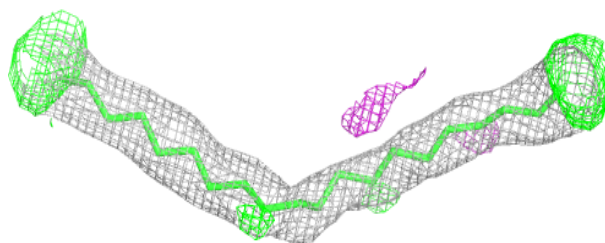
**Electron density around LFA A 319:**

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

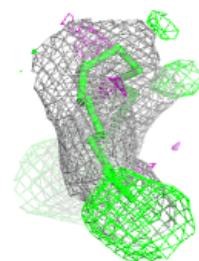
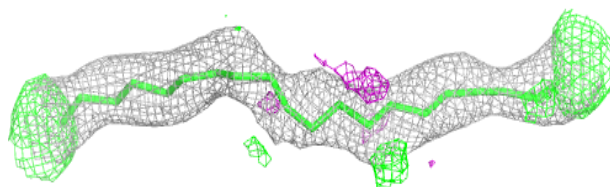
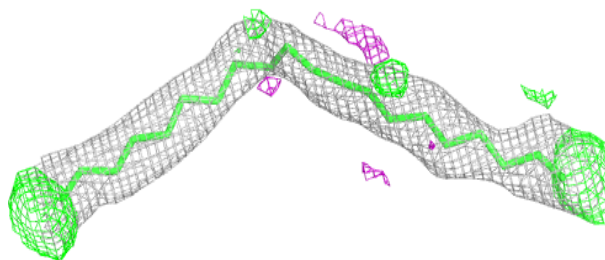


Electron density around LFA D 303:

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

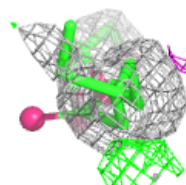
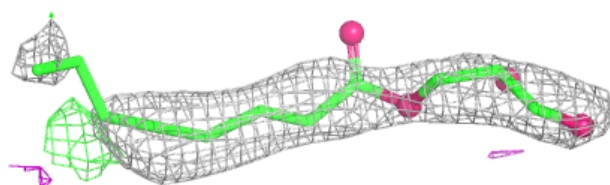
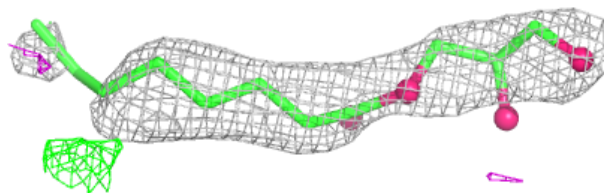
**Electron density around LFA E 302:**

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

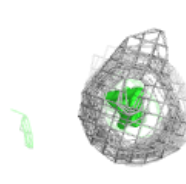
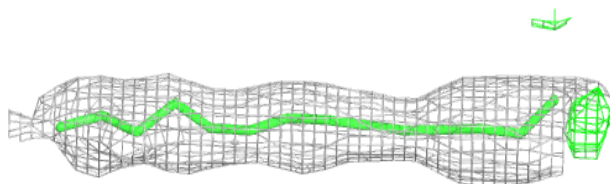
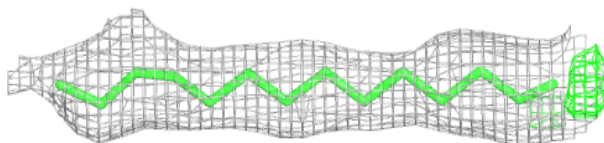


Electron density around OLC E 306:

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

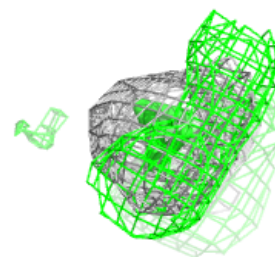
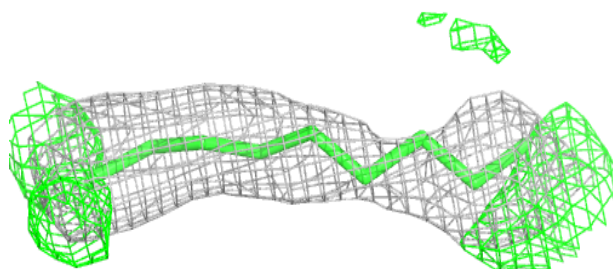
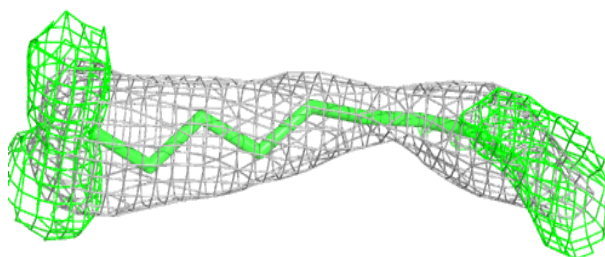
**Electron density around LFA D 320:**

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

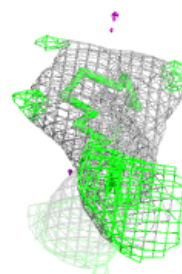
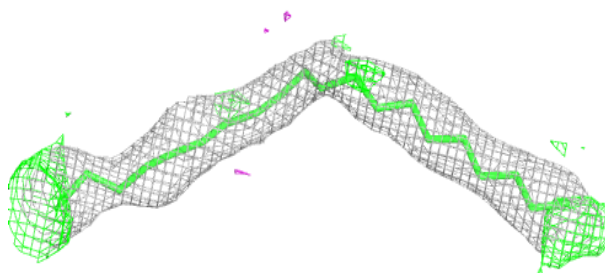


Electron density around LFA A 320:

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

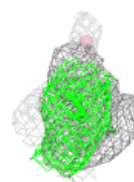
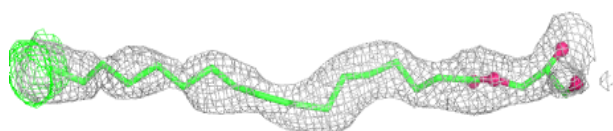
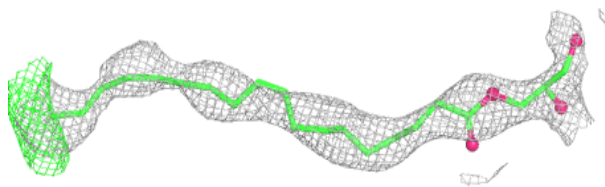
**Electron density around LFA B 303:**

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

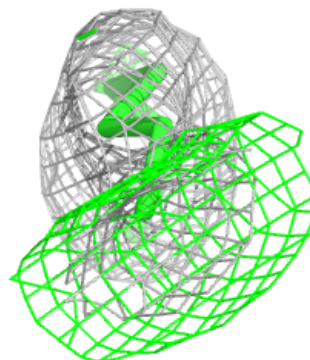
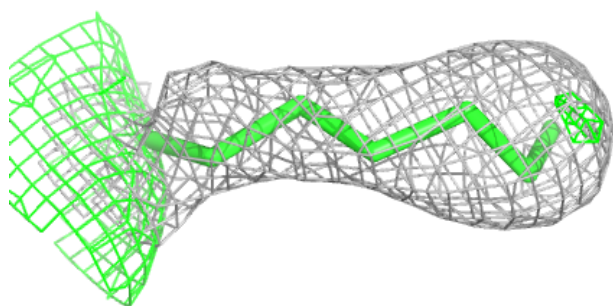
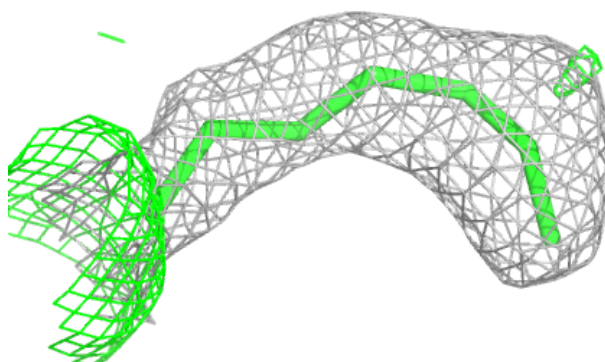


Electron density around OLC B 304:

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

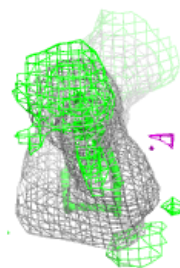
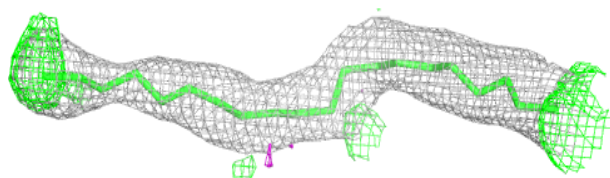
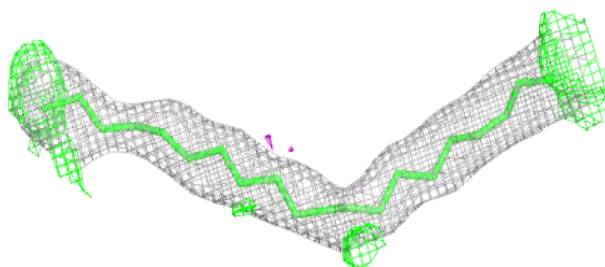
**Electron density around OLC C 310:**

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

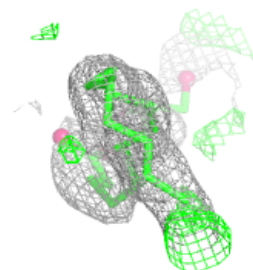
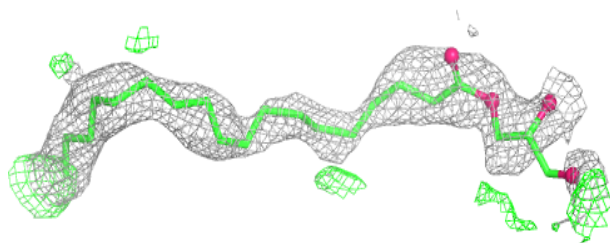
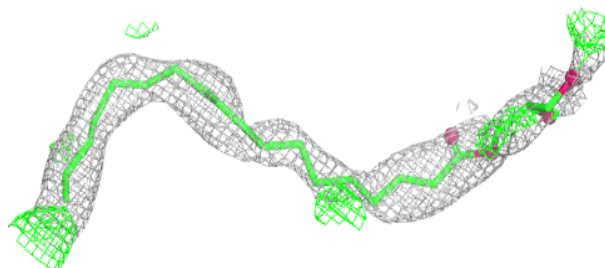


Electron density around LFA C 304:

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

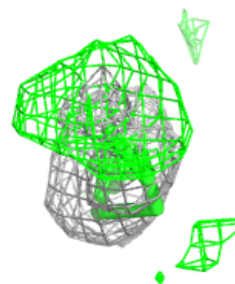
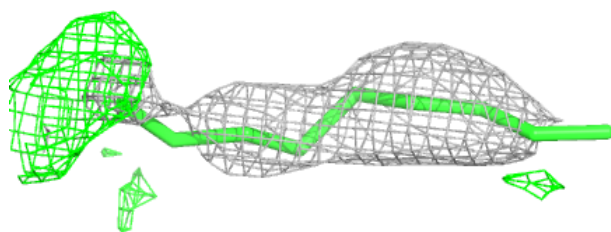
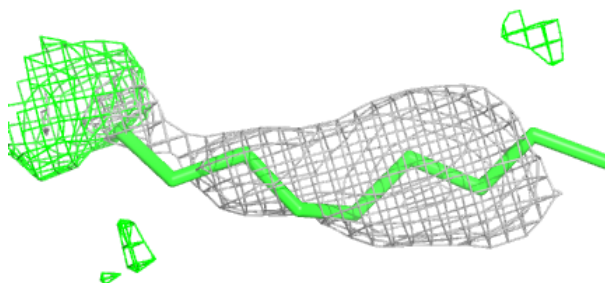
**Electron density around OLC A 305:**

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

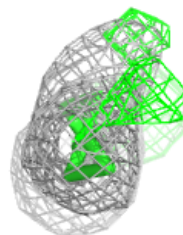
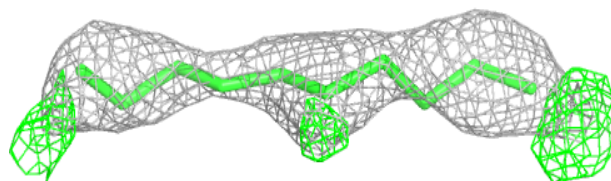
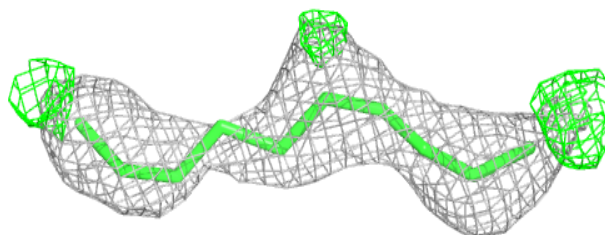


Electron density around LFA B 309:

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

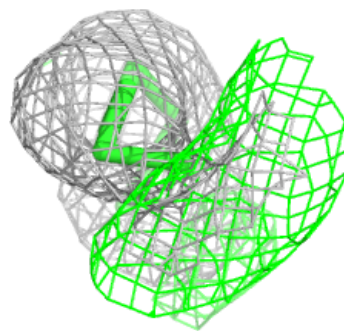
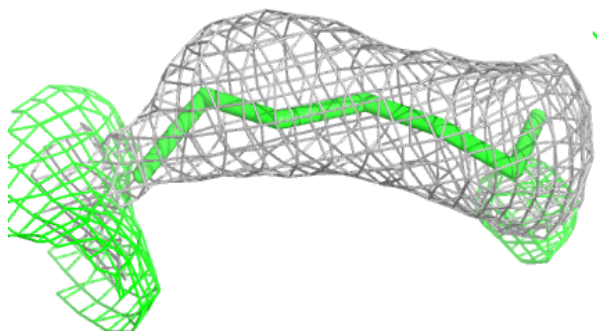
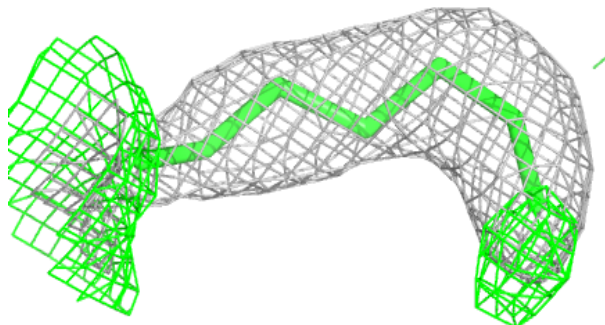
**Electron density around LFA B 311:**

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

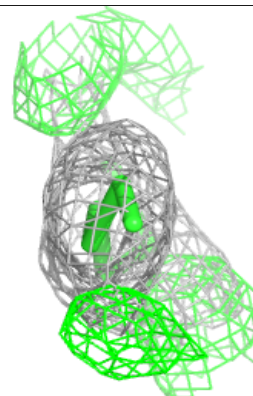
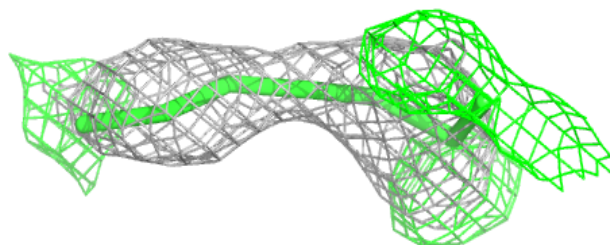
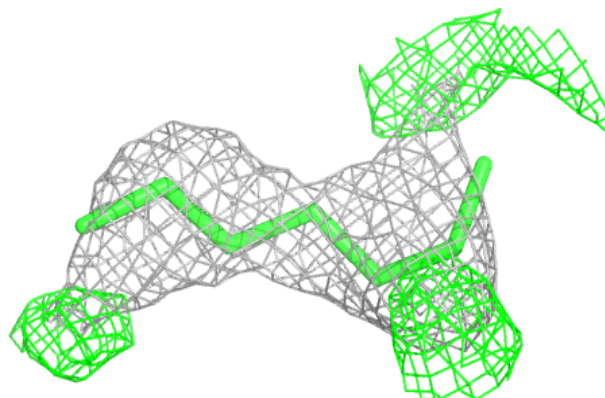


Electron density around OLC D 309:

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

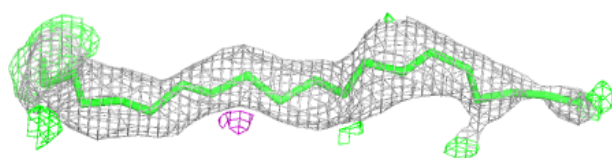
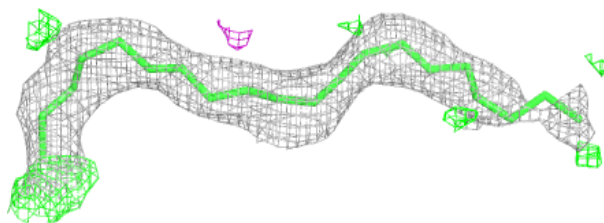
**Electron density around LFA A 308:**

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

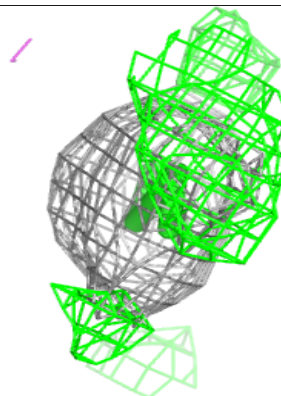
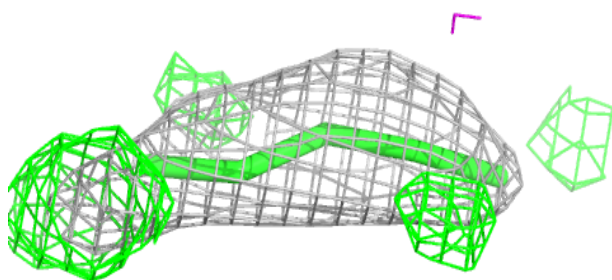
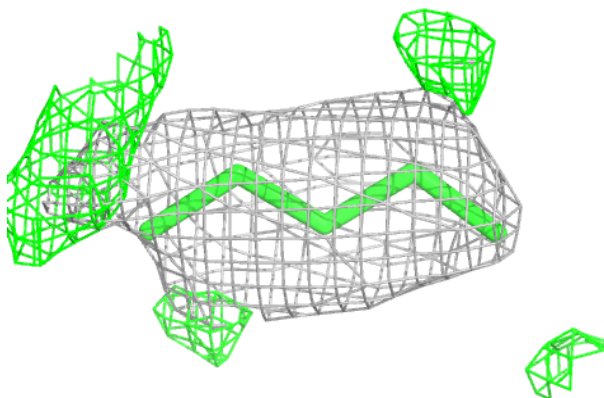


Electron density around LFA D 311:

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

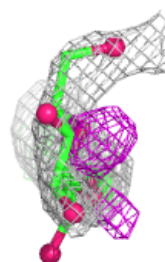
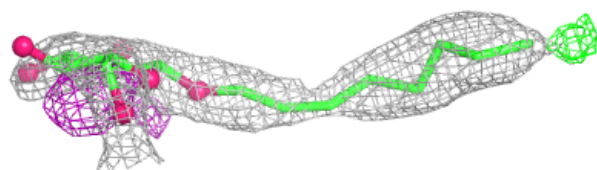
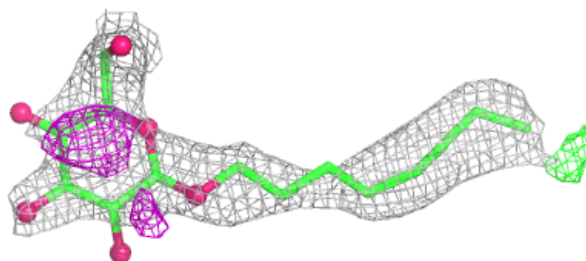
**Electron density around LFA E 314:**

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

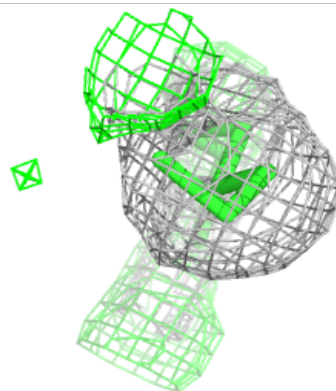
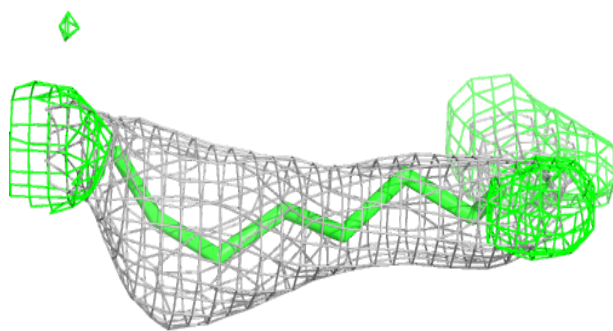
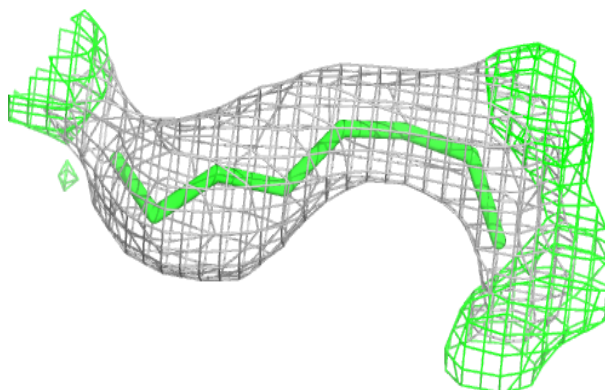


Electron density around BOG B 314:

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

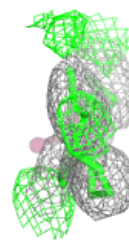
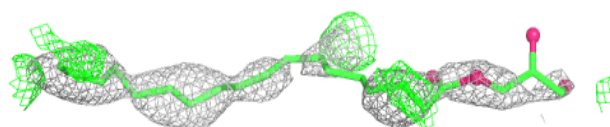
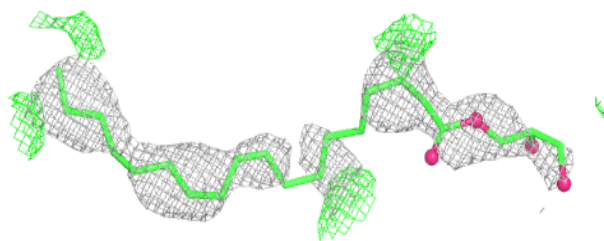
**Electron density around LFA A 309:**

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

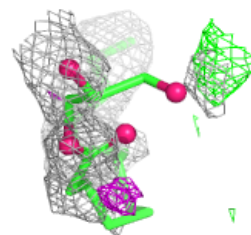
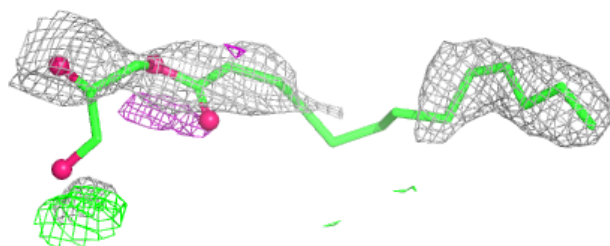
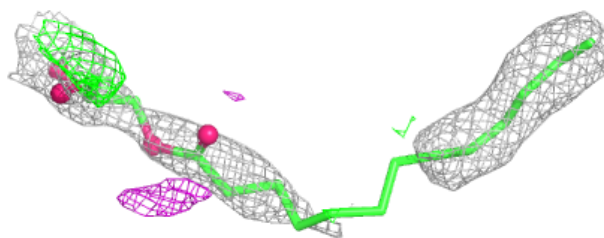


Electron density around OLC A 303:

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

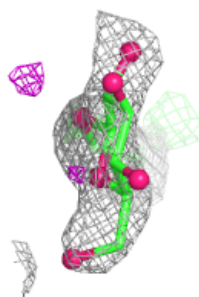
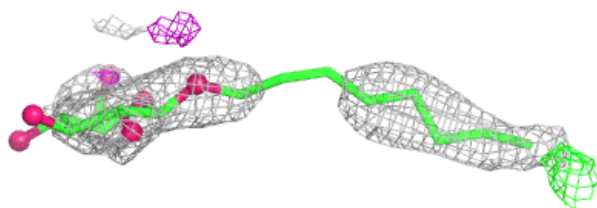
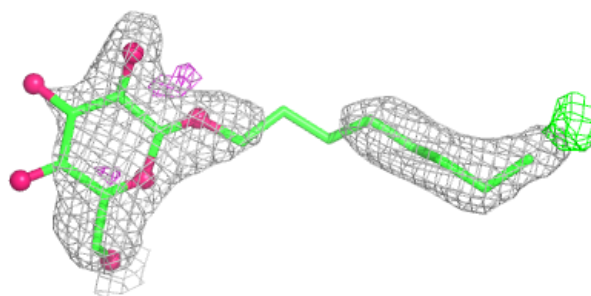
**Electron density around OLC E 310:**

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

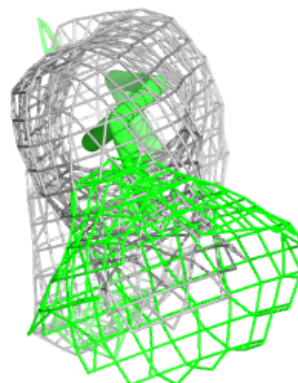
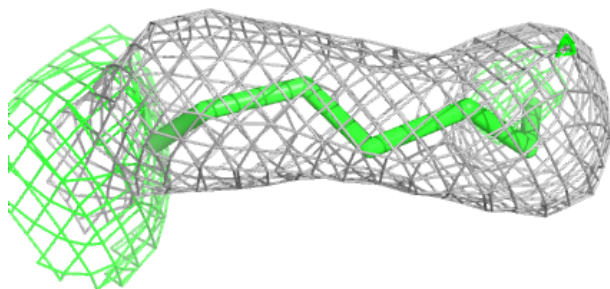
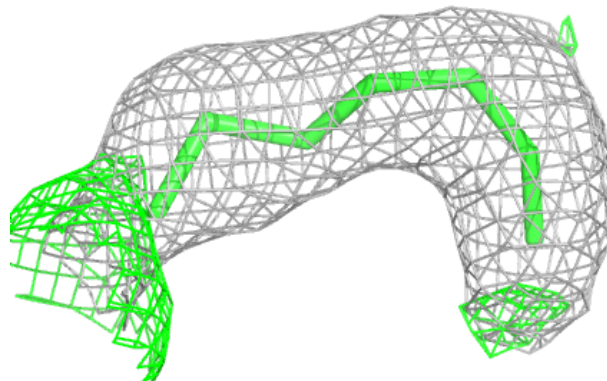


Electron density around BOG A 315:

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

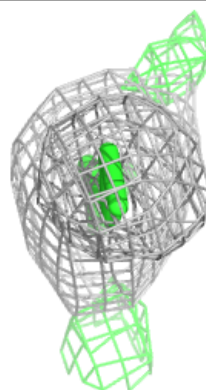
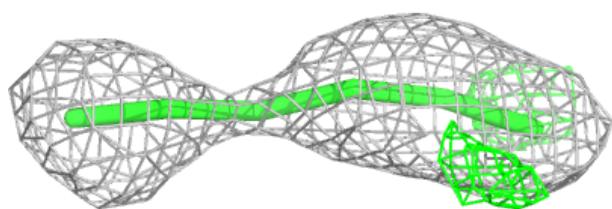
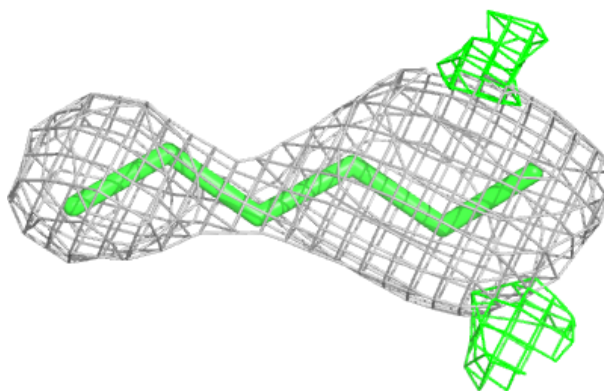
**Electron density around OLC B 308:**

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

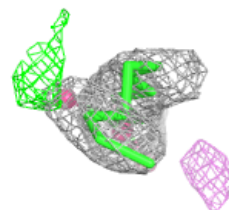
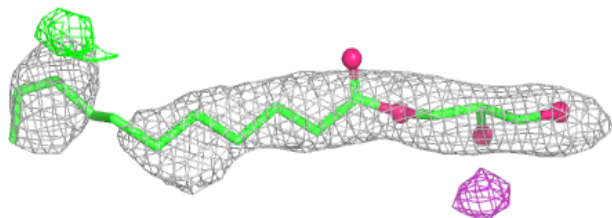
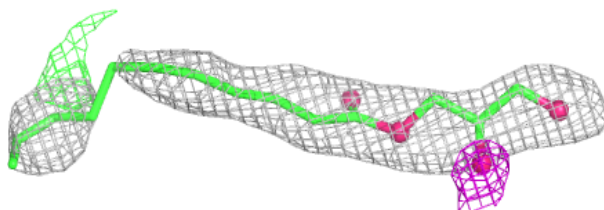


Electron density around LFA C 314:

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

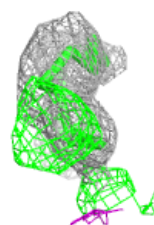
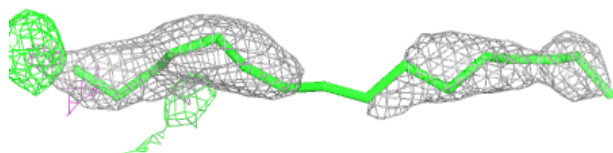
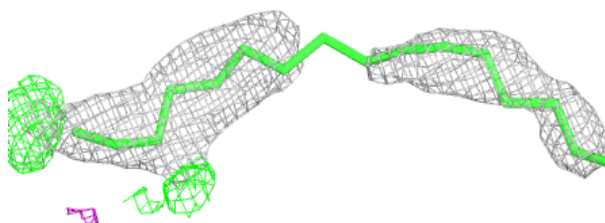
**Electron density around OLC D 306:**

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

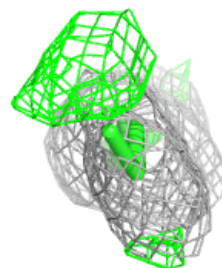
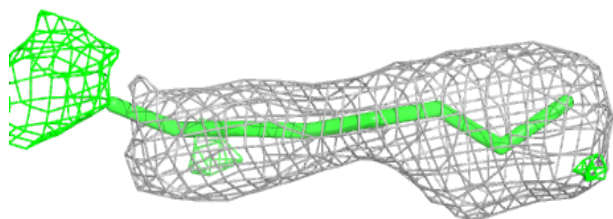
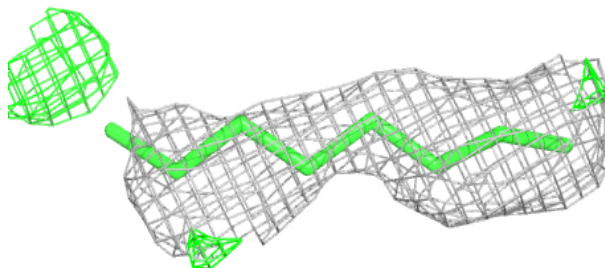


Electron density around LFA A 313:

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

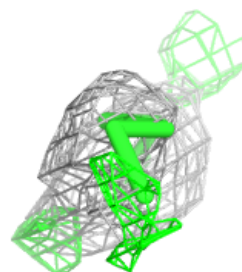
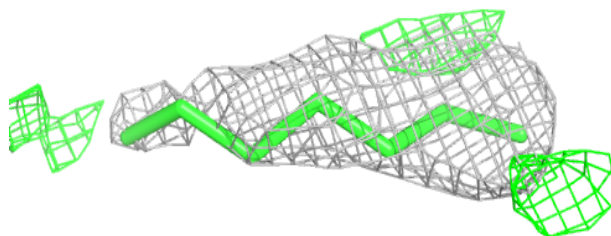
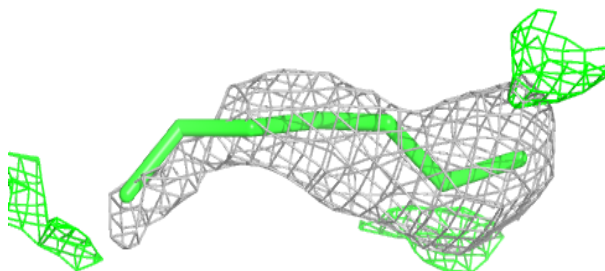
**Electron density around LFA E 311:**

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

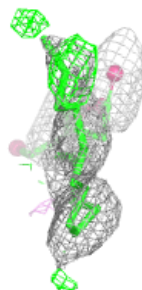
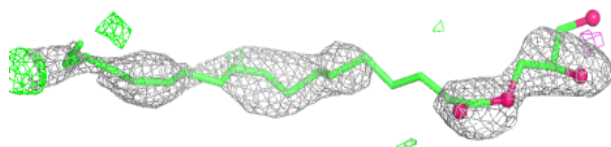
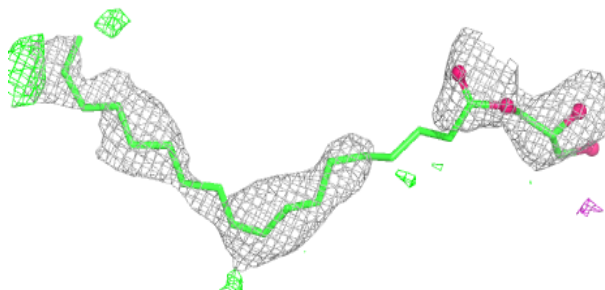


Electron density around LFA C 311:

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

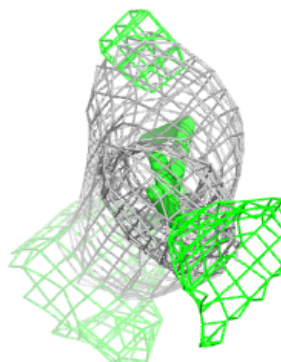
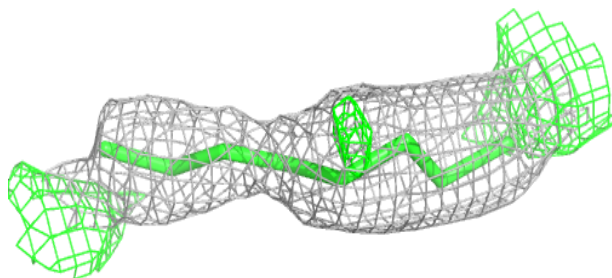
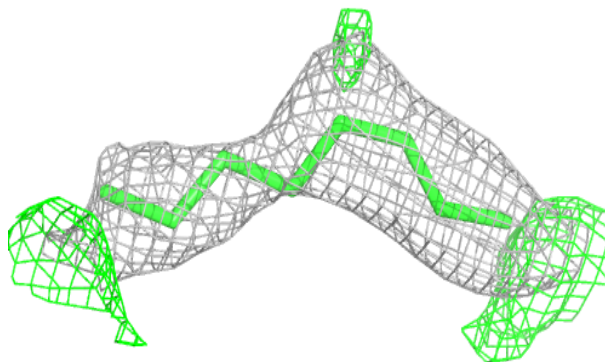
**Electron density around OLC D 305:**

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

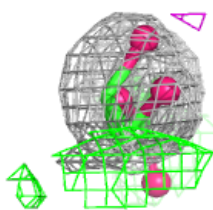
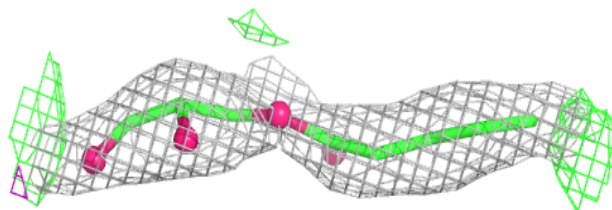
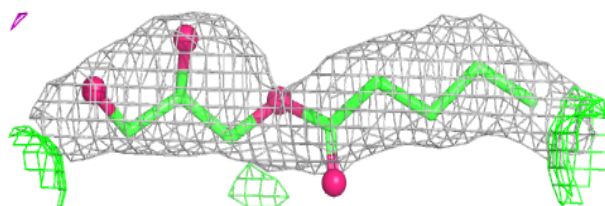


Electron density around OLC E 303:

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

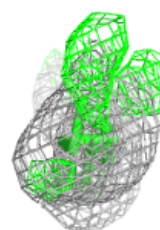
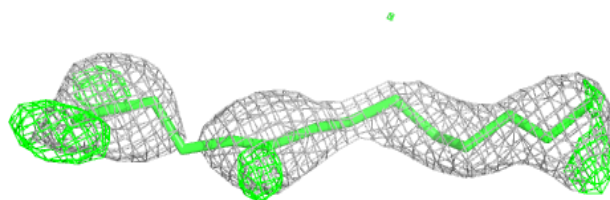
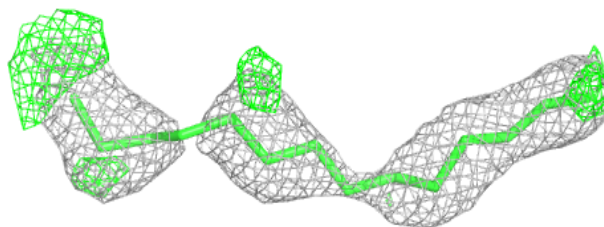
**Electron density around OLC C 303:**

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

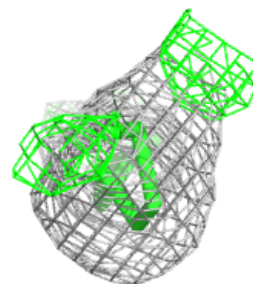
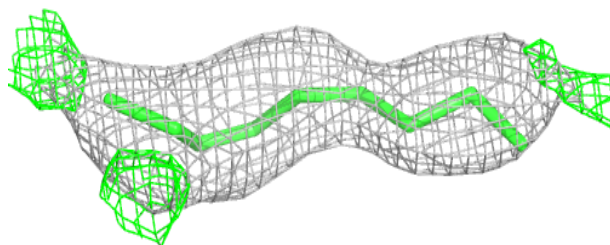
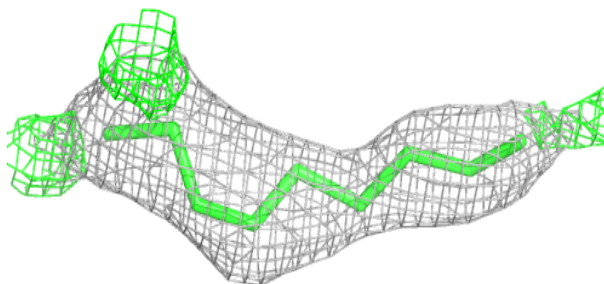


Electron density around LFA E 312:

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

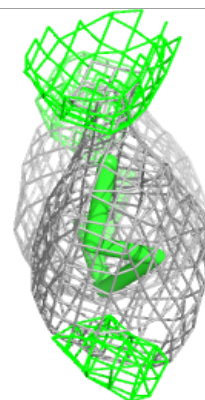
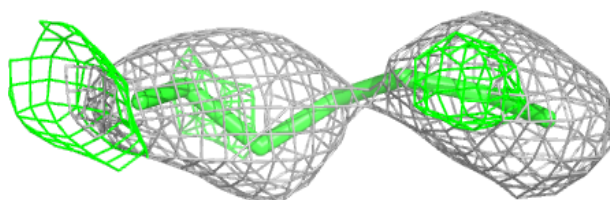
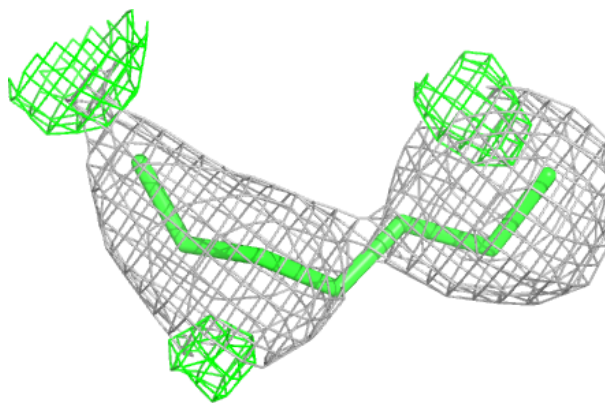
**Electron density around OLC A 301:**

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

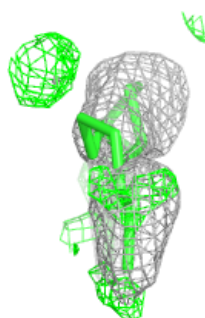
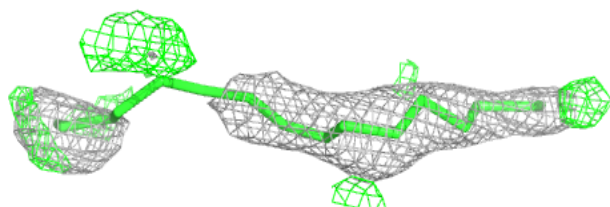
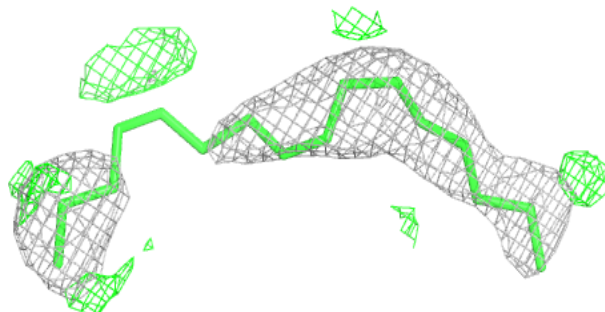


Electron density around LFA D 315:

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

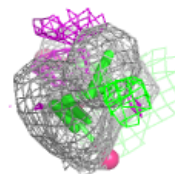
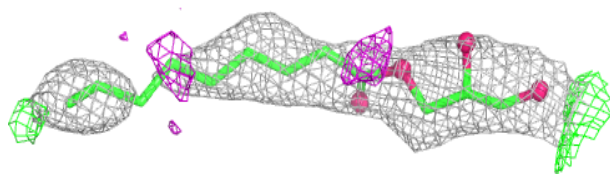
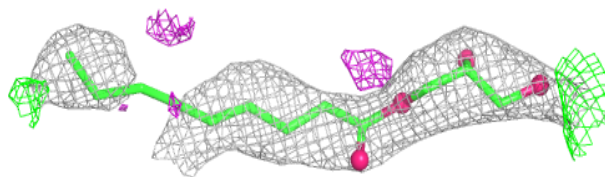
**Electron density around OLC E 304:**

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

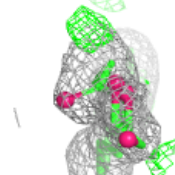
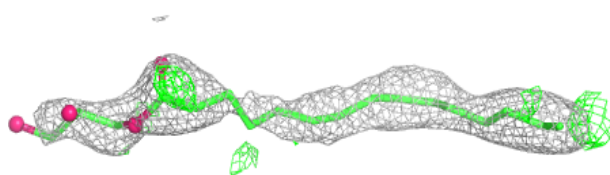
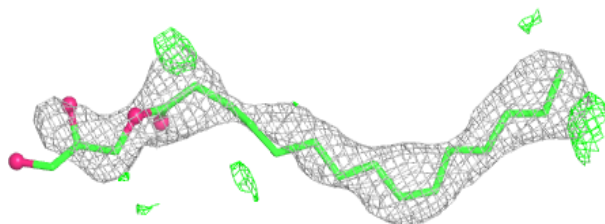


Electron density around OLC D 302:

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

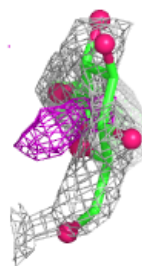
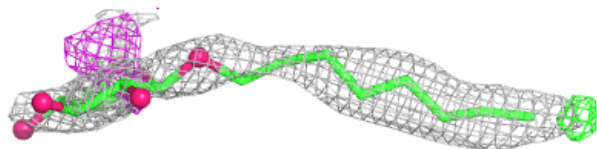
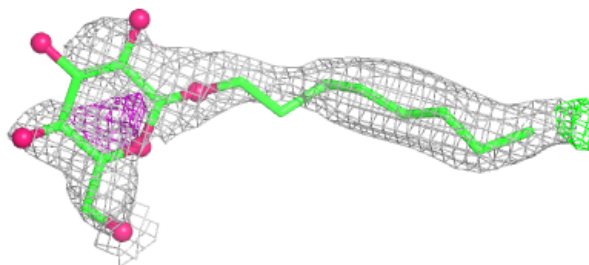
**Electron density around OLC C 306:**

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

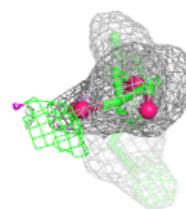
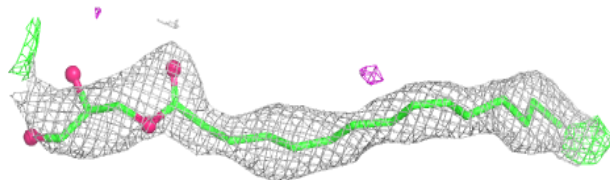
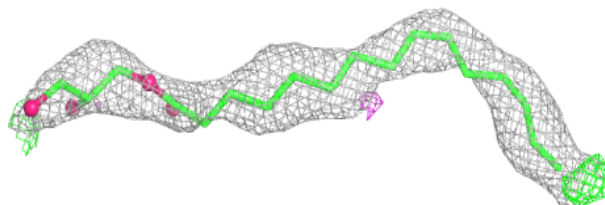


Electron density around BOG E 316:

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

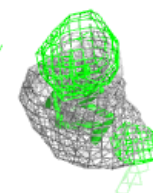
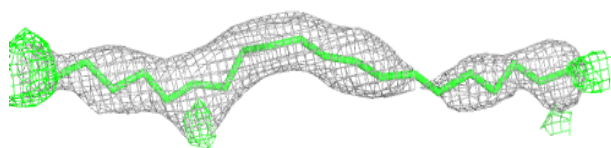
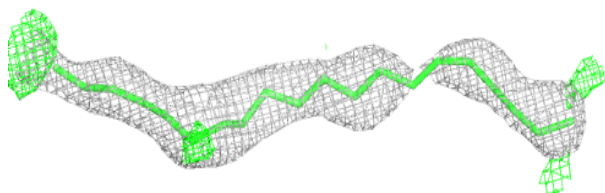
**Electron density around OLC E 309:**

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

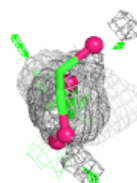
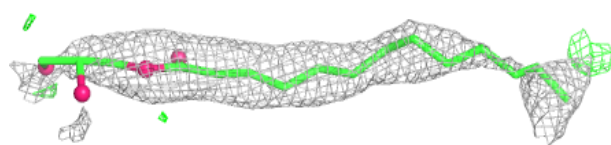
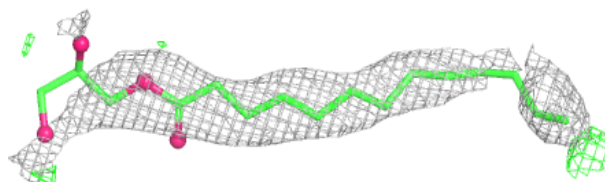


Electron density around LFA D 312:

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

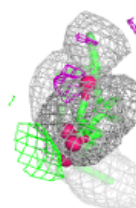
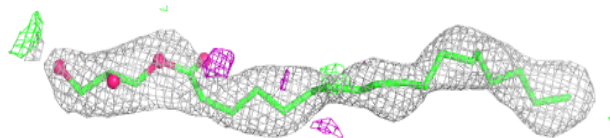
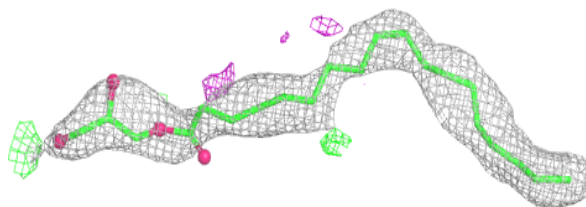
**Electron density around OLC C 307:**

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

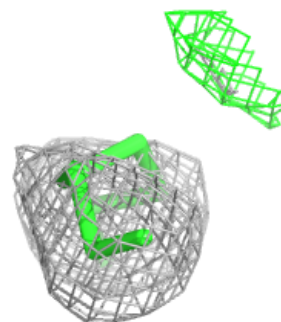
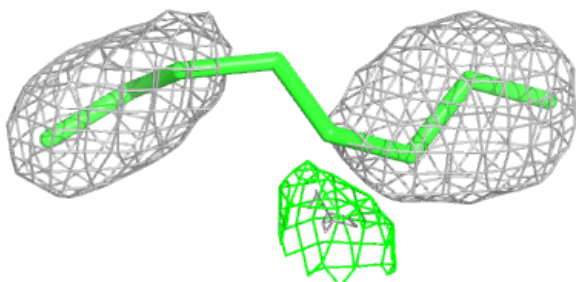
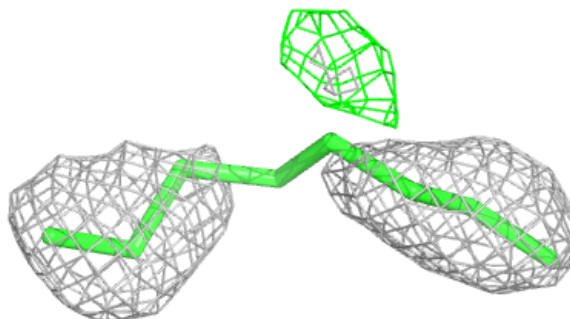


Electron density around OLC D 310:

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

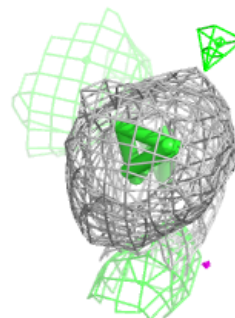
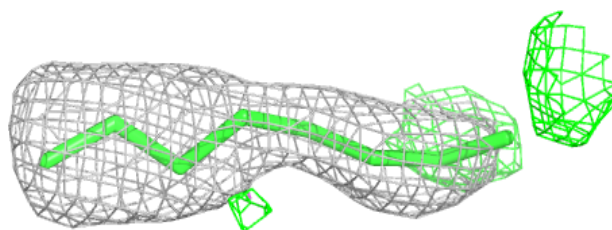
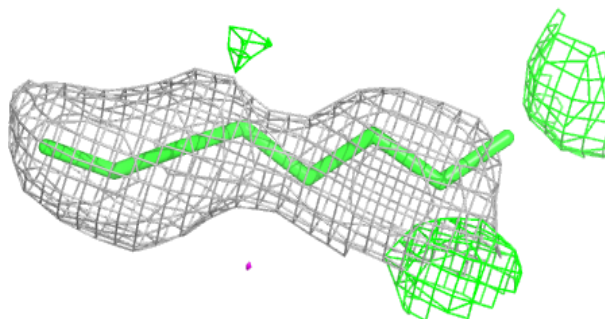
**Electron density around LFA A 310:**

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

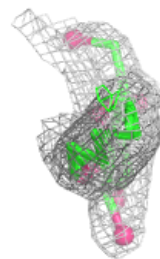
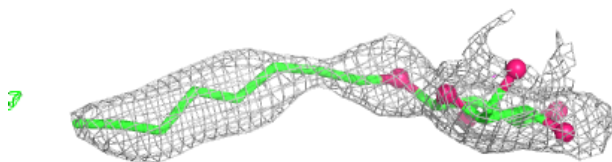
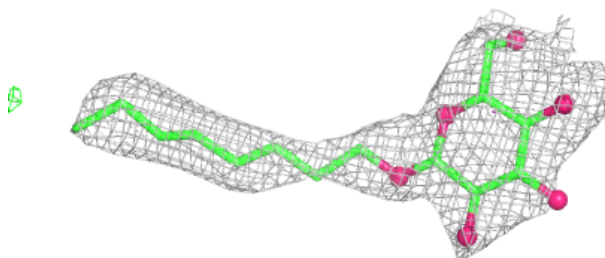


Electron density around LFA B 310:

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

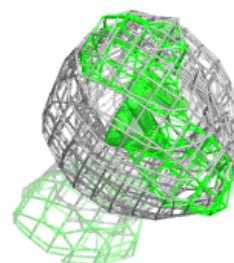
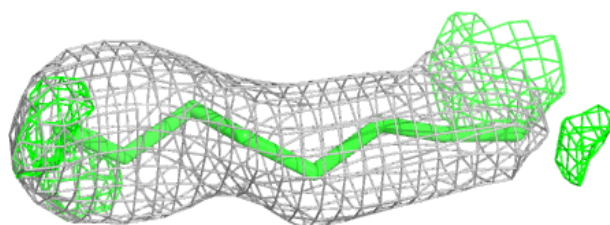
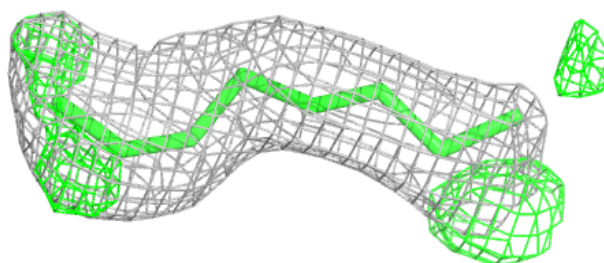
**Electron density around BOG C 317:**

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

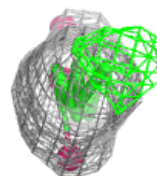
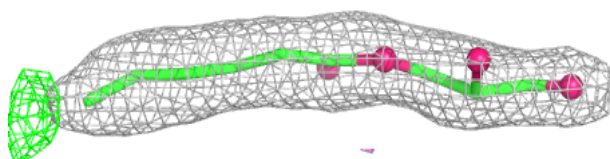
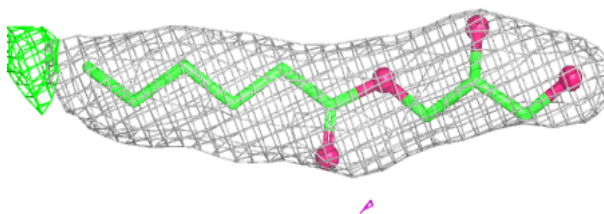


Electron density around LFA C 312:

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

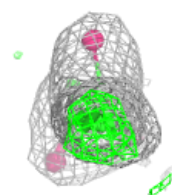
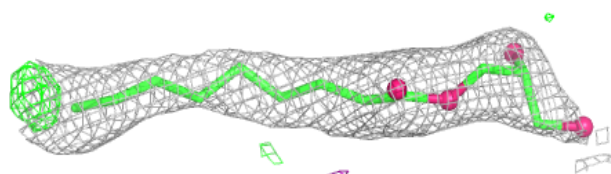
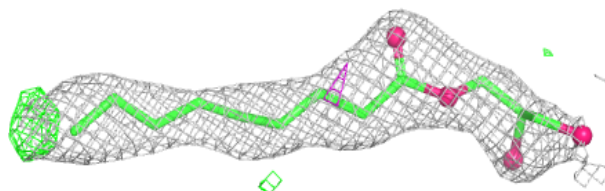
**Electron density around OLC A 304:**

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



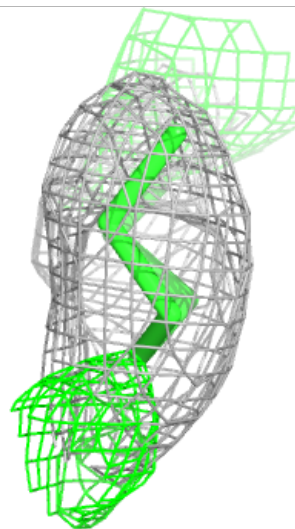
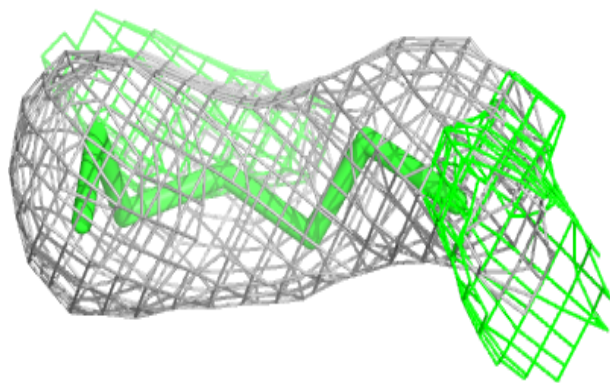
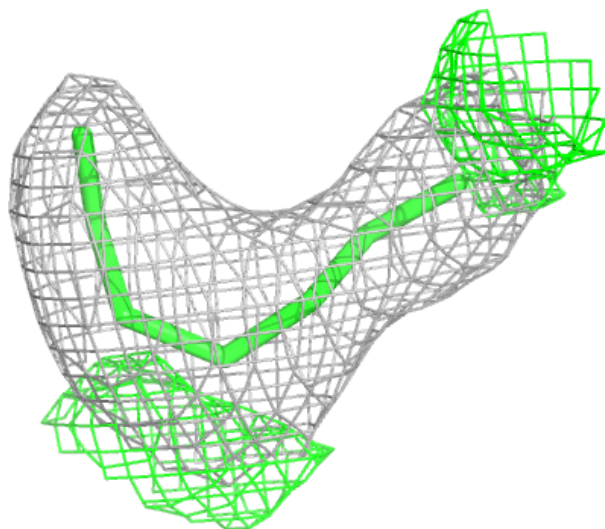
Electron density around OLC C 309:

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



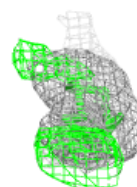
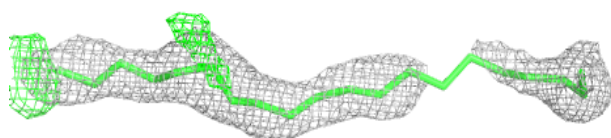
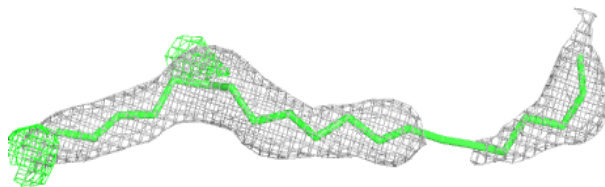
Electron density around OLC A 307:

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

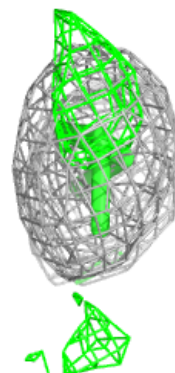
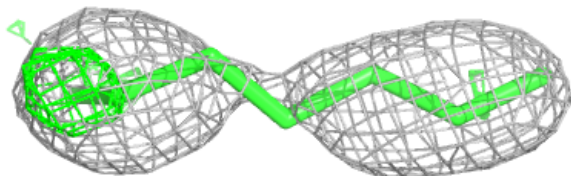
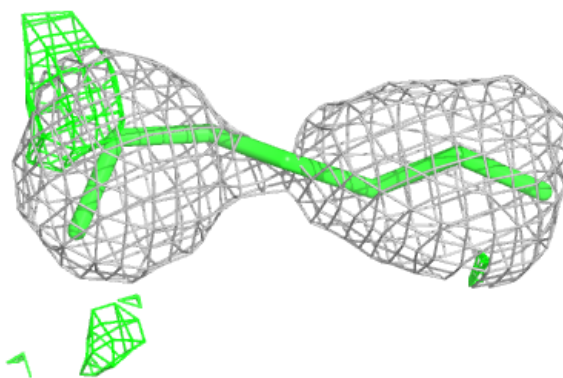


Electron density around LFA C 313:

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

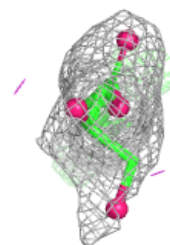
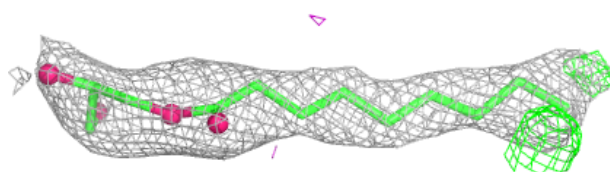
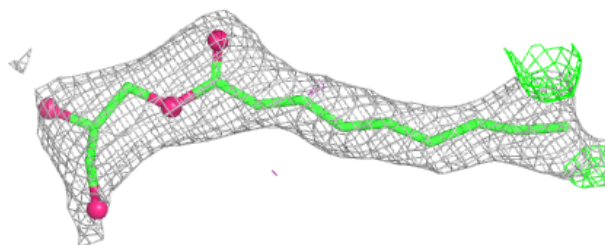
**Electron density around LFA B 312:**

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

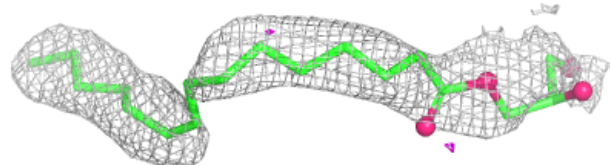
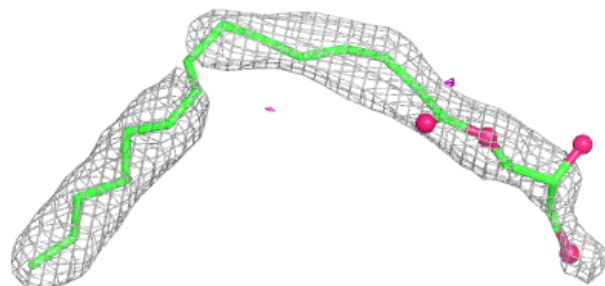


Electron density around OLC B 307:

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

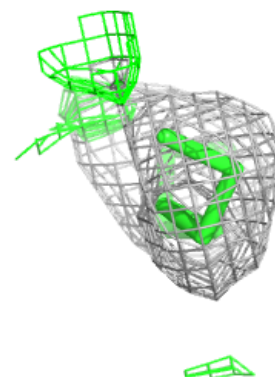
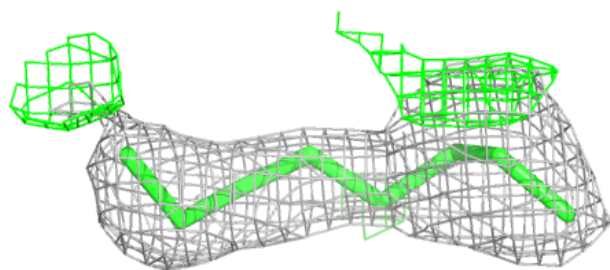
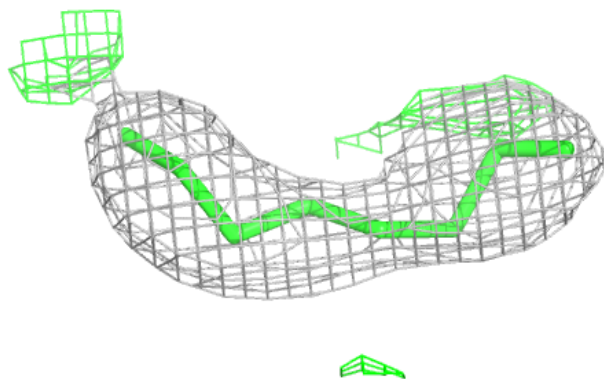
**Electron density around OLC C 308:**

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

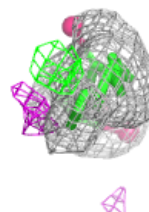
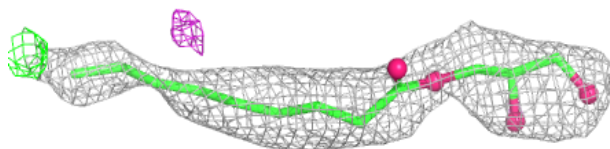
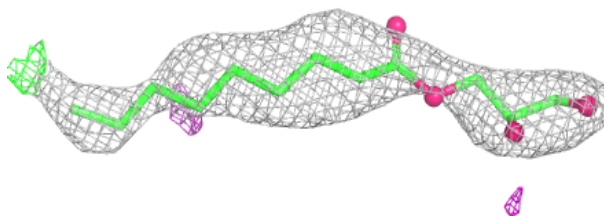


Electron density around LFA D 313:

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

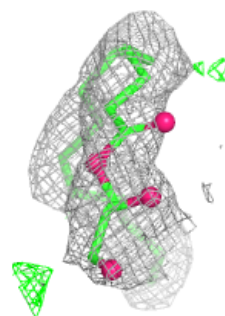
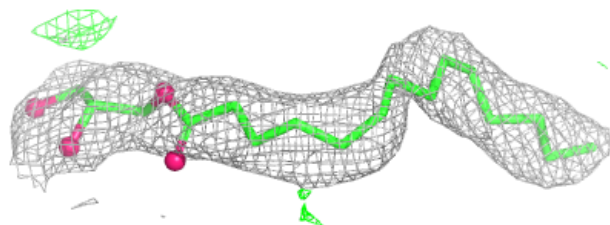
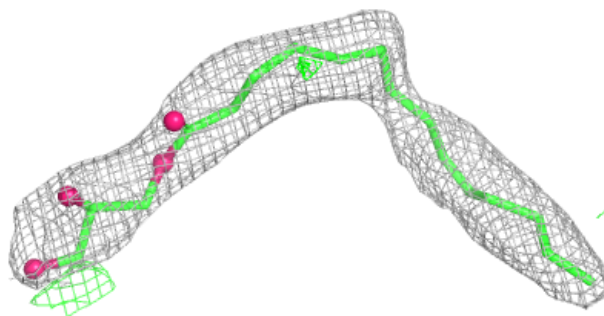
**Electron density around OLC B 302:**

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

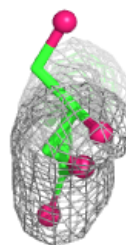
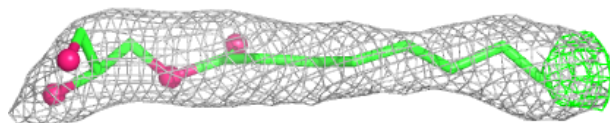
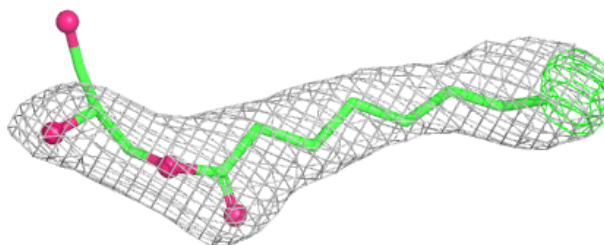


Electron density around OLC B 306:

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

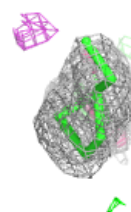
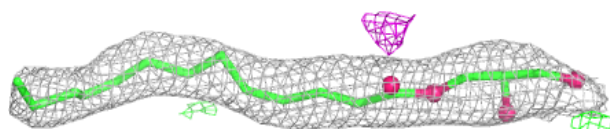
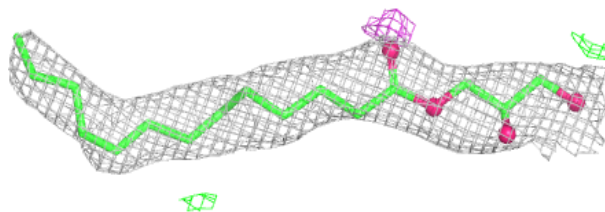
**Electron density around OLC A 306:**

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

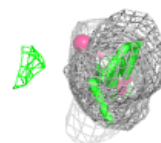
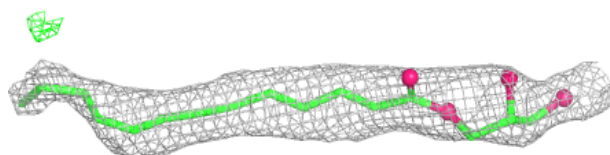
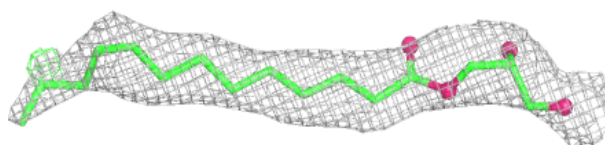


Electron density around OLC E 305:

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

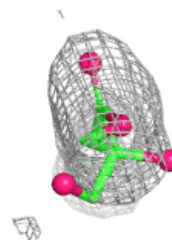
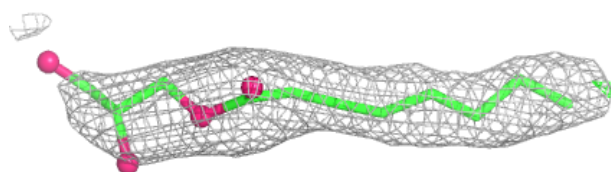
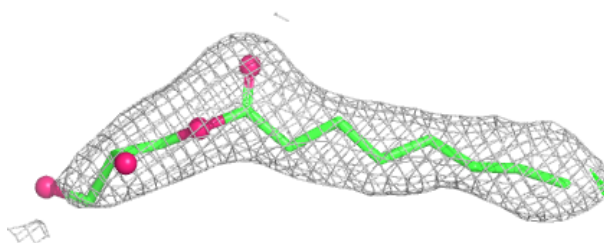
**Electron density around OLC B 305:**

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

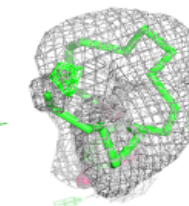
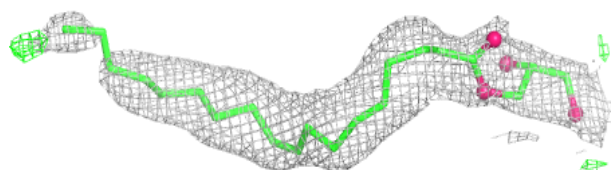
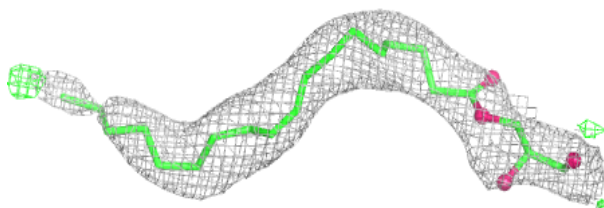


Electron density around OLC E 307:

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

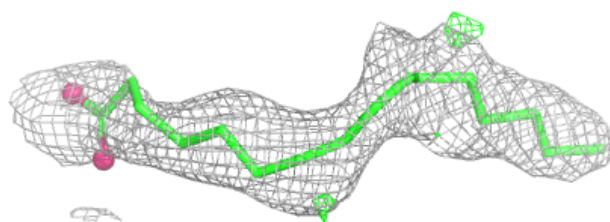
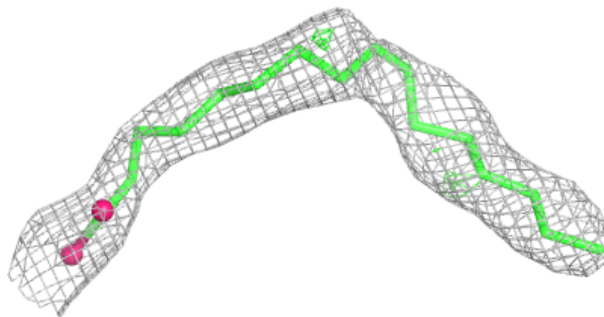
**Electron density around OLC E 301:**

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

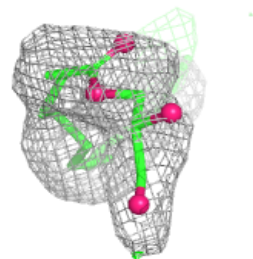
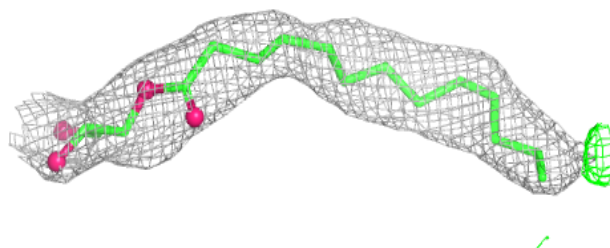
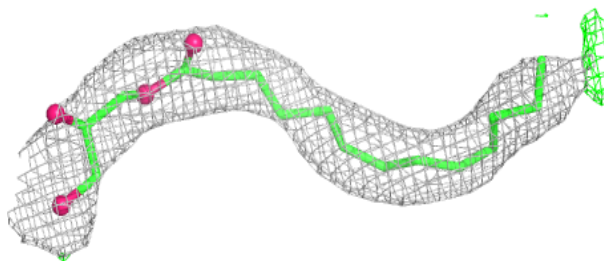


Electron density around OLC D 307:

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

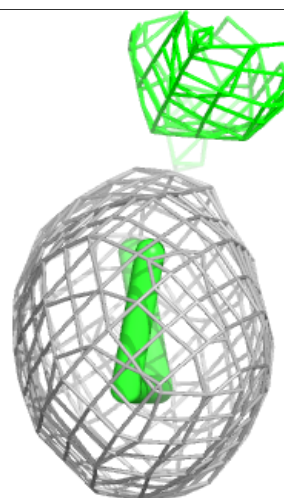
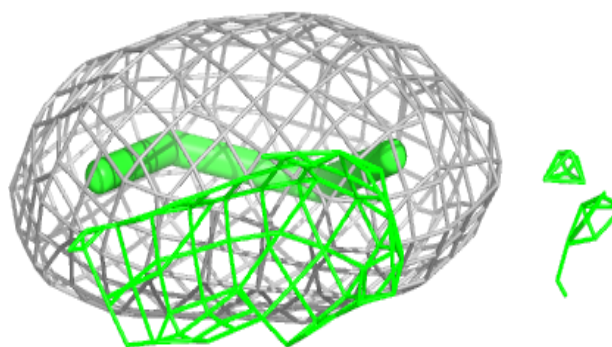
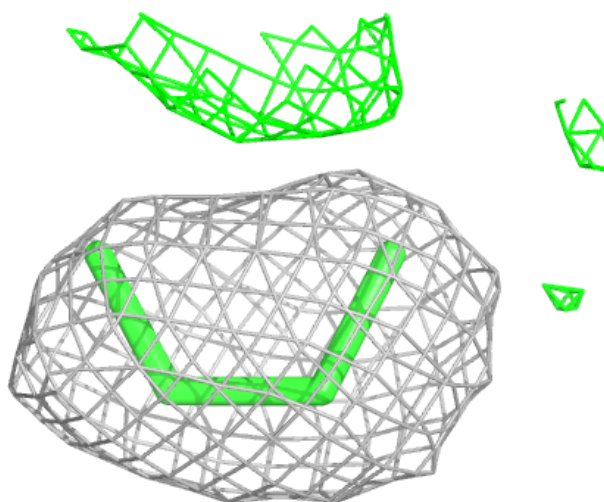
**Electron density around OLC C 302:**

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



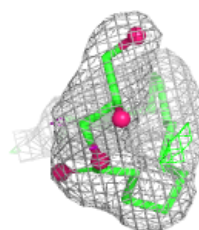
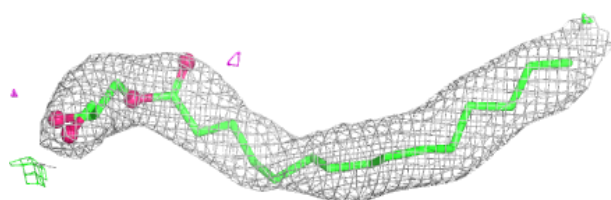
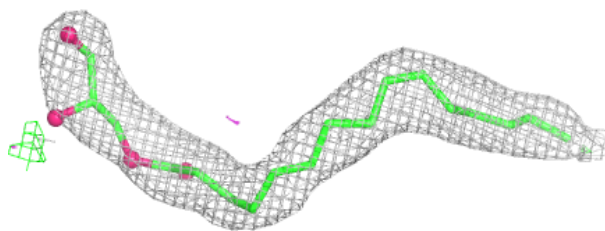
Electron density around LFA E 313:

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

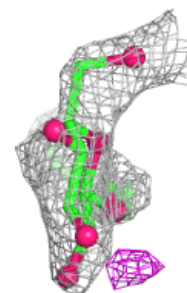
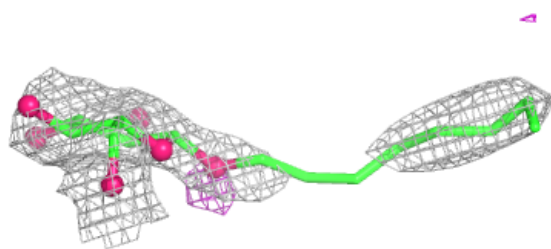
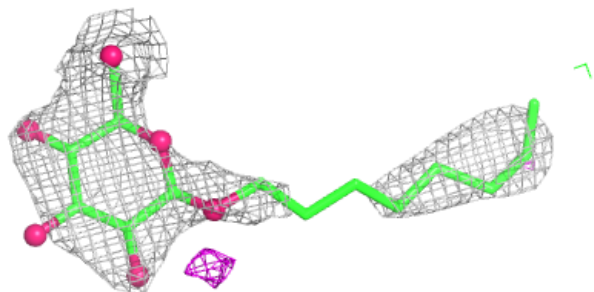


Electron density around OLC B 301:

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

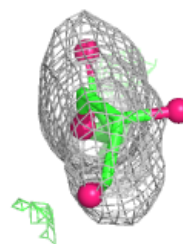
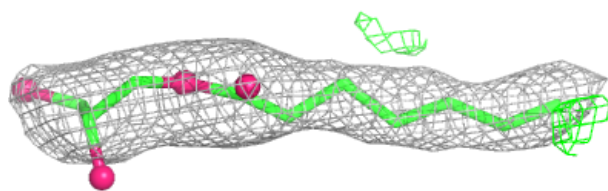
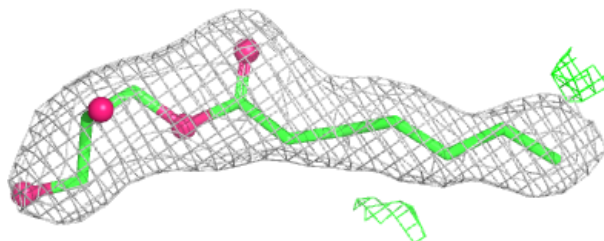
**Electron density around BOG D 318:**

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

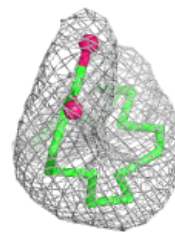
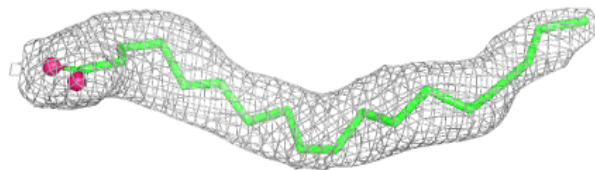
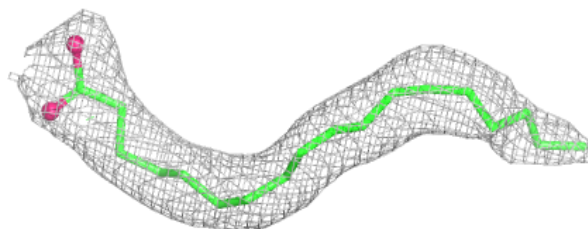


Electron density around OLC D 308:

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

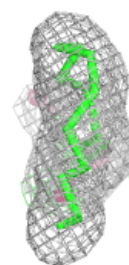
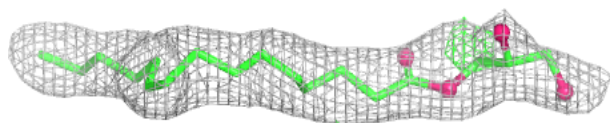
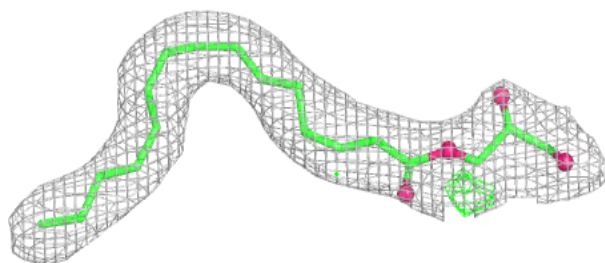
**Electron density around OLC A 318:**

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

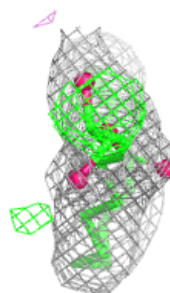
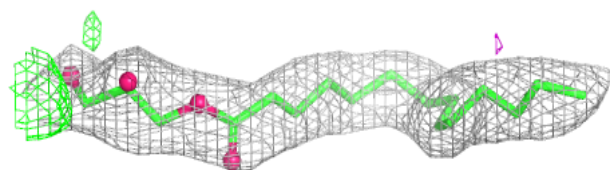
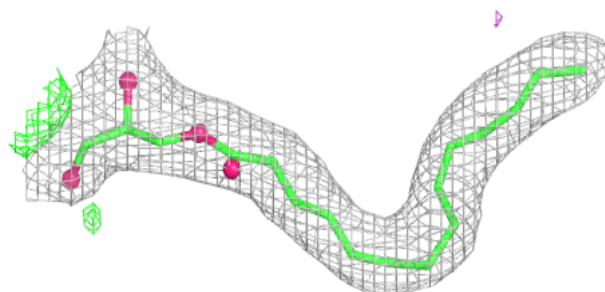


Electron density around OLC A 302:

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

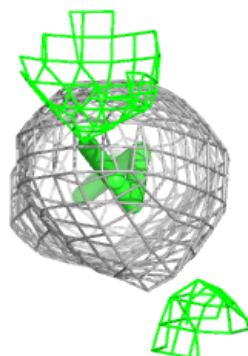
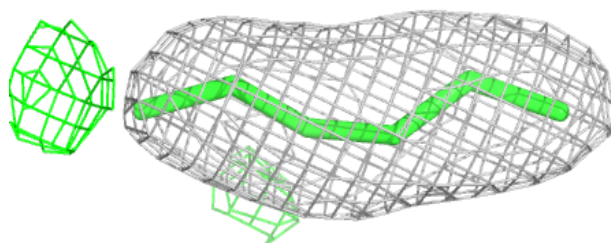
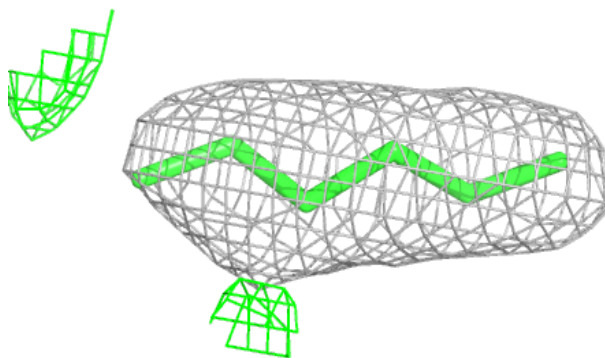
**Electron density around OLC C 301:**

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

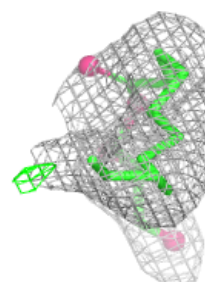
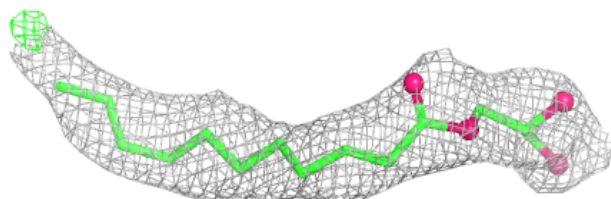
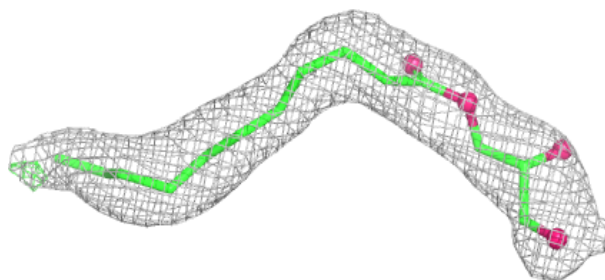


Electron density around LFA A 312:

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

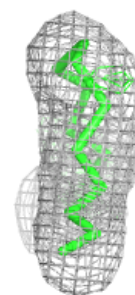
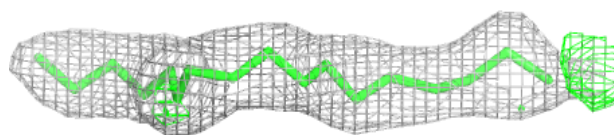
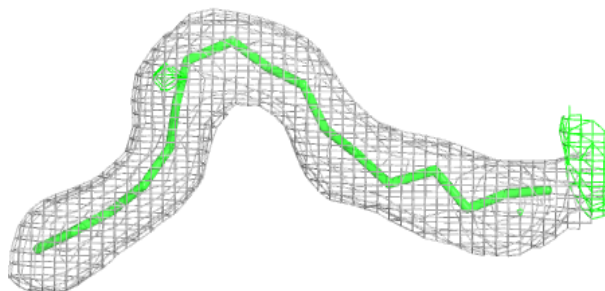
**Electron density around OLC D 301:**

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

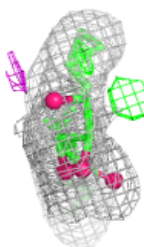
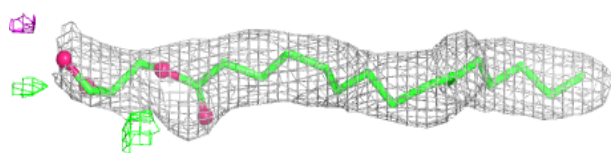
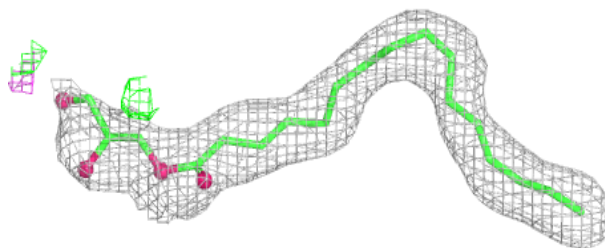


Electron density around LFA D 314:

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

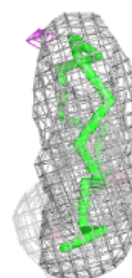
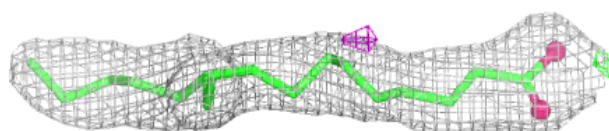
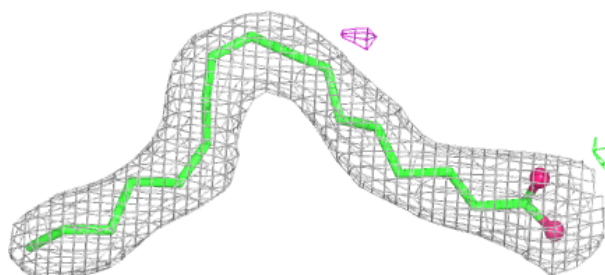
**Electron density around OLC C 305:**

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

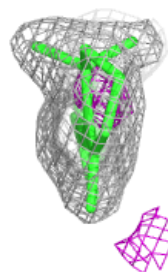
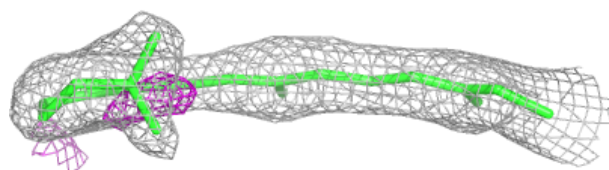
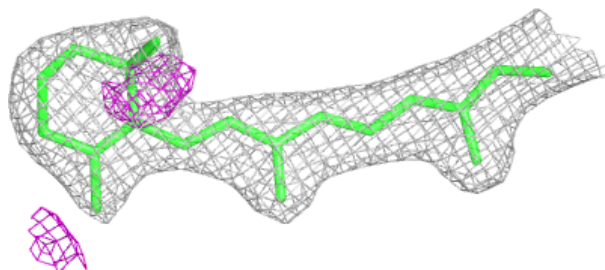


Electron density around OLC A 317:

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

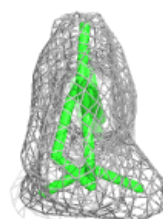
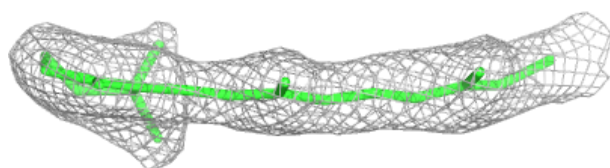
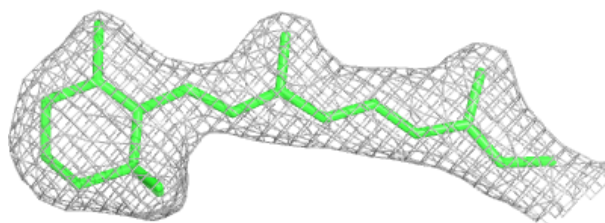
**Electron density around RET A 316:**

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

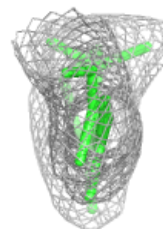
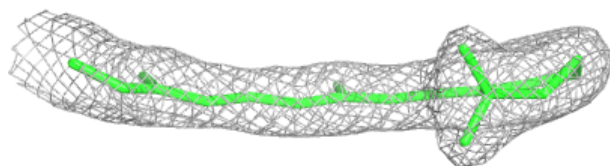
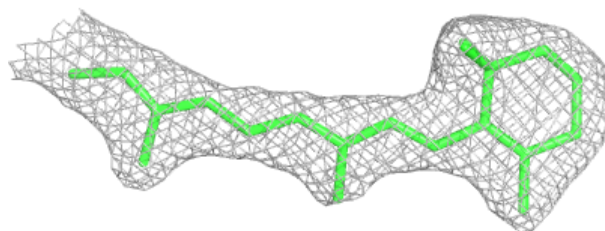


Electron density around RET B 315:

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

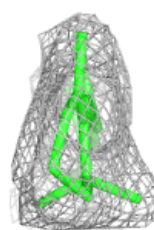
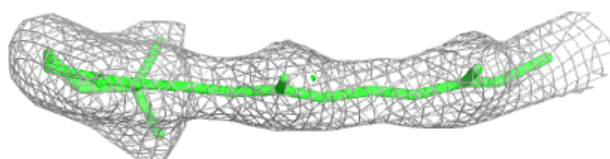
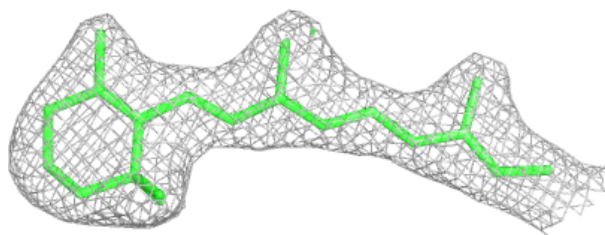
**Electron density around RET D 319:**

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

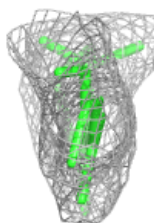
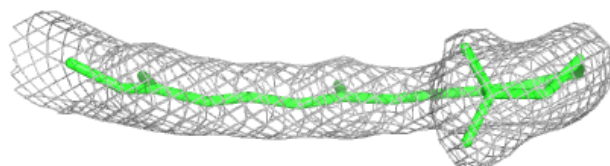
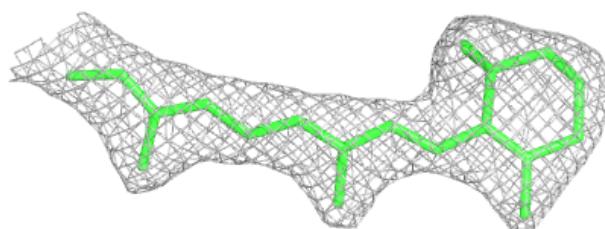


Electron density around RET E 317:

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

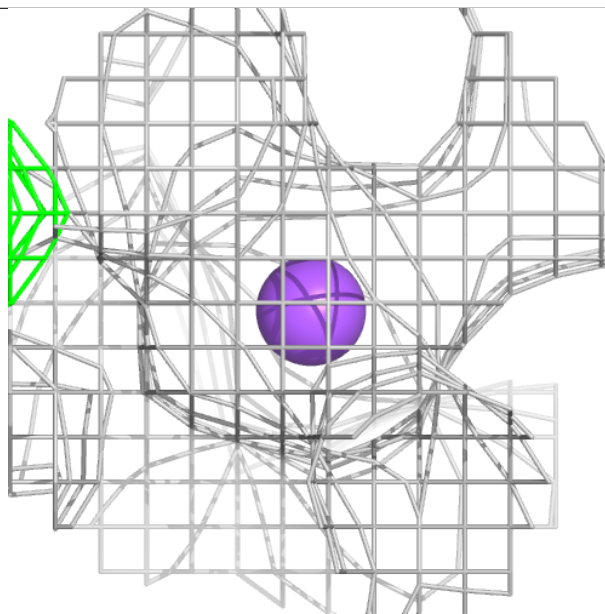
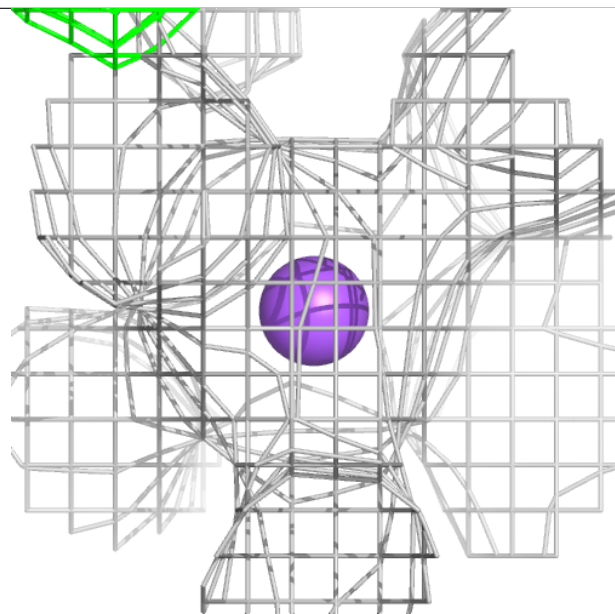
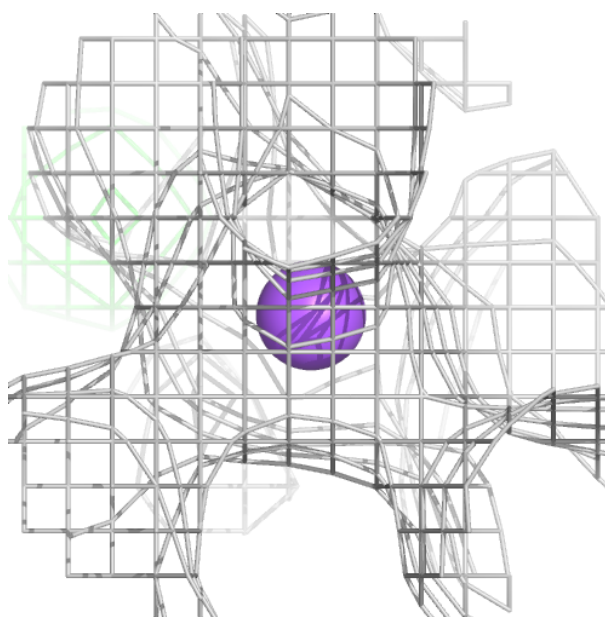
**Electron density around RET C 318:**

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



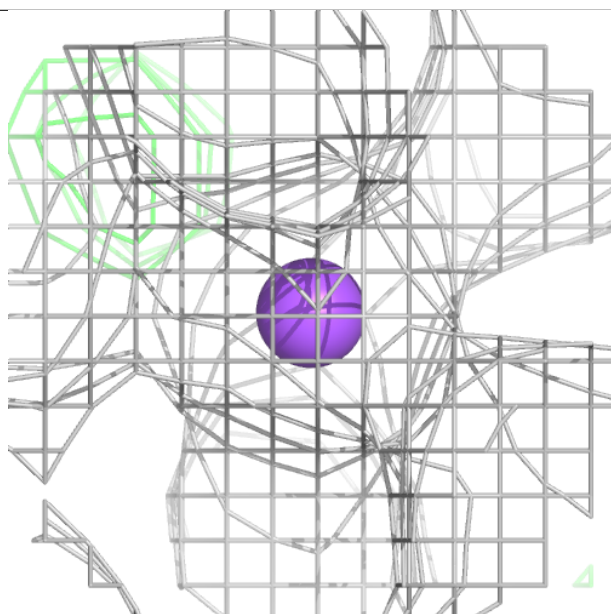
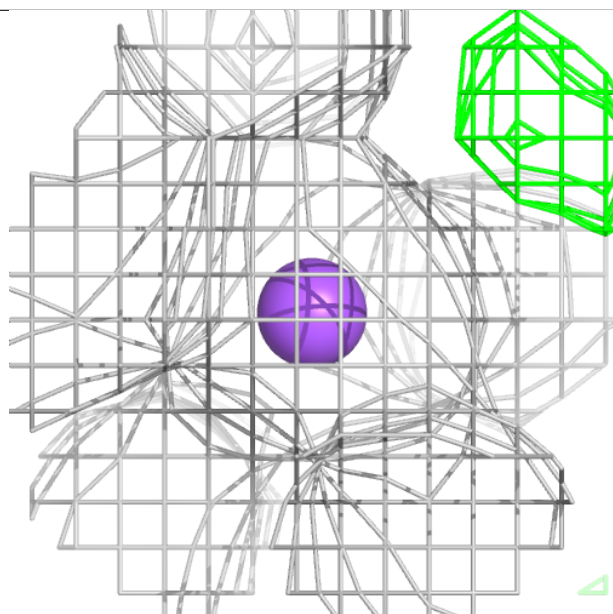
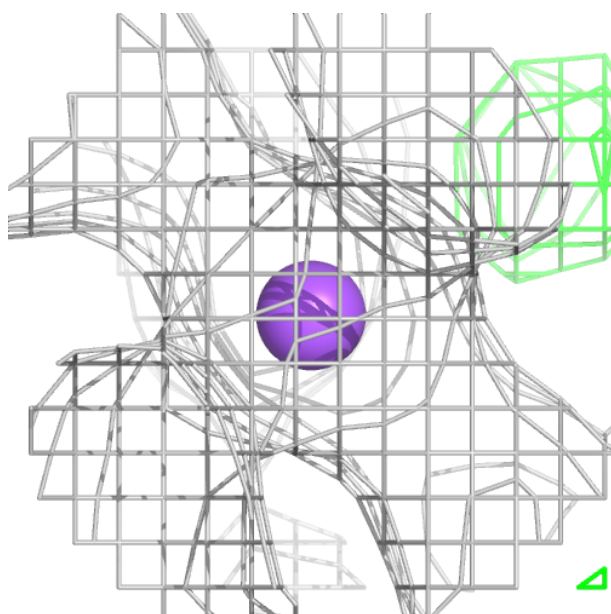
Electron density around NA A 314:

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



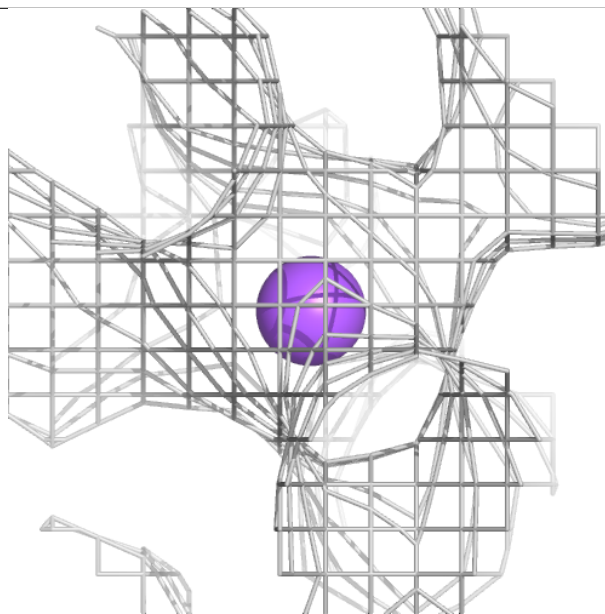
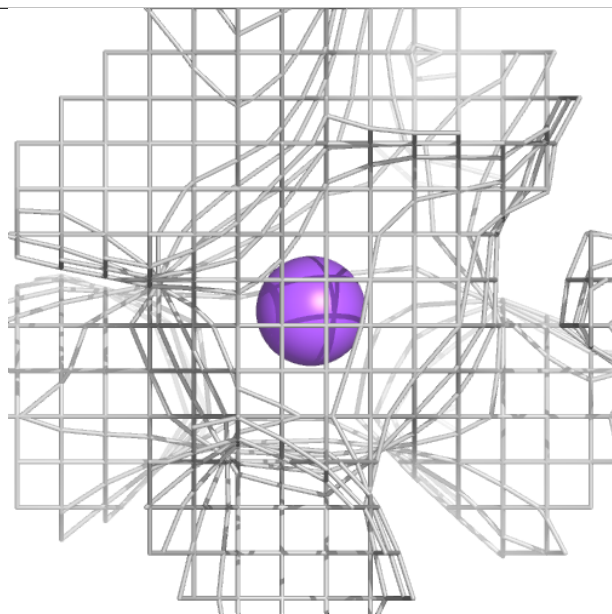
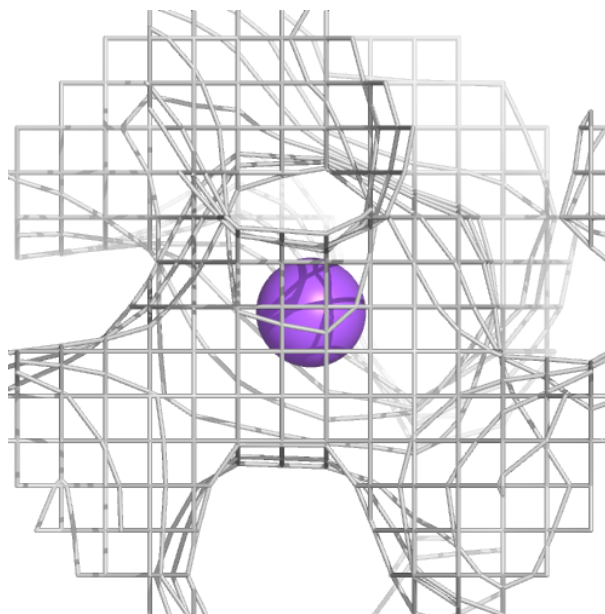
Electron density around NA D 317:

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



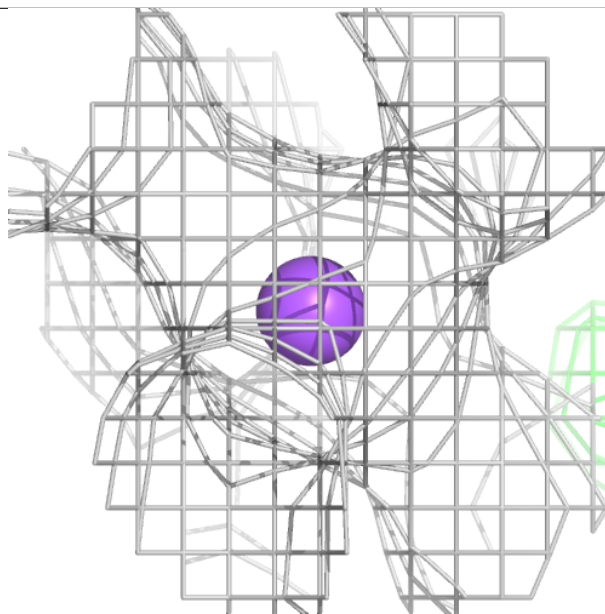
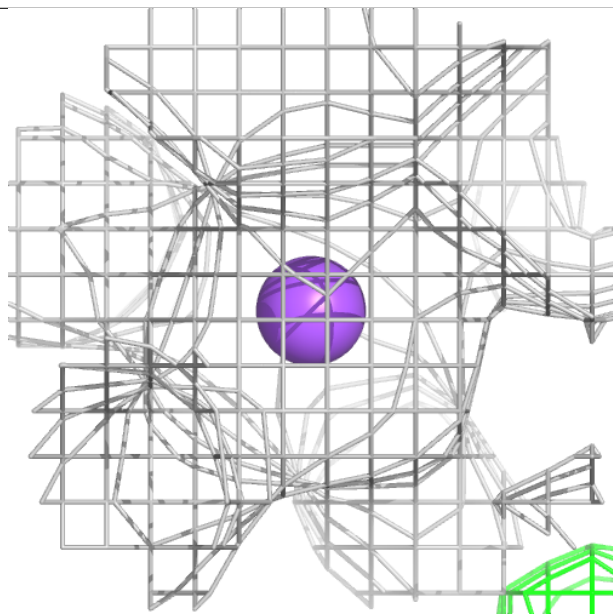
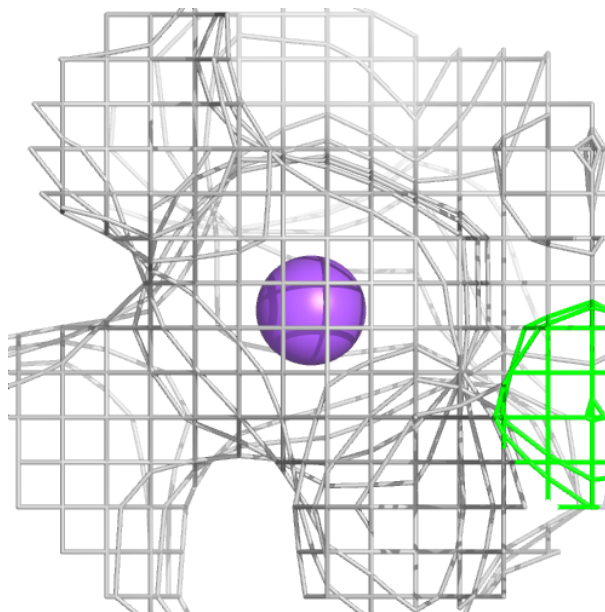
Electron density around NA B 313:

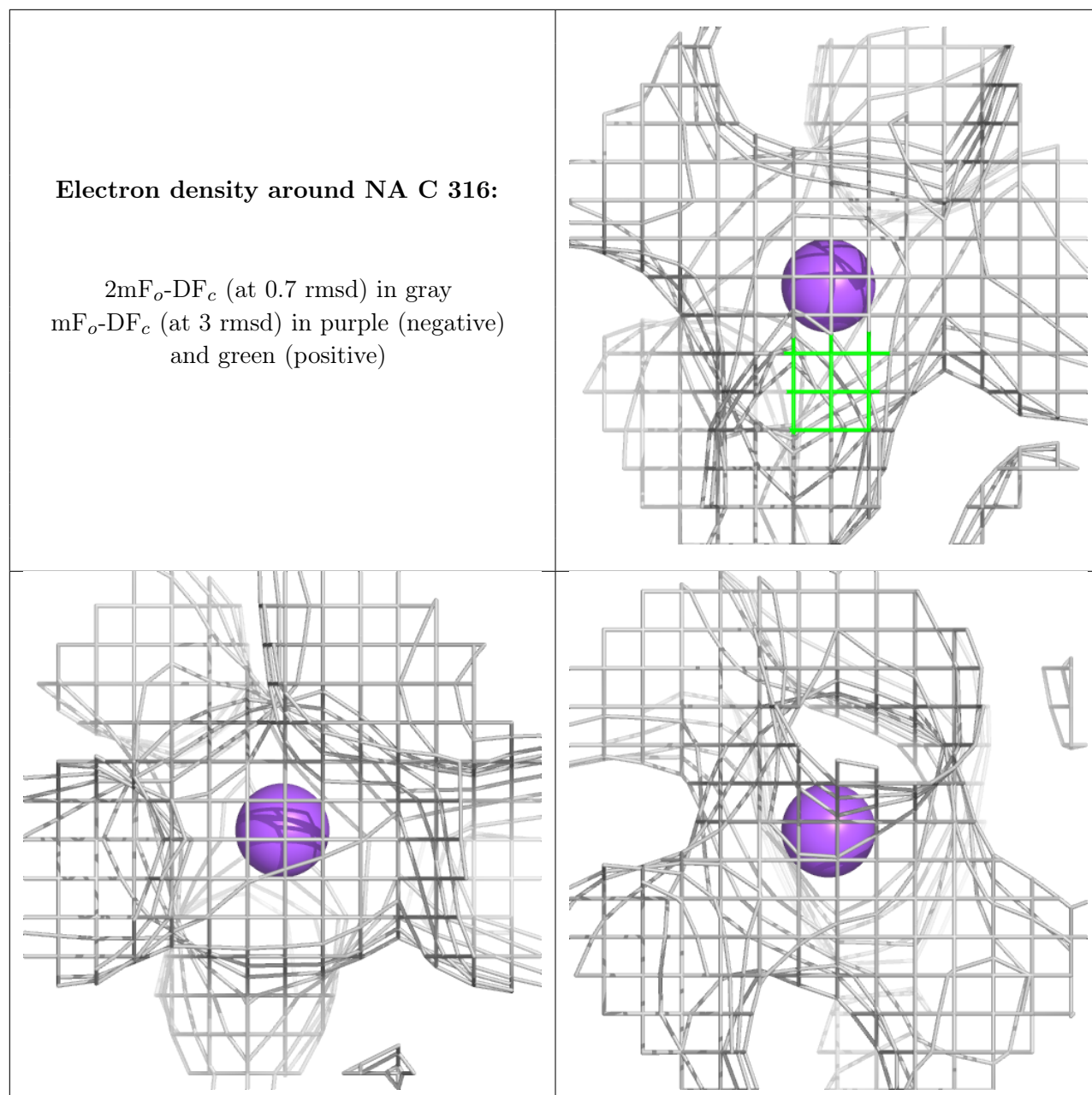
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NA 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.