



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:18 AM UTC

PDB ID : 6YC3 / pdb_00006yc3
Title : Crystal structure 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 : 2.00 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

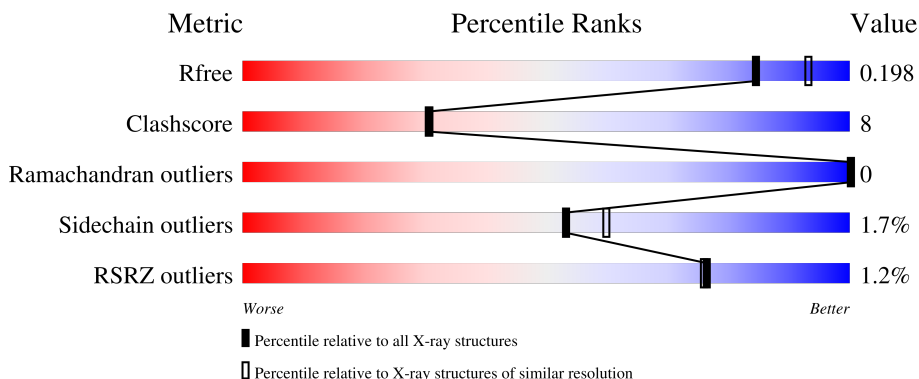
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	273	2% 87% 13%
1	B	273	82% 17%
1	C	273	2% 84% 15%
1	D	273	2% 86% 14%
1	E	273	2% 84% 15%

2 Entry composition [i](#)

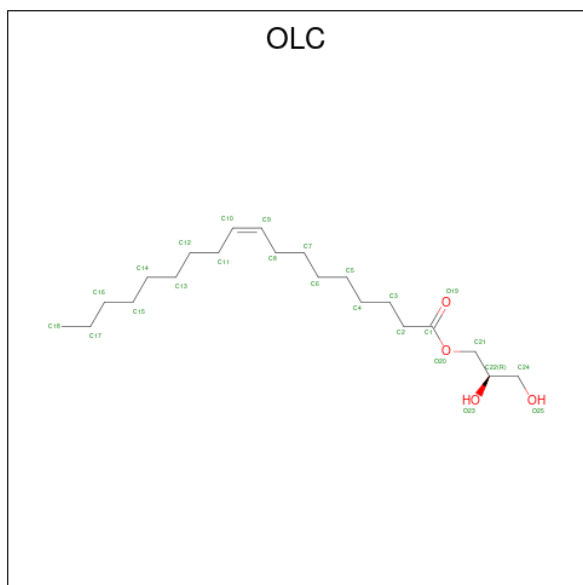
There are 7 unique types of molecules in this entry. The entry contains 12886 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3	0
			2193	1459	333	392	9			
1	B	273	Total	C	N	O	S	0	3	0
			2194	1457	335	393	9			
1	C	273	Total	C	N	O	S	0	3	0
			2186	1455	332	390	9			
1	D	273	Total	C	N	O	S	0	3	0
			2192	1457	334	392	9			
1	E	273	Total	C	N	O	S	0	3	0
			2194	1459	334	392	9			

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			9	9		

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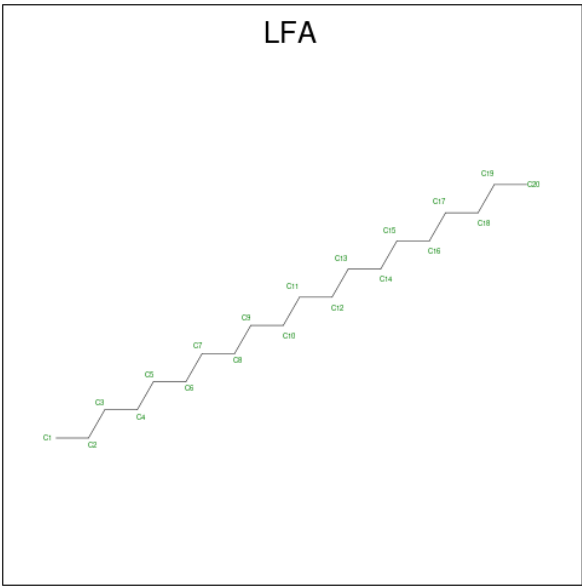
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			22	18	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			13	9	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			15	11	4		
2	A	1	Total	C		0	0
			7	7			
2	A	1	Total	C	O	0	0
			16	12	4		
2	A	1	Total	C	O	0	0
			19	17	2		
2	A	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			22	18	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			21	17	4		
2	B	1	Total	C	O	0	0
			16	12	4		
2	B	1	Total	C		0	0
			7	7			
2	C	1	Total	C	O	0	0
			21	17	4		
2	C	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			12	8	4		
2	C	1	Total	C	O	0	0
			23	19	4		
2	C	1	Total	C	O	0	0
			22	18	4		
2	C	1	Total	C	O	0	0
			20	16	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C 7 7	0	0
2	C	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
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: C₂₀H₄₂).



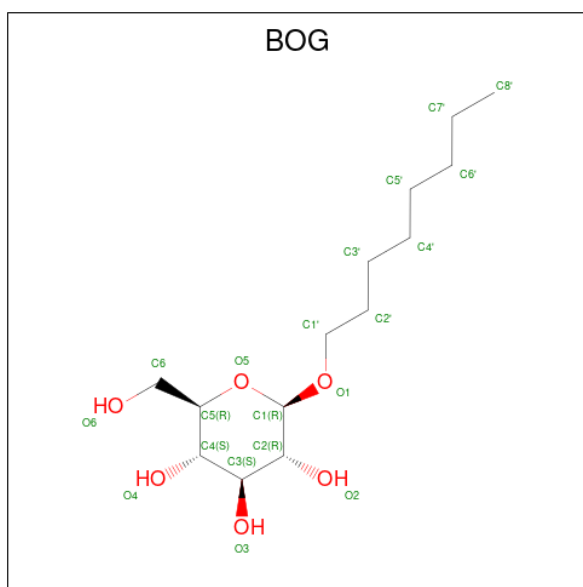
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 20 20	0	0
3	A	1	Total C 9 9	0	0
3	B	1	Total C 20 20	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total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

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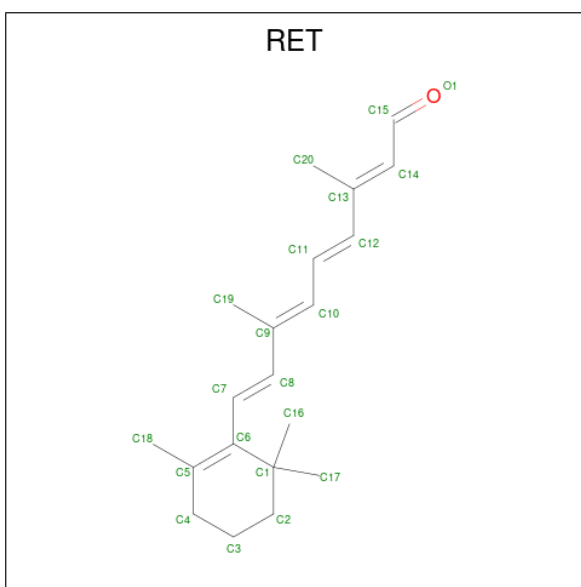
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 4 4	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 4 4	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	E	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 octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



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

- Molecule 5 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Na 2 2	0	0
6	B	2	Total Na 2 2	0	0
6	C	2	Total Na 2 2	0	0
6	D	2	Total Na 2 2	0	0
6	E	2	Total Na 2 2	0	0

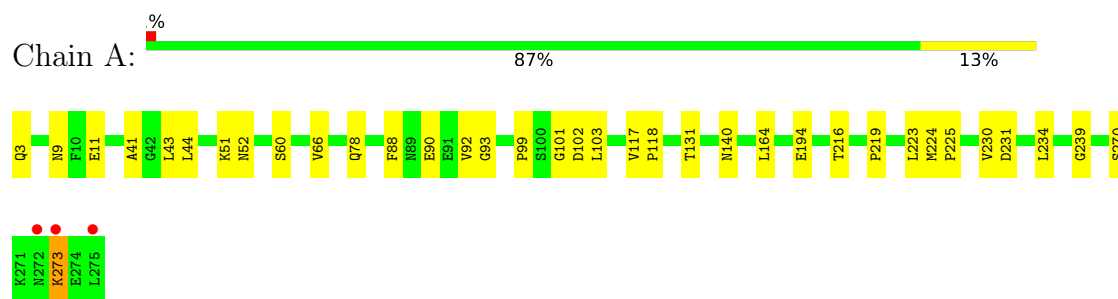
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	123	Total 123	O 123	0	0
7	B	123	Total 123	O 123	0	0
7	C	123	Total 123	O 123	0	0
7	D	107	Total 107	O 107	0	0
7	E	131	Total 131	O 131	0	0

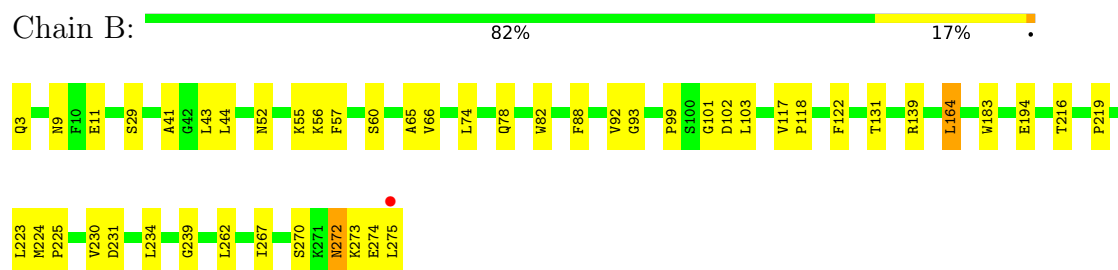
3 Residue-property plots [i](#)

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

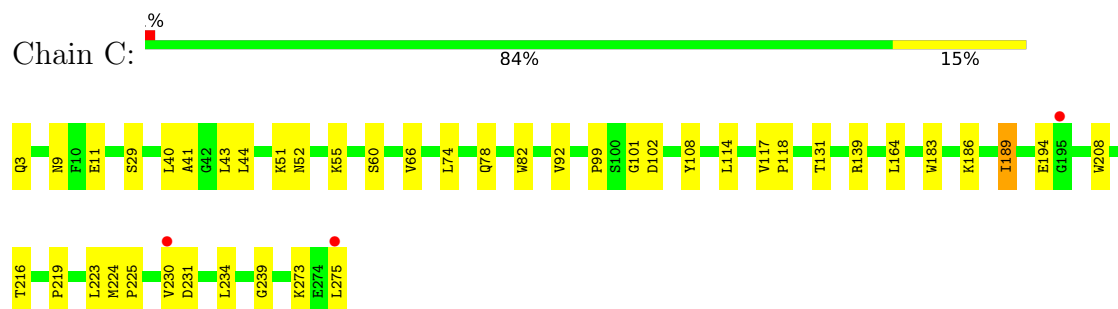
• Molecule 1: Sodium pumping rhodopsin



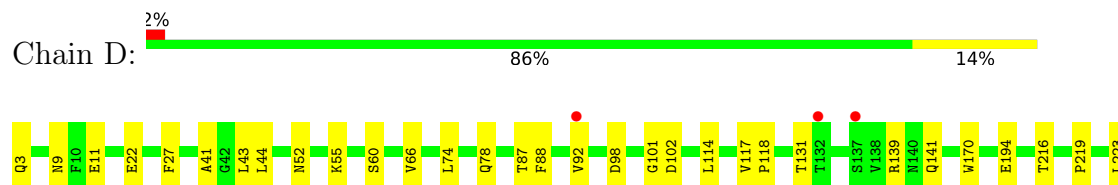
• Molecule 1: Sodium pumping rhodopsin

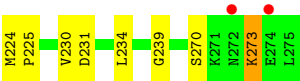


• Molecule 1: Sodium pumping rhodopsin

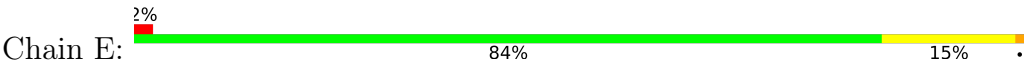


• Molecule 1: Sodium pumping rhodopsin





● Molecule 1: Sodium pumping rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.87Å 240.32Å 135.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.8 (20.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.168 , 0.195 0.171 , 0.198	Depositor DCC
R_{free} test set	7217 reflections (4.27%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12886	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% 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, OLC, BOG, RET, LFA

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	0.93	0/2251	1.40	0/3060
1	B	0.93	0/2252	1.39	0/3062
1	C	0.93	0/2244	1.39	0/3051
1	D	0.93	0/2250	1.41	0/3059
1	E	0.93	0/2252	1.39	0/3062
All	All	0.93	0/11249	1.40	0/15294

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	2193	0	2162	28	0
1	B	2194	0	2165	53	0
1	C	2186	0	2155	37	0
1	D	2192	0	2160	38	0
1	E	2194	0	2167	40	0
2	A	171	0	249	4	0
2	B	111	0	157	3	0
2	C	181	0	245	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	136	0	192	5	0
2	E	147	0	209	7	0
3	A	78	0	151	0	0
3	B	58	0	113	5	0
3	C	65	0	127	7	0
3	D	98	0	198	4	0
3	E	65	0	127	3	0
4	A	20	0	28	2	0
4	B	20	0	28	3	0
4	C	20	0	28	2	0
4	D	20	0	28	2	0
4	E	20	0	28	4	0
5	A	20	0	27	3	0
5	B	20	0	27	2	0
5	C	20	0	27	4	0
5	D	20	0	27	3	0
5	E	20	0	27	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
7	A	123	0	0	6	0
7	B	123	0	0	6	0
7	C	123	0	0	8	0
7	D	107	0	0	7	0
7	E	131	0	0	11	0
All	All	12886	0	12852	208	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 8.

All (208) 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)
7:B:494:HOH:O	1:C:99:PRO:HG2	1.56	1.03
1:B:272:ASN:HD22	1:B:272:ASN:N	1.56	1.03
1:B:272:ASN:HD22	1:B:272:ASN:H	0.92	0.89
1:C:55:LYS:NZ	7:C:401:HOH:O	1.94	0.89
1:D:52:ASN:O	1:D:273:LYS:HG3	1.73	0.89
1:B:275:LEU:O	1:B:275:LEU:HD23	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:H	1:B:272:ASN:ND2	1.72	0.86
1:D:231:ASP:N	4:D:316:BOG:O6	2.09	0.82
1:E:198:PRO:HG2	7:E:500:HOH:O	1.81	0.80
1:B:272:ASN:N	1:B:272:ASN:ND2	2.27	0.80
5:A:320:RET:H8	5:A:320:RET:H161	1.65	0.78
1:D:87[B]:THR:HG21	1:D:98:ASP:OD2	1.84	0.78
5:B:313:RET:H8	5:B:313:RET:H161	1.68	0.76
1:A:231:ASP:N	4:A:315:BOG:O6	2.17	0.75
5:D:317:RET:H8	5:D:317:RET:H161	1.68	0.75
1:A:140:ASN:HB3	2:A:303:OLC:H2A	1.69	0.74
1:D:231:ASP:H	4:D:316:BOG:HO6	1.34	0.74
1:E:87[B]:THR:HG21	1:E:98:ASP:OD2	1.88	0.73
1:D:3:GLN:N	7:D:402:HOH:O	2.21	0.72
1:A:164:LEU:HD21	4:A:315:BOG:H2'1	1.73	0.71
1:E:60:SER:OG	7:E:401:HOH:O	2.07	0.70
7:C:423:HOH:O	1:D:3:GLN:HG2	1.92	0.69
1:D:60:SER:OG	7:D:401:HOH:O	2.10	0.69
5:C:317:RET:H8	5:C:317:RET:H161	1.76	0.67
1:B:60:SER:OG	7:B:401:HOH:O	2.12	0.67
1:E:87[B]:THR:HG22	7:E:479:HOH:O	1.95	0.66
5:E:317:RET:H8	5:E:317:RET:H161	1.77	0.66
1:A:131:THR:HG21	1:A:194:GLU:OE1	1.98	0.63
1:B:275:LEU:HD23	1:B:275:LEU:C	2.23	0.63
1:D:87[B]:THR:HG22	7:D:469:HOH:O	1.99	0.62
1:E:189:ILE:HD12	1:E:208:TRP:HB2	1.80	0.62
1:C:189:ILE:HD12	1:C:208:TRP:HB2	1.81	0.62
1:C:131:THR:HG21	1:C:194:GLU:OE1	2.00	0.61
2:C:305:OLC:H14	2:C:318:OLC:H6A	1.83	0.61
1:C:183:TRP:CE3	3:C:311:LFA:H41	2.36	0.60
1:B:131:THR:HG21	1:B:194:GLU:OE1	2.02	0.60
1:B:231:ASP:H	4:B:312:BOG:HO6	1.47	0.59
1:D:131:THR:HG21	1:D:194:GLU:OE1	2.02	0.59
1:E:131:THR:HG21	1:E:194:GLU:OE1	2.02	0.58
1:B:267:ILE:CG2	1:B:275:LEU:HB2	2.33	0.58
1:C:231:ASP:N	4:C:316:BOG:O6	2.23	0.58
1:E:3:GLN:O	7:E:402:HOH:O	2.17	0.58
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.86	0.57
1:D:60:SER:CB	7:D:401:HOH:O	2.51	0.57
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.86	0.57
1:A:3:GLN:HB2	7:E:412:HOH:O	2.05	0.56
1:B:60:SER:CB	7:B:401:HOH:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:442:HOH:O	1:E:55:LYS:HE3	2.04	0.56
1:B:272:ASN:HB2	1:B:273:LYS:HD3	1.88	0.56
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.88	0.56
1:B:273:LYS:O	7:B:402:HOH:O	2.17	0.56
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.88	0.56
3:D:313:LFA:C15	2:E:302:OLC:H21A	2.35	0.55
1:C:186:LYS:HG2	3:C:311:LFA:C5	2.37	0.55
1:E:111:LEU:O	1:E:114:LEU:HB2	2.06	0.55
1:C:29[B]:SER:HG	1:C:82:TRP:CD1	2.25	0.55
1:C:186:LYS:HG2	3:C:311:LFA:H51	1.88	0.54
1:B:56:LYS:HE3	1:B:57:PHE:CZ	2.42	0.54
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.87	0.54
1:B:139:ARG:NH2	2:B:303:OLC:H21A	2.22	0.54
1:D:27:PHE:CE1	2:D:309:OLC:H2A	2.43	0.54
1:E:114:LEU:HD13	1:E:150:ILE:HG21	1.88	0.54
1:E:234:LEU:O	1:E:239:GLY:HA3	2.07	0.53
1:D:234:LEU:O	1:D:239:GLY:HA3	2.08	0.53
1:A:60:SER:OG	7:A:401:HOH:O	2.19	0.53
1:D:273:LYS:N	1:D:273:LYS:HD3	2.24	0.53
1:B:60:SER:HB3	7:B:401:HOH:O	2.09	0.53
1:A:234:LEU:O	1:A:239:GLY:HA3	2.08	0.53
1:C:234:LEU:O	1:C:239:GLY:HA3	2.10	0.52
1:B:234:LEU:O	1:B:239:GLY:HA3	2.08	0.52
3:B:314:LFA:H11	3:E:301:LFA:C1	2.40	0.52
1:E:60:SER:CB	7:E:401:HOH:O	2.58	0.52
1:B:29[B]:SER:HG	1:B:82:TRP:CD1	2.28	0.52
1:B:139:ARG:HH11	2:B:301:OLC:C24	2.23	0.52
1:C:164:LEU:HD21	4:C:316:BOG:H2'1	1.91	0.51
1:E:231:ASP:N	4:E:316:BOG:O6	2.22	0.51
7:B:418:HOH:O	1:C:3:GLN:HB2	2.11	0.51
1:D:60:SER:HB3	7:D:401:HOH:O	2.08	0.51
1:B:52:ASN:O	1:B:273:LYS:HG3	2.11	0.50
1:D:141:GLN:HG2	2:D:304:OLC:H2	1.93	0.50
1:B:44:LEU:HD21	1:C:43:LEU:HD11	1.93	0.50
1:B:41:ALA:HB1	1:C:66:VAL:HG13	1.93	0.49
2:D:309:OLC:H11A	3:D:313:LFA:H12	1.94	0.49
1:B:224:MET:N	1:B:225:PRO:HD2	2.28	0.49
1:A:270:SER:HB3	1:A:273:LYS:HG2	1.94	0.49
5:A:320:RET:H161	5:A:320:RET:C8	2.37	0.49
1:C:224:MET:N	1:C:225:PRO:HD2	2.27	0.49
1:A:101:GLY:O	1:A:102:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:GLY:O	1:C:102:ASP:HB2	2.12	0.49
1:B:267:ILE:HG22	1:B:275:LEU:HB2	1.95	0.49
1:B:139:ARG:NH1	2:B:301:OLC:C24	2.76	0.48
5:C:317:RET:H161	5:C:317:RET:C8	2.41	0.48
1:B:101:GLY:O	1:B:102:ASP:HB2	2.14	0.48
1:A:224:MET:N	1:A:225:PRO:HD2	2.28	0.48
7:D:442:HOH:O	1:E:55:LYS:CE	2.60	0.48
1:B:267:ILE:HG21	1:B:275:LEU:HB2	1.94	0.48
1:D:224:MET:N	1:D:225:PRO:HD2	2.29	0.48
7:A:441:HOH:O	1:B:55:LYS:HE3	2.13	0.47
1:B:183:TRP:CE3	3:B:308:LFA:H182	2.49	0.47
5:D:317:RET:H161	5:D:317:RET:C8	2.38	0.47
1:E:87[B]:THR:HG23	1:E:98:ASP:HB2	1.96	0.47
5:E:317:RET:H161	5:E:317:RET:C8	2.44	0.47
1:C:40:LEU:HD11	3:C:304:LFA:H142	1.97	0.47
5:C:317:RET:H8	5:C:317:RET:H171	1.97	0.47
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.15	0.47
1:C:60:SER:CB	7:C:402:HOH:O	2.63	0.47
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.15	0.47
1:E:224:MET:N	1:E:225:PRO:HD2	2.29	0.47
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.96	0.46
7:A:403:HOH:O	1:B:3:GLN:HG3	2.14	0.46
1:B:231:ASP:N	4:B:312:BOG:O6	2.22	0.46
1:D:27:PHE:HE1	2:D:309:OLC:H2A	1.80	0.46
1:A:44:LEU:HD21	1:B:43:LEU:HD11	1.98	0.46
1:C:183:TRP:CZ3	3:C:311:LFA:H61	2.50	0.46
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.16	0.46
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.97	0.46
1:C:44:LEU:HD21	1:D:43:LEU:HD11	1.96	0.46
1:E:101:GLY:O	1:E:102:ASP:HB2	2.16	0.46
1:E:198:PRO:CD	7:E:500:HOH:O	2.64	0.46
1:E:231:ASP:H	4:E:316:BOG:HO6	1.56	0.46
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.16	0.45
5:B:313:RET:H161	5:B:313:RET:C8	2.38	0.45
2:C:318:OLC:H5A	2:C:318:OLC:H2	1.80	0.45
1:D:87[B]:THR:HG23	1:D:98:ASP:CB	2.46	0.45
1:E:177:PHE:CE1	2:E:305:OLC:H10	2.52	0.45
1:B:223:LEU:C	1:B:225:PRO:HD2	2.42	0.45
1:C:51:LYS:HD3	7:C:479:HOH:O	2.16	0.45
1:C:216:THR:O	1:C:219:PRO:HG2	2.17	0.45
1:D:216:THR:O	1:D:219:PRO:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:C	1:B:275:LEU:CD2	2.90	0.45
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.17	0.45
1:E:198:PRO:CG	7:E:500:HOH:O	2.53	0.45
1:A:90:GLU:CD	1:B:99:PRO:HG3	2.42	0.45
1:D:44:LEU:HD21	1:E:43:LEU:HD11	1.98	0.45
1:E:87[B]:THR:HG23	1:E:98:ASP:CB	2.47	0.45
7:A:403:HOH:O	1:B:3:GLN:CG	2.64	0.45
1:A:44:LEU:HD21	1:B:65:ALA:HB1	1.99	0.44
2:A:302:OLC:H2A	1:B:122:PHE:HE2	1.82	0.44
1:C:51:LYS:HB2	7:C:435:HOH:O	2.17	0.44
1:E:52:ASN:O	1:E:273:LYS:HG3	2.17	0.44
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.99	0.44
1:C:223:LEU:C	1:C:225:PRO:HD2	2.42	0.44
1:A:43:LEU:HD11	1:E:44:LEU:HD21	2.00	0.44
1:D:87[B]:THR:HG23	1:D:98:ASP:HB2	1.99	0.44
1:D:88:PHE:CD2	1:E:99:PRO:HB3	2.53	0.44
1:A:99:PRO:HG3	1:E:90:GLU:CD	2.42	0.44
4:E:316:BOG:H5	7:E:475:HOH:O	2.18	0.44
1:E:159:TYR:CE1	2:E:308:OLC:H21A	2.53	0.44
1:E:216:THR:O	1:E:219:PRO:HG2	2.18	0.44
1:E:223:LEU:C	1:E:225:PRO:HD2	2.43	0.43
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.53	0.43
1:E:198:PRO:HD2	7:E:500:HOH:O	2.18	0.43
1:D:78[A]:GLN:HA	1:D:78[A]:GLN:OE1	2.18	0.43
1:A:78[A]:GLN:HA	1:A:78[A]:GLN:OE1	2.19	0.43
1:E:78[A]:GLN:HA	1:E:78[A]:GLN:OE1	2.19	0.43
1:A:52:ASN:O	1:A:273:LYS:HG3	2.18	0.43
3:C:304:LFA:H172	3:D:301:LFA:H61	2.01	0.43
1:C:78[A]:GLN:HA	1:C:78[A]:GLN:OE1	2.18	0.43
1:B:29[B]:SER:HB3	1:C:108:TYR:HH	1.84	0.43
1:C:60:SER:OG	7:C:402:HOH:O	2.21	0.43
1:D:223:LEU:C	1:D:225:PRO:HD2	2.44	0.43
1:B:78[A]:GLN:HA	1:B:78[A]:GLN:OE1	2.18	0.43
1:B:216:THR:O	1:B:219:PRO:HG2	2.18	0.43
1:C:60:SER:HB3	7:C:402:HOH:O	2.19	0.43
2:C:305:OLC:H13	2:C:318:OLC:H4A	2.01	0.43
1:C:74:LEU:HD22	1:C:74:LEU:HA	1.89	0.42
1:D:270:SER:HB2	1:D:273:LYS:HB2	1.99	0.42
5:E:317:RET:H8	5:E:317:RET:H171	2.00	0.42
1:A:78[B]:GLN:OE1	1:A:78[B]:GLN:HA	2.18	0.42
1:A:223:LEU:C	1:A:225:PRO:HD2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:305:OLC:H10	2:C:305:OLC:H7	1.63	0.42
1:D:22:GLU:HB2	7:E:440:HOH:O	2.20	0.42
1:D:41:ALA:HB1	1:E:66:VAL:HG13	2.00	0.42
1:C:78[B]:GLN:OE1	1:C:78[B]:GLN:HA	2.18	0.42
5:A:320:RET:H11	5:A:320:RET:H191	1.95	0.42
1:B:44:LEU:CD2	1:C:43:LEU:HD11	2.49	0.42
1:B:183:TRP:CZ3	3:B:308:LFA:H182	2.55	0.42
1:C:52:ASN:O	1:C:273:LYS:HG3	2.20	0.42
1:D:74:LEU:HD22	1:D:74:LEU:HA	1.86	0.42
1:C:139:ARG:NH2	3:C:313:LFA:H203	2.35	0.42
2:A:316:OLC:C17	2:E:310:OLC:C10	2.97	0.42
1:B:164:LEU:HD11	4:B:312:BOG:H2'1	2.00	0.42
1:D:87[B]:THR:CG2	1:D:98:ASP:OD2	2.61	0.42
2:C:318:OLC:C24	1:D:139:ARG:NH1	2.83	0.42
5:D:317:RET:H7	5:D:317:RET:H181	1.84	0.42
1:A:60:SER:CB	7:A:401:HOH:O	2.67	0.41
1:A:88:PHE:CZ	1:A:93:GLY:HA2	2.54	0.41
1:B:74:LEU:HD22	1:B:74:LEU:HA	1.84	0.41
1:D:101:GLY:O	1:D:102:ASP:HB2	2.20	0.41
1:E:159:TYR:CZ	2:E:308:OLC:H21A	2.56	0.41
1:B:88:PHE:CZ	1:B:93:GLY:HA2	2.55	0.41
7:C:439:HOH:O	1:D:55:LYS:HE3	2.20	0.41
1:A:140:ASN:HD22	2:A:303:OLC:H21	1.86	0.41
1:D:114:LEU:O	1:D:118:PRO:HG2	2.20	0.41
1:D:170:TRP:CZ2	2:D:305:OLC:H3A	2.56	0.41
1:E:141:GLN:HG2	2:E:305:OLC:H5A	2.02	0.41
3:B:314:LFA:C1	3:E:301:LFA:C1	2.99	0.41
1:B:78[B]:GLN:HA	1:B:78[B]:GLN:OE1	2.21	0.41
1:A:216:THR:O	1:A:219:PRO:HG2	2.21	0.41
3:B:314:LFA:H11	3:E:301:LFA:H12	2.03	0.41
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.97	0.41
1:B:270:SER:HB3	1:B:273:LYS:HG2	2.02	0.41
5:C:317:RET:C8	5:C:317:RET:H171	2.51	0.41
1:C:114:LEU:O	1:C:118:PRO:HG2	2.21	0.40
1:B:274:GLU:O	1:B:275:LEU:HB3	2.21	0.40
1:E:235:TYR:CG	4:E:316:BOG:H62	2.56	0.40
1:A:51:LYS:CD	7:A:469:HOH:O	2.68	0.40
3:D:313:LFA:H151	2:E:302:OLC:H21A	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/273 (101%)	269 (98%)	6 (2%)	0	100	100
1	B	275/273 (101%)	267 (97%)	8 (3%)	0	100	100
1	C	274/273 (100%)	268 (98%)	6 (2%)	0	100	100
1	D	275/273 (101%)	270 (98%)	5 (2%)	0	100	100
1	E	275/273 (101%)	269 (98%)	6 (2%)	0	100	100
All	All	1374/1365 (101%)	1343 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/234 (99%)	228 (98%)	4 (2%)	53	60
1	B	234/234 (100%)	229 (98%)	5 (2%)	47	52
1	C	231/234 (99%)	227 (98%)	4 (2%)	53	60
1	D	232/234 (99%)	229 (99%)	3 (1%)	61	68
1	E	233/234 (100%)	230 (99%)	3 (1%)	61	68
All	All	1162/1170 (99%)	1143 (98%)	19 (2%)	53	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	103	LEU
1	A	230	VAL
1	A	273	LYS
1	B	92	VAL
1	B	103	LEU
1	B	164	LEU
1	B	230	VAL
1	B	272	ASN
1	C	92	VAL
1	C	189	ILE
1	C	230	VAL
1	C	275	LEU
1	D	92	VAL
1	D	230	VAL
1	D	273	LYS
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	141	GLN
1	B	3	GLN
1	B	61	ASN
1	B	272	ASN
1	C	3	GLN
1	C	61	ASN
1	C	123	GLN
1	C	163	ASN
1	D	141	GLN
1	E	3	GLN
1	E	123	GLN
1	E	141	GLN

5.3.3 RNA ⓘ

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 96 ligands modelled in this entry, 10 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	B	301	-	21,21,24	1.00	1 (4%)	22,22,25	0.91	1 (4%)
2	OLC	B	304	-	19,19,24	1.06	1 (5%)	20,20,25	0.99	2 (10%)
2	OLC	E	302	-	24,24,24	0.94	1 (4%)	25,25,25	0.90	1 (4%)
3	LFA	A	319	-	8,8,19	0.09	0	7,7,18	0.08	0
2	OLC	D	306	-	17,17,24	1.14	1 (5%)	17,17,25	0.89	1 (5%)
2	OLC	E	309	-	5,5,24	0.32	0	4,4,25	0.34	0
3	LFA	B	311	-	6,6,19	0.09	0	5,5,18	0.08	0
3	LFA	A	318	-	19,19,19	0.10	0	18,18,18	0.11	0
2	OLC	A	308	-	15,15,24	1.22	1 (6%)	16,16,25	1.03	1 (6%)
2	OLC	C	305	-	22,22,24	0.95	1 (4%)	23,23,25	0.95	1 (4%)
2	OLC	A	316	-	18,18,24	1.09	1 (5%)	18,18,25	0.82	0
3	LFA	D	311	-	19,19,19	0.07	0	18,18,18	0.05	0
3	LFA	B	302	-	19,19,19	0.10	0	18,18,18	0.10	0
2	OLC	E	306	-	19,19,24	1.04	1 (5%)	20,20,25	1.03	2 (10%)
2	OLC	E	307	-	14,14,24	1.21	1 (7%)	15,15,25	1.07	1 (6%)
2	OLC	D	303	-	12,12,24	1.31	1 (8%)	13,13,25	1.06	1 (7%)
2	OLC	E	310	-	21,21,24	1.03	1 (4%)	22,22,25	0.89	1 (4%)
3	LFA	E	313	-	13,13,19	0.08	0	12,12,18	0.06	0
4	BOG	A	315	-	20,20,20	0.54	0	25,25,25	0.60	0
2	OLC	C	307	-	19,19,24	1.05	1 (5%)	20,20,25	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	B	307	-	6,6,24	0.44	0	5,5,25	0.52	0
2	OLC	C	318	-	17,17,24	1.11	1 (5%)	18,18,25	1.03	1 (5%)
2	OLC	D	305	-	17,17,24	1.11	1 (5%)	18,18,25	1.17	2 (11%)
2	OLC	E	308	-	14,14,24	1.16	1 (7%)	15,15,25	1.00	2 (13%)
2	OLC	D	304	-	24,24,24	0.93	1 (4%)	25,25,25	0.84	1 (4%)
3	LFA	E	315	-	4,4,19	0.13	0	3,3,18	0.21	0
3	LFA	C	315	-	3,3,19	0.22	0	2,2,18	0.43	0
2	OLC	D	308	-	6,6,24	0.35	0	5,5,25	0.37	0
3	LFA	D	312	-	7,7,19	0.10	0	6,6,18	0.08	0
2	OLC	E	304	-	7,7,24	0.30	0	6,6,25	0.38	0
2	OLC	A	307	-	6,6,24	0.27	0	5,5,25	0.46	0
3	LFA	D	310	-	19,19,19	0.07	0	18,18,18	0.03	0
2	OLC	A	317	-	19,19,24	1.11	1 (5%)	19,19,25	0.85	0
2	OLC	D	309	-	24,24,24	0.93	1 (4%)	25,25,25	0.82	1 (4%)
5	RET	C	317	1	20,20,21	2.37	4 (20%)	27,27,28	1.08	1 (3%)
2	OLC	A	304	-	12,12,24	1.30	1 (8%)	13,13,25	1.25	2 (15%)
3	LFA	D	314	-	6,6,19	0.10	0	5,5,18	0.09	0
3	LFA	C	312	-	7,7,19	0.09	0	6,6,18	0.08	0
4	BOG	E	316	-	20,20,20	0.54	0	25,25,25	0.56	0
5	RET	D	317	1	20,20,21	2.26	3 (15%)	27,27,28	1.17	2 (7%)
2	OLC	E	311	-	19,19,24	1.08	1 (5%)	20,20,25	0.95	1 (5%)
3	LFA	E	301	-	13,13,19	0.07	0	12,12,18	0.06	0
3	LFA	C	311	-	6,6,19	0.11	0	5,5,18	0.07	0
3	LFA	A	311	-	7,7,19	0.09	0	6,6,18	0.07	0
3	LFA	B	309	-	7,7,19	0.10	0	6,6,18	0.07	0
2	OLC	A	301	-	8,8,24	0.36	0	7,7,25	0.56	0
2	OLC	C	308	-	21,21,24	1.02	1 (4%)	22,22,25	0.94	1 (4%)
3	LFA	D	313	-	16,16,19	0.08	0	15,15,18	0.08	0
3	LFA	D	315	-	5,5,19	0.12	0	4,4,18	0.12	0
3	LFA	B	308	-	8,8,19	0.10	0	7,7,18	0.08	0
3	LFA	C	314	-	5,5,19	0.11	0	4,4,18	0.12	0
3	LFA	A	314	-	15,15,19	0.08	0	14,14,18	0.06	0
2	OLC	A	306	-	14,14,24	1.20	1 (7%)	15,15,25	1.11	2 (13%)
5	RET	E	317	1	20,20,21	2.36	4 (20%)	27,27,28	1.21	3 (11%)
2	OLC	C	303	-	11,11,24	1.43	1 (9%)	12,12,25	1.08	1 (8%)
3	LFA	E	314	-	3,3,19	0.20	0	2,2,18	0.45	0
3	LFA	C	313	-	19,19,19	0.08	0	18,18,18	0.04	0
5	RET	A	320	1	20,20,21	2.46	4 (20%)	27,27,28	1.15	3 (11%)
2	OLC	C	310	-	6,6,24	0.29	0	5,5,25	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	A	305	-	24,24,24	0.99	1 (4%)	25,25,25	0.91	1 (4%)
3	LFA	E	303	-	19,19,19	0.11	0	18,18,18	0.11	0
3	LFA	A	309	-	6,6,19	0.11	0	5,5,18	0.08	0
4	BOG	B	312	-	20,20,20	0.56	1 (5%)	25,25,25	0.67	0
3	LFA	C	304	-	19,19,19	0.08	0	18,18,18	0.10	0
2	OLC	C	309	-	15,15,24	1.17	1 (6%)	16,16,25	0.87	1 (6%)
3	LFA	B	310	-	9,9,19	0.08	0	8,8,18	0.08	0
3	LFA	A	313	-	5,5,19	0.12	0	4,4,18	0.11	0
3	LFA	E	312	-	7,7,19	0.09	0	6,6,18	0.08	0
2	OLC	D	302	-	15,15,24	1.25	1 (6%)	16,16,25	1.11	2 (12%)
2	OLC	B	306	-	15,15,24	1.14	1 (6%)	16,16,25	1.05	2 (12%)
3	LFA	A	312	-	3,3,19	0.22	0	2,2,18	0.45	0
3	LFA	A	310	-	7,7,19	0.10	0	6,6,18	0.09	0
2	OLC	E	305	-	15,15,24	0.28	0	14,14,25	0.50	0
2	OLC	A	302	-	21,21,24	0.97	1 (4%)	22,22,25	0.93	2 (9%)
2	OLC	B	305	-	20,20,24	1.04	1 (5%)	21,21,25	0.97	1 (4%)
4	BOG	C	316	-	20,20,20	0.53	0	25,25,25	0.61	0
3	LFA	B	314	-	3,3,19	0.20	0	2,2,18	0.45	0
2	OLC	C	301	-	20,20,24	1.01	1 (5%)	21,21,25	0.97	1 (4%)
2	OLC	C	302	-	19,19,24	1.07	1 (5%)	20,20,25	0.94	2 (10%)
4	BOG	D	316	-	20,20,20	0.53	0	25,25,25	0.63	0
2	OLC	D	307	-	13,13,24	1.22	1 (7%)	14,14,25	0.98	2 (14%)
3	LFA	D	301	-	19,19,19	0.10	0	18,18,18	0.12	0
2	OLC	B	303	-	24,24,24	0.95	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	A	303	-	24,24,24	0.97	1 (4%)	25,25,25	0.87	1 (4%)
5	RET	B	313	1	20,20,21	2.46	4 (20%)	27,27,28	1.14	1 (3%)
2	OLC	C	306	-	21,21,24	1.02	1 (4%)	22,22,25	0.94	1 (4%)

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	B	301	-	-	10/21/21/24	-
2	OLC	B	304	-	-	5/19/19/24	-
2	OLC	E	302	-	-	15/24/24/24	-
3	LFA	A	319	-	-	3/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	D	306	-	-	5/15/15/24	-
2	OLC	E	309	-	-	1/3/3/24	-
3	LFA	B	311	-	-	1/4/4/17	-
3	LFA	A	318	-	-	10/17/17/17	-
2	OLC	A	308	-	-	6/15/15/24	-
2	OLC	C	305	-	-	11/22/22/24	-
2	OLC	A	316	-	-	6/16/16/24	-
3	LFA	D	311	-	-	9/17/17/17	-
3	LFA	B	302	-	-	6/17/17/17	-
2	OLC	E	306	-	-	5/19/19/24	-
2	OLC	E	307	-	-	6/14/14/24	-
2	OLC	D	303	-	-	4/12/12/24	-
2	OLC	E	310	-	-	7/21/21/24	-
3	LFA	E	313	-	-	4/11/11/17	-
4	BOG	A	315	-	-	3/11/31/31	0/1/1/1
2	OLC	C	307	-	-	4/19/19/24	-
2	OLC	B	307	-	-	2/4/4/24	-
2	OLC	C	318	-	-	6/17/17/24	-
2	OLC	D	305	-	-	7/17/17/24	-
2	OLC	E	308	-	-	10/14/14/24	-
2	OLC	D	304	-	-	10/24/24/24	-
3	LFA	E	315	-	-	1/2/2/17	-
3	LFA	C	315	-	-	1/1/1/17	-
2	OLC	D	308	-	-	3/4/4/24	-
3	LFA	D	312	-	-	4/5/5/17	-
2	OLC	E	304	-	-	2/5/5/24	-
2	OLC	A	307	-	-	3/4/4/24	-
3	LFA	D	310	-	-	11/17/17/17	-
2	OLC	A	317	-	-	8/17/17/24	-
2	OLC	D	309	-	-	13/24/24/24	-
5	RET	C	317	1	-	2/13/30/31	0/1/1/1
2	OLC	A	304	-	-	0/12/12/24	-
3	LFA	D	314	-	-	3/4/4/17	-
3	LFA	C	312	-	-	5/5/5/17	-
4	BOG	E	316	-	-	9/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	RET	D	317	1	-	2/13/30/31	0/1/1/1
2	OLC	E	311	-	-	12/19/19/24	-
3	LFA	E	301	-	-	4/11/11/17	-
3	LFA	C	311	-	-	2/4/4/17	-
3	LFA	A	311	-	-	2/5/5/17	-
3	LFA	B	309	-	-	3/5/5/17	-
2	OLC	A	301	-	-	4/6/6/24	-
2	OLC	C	308	-	-	11/21/21/24	-
3	LFA	D	313	-	-	10/14/14/17	-
3	LFA	D	315	-	-	1/3/3/17	-
3	LFA	B	308	-	-	2/6/6/17	-
3	LFA	C	314	-	-	0/3/3/17	-
3	LFA	A	314	-	-	9/13/13/17	-
2	OLC	A	306	-	-	8/14/14/24	-
5	RET	E	317	1	-	3/13/30/31	0/1/1/1
2	OLC	C	303	-	-	5/11/11/24	-
3	LFA	E	314	-	-	1/1/1/17	-
3	LFA	C	313	-	-	13/17/17/17	-
5	RET	A	320	1	-	2/13/30/31	0/1/1/1
2	OLC	C	310	-	-	3/4/4/24	-
2	OLC	A	305	-	-	17/24/24/24	-
3	LFA	E	303	-	-	11/17/17/17	-
3	LFA	A	309	-	-	2/4/4/17	-
4	BOG	B	312	-	-	5/11/31/31	0/1/1/1
3	LFA	C	304	-	-	12/17/17/17	-
2	OLC	C	309	-	-	6/15/15/24	-
3	LFA	B	310	-	-	3/7/7/17	-
3	LFA	A	313	-	-	2/3/3/17	-
3	LFA	E	312	-	-	2/5/5/17	-
2	OLC	D	302	-	-	8/15/15/24	-
2	OLC	B	306	-	-	3/15/15/24	-
3	LFA	A	312	-	-	0/1/1/17	-
3	LFA	A	310	-	-	1/5/5/17	-
2	OLC	E	305	-	-	7/13/13/24	-
2	OLC	A	302	-	-	10/21/21/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	305	-	-	11/20/20/24	-
4	BOG	C	316	-	-	3/11/31/31	0/1/1/1
3	LFA	B	314	-	-	0/1/1/17	-
2	OLC	C	301	-	-	7/20/20/24	-
2	OLC	C	302	-	-	9/19/19/24	-
4	BOG	D	316	-	-	4/11/31/31	0/1/1/1
2	OLC	D	307	-	-	7/13/13/24	-
3	LFA	D	301	-	-	7/17/17/17	-
2	OLC	B	303	-	-	12/24/24/24	-
2	OLC	A	303	-	-	12/24/24/24	-
5	RET	B	313	1	-	2/13/30/31	0/1/1/1
2	OLC	C	306	-	-	6/21/21/24	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	320	RET	C14-C13	9.54	1.40	1.33
5	B	313	RET	C14-C13	9.50	1.40	1.33
5	C	317	RET	C14-C13	9.14	1.40	1.33
5	E	317	RET	C14-C13	9.02	1.39	1.33
5	D	317	RET	C14-C13	8.61	1.39	1.33
2	A	317	OLC	O20-C1	4.72	1.46	1.30
2	D	302	OLC	O20-C1	4.62	1.46	1.33
2	D	306	OLC	O20-C1	4.56	1.45	1.30
2	A	305	OLC	O20-C1	4.54	1.46	1.33
2	C	303	OLC	O20-C1	4.54	1.46	1.33
2	A	308	OLC	O20-C1	4.53	1.46	1.33
2	A	316	OLC	O20-C1	4.52	1.45	1.30
2	A	303	OLC	O20-C1	4.47	1.46	1.33
2	E	310	OLC	O20-C1	4.44	1.46	1.33
2	E	311	OLC	O20-C1	4.44	1.46	1.33
2	C	306	OLC	O20-C1	4.42	1.46	1.33
2	C	308	OLC	O20-C1	4.42	1.46	1.33
2	B	305	OLC	O20-C1	4.42	1.46	1.33
2	C	302	OLC	O20-C1	4.38	1.46	1.33
2	E	302	OLC	O20-C1	4.36	1.46	1.33
2	E	307	OLC	O20-C1	4.36	1.46	1.33
2	C	307	OLC	O20-C1	4.36	1.46	1.33
2	D	303	OLC	O20-C1	4.35	1.46	1.33
2	E	306	OLC	O20-C1	4.35	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	304	OLC	O20-C1	4.33	1.46	1.33
2	B	303	OLC	O20-C1	4.33	1.46	1.33
2	D	305	OLC	O20-C1	4.33	1.46	1.33
2	A	304	OLC	O20-C1	4.33	1.46	1.33
2	C	309	OLC	O20-C1	4.32	1.45	1.33
2	C	301	OLC	O20-C1	4.32	1.45	1.33
2	C	318	OLC	O20-C1	4.31	1.45	1.33
2	B	301	OLC	O20-C1	4.30	1.45	1.33
2	D	309	OLC	O20-C1	4.29	1.45	1.33
2	D	304	OLC	O20-C1	4.28	1.45	1.33
2	A	306	OLC	O20-C1	4.23	1.45	1.33
2	C	305	OLC	O20-C1	4.16	1.45	1.33
2	B	306	OLC	O20-C1	4.15	1.45	1.33
2	D	307	OLC	O20-C1	4.14	1.45	1.33
2	A	302	OLC	O20-C1	4.10	1.45	1.33
2	E	308	OLC	O20-C1	4.07	1.45	1.33
5	A	320	RET	C10-C9	2.57	1.41	1.35
5	C	317	RET	C10-C9	2.52	1.41	1.35
5	B	313	RET	C12-C13	-2.50	1.40	1.46
5	C	317	RET	C8-C9	-2.45	1.40	1.46
5	D	317	RET	C10-C9	2.44	1.41	1.35
5	A	320	RET	C8-C9	-2.42	1.40	1.46
5	E	317	RET	C10-C9	2.37	1.41	1.35
5	B	313	RET	C8-C9	-2.36	1.40	1.46
5	E	317	RET	C8-C9	-2.32	1.41	1.46
5	B	313	RET	C10-C9	2.27	1.41	1.35
5	D	317	RET	C8-C9	-2.18	1.41	1.46
5	A	320	RET	C12-C13	-2.10	1.41	1.46
5	E	317	RET	C12-C13	-2.08	1.41	1.46
4	B	312	BOG	O1-C1	2.03	1.43	1.40
5	C	317	RET	C12-C13	-2.01	1.41	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	317	RET	C19-C9-C10	-3.55	117.06	122.82
5	D	317	RET	C19-C9-C10	-3.53	117.10	122.82
5	B	313	RET	C19-C9-C10	-3.51	117.13	122.82
5	A	320	RET	C19-C9-C10	-3.39	117.33	122.82
2	D	305	OLC	O20-C1-C2	3.30	121.90	111.83
2	A	304	OLC	O20-C1-C2	3.30	121.89	111.83
2	D	302	OLC	O20-C1-C2	3.19	121.56	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	306	OLC	O20-C1-C2	3.19	121.55	111.83
5	C	317	RET	C19-C9-C10	-3.15	117.71	122.82
2	A	305	OLC	O20-C1-C2	3.03	121.07	111.83
2	C	308	OLC	O20-C1-C2	3.02	121.05	111.83
2	A	306	OLC	O20-C1-C2	3.00	120.99	111.83
2	C	301	OLC	O20-C1-C2	3.00	120.99	111.83
2	B	305	OLC	O20-C1-C2	2.98	120.93	111.83
2	A	302	OLC	O20-C1-C2	2.98	120.91	111.83
2	B	303	OLC	O20-C1-C2	2.92	120.74	111.83
2	B	304	OLC	O20-C1-C2	2.92	120.74	111.83
2	E	311	OLC	O20-C1-C2	2.92	120.74	111.83
2	A	308	OLC	O20-C1-C2	2.92	120.73	111.83
2	C	302	OLC	O20-C1-C2	2.91	120.71	111.83
2	C	307	OLC	O20-C1-C2	2.90	120.67	111.83
2	E	307	OLC	O20-C1-C2	2.89	120.65	111.83
2	C	306	OLC	O20-C1-C2	2.86	120.56	111.83
2	C	318	OLC	O20-C1-C2	2.82	120.43	111.83
2	A	303	OLC	O20-C1-C2	2.82	120.42	111.83
2	E	310	OLC	O20-C1-C2	2.79	120.35	111.83
2	B	301	OLC	O20-C1-C2	2.78	120.32	111.83
2	E	302	OLC	O20-C1-C2	2.78	120.30	111.83
2	D	303	OLC	O20-C1-C2	2.74	120.18	111.83
2	C	305	OLC	O20-C1-C2	2.71	120.09	111.83
2	B	306	OLC	O20-C1-C2	2.70	120.07	111.83
2	C	303	OLC	O20-C1-C2	2.69	120.05	111.83
2	D	309	OLC	O20-C1-C2	2.64	119.89	111.83
2	D	307	OLC	O20-C1-C2	2.60	119.77	111.83
2	E	308	OLC	O20-C1-C2	2.58	119.69	111.83
2	D	304	OLC	O20-C1-C2	2.55	119.61	111.83
2	A	302	OLC	O20-C1-O19	-2.50	117.38	123.63
2	A	304	OLC	O20-C1-O19	-2.44	117.54	123.63
2	E	308	OLC	O20-C1-O19	-2.38	117.66	123.63
5	D	317	RET	C8-C9-C10	2.28	122.59	119.01
2	A	306	OLC	O20-C1-O19	-2.24	118.02	123.63
2	C	309	OLC	O20-C1-C2	2.22	118.61	111.83
5	A	320	RET	C8-C9-C10	2.19	122.46	119.01
2	D	305	OLC	O20-C1-O19	-2.17	118.19	123.63
5	E	317	RET	C19-C9-C8	2.17	121.40	118.09
2	B	306	OLC	O20-C1-O19	-2.09	118.39	123.63
2	E	306	OLC	O20-C1-O19	-2.09	118.40	123.63
2	B	304	OLC	O20-C1-O19	-2.08	118.42	123.63
2	C	302	OLC	O20-C1-O19	-2.07	118.45	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	OLC	O20-C1-O19	-2.07	118.46	123.63
5	A	320	RET	C2-C1-C6	2.05	113.42	110.44
2	D	307	OLC	O20-C1-O19	-2.05	118.51	123.63
5	E	317	RET	C2-C1-C6	2.02	113.37	110.44
2	D	306	OLC	O20-C1-C2	2.02	120.38	114.00

There are no chirality outliers.

All (487) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	OLC	C21-C22-C24-O25
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	306	OLC	O20-C21-C22-C24
2	A	308	OLC	C21-C22-C24-O25
2	B	304	OLC	C10-C11-C12-C13
2	C	301	OLC	C21-C22-C24-O25
2	C	302	OLC	C10-C11-C12-C13
2	C	303	OLC	C21-C22-C24-O25
2	C	303	OLC	O20-C21-C22-O23
2	C	306	OLC	O20-C21-C22-C24
2	C	306	OLC	O20-C21-C22-O23
2	C	307	OLC	C21-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	304	OLC	C21-C22-C24-O25
2	D	305	OLC	O20-C21-C22-O23
2	D	307	OLC	C21-C22-C24-O25
2	D	307	OLC	O23-C22-C24-O25
2	D	309	OLC	C21-C22-C24-O25
2	D	309	OLC	O23-C22-C24-O25
2	E	306	OLC	C10-C11-C12-C13
2	E	307	OLC	O20-C21-C22-O23
2	E	308	OLC	O20-C21-C22-C24
2	E	308	OLC	O20-C21-C22-O23
2	E	311	OLC	O20-C21-C22-C24
3	C	315	LFA	C17-C18-C19-C20
3	E	314	LFA	C17-C18-C19-C20
4	E	316	BOG	C2-C1-O1-C1'
5	B	313	RET	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
5	C	317	RET	C20-C13-C14-C15
5	E	317	RET	C20-C13-C14-C15
2	C	305	OLC	O19-C1-O20-C21
2	C	318	OLC	O19-C1-O20-C21
2	D	304	OLC	O19-C1-O20-C21
2	D	304	OLC	C2-C1-O20-C21
2	A	303	OLC	C2-C1-O20-C21
2	B	304	OLC	C2-C1-O20-C21
2	B	306	OLC	C2-C1-O20-C21
2	C	305	OLC	C2-C1-O20-C21
2	C	318	OLC	C2-C1-O20-C21
2	E	308	OLC	C2-C1-O20-C21
2	A	305	OLC	O19-C1-O20-C21
2	A	306	OLC	O19-C1-O20-C21
2	A	306	OLC	C2-C1-O20-C21
2	A	306	OLC	O20-C21-C22-O23
2	E	302	OLC	O20-C21-C22-O23
4	E	316	BOG	O5-C5-C6-O6
2	E	308	OLC	O19-C1-O20-C21
2	A	305	OLC	C2-C1-O20-C21
2	A	303	OLC	O19-C1-O20-C21
2	B	304	OLC	O19-C1-O20-C21
2	B	306	OLC	O19-C1-O20-C21
2	E	302	OLC	C12-C13-C14-C15
2	B	301	OLC	C2-C1-O20-C21
2	C	309	OLC	C2-C1-O20-C21
2	D	302	OLC	C2-C1-O20-C21
2	D	309	OLC	C2-C1-O20-C21
4	E	316	BOG	C4-C5-C6-O6
2	E	311	OLC	O20-C21-C22-O23
2	B	301	OLC	O19-C1-O20-C21
2	C	309	OLC	O19-C1-O20-C21
4	B	312	BOG	O5-C5-C6-O6
2	A	302	OLC	O23-C22-C24-O25
2	A	308	OLC	O23-C22-C24-O25
2	D	304	OLC	O23-C22-C24-O25
2	C	302	OLC	C1-C2-C3-C4
4	B	312	BOG	C4-C5-C6-O6
2	D	307	OLC	C1-C2-C3-C4
2	E	311	OLC	C1-C2-C3-C4
2	D	309	OLC	O19-C1-O20-C21
4	E	316	BOG	O5-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
2	A	303	OLC	C1-C2-C3-C4
2	D	302	OLC	O19-C1-O20-C21
2	B	303	OLC	O20-C21-C22-O23
2	C	302	OLC	O20-C21-C22-O23
2	E	310	OLC	O20-C21-C22-O23
2	E	302	OLC	C1-C2-C3-C4
2	E	305	OLC	C4-C5-C6-C7
2	D	309	OLC	C1-C2-C3-C4
2	B	303	OLC	O20-C21-C22-C24
2	C	302	OLC	O20-C21-C22-C24
2	D	302	OLC	O20-C21-C22-C24
2	E	307	OLC	O20-C21-C22-C24
2	E	310	OLC	O20-C21-C22-C24
4	D	316	BOG	O5-C5-C6-O6
2	A	305	OLC	C21-C22-C24-O25
2	B	305	OLC	C21-C22-C24-O25
2	D	303	OLC	C21-C22-C24-O25
2	E	302	OLC	C21-C22-C24-O25
2	E	308	OLC	C21-C22-C24-O25
4	E	316	BOG	O1-C1'-C2'-C3'
4	D	316	BOG	C4-C5-C6-O6
2	D	303	OLC	C1-C2-C3-C4
4	B	312	BOG	C1'-C2'-C3'-C4'
4	D	316	BOG	C1'-C2'-C3'-C4'
4	A	315	BOG	C1'-C2'-C3'-C4'
2	C	302	OLC	C5-C6-C7-C8
2	E	306	OLC	C5-C6-C7-C8
3	B	309	LFA	C3-C4-C5-C6
3	C	312	LFA	C16-C17-C18-C19
3	D	313	LFA	C5-C6-C7-C8
3	E	313	LFA	C9-C10-C11-C12
2	A	317	OLC	C13-C14-C15-C16
2	E	308	OLC	C2-C3-C4-C5
4	E	316	BOG	C2'-C3'-C4'-C5'
2	A	302	OLC	C3-C4-C5-C6
2	C	301	OLC	C5-C6-C7-C8
2	C	305	OLC	C4-C5-C6-C7
2	B	305	OLC	O23-C22-C24-O25
2	C	301	OLC	O23-C22-C24-O25
2	C	303	OLC	O23-C22-C24-O25
2	C	307	OLC	O23-C22-C24-O25
2	E	302	OLC	O23-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
4	E	316	BOG	C2'-C1'-O1-C1
2	C	305	OLC	C3-C4-C5-C6
2	D	306	OLC	C2-C3-C4-C5
2	A	303	OLC	C13-C14-C15-C16
2	A	307	OLC	C4-C5-C6-C7
2	A	317	OLC	C11-C12-C13-C14
3	D	310	LFA	C6-C7-C8-C9
3	D	312	LFA	C2-C3-C4-C5
2	A	305	OLC	C13-C14-C15-C16
2	D	304	OLC	C4-C5-C6-C7
2	D	309	OLC	C2-C3-C4-C5
3	A	309	LFA	C16-C17-C18-C19
3	A	314	LFA	C10-C11-C12-C13
3	C	312	LFA	C15-C16-C17-C18
3	D	301	LFA	C11-C10-C9-C8
3	E	313	LFA	C13-C14-C15-C16
2	E	304	OLC	C4-C5-C6-C7
3	D	301	LFA	C9-C10-C11-C12
2	A	317	OLC	C5-C6-C7-C8
2	C	306	OLC	C3-C4-C5-C6
2	E	306	OLC	C3-C4-C5-C6
2	A	316	OLC	C6-C7-C8-C9
2	C	302	OLC	C3-C4-C5-C6
3	C	304	LFA	C7-C8-C9-C10
3	D	310	LFA	C2-C3-C4-C5
3	D	310	LFA	C7-C8-C9-C10
2	B	305	OLC	C2-C3-C4-C5
2	C	309	OLC	C3-C4-C5-C6
3	D	311	LFA	C11-C12-C13-C14
3	B	308	LFA	C14-C15-C16-C17
3	A	314	LFA	C4-C5-C6-C7
3	D	301	LFA	C12-C13-C14-C15
2	C	308	OLC	C2-C3-C4-C5
3	D	311	LFA	C14-C15-C16-C17
3	E	301	LFA	C2-C3-C4-C5
2	D	305	OLC	C2-C1-O20-C21
2	C	303	OLC	O20-C21-C22-C24
2	C	310	OLC	C5-C6-C7-C8
2	E	302	OLC	C13-C14-C15-C16
2	A	317	OLC	C12-C13-C14-C15
3	B	302	LFA	C16-C17-C18-C19
3	C	304	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	D	310	LFA	C15-C16-C17-C18
2	C	301	OLC	C4-C5-C6-C7
2	E	310	OLC	C11-C12-C13-C14
3	A	314	LFA	C3-C4-C5-C6
2	B	303	OLC	C4-C5-C6-C7
3	D	313	LFA	C11-C12-C13-C14
3	E	301	LFA	C3-C4-C5-C6
2	A	301	OLC	C7-C8-C9-C10
3	E	313	LFA	C14-C15-C16-C17
2	D	306	OLC	C1-C2-C3-C4
3	D	313	LFA	C7-C8-C9-C10
2	A	305	OLC	C10-C11-C12-C13
2	B	303	OLC	C10-C11-C12-C13
2	D	306	OLC	C10-C11-C12-C13
3	A	310	LFA	C1-C2-C3-C4
2	D	309	OLC	C13-C14-C15-C16
2	A	305	OLC	C4-C5-C6-C7
2	D	309	OLC	C11-C12-C13-C14
3	E	303	LFA	C10-C11-C12-C13
4	C	316	BOG	C1'-C2'-C3'-C4'
3	D	312	LFA	C4-C5-C6-C7
2	E	305	OLC	C5-C6-C7-C8
2	E	311	OLC	C4-C5-C6-C7
3	D	311	LFA	C13-C14-C15-C16
3	B	308	LFA	C16-C17-C18-C19
3	B	309	LFA	C2-C3-C4-C5
3	D	310	LFA	C3-C4-C5-C6
2	B	303	OLC	C1-C2-C3-C4
3	A	311	LFA	C16-C17-C18-C19
2	A	302	OLC	C10-C11-C12-C13
2	C	318	OLC	C6-C7-C8-C9
3	D	314	LFA	C16-C17-C18-C19
2	C	305	OLC	C7-C8-C9-C10
2	E	307	OLC	C4-C5-C6-C7
3	E	301	LFA	C4-C5-C6-C7
2	D	307	OLC	C2-C3-C4-C5
3	C	304	LFA	C13-C14-C15-C16
2	A	305	OLC	C2-C3-C4-C5
2	A	316	OLC	C3-C4-C5-C6
3	A	314	LFA	C7-C8-C9-C10
3	A	318	LFA	C16-C17-C18-C19
2	E	308	OLC	O23-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
2	D	305	OLC	O19-C1-O20-C21
3	B	310	LFA	C5-C6-C7-C8
3	C	313	LFA	C13-C14-C15-C16
4	E	316	BOG	C1'-C2'-C3'-C4'
3	C	311	LFA	C2-C3-C4-C5
3	C	313	LFA	C12-C13-C14-C15
2	A	302	OLC	C6-C7-C8-C9
2	B	307	OLC	C6-C7-C8-C9
2	C	307	OLC	C6-C7-C8-C9
2	E	311	OLC	C6-C7-C8-C9
2	E	302	OLC	C14-C15-C16-C17
2	B	305	OLC	C2-C1-O20-C21
3	A	319	LFA	C3-C4-C5-C6
2	A	305	OLC	C6-C7-C8-C9
2	A	305	OLC	C11-C12-C13-C14
3	A	314	LFA	C11-C12-C13-C14
2	E	306	OLC	C4-C5-C6-C7
3	D	313	LFA	C3-C4-C5-C6
2	A	316	OLC	C11-C12-C13-C14
3	A	318	LFA	C7-C8-C9-C10
3	D	313	LFA	C13-C14-C15-C16
3	E	313	LFA	C15-C16-C17-C18
3	B	311	LFA	C15-C16-C17-C18
3	A	318	LFA	C13-C14-C15-C16
3	E	312	LFA	C16-C17-C18-C19
3	A	313	LFA	C2-C3-C4-C5
3	B	302	LFA	C11-C10-C9-C8
2	C	305	OLC	C12-C13-C14-C15
5	E	317	RET	C10-C11-C12-C13
2	B	301	OLC	C10-C11-C12-C13
2	B	305	OLC	C10-C11-C12-C13
2	C	308	OLC	C6-C7-C8-C9
3	E	303	LFA	C6-C7-C8-C9
2	C	308	OLC	C1-C2-C3-C4
3	D	311	LFA	C4-C5-C6-C7
3	E	303	LFA	C7-C8-C9-C10
3	D	313	LFA	C14-C15-C16-C17
2	A	308	OLC	C2-C1-O20-C21
2	C	301	OLC	C2-C1-O20-C21
3	A	311	LFA	C14-C15-C16-C17
5	A	320	RET	C12-C13-C14-C15
5	B	313	RET	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
5	C	317	RET	C12-C13-C14-C15
5	D	317	RET	C12-C13-C14-C15
5	E	317	RET	C12-C13-C14-C15
3	C	304	LFA	C16-C17-C18-C19
3	B	302	LFA	C6-C7-C8-C9
3	D	310	LFA	C9-C10-C11-C12
2	C	308	OLC	C5-C6-C7-C8
2	E	308	OLC	C3-C4-C5-C6
2	D	308	OLC	C2-C3-C4-C5
3	B	310	LFA	C7-C8-C9-C10
3	D	311	LFA	C1-C2-C3-C4
3	A	318	LFA	C6-C7-C8-C9
3	D	311	LFA	C3-C4-C5-C6
3	E	303	LFA	C9-C10-C11-C12
4	B	312	BOG	C5'-C6'-C7'-C8'
2	A	307	OLC	C6-C7-C8-C9
2	D	304	OLC	C3-C4-C5-C6
2	E	302	OLC	C4-C5-C6-C7
3	C	304	LFA	C15-C16-C17-C18
4	A	315	BOG	C5'-C6'-C7'-C8'
2	C	302	OLC	C4-C5-C6-C7
3	D	310	LFA	C1-C2-C3-C4
3	A	319	LFA	C4-C5-C6-C7
2	A	316	OLC	C14-C15-C16-C17
2	B	307	OLC	C4-C5-C6-C7
3	D	314	LFA	C15-C16-C17-C18
2	A	305	OLC	C14-C15-C16-C17
3	C	313	LFA	C11-C12-C13-C14
2	D	303	OLC	O23-C22-C24-O25
2	D	305	OLC	O20-C21-C22-C24
2	A	317	OLC	C2-C3-C4-C5
2	A	316	OLC	C13-C14-C15-C16
2	A	301	OLC	C10-C11-C12-C13
2	B	303	OLC	C14-C15-C16-C17
2	D	307	OLC	C3-C4-C5-C6
3	C	313	LFA	C9-C10-C11-C12
4	C	316	BOG	C5'-C6'-C7'-C8'
2	A	303	OLC	C15-C16-C17-C18
2	D	303	OLC	C3-C4-C5-C6
5	A	320	RET	C20-C13-C14-C15
5	D	317	RET	C20-C13-C14-C15
2	B	305	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	A	307	OLC	C5-C6-C7-C8
3	C	311	LFA	C4-C5-C6-C7
3	D	301	LFA	C10-C11-C12-C13
3	C	313	LFA	C14-C15-C16-C17
3	C	304	LFA	C3-C4-C5-C6
3	C	313	LFA	C15-C16-C17-C18
3	A	309	LFA	C17-C18-C19-C20
3	C	312	LFA	C17-C18-C19-C20
2	C	310	OLC	C6-C7-C8-C9
2	D	309	OLC	C12-C13-C14-C15
2	C	302	OLC	C6-C7-C8-C9
2	A	305	OLC	C3-C4-C5-C6
3	D	310	LFA	C11-C12-C13-C14
2	B	303	OLC	C5-C6-C7-C8
2	B	303	OLC	C13-C14-C15-C16
2	D	304	OLC	C15-C16-C17-C18
3	D	312	LFA	C1-C2-C3-C4
2	B	301	OLC	C5-C6-C7-C8
2	D	309	OLC	C4-C5-C6-C7
2	A	302	OLC	C2-C3-C4-C5
2	B	305	OLC	O20-C21-C22-C24
2	D	305	OLC	C2-C3-C4-C5
3	A	314	LFA	C5-C6-C7-C8
2	A	308	OLC	O19-C1-O20-C21
3	D	311	LFA	C12-C13-C14-C15
2	C	309	OLC	C2-C3-C4-C5
2	C	305	OLC	C11-C12-C13-C14
2	D	302	OLC	C5-C6-C7-C8
3	D	301	LFA	C7-C8-C9-C10
3	C	304	LFA	C12-C13-C14-C15
2	C	301	OLC	O19-C1-O20-C21
3	D	311	LFA	C10-C11-C12-C13
2	E	311	OLC	C2-C1-O20-C21
2	D	309	OLC	C5-C6-C7-C8
2	E	311	OLC	C2-C3-C4-C5
2	A	303	OLC	C21-C22-C24-O25
2	A	306	OLC	C21-C22-C24-O25
3	D	310	LFA	C17-C18-C19-C20
2	E	305	OLC	C6-C7-C8-C9
2	A	305	OLC	C12-C13-C14-C15
4	E	316	BOG	C5'-C6'-C7'-C8'
3	D	312	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	306	OLC	C5-C6-C7-C8
2	E	311	OLC	C5-C6-C7-C8
2	B	303	OLC	C3-C4-C5-C6
3	C	312	LFA	C13-C14-C15-C16
3	C	312	LFA	C14-C15-C16-C17
3	E	303	LFA	C4-C5-C6-C7
3	A	318	LFA	C12-C13-C14-C15
2	E	310	OLC	C4-C5-C6-C7
3	E	303	LFA	C15-C16-C17-C18
2	C	306	OLC	C5-C6-C7-C8
2	C	306	OLC	C4-C5-C6-C7
2	D	302	OLC	C6-C7-C8-C9
3	C	313	LFA	C4-C5-C6-C7
3	C	313	LFA	C10-C11-C12-C13
2	C	318	OLC	C1-C2-C3-C4
2	A	303	OLC	C14-C15-C16-C17
2	E	305	OLC	C13-C14-C15-C16
2	C	305	OLC	C6-C7-C8-C9
2	E	311	OLC	O19-C1-O20-C21
3	E	303	LFA	C11-C10-C9-C8
3	B	302	LFA	C10-C11-C12-C13
2	C	307	OLC	C5-C6-C7-C8
3	E	303	LFA	C11-C12-C13-C14
4	D	316	BOG	C3'-C4'-C5'-C6'
2	B	305	OLC	C5-C6-C7-C8
2	A	302	OLC	C5-C6-C7-C8
2	B	304	OLC	C4-C5-C6-C7
3	A	318	LFA	C10-C11-C12-C13
4	B	312	BOG	C3'-C4'-C5'-C6'
3	C	304	LFA	C1-C2-C3-C4
2	D	308	OLC	C5-C6-C7-C8
2	C	308	OLC	C11-C12-C13-C14
2	C	308	OLC	C4-C5-C6-C7
3	D	314	LFA	C14-C15-C16-C17
2	D	306	OLC	C5-C6-C7-C8
2	B	305	OLC	C7-C8-C9-C10
2	E	306	OLC	C9-C10-C11-C12
3	A	318	LFA	C11-C12-C13-C14
3	B	302	LFA	C9-C10-C11-C12
2	C	318	OLC	C2-C3-C4-C5
2	A	303	OLC	C9-C10-C11-C12
2	E	302	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	318	LFA	C14-C15-C16-C17
3	A	318	LFA	C11-C10-C9-C8
4	C	316	BOG	C3'-C4'-C5'-C6'
2	D	308	OLC	C4-C5-C6-C7
2	A	305	OLC	O23-C22-C24-O25
2	E	307	OLC	O23-C22-C24-O25
2	C	310	OLC	C3-C4-C5-C6
2	E	309	OLC	C3-C4-C5-C6
2	C	309	OLC	C4-C5-C6-C7
2	A	305	OLC	C15-C16-C17-C18
2	C	309	OLC	C6-C7-C8-C9
2	B	304	OLC	C9-C10-C11-C12
2	E	302	OLC	C7-C8-C9-C10
2	E	311	OLC	C9-C10-C11-C12
2	A	308	OLC	C1-C2-C3-C4
2	D	305	OLC	C3-C4-C5-C6
2	E	310	OLC	C1-C2-C3-C4
3	D	313	LFA	C2-C3-C4-C5
2	C	303	OLC	C1-C2-C3-C4
3	A	314	LFA	C13-C14-C15-C16
2	E	311	OLC	C3-C4-C5-C6
2	C	308	OLC	C10-C11-C12-C13
2	B	301	OLC	C6-C7-C8-C9
2	D	304	OLC	C13-C14-C15-C16
2	B	301	OLC	O20-C21-C22-C24
3	D	313	LFA	C11-C10-C9-C8
3	C	313	LFA	C7-C8-C9-C10
2	E	310	OLC	C7-C8-C9-C10
2	B	305	OLC	C4-C5-C6-C7
2	D	305	OLC	C5-C6-C7-C8
3	E	312	LFA	C17-C18-C19-C20
2	A	301	OLC	C11-C12-C13-C14
2	A	317	OLC	C7-C8-C9-C10
3	C	313	LFA	C11-C10-C9-C8
3	C	304	LFA	C14-C15-C16-C17
3	A	319	LFA	C1-C2-C3-C4
2	B	306	OLC	C5-C6-C7-C8
2	E	302	OLC	C3-C4-C5-C6
3	E	315	LFA	C17-C18-C19-C20
2	A	305	OLC	C9-C10-C11-C12
2	C	318	OLC	C7-C8-C9-C10
2	D	304	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
3	C	313	LFA	C6-C7-C8-C9
2	A	306	OLC	O23-C22-C24-O25
3	E	303	LFA	C17-C18-C19-C20
2	A	308	OLC	C3-C4-C5-C6
3	D	301	LFA	C3-C4-C5-C6
3	D	311	LFA	C5-C6-C7-C8
2	C	308	OLC	C7-C8-C9-C10
3	D	310	LFA	C16-C17-C18-C19
2	C	305	OLC	C10-C11-C12-C13
3	D	301	LFA	C4-C5-C6-C7
3	A	314	LFA	C11-C10-C9-C8
2	E	304	OLC	C2-C3-C4-C5
3	E	303	LFA	C5-C6-C7-C8
3	E	303	LFA	C14-C15-C16-C17
2	B	303	OLC	C7-C8-C9-C10
2	D	302	OLC	C4-C5-C6-C7
2	E	305	OLC	C7-C8-C9-C10
3	C	304	LFA	C4-C5-C6-C7
3	D	315	LFA	C3-C4-C5-C6
3	A	313	LFA	C1-C2-C3-C4
2	A	301	OLC	C9-C10-C11-C12
2	D	304	OLC	C9-C10-C11-C12
2	E	302	OLC	O20-C21-C22-C24
3	C	313	LFA	C16-C17-C18-C19
2	A	303	OLC	C7-C8-C9-C10
2	B	301	OLC	C7-C8-C9-C10
2	C	301	OLC	C7-C8-C9-C10
2	D	309	OLC	C7-C8-C9-C10
2	D	302	OLC	C1-C2-C3-C4
2	A	317	OLC	C9-C10-C11-C12
2	E	305	OLC	C9-C10-C11-C12
3	A	318	LFA	C2-C3-C4-C5
2	B	305	OLC	O20-C21-C22-O23
3	B	309	LFA	C5-C6-C7-C8
3	B	310	LFA	C1-C2-C3-C4
2	E	308	OLC	C4-C5-C6-C7
2	A	302	OLC	C9-C10-C11-C12
3	C	313	LFA	C3-C4-C5-C6
3	D	310	LFA	C14-C15-C16-C17
2	D	309	OLC	C10-C11-C12-C13
3	C	304	LFA	C9-C10-C11-C12
2	D	307	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
2	C	305	OLC	C9-C10-C11-C12
2	D	306	OLC	C7-C8-C9-C10
2	A	303	OLC	O20-C1-C2-C3
2	C	306	OLC	C9-C10-C11-C12
2	B	303	OLC	C6-C7-C8-C9
2	E	302	OLC	O20-C1-C2-C3
2	C	308	OLC	C12-C13-C14-C15
2	B	301	OLC	C3-C4-C5-C6
2	E	307	OLC	C3-C4-C5-C6
2	C	302	OLC	C7-C8-C9-C10
2	A	302	OLC	O20-C1-C2-C3
3	B	302	LFA	C7-C8-C9-C10
2	E	305	OLC	C3-C4-C5-C6
2	E	307	OLC	O20-C1-C2-C3
2	C	305	OLC	C2-C3-C4-C5
2	E	302	OLC	C2-C3-C4-C5
3	C	304	LFA	C17-C18-C19-C20
2	A	316	OLC	C12-C13-C14-C15
2	A	317	OLC	C15-C16-C17-C18
3	E	301	LFA	C6-C7-C8-C9
4	A	315	BOG	C3'-C4'-C5'-C6'
2	A	306	OLC	C2-C3-C4-C5
3	A	314	LFA	C9-C10-C11-C12
3	D	313	LFA	C4-C5-C6-C7
2	E	308	OLC	C5-C6-C7-C8
2	E	302	OLC	O19-C1-C2-C3
2	A	302	OLC	O19-C1-C2-C3
2	E	311	OLC	O23-C22-C24-O25
2	D	307	OLC	C4-C5-C6-C7
2	A	303	OLC	O19-C1-C2-C3
2	B	301	OLC	C11-C12-C13-C14
2	B	301	OLC	C12-C13-C14-C15
2	B	303	OLC	C9-C10-C11-C12
3	D	313	LFA	C6-C7-C8-C9
2	E	310	OLC	O20-C1-C2-C3

There are no ring outliers.

32 monomers are involved in 63 short contacts:

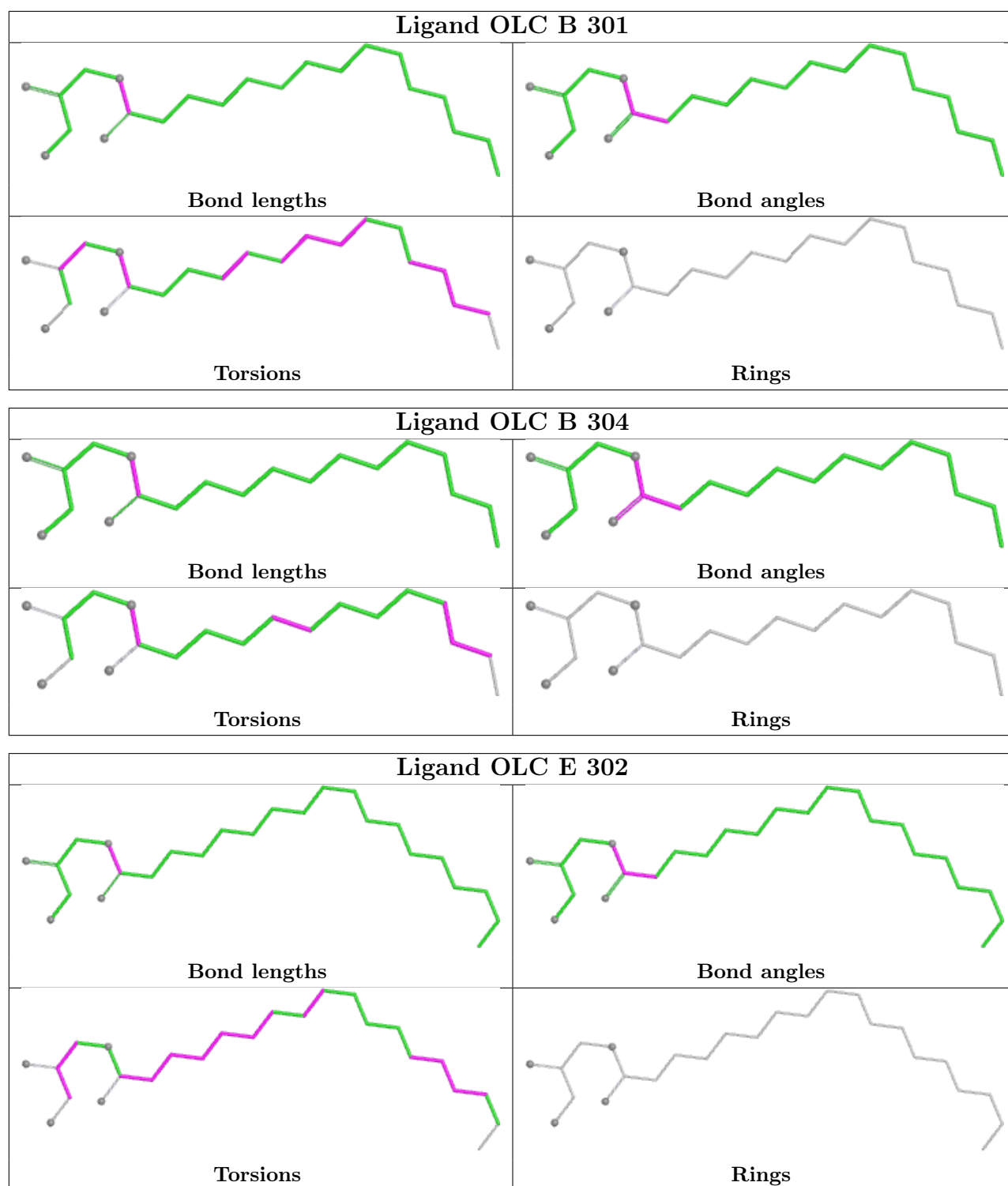
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	OLC	2	0
2	E	302	OLC	2	0

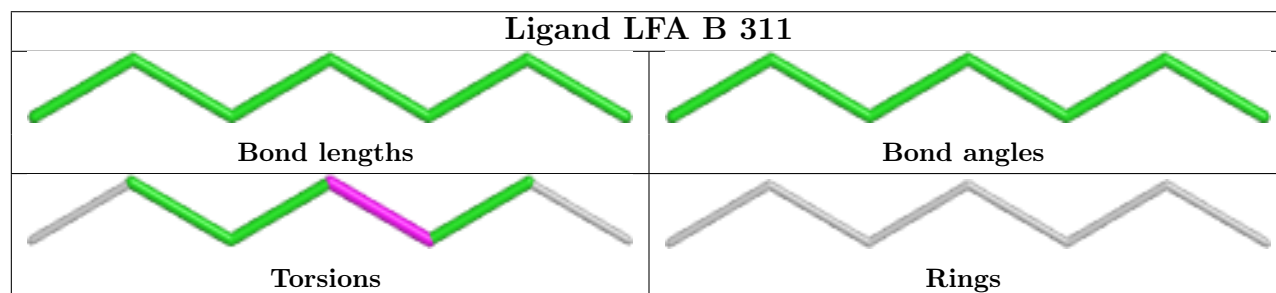
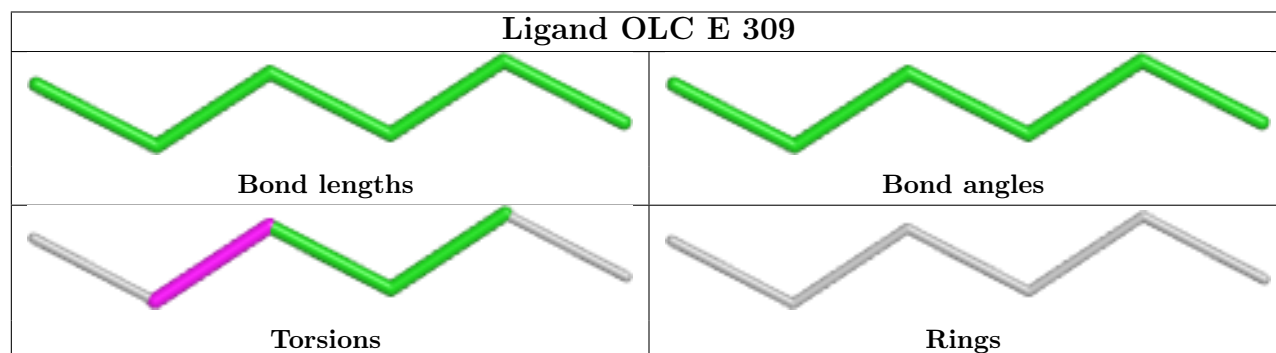
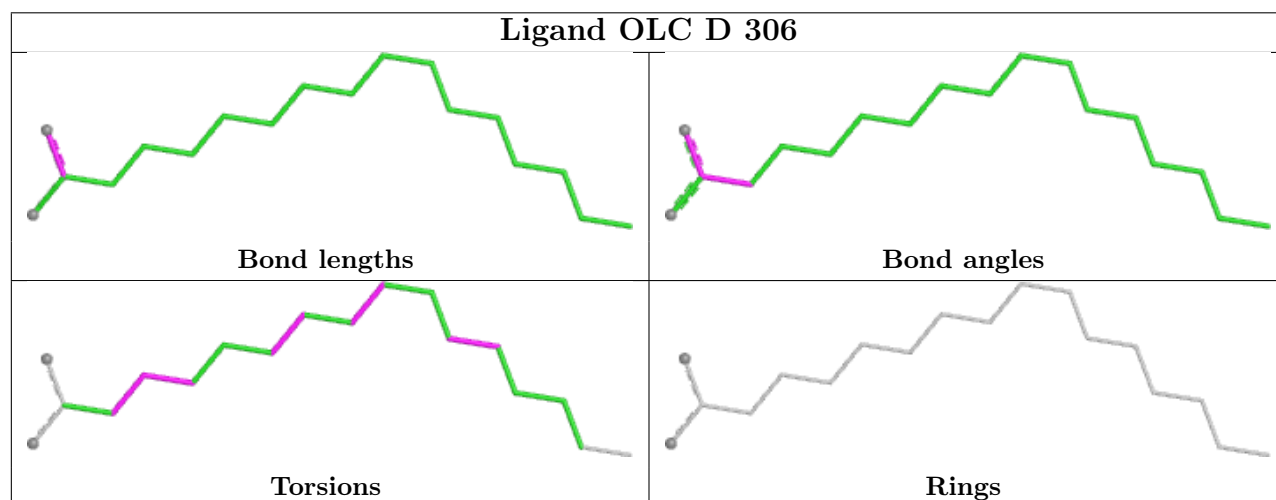
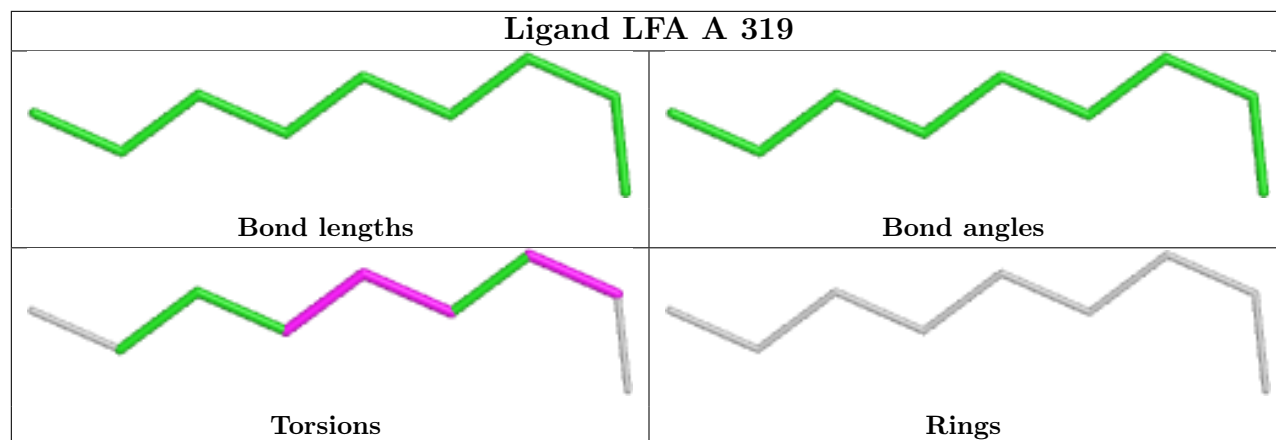
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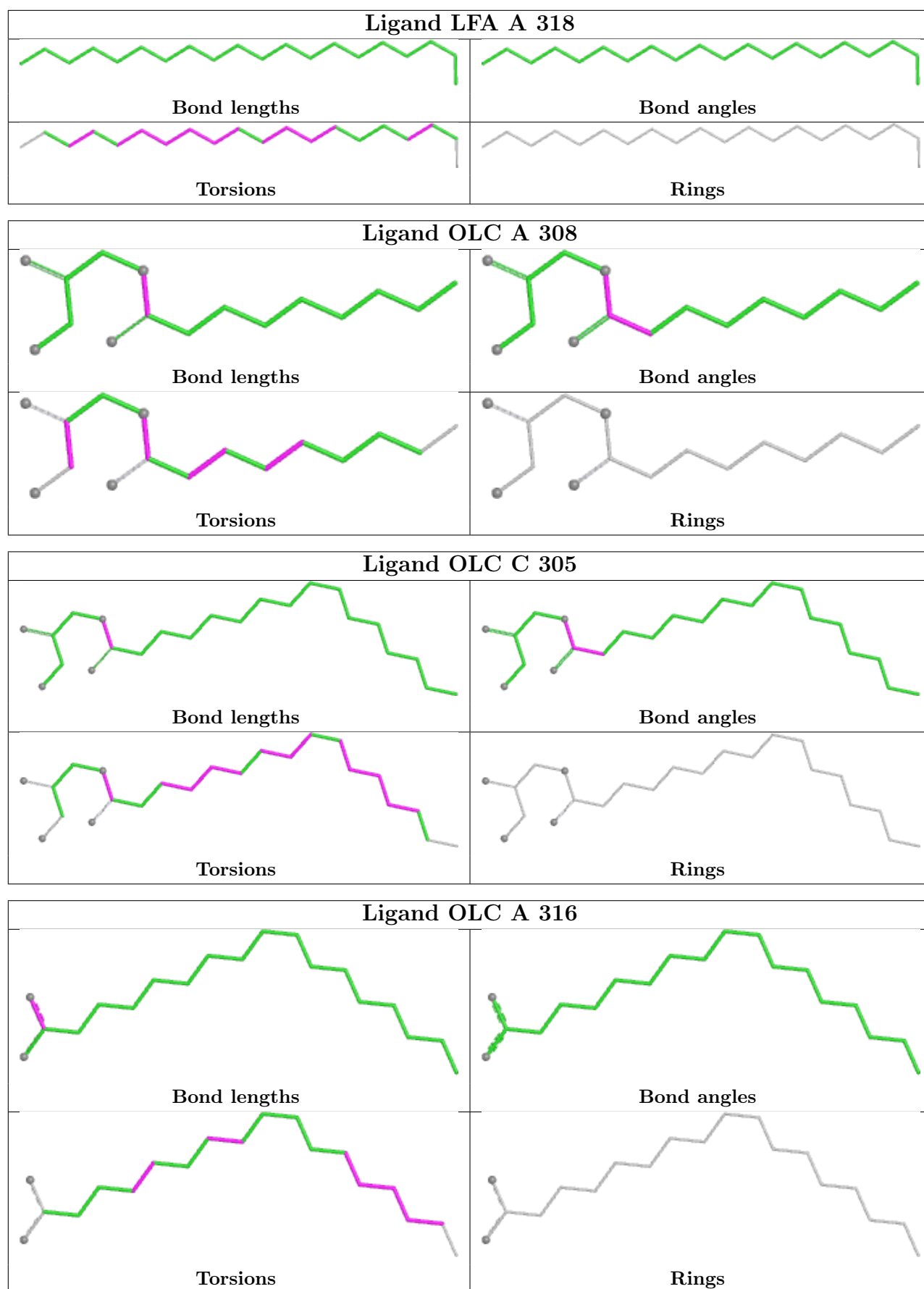
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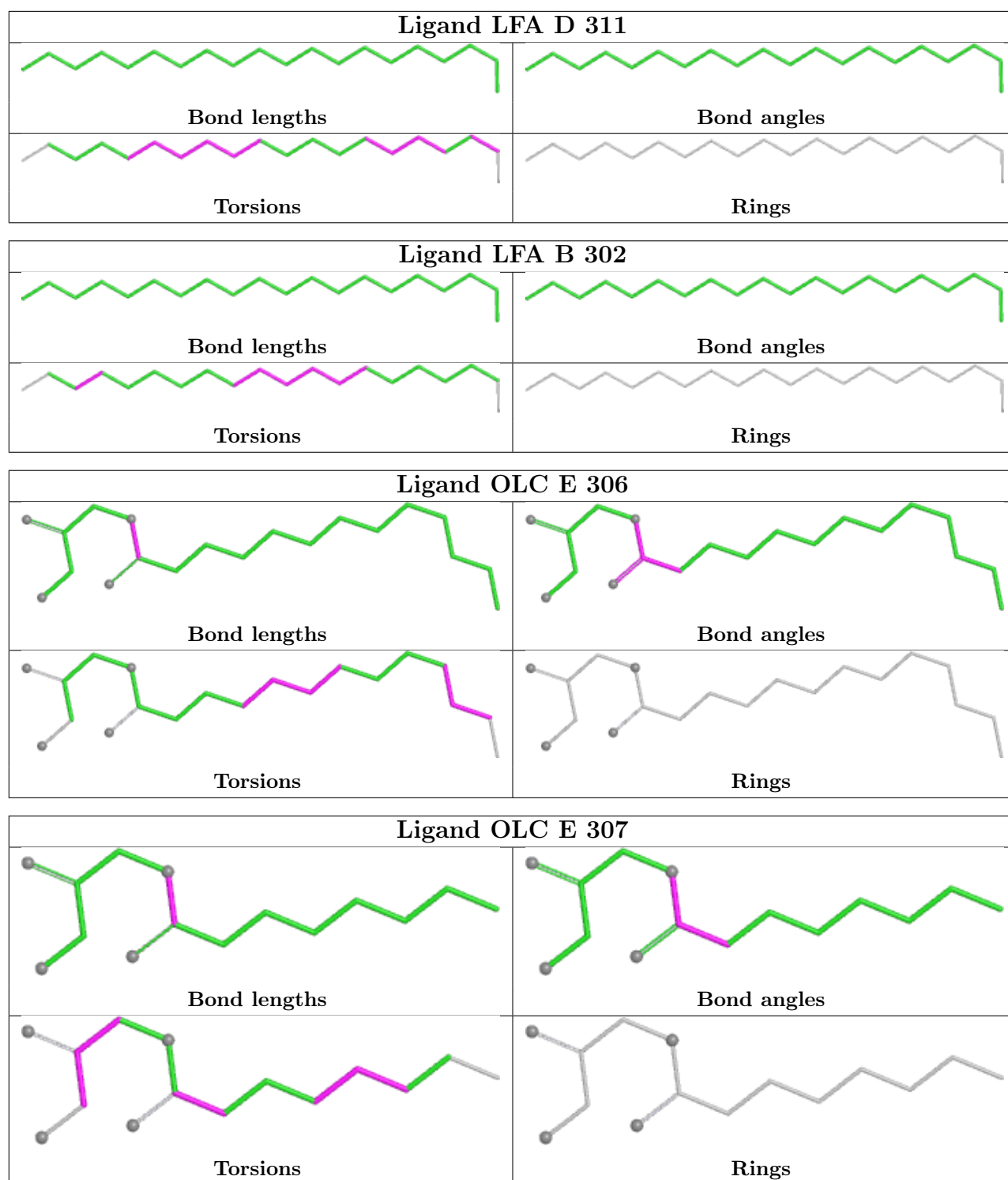
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	305	OLC	3	0
2	A	316	OLC	1	0
2	E	310	OLC	1	0
4	A	315	BOG	2	0
2	C	318	OLC	4	0
2	D	305	OLC	1	0
2	E	308	OLC	2	0
2	D	304	OLC	1	0
2	D	309	OLC	3	0
5	C	317	RET	4	0
4	E	316	BOG	4	0
5	D	317	RET	3	0
3	E	301	LFA	3	0
3	C	311	LFA	4	0
3	D	313	LFA	3	0
3	B	308	LFA	2	0
5	E	317	RET	3	0
3	C	313	LFA	1	0
5	A	320	RET	3	0
4	B	312	BOG	3	0
3	C	304	LFA	2	0
2	E	305	OLC	2	0
2	A	302	OLC	1	0
4	C	316	BOG	2	0
3	B	314	LFA	3	0
4	D	316	BOG	2	0
3	D	301	LFA	1	0
2	B	303	OLC	1	0
2	A	303	OLC	2	0
5	B	313	RET	2	0

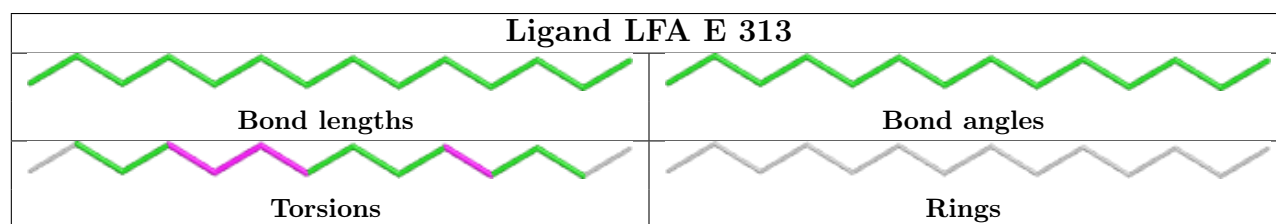
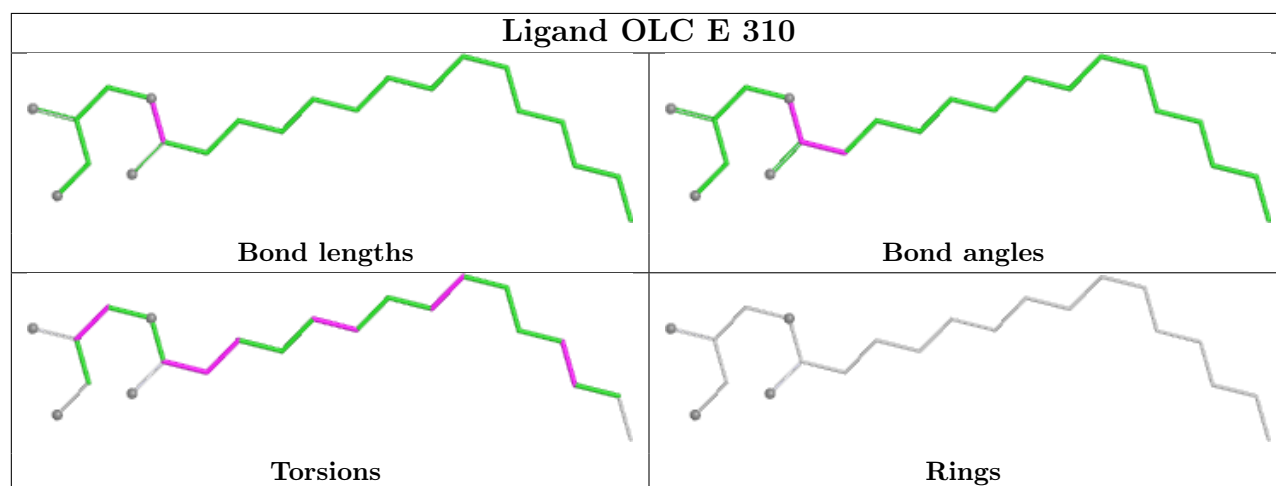
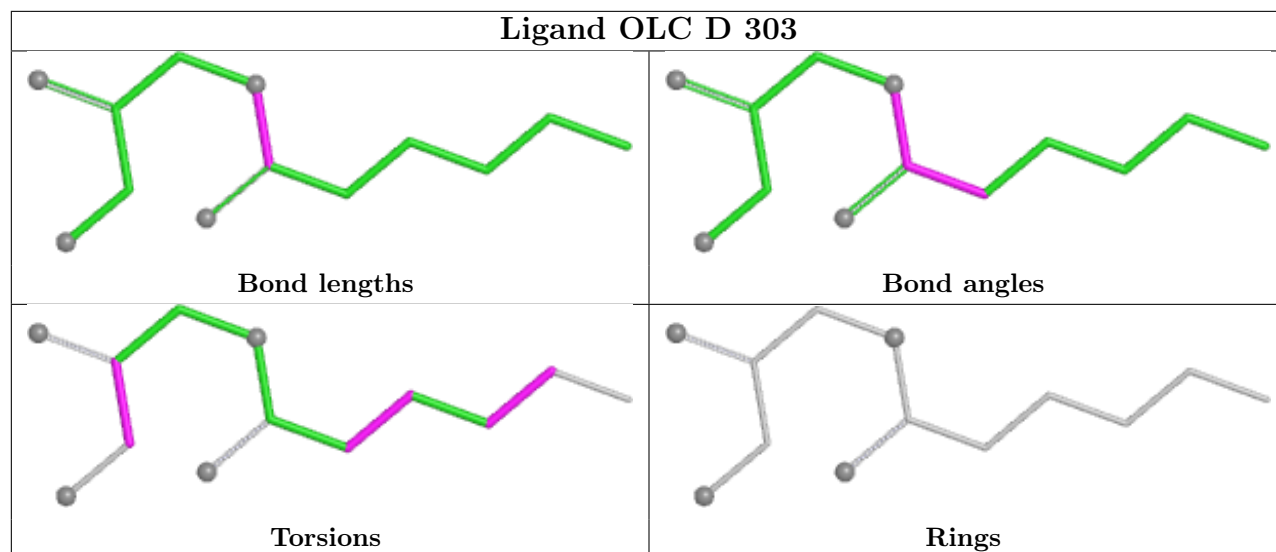
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

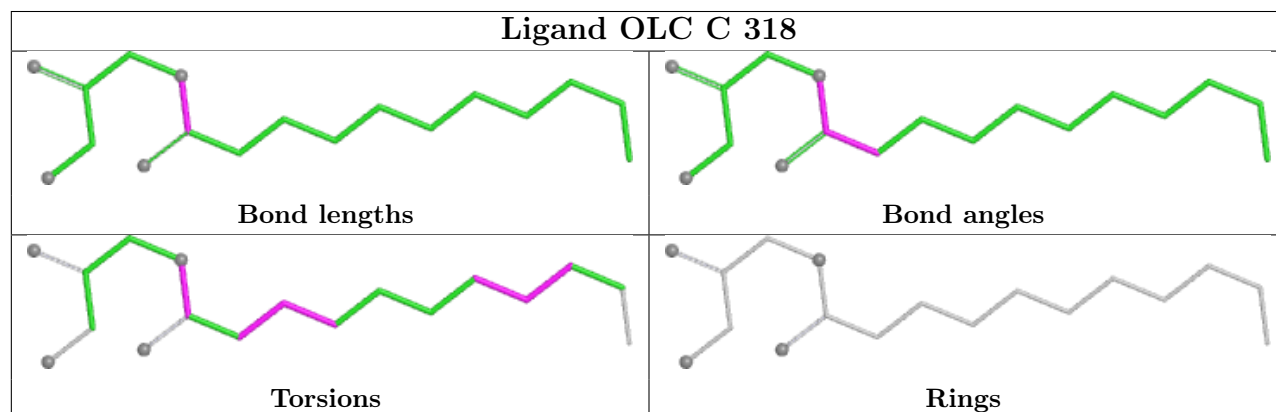
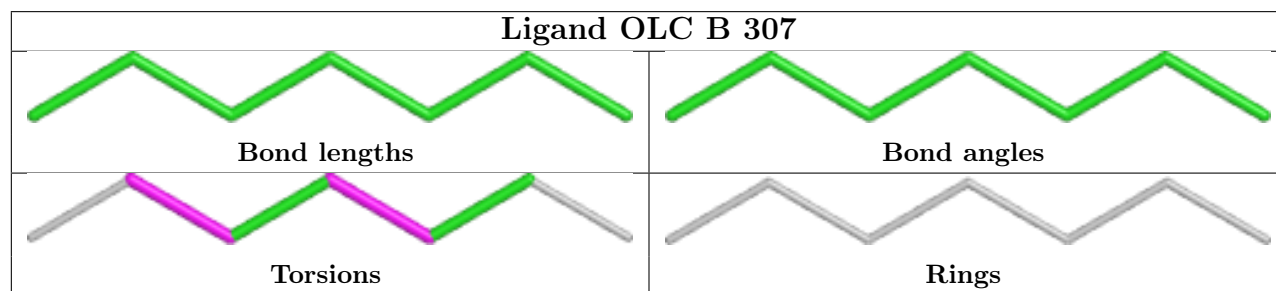
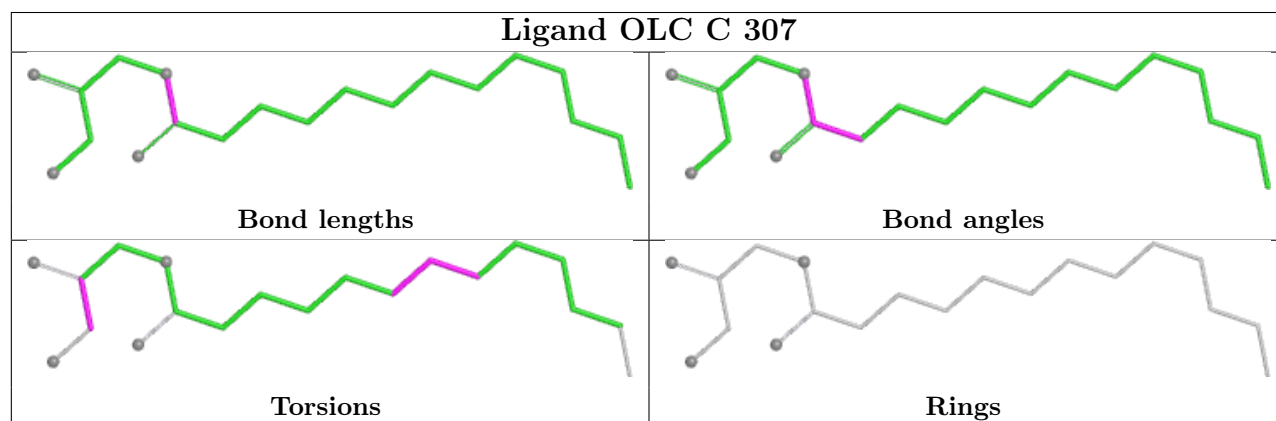
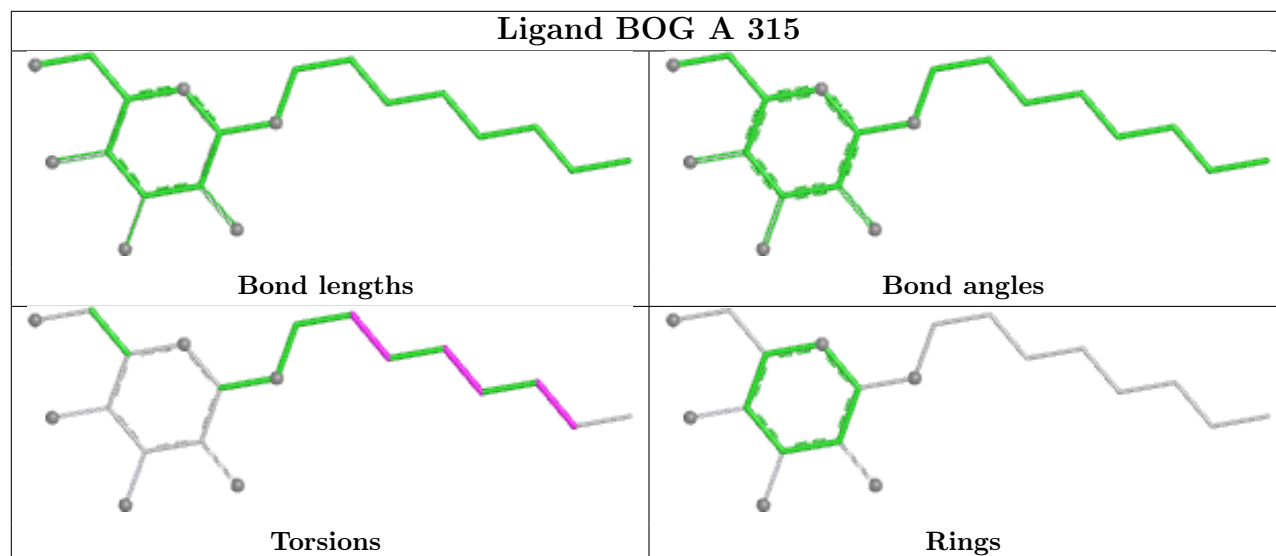


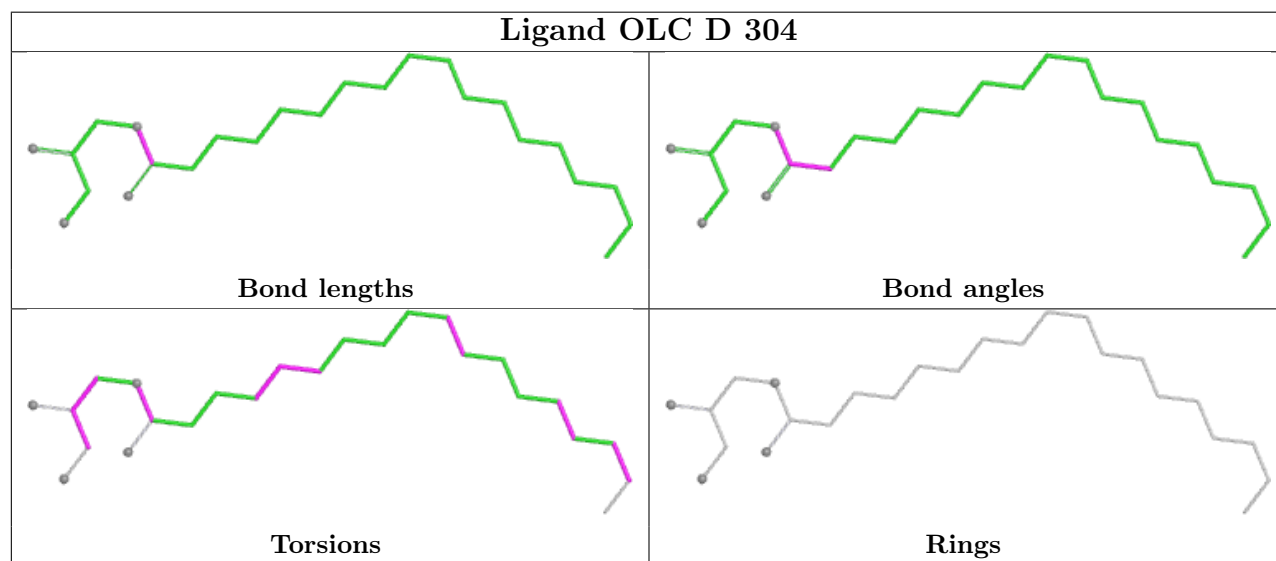
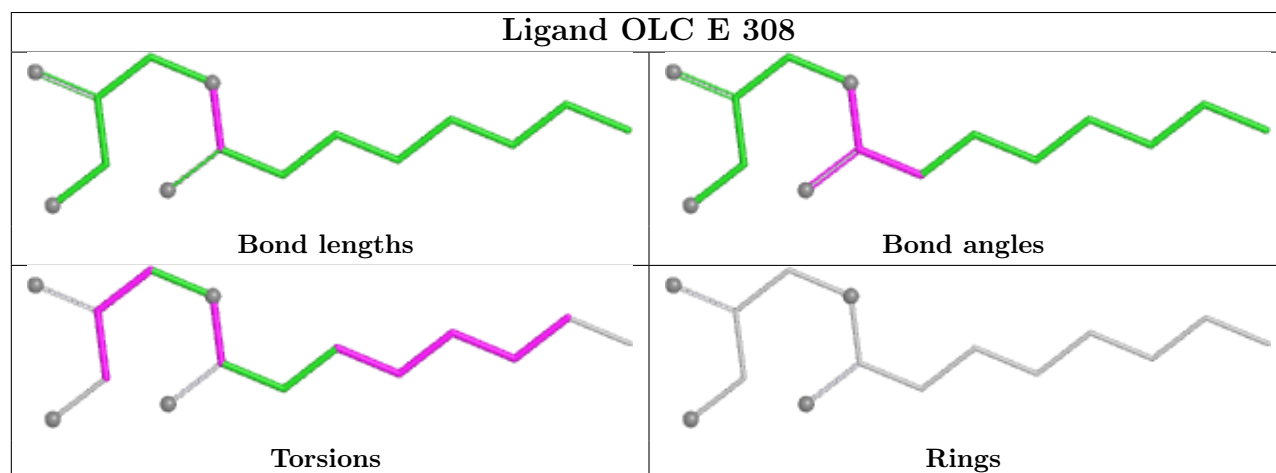
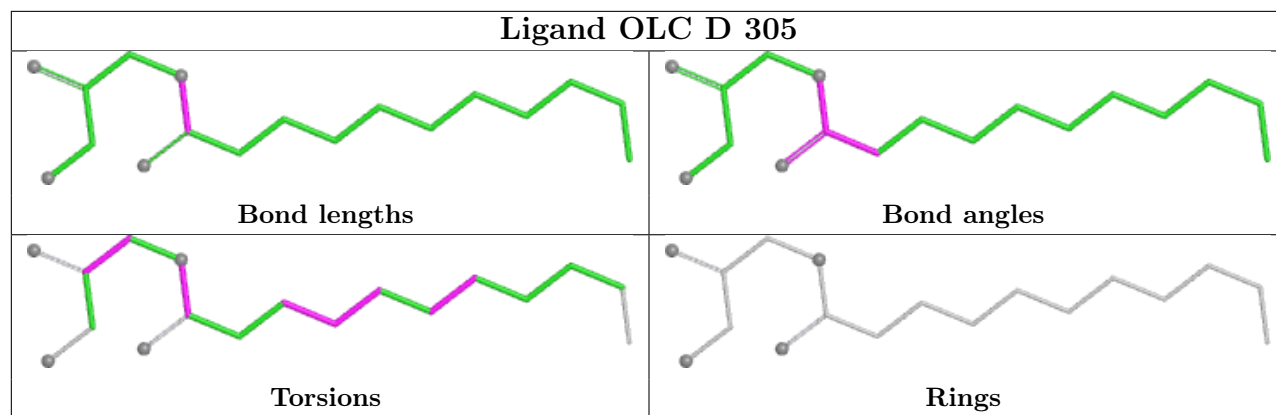


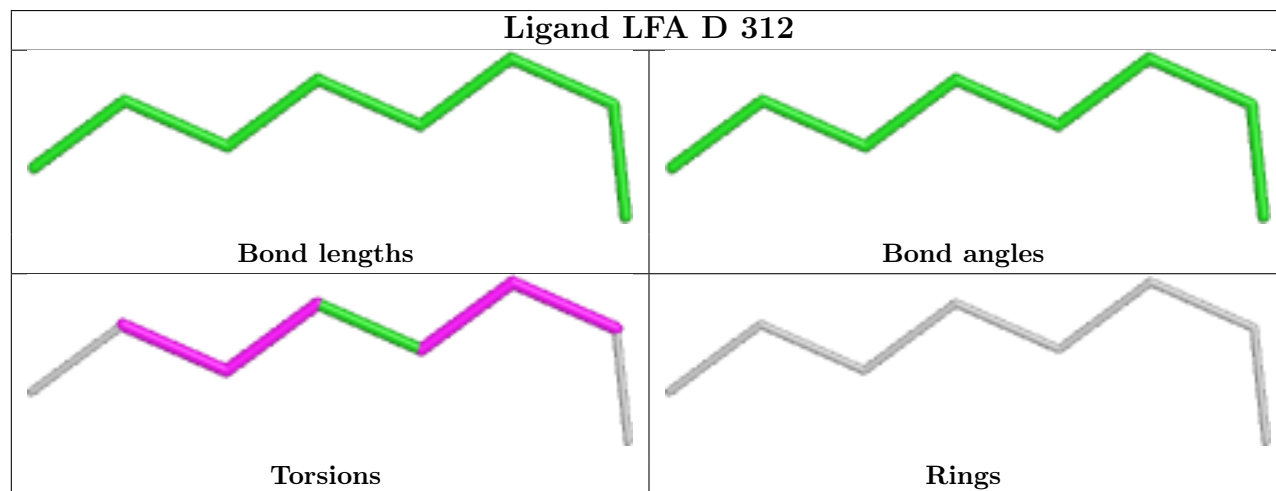
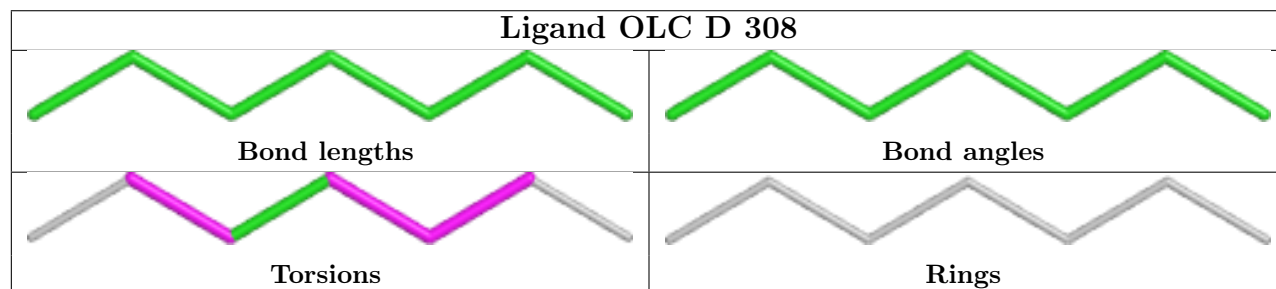
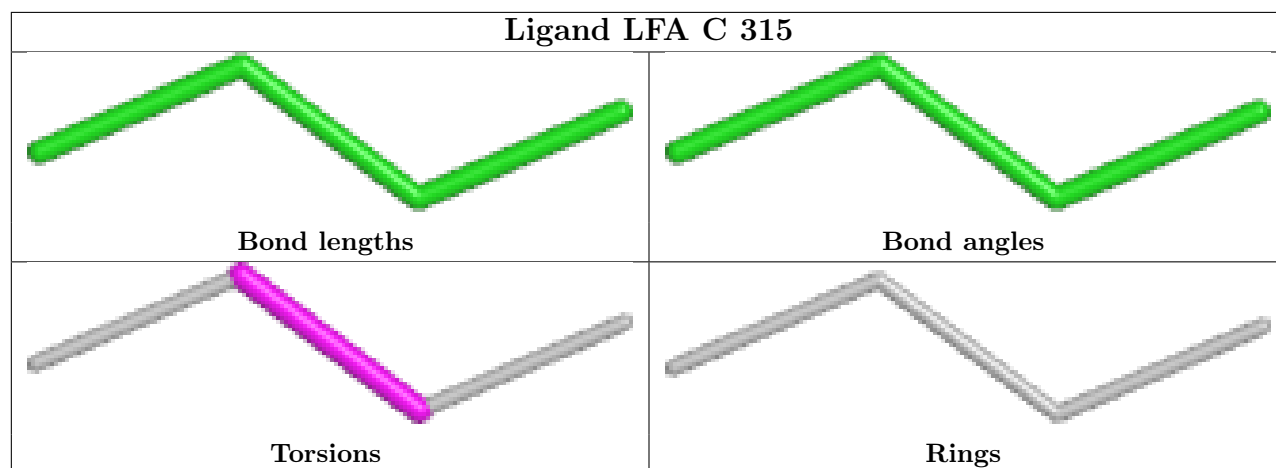
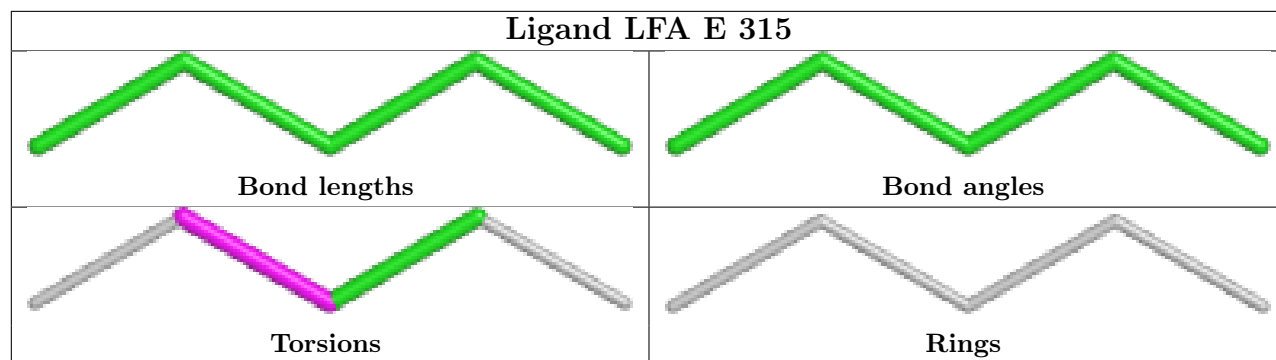


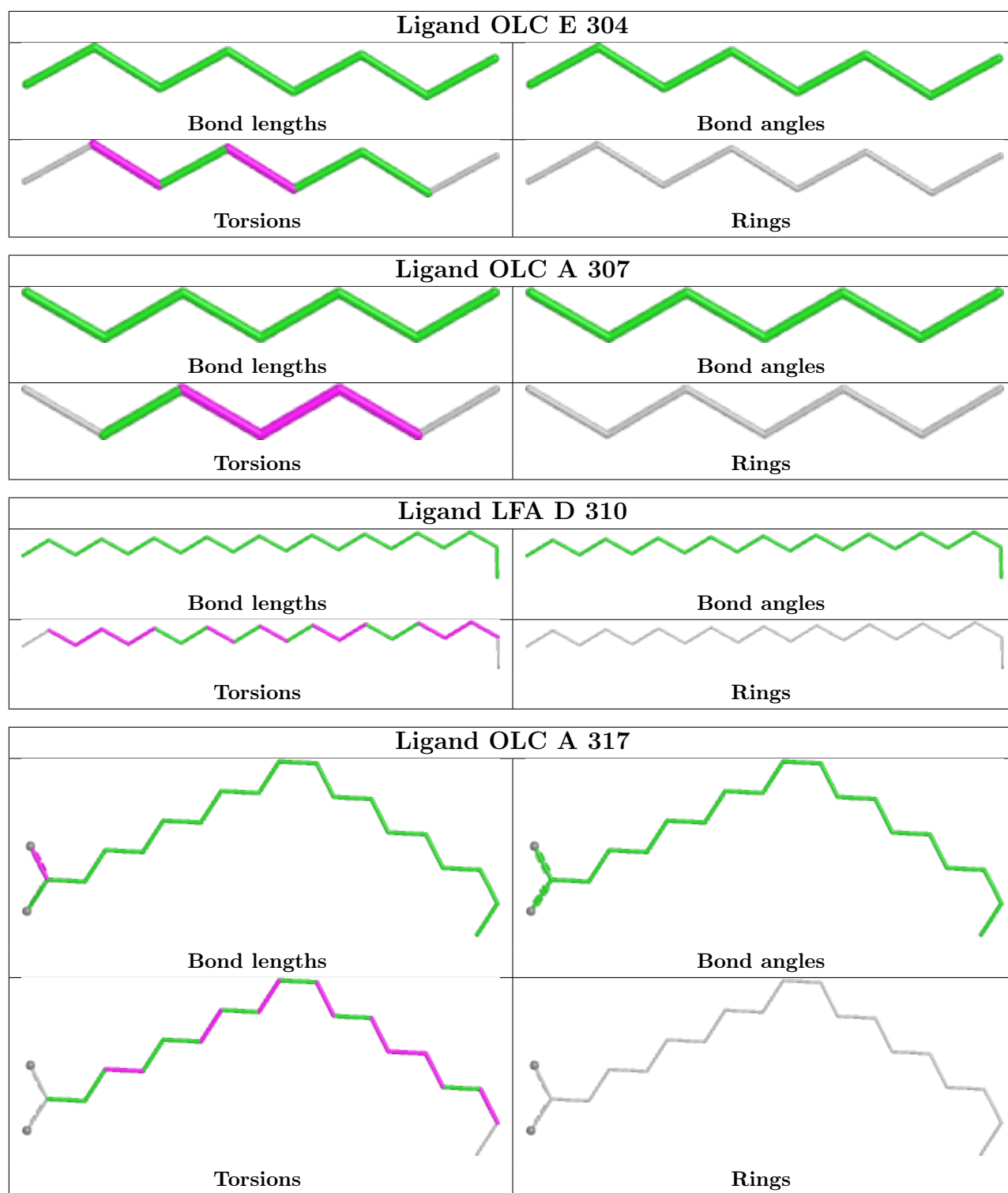


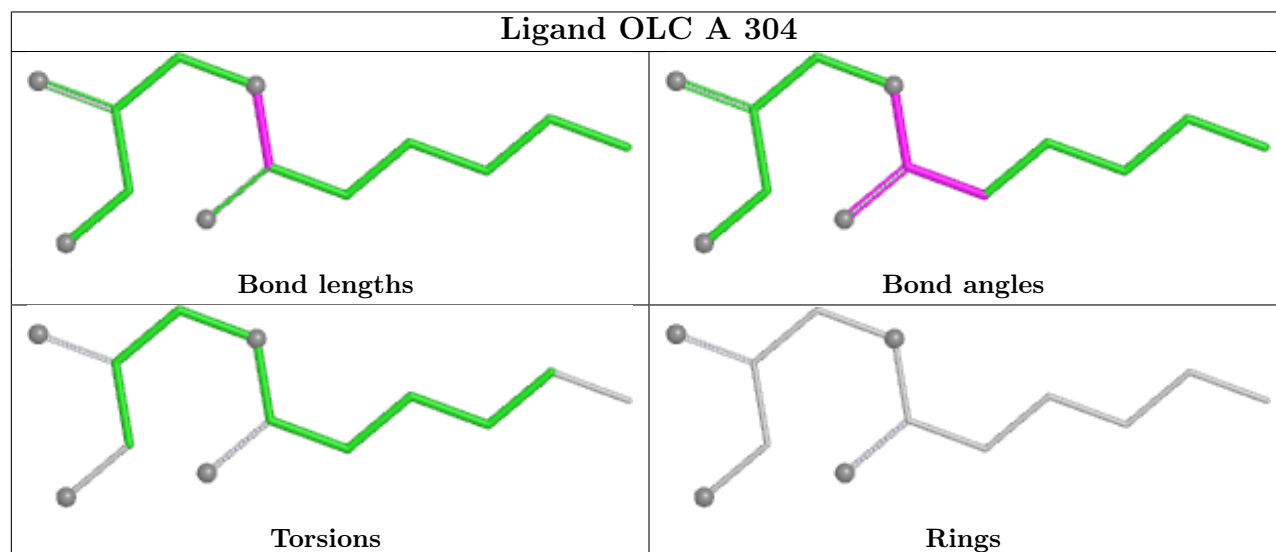
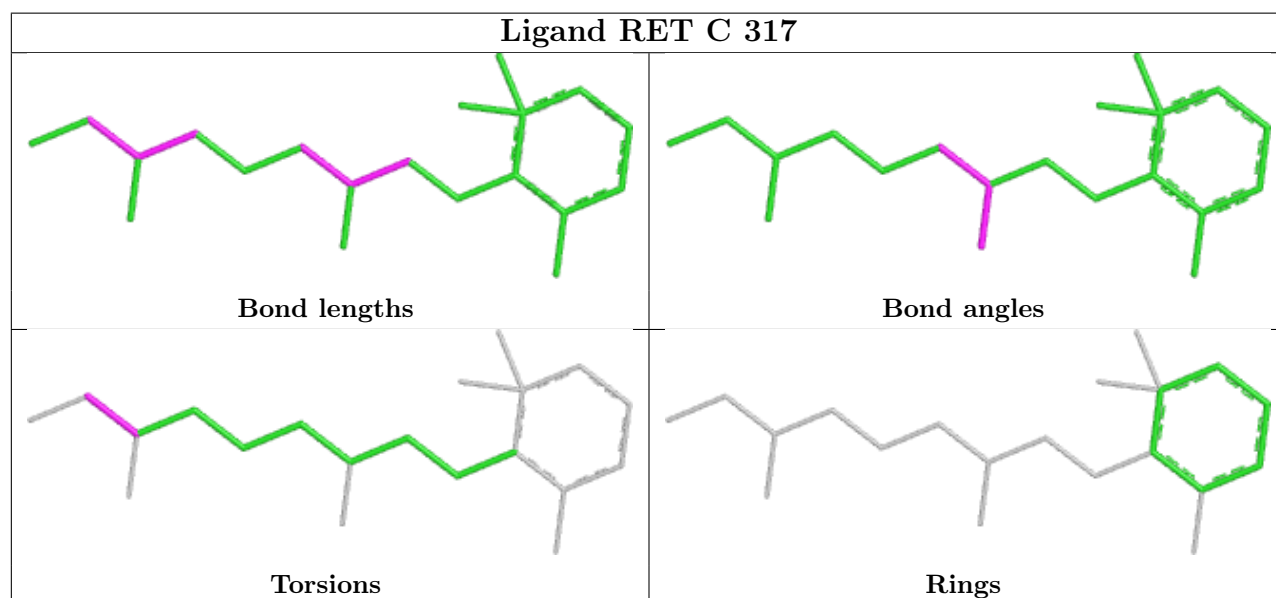
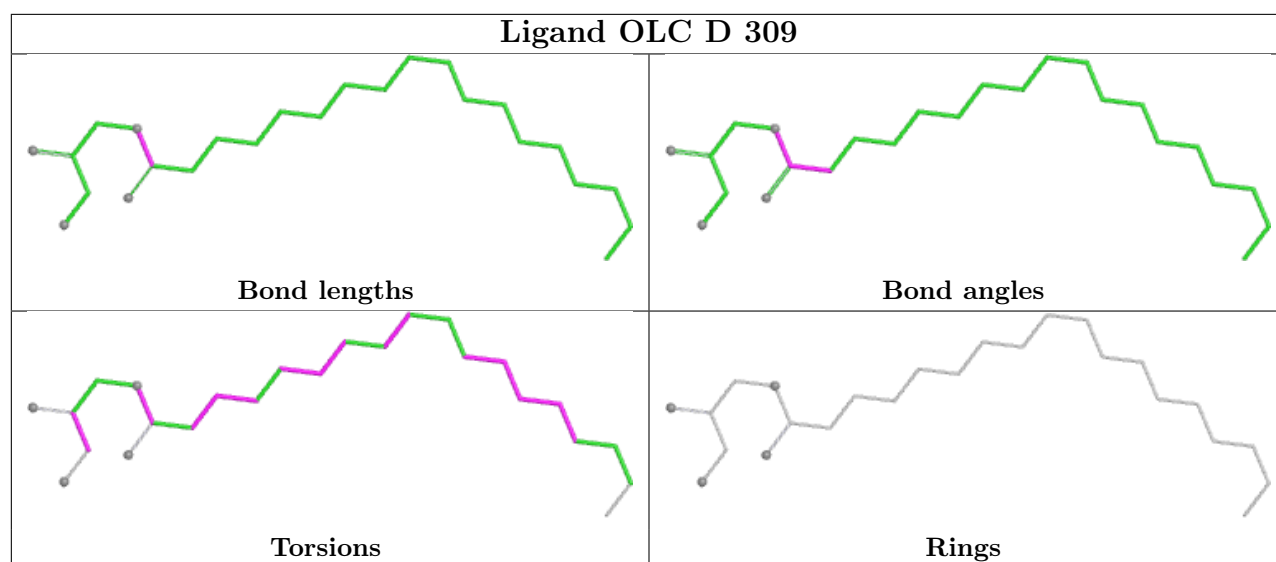


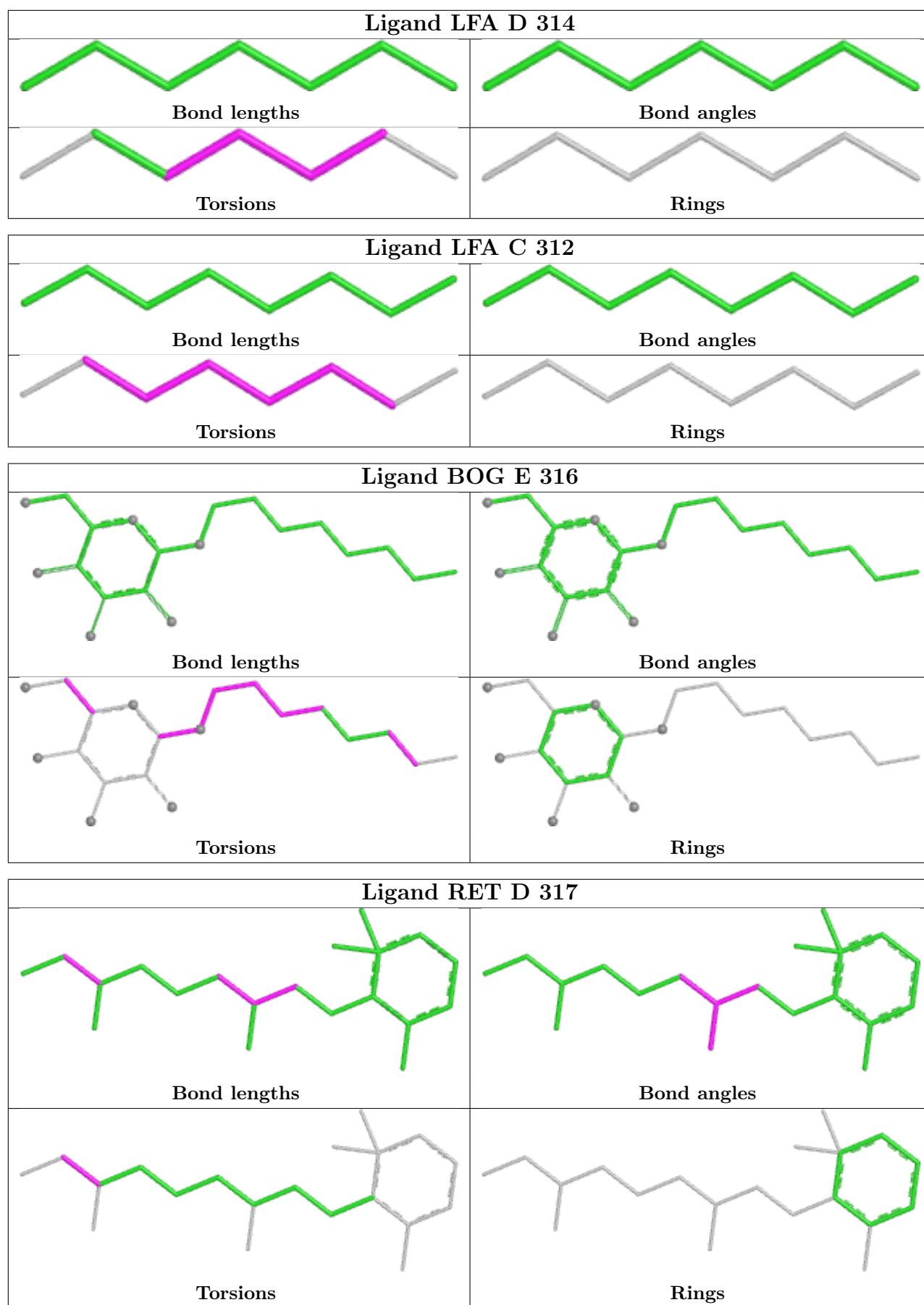


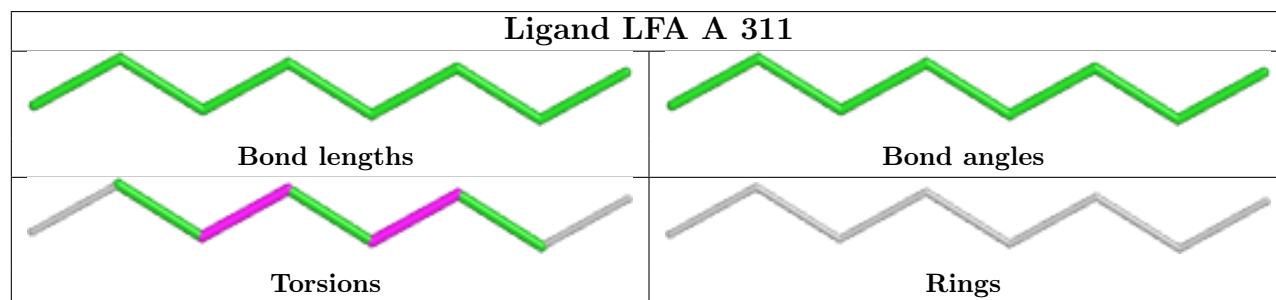
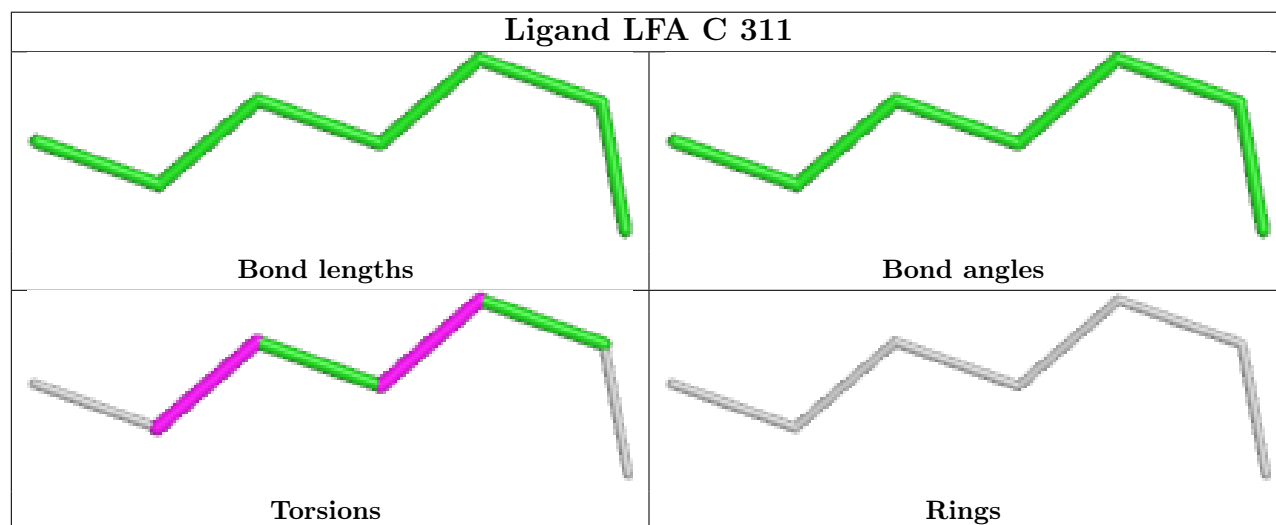
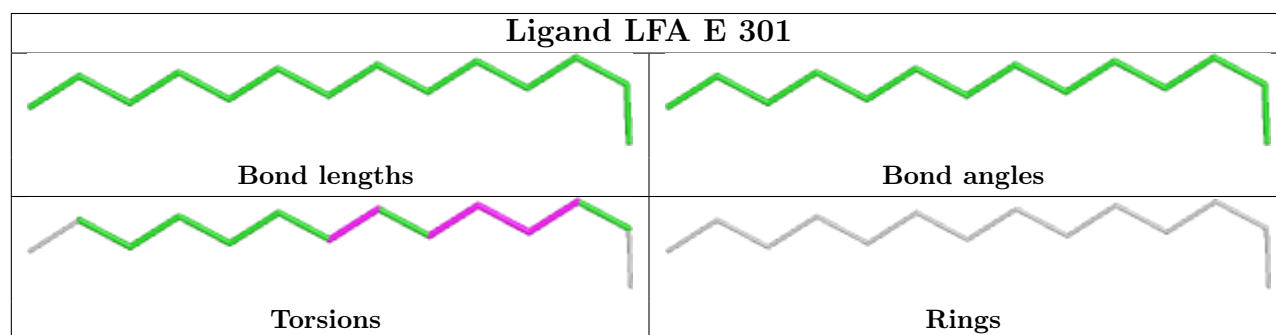
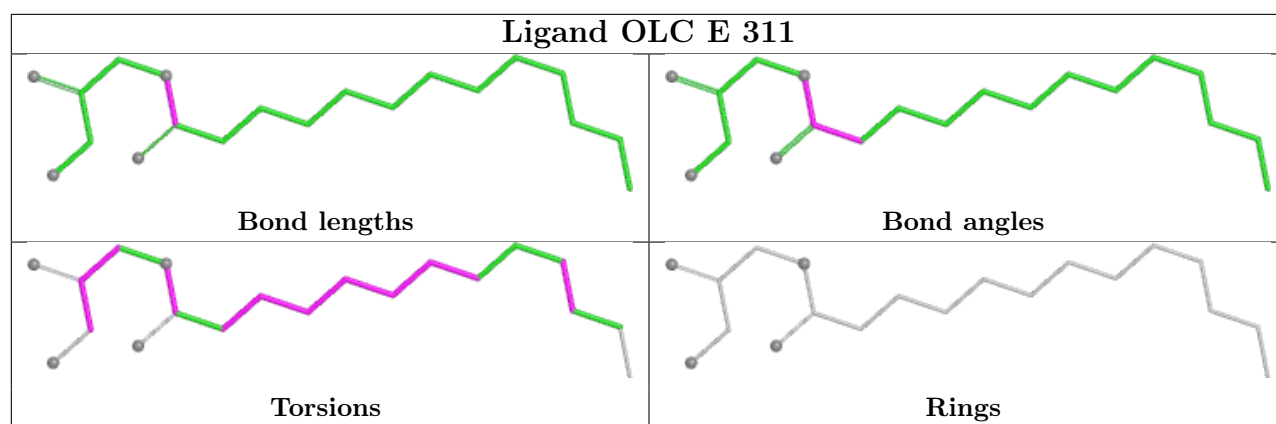


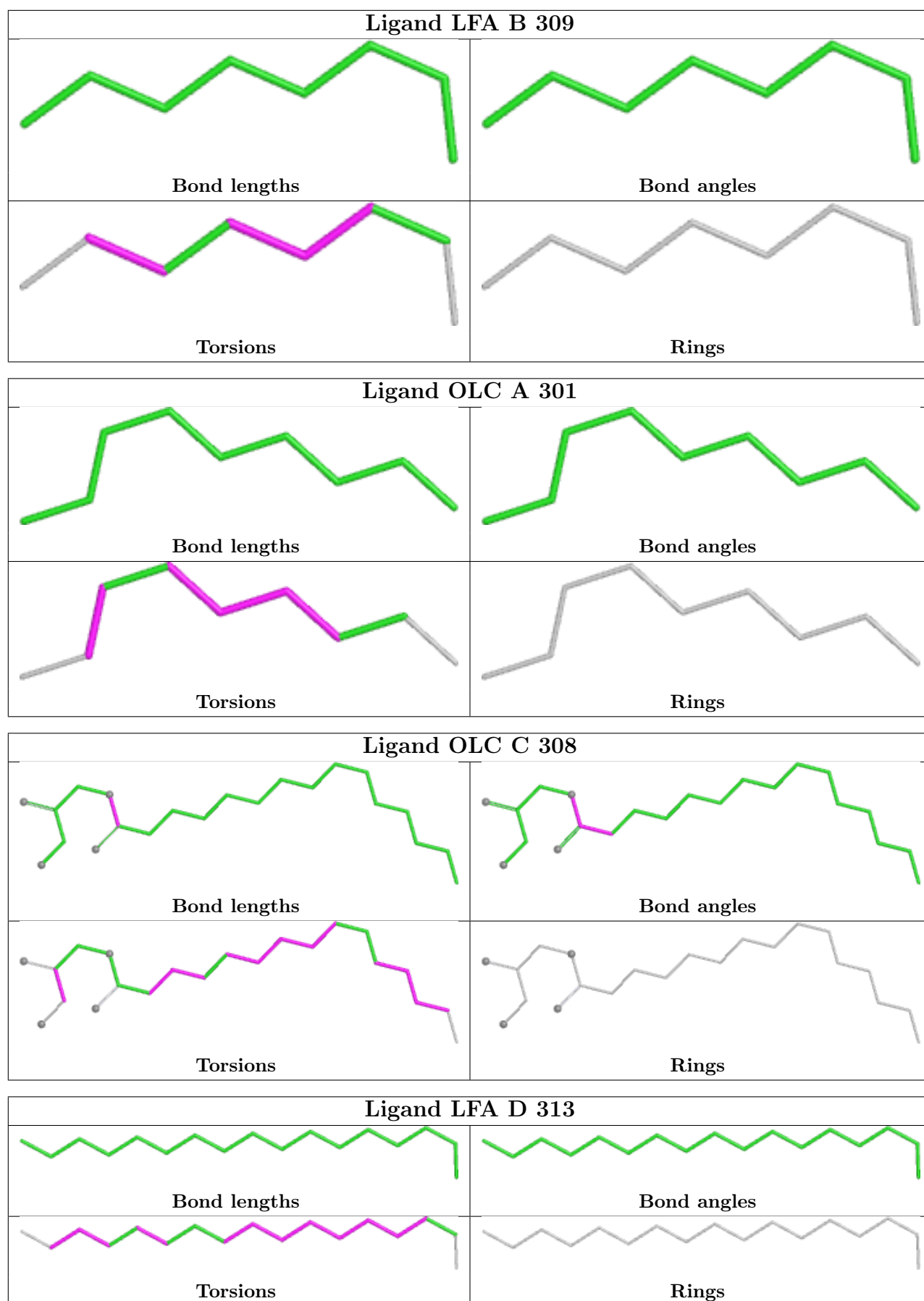


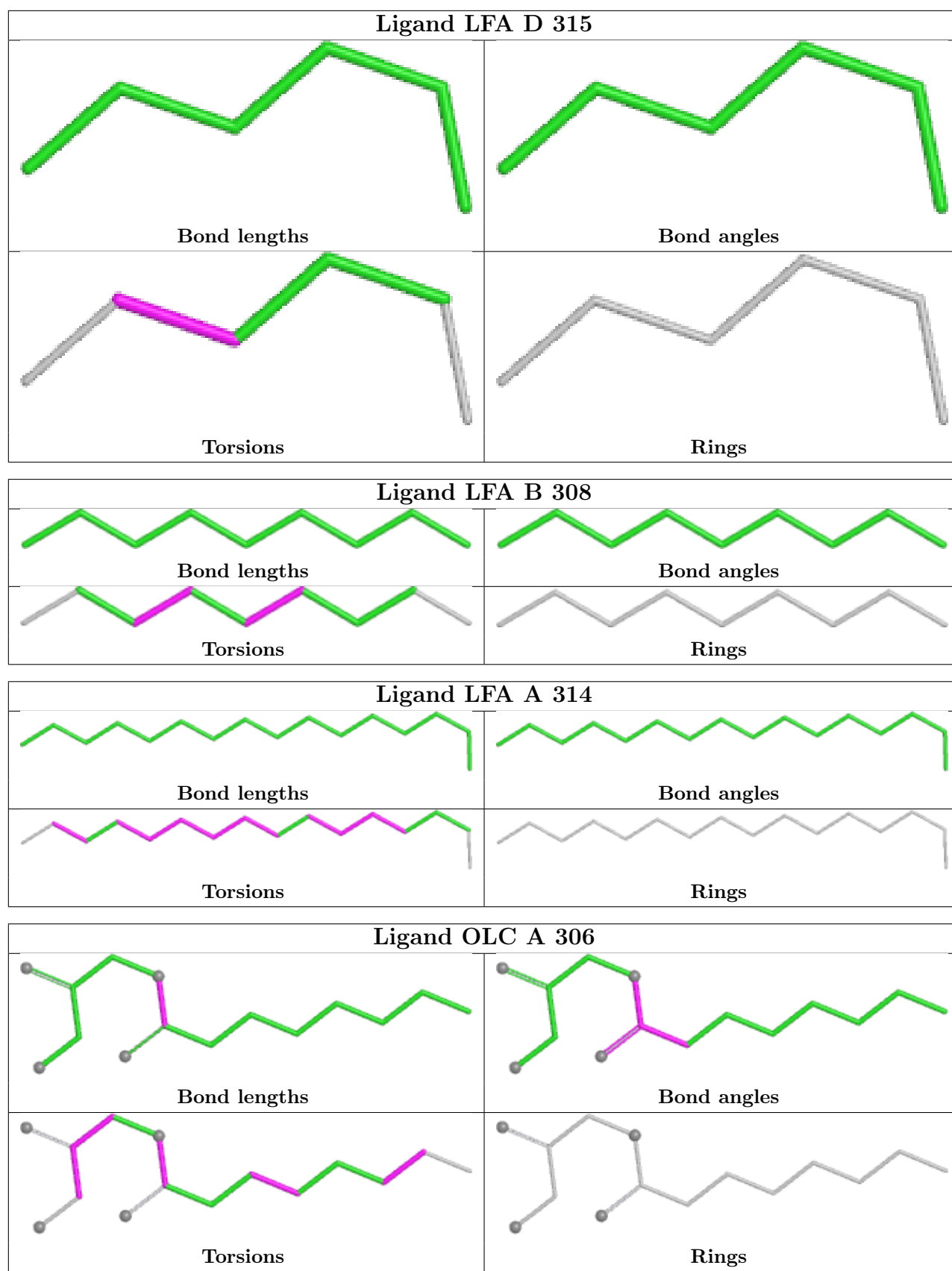


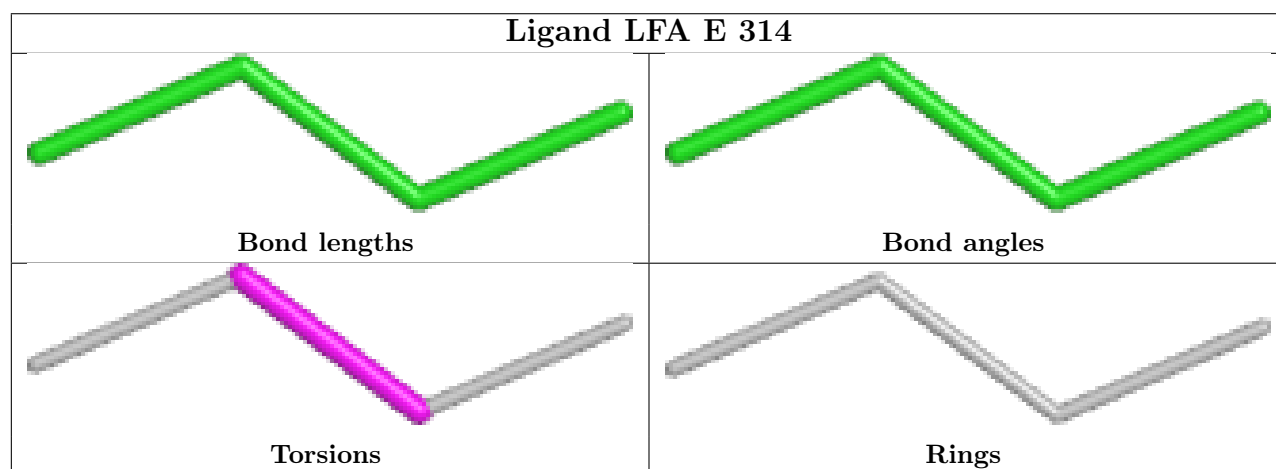
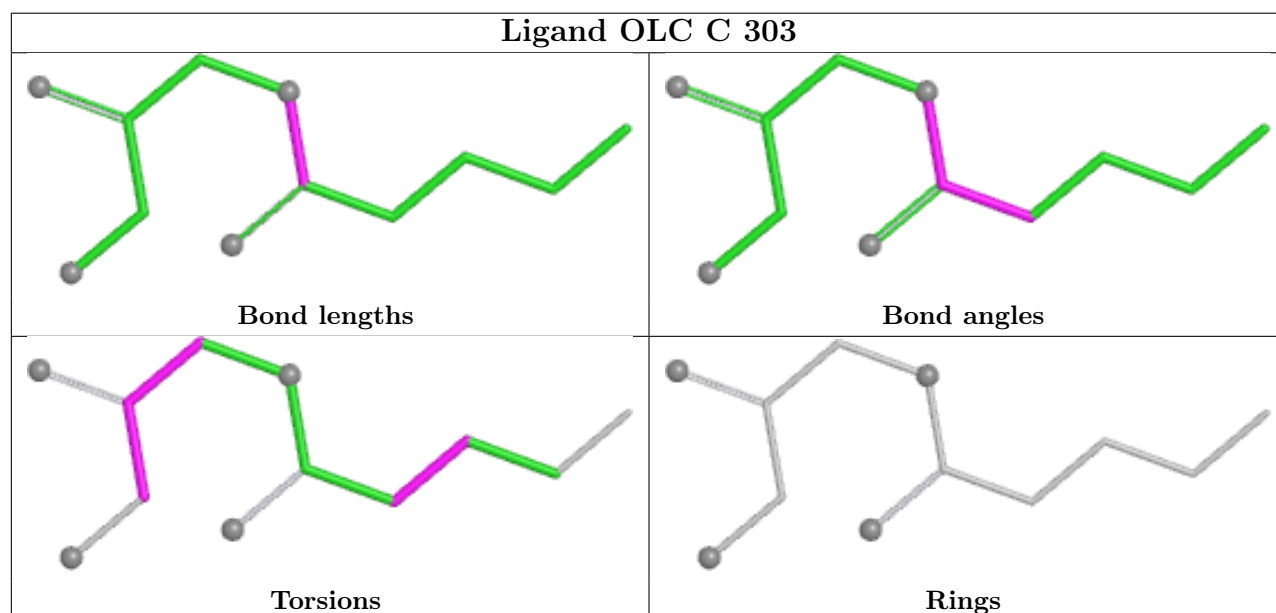
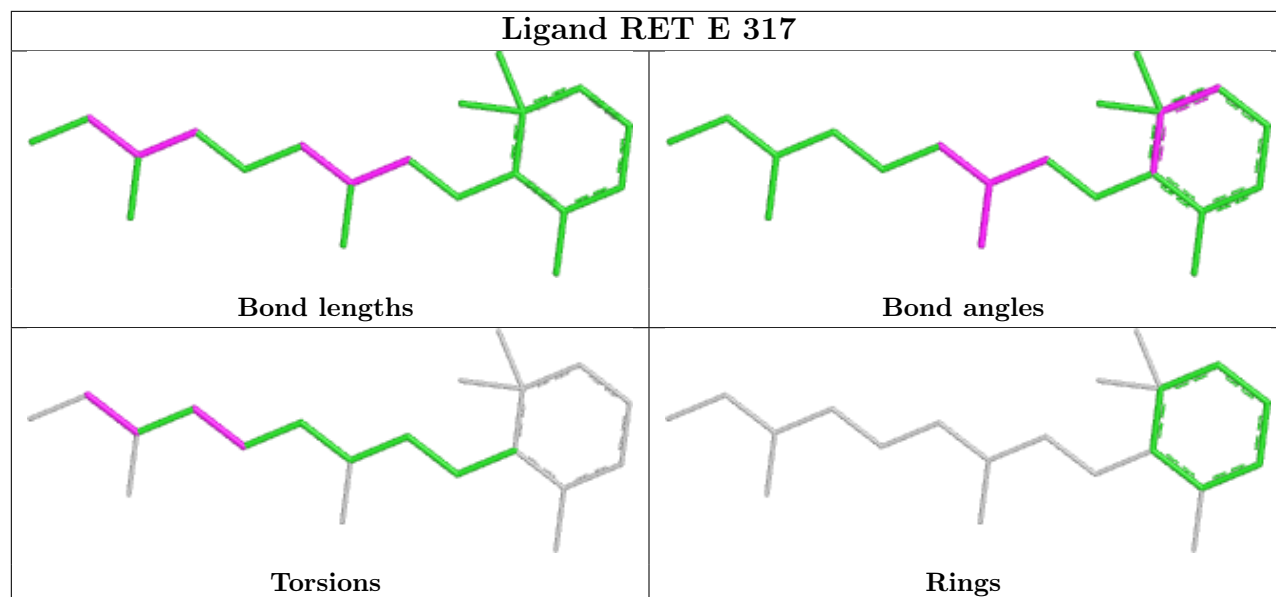


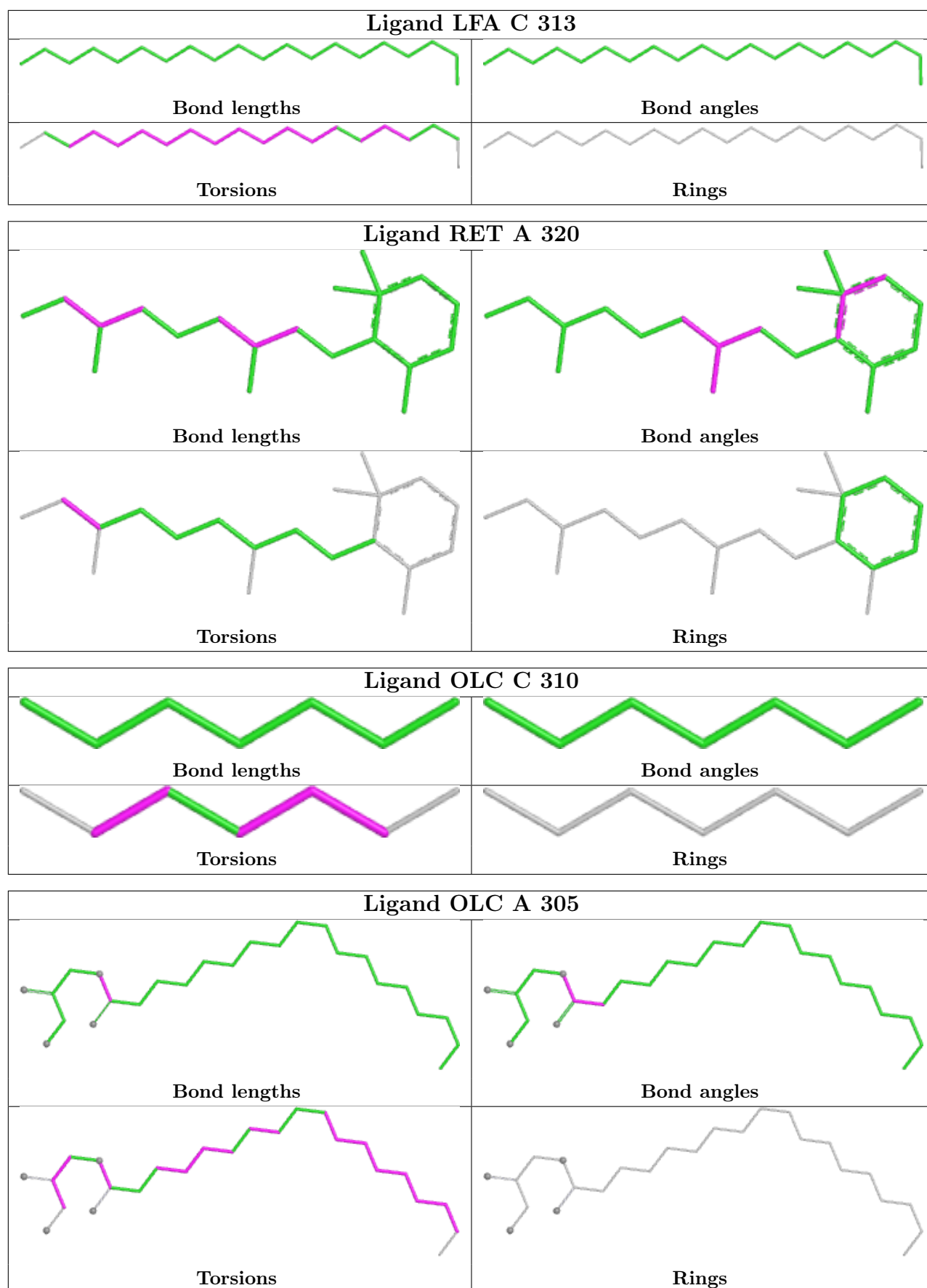


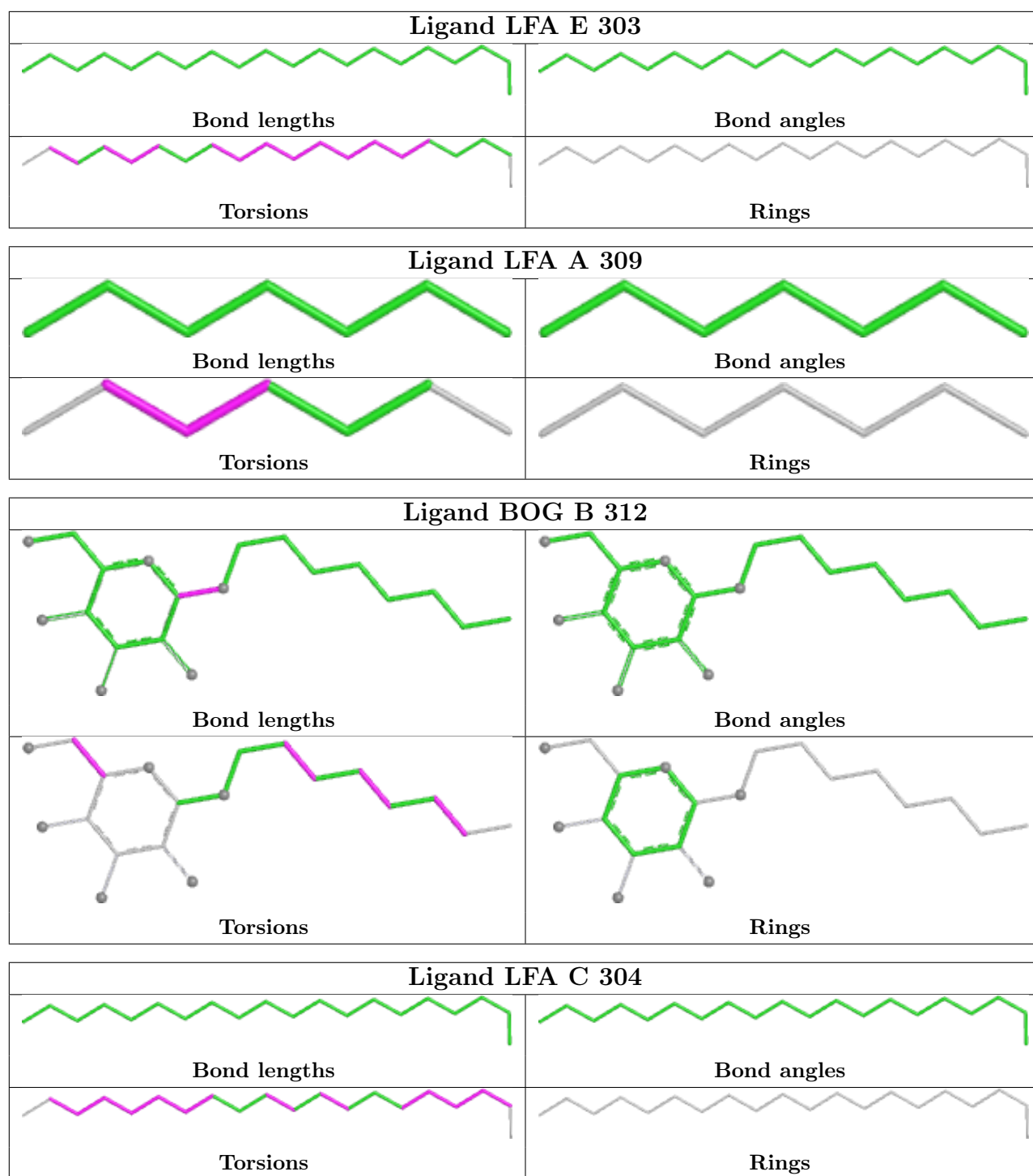


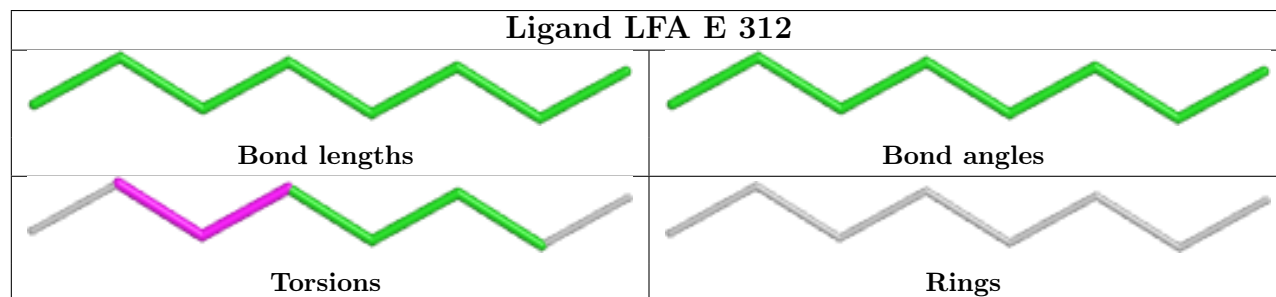
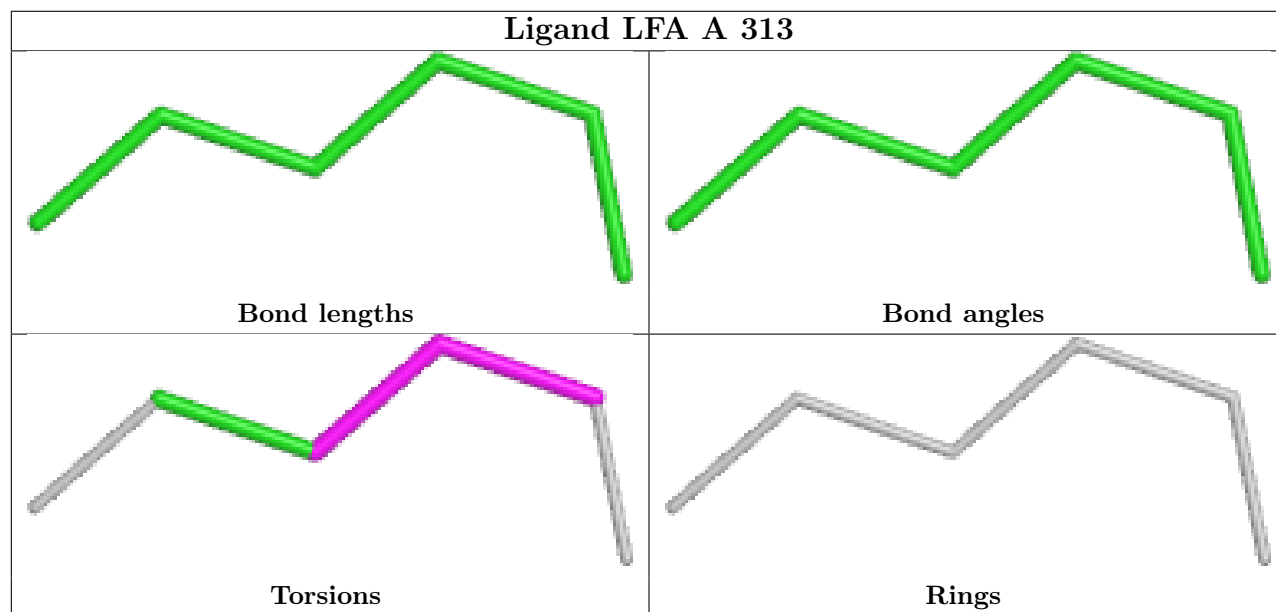
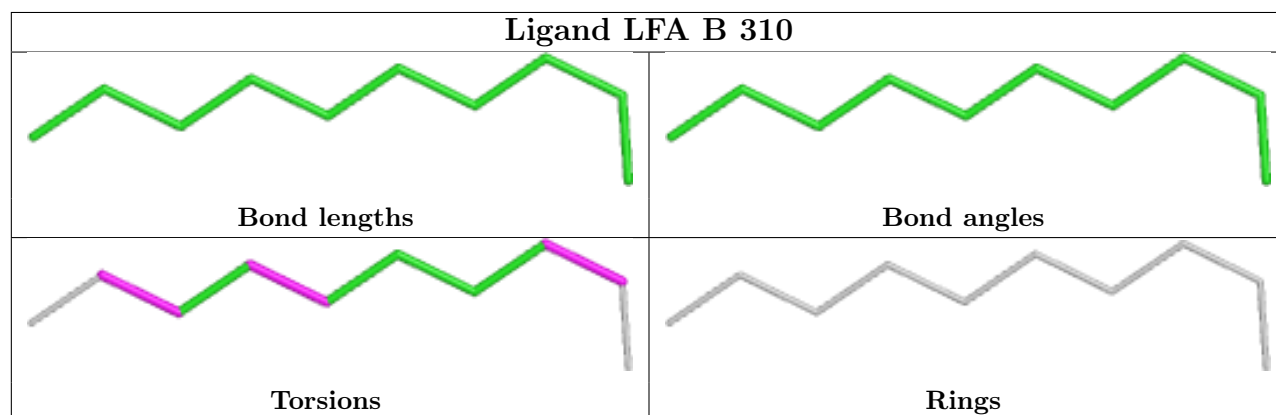
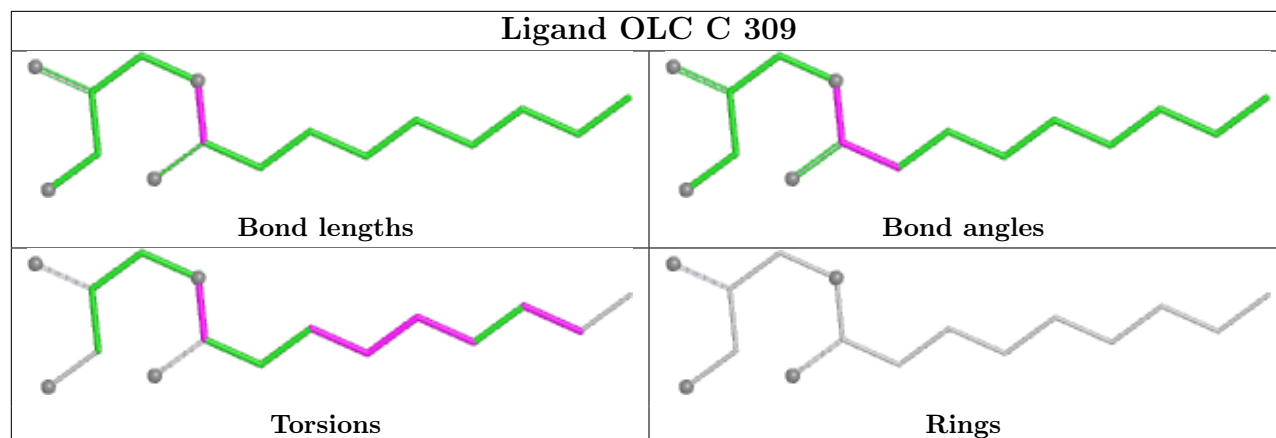


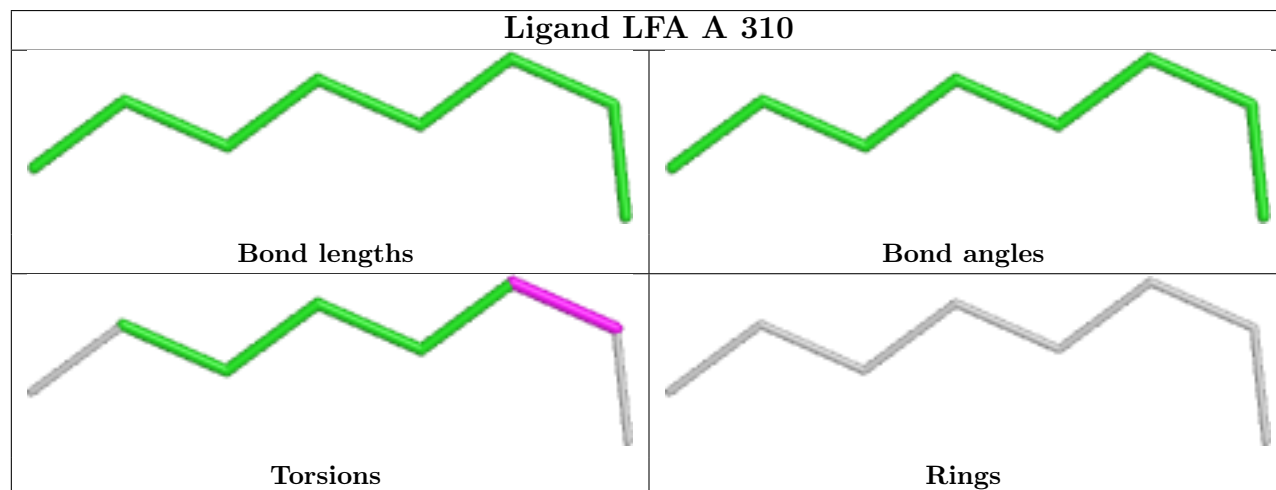
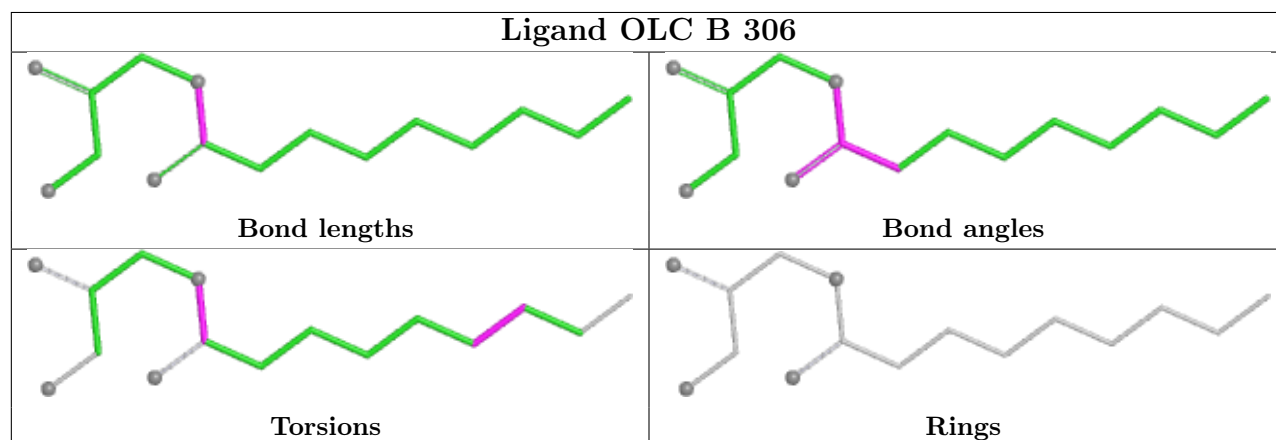
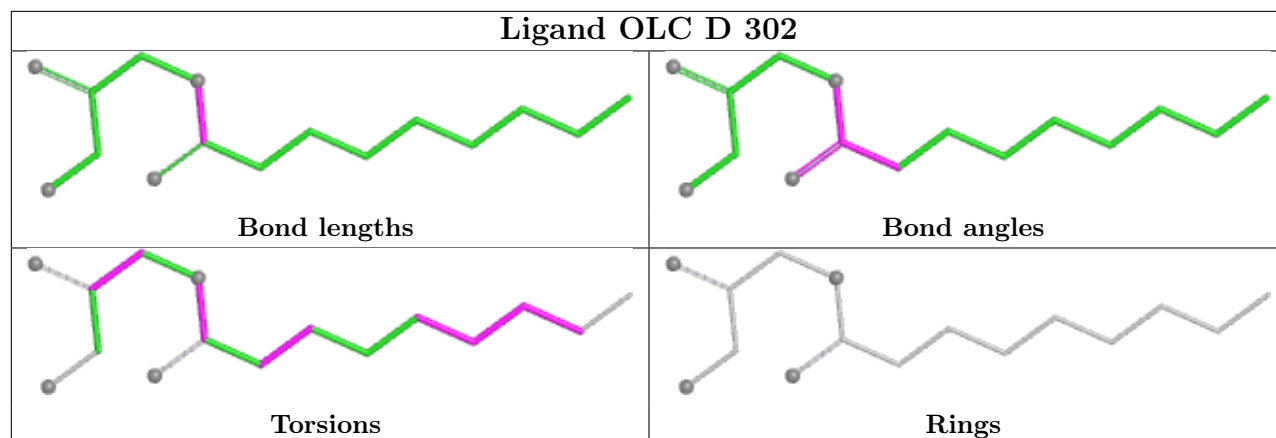


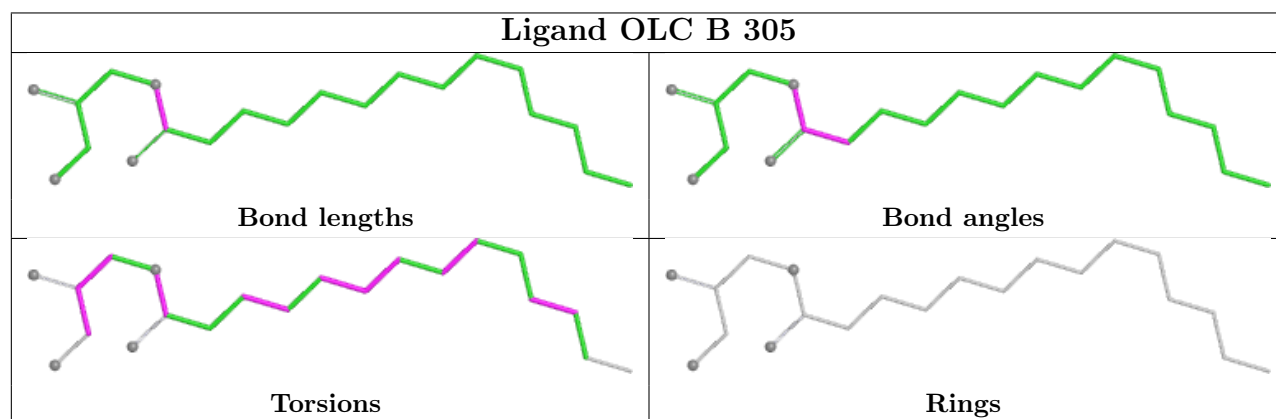
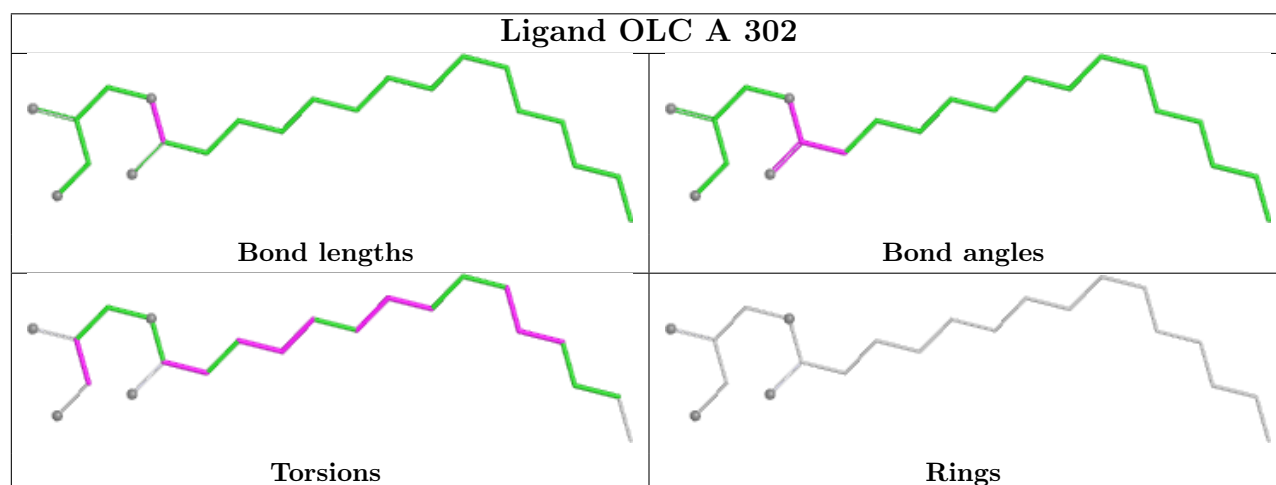
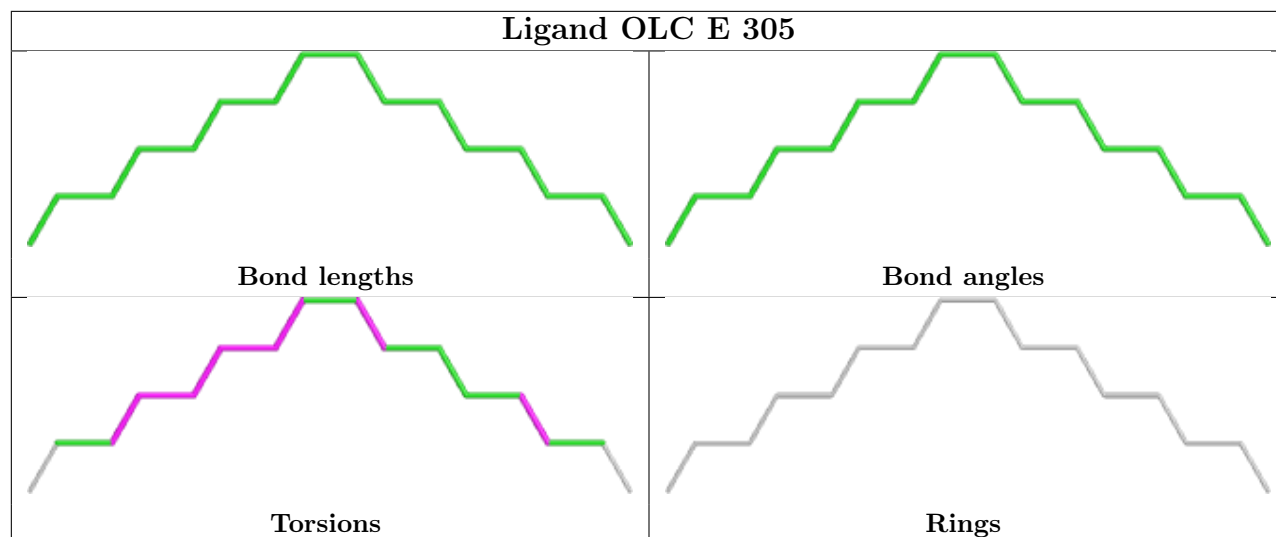


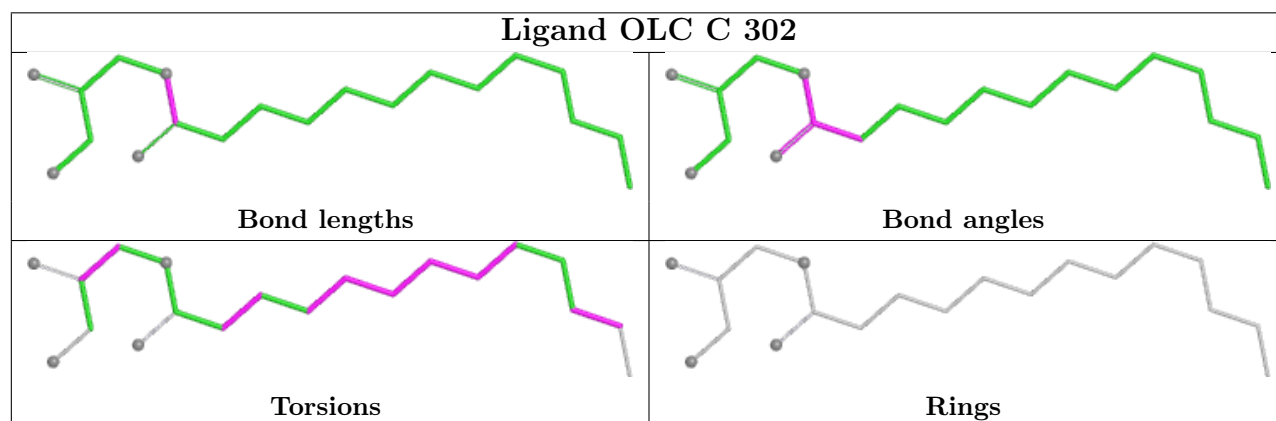
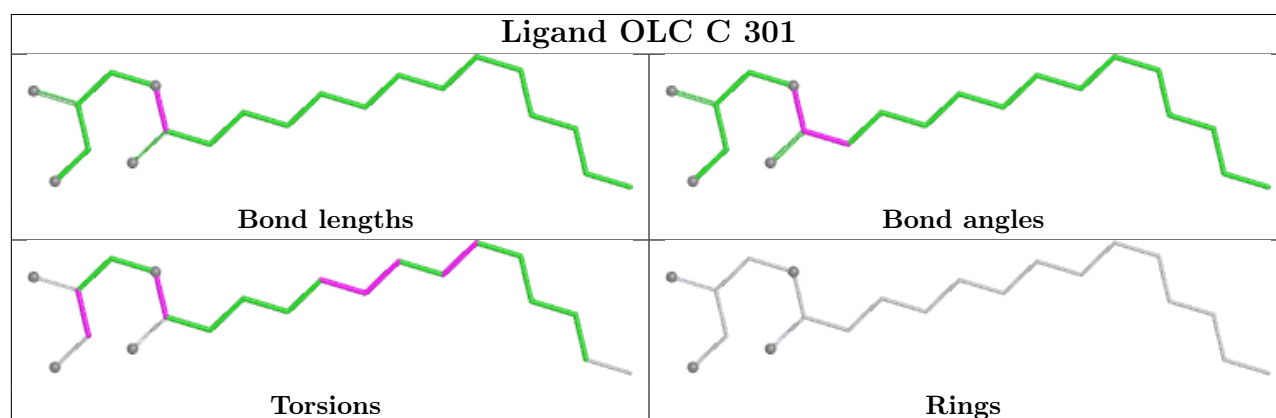
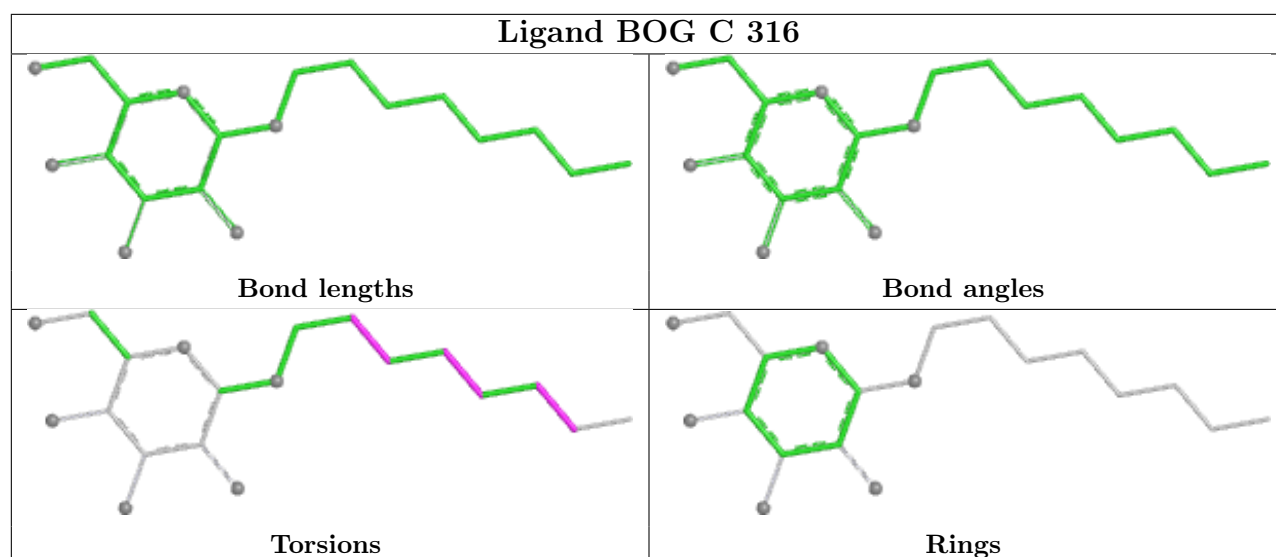


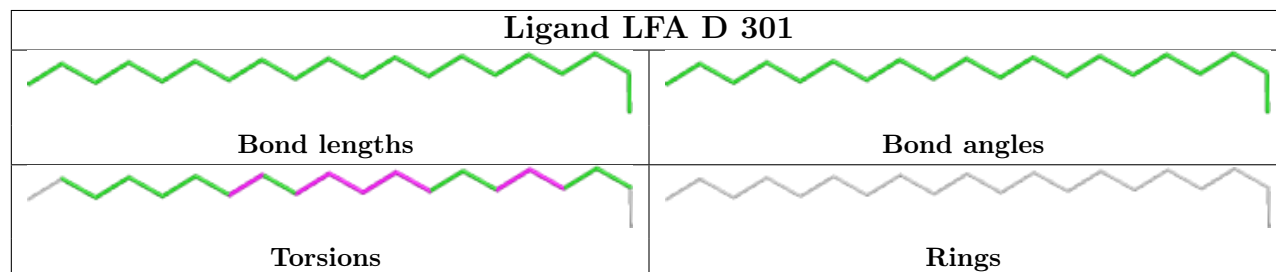
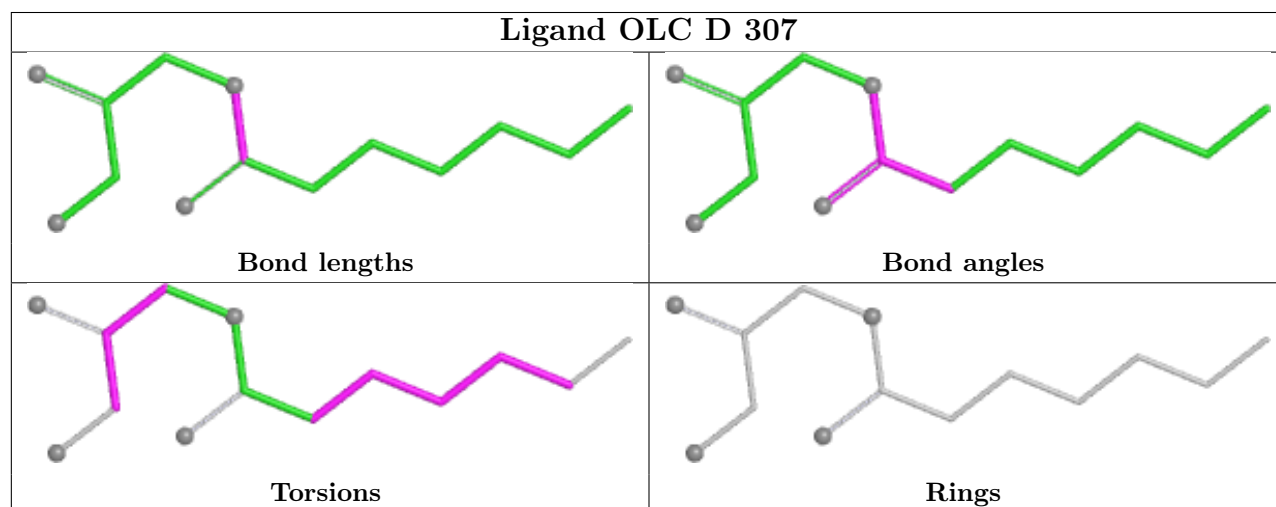
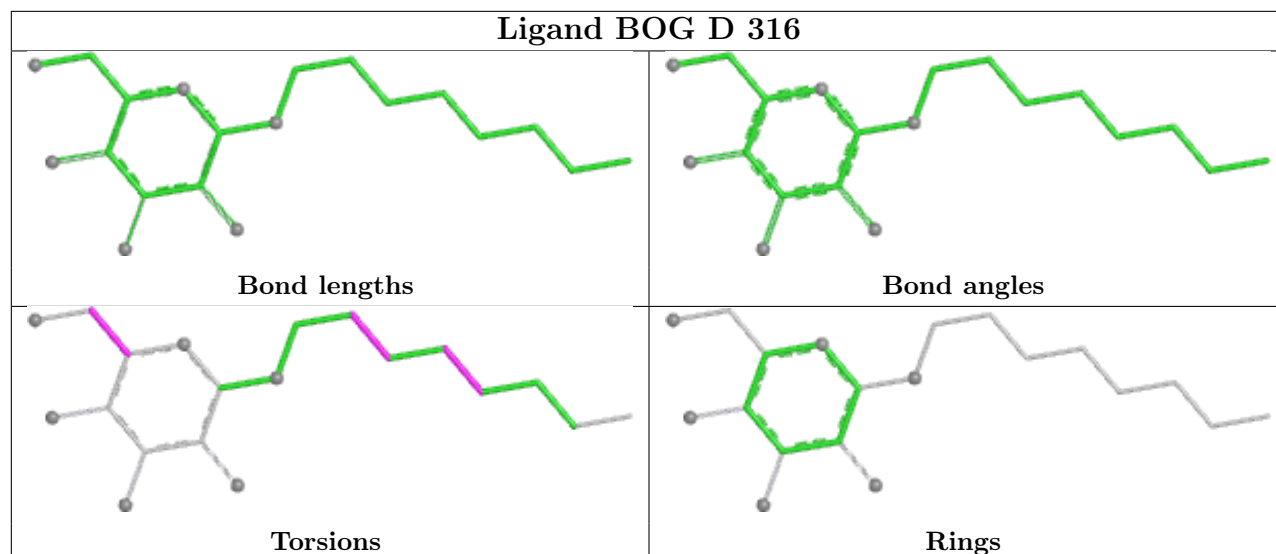


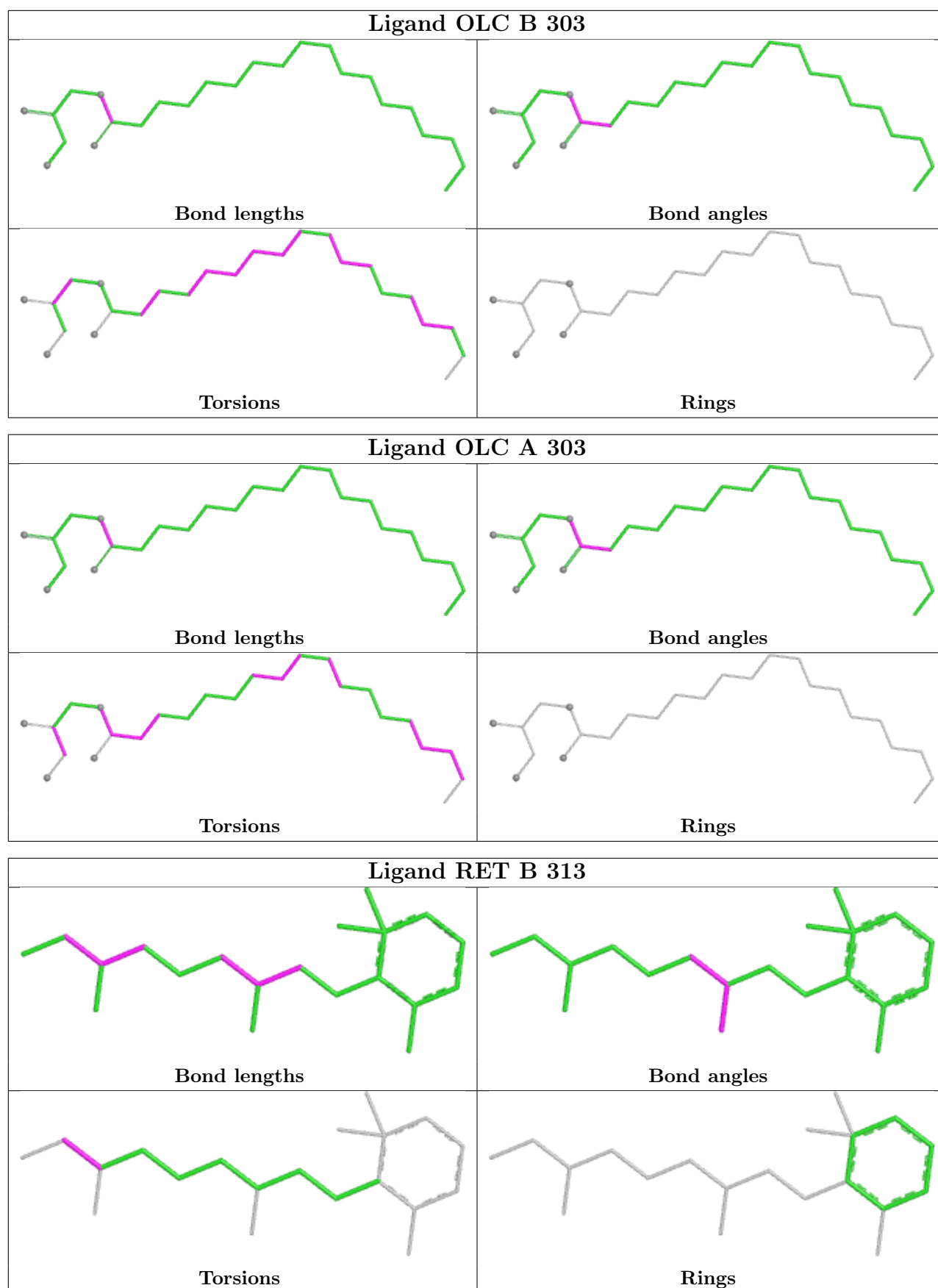


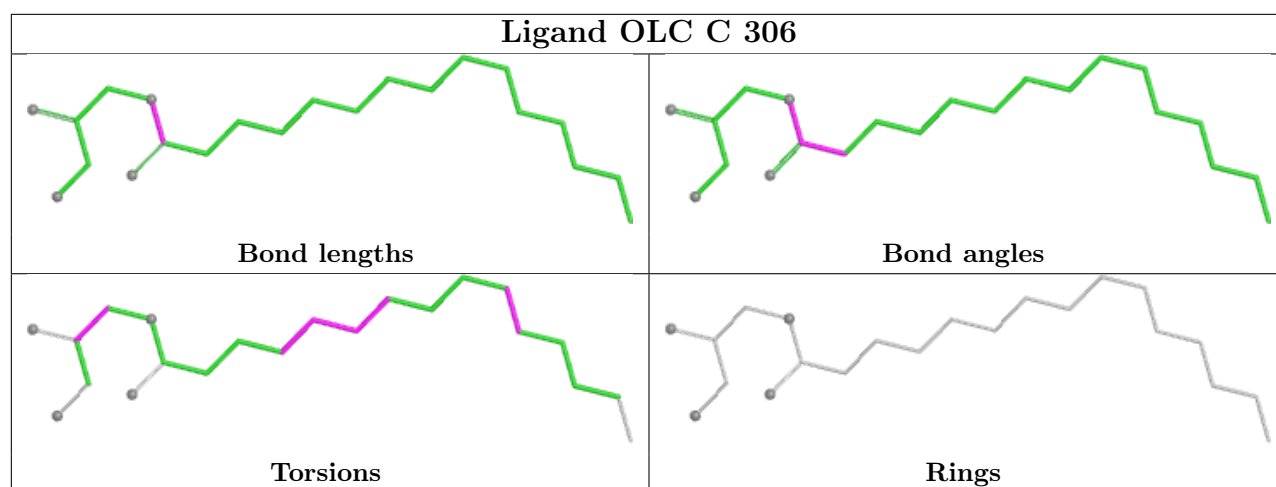












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/273 (100%)	-0.11	3 (1%) 78 77	12, 44, 65, 122	3 (1%)
1	B	273/273 (100%)	-0.08	1 (0%) 88 88	13, 45, 65, 118	3 (1%)
1	C	273/273 (100%)	-0.09	3 (1%) 78 77	19, 44, 66, 127	3 (1%)
1	D	273/273 (100%)	0.01	5 (1%) 67 67	12, 45, 70, 129	3 (1%)
1	E	273/273 (100%)	-0.07	5 (1%) 67 67	12, 44, 67, 124	3 (1%)
All	All	1365/1365 (100%)	-0.07	17 (1%) 76 76	12, 44, 67, 129	15 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	275	LEU	3.4
1	B	275	LEU	3.0
1	C	275	LEU	2.9
1	A	275	LEU	2.6
1	E	274	GLU	2.6
1	D	272	ASN	2.4
1	E	272	ASN	2.4
1	E	92	VAL	2.4
1	E	273	LYS	2.3
1	A	272	ASN	2.2
1	D	132	THR	2.2
1	D	92	VAL	2.1
1	D	137	SER	2.1
1	C	230	VAL	2.1
1	A	273	LYS	2.1
1	D	274	GLU	2.0
1	C	195	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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	303	13/25	0.63	0.15	98,114,134,162	0
2	OLC	E	307	15/25	0.66	0.18	77,93,123,123	0
3	LFA	E	301	14/20	0.67	0.13	95,104,119,121	0
3	LFA	A	318	20/20	0.68	0.14	59,69,80,83	0
3	LFA	A	319	9/20	0.69	0.21	76,79,94,95	0
2	OLC	B	303	25/25	0.70	0.17	77,96,107,113	0
3	LFA	E	303	20/20	0.70	0.14	57,73,92,92	0
3	LFA	B	302	20/20	0.71	0.14	53,73,87,97	0
3	LFA	D	301	20/20	0.71	0.14	57,70,97,97	0
3	LFA	C	304	20/20	0.73	0.14	57,72,84,88	0
2	OLC	A	305	25/25	0.73	0.16	80,98,107,111	0
4	BOG	B	312	20/20	0.73	0.16	73,89,103,104	0
3	LFA	B	310	10/20	0.74	0.25	79,95,103,105	0
2	OLC	A	303	25/25	0.74	0.20	79,90,106,137	0
3	LFA	D	310	20/20	0.75	0.18	82,93,102,106	0
2	OLC	E	311	20/25	0.75	0.15	60,105,126,126	0
3	LFA	C	315	4/20	0.75	0.23	76,76,81,87	0
4	BOG	A	315	20/20	0.75	0.15	71,97,111,113	0
3	LFA	A	312	4/20	0.75	0.22	79,82,84,86	0
4	BOG	E	316	20/20	0.75	0.14	69,89,103,112	0
3	LFA	D	315	6/20	0.76	0.19	86,90,96,102	0
2	OLC	C	306	22/25	0.76	0.20	79,95,113,118	0
3	LFA	C	311	7/20	0.77	0.21	74,84,96,99	0
2	OLC	D	309	25/25	0.77	0.17	67,86,112,130	0
2	OLC	D	308	7/25	0.78	0.18	64,75,83,85	0
2	OLC	D	302	16/25	0.78	0.16	66,88,94,111	0
3	LFA	D	314	7/20	0.78	0.20	78,84,96,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	E	305	16/25	0.79	0.20	76,88,96,99	0
3	LFA	A	314	16/20	0.79	0.20	83,98,106,108	0
4	BOG	C	316	20/20	0.79	0.14	64,82,99,100	0
3	LFA	A	309	7/20	0.79	0.24	80,82,90,92	0
2	OLC	E	310	22/25	0.80	0.17	68,88,107,117	0
2	OLC	D	305	18/25	0.80	0.17	77,90,111,125	0
2	OLC	B	307	7/25	0.80	0.19	69,77,86,86	0
2	OLC	C	302	20/25	0.80	0.14	67,83,89,96	0
2	OLC	E	304	8/25	0.80	0.17	67,71,90,90	0
2	OLC	C	303	12/25	0.80	0.15	72,88,121,133	0
2	OLC	D	304	25/25	0.80	0.19	77,97,108,124	0
3	LFA	D	311	20/20	0.80	0.16	78,89,99,104	0
2	OLC	A	306	15/25	0.81	0.16	65,76,100,125	0
3	LFA	B	308	9/20	0.81	0.19	82,92,103,107	0
3	LFA	C	314	6/20	0.81	0.21	61,70,84,84	0
2	OLC	E	306	20/25	0.81	0.15	72,89,105,116	0
3	LFA	B	311	7/20	0.81	0.26	75,77,95,108	0
3	LFA	E	312	8/20	0.82	0.18	68,85,93,94	0
2	OLC	A	304	13/25	0.82	0.14	65,72,90,91	0
2	OLC	C	307	20/25	0.82	0.15	70,95,111,114	0
2	OLC	E	309	6/25	0.82	0.18	61,74,80,86	0
3	LFA	D	312	8/20	0.82	0.21	75,93,104,107	0
2	OLC	D	306	18/25	0.83	0.15	53,86,104,111	0
2	OLC	C	308	22/25	0.83	0.15	53,90,109,116	0
2	OLC	C	310	7/25	0.83	0.17	70,70,84,94	0
6	NA	E	319	1/1	0.83	0.33	66,66,66,66	0
3	LFA	A	310	8/20	0.84	0.18	75,80,84,84	0
3	LFA	A	311	8/20	0.84	0.22	70,85,101,103	0
2	OLC	C	309	16/25	0.84	0.14	61,84,92,94	0
2	OLC	E	302	25/25	0.84	0.13	70,82,129,140	0
3	LFA	B	309	8/20	0.84	0.17	68,82,87,92	0
2	OLC	B	301	22/25	0.85	0.12	70,82,101,108	0
2	OLC	A	308	16/25	0.85	0.13	65,83,127,132	0
4	BOG	D	316	20/20	0.85	0.13	69,83,100,100	0
2	OLC	E	308	15/25	0.85	0.15	60,73,85,86	0
2	OLC	B	305	21/25	0.85	0.13	55,87,118,133	0
3	LFA	C	313	20/20	0.86	0.15	70,88,106,108	0
2	OLC	B	306	16/25	0.86	0.12	61,85,96,116	0
2	OLC	A	301	9/25	0.86	0.15	66,77,89,92	0
2	OLC	A	307	7/25	0.86	0.16	76,81,86,88	0
3	LFA	E	313	14/20	0.86	0.19	74,89,103,104	0
3	LFA	E	314	4/20	0.86	0.21	67,70,79,79	0

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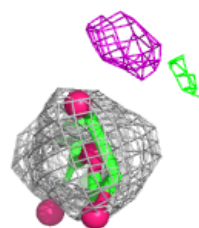
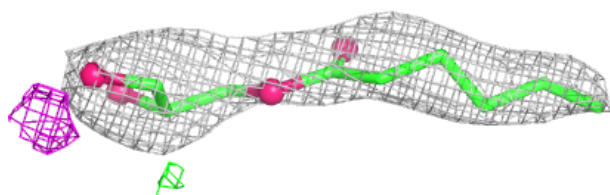
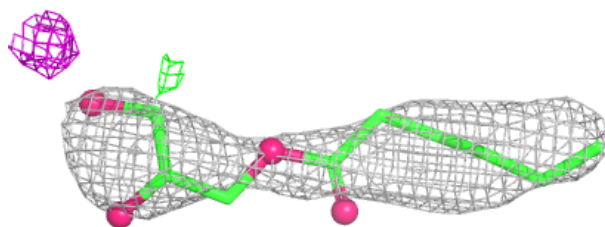
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	B	304	20/25	0.87	0.14	65,88,108,116	0
3	LFA	E	315	5/20	0.87	0.19	83,85,87,91	0
2	OLC	C	318	18/25	0.87	0.12	67,81,98,110	0
2	OLC	A	317	20/25	0.87	0.12	66,76,96,97	0
2	OLC	D	307	14/25	0.88	0.12	59,76,94,97	0
2	OLC	A	302	22/25	0.88	0.13	45,67,107,111	0
6	NA	B	316	1/1	0.88	0.26	76,76,76,76	0
3	LFA	C	312	8/20	0.88	0.20	72,85,88,90	0
3	LFA	D	313	17/20	0.90	0.12	56,62,83,91	0
2	OLC	C	301	21/25	0.90	0.12	51,64,90,96	0
6	NA	A	322	1/1	0.90	0.20	78,78,78,78	0
3	LFA	B	314	4/20	0.90	0.08	84,87,90,92	0
6	NA	C	320	1/1	0.90	0.21	70,70,70,70	0
2	OLC	C	305	23/25	0.90	0.12	49,66,106,120	0
6	NA	D	319	1/1	0.91	0.18	71,71,71,71	0
3	LFA	A	313	6/20	0.93	0.13	64,69,81,93	0
5	RET	C	317	20/21	0.94	0.09	36,43,47,49	0
5	RET	D	317	20/21	0.94	0.10	39,43,48,49	0
5	RET	E	317	20/21	0.94	0.08	37,43,45,49	0
5	RET	A	320	20/21	0.94	0.08	38,43,45,46	0
2	OLC	A	316	19/25	0.95	0.09	51,59,74,75	0
5	RET	B	313	20/21	0.95	0.08	37,43,49,52	0
6	NA	A	321	1/1	0.98	0.10	39,39,39,39	0
6	NA	E	318	1/1	0.98	0.08	39,39,39,39	0
6	NA	B	315	1/1	0.98	0.06	39,39,39,39	0
6	NA	D	318	1/1	0.99	0.14	38,38,38,38	0
6	NA	C	319	1/1	0.99	0.08	39,39,39,39	0

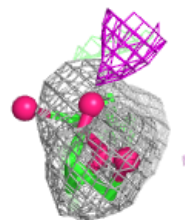
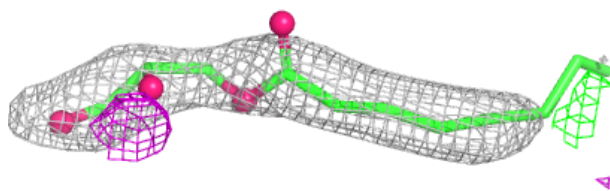
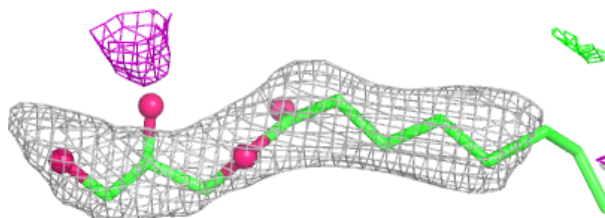
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC D 303:

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

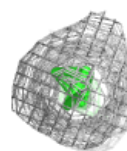
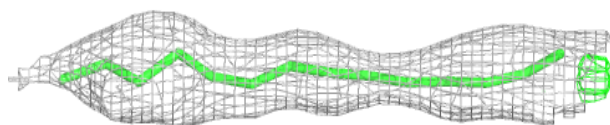
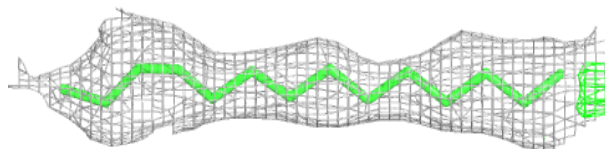
**Electron density around OLC E 307:**

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

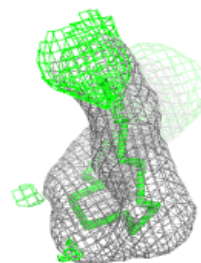
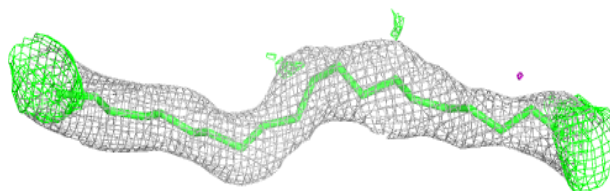
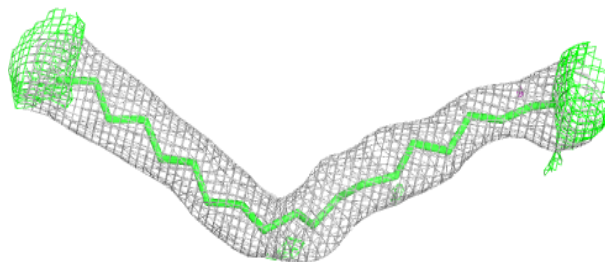


Electron density around LFA E 301:

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

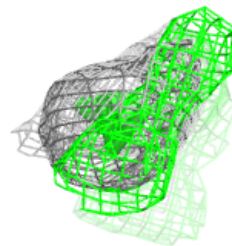
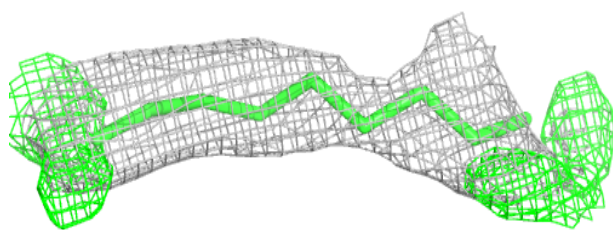
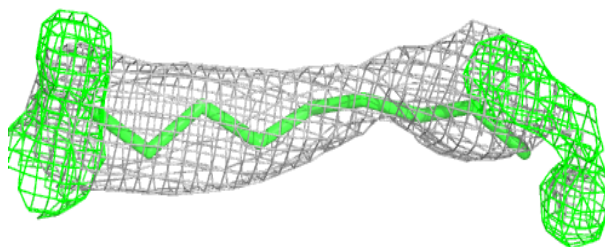
**Electron density around LFA A 318:**

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

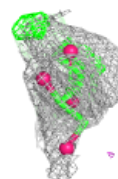
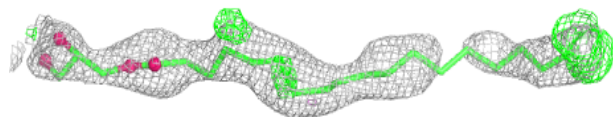
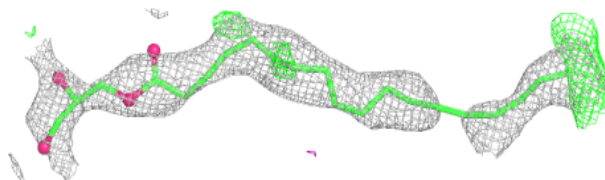


Electron density around LFA A 319:

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

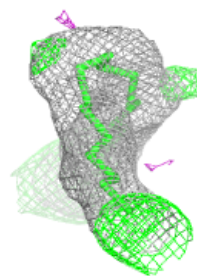
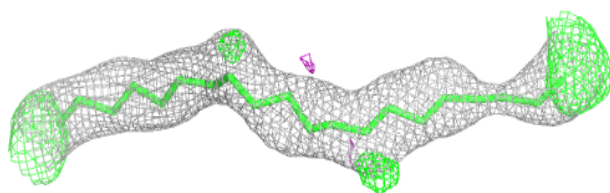
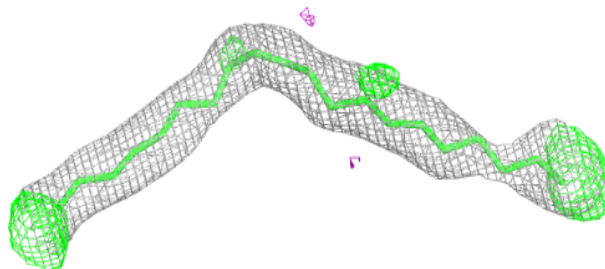
**Electron density around OLC B 303:**

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

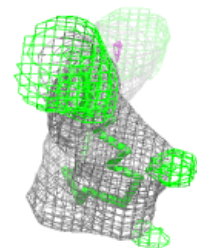
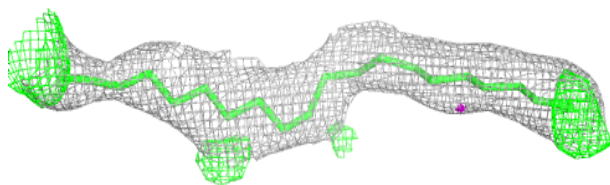
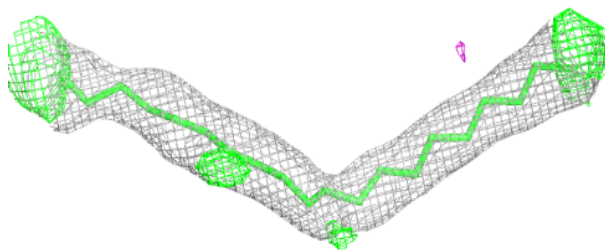


Electron density around LFA E 303:

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

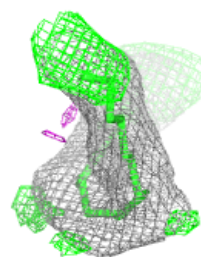
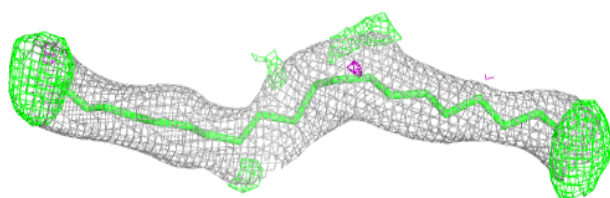
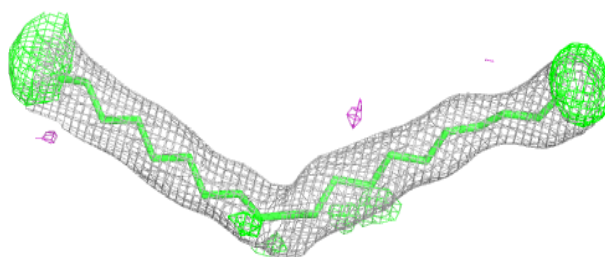
**Electron density around LFA B 302:**

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

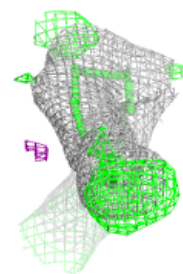
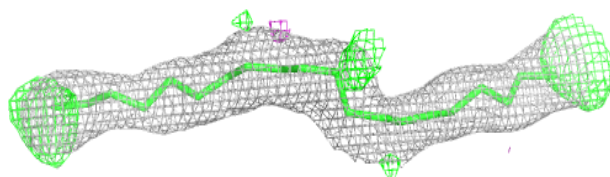
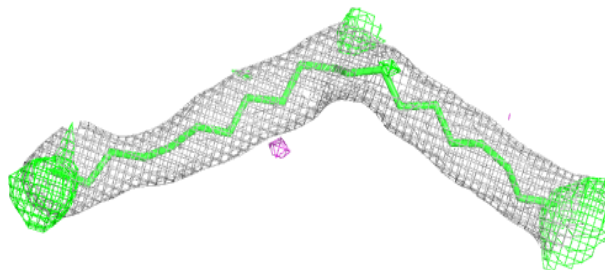


Electron density around LFA D 301:

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

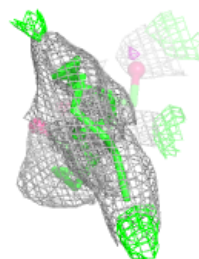
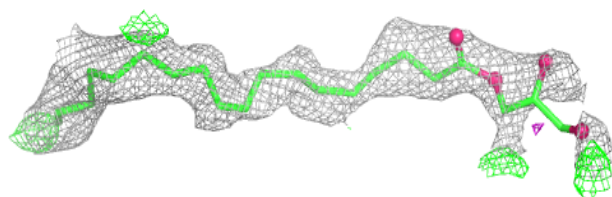
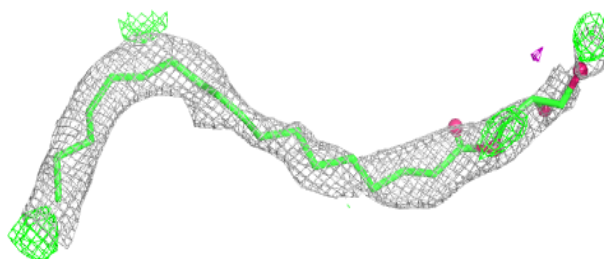
**Electron density around LFA C 304:**

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

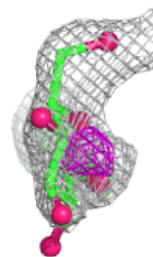
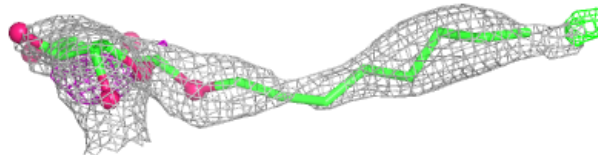
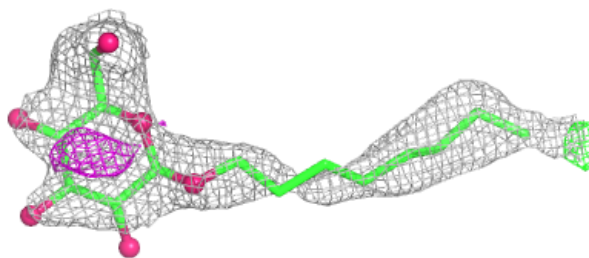


Electron density around OLC A 305:

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

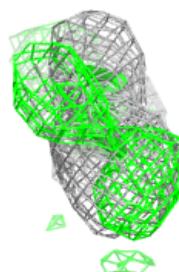
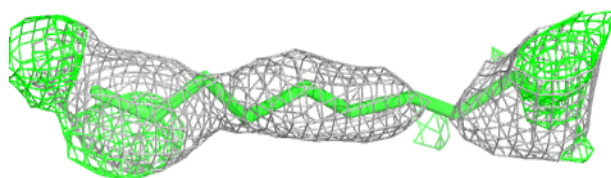
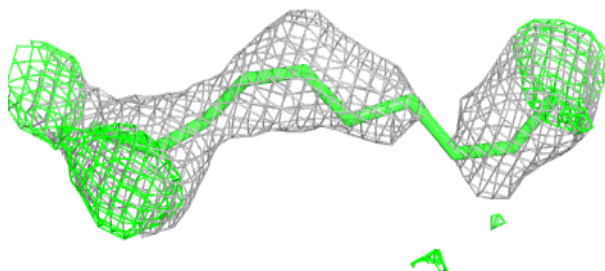
**Electron density around BOG B 312:**

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

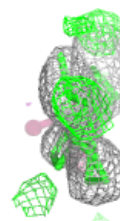
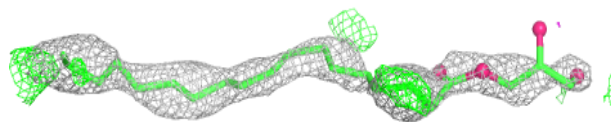
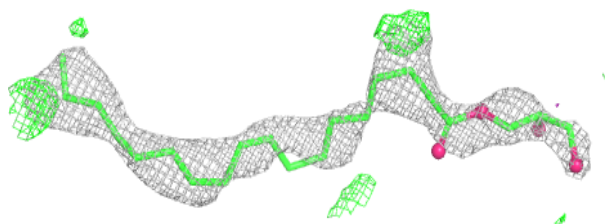


Electron density around LFA B 310:

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

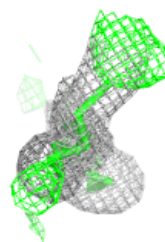
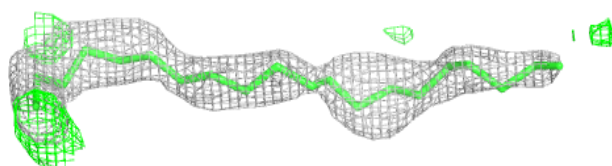
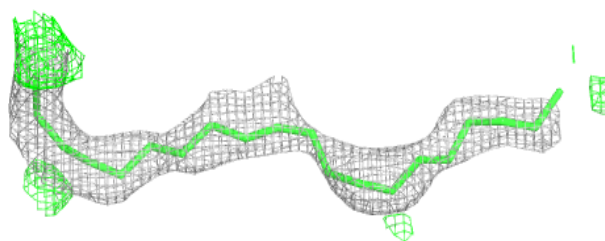
**Electron density around OLC A 303:**

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

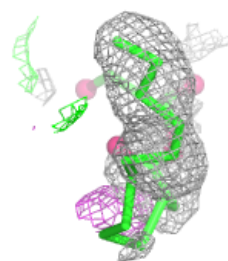
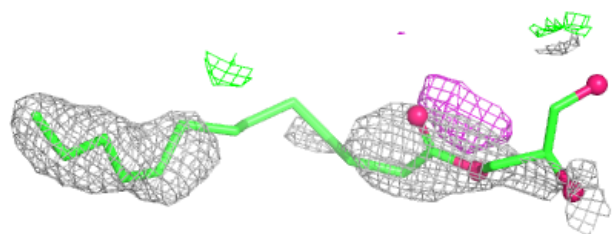
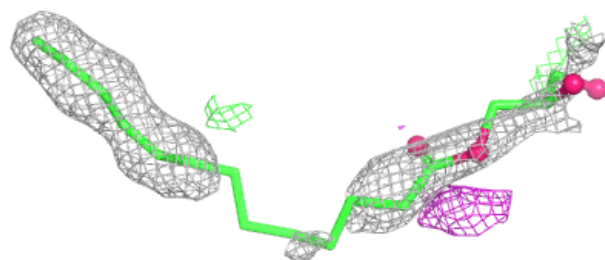


Electron density around LFA D 310:

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

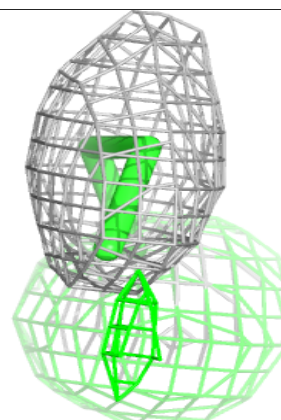
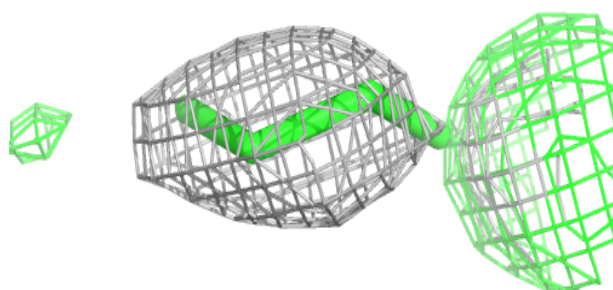
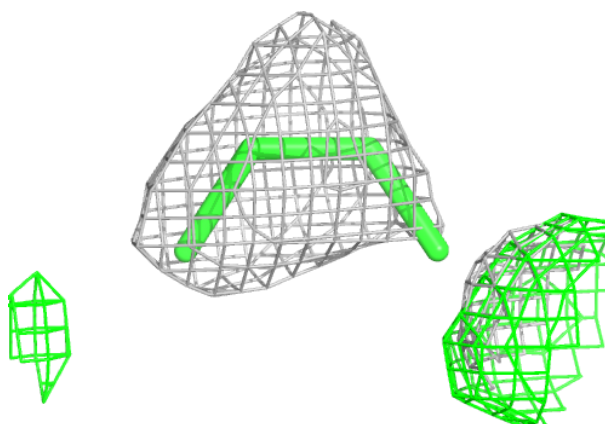
**Electron density around OLC E 311:**

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

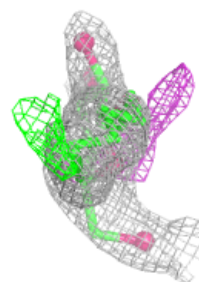
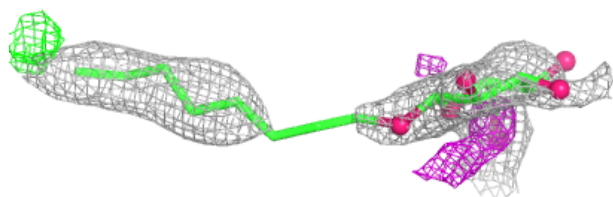
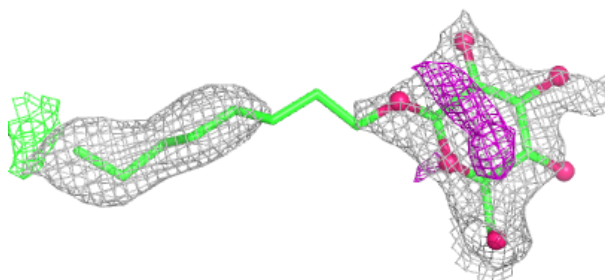


Electron density around LFA C 315:

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

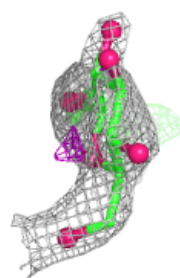
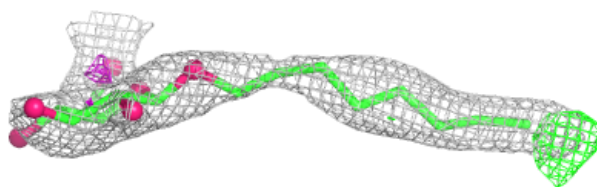
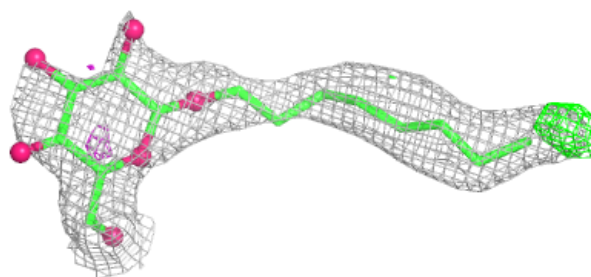
**Electron density around BOG A 315:**

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

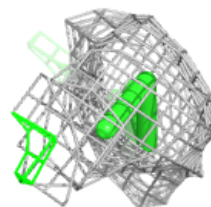
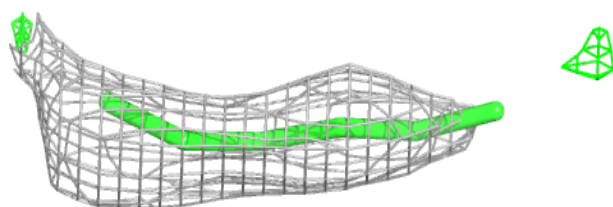
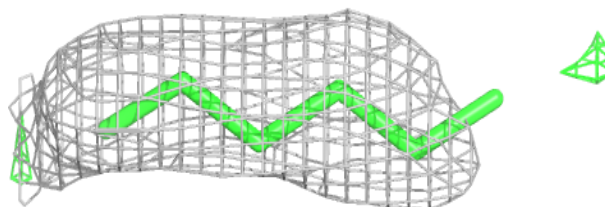


Electron density around BOG E 316:

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

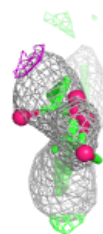
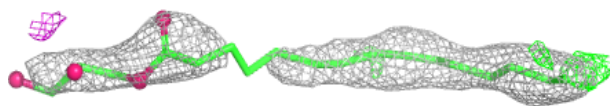
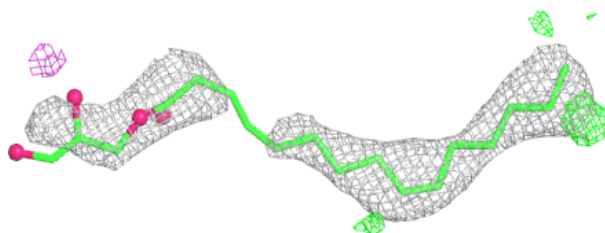
**Electron density around LFA D 315:**

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

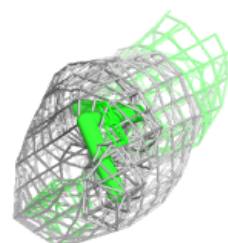
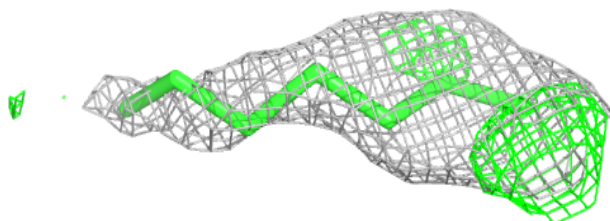
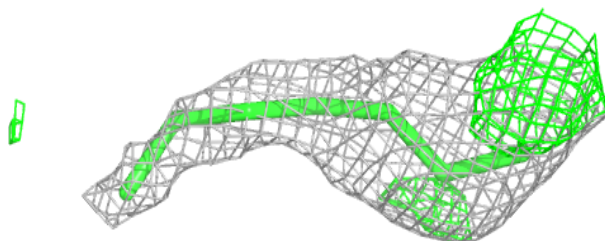


Electron density around OLC C 306:

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

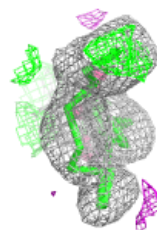
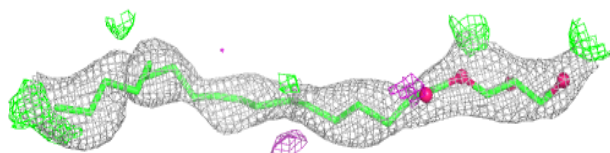
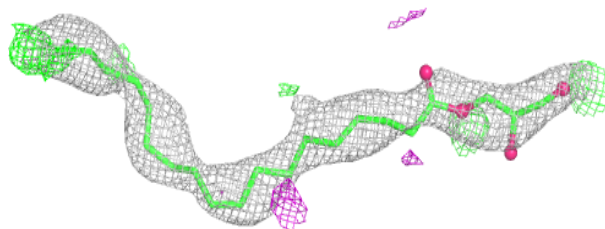
**Electron density around LFA C 311:**

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

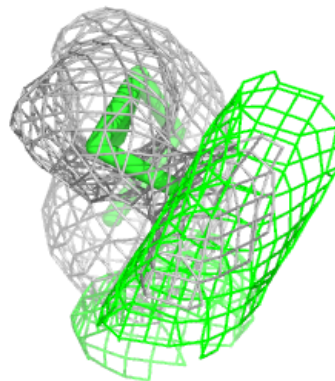
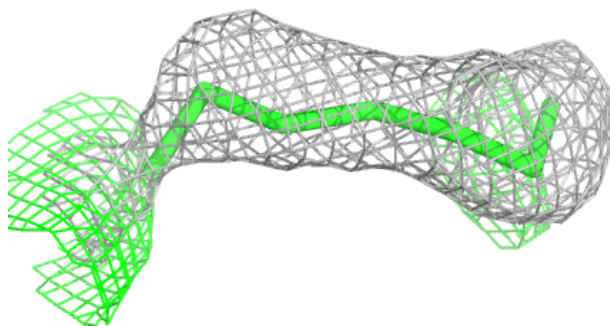
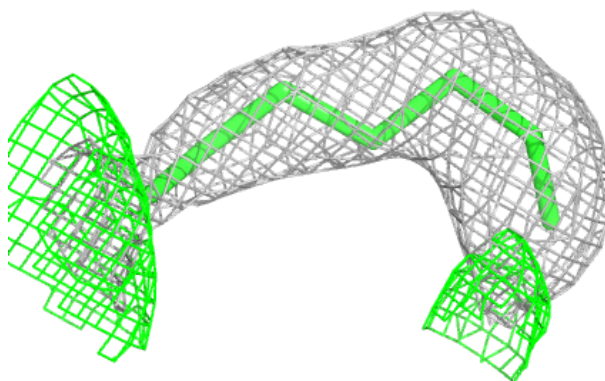


Electron density around OLC D 309:

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

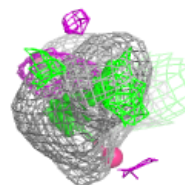
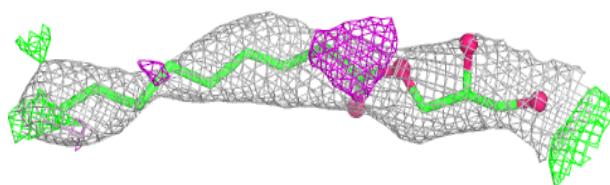
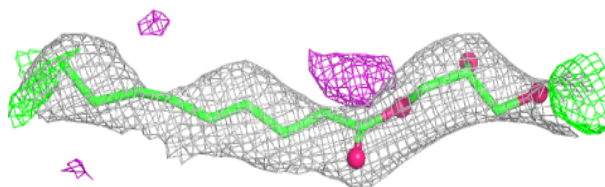
**Electron density around OLC D 308:**

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

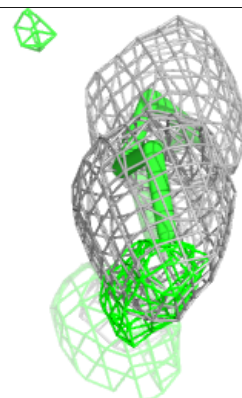
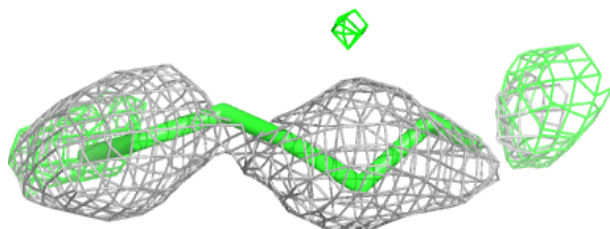
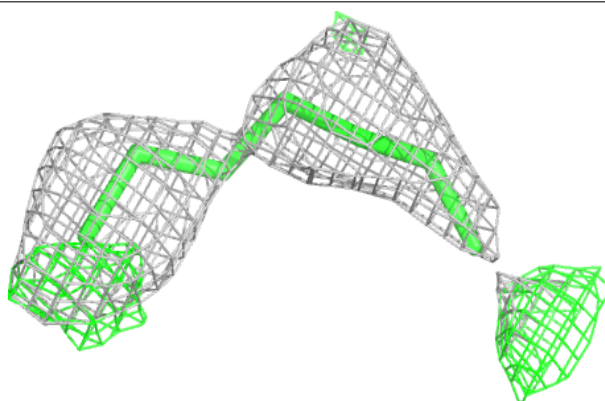


Electron density around OLC D 302:

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

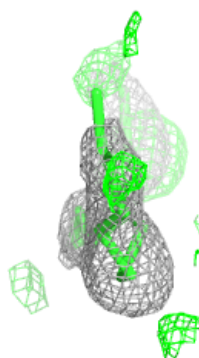
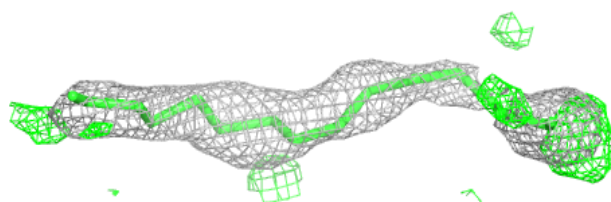
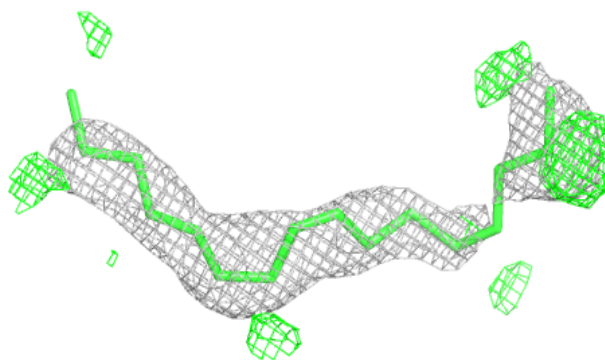
**Electron density around LFA D 314:**

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

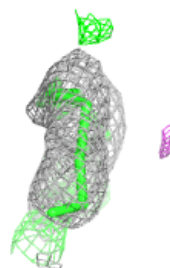
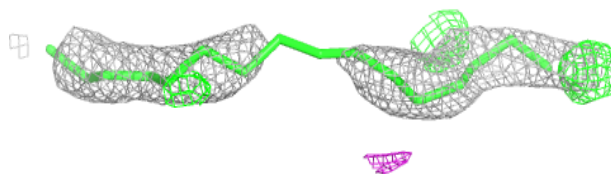
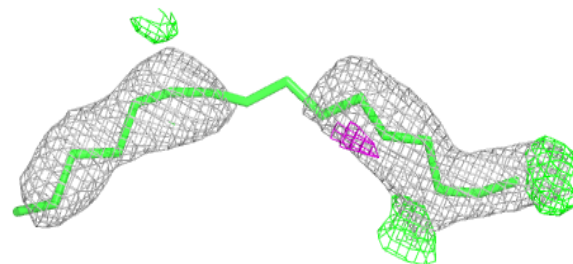


Electron density around OLC E 305:

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

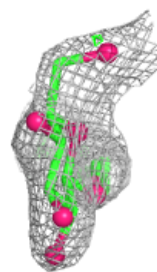
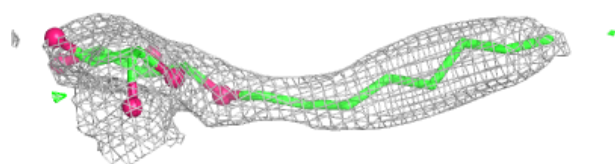
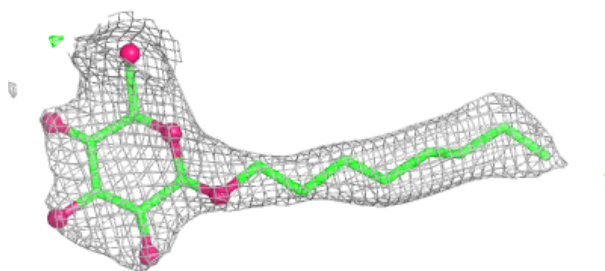
**Electron density around LFA A 314:**

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

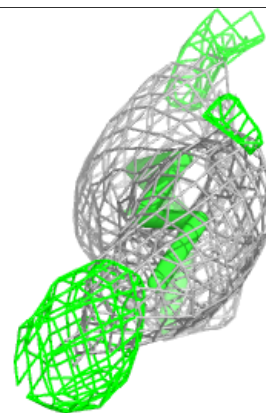
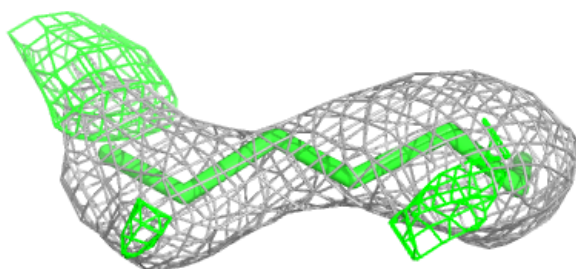
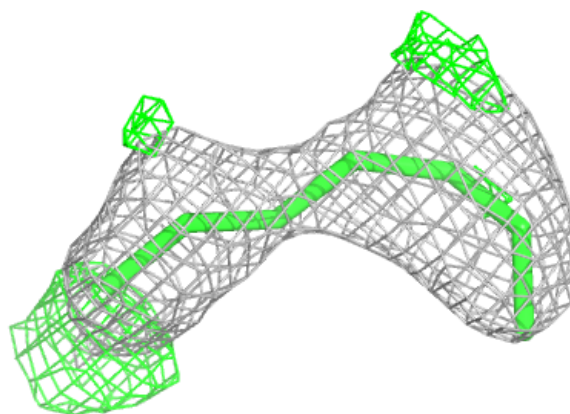


Electron density around BOG C 316:

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

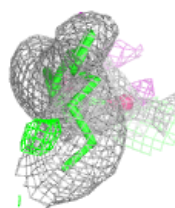
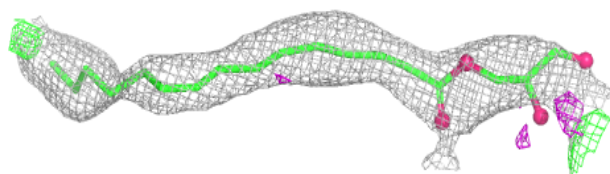
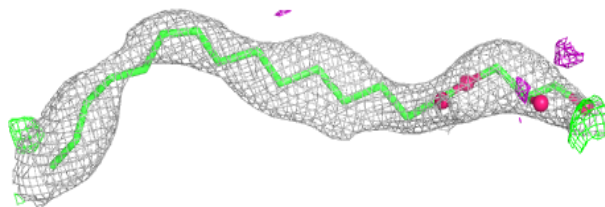
**Electron density around LFA A 309:**

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

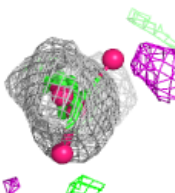
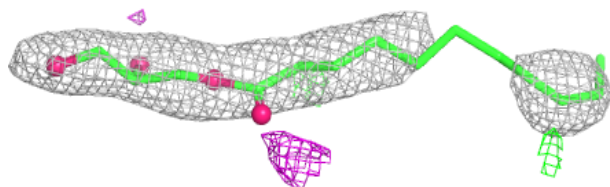
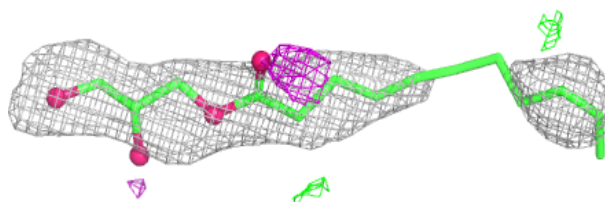


Electron density around OLC E 310:

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

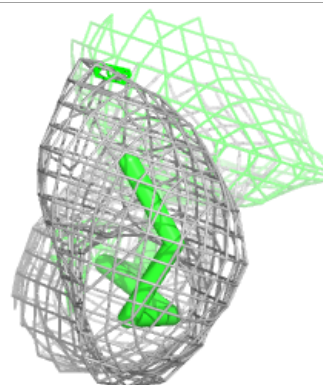
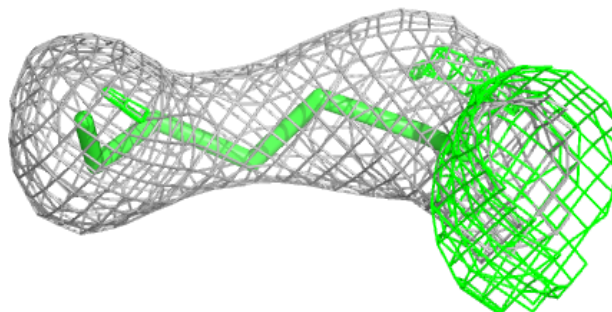
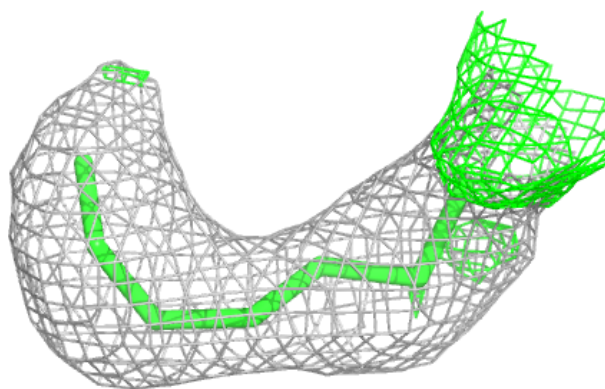
**Electron density around OLC D 305:**

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

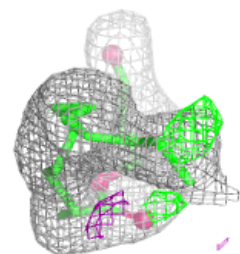
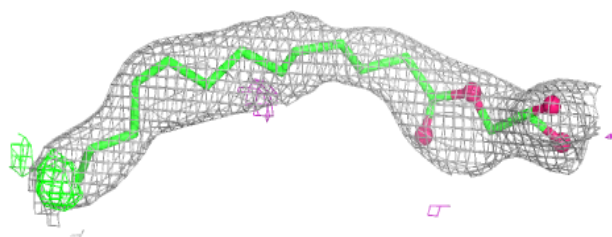
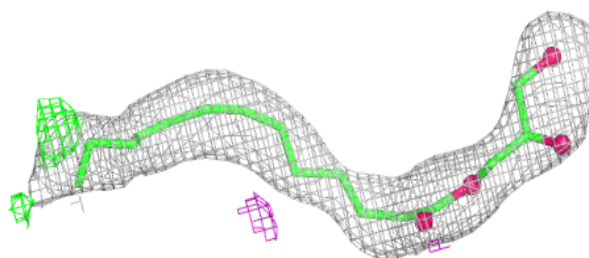


Electron density around OLC B 307:

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

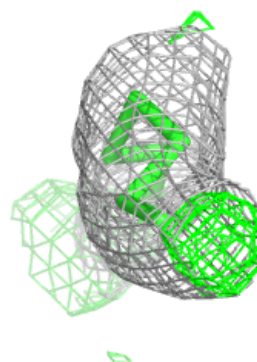
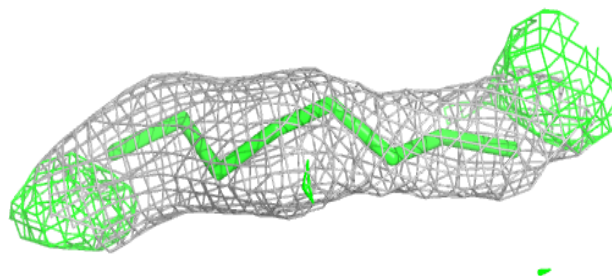
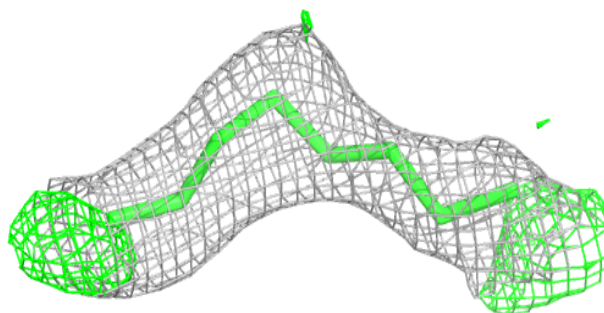
**Electron density around OLC C 302:**

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

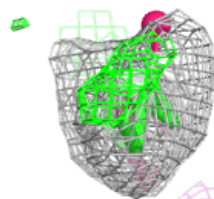
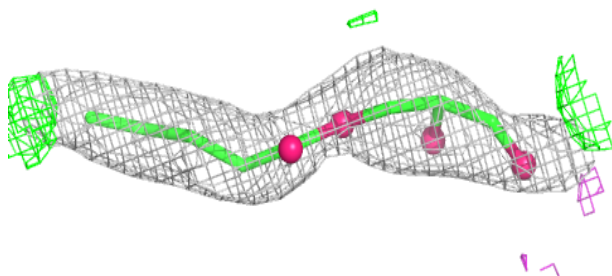
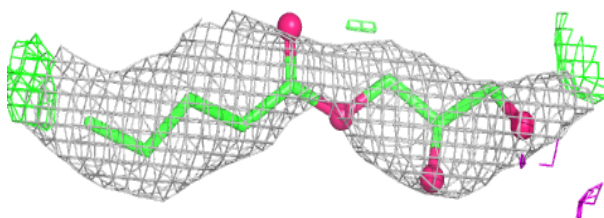


Electron density around OLC E 304:

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

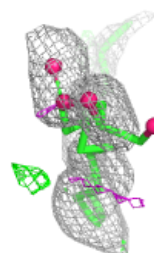
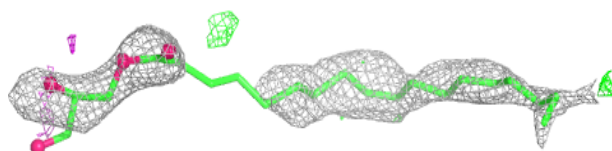
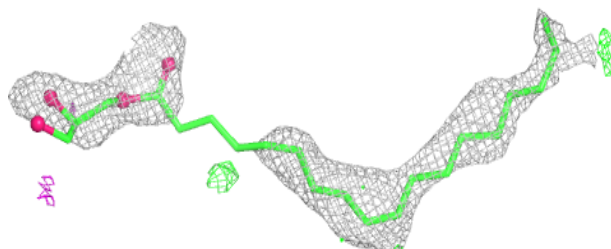
**Electron density around OLC C 303:**

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

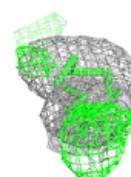
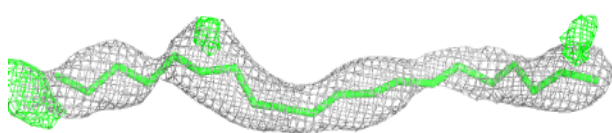
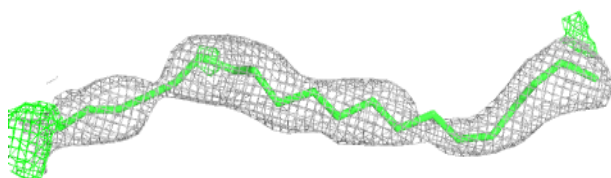


Electron density around OLC D 304:

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

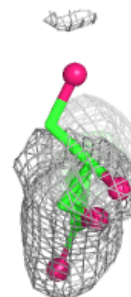
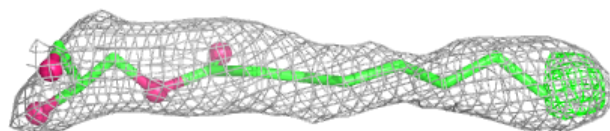
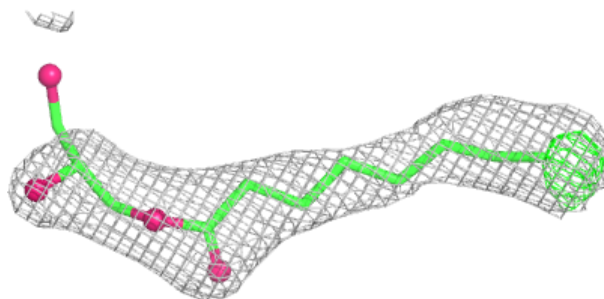
**Electron density around LFA D 311:**

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

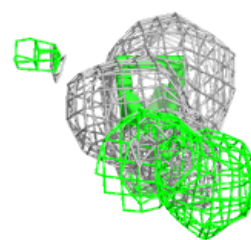
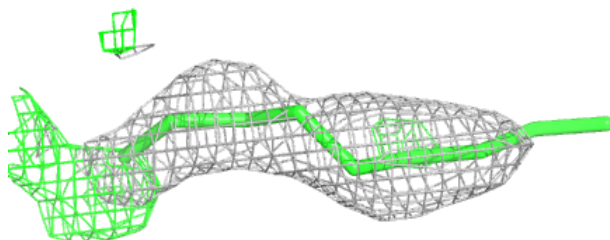
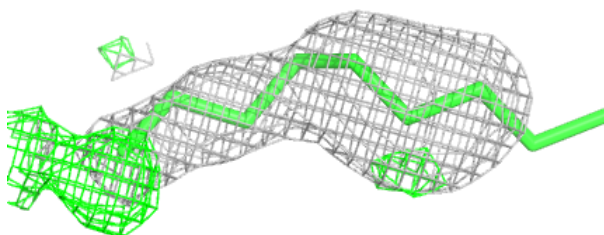


Electron density around OLC A 306:

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

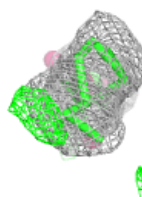
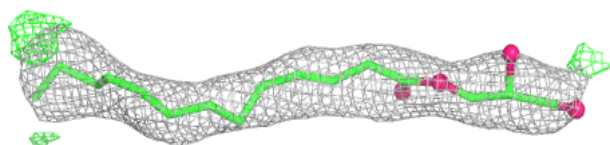
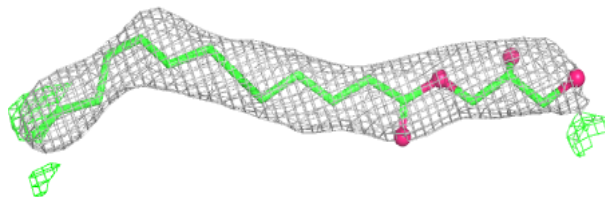
**Electron density around LFA B 308:**

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

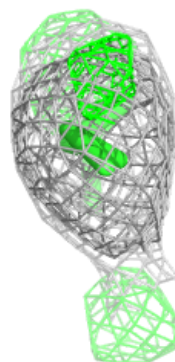
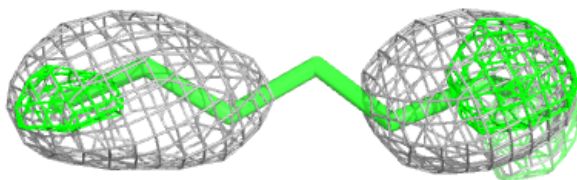
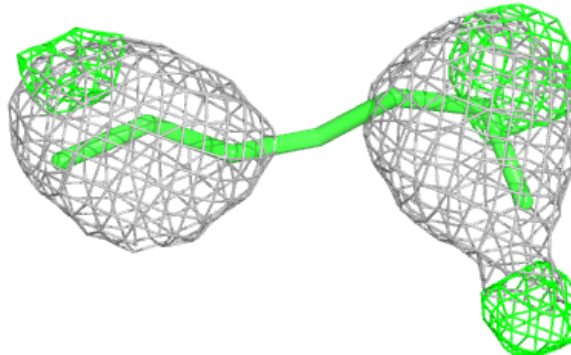


Electron density around OLC E 306:

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

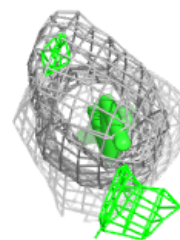
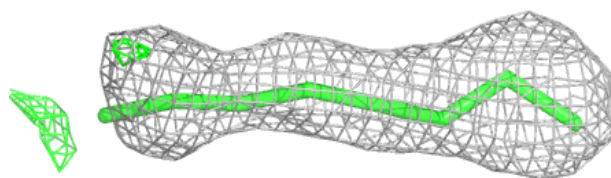
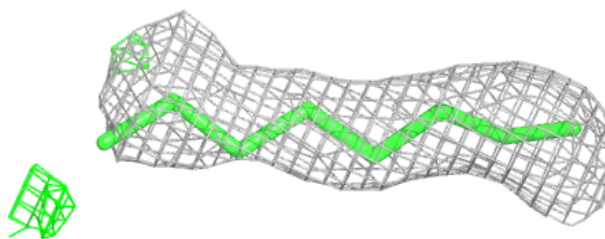
**Electron density around LFA B 311:**

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

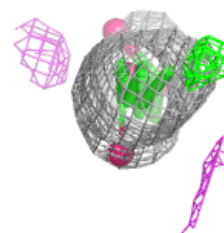
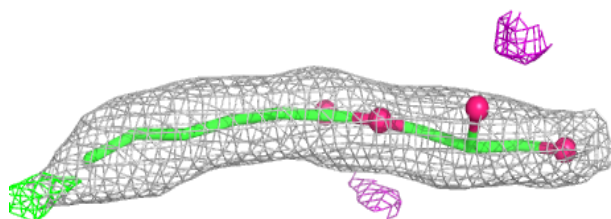
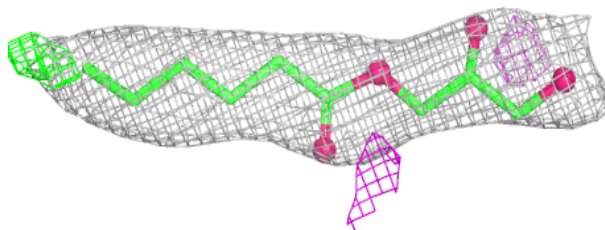


Electron density around LFA E 312:

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

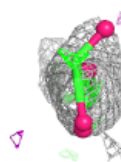
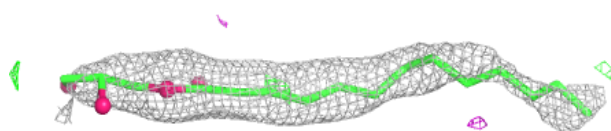
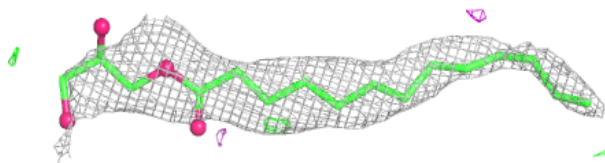
**Electron density around OLC A 304:**

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

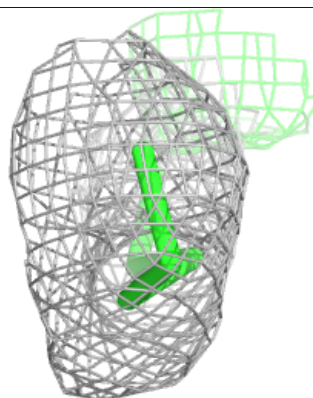
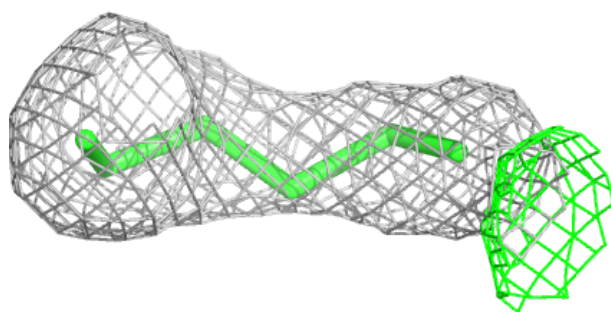
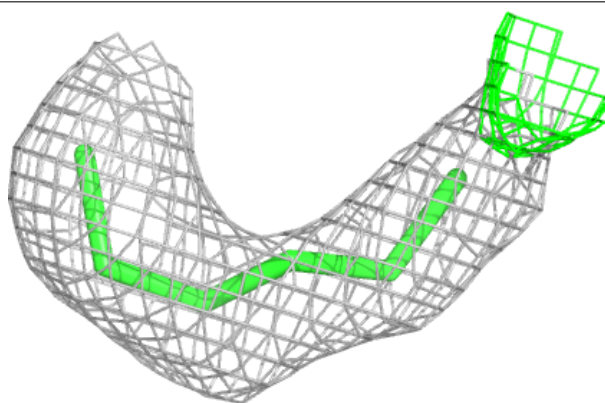


Electron density around OLC C 307:

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

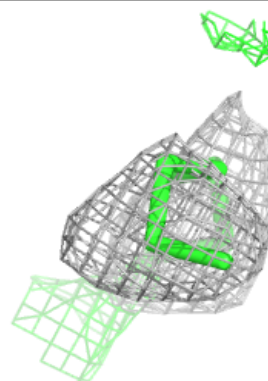
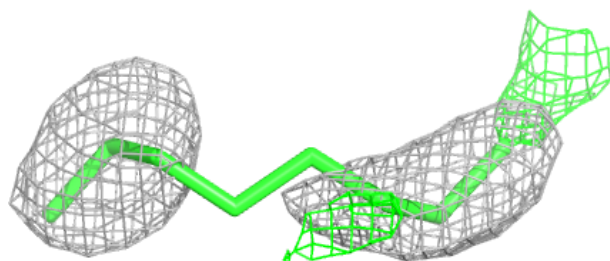
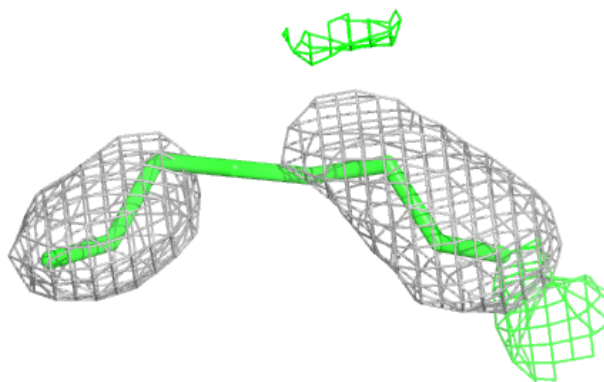
**Electron density around OLC E 309:**

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

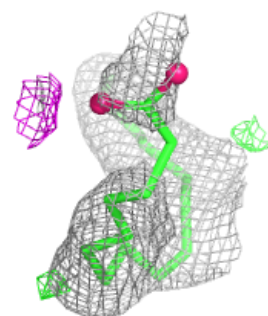
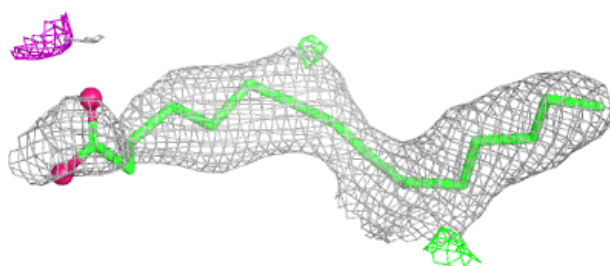
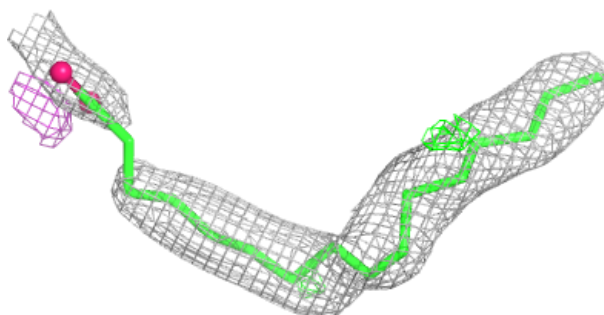


Electron density around LFA D 312:

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

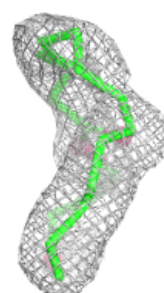
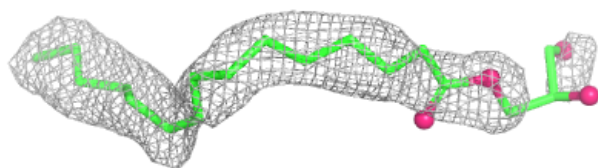
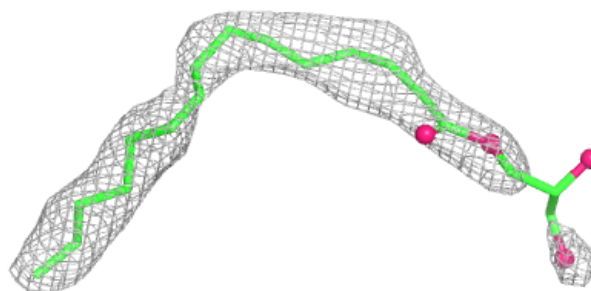
**Electron density around OLC D 306:**

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

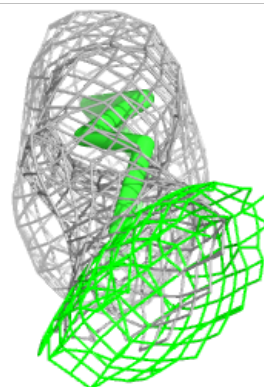
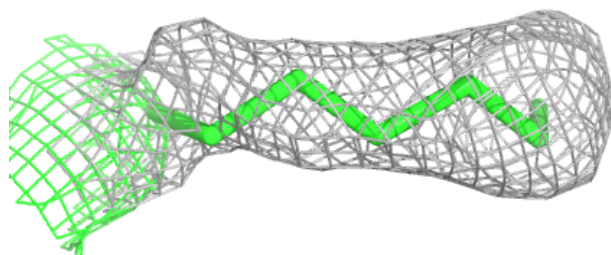
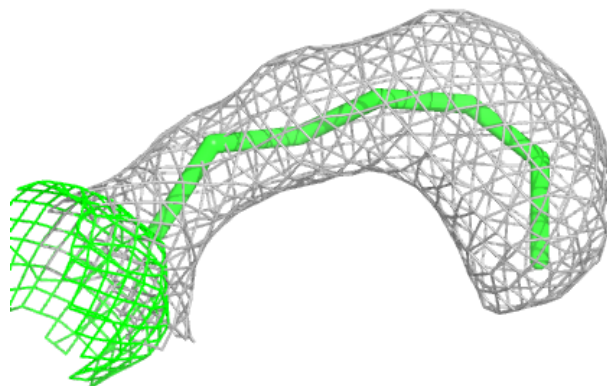


Electron density around OLC C 308:

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

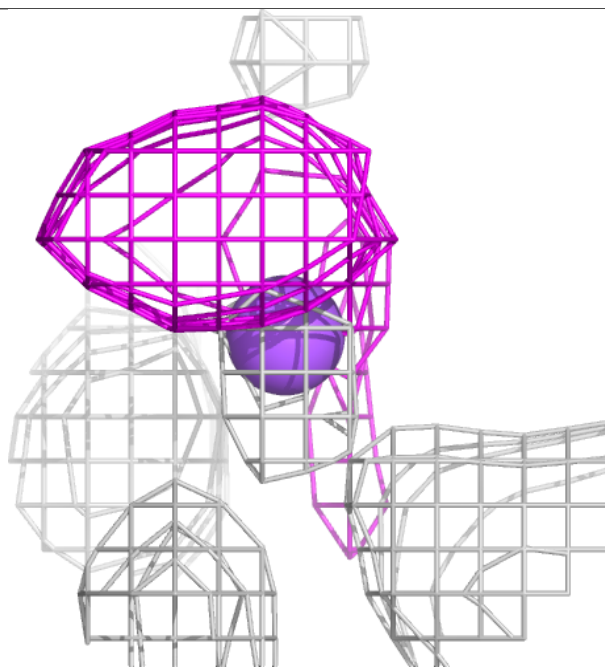
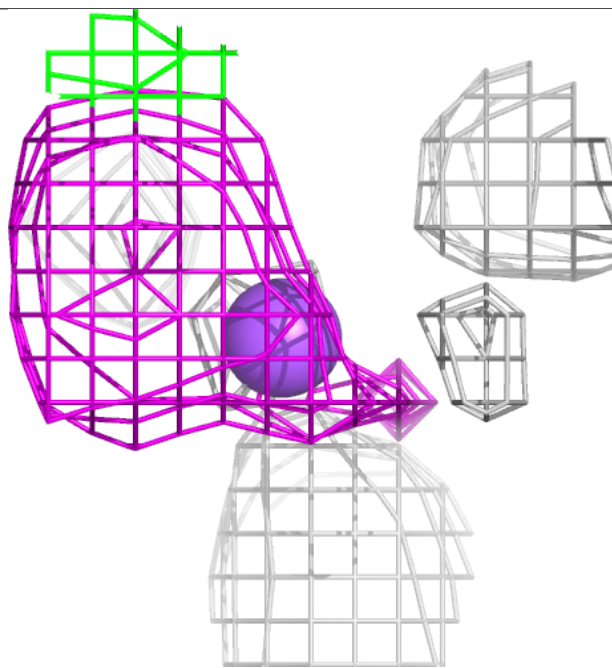
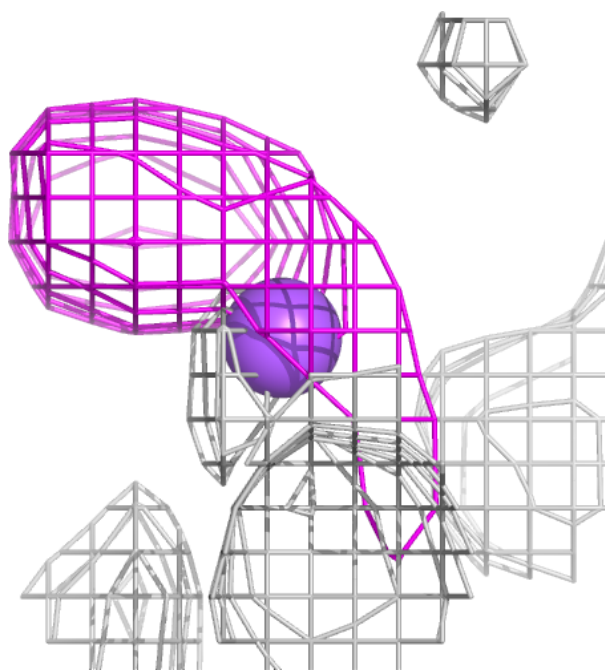
**Electron density around OLC C 310:**

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



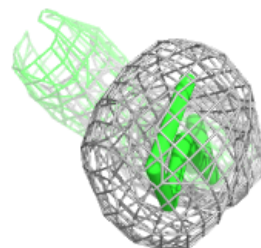
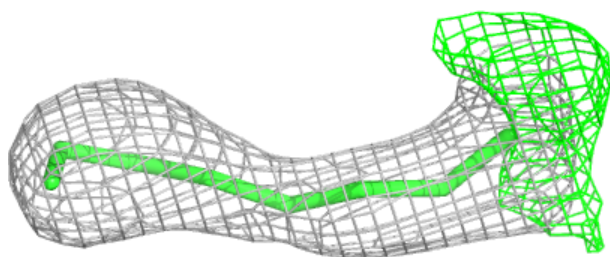
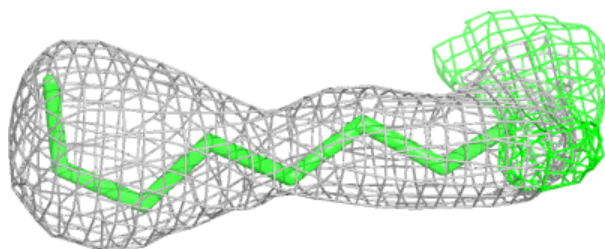
Electron density around NA E 319:

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

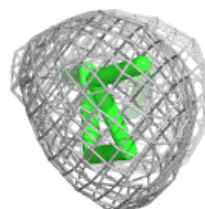
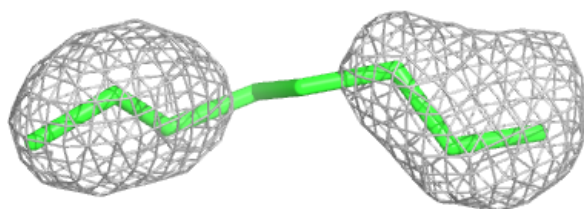
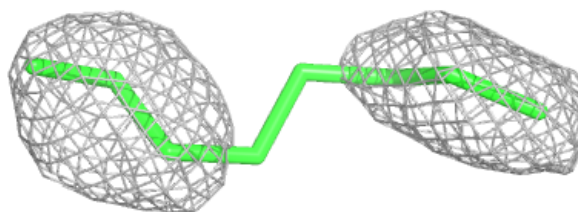


Electron density around LFA A 310:

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

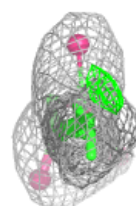
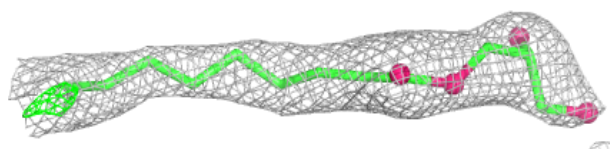
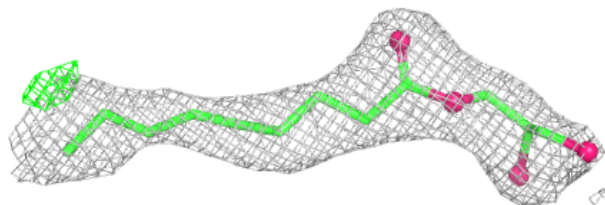
**Electron density around LFA A 311:**

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

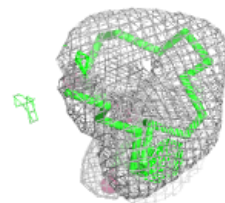
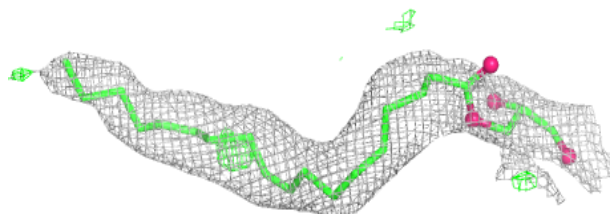
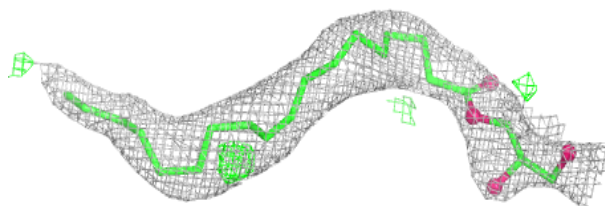


Electron density around OLC C 309:

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

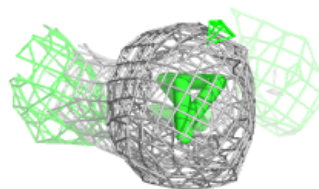
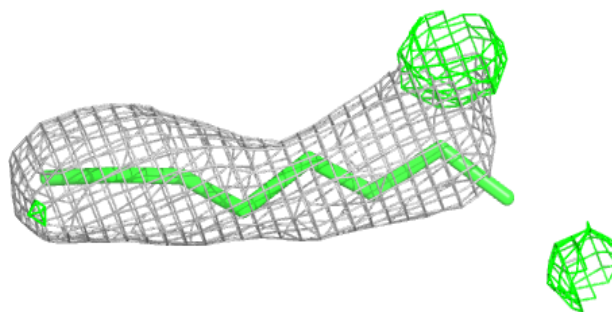
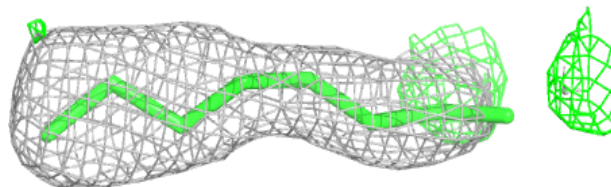
**Electron density around OLC E 302:**

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

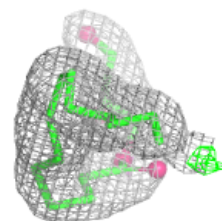
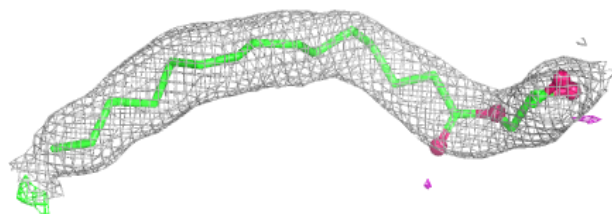
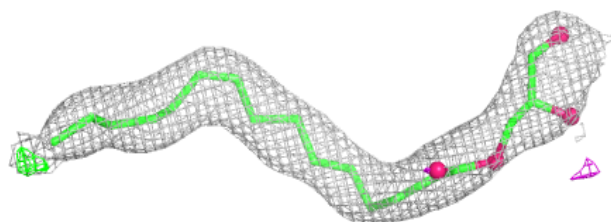


Electron density around LFA B 309:

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

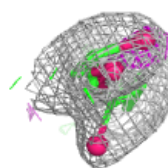
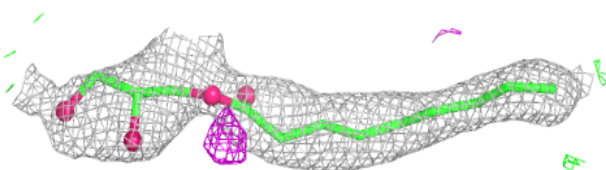
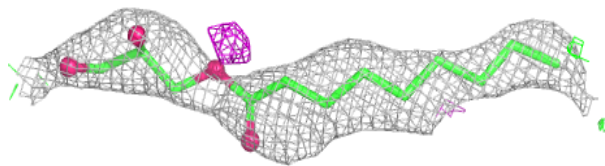
**Electron density around OLC B 301:**

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

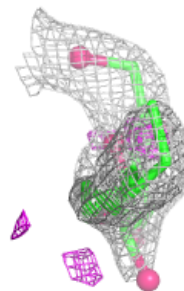
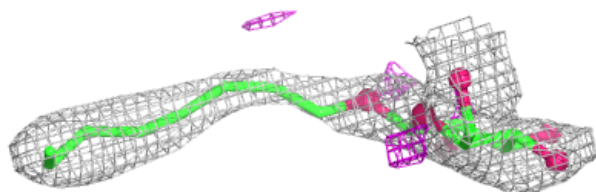
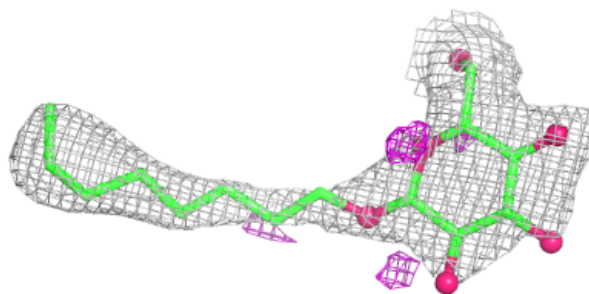


Electron density around OLC A 308:

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

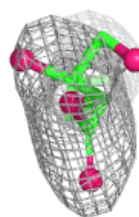
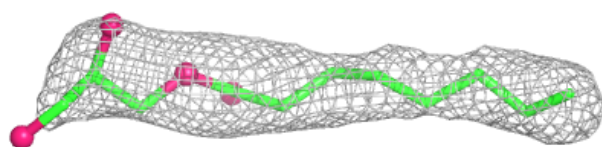
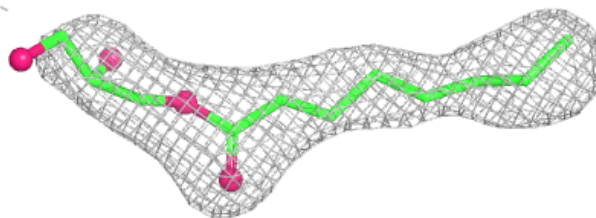
**Electron density around BOG D 316:**

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

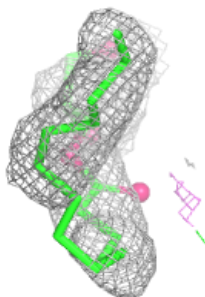
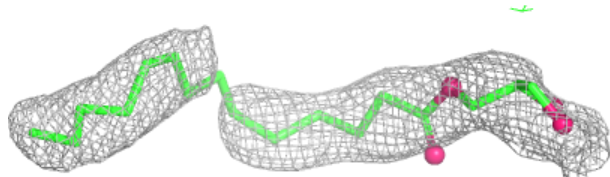
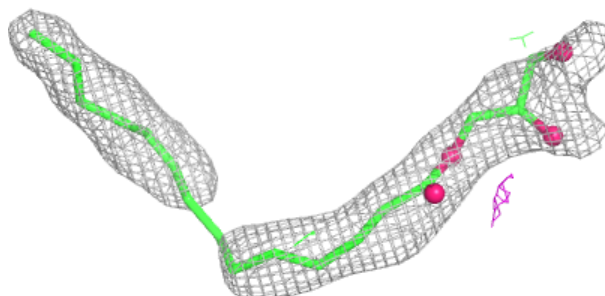


Electron density around OLC E 308:

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

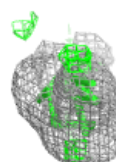
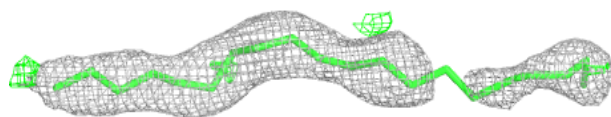
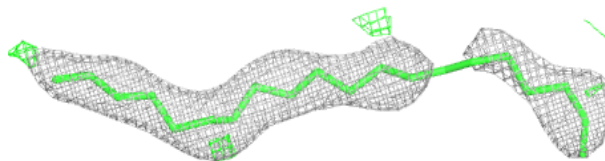
**Electron density around OLC B 305:**

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

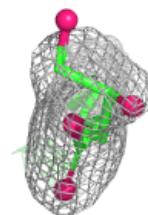
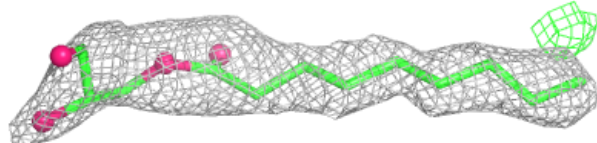
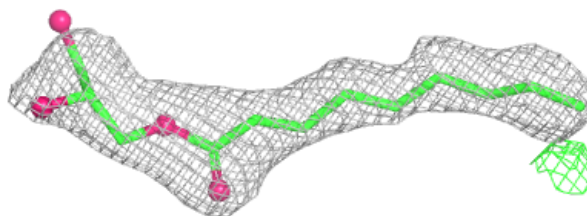


Electron density around LFA C 313:

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

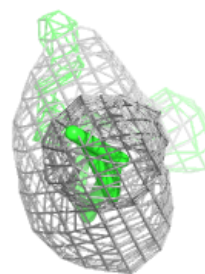
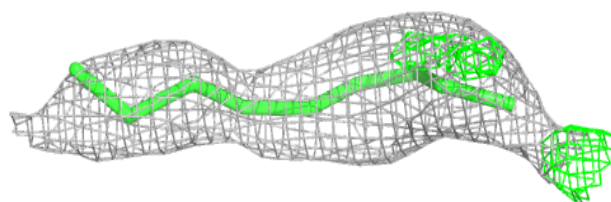
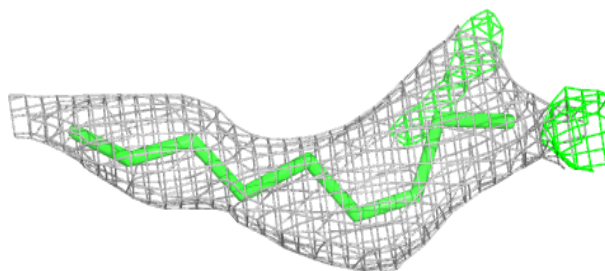
**Electron density around OLC B 306:**

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



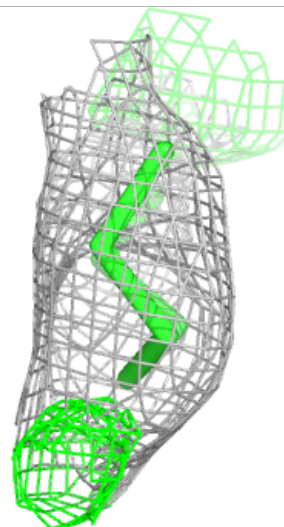
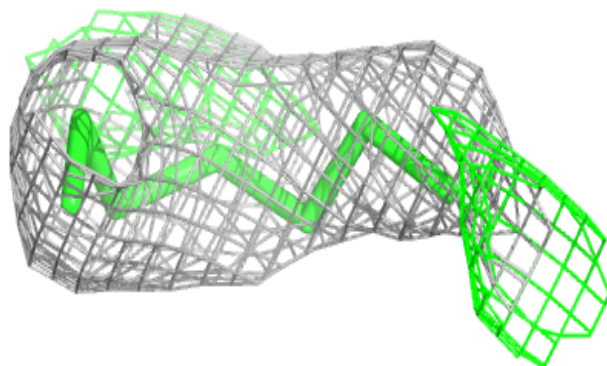
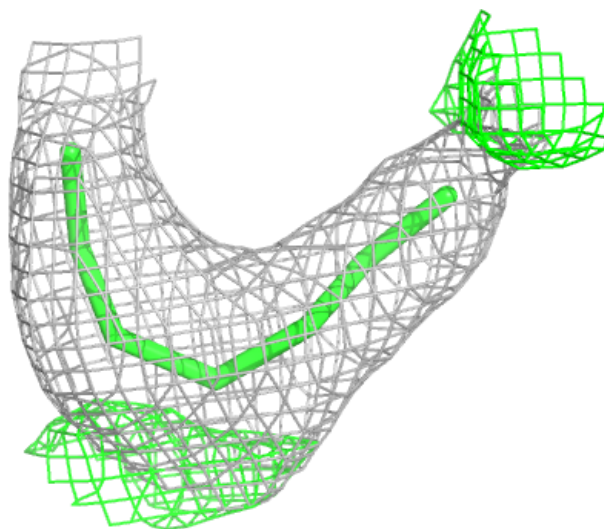
Electron density around OLC A 301:

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



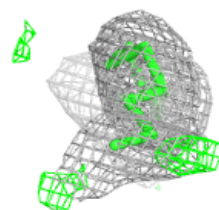
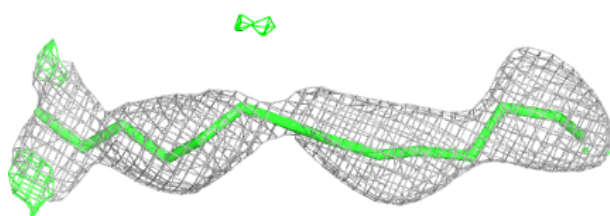
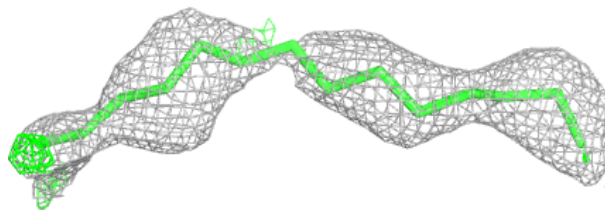
Electron density around OLC A 307:

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



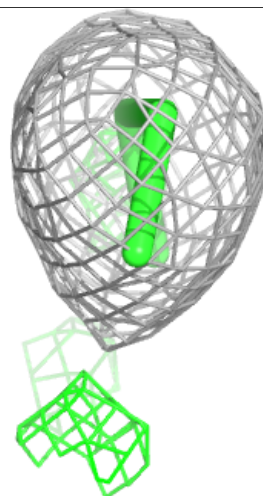
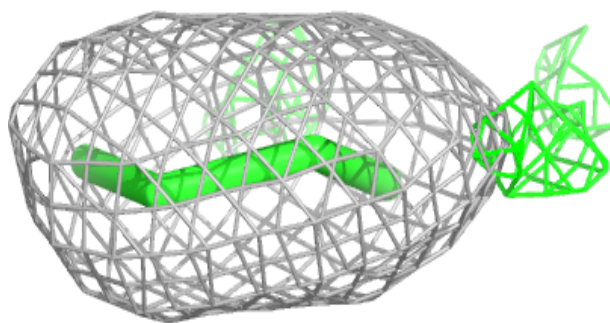
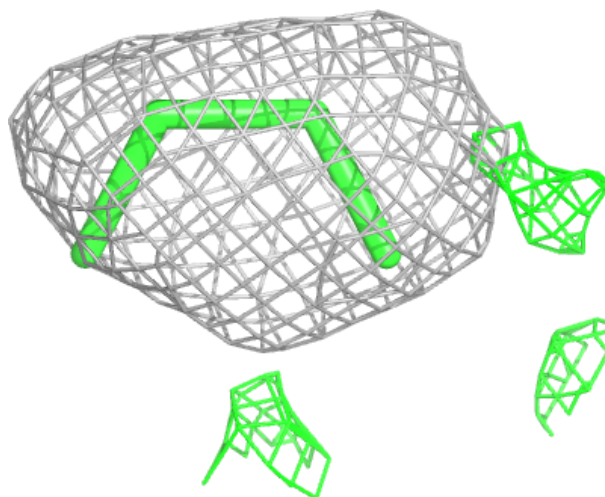
Electron density around LFA E 313:

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



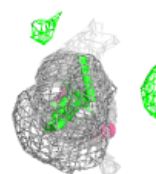
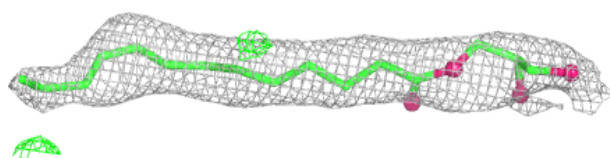
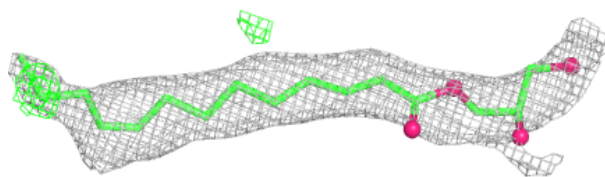
Electron density around LFA E 314:

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

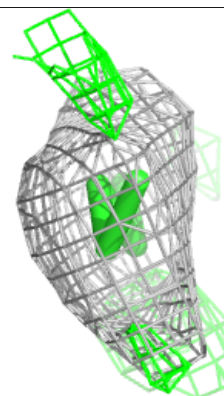
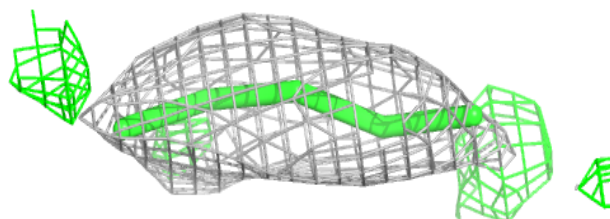
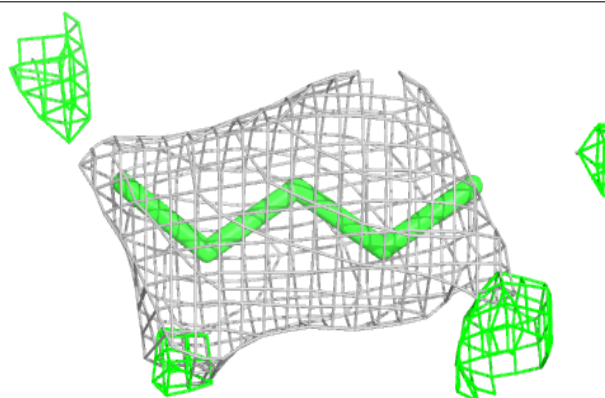


Electron density around OLC B 304:

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

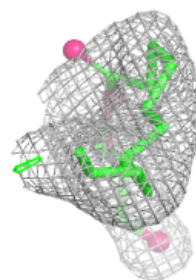
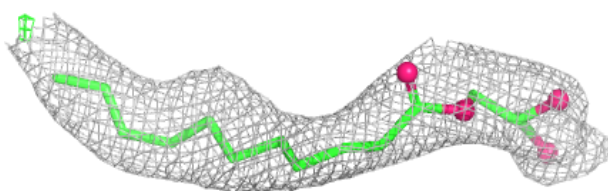
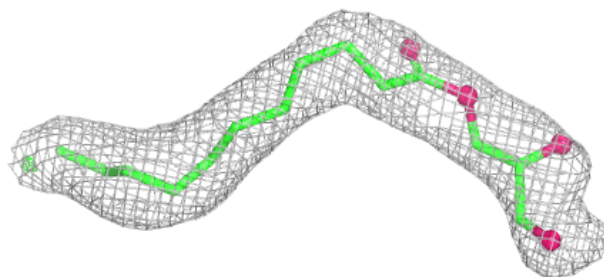
**Electron density around LFA E 315:**

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

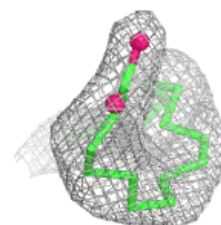
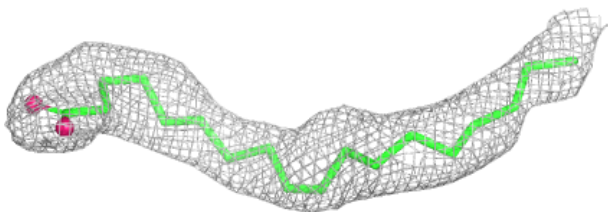
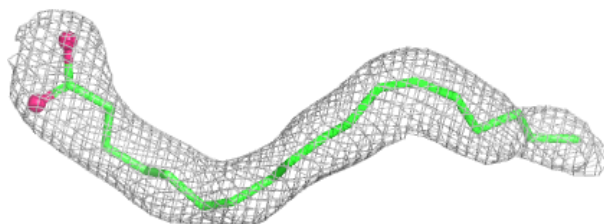


Electron density around OLC C 318:

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

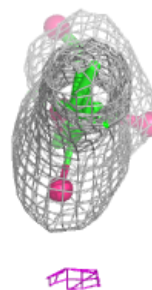
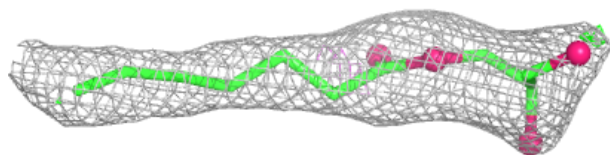
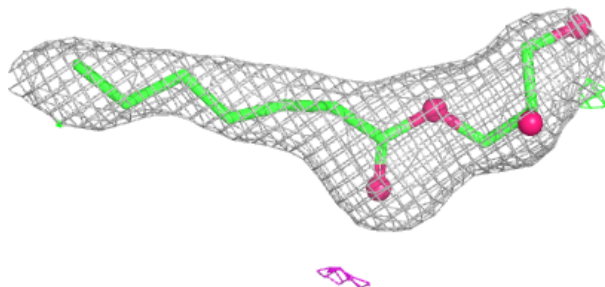
**Electron density around OLC A 317:**

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

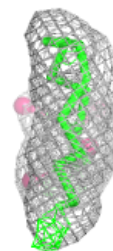
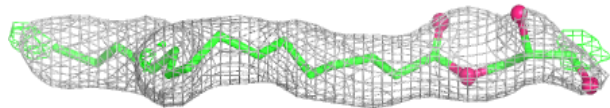
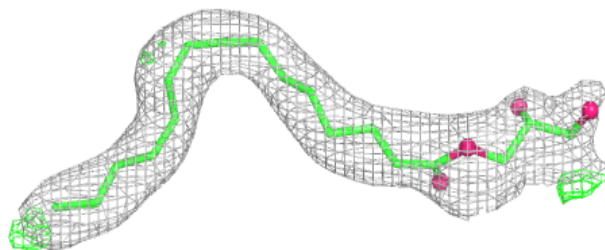


Electron density around OLC D 307:

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

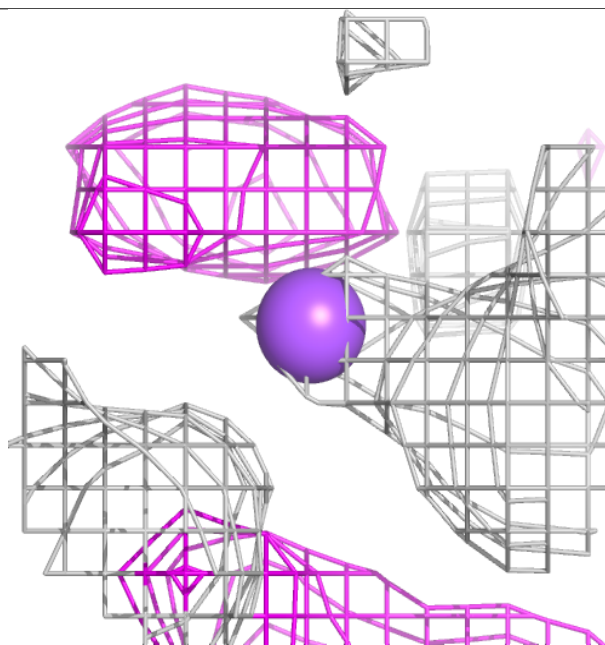
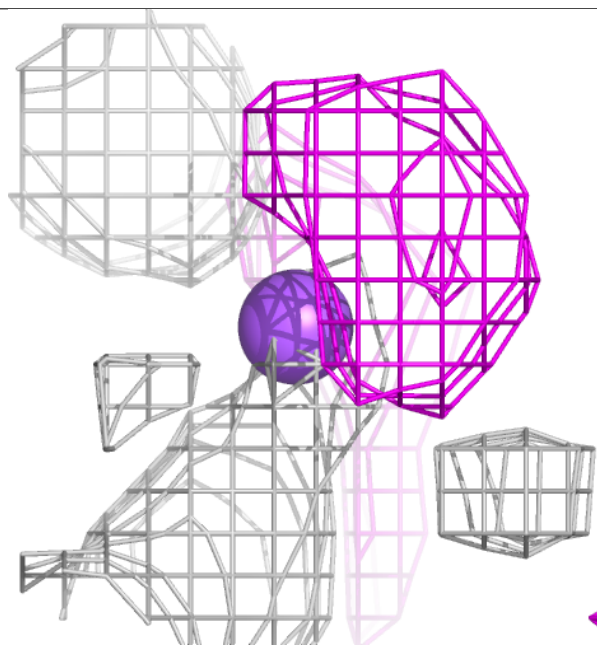
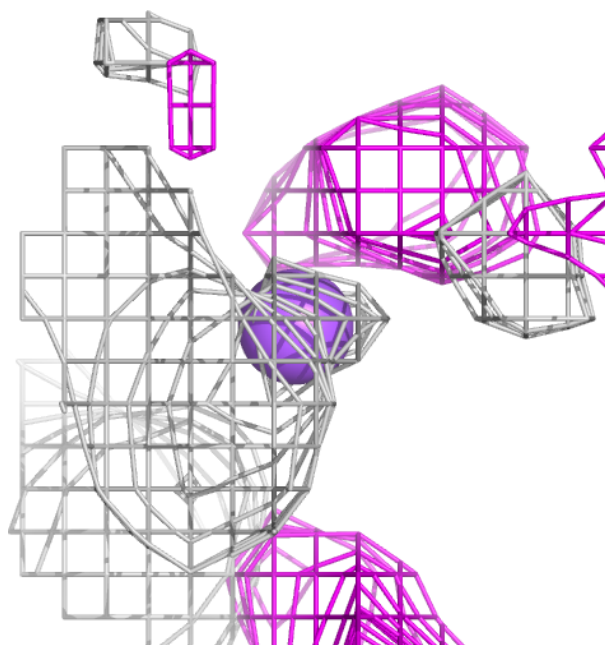
**Electron density around OLC A 302:**

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



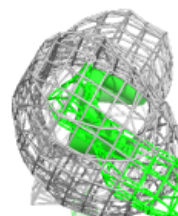
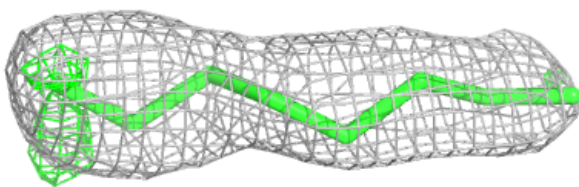
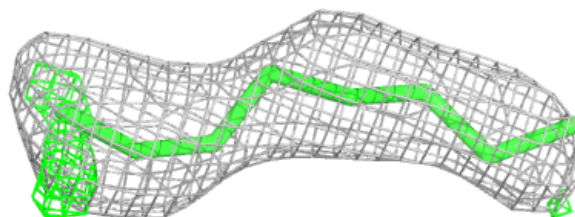
Electron density around NA B 316:

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

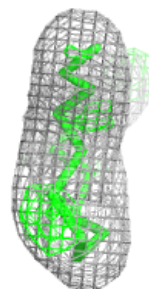
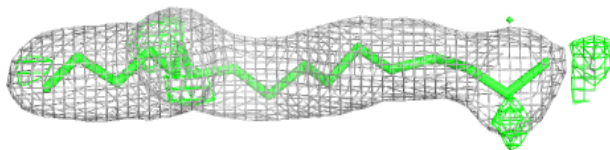
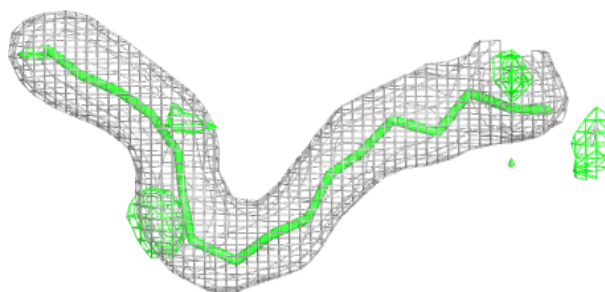


Electron density around LFA C 312:

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

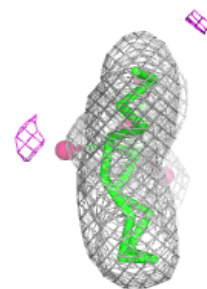
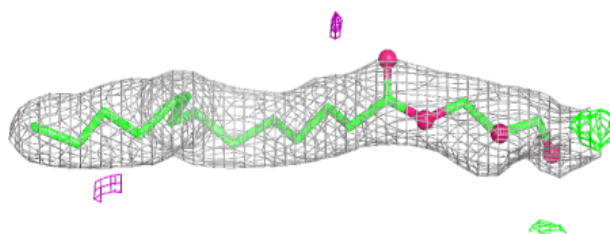
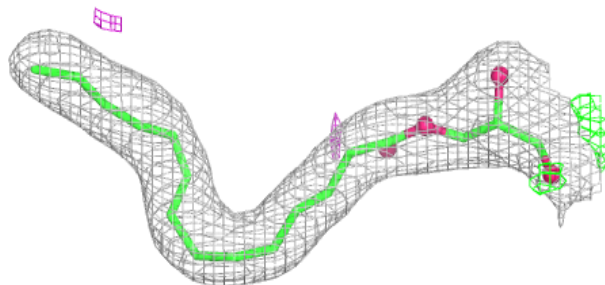
**Electron density around LFA D 313:**

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



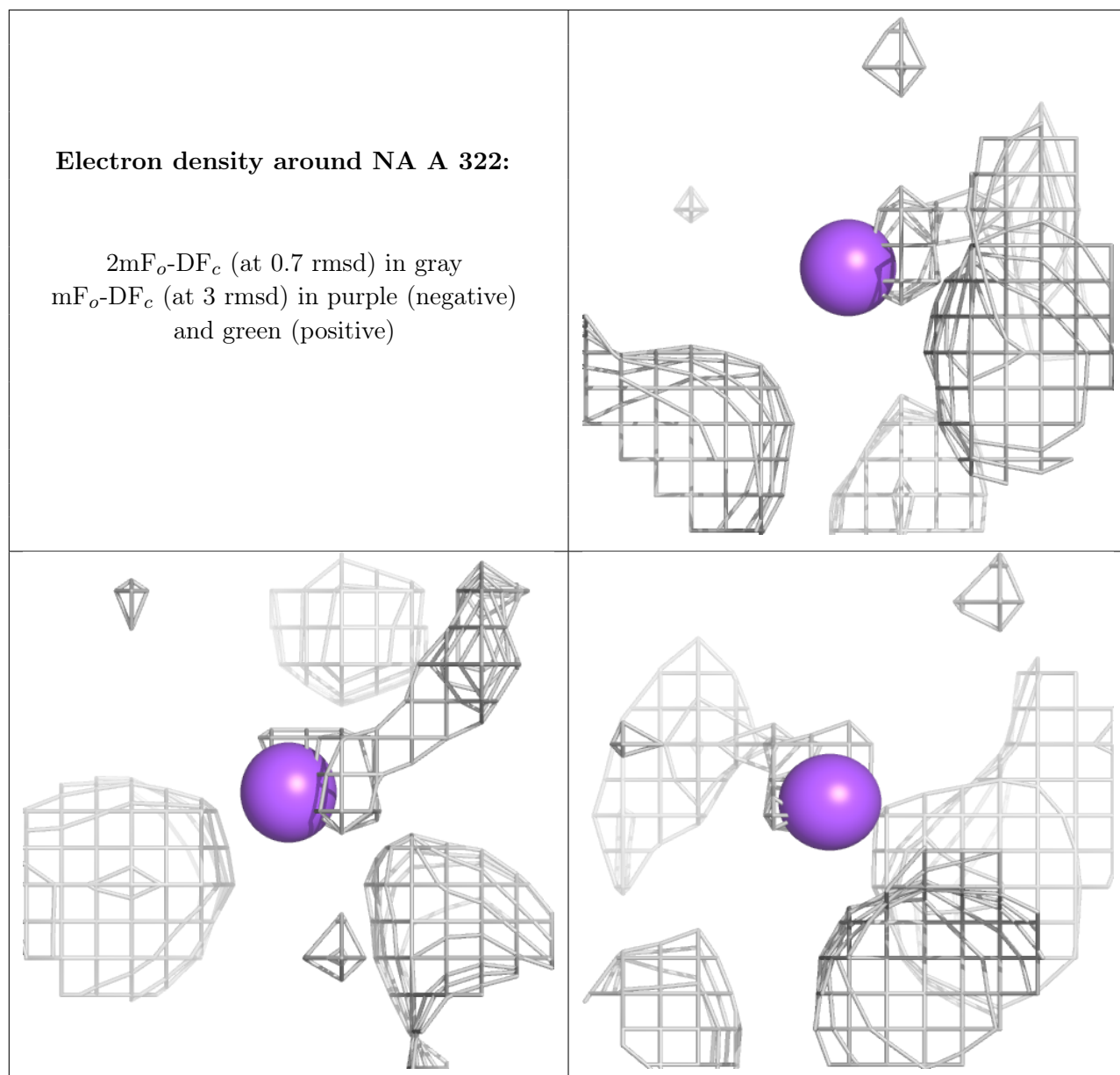
Electron density around OLC C 301:

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



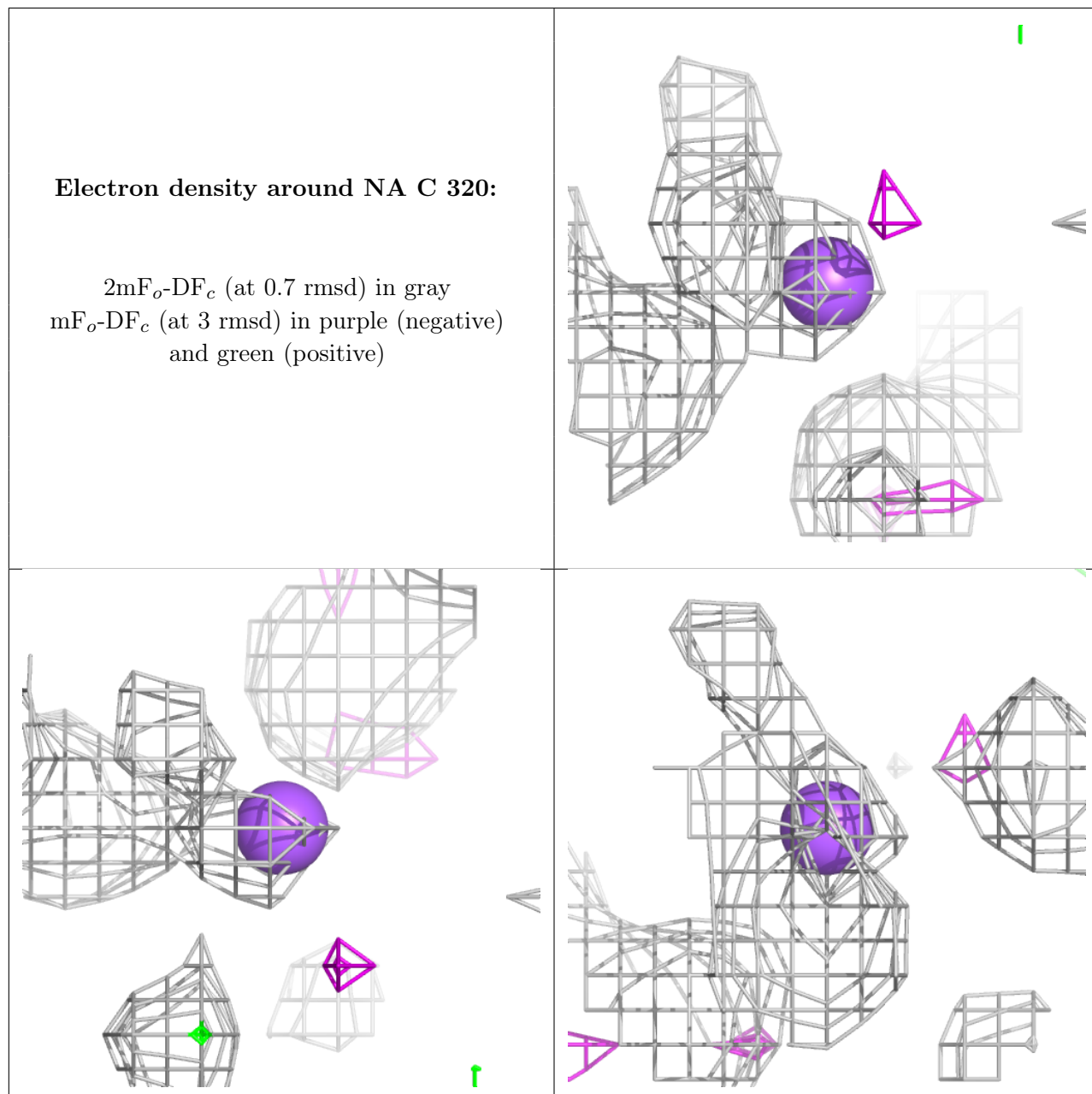
Electron density around NA A 322:

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



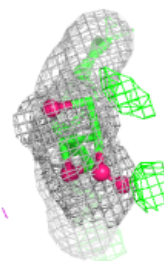
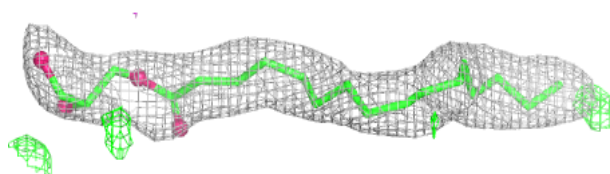
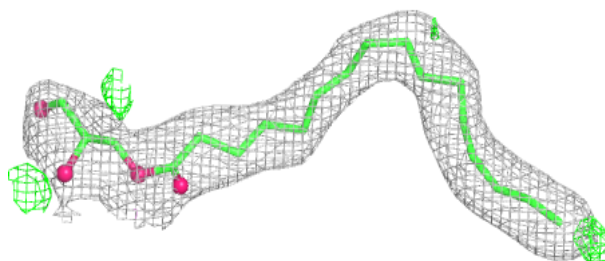
Electron density around NA C 320:

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



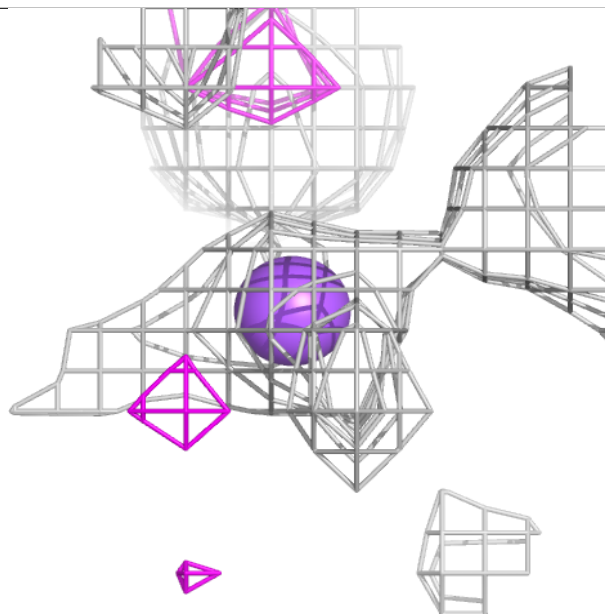
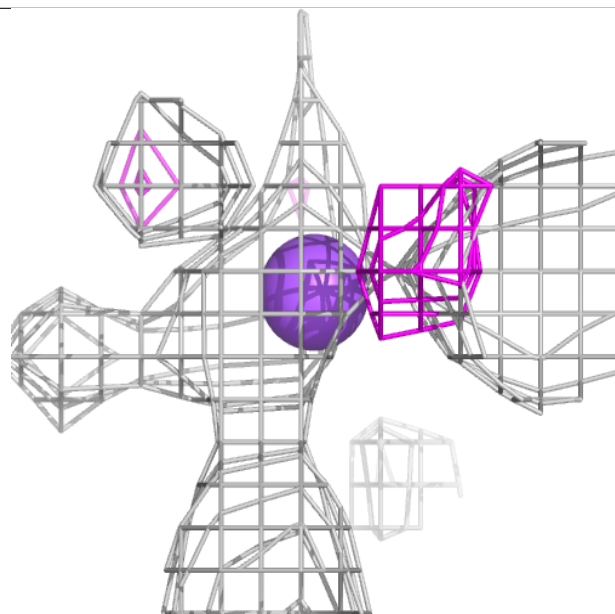
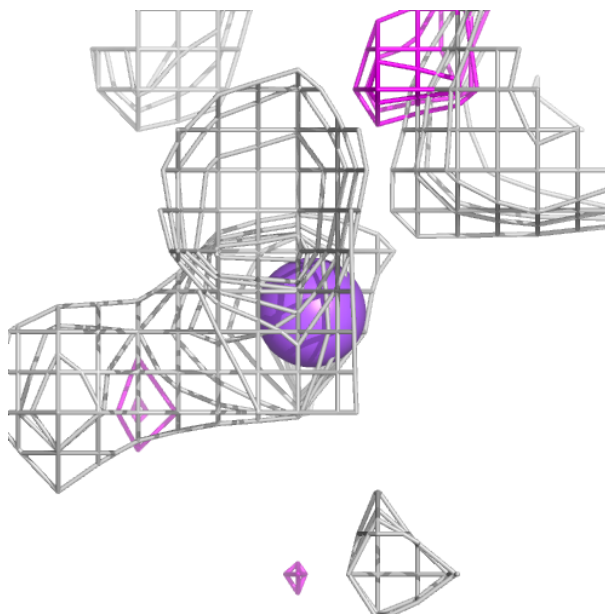
Electron density around OLC C 305:

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



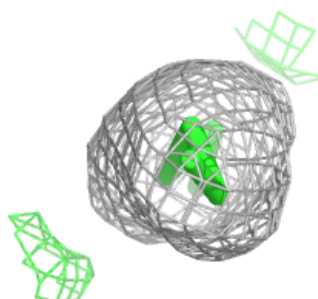
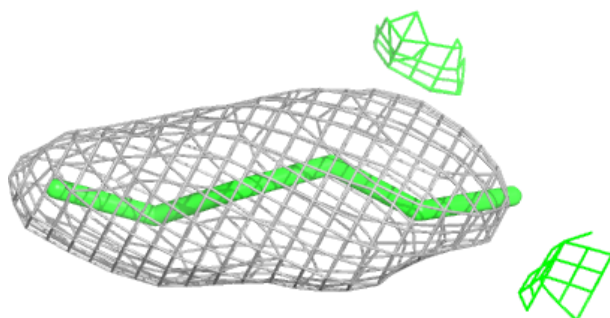
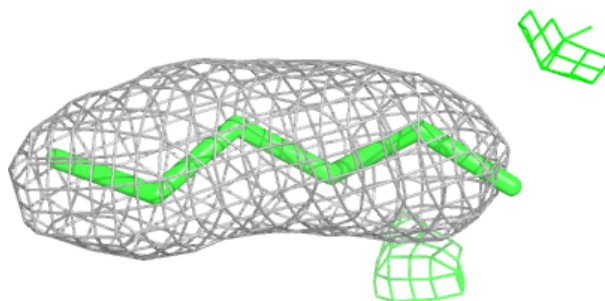
Electron density around NA D 319:

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

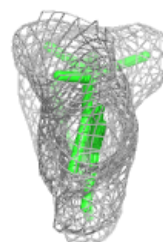
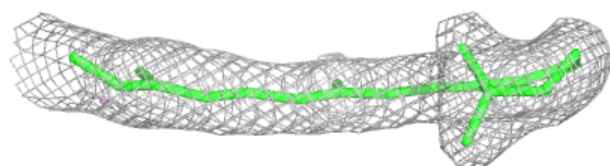
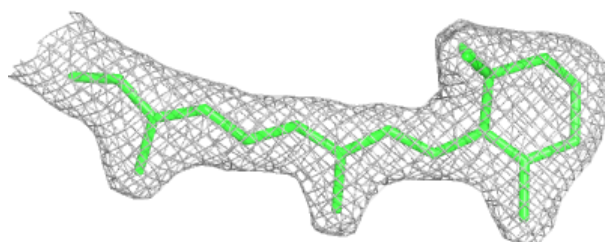


Electron density around LFA A 313:

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

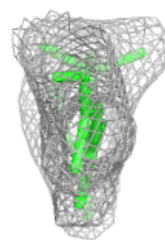
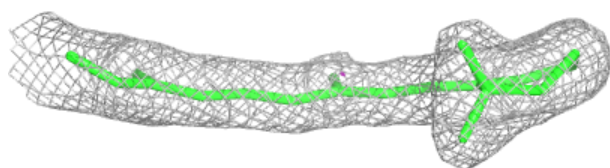
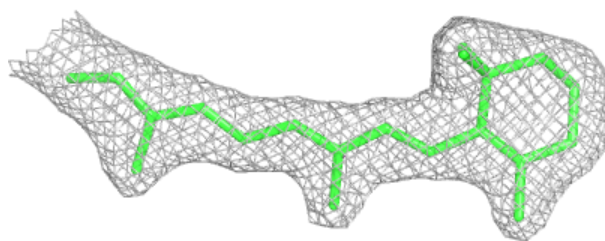
**Electron density around RET C 317:**

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

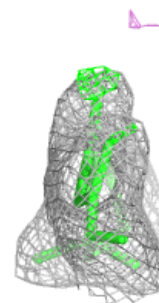
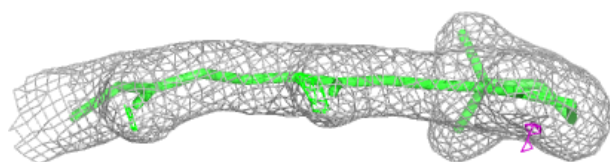
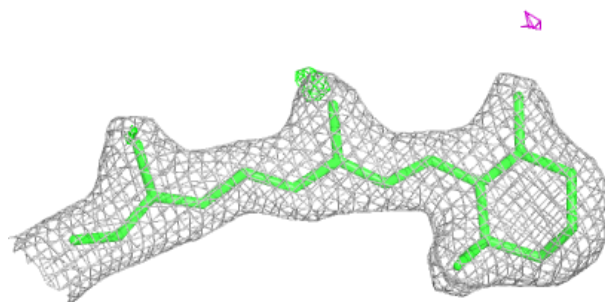


Electron density around RET D 317:

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

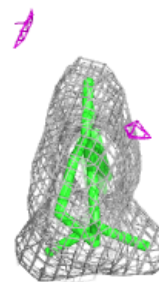
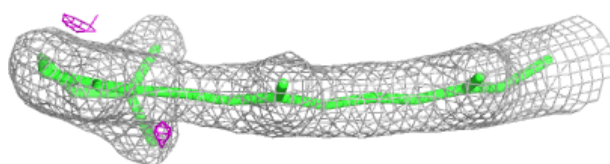
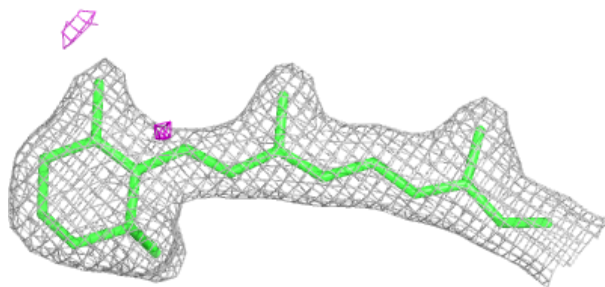
**Electron density around RET E 317:**

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

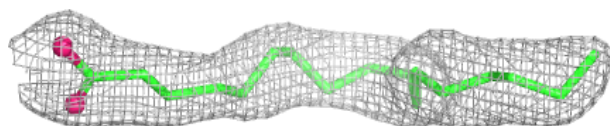
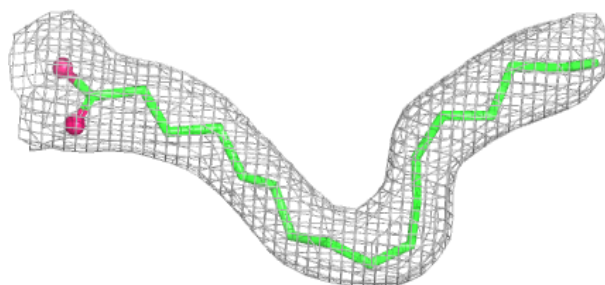


Electron density around RET A 320:

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

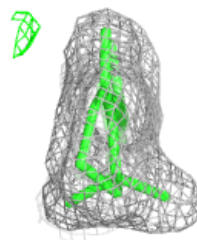
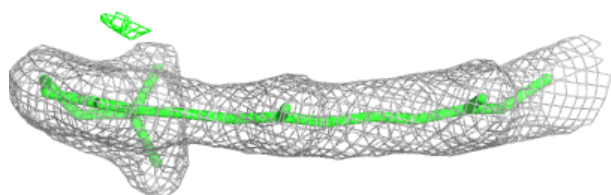
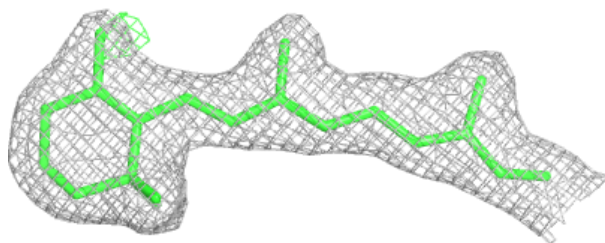
**Electron density around OLC A 316:**

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



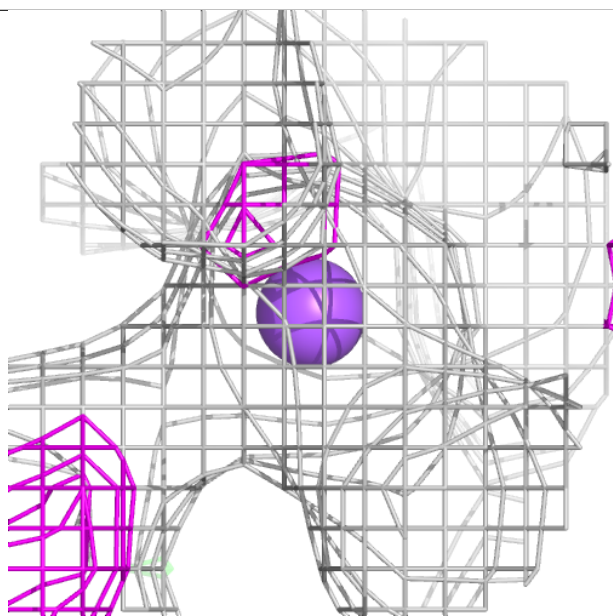
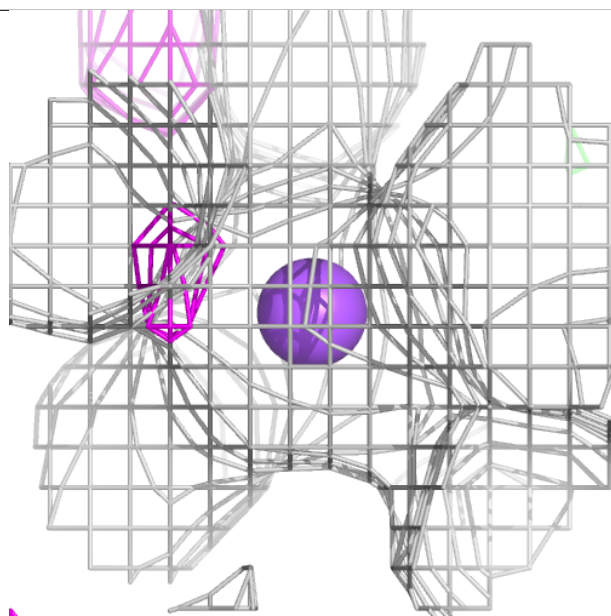
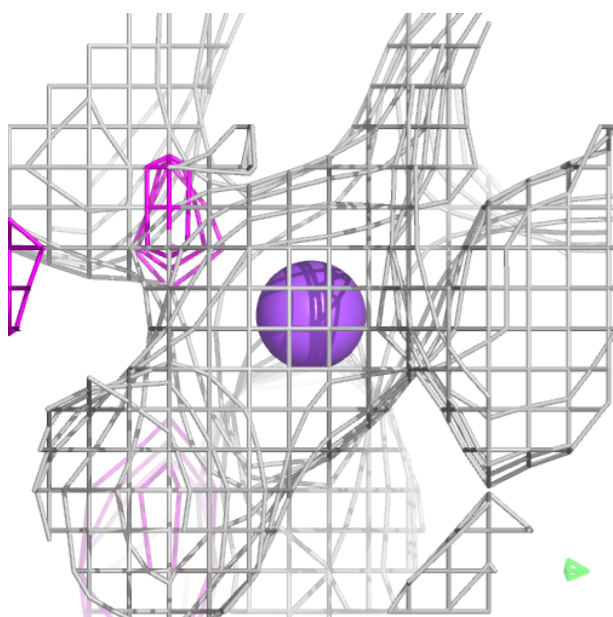
Electron density around RET B 313:

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



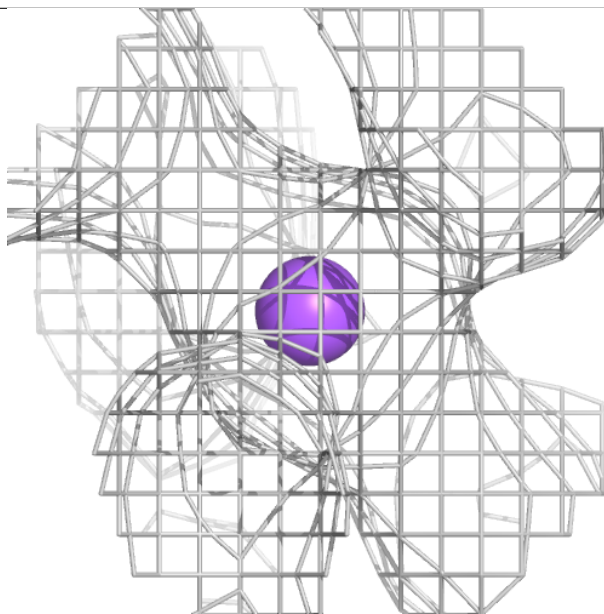
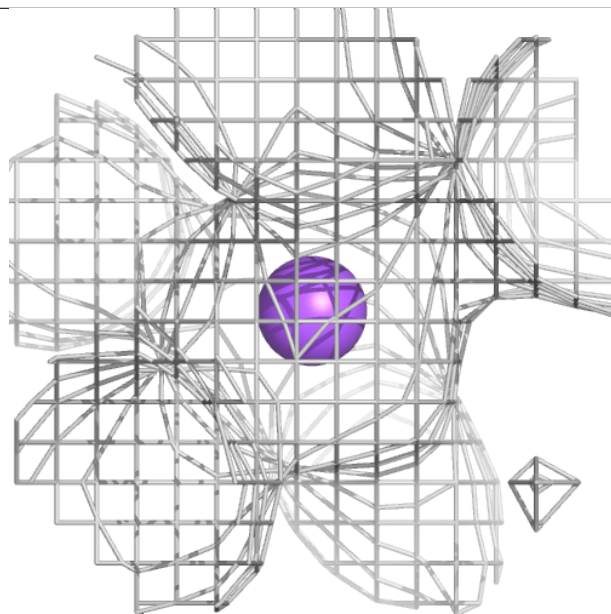
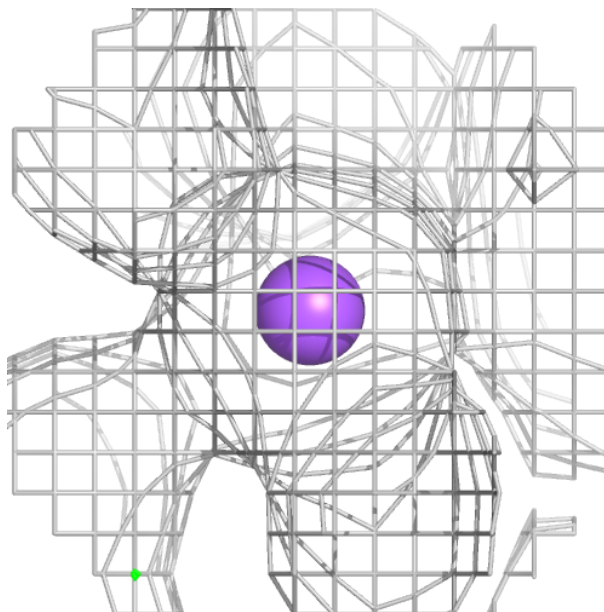
Electron density around NA A 321:

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



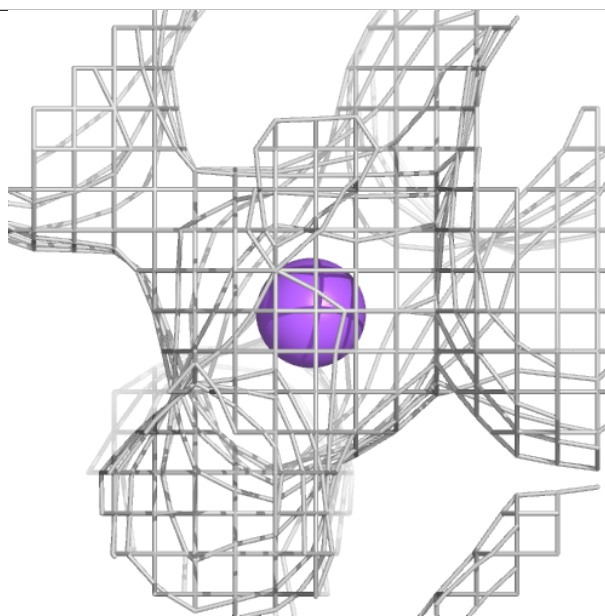
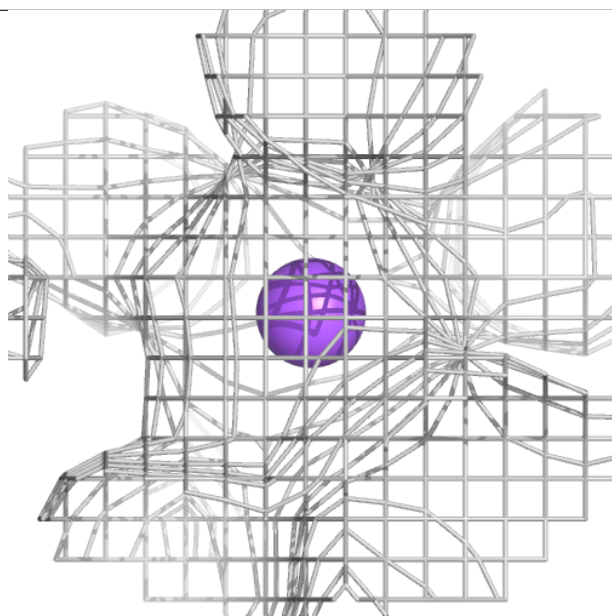
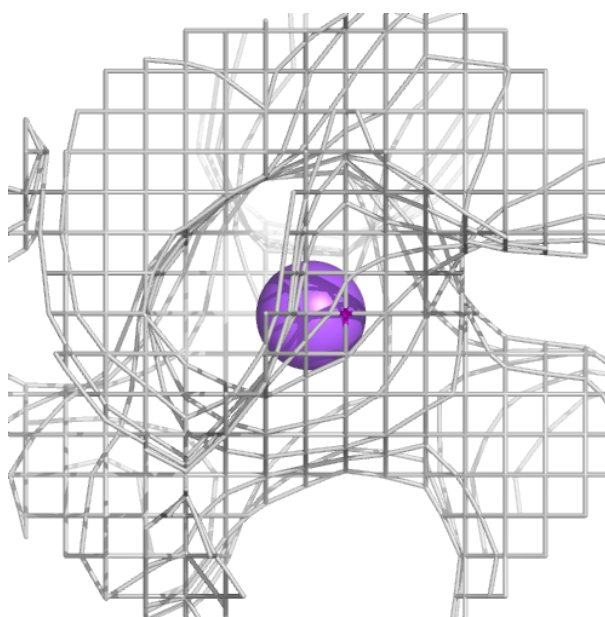
Electron density around NA E 318:

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



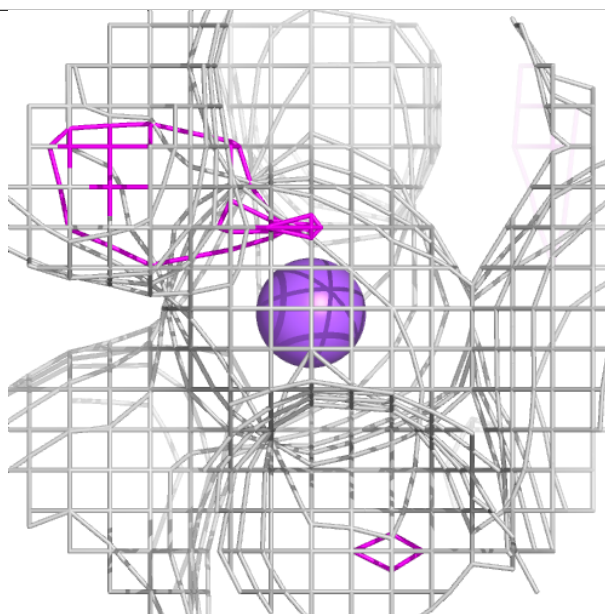
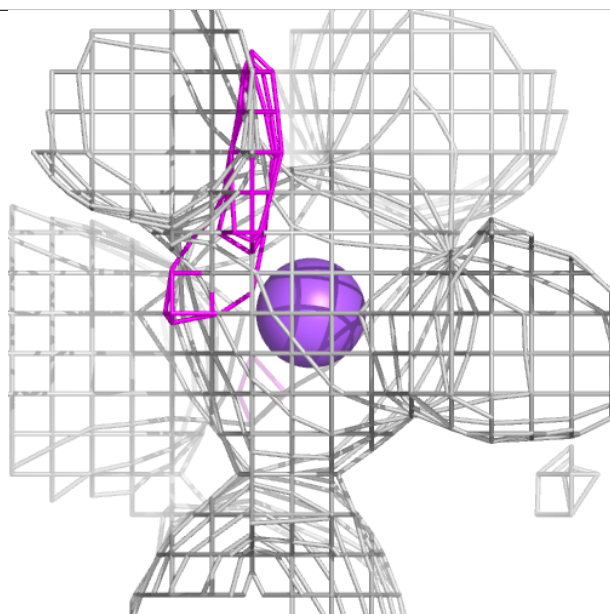
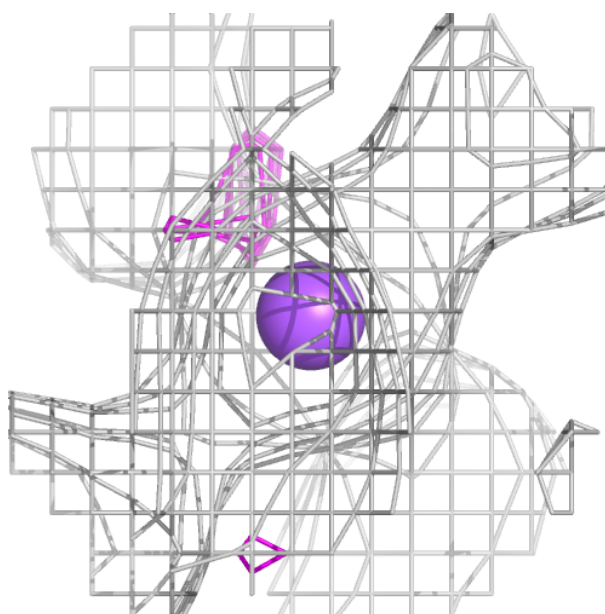
Electron density around NA B 315:

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



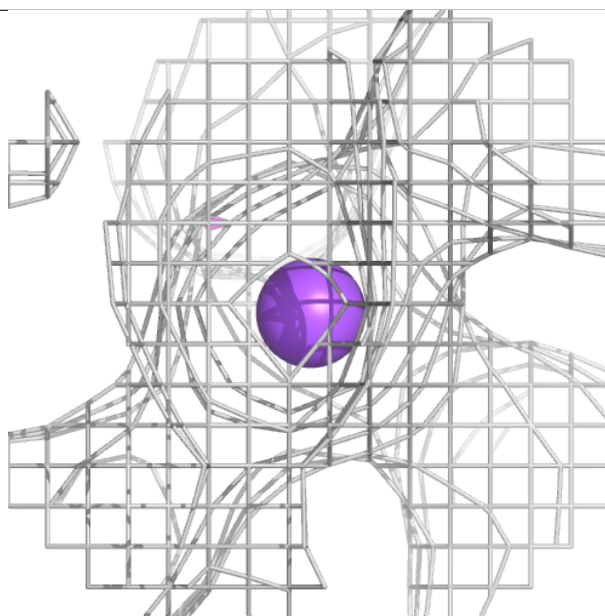
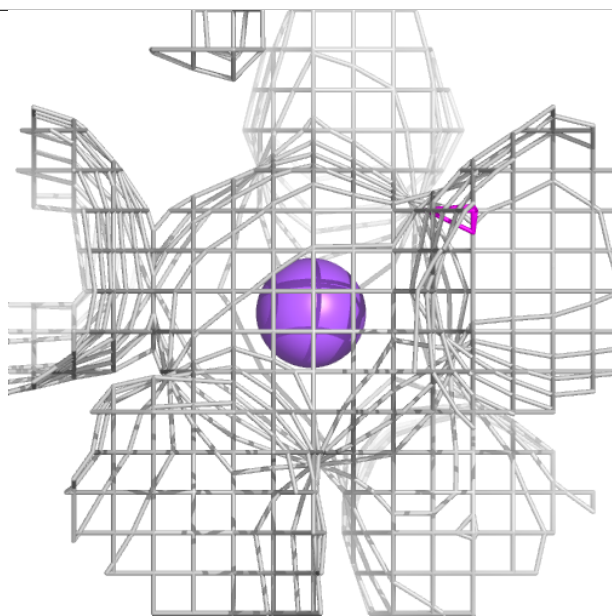
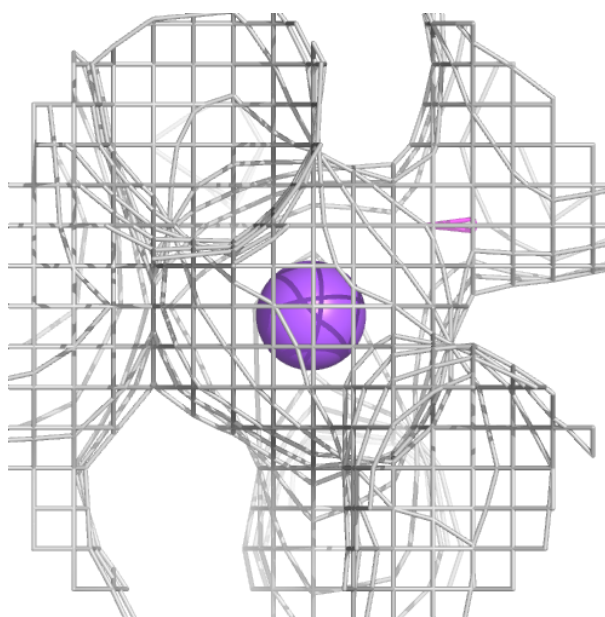
Electron density around NA D 318:

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



Electron density around NA C 319:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.