



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:31 am BST

PDB ID : 3POX
Title : Crystal Structure of E.coli OmpF porin in lipidic cubic phase: space group P1
Authors : Efremov, R.G.; Sazanov, L.A.
Deposited on : 2010-11-23
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

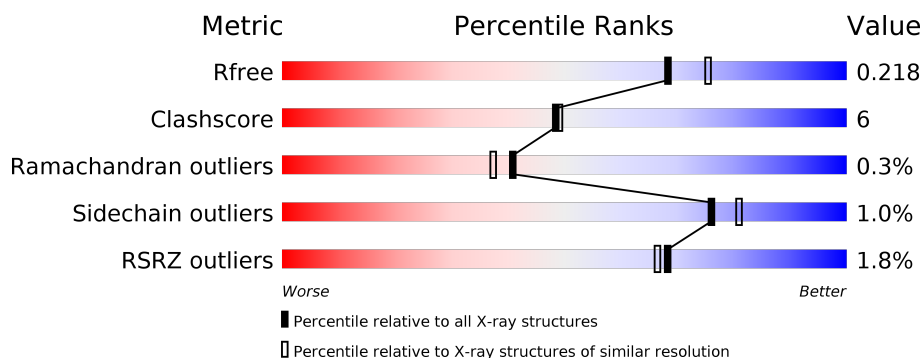
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	340	<div> <div>0%</div> <div>88% 12%</div> </div>
1	B	340	<div> <div>2%</div> <div>86% 13%</div> </div>
1	C	340	<div> <div>2%</div> <div>90% 10%</div> </div>
1	D	340	<div> <div>2%</div> <div>90% 10%</div> </div>
1	E	340	<div> <div>89% 10%</div> </div>
1	F	340	<div> <div>3%</div> <div>89% 11%</div> </div>

2 Entry composition [i](#)

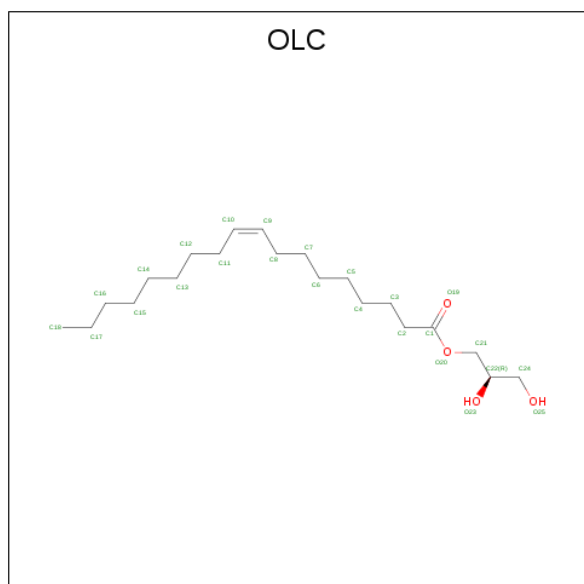
There are 5 unique types of molecules in this entry. The entry contains 18507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OmpF protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	B	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	D	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	F	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C 14 14	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 8 8	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 14 14	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 14 14	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C O 25 21 4	0	0
2	C	1	Total C 12 12	0	0
2	D	1	Total C 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C 12 12	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 8 8	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 12 12	0	0
2	E	1	Total C 12 12	0	0
2	E	1	Total C 14 14	0	0
2	E	1	Total C 10 10	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 12 12	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 14 14	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 10 10	0	0
2	F	1	Total C 12 12	0	0

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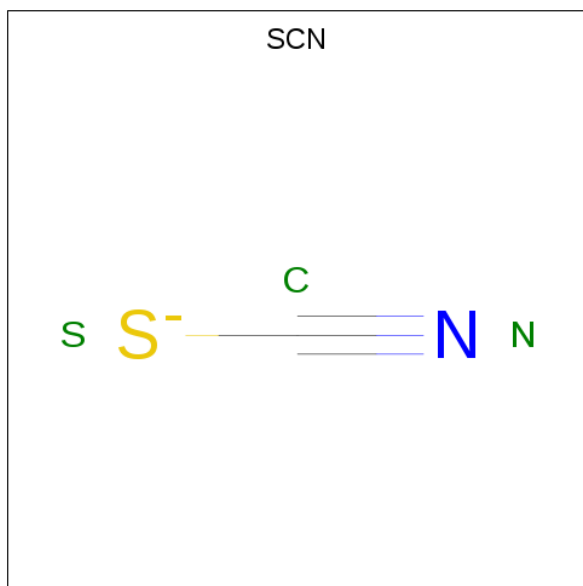
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C 8 8	0	0
2	F	1	Total C 14 14	0	0
2	F	1	Total C 14 14	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	4	Total K 4 4	0	0
3	E	3	Total K 3 3	0	0
3	B	3	Total K 3 3	0	0
3	C	4	Total K 4 4	0	0
3	A	3	Total K 3 3	0	0
3	F	3	Total K 3 3	0	0

- Molecule 4 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N S 3 1 1 1	0	0
4	B	1	Total C N S 3 1 1 1	0	0
4	D	1	Total C N S 3 1 1 1	0	0
4	E	1	Total C N S 3 1 1 1	0	0
4	E	1	Total C N S 3 1 1 1	0	0
4	F	1	Total C N S 3 1 1 1	0	0

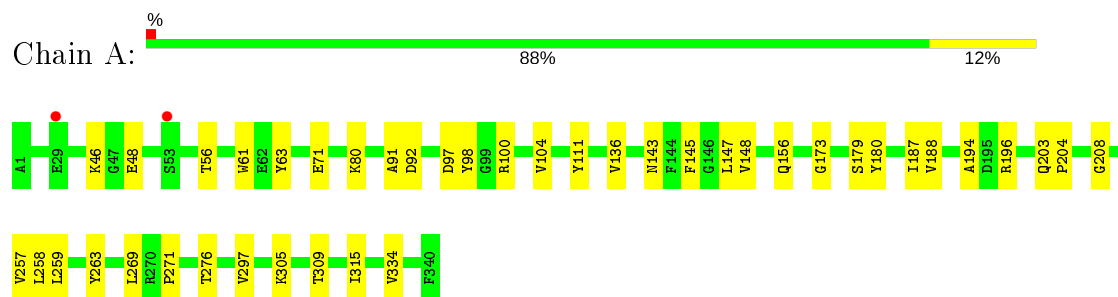
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	267	Total O 267 267	0	0
5	B	236	Total O 236 236	0	0
5	C	257	Total O 257 257	0	0
5	D	272	Total O 272 272	0	0
5	E	278	Total O 278 278	0	0
5	F	212	Total O 212 212	0	0

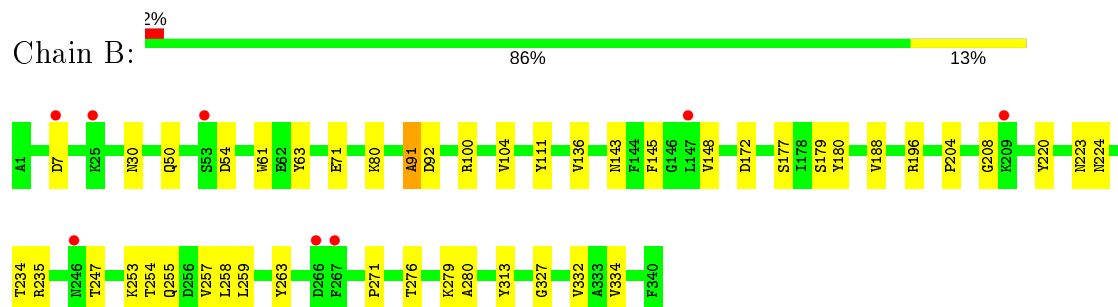
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

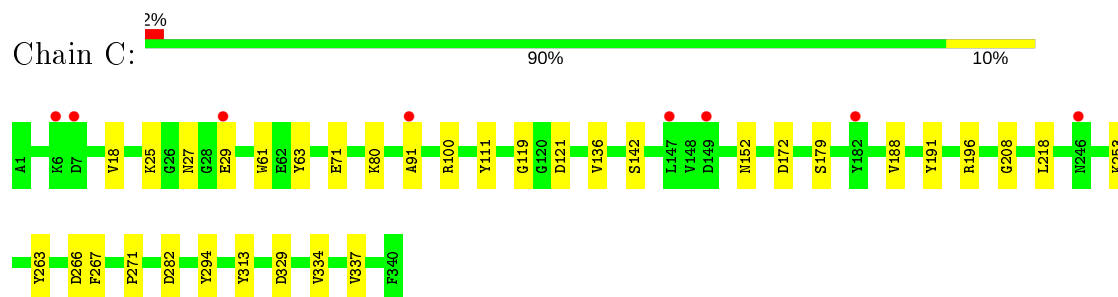
- Molecule 1: OmpF protein



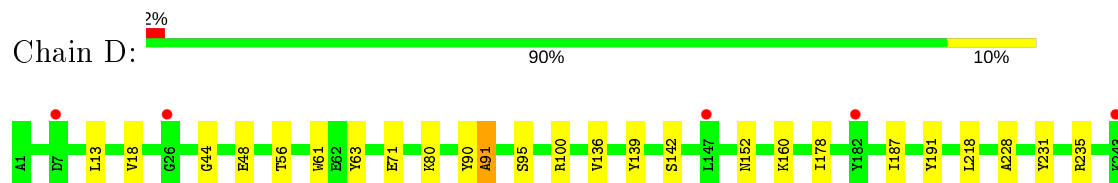
- Molecule 1: OmpF protein



- Molecule 1: OmpF protein



- Molecule 1: OmpF protein





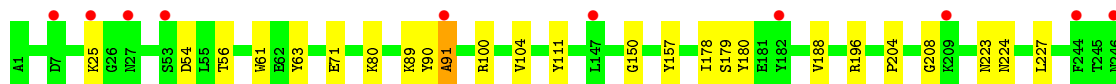
- Molecule 1: OmpF protein

Chain E: 89% 10%



- Molecule 1: OmpF protein

Chain F: 3% 89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.57Å 86.02Å 116.56Å 83.28° 78.46° 89.89°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.00) 96.6 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.188 , 0.225 0.181 , 0.218	Depositor DCC
R_{free} test set	9832 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18507	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% 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: K, OLC, SCN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/2683	0.56	0/3628
1	B	0.39	0/2683	0.54	0/3628
1	C	0.40	0/2683	0.55	0/3628
1	D	0.40	0/2683	0.55	0/3628
1	E	0.43	0/2683	0.57	0/3628
1	F	0.36	0/2683	0.53	0/3628
All	All	0.40	0/16098	0.55	0/21768

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	2627	0	2444	35	0
1	B	2627	0	2444	36	0
1	C	2627	0	2444	27	0
1	D	2627	0	2444	26	0
1	E	2627	0	2444	26	0
1	F	2627	0	2444	28	0
2	A	342	0	531	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	205	0	321	5	0
2	C	323	0	499	18	0
2	D	109	0	167	8	0
2	E	118	0	183	19	0
2	F	88	0	135	9	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	D	3	0	0	0	0
4	E	6	0	0	0	0
4	F	3	0	0	0	0
5	A	267	0	0	2	0
5	B	236	0	0	4	0
5	C	257	0	0	1	0
5	D	272	0	0	1	0
5	E	278	0	0	2	0
5	F	212	0	0	0	0
All	All	18507	0	16500	201	0

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

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:SER:HB2	1:B:188:VAL:HG22	1.53	0.90
2:A:341:OLC:H2	2:A:361:OLC:O19	1.73	0.88
1:A:297:VAL:HG12	2:A:361:OLC:H13	1.58	0.85
1:A:258:LEU:CD1	1:A:276:THR:HG23	2.07	0.84
2:A:359:OLC:H24	1:B:172:ASP:OD1	1.79	0.83
1:C:179:SER:CB	1:C:188:VAL:HG12	2.09	0.83
2:C:363:OLC:H22	5:C:546:HOH:O	1.77	0.82
1:C:172:ASP:OD1	2:C:359:OLC:H24	1.80	0.81
2:A:360:OLC:C12	2:A:365:OLC:H3	2.12	0.79
1:E:334:VAL:CG2	2:E:347:OLC:H9	2.13	0.79
1:C:179:SER:HB2	1:C:188:VAL:HG12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:OLC:H7A	2:C:349:OLC:H2A	1.66	0.77
2:E:346:OLC:H3	2:F:347:OLC:H6A	1.68	0.74
1:F:178:ILE:HG13	2:F:342:OLC:H4	1.68	0.74
2:B:344:OLC:H9	2:B:345:OLC:H21	1.68	0.73
1:E:334:VAL:HG22	2:E:347:OLC:H9	1.70	0.73
2:A:360:OLC:C11	2:A:365:OLC:H3	2.19	0.73
1:D:18:VAL:HG13	1:D:337:VAL:HG22	1.71	0.73
1:B:71:GLU:HB3	1:C:80:LYS:HD2	1.71	0.72
1:F:179:SER:HB2	1:F:188:VAL:HG22	1.71	0.72
1:C:18:VAL:HG13	1:C:337:VAL:HG22	1.73	0.70
1:C:111:TYR:OH	1:C:188:VAL:HG13	1.92	0.70
1:B:111:TYR:OH	1:B:188:VAL:HG23	1.92	0.70
1:F:54:ASP:HB3	1:F:91:ALA:HB2	1.73	0.69
2:A:360:OLC:H11A	2:A:365:OLC:H3	1.75	0.69
1:D:160:LYS:HE2	5:D:1294:HOH:O	1.93	0.69
2:C:353:OLC:H2A	2:C:363:OLC:H18	1.75	0.68
1:C:179:SER:HB3	1:C:188:VAL:HG12	1.75	0.67
1:F:258:LEU:CD1	1:F:276:THR:HG23	2.25	0.67
1:B:179:SER:CB	1:B:188:VAL:HG22	2.25	0.66
1:E:262:GLN:HG2	1:E:272:SER:HB2	1.78	0.65
1:B:334:VAL:CG2	2:C:359:OLC:H12	2.28	0.64
1:E:330:ASP:H	2:E:344:OLC:C1	2.09	0.64
1:D:178:ILE:HG13	2:D:342:OLC:H11	1.78	0.64
1:E:334:VAL:HG23	2:E:347:OLC:H12A	1.78	0.63
1:A:271:PRO:HB3	2:A:361:OLC:H18B	1.81	0.63
1:F:179:SER:CB	1:F:188:VAL:HG22	2.30	0.62
2:A:361:OLC:H18	2:A:365:OLC:C1	2.30	0.61
1:B:258:LEU:CD1	1:B:276:THR:HG23	2.30	0.61
1:E:299:ALA:HB3	2:E:347:OLC:H18B	1.79	0.61
1:A:196:ARG:HD3	1:A:208:GLY:O	1.99	0.61
1:A:179:SER:HB3	1:A:188:VAL:HG22	1.83	0.61
1:F:286:ILE:HG23	1:F:323:LYS:HD3	1.83	0.60
1:A:111:TYR:OH	1:A:188:VAL:HG23	2.01	0.60
1:A:179:SER:CB	1:A:188:VAL:HG22	2.30	0.59
2:E:347:OLC:C11	2:E:348:OLC:H3	2.32	0.59
1:A:334:VAL:HG12	2:A:359:OLC:H8A	1.84	0.59
1:E:334:VAL:CG2	2:E:347:OLC:H12A	2.33	0.58
1:D:267:PHE:HB2	2:D:349:OLC:H22	1.84	0.58
1:D:80:LYS:HD2	1:F:71:GLU:HB3	1.84	0.58
1:A:258:LEU:HD12	1:A:276:THR:HG23	1.85	0.57
1:A:309:THR:OG1	2:A:359:OLC:H11A	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TYR:CE1	2:B:350:OLC:H5	2.40	0.57
2:E:347:OLC:H11A	2:E:348:OLC:H3	1.86	0.57
1:E:253:LYS:HE2	1:E:282:ASP:OD2	2.04	0.57
2:C:347:OLC:H5	2:C:358:OLC:O19	2.04	0.57
2:A:356:OLC:H7	1:C:334:VAL:HG12	1.87	0.56
1:B:71:GLU:CB	1:C:80:LYS:HD2	2.35	0.56
1:F:157:TYR:CZ	2:F:347:OLC:H8	2.40	0.56
1:F:259:LEU:HD11	2:F:344:OLC:H7A	1.86	0.56
1:A:263:TYR:O	1:A:271:PRO:HD2	2.05	0.56
1:E:299:ALA:HB3	2:E:347:OLC:C18	2.36	0.56
1:F:257:VAL:O	1:F:258:LEU:HD13	2.05	0.56
1:F:258:LEU:HD12	1:F:276:THR:HG23	1.88	0.56
2:F:341:OLC:C1	2:F:342:OLC:H2A	2.36	0.56
1:B:204:PRO:HG2	1:B:247:THR:HG23	1.88	0.55
1:A:100:ARG:NH2	1:C:71:GLU:HG3	2.20	0.55
1:F:196:ARG:HD3	1:F:208:GLY:O	2.06	0.55
2:A:341:OLC:H4	2:A:361:OLC:H3A	1.88	0.55
1:C:191:TYR:HE2	2:C:352:OLC:H5	1.71	0.55
2:E:347:OLC:H11A	2:E:348:OLC:C3	2.38	0.54
1:D:178:ILE:HG12	2:D:342:OLC:H14	1.89	0.54
1:F:253:LYS:HE2	1:F:282:ASP:OD2	2.07	0.54
1:A:92:ASP:O	1:A:145:PHE:HA	2.08	0.54
1:A:257:VAL:O	1:A:258:LEU:HD13	2.08	0.53
1:B:196:ARG:HD3	1:B:208:GLY:O	2.08	0.53
1:C:266:ASP:N	2:C:362:OLC:H24	2.23	0.53
1:B:334:VAL:HG22	2:C:359:OLC:H12	1.91	0.53
2:E:347:OLC:C10	2:E:348:OLC:H3	2.38	0.53
1:E:46:LYS:HG2	5:E:1092:HOH:O	2.08	0.52
1:A:180:TYR:HB2	2:A:349:OLC:H12A	1.90	0.52
1:D:61:TRP:CZ2	1:D:63:TYR:HB2	2.45	0.52
1:E:179:SER:HB3	1:E:188:VAL:HG23	1.92	0.52
1:E:263:TYR:O	1:E:271:PRO:HD2	2.10	0.52
1:F:111:TYR:OH	1:F:188:VAL:HG23	2.10	0.52
1:F:223:ASN:O	1:F:224:ASN:HB2	2.10	0.52
1:D:235:ARG:HD3	1:D:253:LYS:HG2	1.93	0.51
1:B:313:TYR:CE2	1:B:332:VAL:HG22	2.46	0.51
1:B:71:GLU:HG3	1:C:100:ARG:NH2	2.26	0.51
1:D:259:LEU:HB3	2:D:346:OLC:H6A	1.93	0.51
2:E:347:OLC:H10	2:E:348:OLC:H3	1.91	0.51
1:B:111:TYR:OH	1:B:188:VAL:CG2	2.58	0.51
1:B:54:ASP:HB3	1:B:91:ALA:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ARG:HD3	1:C:208:GLY:O	2.10	0.50
1:A:71:GLU:HG3	1:B:100:ARG:NH2	2.26	0.50
1:E:48:GLU:HG3	1:E:56:THR:CG2	2.42	0.50
2:C:360:OLC:H12A	2:C:360:OLC:H8A	1.93	0.50
1:E:92:ASP:O	1:E:145:PHE:HA	2.12	0.50
1:A:173:GLY:HA3	1:A:194:ALA:HB2	1.93	0.50
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.47	0.50
1:A:271:PRO:HB2	2:A:343:OLC:H2	1.94	0.50
1:F:178:ILE:CG1	2:F:342:OLC:H4	2.39	0.50
1:F:111:TYR:CZ	1:F:188:VAL:HG23	2.47	0.49
1:C:111:TYR:CZ	1:C:188:VAL:HG13	2.47	0.49
1:E:18:VAL:HG13	1:E:337:VAL:HG22	1.95	0.49
2:A:349:OLC:H21	5:A:425:HOH:O	2.13	0.49
1:C:25:LYS:HE3	1:C:329:ASP:CG	2.33	0.49
1:C:263:TYR:O	1:C:271:PRO:HD2	2.14	0.48
2:C:347:OLC:H3	2:C:358:OLC:O19	2.13	0.48
1:F:204:PRO:HG2	1:F:247:THR:HG23	1.95	0.48
1:A:143:ASN:HA	1:A:148:VAL:O	2.13	0.48
1:C:266:ASP:H	2:C:362:OLC:H24	1.79	0.48
1:D:336:ILE:HB	2:E:341:OLC:H9	1.95	0.48
1:A:271:PRO:CB	2:A:361:OLC:H18B	2.41	0.48
2:E:343:OLC:H2A	2:E:344:OLC:H5	1.96	0.48
1:B:223:ASN:O	1:B:224:ASN:HB2	2.13	0.47
1:D:142:SER:HA	1:D:152:ASN:OD1	2.14	0.47
1:E:270:ARG:NH2	5:E:641:HOH:O	2.47	0.47
1:B:255:GLN:NE2	5:B:956:HOH:O	2.48	0.47
1:F:180:TYR:HB2	2:F:343:OLC:C1	2.45	0.47
1:B:263:TYR:O	1:B:271:PRO:HD2	2.13	0.47
1:B:143:ASN:HA	1:B:148:VAL:O	2.15	0.47
1:C:25:LYS:HE3	1:C:329:ASP:OD1	2.14	0.47
1:A:187:ILE:HG12	2:A:349:OLC:H16	1.95	0.47
1:B:313:TYR:CD2	1:B:332:VAL:HG22	2.49	0.47
1:B:7:ASP:HB2	5:B:661:HOH:O	2.15	0.47
1:E:196:ARG:HD3	1:E:208:GLY:O	2.15	0.46
1:B:259:LEU:HD11	2:B:351:OLC:H8	1.97	0.46
1:A:258:LEU:HD11	1:A:276:THR:HG23	1.91	0.46
2:B:351:OLC:O19	2:B:351:OLC:C4	2.62	0.46
1:A:147:LEU:HD11	2:A:353:OLC:H3	1.98	0.46
1:B:92:ASP:O	1:B:145:PHE:HA	2.15	0.46
1:F:56:THR:HB	1:F:89:LYS:HG2	1.96	0.46
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TYR:CZ	1:A:188:VAL:HG23	2.51	0.45
2:A:361:OLC:H22	5:A:397:HOH:O	2.16	0.45
1:B:234:THR:O	1:B:235:ARG:HD3	2.17	0.45
1:A:179:SER:HB2	1:A:188:VAL:HG22	1.97	0.45
1:B:111:TYR:CZ	1:B:188:VAL:HG23	2.51	0.45
1:C:191:TYR:CE2	2:C:352:OLC:H5	2.52	0.45
1:D:270:ARG:O	1:D:270:ARG:HG2	2.17	0.45
1:D:48:GLU:HG3	1:D:56:THR:CG2	2.46	0.45
1:B:257:VAL:O	1:B:258:LEU:HD13	2.16	0.45
2:C:363:OLC:H5A	2:C:363:OLC:H8A	1.61	0.45
1:B:220:TYR:OH	2:B:345:OLC:H21A	2.17	0.44
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.53	0.44
1:F:150:GLY:O	1:F:180:TYR:HA	2.17	0.44
1:B:50:GLN:NE2	5:B:1263:HOH:O	2.50	0.44
1:E:223:ASN:O	1:E:225:ILE:HG13	2.17	0.44
1:D:231:TYR:HB2	2:D:348:OLC:H3	1.99	0.44
1:D:178:ILE:CG1	2:D:342:OLC:H14	2.47	0.44
1:B:30:ASN:ND2	1:B:327:GLY:HA2	2.32	0.44
1:D:187:ILE:HG13	1:D:218:LEU:HD23	2.00	0.44
1:D:263:TYR:O	1:D:271:PRO:HD2	2.17	0.44
1:C:119:GLY:HA2	1:C:294:TYR:OH	2.18	0.43
1:A:98:TYR:CE1	2:A:356:OLC:H4A	2.53	0.43
1:C:142:SER:HA	1:C:152:ASN:OD1	2.18	0.43
1:C:218:LEU:HG	2:C:349:OLC:H9	1.99	0.43
1:C:267:PHE:HB2	2:C:360:OLC:H21	1.99	0.43
2:A:345:OLC:H3	2:A:362:OLC:H4	2.00	0.43
1:D:100:ARG:NH2	1:F:71:GLU:HG3	2.34	0.43
1:F:227:LEU:HB3	2:F:345:OLC:H5A	1.99	0.43
1:A:258:LEU:O	1:A:259:LEU:HD23	2.17	0.43
1:C:27:ASN:OD1	1:C:29:GLU:HB2	2.19	0.43
1:E:181:GLU:HA	1:E:185:PHE:O	2.19	0.43
1:F:61:TRP:CZ2	1:F:63:TYR:HB2	2.54	0.43
1:D:71:GLU:HG2	1:E:80:LYS:HG3	2.00	0.42
1:D:228:ALA:HB3	1:D:260:VAL:CG2	2.49	0.42
1:F:262:GLN:OE1	1:F:270:ARG:NH1	2.48	0.42
1:E:309:THR:HG21	2:E:348:OLC:H5A	2.01	0.42
1:F:25:LYS:HE3	1:F:329:ASP:OD1	2.19	0.42
1:C:253:LYS:HE2	1:C:282:ASP:OD2	2.19	0.42
1:B:104:VAL:HG22	1:B:177:SER:HB3	2.02	0.42
1:A:104:VAL:HG13	1:A:156:GLN:CD	2.40	0.42
1:D:13:LEU:HD12	1:D:44:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:GLU:HG3	1:F:100:ARG:NH2	2.35	0.42
1:B:254:THR:HA	1:B:279:LYS:O	2.20	0.42
1:E:173:GLY:HA3	1:E:194:ALA:HB2	2.02	0.42
1:B:204:PRO:HB2	1:B:247:THR:HG21	2.02	0.41
1:A:305:LYS:NZ	5:B:661:HOH:O	2.52	0.41
1:E:25:LYS:HD3	2:E:344:OLC:H2	2.02	0.41
1:E:90:TYR:O	1:E:91:ALA:C	2.58	0.41
1:E:203:GLN:HA	1:E:204:PRO:HD3	1.94	0.41
1:F:54:ASP:HB2	1:F:90:TYR:HE1	1.85	0.41
1:A:315:ILE:HG12	2:A:361:OLC:H3	2.03	0.41
2:C:352:OLC:H10	2:C:363:OLC:H15A	2.03	0.41
1:D:191:TYR:CE1	2:D:345:OLC:H5A	2.56	0.41
1:D:48:GLU:HG3	1:D:56:THR:HG21	2.03	0.41
2:A:344:OLC:C10	2:A:344:OLC:H6	2.51	0.40
1:D:90:TYR:O	1:D:91:ALA:C	2.60	0.40
1:A:203:GLN:HA	1:A:204:PRO:HD3	1.92	0.40
2:E:346:OLC:H5	2:F:347:OLC:C9	2.51	0.40
1:A:46:LYS:HB3	1:A:46:LYS:HE2	1.77	0.40
1:D:95:SER:O	1:D:139:TYR:HA	2.21	0.40
2:E:342:OLC:H4	2:E:342:OLC:H7	1.89	0.40
2:A:360:OLC:H11A	2:A:365:OLC:C3	2.47	0.40
2:C:348:OLC:H7A	2:C:349:OLC:C2	2.45	0.40
1:D:178:ILE:CG1	2:D:342:OLC:H11	2.48	0.40
1:A:269:LEU:HG	1:A:271:PRO:HD3	2.03	0.40
1:A:48:GLU:HG2	1:A:56:THR:CG2	2.52	0.40
1:B:253:LYS:O	1:B:280:ALA:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	41	37
1	B	338/340 (99%)	323 (96%)	14 (4%)	1 (0%)	41	37
1	C	338/340 (99%)	324 (96%)	13 (4%)	1 (0%)	41	37
1	D	338/340 (99%)	327 (97%)	10 (3%)	1 (0%)	41	37
1	E	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	41	37
1	F	338/340 (99%)	321 (95%)	16 (5%)	1 (0%)	41	37
All	All	2028/2040 (99%)	1945 (96%)	77 (4%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	91	ALA
1	A	91	ALA
1	F	91	ALA
1	D	91	ALA
1	B	91	ALA
1	C	91	ALA

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	263/263 (100%)	260 (99%)	3 (1%)	73	78
1	B	263/263 (100%)	261 (99%)	2 (1%)	81	86
1	C	263/263 (100%)	260 (99%)	3 (1%)	73	78
1	D	263/263 (100%)	262 (100%)	1 (0%)	91	93
1	E	263/263 (100%)	260 (99%)	3 (1%)	73	78
1	F	263/263 (100%)	260 (99%)	3 (1%)	73	78
All	All	1578/1578 (100%)	1563 (99%)	15 (1%)	76	81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	97	ASP
1	A	136	VAL
1	B	80	LYS
1	B	136	VAL
1	C	121	ASP
1	C	136	VAL
1	C	313	TYR
1	D	136	VAL
1	E	80	LYS
1	E	136	VAL
1	E	210	LYS
1	F	80	LYS
1	F	104	VAL
1	F	313	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	60	GLN
1	B	30	ASN
1	B	50	GLN
1	B	60	GLN
1	C	30	ASN
1	C	50	GLN
1	C	60	GLN
1	D	30	ASN
1	D	60	GLN
1	E	60	GLN
1	F	30	ASN
1	F	60	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 114 ligands modelled in this entry, 20 are monoatomic - leaving 94 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	C	348	-	11,11,24	1.17	1 (9%)	9,10,25	0.72	0
2	OLC	A	353	-	7,7,24	0.20	0	6,6,25	0.55	0
2	OLC	B	352	-	15,15,24	0.97	1 (6%)	14,14,25	1.12	1 (7%)
2	OLC	C	342	-	7,7,24	0.22	0	6,6,25	0.58	0
2	OLC	A	349	-	24,24,24	1.33	4 (16%)	25,25,25	1.10	2 (8%)
4	SCN	E	352	-	1,2,2	1.00	0	0,1,1	0.00	-
2	OLC	A	342	-	7,7,24	0.22	0	6,6,25	0.58	0
2	OLC	E	345	-	13,13,24	1.09	1 (7%)	12,12,25	0.79	0
2	OLC	C	361	-	11,11,24	1.20	1 (9%)	9,10,25	0.77	0
2	OLC	A	347	-	7,7,24	0.24	0	6,6,25	0.52	0
2	OLC	B	342	-	13,13,24	1.06	1 (7%)	12,12,25	0.86	0
2	OLC	A	344	-	9,9,24	1.24	1 (11%)	8,8,25	0.96	1 (12%)
2	OLC	D	341	-	4,4,24	0.26	0	3,3,25	0.35	0
2	OLC	C	347	-	9,9,24	1.20	1 (11%)	8,8,25	1.08	1 (12%)
2	OLC	C	343	-	7,7,24	0.22	0	6,6,25	0.53	0
2	OLC	A	351	-	13,13,24	1.06	1 (7%)	12,12,25	0.82	0
2	OLC	D	343	-	7,7,24	0.22	0	6,6,25	0.56	0
2	OLC	C	357	-	13,13,24	1.13	1 (7%)	12,12,25	0.72	0
2	OLC	A	343	-	7,7,24	0.23	0	6,6,25	0.57	0
2	OLC	D	349	3	24,24,24	1.29	4 (16%)	25,25,25	1.22	3 (12%)
2	OLC	C	349	-	9,9,24	1.19	1 (11%)	8,8,25	1.13	1 (12%)
2	OLC	B	351	-	24,24,24	1.28	4 (16%)	25,25,25	1.07	1 (4%)
2	OLC	B	347	-	13,13,24	1.07	1 (7%)	12,12,25	0.90	1 (8%)
2	OLC	A	357	-	9,9,24	1.21	1 (11%)	8,8,25	0.92	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	C	362	-	24,24,24	1.35	4 (16%)	25,25,25	1.39	3 (12%)
2	OLC	C	354	-	9,9,24	1.20	1 (11%)	8,8,25	1.01	1 (12%)
2	OLC	C	350	-	13,13,24	1.06	1 (7%)	12,12,25	0.89	0
2	OLC	D	346	-	11,11,24	1.19	1 (9%)	9,10,25	0.83	0
2	OLC	A	363	-	11,11,24	1.26	1 (9%)	9,10,25	0.66	0
2	OLC	B	344	-	9,9,24	1.22	1 (11%)	8,8,25	0.92	1 (12%)
2	OLC	C	364	-	11,11,24	1.19	1 (9%)	9,10,25	0.84	0
2	OLC	C	353	-	9,9,24	1.20	1 (11%)	8,8,25	1.00	1 (12%)
2	OLC	A	350	-	13,13,24	1.09	1 (7%)	12,12,25	0.83	0
2	OLC	B	354	-	7,7,24	0.44	0	6,6,25	0.69	0
2	OLC	A	345	-	7,7,24	0.27	0	6,6,25	0.48	0
2	OLC	E	343	-	11,11,24	1.19	1 (9%)	9,10,25	0.76	0
2	OLC	C	346	-	9,9,24	1.19	1 (11%)	8,8,25	1.10	1 (12%)
2	OLC	F	346	-	7,7,24	0.22	0	6,6,25	0.65	0
2	OLC	C	358	-	24,24,24	1.34	4 (16%)	25,25,25	1.17	1 (4%)
2	OLC	F	348	-	13,13,24	1.15	1 (7%)	12,12,25	0.85	0
2	OLC	D	348	-	7,7,24	0.17	0	6,6,25	0.84	0
2	OLC	C	363	-	24,24,24	1.33	4 (16%)	25,25,25	1.37	2 (8%)
2	OLC	C	356	-	7,7,24	0.26	0	6,6,25	0.40	0
2	OLC	E	348	-	11,11,24	1.26	1 (9%)	9,10,25	0.59	0
2	OLC	A	356	-	24,24,24	1.35	4 (16%)	25,25,25	1.27	3 (12%)
2	OLC	B	353	-	7,7,24	0.34	0	6,6,25	0.46	0
2	OLC	B	348	-	13,13,24	1.05	1 (7%)	12,12,25	0.89	1 (8%)
2	OLC	C	359	-	24,24,24	1.34	4 (16%)	25,25,25	1.27	3 (12%)
2	OLC	C	355	-	9,9,24	1.19	1 (11%)	8,8,25	1.00	1 (12%)
4	SCN	E	353	-	1,2,2	1.05	0	0,1,1	0.00	-
2	OLC	D	347	-	7,7,24	0.31	0	6,6,25	0.50	0
2	OLC	A	361	-	24,24,24	1.46	4 (16%)	25,25,25	1.34	2 (8%)
4	SCN	B	358	-	1,2,2	0.99	0	0,1,1	0.00	-
2	OLC	C	344	-	7,7,24	0.28	0	6,6,25	0.45	0
2	OLC	A	364	-	11,11,24	1.20	1 (9%)	9,10,25	0.75	0
2	OLC	A	360	-	11,11,24	1.15	1 (9%)	9,10,25	0.75	0
2	OLC	B	349	-	7,7,24	0.24	0	6,6,25	0.47	0
2	OLC	C	341	-	9,9,24	1.19	1 (11%)	8,8,25	1.00	1 (12%)
2	OLC	F	347	-	13,13,24	1.07	1 (7%)	12,12,25	0.84	0
2	OLC	A	352	-	9,9,24	1.21	1 (11%)	8,8,25	0.94	1 (12%)
2	OLC	C	360	3	24,24,24	1.39	4 (16%)	25,25,25	1.01	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	F	342	-	13,13,24	1.10	1 (7%)	12,12,25	0.79	1 (8%)
2	OLC	C	351	-	7,7,24	0.24	0	6,6,25	0.49	0
2	OLC	A	346	-	24,24,24	1.37	4 (16%)	25,25,25	1.21	3 (12%)
2	OLC	E	341	-	24,24,24	1.33	4 (16%)	25,25,25	1.41	3 (12%)
2	OLC	F	344	-	9,9,24	1.19	1 (11%)	8,8,25	1.03	1 (12%)
2	OLC	A	354	-	7,7,24	0.24	0	6,6,25	0.53	0
4	SCN	A	369	-	1,2,2	1.09	0	0,1,1	0.00	-
2	OLC	D	345	-	9,9,24	1.19	1 (11%)	8,8,25	1.05	1 (12%)
2	OLC	F	341	-	7,7,24	0.25	0	6,6,25	0.47	0
2	OLC	F	345	-	11,11,24	1.16	1 (9%)	9,10,25	0.76	0
2	OLC	E	342	-	7,7,24	0.23	0	6,6,25	0.61	0
2	OLC	C	352	-	11,11,24	1.16	1 (9%)	9,10,25	0.69	0
2	OLC	A	348	-	9,9,24	1.20	1 (11%)	8,8,25	0.97	1 (12%)
2	OLC	A	365	-	7,7,24	0.45	0	6,6,25	0.79	0
2	OLC	E	347	-	24,24,24	1.38	4 (16%)	25,25,25	1.15	2 (8%)
2	OLC	A	355	-	9,9,24	1.21	1 (11%)	8,8,25	1.01	1 (12%)
2	OLC	F	343	-	7,7,24	0.22	0	6,6,25	0.63	0
2	OLC	B	343	-	7,7,24	0.23	0	6,6,25	0.46	0
4	SCN	F	352	-	1,2,2	0.90	0	0,1,1	0.00	-
2	OLC	B	346	-	24,24,24	1.36	4 (16%)	25,25,25	1.42	3 (12%)
2	OLC	C	345	-	11,11,24	1.18	1 (9%)	9,10,25	0.63	0
2	OLC	E	346	-	9,9,24	1.20	1 (11%)	8,8,25	0.99	1 (12%)
2	OLC	D	344	-	7,7,24	0.22	0	6,6,25	0.50	0
2	OLC	B	345	-	24,24,24	1.36	4 (16%)	25,25,25	1.04	2 (8%)
2	OLC	B	341	-	4,4,24	0.22	0	3,3,25	0.44	0
2	OLC	B	350	-	24,24,24	1.35	4 (16%)	25,25,25	1.05	1 (4%)
4	SCN	D	354	-	1,2,2	1.14	0	0,1,1	0.00	-
2	OLC	A	358	-	24,24,24	1.35	4 (16%)	25,25,25	1.13	2 (8%)
2	OLC	E	344	-	11,11,24	1.14	1 (9%)	9,10,25	0.83	0
2	OLC	D	342	-	24,24,24	1.37	4 (16%)	25,25,25	1.05	2 (8%)
2	OLC	A	359	-	24,24,24	1.30	4 (16%)	25,25,25	1.01	2 (8%)
2	OLC	A	362	-	13,13,24	1.11	1 (7%)	12,12,25	0.92	1 (8%)
2	OLC	A	341	-	7,7,24	0.23	0	6,6,25	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	348	-	-	2/9/9/24	-
2	OLC	A	353	-	-	0/5/5/24	-
2	OLC	B	352	-	-	9/13/13/24	-
2	OLC	C	342	-	-	2/5/5/24	-
2	OLC	A	349	-	-	11/24/24/24	-
2	OLC	A	342	-	-	1/5/5/24	-
2	OLC	E	345	-	-	7/11/11/24	-
2	OLC	C	361	-	-	4/9/9/24	-
2	OLC	A	347	-	-	3/5/5/24	-
2	OLC	B	342	-	-	3/11/11/24	-
2	OLC	A	344	-	-	0/7/7/24	-
2	OLC	D	341	-	-	0/2/2/24	-
2	OLC	C	347	-	-	2/7/7/24	-
2	OLC	C	343	-	-	0/5/5/24	-
2	OLC	A	351	-	-	1/11/11/24	-
2	OLC	D	343	-	-	0/5/5/24	-
2	OLC	C	357	-	-	2/11/11/24	-
2	OLC	A	343	-	-	2/5/5/24	-
2	OLC	D	349	3	-	14/24/24/24	-
2	OLC	C	349	-	-	4/7/7/24	-
2	OLC	B	351	-	-	16/24/24/24	-
2	OLC	B	347	-	-	1/11/11/24	-
2	OLC	A	357	-	-	4/7/7/24	-
2	OLC	C	362	-	-	15/24/24/24	-
2	OLC	C	354	-	-	1/7/7/24	-
2	OLC	C	350	-	-	3/11/11/24	-
2	OLC	D	346	-	-	4/9/9/24	-
2	OLC	A	363	-	-	6/9/9/24	-
2	OLC	B	344	-	-	2/7/7/24	-
2	OLC	C	364	-	-	5/9/9/24	-
2	OLC	C	353	-	-	3/7/7/24	-
2	OLC	A	350	-	-	4/11/11/24	-
2	OLC	B	354	-	-	2/5/5/24	-
2	OLC	A	345	-	-	1/5/5/24	-
2	OLC	E	343	-	-	4/9/9/24	-
2	OLC	C	346	-	-	3/7/7/24	-
2	OLC	F	346	-	-	0/5/5/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	358	-	-	8/24/24/24	-
2	OLC	F	348	-	-	6/11/11/24	-
2	OLC	D	348	-	-	3/5/5/24	-
2	OLC	C	363	-	-	12/24/24/24	-
2	OLC	C	356	-	-	0/5/5/24	-
2	OLC	E	348	-	-	6/9/9/24	-
2	OLC	A	356	-	-	5/24/24/24	-
2	OLC	B	353	-	-	1/5/5/24	-
2	OLC	B	348	-	-	3/11/11/24	-
2	OLC	C	359	-	-	12/24/24/24	-
2	OLC	C	355	-	-	1/7/7/24	-
2	OLC	D	347	-	-	3/5/5/24	-
2	OLC	A	361	-	-	15/24/24/24	-
2	OLC	C	344	-	-	1/5/5/24	-
2	OLC	A	364	-	-	6/9/9/24	-
2	OLC	A	360	-	-	2/9/9/24	-
2	OLC	B	349	-	-	0/5/5/24	-
2	OLC	C	341	-	-	1/7/7/24	-
2	OLC	F	347	-	-	4/11/11/24	-
2	OLC	A	352	-	-	3/7/7/24	-
2	OLC	C	360	3	-	17/24/24/24	-
2	OLC	F	342	-	-	4/11/11/24	-
2	OLC	C	351	-	-	0/5/5/24	-
2	OLC	A	346	-	-	7/24/24/24	-
2	OLC	E	341	-	-	11/24/24/24	-
2	OLC	F	344	-	-	1/7/7/24	-
2	OLC	A	354	-	-	4/5/5/24	-
2	OLC	D	345	-	-	1/7/7/24	-
2	OLC	F	341	-	-	0/5/5/24	-
2	OLC	F	345	-	-	4/9/9/24	-
2	OLC	E	342	-	-	2/5/5/24	-
2	OLC	C	352	-	-	6/9/9/24	-
2	OLC	A	348	-	-	5/7/7/24	-
2	OLC	A	365	-	-	3/5/5/24	-
2	OLC	E	347	-	-	8/24/24/24	-
2	OLC	A	355	-	-	2/7/7/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	F	343	-	-	0/5/5/24	-
2	OLC	B	343	-	-	0/5/5/24	-
2	OLC	B	346	-	-	10/24/24/24	-
2	OLC	C	345	-	-	1/9/9/24	-
2	OLC	E	346	-	-	2/7/7/24	-
2	OLC	D	344	-	-	2/5/5/24	-
2	OLC	B	345	-	-	9/24/24/24	-
2	OLC	B	341	-	-	1/2/2/24	-
2	OLC	B	350	-	-	18/24/24/24	-
2	OLC	A	358	-	-	16/24/24/24	-
2	OLC	E	344	-	-	4/9/9/24	-
2	OLC	D	342	-	-	11/24/24/24	-
2	OLC	A	359	-	-	10/24/24/24	-
2	OLC	A	362	-	-	6/11/11/24	-
2	OLC	A	341	-	-	0/5/5/24	-

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	OLC	O20-C1	4.89	1.47	1.33
2	C	360	OLC	O20-C1	4.66	1.47	1.33
2	E	347	OLC	O20-C1	4.56	1.46	1.33
2	D	342	OLC	O20-C1	4.50	1.46	1.33
2	B	346	OLC	O20-C1	4.45	1.46	1.33
2	A	346	OLC	O20-C1	4.40	1.46	1.33
2	A	356	OLC	O20-C1	4.38	1.46	1.33
2	B	345	OLC	O20-C1	4.36	1.46	1.33
2	C	362	OLC	O20-C1	4.26	1.45	1.33
2	C	363	OLC	O20-C1	4.23	1.45	1.33
2	A	358	OLC	O20-C1	4.22	1.45	1.33
2	B	350	OLC	O20-C1	4.19	1.45	1.33
2	A	359	OLC	O20-C1	4.11	1.45	1.33
2	A	349	OLC	O20-C1	4.11	1.45	1.33
2	C	359	OLC	O20-C1	4.09	1.45	1.33
2	E	341	OLC	O20-C1	4.08	1.45	1.33
2	C	358	OLC	O20-C1	4.08	1.45	1.33
2	A	363	OLC	C9-C10	3.97	1.54	1.31
2	E	348	OLC	C9-C10	3.93	1.54	1.31
2	B	351	OLC	O20-C1	3.91	1.44	1.33
2	F	348	OLC	C9-C10	3.91	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	361	OLC	C9-C10	3.88	1.54	1.31
2	C	357	OLC	C9-C10	3.84	1.54	1.31
2	C	364	OLC	C9-C10	3.81	1.53	1.31
2	A	362	OLC	C9-C10	3.79	1.53	1.31
2	D	346	OLC	C9-C10	3.78	1.53	1.31
2	A	364	OLC	C9-C10	3.77	1.53	1.31
2	D	349	OLC	O20-C1	3.77	1.44	1.33
2	F	342	OLC	C9-C10	3.76	1.53	1.31
2	E	343	OLC	C9-C10	3.75	1.53	1.31
2	A	350	OLC	C9-C10	3.74	1.53	1.31
2	E	345	OLC	C9-C10	3.73	1.53	1.31
2	C	345	OLC	C9-C10	3.71	1.53	1.31
2	B	347	OLC	C9-C10	3.71	1.53	1.31
2	F	347	OLC	C9-C10	3.70	1.53	1.31
2	C	348	OLC	C9-C10	3.69	1.53	1.31
2	A	360	OLC	C9-C10	3.68	1.53	1.31
2	C	350	OLC	C9-C10	3.68	1.53	1.31
2	A	351	OLC	C9-C10	3.68	1.53	1.31
2	B	342	OLC	C9-C10	3.67	1.53	1.31
2	F	345	OLC	C9-C10	3.67	1.53	1.31
2	C	352	OLC	C9-C10	3.66	1.53	1.31
2	E	344	OLC	C9-C10	3.66	1.53	1.31
2	B	348	OLC	C9-C10	3.63	1.52	1.31
2	A	344	OLC	C10-C9	3.56	1.52	1.28
2	B	352	OLC	C9-C10	3.53	1.52	1.31
2	A	357	OLC	C10-C9	3.51	1.52	1.28
2	B	344	OLC	C10-C9	3.47	1.52	1.28
2	A	348	OLC	C10-C9	3.47	1.52	1.28
2	A	355	OLC	C10-C9	3.47	1.52	1.28
2	A	352	OLC	C10-C9	3.47	1.52	1.28
2	C	349	OLC	C10-C9	3.45	1.51	1.28
2	C	354	OLC	C10-C9	3.45	1.51	1.28
2	E	346	OLC	C10-C9	3.45	1.51	1.28
2	C	346	OLC	C10-C9	3.45	1.51	1.28
2	C	347	OLC	C10-C9	3.44	1.51	1.28
2	C	355	OLC	C10-C9	3.44	1.51	1.28
2	C	353	OLC	C10-C9	3.44	1.51	1.28
2	C	341	OLC	C10-C9	3.43	1.51	1.28
2	D	345	OLC	C10-C9	3.43	1.51	1.28
2	F	344	OLC	C10-C9	3.43	1.51	1.28
2	C	358	OLC	C11-C10	-3.06	1.32	1.50
2	E	341	OLC	C11-C10	-3.03	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	OLC	C8-C9	-3.02	1.33	1.50
2	B	350	OLC	C11-C10	-3.01	1.33	1.50
2	E	341	OLC	C8-C9	-3.01	1.33	1.50
2	D	349	OLC	C9-C10	2.98	1.49	1.31
2	C	359	OLC	C11-C10	-2.97	1.33	1.50
2	A	356	OLC	C11-C10	-2.97	1.33	1.50
2	A	349	OLC	C11-C10	-2.97	1.33	1.50
2	A	346	OLC	C11-C10	-2.97	1.33	1.50
2	C	358	OLC	C8-C9	-2.95	1.33	1.50
2	E	347	OLC	C8-C9	-2.94	1.33	1.50
2	B	345	OLC	C11-C10	-2.93	1.33	1.50
2	A	358	OLC	C11-C10	-2.93	1.33	1.50
2	B	346	OLC	C11-C10	-2.93	1.33	1.50
2	A	358	OLC	C8-C9	-2.93	1.33	1.50
2	C	359	OLC	C8-C9	-2.90	1.33	1.50
2	B	346	OLC	C8-C9	-2.89	1.33	1.50
2	A	349	OLC	C8-C9	-2.89	1.33	1.50
2	C	363	OLC	C8-C9	-2.87	1.33	1.50
2	A	346	OLC	C8-C9	-2.86	1.34	1.50
2	B	345	OLC	C8-C9	-2.85	1.34	1.50
2	A	361	OLC	C11-C10	-2.85	1.34	1.50
2	A	356	OLC	C8-C9	-2.84	1.34	1.50
2	C	362	OLC	C11-C10	-2.83	1.34	1.50
2	D	342	OLC	C8-C9	-2.81	1.34	1.50
2	C	363	OLC	C11-C10	-2.80	1.34	1.50
2	C	362	OLC	C8-C9	-2.78	1.34	1.50
2	D	342	OLC	C11-C10	-2.77	1.34	1.50
2	E	347	OLC	C11-C10	-2.76	1.34	1.50
2	C	360	OLC	C9-C10	2.74	1.47	1.31
2	C	360	OLC	C8-C9	-2.74	1.34	1.50
2	A	361	OLC	C8-C9	-2.72	1.34	1.50
2	C	360	OLC	C11-C10	-2.72	1.34	1.50
2	A	359	OLC	C11-C10	-2.71	1.34	1.50
2	B	351	OLC	C8-C9	-2.71	1.34	1.50
2	A	361	OLC	C9-C10	2.70	1.47	1.31
2	B	351	OLC	C9-C10	2.70	1.47	1.31
2	A	359	OLC	C8-C9	-2.69	1.34	1.50
2	C	362	OLC	C9-C10	2.68	1.47	1.31
2	B	351	OLC	C11-C10	-2.61	1.35	1.50
2	D	342	OLC	C9-C10	2.60	1.46	1.31
2	A	346	OLC	C9-C10	2.59	1.46	1.31
2	A	359	OLC	C9-C10	2.55	1.46	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	349	OLC	C8-C9	-2.54	1.35	1.50
2	C	359	OLC	C9-C10	2.54	1.46	1.31
2	A	349	OLC	C9-C10	2.54	1.46	1.31
2	A	358	OLC	C9-C10	2.54	1.46	1.31
2	E	347	OLC	C9-C10	2.52	1.46	1.31
2	B	345	OLC	C9-C10	2.50	1.46	1.31
2	D	349	OLC	C11-C10	-2.50	1.36	1.50
2	E	341	OLC	C9-C10	2.48	1.46	1.31
2	B	350	OLC	C9-C10	2.48	1.46	1.31
2	C	363	OLC	C9-C10	2.44	1.45	1.31
2	C	358	OLC	C9-C10	2.43	1.45	1.31
2	A	356	OLC	C9-C10	2.41	1.45	1.31
2	B	346	OLC	C9-C10	2.41	1.45	1.31

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	OLC	O20-C1-C2	4.60	126.35	111.91
2	C	362	OLC	O20-C1-C2	4.09	124.75	111.91
2	E	341	OLC	O20-C1-C2	4.07	124.68	111.91
2	B	346	OLC	O20-C1-C2	3.99	124.42	111.91
2	C	363	OLC	O20-C1-C2	3.80	123.85	111.91
2	A	356	OLC	O20-C1-C2	3.80	123.83	111.91
2	C	362	OLC	O20-C1-O19	-3.58	114.55	123.59
2	A	358	OLC	O20-C1-C2	3.56	123.07	111.91
2	C	359	OLC	O20-C1-C2	3.54	123.00	111.91
2	D	349	OLC	O20-C1-C2	3.53	123.00	111.91
2	E	347	OLC	O20-C1-C2	3.53	122.99	111.91
2	A	361	OLC	O20-C1-O19	-3.45	114.87	123.59
2	C	363	OLC	O20-C1-O19	-3.27	115.34	123.59
2	A	346	OLC	O20-C1-C2	3.26	122.13	111.91
2	B	345	OLC	O20-C1-C2	3.15	121.80	111.91
2	D	349	OLC	O20-C1-O19	-3.14	115.67	123.59
2	E	341	OLC	C3-C2-C1	-3.07	102.47	113.62
2	A	349	OLC	O20-C1-C2	3.03	121.41	111.91
2	A	359	OLC	O20-C1-C2	2.96	121.19	111.91
2	C	360	OLC	O20-C1-C2	2.95	121.16	111.91
2	D	342	OLC	O20-C1-C2	2.93	121.11	111.91
2	B	346	OLC	O20-C1-O19	-2.74	116.68	123.59
2	B	351	OLC	O20-C1-C2	2.70	120.37	111.91
2	C	359	OLC	O20-C1-O19	-2.64	116.92	123.59
2	A	356	OLC	O20-C1-O19	-2.63	116.95	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	358	OLC	O20-C1-C2	2.62	120.14	111.91
2	A	349	OLC	O20-C1-O19	-2.53	117.21	123.59
2	E	341	OLC	O20-C1-O19	-2.52	117.23	123.59
2	C	349	OLC	C8-C9-C10	-2.47	110.08	126.84
2	D	345	OLC	C8-C9-C10	-2.43	110.29	126.84
2	C	346	OLC	C8-C9-C10	-2.39	110.56	126.84
2	A	355	OLC	C8-C9-C10	-2.34	110.94	126.84
2	E	346	OLC	C8-C9-C10	-2.33	110.99	126.84
2	C	359	OLC	C21-O20-C1	2.33	125.73	117.12
2	A	344	OLC	C8-C9-C10	-2.32	111.06	126.84
2	C	355	OLC	C8-C9-C10	-2.31	111.16	126.84
2	A	358	OLC	O20-C1-O19	-2.30	117.78	123.59
2	C	353	OLC	C8-C9-C10	-2.29	111.24	126.84
2	A	362	OLC	C8-C9-C10	-2.29	107.15	124.73
2	D	349	OLC	C12-C11-C10	2.28	125.51	112.43
2	F	344	OLC	C8-C9-C10	-2.28	111.35	126.84
2	A	348	OLC	C8-C9-C10	-2.28	111.35	126.84
2	A	346	OLC	O20-C1-O19	-2.28	117.84	123.59
2	C	354	OLC	C8-C9-C10	-2.25	111.55	126.84
2	C	347	OLC	C8-C9-C10	-2.23	111.66	126.84
2	A	357	OLC	C8-C9-C10	-2.23	111.70	126.84
2	B	344	OLC	C8-C9-C10	-2.22	111.72	126.84
2	A	359	OLC	O20-C1-O19	-2.21	118.00	123.59
2	A	352	OLC	C8-C9-C10	-2.20	111.87	126.84
2	C	341	OLC	C8-C9-C10	-2.19	111.97	126.84
2	B	347	OLC	C8-C9-C10	-2.16	108.17	124.73
2	E	347	OLC	O20-C1-O19	-2.13	118.23	123.59
2	A	356	OLC	C3-C2-C1	-2.12	105.91	113.62
2	C	362	OLC	C3-C2-C1	-2.12	105.91	113.62
2	B	350	OLC	O20-C1-C2	2.10	118.50	111.91
2	B	348	OLC	C11-C10-C9	-2.07	108.81	124.73
2	B	346	OLC	C3-C2-C1	-2.07	106.10	113.62
2	D	342	OLC	O20-C1-O19	-2.05	118.42	123.59
2	C	360	OLC	O20-C1-O19	-2.03	118.46	123.59
2	F	342	OLC	C8-C9-C10	-2.03	109.13	124.73
2	B	345	OLC	O20-C1-O19	-2.03	118.48	123.59
2	A	346	OLC	C3-C2-C1	-2.02	106.26	113.62
2	B	352	OLC	C11-C10-C9	-2.02	109.20	124.73

There are no chirality outliers.

All (398) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	349	OLC	O20-C21-C22-C24
2	A	349	OLC	O20-C21-C22-O23
2	D	349	OLC	O23-C22-C24-O25
2	B	351	OLC	C11-C10-C9-C8
2	B	351	OLC	C21-C22-C24-O25
2	C	362	OLC	O20-C21-C22-C24
2	C	362	OLC	O20-C21-C22-O23
2	D	346	OLC	C9-C10-C11-C12
2	A	363	OLC	C11-C10-C9-C8
2	A	363	OLC	C9-C10-C11-C12
2	C	358	OLC	C2-C1-O20-C21
2	C	358	OLC	O19-C1-O20-C21
2	C	359	OLC	C21-C22-C24-O25
2	C	359	OLC	O20-C21-C22-O23
2	C	359	OLC	C2-C1-O20-C21
2	C	359	OLC	O19-C1-O20-C21
2	A	361	OLC	C11-C10-C9-C8
2	A	364	OLC	C9-C10-C11-C12
2	C	360	OLC	C11-C10-C9-C8
2	C	360	OLC	O20-C21-C22-C24
2	C	360	OLC	O20-C21-C22-O23
2	C	360	OLC	O19-C1-O20-C21
2	E	347	OLC	C2-C1-O20-C21
2	E	347	OLC	O19-C1-O20-C21
2	B	346	OLC	O20-C21-C22-C24
2	B	350	OLC	C2-C1-O20-C21
2	B	350	OLC	O19-C1-O20-C21
2	A	358	OLC	O20-C21-C22-C24
2	A	358	OLC	O20-C21-C22-O23
2	E	344	OLC	C9-C10-C11-C12
2	D	342	OLC	C2-C1-O20-C21
2	D	342	OLC	O19-C1-O20-C21
2	A	358	OLC	O19-C1-O20-C21
2	C	360	OLC	C2-C1-O20-C21
2	B	351	OLC	O19-C1-O20-C21
2	B	351	OLC	C2-C1-O20-C21
2	C	362	OLC	C2-C1-O20-C21
2	A	358	OLC	C2-C1-O20-C21
2	A	361	OLC	O19-C1-O20-C21
2	B	352	OLC	C11-C10-C9-C8
2	C	361	OLC	C11-C10-C9-C8
2	A	359	OLC	C11-C12-C13-C14
2	C	362	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	B	346	OLC	O20-C21-C22-O23
2	A	361	OLC	C2-C1-O20-C21
2	A	349	OLC	C2-C1-O20-C21
2	E	341	OLC	O20-C21-C22-C24
2	E	341	OLC	O20-C21-C22-O23
2	D	342	OLC	O23-C22-C24-O25
2	A	349	OLC	O19-C1-O20-C21
2	D	349	OLC	C1-C2-C3-C4
2	C	358	OLC	C1-C2-C3-C4
2	E	347	OLC	C1-C2-C3-C4
2	F	344	OLC	C7-C8-C9-C10
2	A	359	OLC	C1-C2-C3-C4
2	B	350	OLC	C11-C10-C9-C8
2	C	363	OLC	C5-C6-C7-C8
2	A	343	OLC	C1-C2-C3-C4
2	E	347	OLC	C6-C7-C8-C9
2	A	361	OLC	C5-C6-C7-C8
2	A	364	OLC	C5-C6-C7-C8
2	C	349	OLC	C4-C5-C6-C7
2	C	358	OLC	C11-C10-C9-C8
2	A	358	OLC	C1-C2-C3-C4
2	B	351	OLC	C14-C15-C16-C17
2	C	364	OLC	C2-C3-C4-C5
2	C	363	OLC	C2-C3-C4-C5
2	A	361	OLC	C14-C15-C16-C17
2	A	358	OLC	C2-C3-C4-C5
2	A	349	OLC	C11-C12-C13-C14
2	C	363	OLC	C3-C4-C5-C6
2	C	362	OLC	C3-C4-C5-C6
2	A	356	OLC	C2-C3-C4-C5
2	A	362	OLC	C2-C3-C4-C5
2	D	349	OLC	C2-C3-C4-C5
2	D	348	OLC	C3-C4-C5-C6
2	D	347	OLC	C4-C5-C6-C7
2	D	349	OLC	C21-C22-C24-O25
2	B	350	OLC	C21-C22-C24-O25
2	D	342	OLC	C21-C22-C24-O25
2	C	360	OLC	C6-C7-C8-C9
2	A	358	OLC	C6-C7-C8-C9
2	C	357	OLC	C4-C5-C6-C7
2	C	349	OLC	C3-C4-C5-C6
2	C	362	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	E	348	OLC	C4-C5-C6-C7
2	A	361	OLC	C2-C3-C4-C5
2	D	342	OLC	C5-C6-C7-C8
2	C	361	OLC	C4-C5-C6-C7
2	A	347	OLC	C2-C3-C4-C5
2	A	363	OLC	C2-C3-C4-C5
2	A	346	OLC	C14-C15-C16-C17
2	B	352	OLC	C12-C13-C14-C15
2	A	346	OLC	C3-C4-C5-C6
2	C	362	OLC	C14-C15-C16-C17
2	A	364	OLC	C2-C3-C4-C5
2	C	352	OLC	C4-C5-C6-C7
2	B	352	OLC	C4-C5-C6-C7
2	C	342	OLC	C2-C3-C4-C5
2	A	356	OLC	C11-C12-C13-C14
2	A	349	OLC	C1-C2-C3-C4
2	C	364	OLC	C11-C10-C9-C8
2	F	345	OLC	C11-C10-C9-C8
2	A	359	OLC	C11-C10-C9-C8
2	C	363	OLC	C1-C2-C3-C4
2	C	361	OLC	C5-C6-C7-C8
2	B	351	OLC	O23-C22-C24-O25
2	B	350	OLC	O23-C22-C24-O25
2	D	348	OLC	C2-C3-C4-C5
2	C	363	OLC	C4-C5-C6-C7
2	A	361	OLC	C3-C4-C5-C6
2	C	350	OLC	C6-C7-C8-C9
2	C	363	OLC	C10-C11-C12-C13
2	C	352	OLC	C6-C7-C8-C9
2	B	352	OLC	C2-C3-C4-C5
2	E	348	OLC	C2-C3-C4-C5
2	A	361	OLC	C12-C13-C14-C15
2	E	345	OLC	C2-C3-C4-C5
2	A	363	OLC	C5-C6-C7-C8
2	A	361	OLC	C4-C5-C6-C7
2	A	358	OLC	C4-C5-C6-C7
2	C	363	OLC	C11-C12-C13-C14
2	A	357	OLC	C3-C4-C5-C6
2	E	343	OLC	C9-C10-C11-C12
2	B	352	OLC	C1-C2-C3-C4
2	C	359	OLC	C11-C10-C9-C8
2	B	351	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	B	351	OLC	C10-C11-C12-C13
2	A	361	OLC	C10-C11-C12-C13
2	C	360	OLC	C10-C11-C12-C13
2	A	346	OLC	C1-C2-C3-C4
2	D	349	OLC	C2-C1-O20-C21
2	C	359	OLC	O20-C21-C22-C24
2	A	348	OLC	C3-C4-C5-C6
2	D	342	OLC	C2-C3-C4-C5
2	B	348	OLC	C4-C5-C6-C7
2	A	354	OLC	C4-C5-C6-C7
2	B	352	OLC	C10-C11-C12-C13
2	A	357	OLC	C6-C7-C8-C9
2	F	348	OLC	C10-C11-C12-C13
2	C	362	OLC	C11-C12-C13-C14
2	B	351	OLC	C5-C6-C7-C8
2	F	345	OLC	C2-C3-C4-C5
2	E	344	OLC	C3-C4-C5-C6
2	A	351	OLC	C9-C10-C11-C12
2	B	345	OLC	C11-C12-C13-C14
2	C	360	OLC	C14-C15-C16-C17
2	B	351	OLC	C6-C7-C8-C9
2	A	357	OLC	C4-C5-C6-C7
2	C	362	OLC	C12-C13-C14-C15
2	E	345	OLC	C1-C2-C3-C4
2	D	349	OLC	O19-C1-O20-C21
2	B	351	OLC	C11-C12-C13-C14
2	E	348	OLC	C1-C2-C3-C4
2	C	360	OLC	C11-C12-C13-C14
2	A	354	OLC	C1-C2-C3-C4
2	A	358	OLC	C14-C15-C16-C17
2	C	360	OLC	C5-C6-C7-C8
2	C	352	OLC	C3-C4-C5-C6
2	E	345	OLC	C10-C11-C12-C13
2	F	342	OLC	C6-C7-C8-C9
2	B	350	OLC	C6-C7-C8-C9
2	A	342	OLC	C5-C6-C7-C8
2	E	341	OLC	C13-C14-C15-C16
2	A	364	OLC	C4-C5-C6-C7
2	B	345	OLC	C2-C1-O20-C21
2	A	347	OLC	C5-C6-C7-C8
2	B	351	OLC	C15-C16-C17-C18
2	A	365	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	D	342	OLC	C13-C14-C15-C16
2	D	346	OLC	C11-C10-C9-C8
2	B	345	OLC	C4-C5-C6-C7
2	F	348	OLC	C11-C12-C13-C14
2	A	365	OLC	C1-C2-C3-C4
2	B	350	OLC	C5-C6-C7-C8
2	A	354	OLC	C3-C4-C5-C6
2	C	359	OLC	C14-C15-C16-C17
2	B	345	OLC	C15-C16-C17-C18
2	B	351	OLC	C2-C3-C4-C5
2	F	342	OLC	C5-C6-C7-C8
2	B	351	OLC	C3-C4-C5-C6
2	A	348	OLC	C4-C5-C6-C7
2	B	350	OLC	C1-C2-C3-C4
2	E	341	OLC	C2-C3-C4-C5
2	A	359	OLC	C2-C3-C4-C5
2	C	350	OLC	C4-C5-C6-C7
2	E	345	OLC	C11-C12-C13-C14
2	B	352	OLC	C13-C14-C15-C16
2	E	346	OLC	C3-C4-C5-C6
2	A	350	OLC	C11-C12-C13-C14
2	D	349	OLC	C11-C12-C13-C14
2	A	360	OLC	C11-C10-C9-C8
2	B	350	OLC	O20-C21-C22-C24
2	B	345	OLC	C12-C13-C14-C15
2	A	359	OLC	O23-C22-C24-O25
2	B	345	OLC	O19-C1-O20-C21
2	C	360	OLC	C15-C16-C17-C18
2	A	365	OLC	C3-C4-C5-C6
2	F	348	OLC	C1-C2-C3-C4
2	C	360	OLC	C12-C13-C14-C15
2	B	346	OLC	C6-C7-C8-C9
2	E	341	OLC	C4-C5-C6-C7
2	C	357	OLC	C7-C8-C9-C10
2	C	344	OLC	C5-C6-C7-C8
2	A	361	OLC	C15-C16-C17-C18
2	A	361	OLC	C1-C2-C3-C4
2	C	348	OLC	C9-C10-C11-C12
2	C	364	OLC	C9-C10-C11-C12
2	E	348	OLC	C9-C10-C11-C12
2	F	345	OLC	C9-C10-C11-C12
2	C	352	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	363	OLC	C1-C2-C3-C4
2	D	347	OLC	C5-C6-C7-C8
2	C	352	OLC	C2-C3-C4-C5
2	B	346	OLC	C11-C12-C13-C14
2	A	362	OLC	C11-C12-C13-C14
2	A	362	OLC	C5-C6-C7-C8
2	E	348	OLC	C3-C4-C5-C6
2	B	352	OLC	C11-C12-C13-C14
2	C	347	OLC	C7-C8-C9-C10
2	A	356	OLC	C4-C5-C6-C7
2	D	346	OLC	C3-C4-C5-C6
2	A	346	OLC	C15-C16-C17-C18
2	C	359	OLC	O23-C22-C24-O25
2	C	362	OLC	C10-C11-C12-C13
2	F	348	OLC	C6-C7-C8-C9
2	B	345	OLC	C6-C7-C8-C9
2	C	353	OLC	C3-C4-C5-C6
2	A	349	OLC	C5-C6-C7-C8
2	D	342	OLC	C1-C2-C3-C4
2	D	349	OLC	C13-C14-C15-C16
2	C	364	OLC	C3-C4-C5-C6
2	C	358	OLC	C5-C6-C7-C8
2	B	353	OLC	C4-C5-C6-C7
2	E	341	OLC	C15-C16-C17-C18
2	F	347	OLC	C11-C12-C13-C14
2	C	363	OLC	C12-C13-C14-C15
2	B	354	OLC	C1-C2-C3-C4
2	C	360	OLC	C3-C4-C5-C6
2	C	349	OLC	C7-C8-C9-C10
2	C	354	OLC	C7-C8-C9-C10
2	B	344	OLC	C7-C8-C9-C10
2	A	352	OLC	C7-C8-C9-C10
2	A	358	OLC	C15-C16-C17-C18
2	C	364	OLC	C6-C7-C8-C9
2	C	359	OLC	C6-C7-C8-C9
2	A	346	OLC	C10-C11-C12-C13
2	A	359	OLC	C6-C7-C8-C9
2	A	355	OLC	C2-C3-C4-C5
2	A	361	OLC	C11-C12-C13-C14
2	D	348	OLC	C1-C2-C3-C4
2	A	358	OLC	C3-C4-C5-C6
2	A	364	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	F	348	OLC	C9-C10-C11-C12
2	D	342	OLC	C4-C5-C6-C7
2	E	341	OLC	C11-C12-C13-C14
2	C	362	OLC	C9-C10-C11-C12
2	A	356	OLC	C9-C10-C11-C12
2	C	360	OLC	C7-C8-C9-C10
2	B	350	OLC	C7-C8-C9-C10
2	A	358	OLC	C7-C8-C9-C10
2	D	342	OLC	C9-C10-C11-C12
2	B	354	OLC	C2-C3-C4-C5
2	C	347	OLC	C5-C6-C7-C8
2	A	349	OLC	C9-C10-C11-C12
2	B	342	OLC	C7-C8-C9-C10
2	C	358	OLC	C9-C10-C11-C12
2	C	358	OLC	C7-C8-C9-C10
2	C	363	OLC	C9-C10-C11-C12
2	C	363	OLC	C7-C8-C9-C10
2	A	361	OLC	C7-C8-C9-C10
2	A	346	OLC	C9-C10-C11-C12
2	E	341	OLC	C9-C10-C11-C12
2	E	347	OLC	C7-C8-C9-C10
2	B	345	OLC	C9-C10-C11-C12
2	B	350	OLC	C9-C10-C11-C12
2	A	358	OLC	C9-C10-C11-C12
2	A	359	OLC	C7-C8-C9-C10
2	A	350	OLC	C5-C6-C7-C8
2	E	342	OLC	C1-C2-C3-C4
2	D	349	OLC	O20-C21-C22-O23
2	B	351	OLC	C7-C8-C9-C10
2	C	362	OLC	C7-C8-C9-C10
2	C	350	OLC	C9-C10-C11-C12
2	B	346	OLC	C9-C10-C11-C12
2	C	358	OLC	C15-C16-C17-C18
2	E	348	OLC	C7-C8-C9-C10
2	A	361	OLC	C9-C10-C11-C12
2	D	344	OLC	C5-C6-C7-C8
2	E	343	OLC	C1-C2-C3-C4
2	A	347	OLC	C4-C5-C6-C7
2	B	350	OLC	C2-C3-C4-C5
2	B	346	OLC	C21-C22-C24-O25
2	D	349	OLC	C9-C10-C11-C12
2	D	349	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	C	362	OLC	C15-C16-C17-C18
2	C	363	OLC	C11-C10-C9-C8
2	A	358	OLC	C11-C12-C13-C14
2	C	346	OLC	C1-C2-C3-C4
2	A	348	OLC	C2-C3-C4-C5
2	C	355	OLC	C7-C8-C9-C10
2	C	341	OLC	C7-C8-C9-C10
2	C	349	OLC	C1-C2-C3-C4
2	A	362	OLC	C10-C11-C12-C13
2	B	350	OLC	C3-C4-C5-C6
2	A	343	OLC	C3-C4-C5-C6
2	C	353	OLC	C2-C3-C4-C5
2	D	349	OLC	C15-C16-C17-C18
2	D	344	OLC	C4-C5-C6-C7
2	C	346	OLC	C3-C4-C5-C6
2	A	348	OLC	C5-C6-C7-C8
2	B	342	OLC	C3-C4-C5-C6
2	B	350	OLC	C14-C15-C16-C17
2	D	345	OLC	C7-C8-C9-C10
2	A	348	OLC	C7-C8-C9-C10
2	F	347	OLC	C1-C2-C3-C4
2	D	349	OLC	C11-C10-C9-C8
2	A	357	OLC	C5-C6-C7-C8
2	F	342	OLC	C9-C10-C11-C12
2	C	346	OLC	C7-C8-C9-C10
2	E	346	OLC	C7-C8-C9-C10
2	A	359	OLC	C21-C22-C24-O25
2	E	341	OLC	C11-C10-C9-C8
2	B	352	OLC	C9-C10-C11-C12
2	B	342	OLC	C9-C10-C11-C12
2	F	345	OLC	C7-C8-C9-C10
2	B	346	OLC	O23-C22-C24-O25
2	A	349	OLC	O20-C1-C2-C3
2	D	347	OLC	C3-C4-C5-C6
2	C	360	OLC	C13-C14-C15-C16
2	C	353	OLC	C7-C8-C9-C10
2	A	355	OLC	C7-C8-C9-C10
2	A	363	OLC	C7-C8-C9-C10
2	B	348	OLC	C9-C10-C11-C12
2	E	344	OLC	C4-C5-C6-C7
2	C	363	OLC	C14-C15-C16-C17
2	F	342	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	C	362	OLC	C6-C7-C8-C9
2	C	362	OLC	C13-C14-C15-C16
2	B	346	OLC	O19-C1-O20-C21
2	E	345	OLC	C9-C10-C11-C12
2	D	346	OLC	C7-C8-C9-C10
2	B	348	OLC	C7-C8-C9-C10
2	A	360	OLC	C7-C8-C9-C10
2	C	352	OLC	C7-C8-C9-C10
2	E	344	OLC	C7-C8-C9-C10
2	E	341	OLC	C12-C13-C14-C15
2	B	344	OLC	C2-C3-C4-C5
2	C	359	OLC	C12-C13-C14-C15
2	A	350	OLC	C7-C8-C9-C10
2	C	342	OLC	C3-C4-C5-C6
2	A	358	OLC	O20-C1-C2-C3
2	E	342	OLC	C5-C6-C7-C8
2	B	347	OLC	C9-C10-C11-C12
2	A	350	OLC	C9-C10-C11-C12
2	A	364	OLC	C7-C8-C9-C10
2	F	347	OLC	C9-C10-C11-C12
2	D	349	OLC	C4-C5-C6-C7
2	C	360	OLC	C4-C5-C6-C7
2	A	362	OLC	C9-C10-C11-C12
2	A	362	OLC	C7-C8-C9-C10
2	E	343	OLC	C11-C10-C9-C8
2	B	350	OLC	O20-C21-C22-O23
2	E	347	OLC	C2-C3-C4-C5
2	A	352	OLC	C4-C5-C6-C7
2	C	345	OLC	C7-C8-C9-C10
2	A	358	OLC	O19-C1-C2-C3
2	A	349	OLC	C7-C8-C9-C10
2	A	346	OLC	C7-C8-C9-C10
2	E	341	OLC	C7-C8-C9-C10
2	B	345	OLC	C7-C8-C9-C10
2	D	342	OLC	C7-C8-C9-C10
2	A	359	OLC	C9-C10-C11-C12
2	A	356	OLC	C7-C8-C9-C10
2	F	347	OLC	C7-C8-C9-C10
2	A	359	OLC	C12-C13-C14-C15
2	B	346	OLC	C2-C1-O20-C21
2	A	349	OLC	O19-C1-C2-C3
2	E	347	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	A	354	OLC	C2-C3-C4-C5
2	B	351	OLC	C9-C10-C11-C12
2	C	359	OLC	C9-C10-C11-C12
2	C	359	OLC	C7-C8-C9-C10
2	E	345	OLC	C4-C5-C6-C7
2	B	350	OLC	O20-C1-C2-C3
2	F	348	OLC	C4-C5-C6-C7
2	E	345	OLC	C7-C8-C9-C10
2	C	360	OLC	C9-C10-C11-C12
2	E	347	OLC	C9-C10-C11-C12
2	B	346	OLC	C7-C8-C9-C10
2	A	352	OLC	C2-C3-C4-C5
2	A	345	OLC	C5-C6-C7-C8
2	E	343	OLC	C2-C3-C4-C5
2	B	341	OLC	C2-C3-C4-C5
2	C	361	OLC	C9-C10-C11-C12
2	C	348	OLC	C7-C8-C9-C10
2	B	350	OLC	C11-C12-C13-C14
2	B	350	OLC	O19-C1-C2-C3

There are no ring outliers.

44 monomers are involved in 81 short contacts:

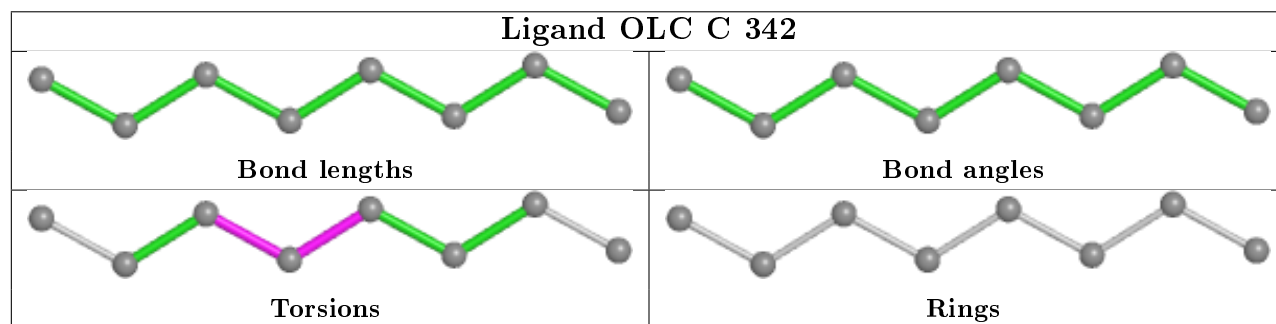
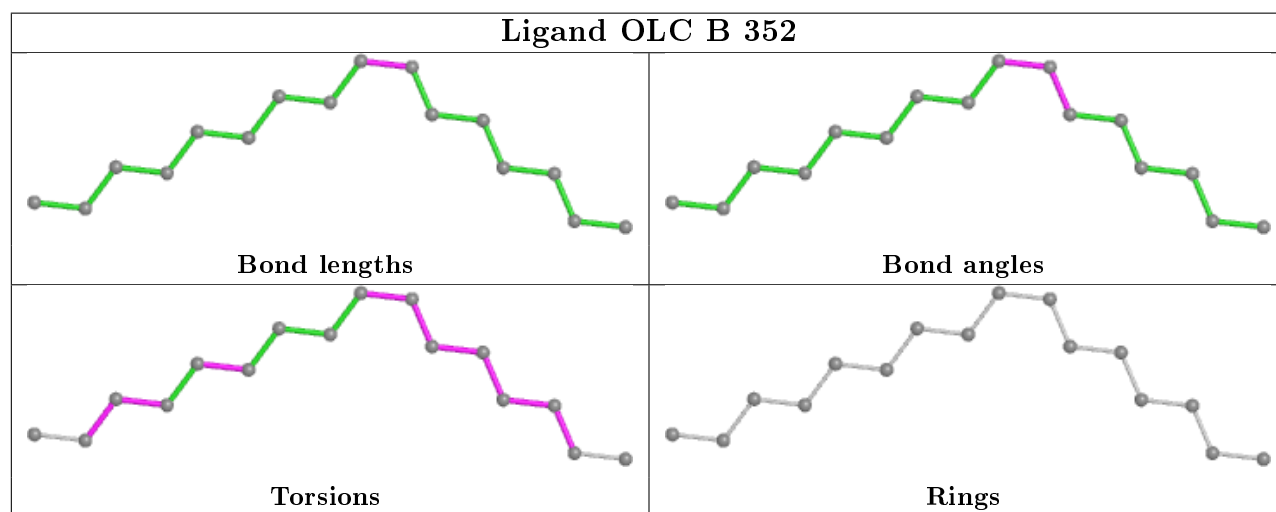
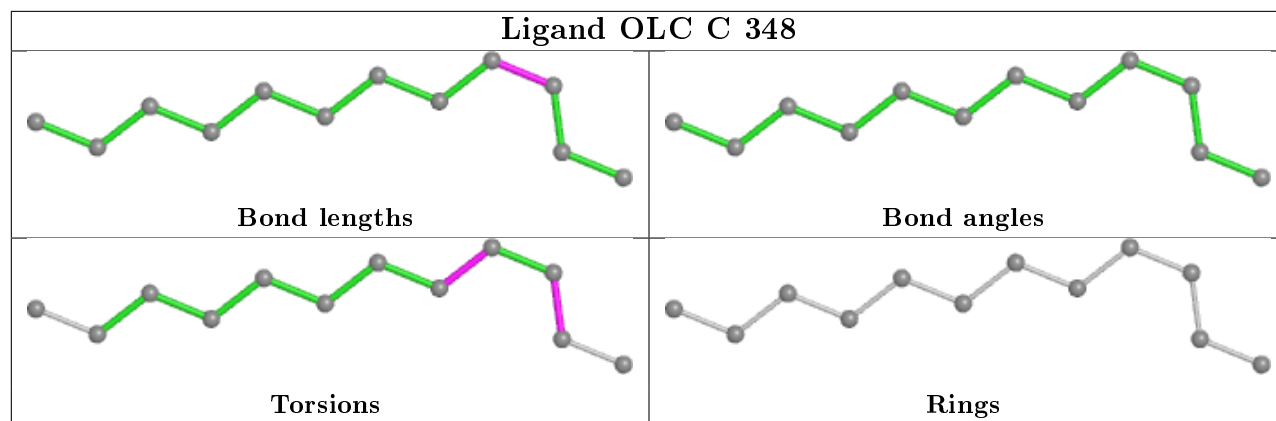
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	348	OLC	2	0
2	A	353	OLC	1	0
2	A	349	OLC	3	0
2	A	344	OLC	1	0
2	C	347	OLC	2	0
2	A	343	OLC	1	0
2	D	349	OLC	1	0
2	C	349	OLC	3	0
2	B	351	OLC	2	0
2	C	362	OLC	2	0
2	D	346	OLC	1	0
2	B	344	OLC	1	0
2	C	353	OLC	1	0
2	A	345	OLC	1	0
2	E	343	OLC	1	0
2	C	358	OLC	2	0
2	D	348	OLC	1	0
2	C	363	OLC	4	0

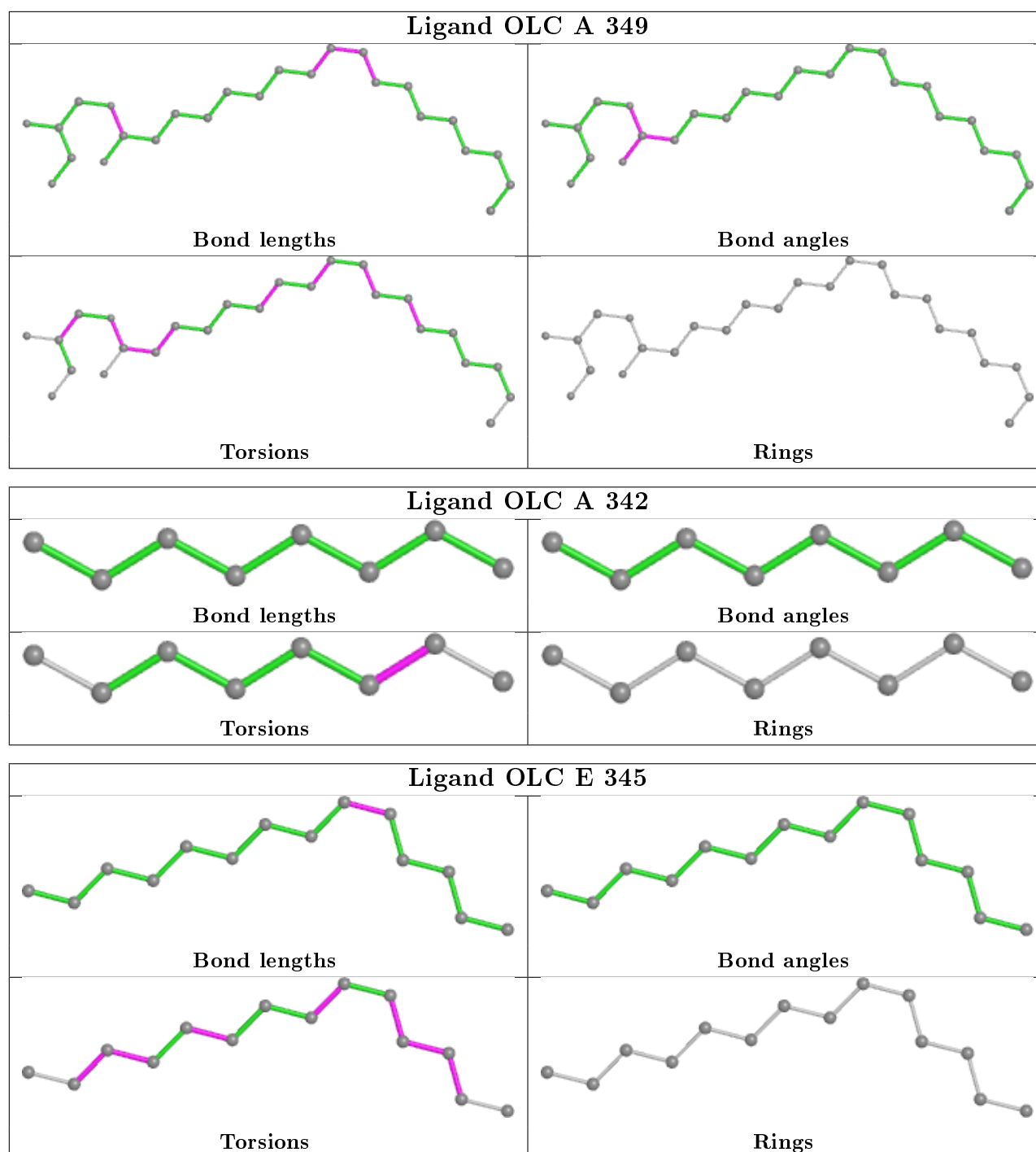
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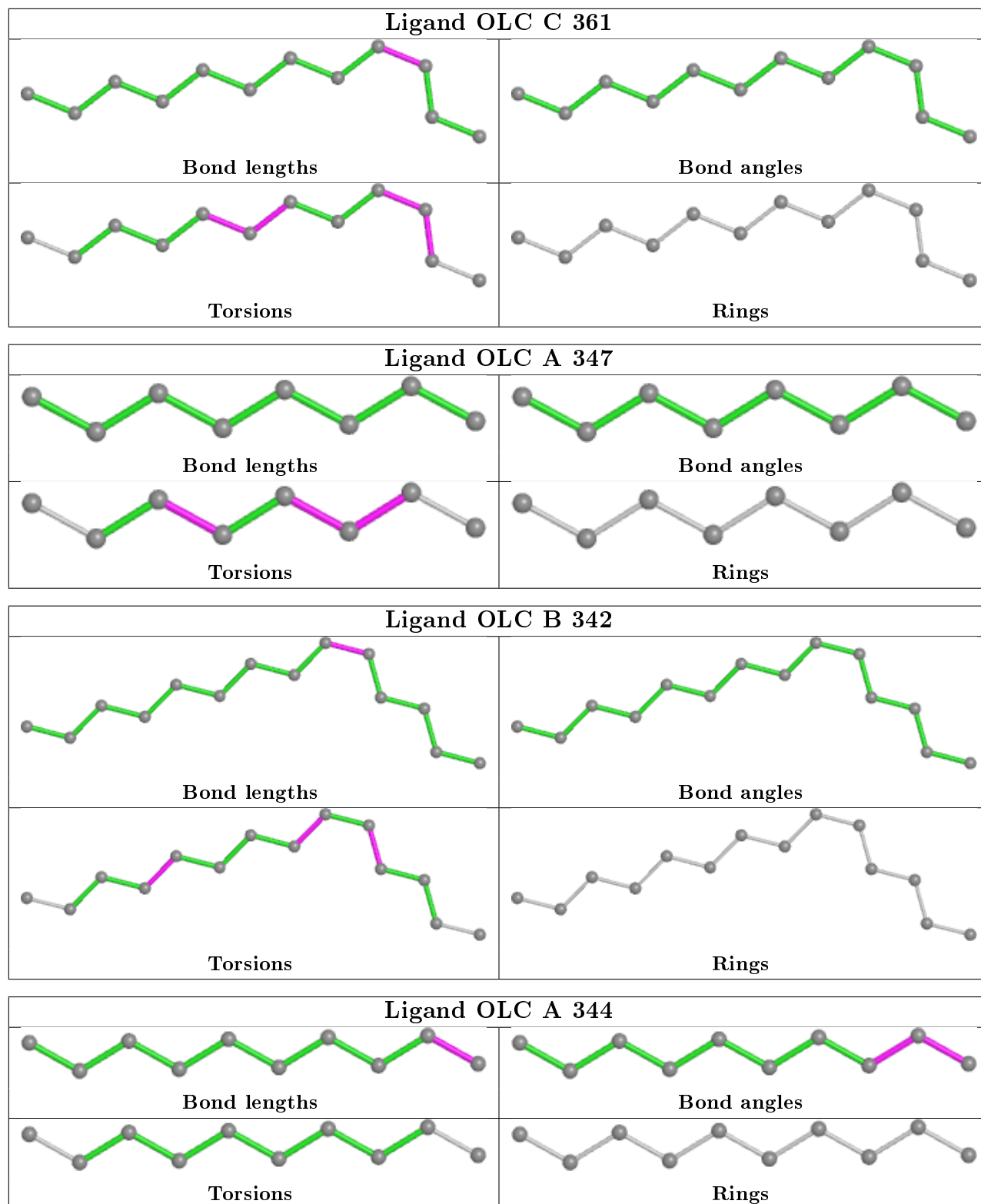
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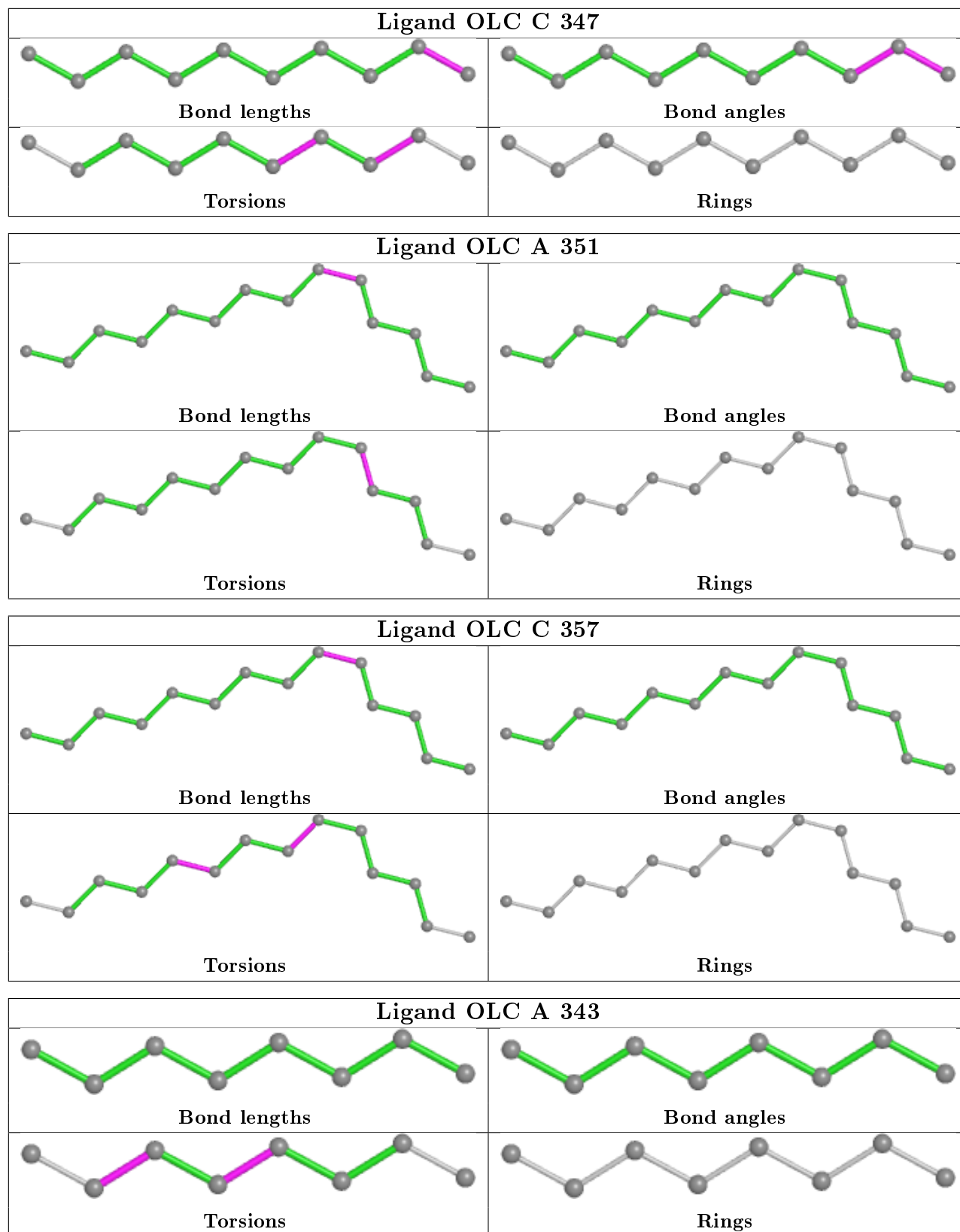
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	348	OLC	6	0
2	A	356	OLC	2	0
2	C	359	OLC	3	0
2	A	361	OLC	8	0
2	A	360	OLC	4	0
2	F	347	OLC	3	0
2	C	360	OLC	2	0
2	F	342	OLC	3	0
2	E	341	OLC	1	0
2	F	344	OLC	1	0
2	D	345	OLC	1	0
2	F	341	OLC	1	0
2	F	345	OLC	1	0
2	E	342	OLC	1	0
2	C	352	OLC	3	0
2	A	365	OLC	5	0
2	E	347	OLC	11	0
2	F	343	OLC	1	0
2	E	346	OLC	2	0
2	B	345	OLC	2	0
2	B	350	OLC	1	0
2	E	344	OLC	3	0
2	D	342	OLC	4	0
2	A	359	OLC	3	0
2	A	362	OLC	1	0
2	A	341	OLC	2	0

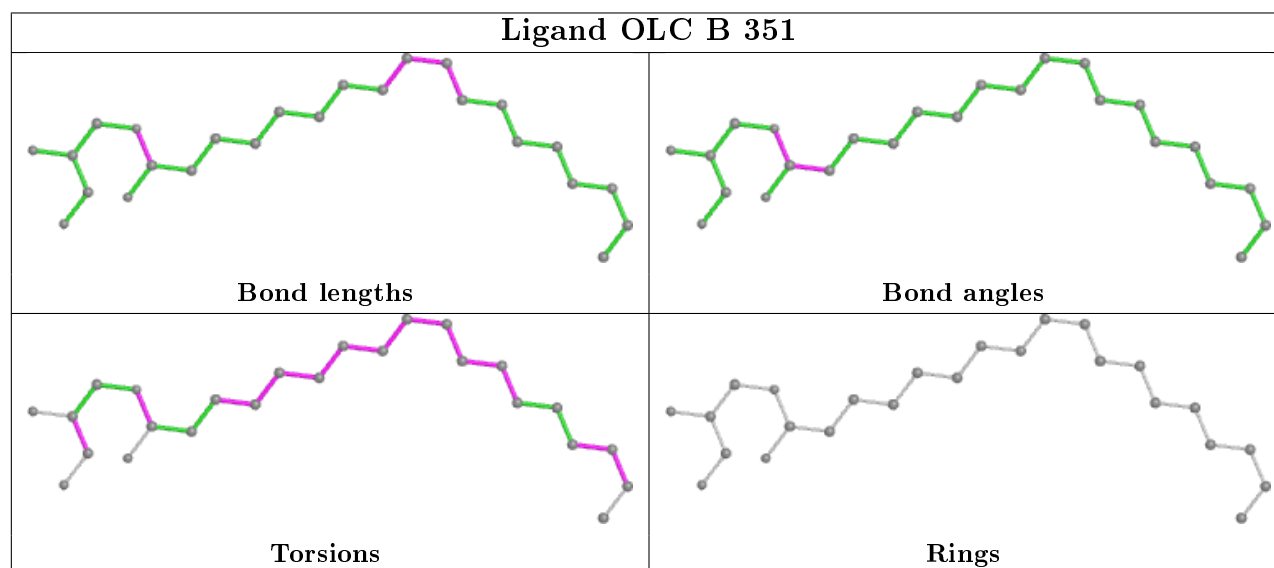
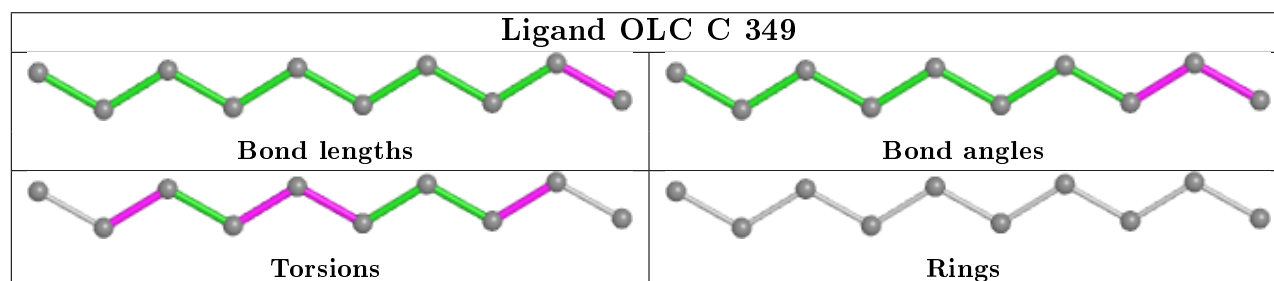
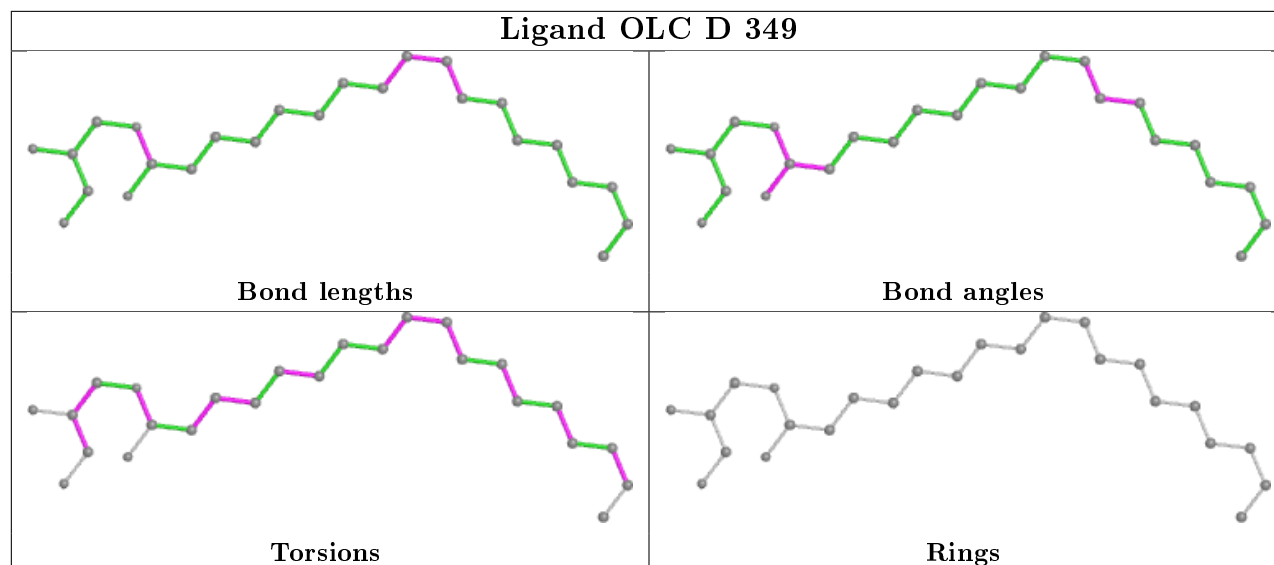
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

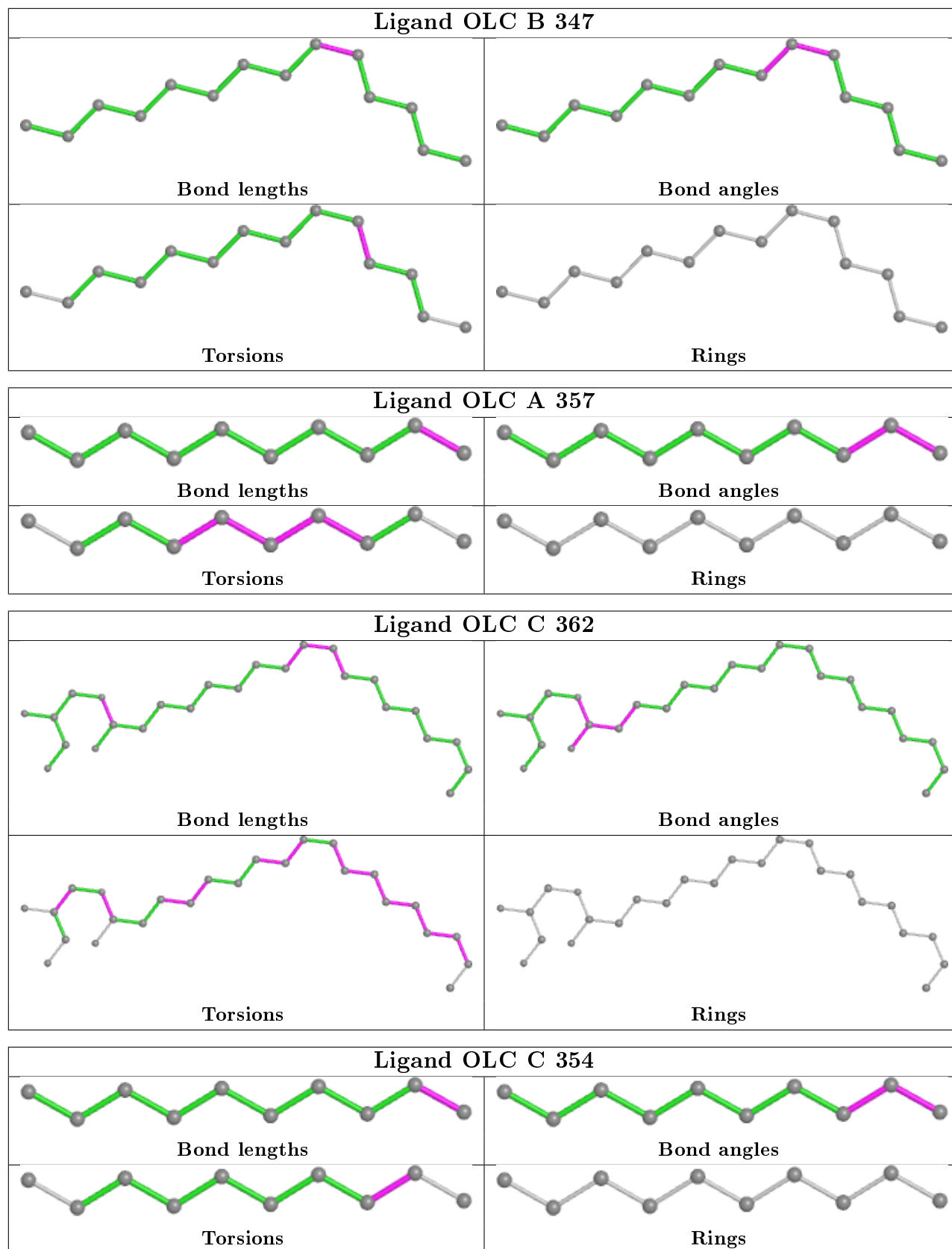


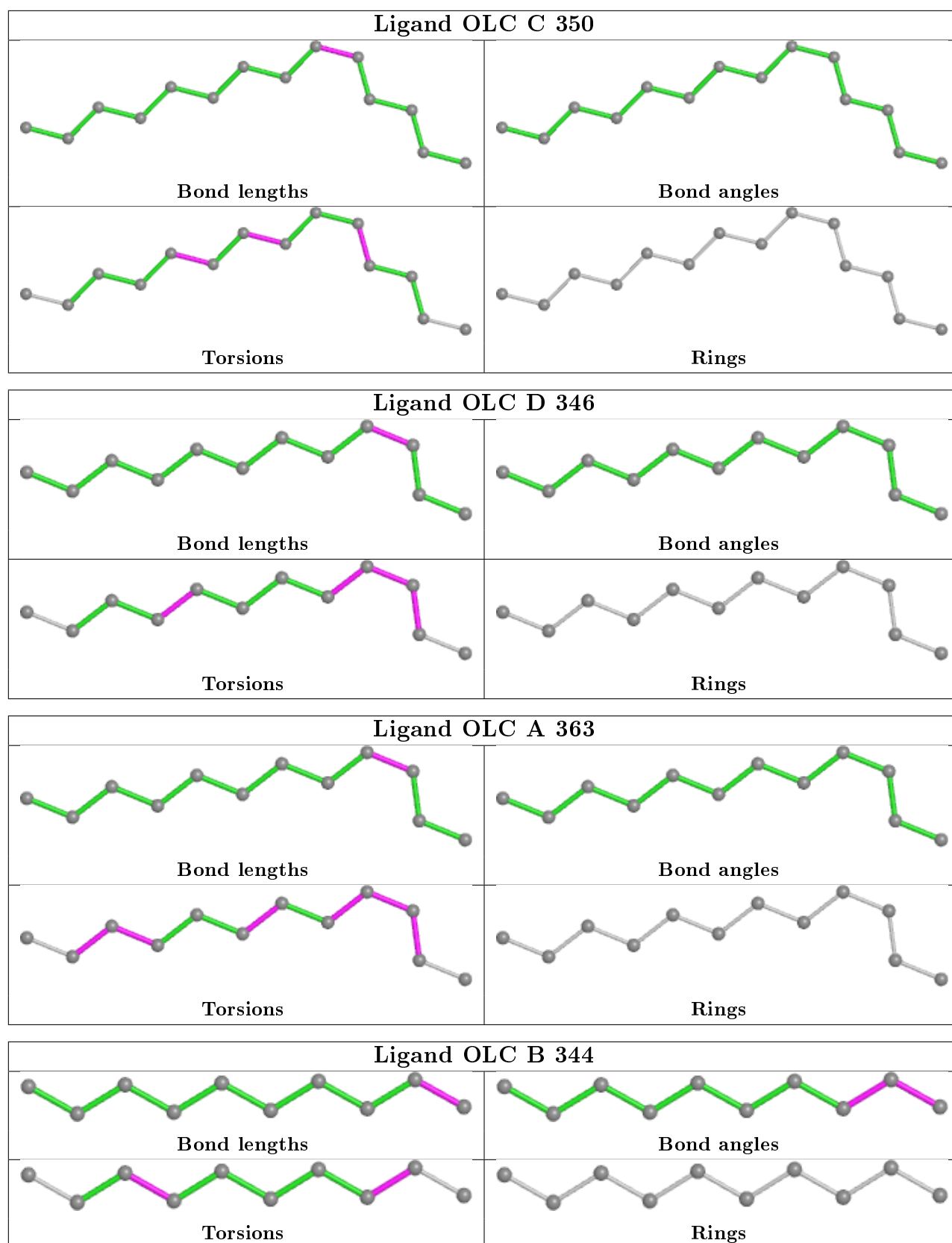


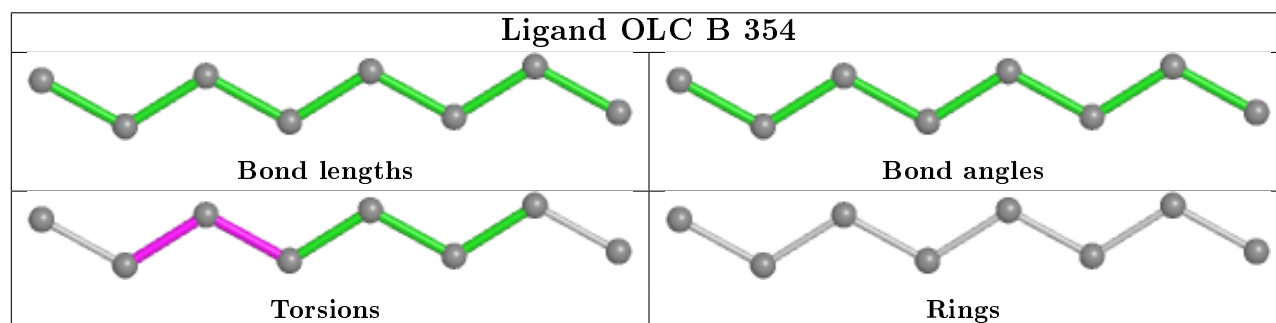
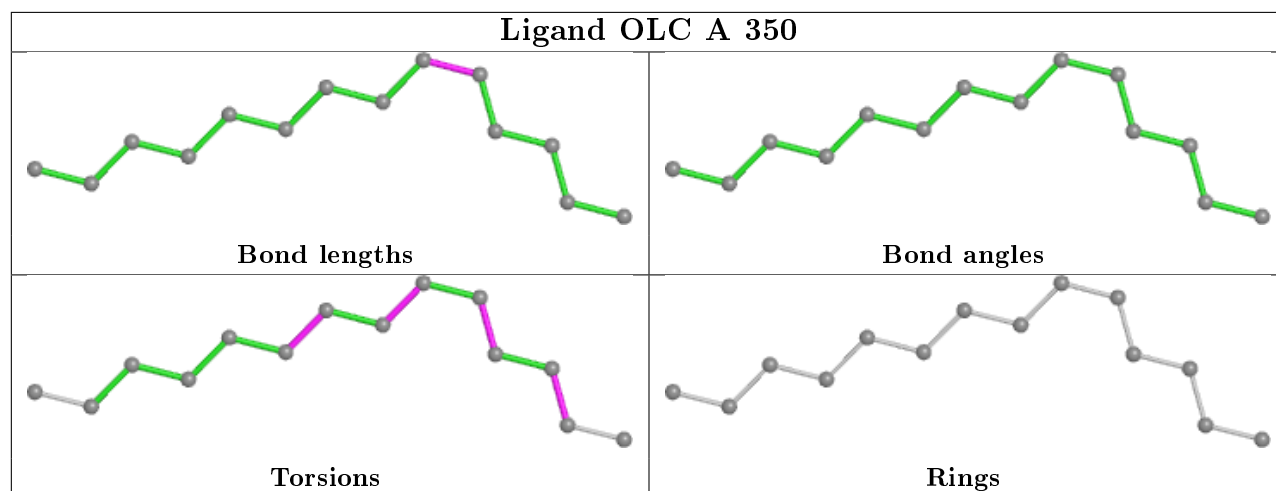
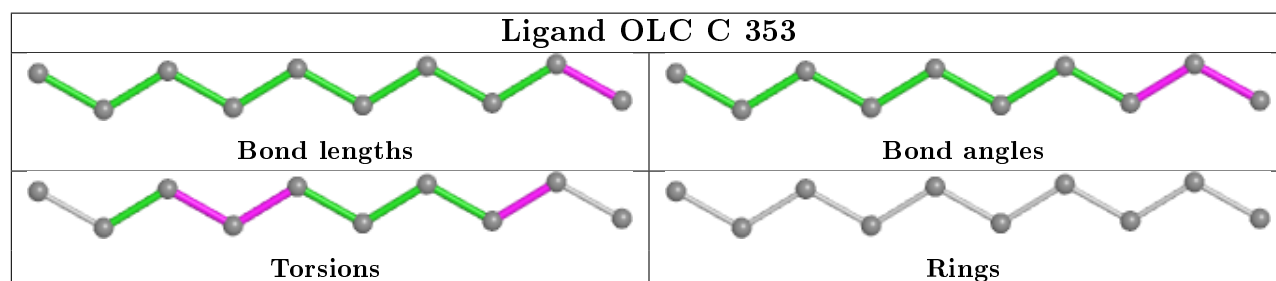
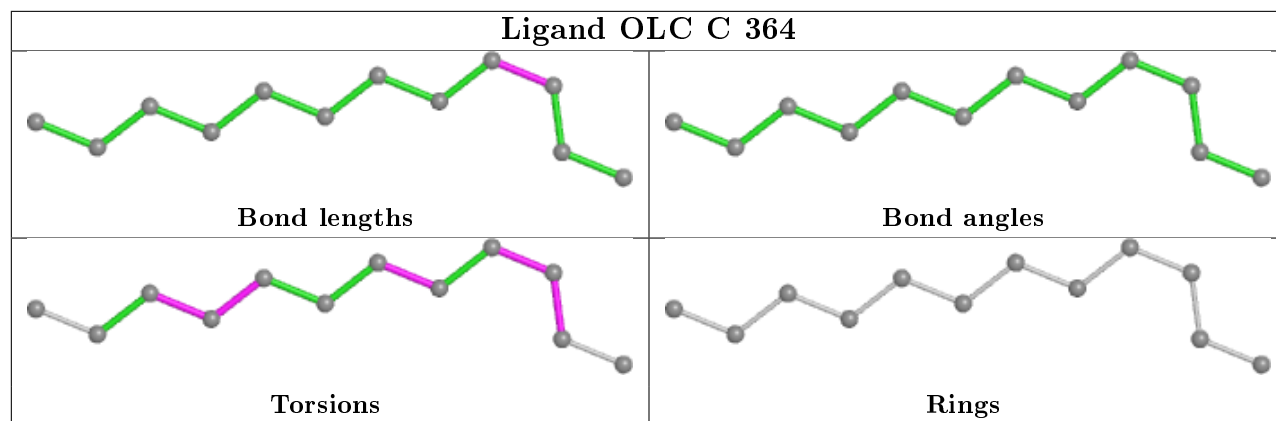


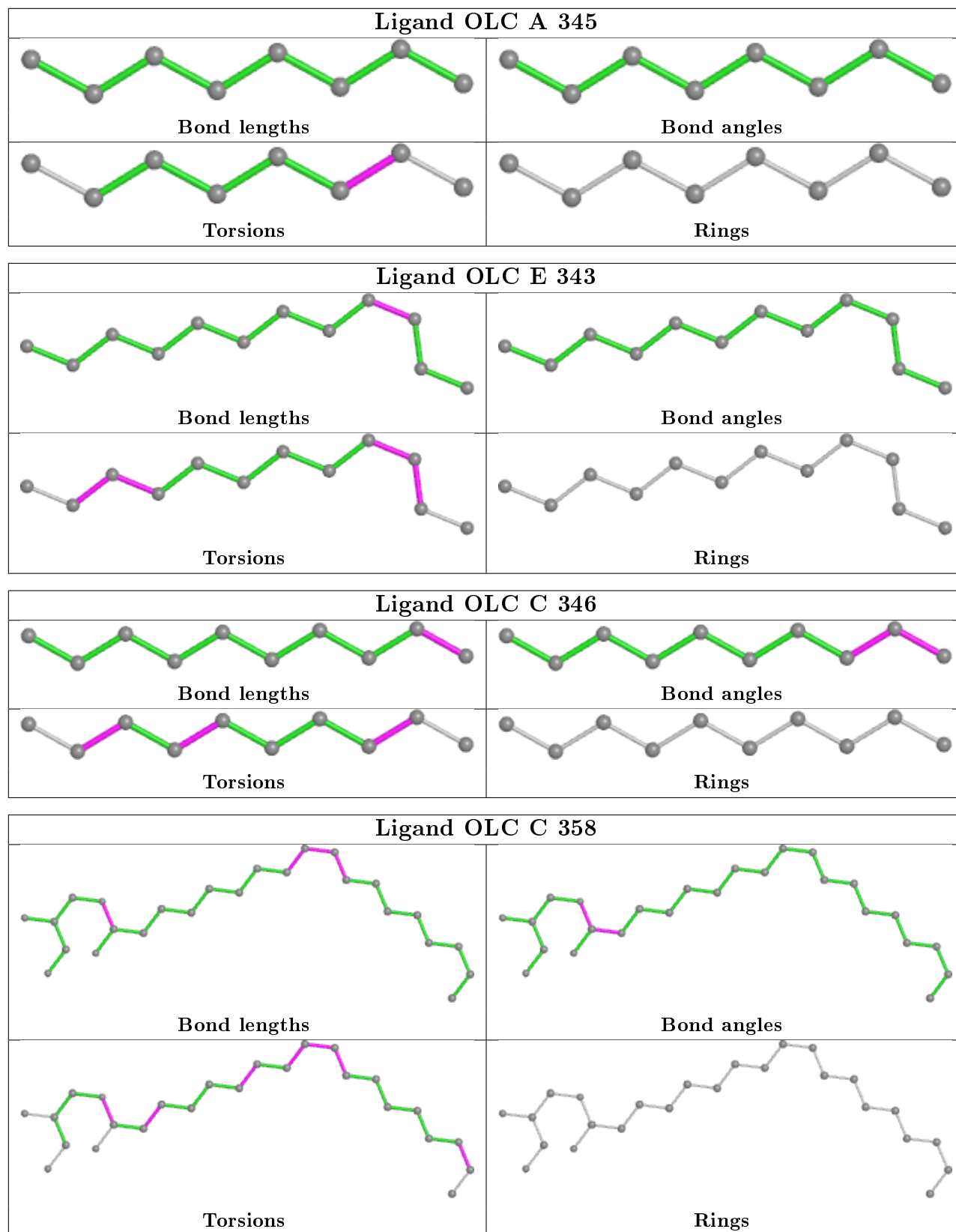


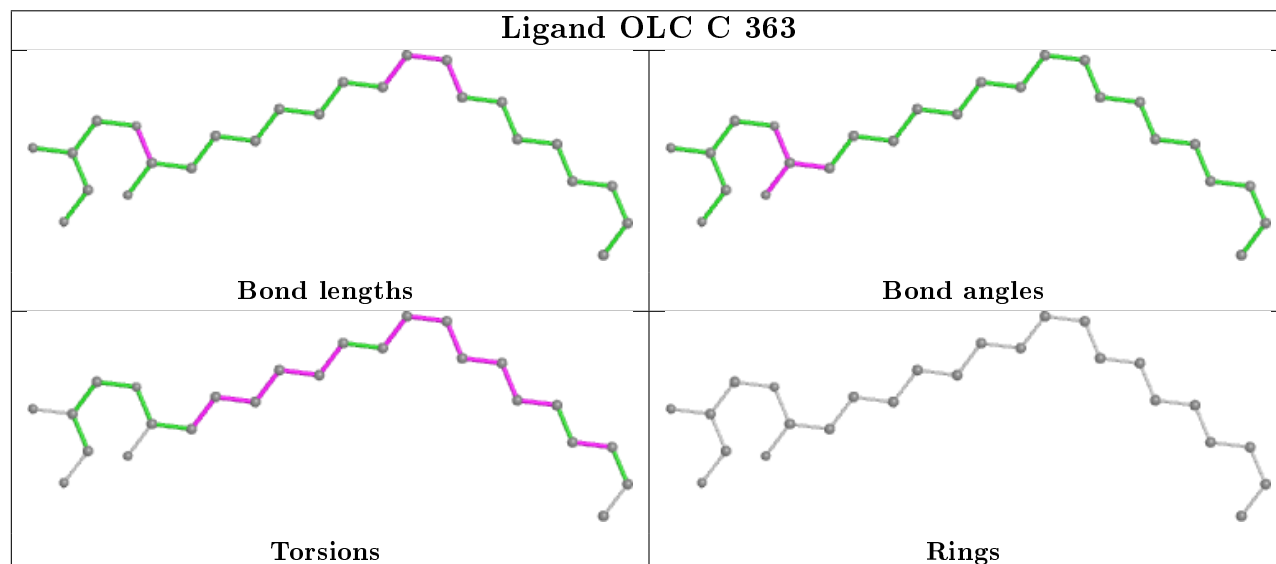
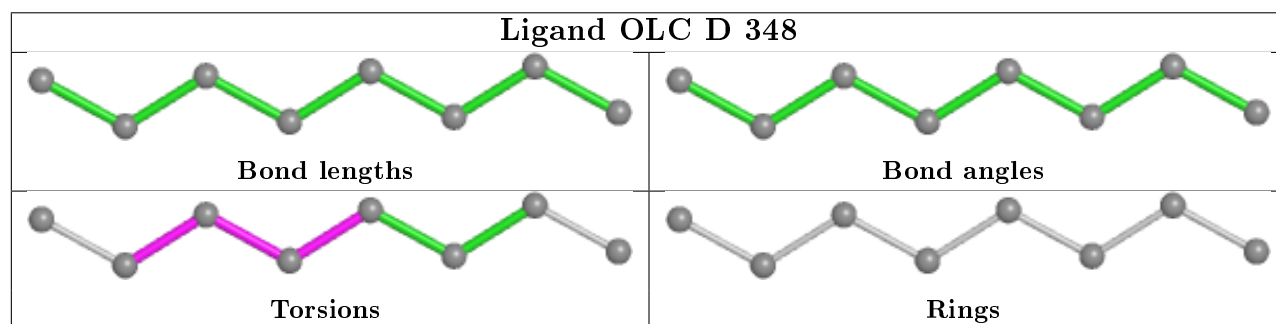
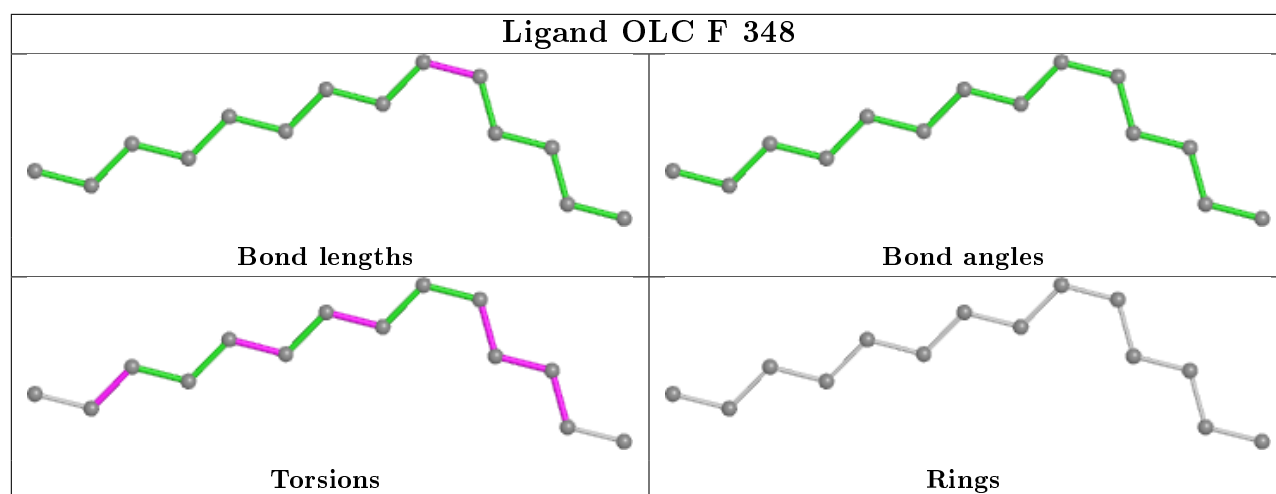


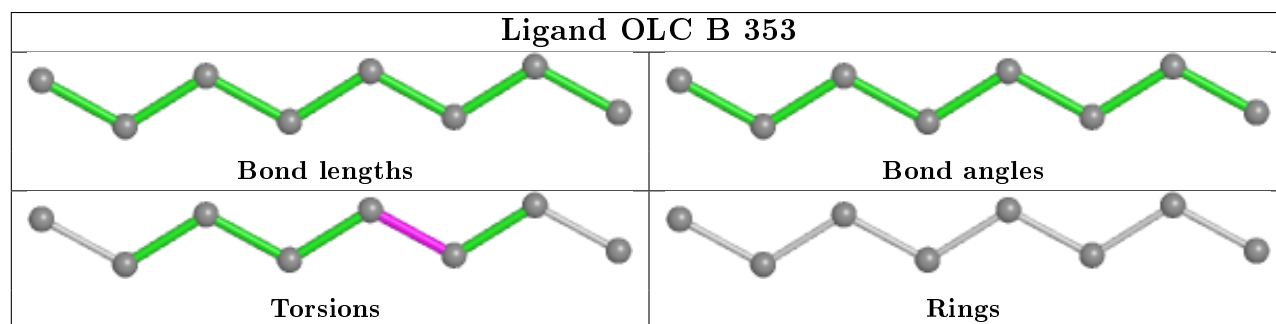
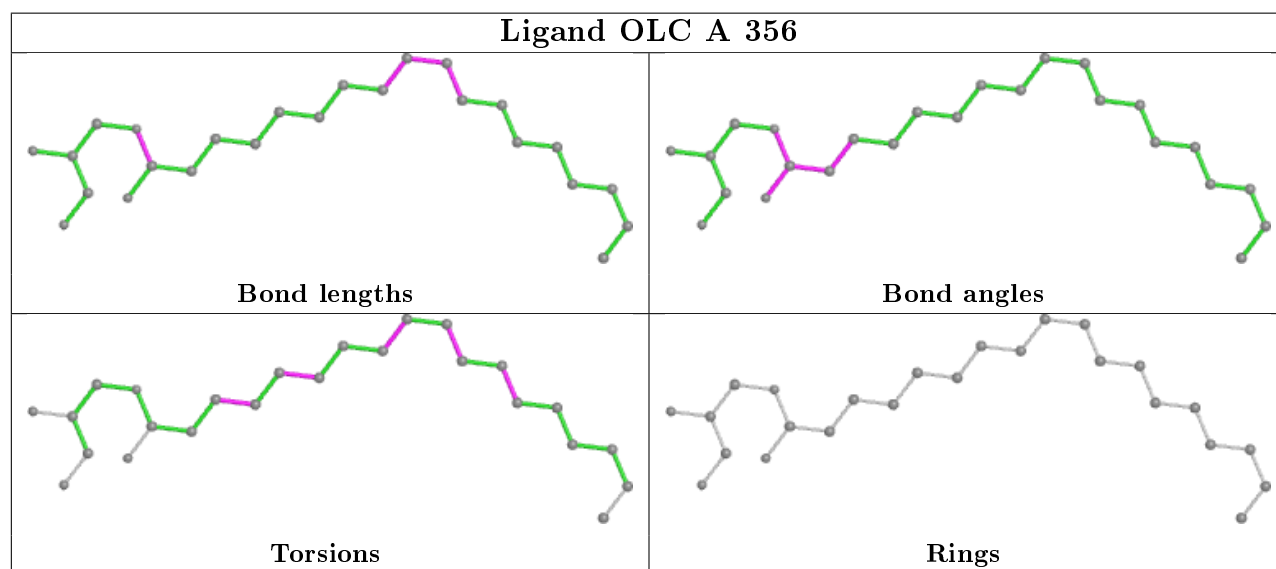
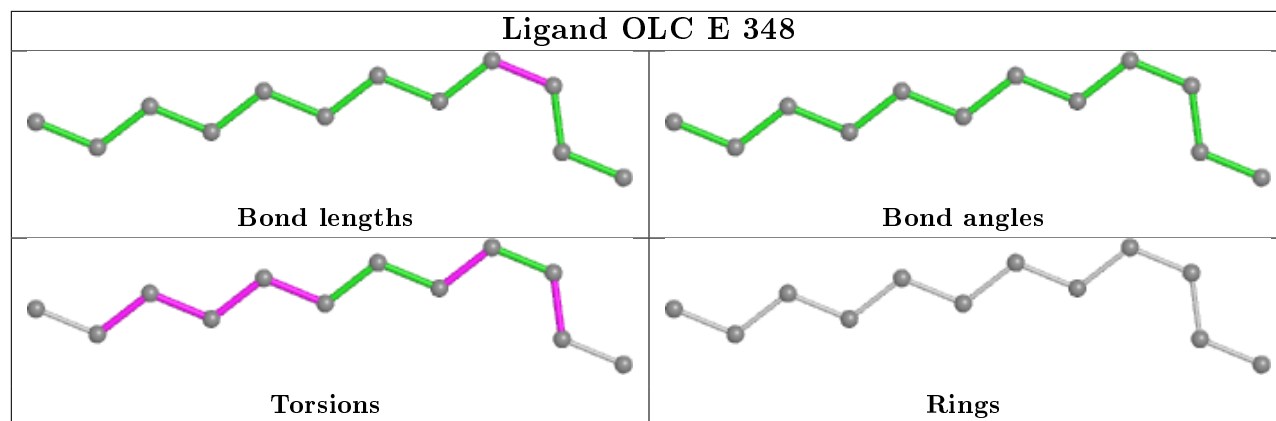


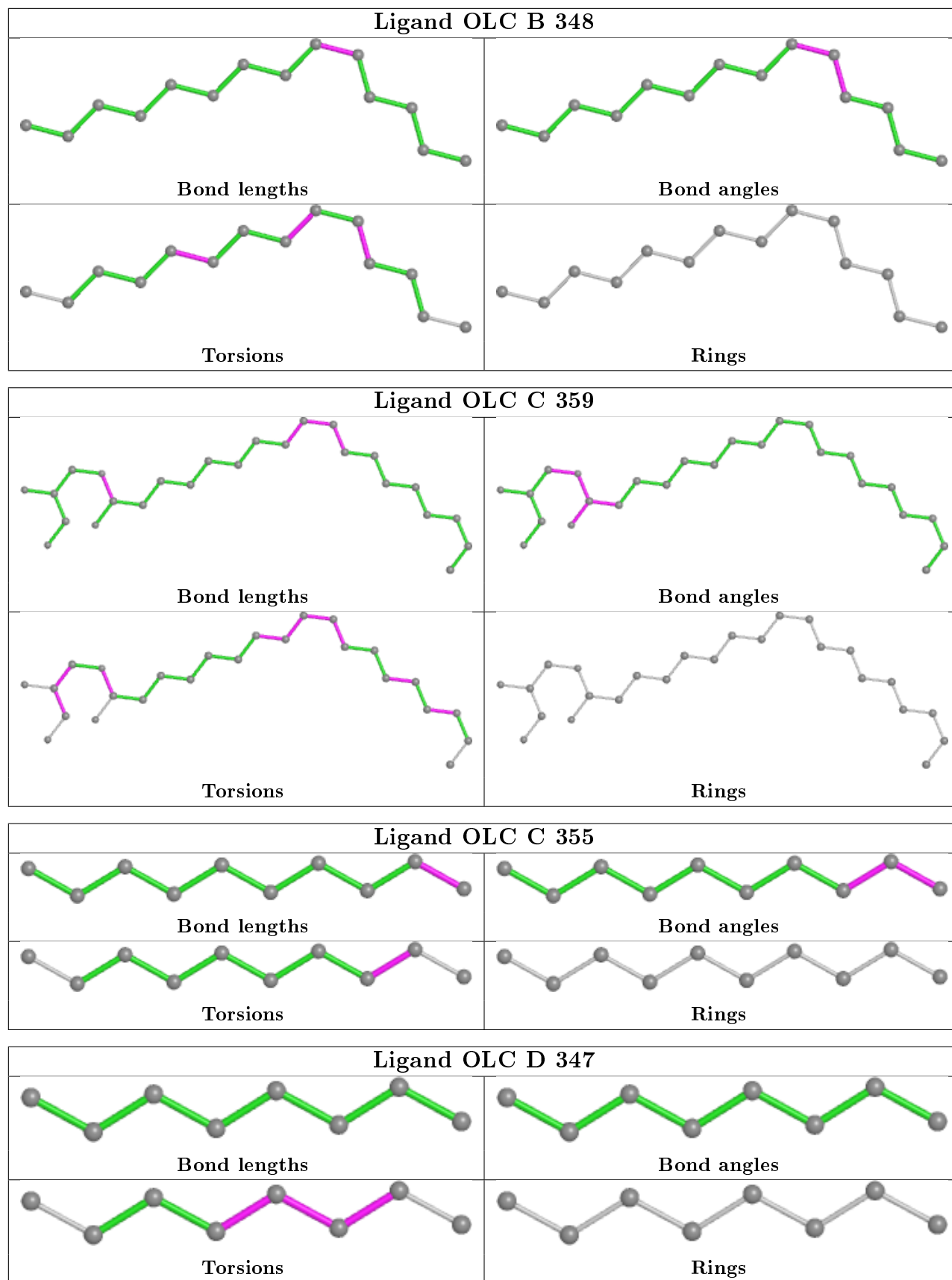


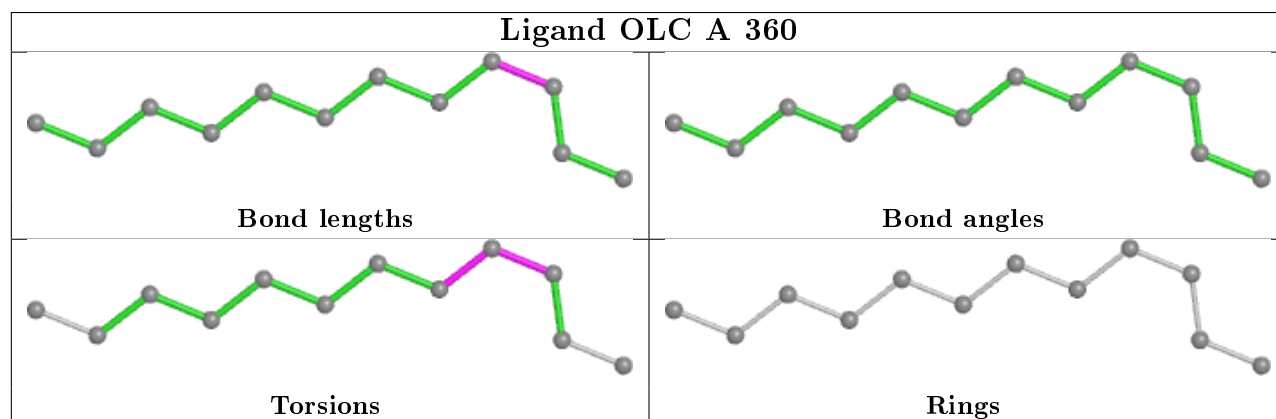
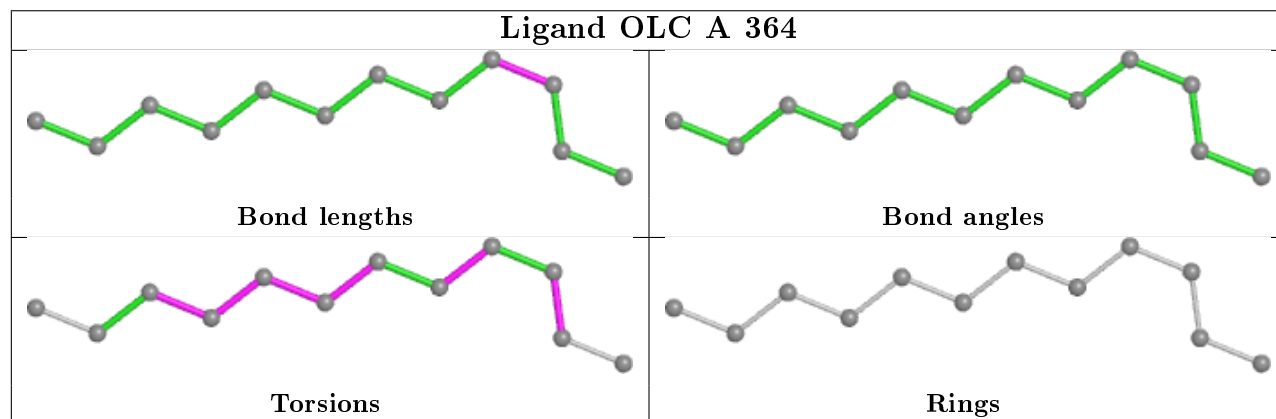
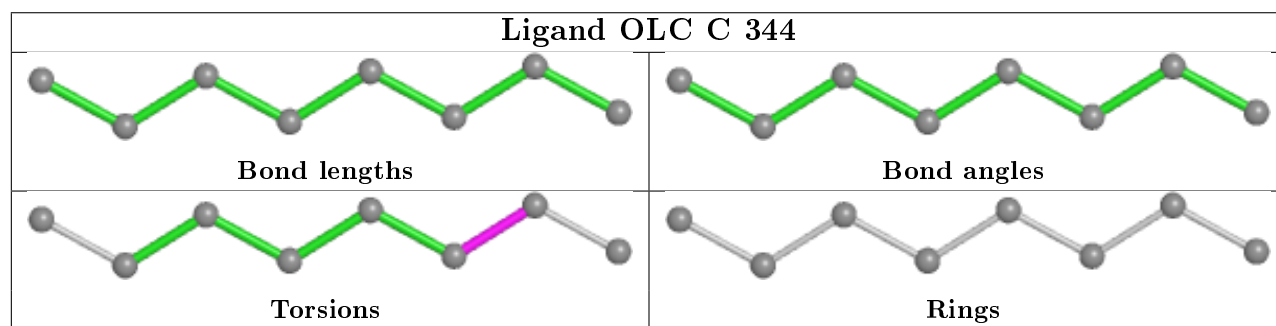
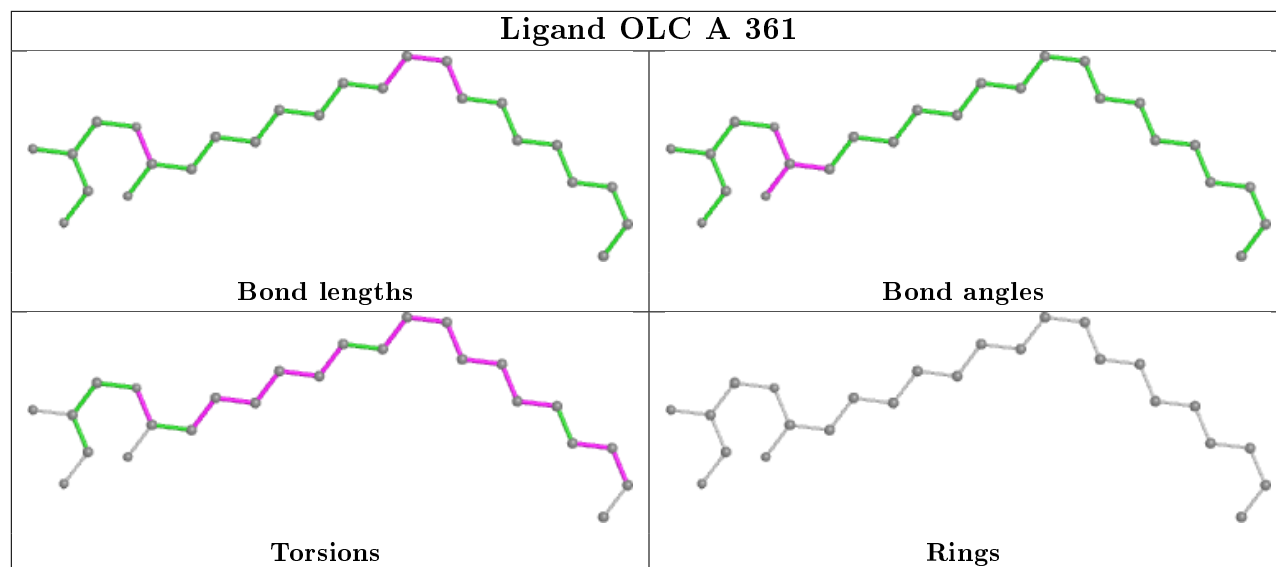


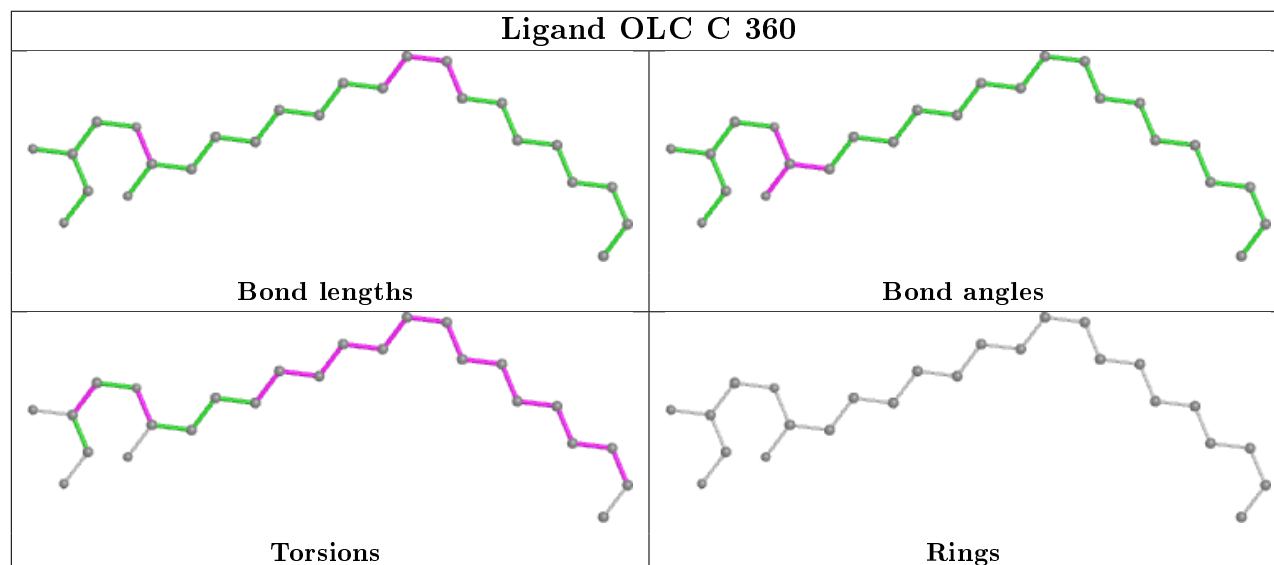
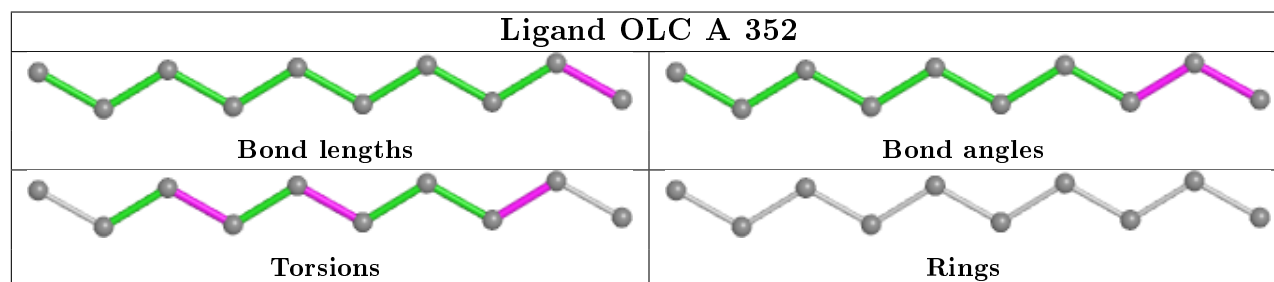
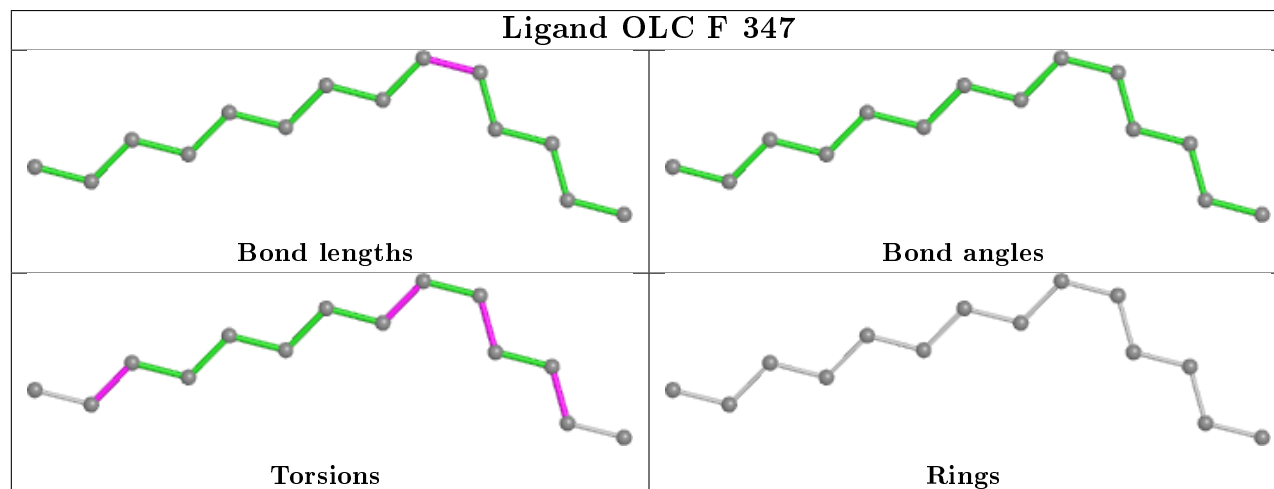
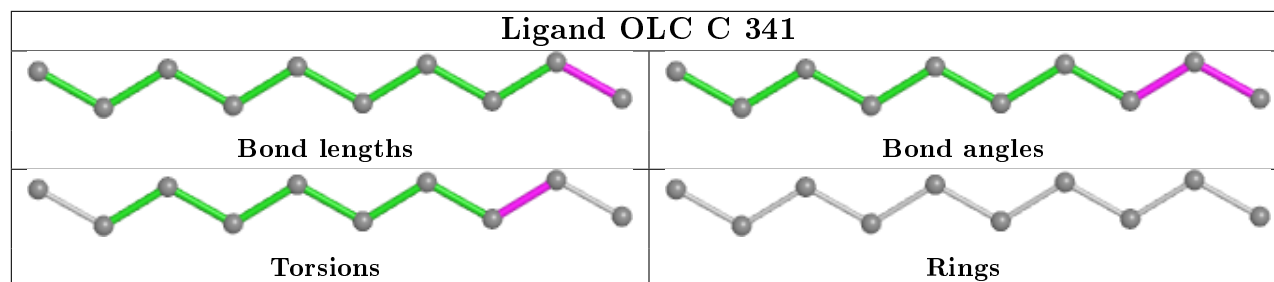


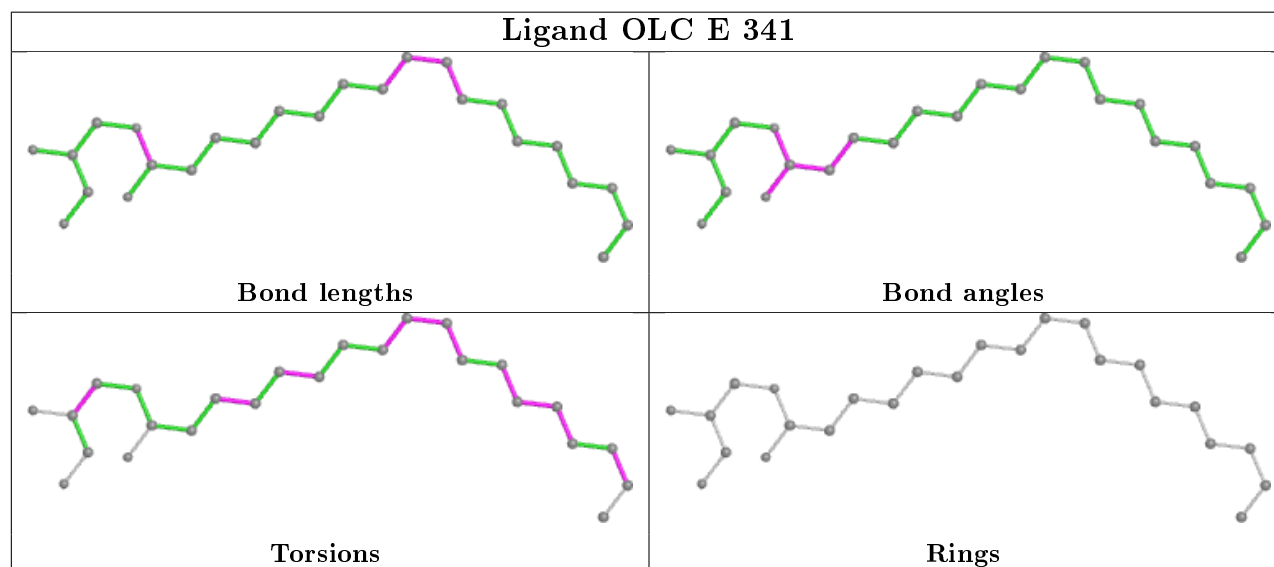
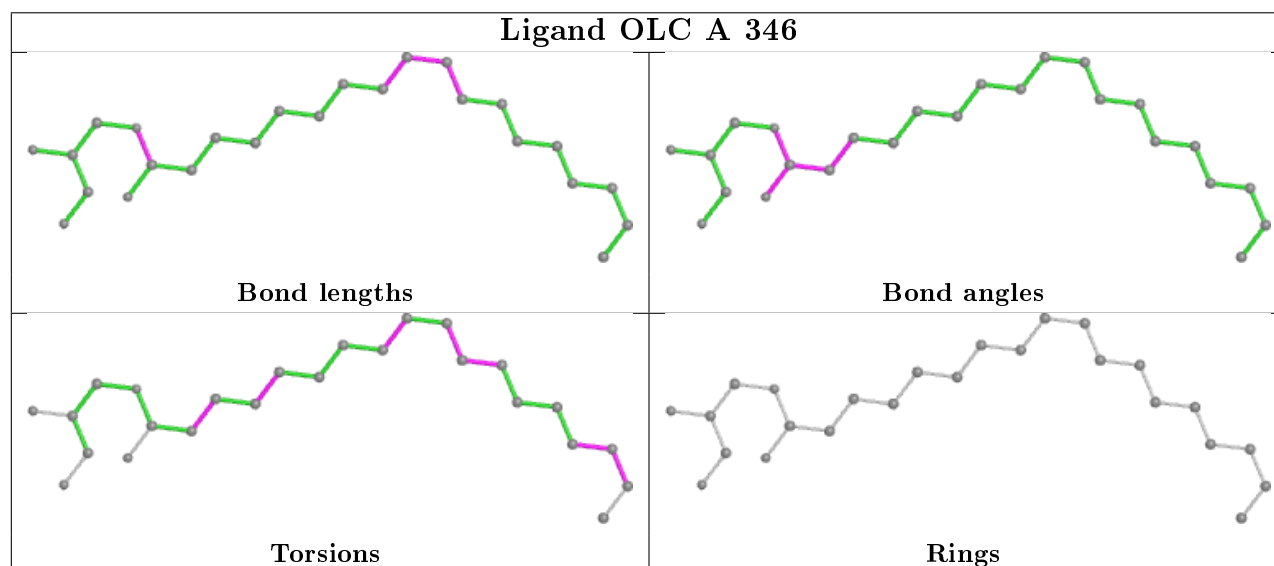
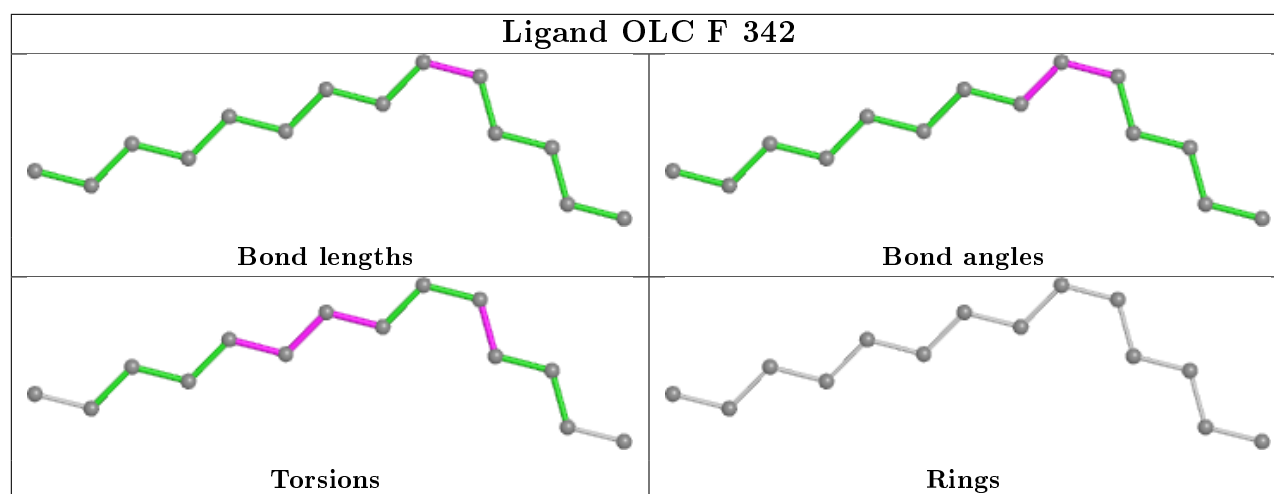


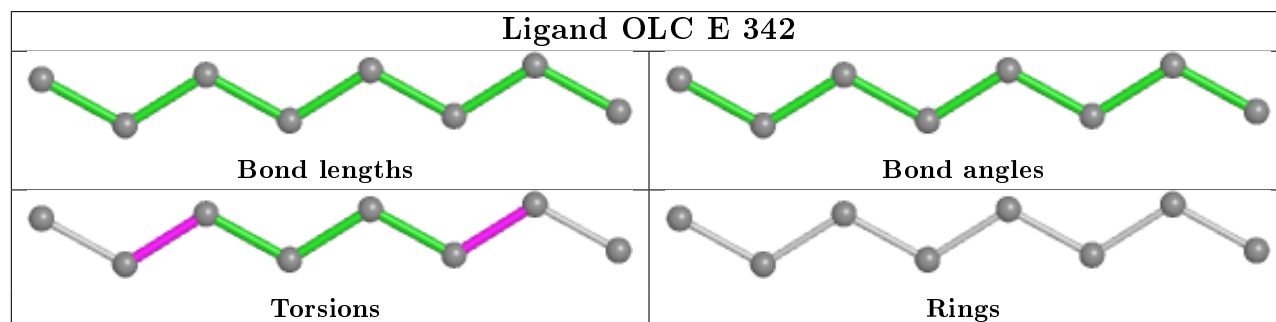
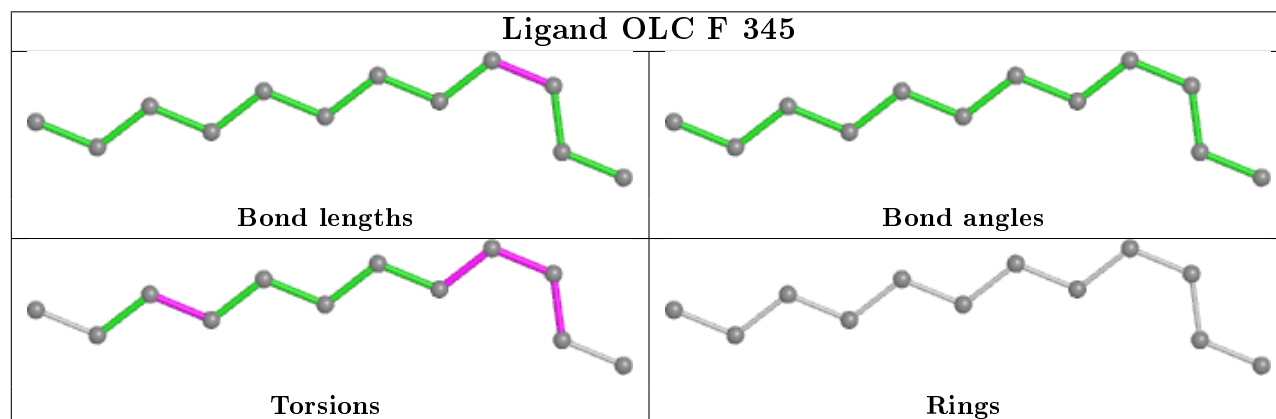
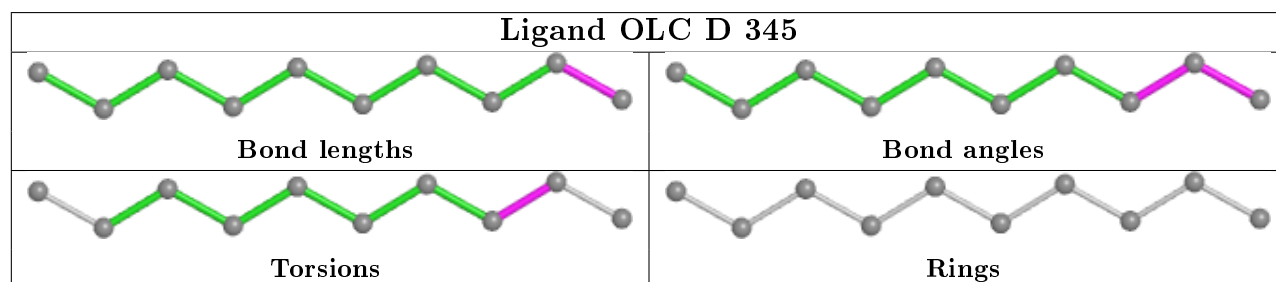
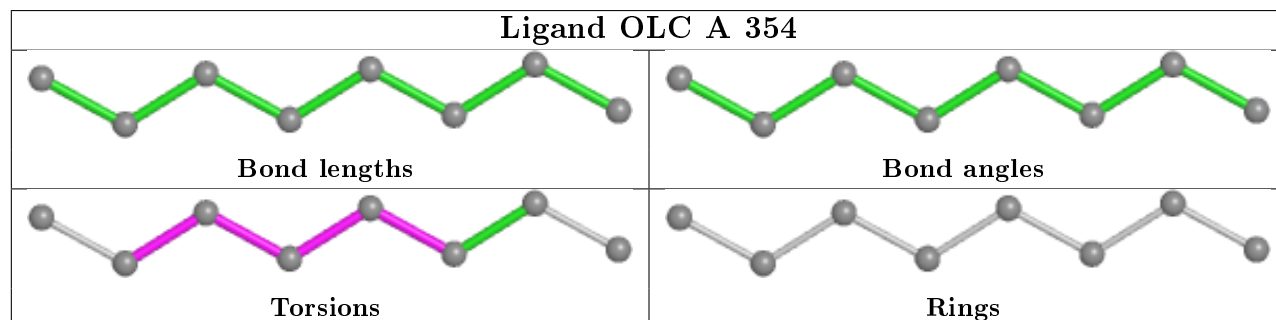
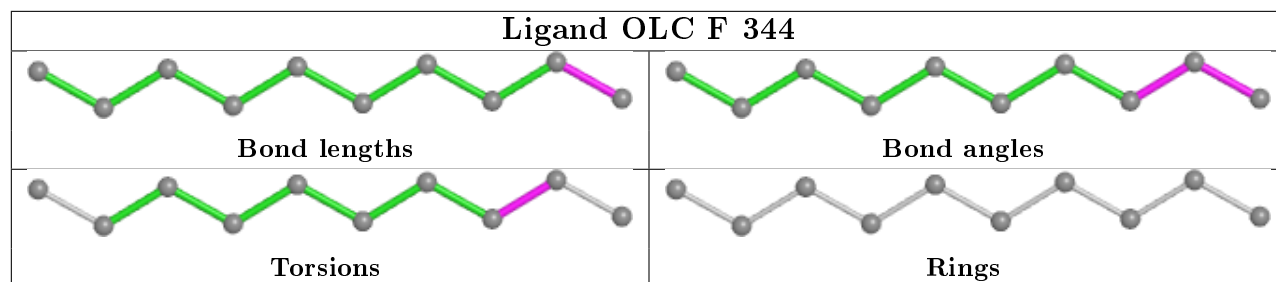


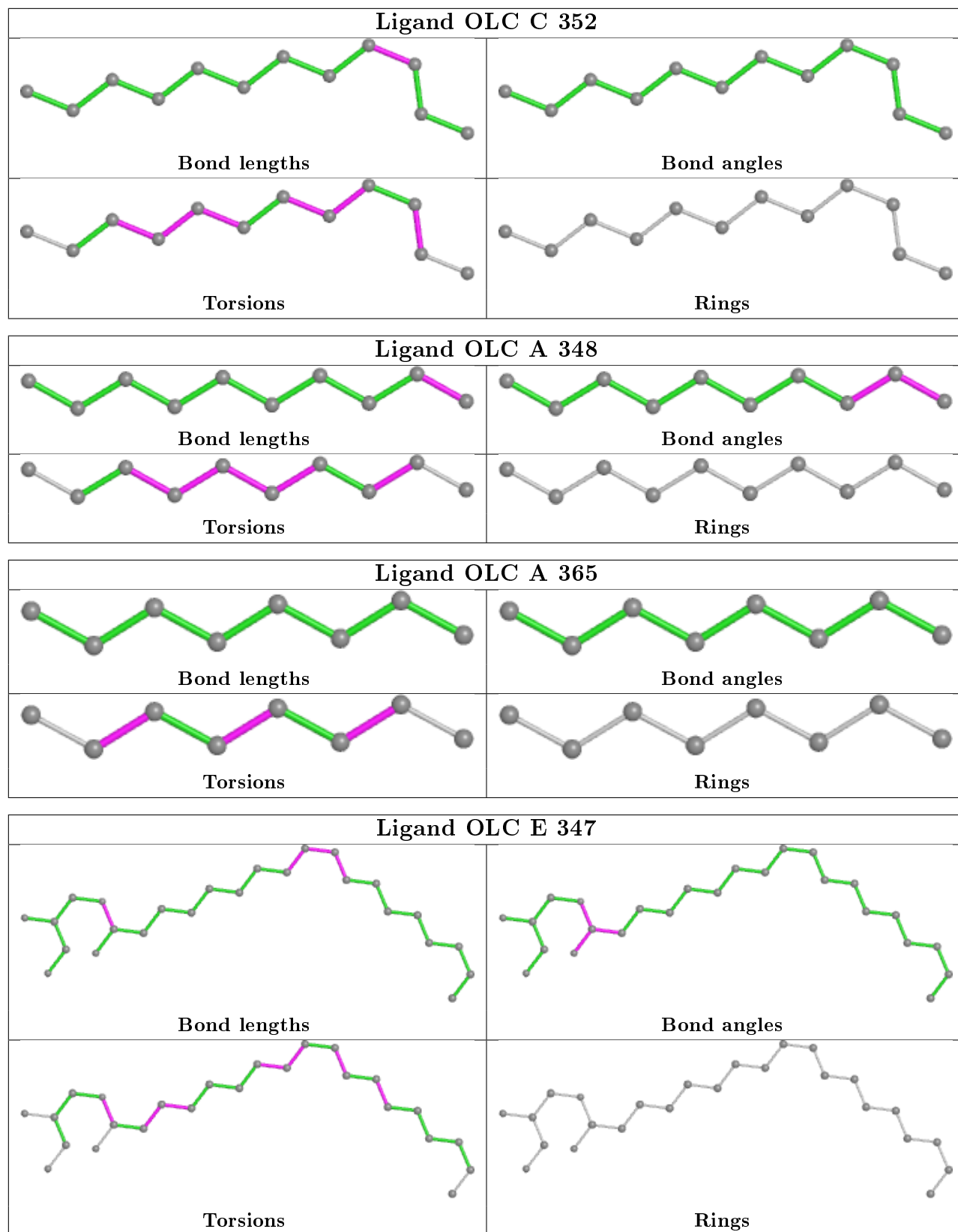


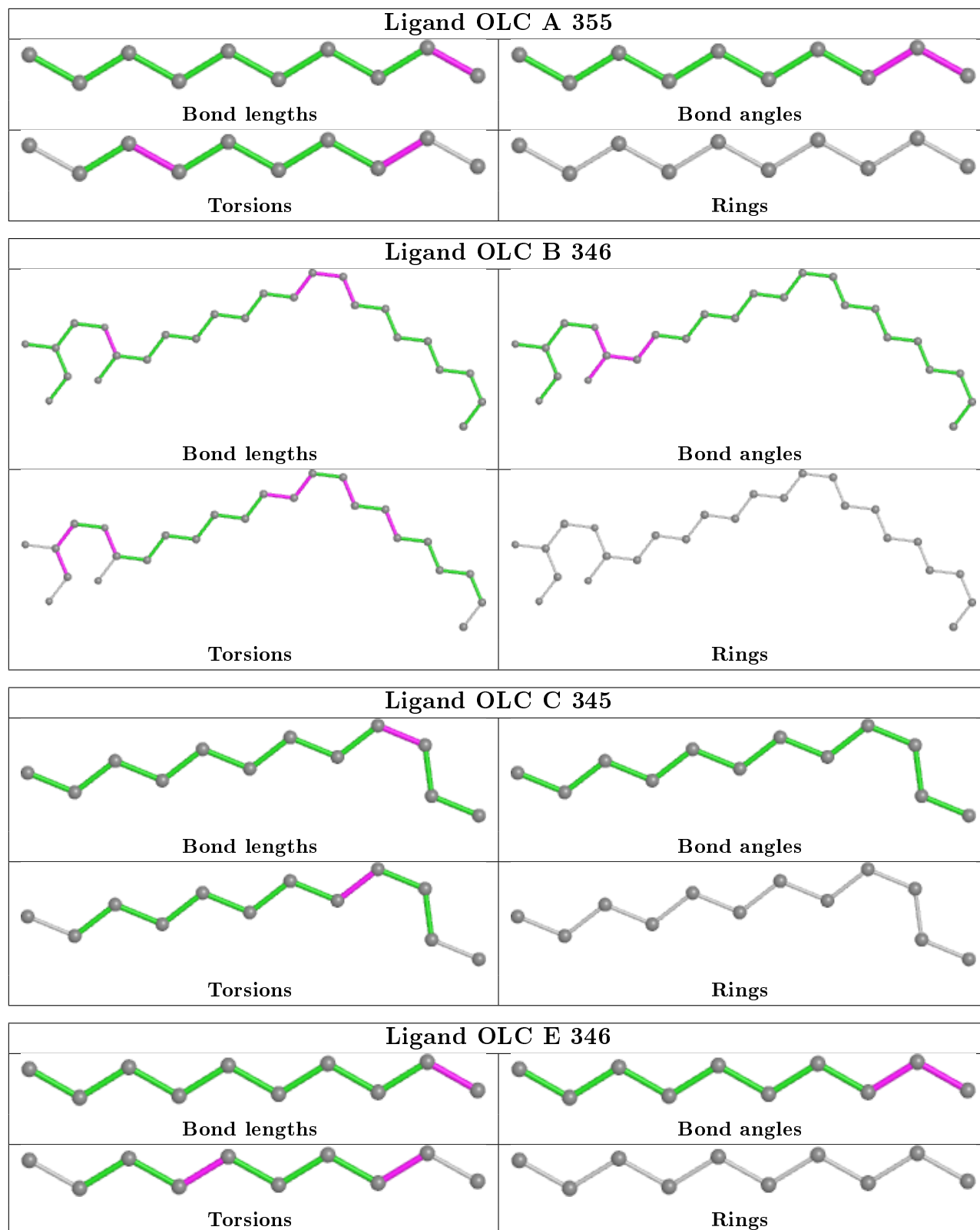


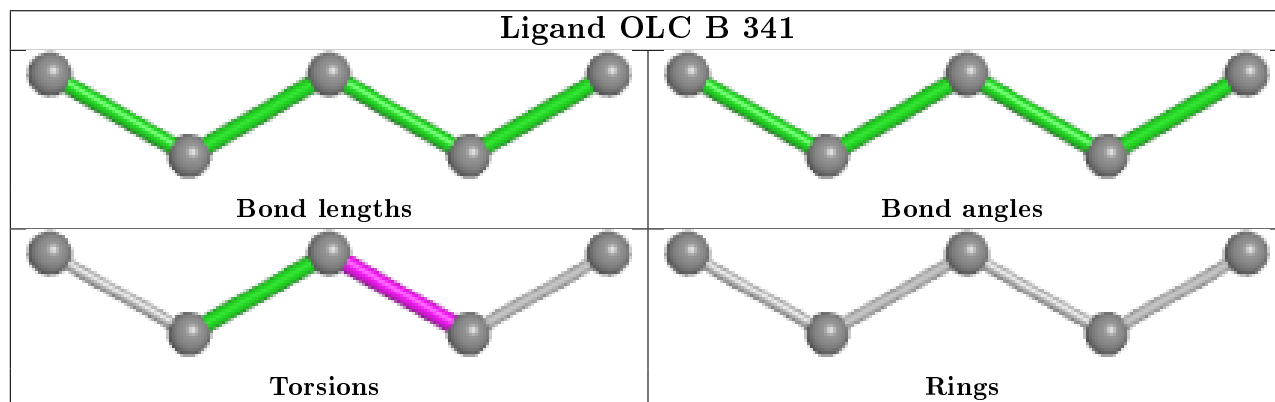
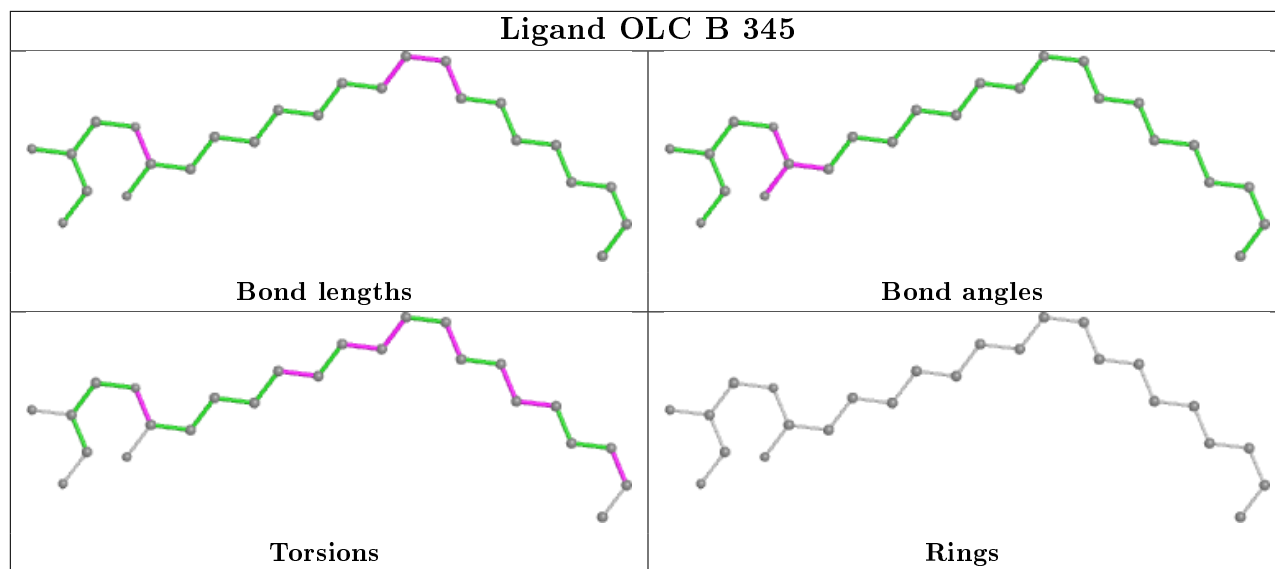
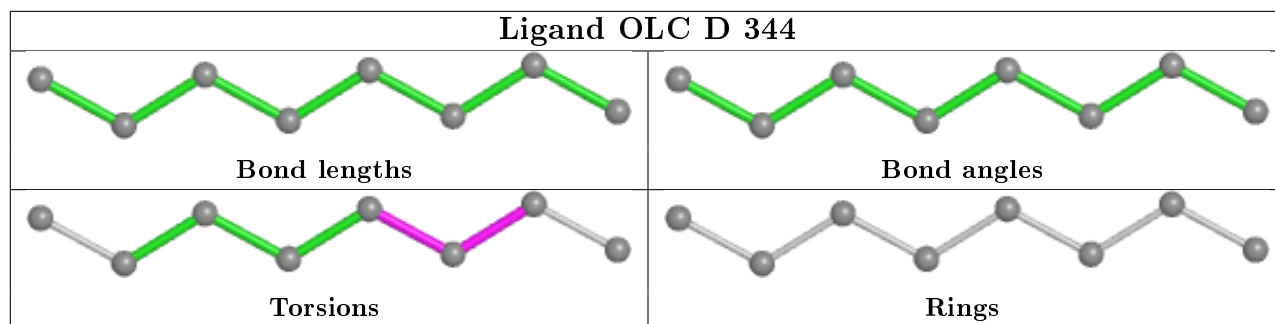


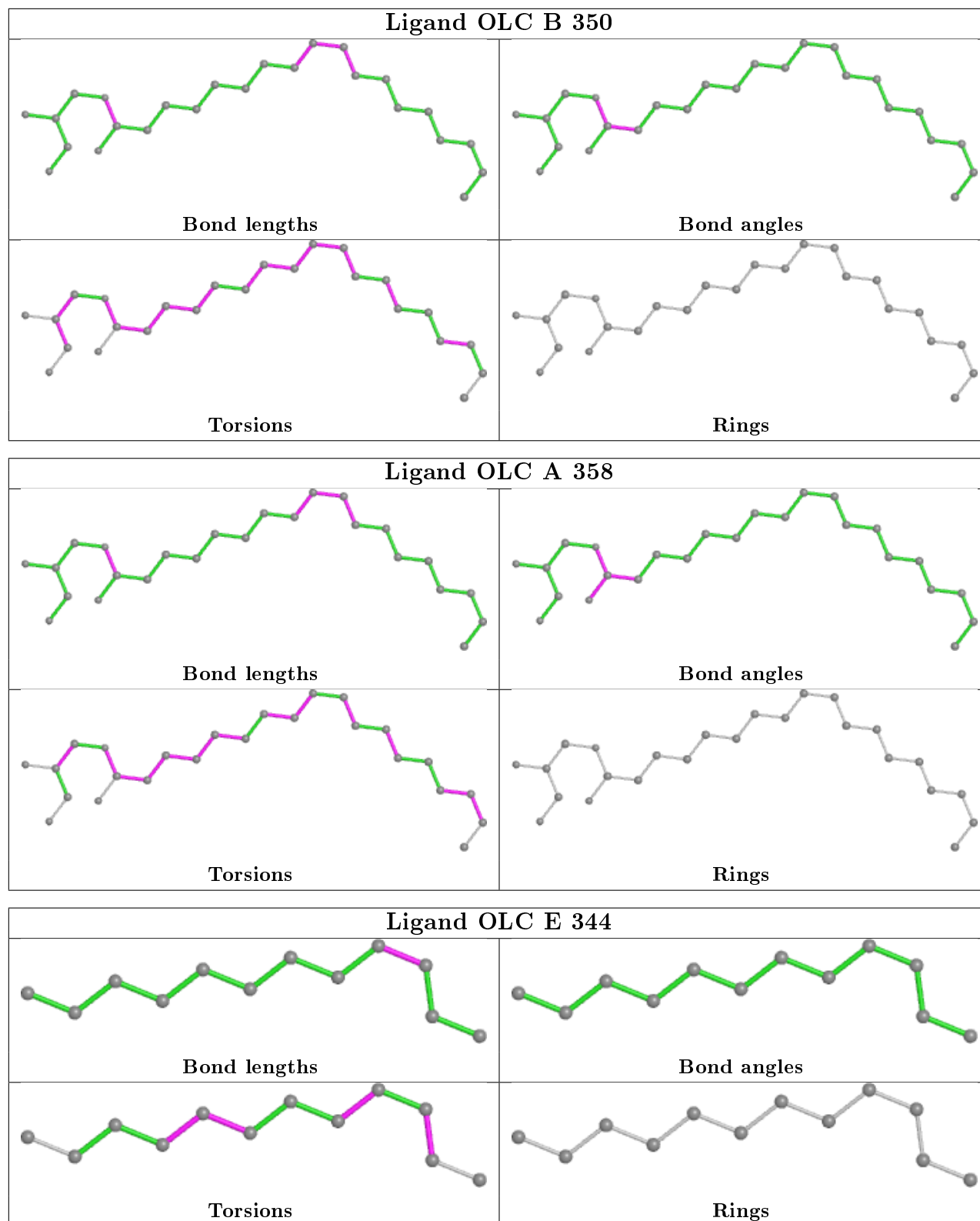


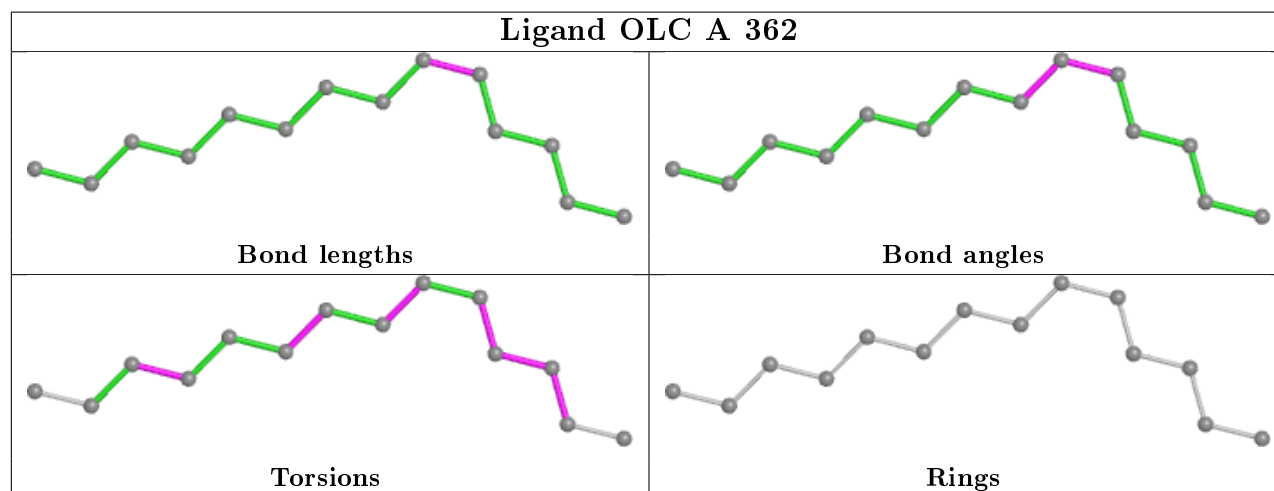
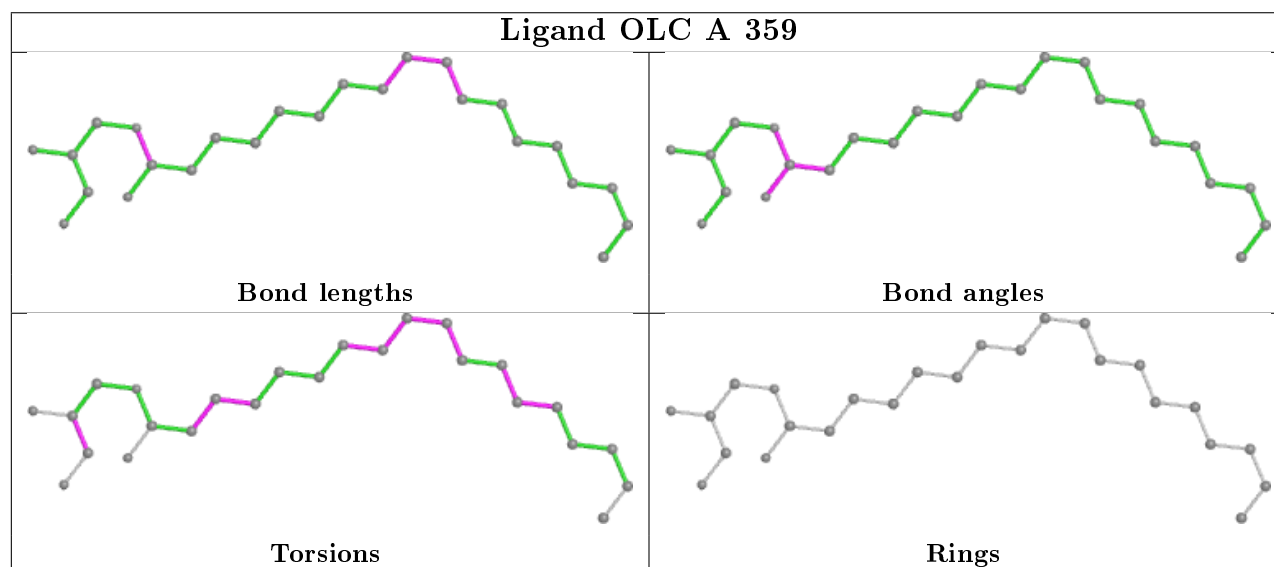
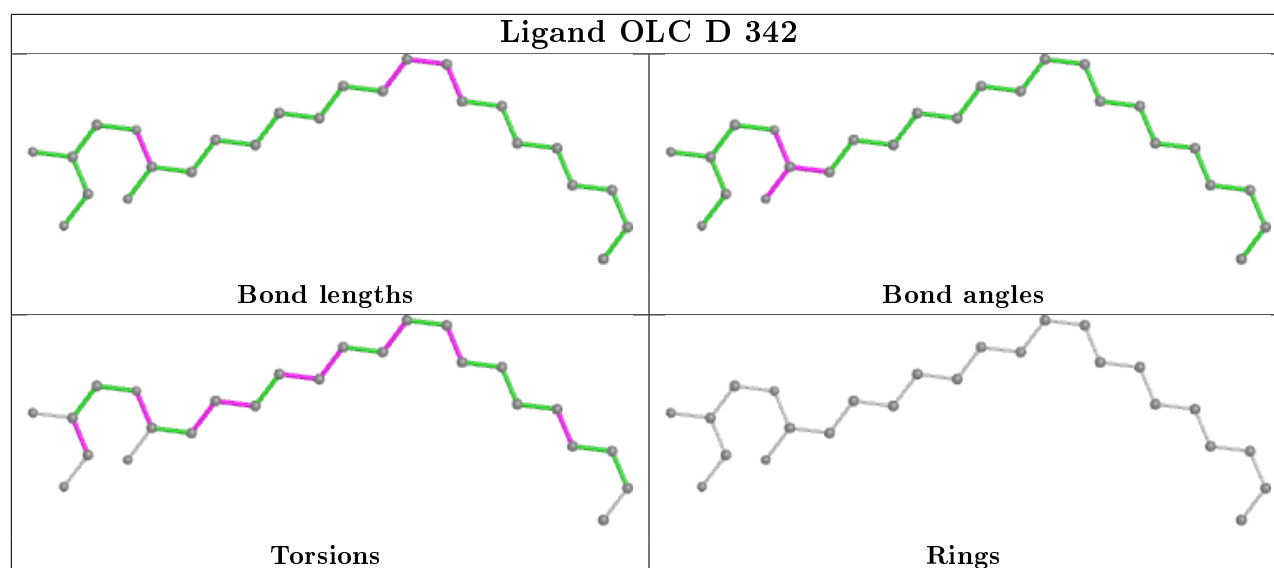












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	340/340 (100%)	-0.50	2 (0%) 89 88	11, 19, 38, 53	0
1	B	340/340 (100%)	-0.32	8 (2%) 59 57	14, 25, 46, 59	0
1	C	340/340 (100%)	-0.37	8 (2%) 59 57	13, 22, 40, 53	0
1	D	340/340 (100%)	-0.41	6 (1%) 68 66	12, 21, 42, 56	0
1	E	340/340 (100%)	-0.50	1 (0%) 94 93	11, 20, 38, 51	0
1	F	340/340 (100%)	-0.21	11 (3%) 47 46	13, 27, 49, 65	0
All	All	2040/2040 (100%)	-0.39	36 (1%) 68 66	11, 22, 44, 65	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ASN	3.6
1	F	246	ASN	3.3
1	F	147	LEU	3.3
1	F	182	TYR	3.2
1	C	147	LEU	3.1
1	F	7	ASP	3.1
1	C	7	ASP	3.0
1	A	29	GLU	2.9
1	C	6	LYS	2.9
1	F	285	GLY	2.8
1	C	91	ALA	2.8
1	B	25	LYS	2.7
1	D	147	LEU	2.7
1	D	7	ASP	2.7
1	B	7	ASP	2.7
1	D	182	TYR	2.6
1	F	27	ASN	2.6
1	D	246	ASN	2.5
1	F	244	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	25	LYS	2.4
1	F	209	LYS	2.4
1	E	29	GLU	2.3
1	C	182	TYR	2.3
1	B	147	LEU	2.3
1	B	267	PHE	2.3
1	C	246	ASN	2.3
1	A	53	SER	2.2
1	B	209	LYS	2.2
1	F	91	ALA	2.2
1	F	53	SER	2.2
1	D	26	GLY	2.1
1	D	243	LYS	2.1
1	C	29	GLU	2.0
1	B	266	ASP	2.0
1	C	149	ASP	2.0
1	B	53	SER	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 carbohydrates 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	E	345	14/25	0.60	0.21	32,50,57,59	0
2	OLC	B	348	14/25	0.63	0.27	50,58,61,61	0
2	OLC	F	342	14/25	0.63	0.24	50,52,58,59	0
2	OLC	D	342	25/25	0.64	0.23	45,51,70,75	0
2	OLC	A	358	25/25	0.68	0.24	49,55,61,64	0
2	OLC	B	351	25/25	0.68	0.21	37,46,61,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	D	349	25/25	0.69	0.18	39,49,54,55	0
2	OLC	B	341	5/25	0.70	0.18	42,44,47,47	0
2	OLC	A	360	12/25	0.70	0.32	49,54,68,68	0
2	OLC	B	342	14/25	0.70	0.30	51,56,62,64	0
2	OLC	A	365	8/25	0.71	0.26	44,48,60,60	0
2	OLC	B	350	25/25	0.71	0.22	34,49,60,71	0
2	OLC	C	352	12/25	0.72	0.25	51,56,59,59	0
2	OLC	C	348	12/25	0.73	0.26	50,55,59,59	0
2	OLC	E	344	12/25	0.73	0.29	29,54,59,59	0
2	OLC	C	351	8/25	0.73	0.27	53,56,60,60	0
2	OLC	F	344	10/25	0.74	0.22	49,57,62,63	0
2	OLC	C	363	25/25	0.74	0.21	38,46,56,66	0
2	OLC	C	356	8/25	0.74	0.27	35,50,58,59	0
2	OLC	C	357	14/25	0.74	0.18	28,46,50,51	0
2	OLC	E	346	10/25	0.75	0.21	58,60,62,62	0
2	OLC	D	345	10/25	0.75	0.18	39,45,49,51	0
2	OLC	C	362	25/25	0.76	0.22	27,41,58,60	0
2	OLC	A	361	25/25	0.76	0.23	40,53,64,67	0
2	OLC	C	354	10/25	0.76	0.34	60,64,67,67	0
2	OLC	B	354	8/25	0.77	0.15	36,48,60,64	0
2	OLC	C	347	10/25	0.77	0.23	49,50,62,63	0
2	OLC	C	350	14/25	0.77	0.19	37,49,53,55	0
2	OLC	D	346	12/25	0.78	0.16	32,36,41,43	0
2	OLC	C	345	12/25	0.78	0.17	37,43,49,49	0
2	OLC	F	341	8/25	0.78	0.22	40,44,48,52	0
2	OLC	A	344	10/25	0.78	0.18	29,42,49,49	0
2	OLC	A	345	8/25	0.79	0.14	35,44,47,49	0
2	OLC	A	355	10/25	0.79	0.22	40,51,66,66	0
2	OLC	F	347	14/25	0.79	0.34	49,60,63,64	0
2	OLC	F	348	14/25	0.80	0.16	36,43,50,50	0
2	OLC	A	350	14/25	0.80	0.17	31,35,46,47	0
2	OLC	C	344	8/25	0.80	0.18	40,44,53,55	0
2	OLC	E	343	12/25	0.80	0.15	40,48,52,54	0
2	OLC	B	349	8/25	0.80	0.14	43,45,49,50	0
2	OLC	F	345	12/25	0.80	0.19	37,46,57,57	0
2	OLC	B	353	8/25	0.80	0.22	35,41,49,50	0
2	OLC	C	360	25/25	0.80	0.16	23,40,72,74	0
2	OLC	A	349	25/25	0.81	0.19	36,42,56,63	0
2	OLC	A	363	12/25	0.81	0.15	31,39,47,48	0
2	OLC	C	353	10/25	0.81	0.28	54,56,62,63	0
2	OLC	F	346	8/25	0.81	0.15	40,45,50,51	0
2	OLC	F	343	8/25	0.81	0.22	48,55,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	A	351	14/25	0.81	0.16	42,50,56,56	0
2	OLC	C	358	25/25	0.82	0.18	31,39,63,66	0
2	OLC	C	341	10/25	0.82	0.13	36,40,55,59	0
2	OLC	A	346	25/25	0.82	0.17	35,44,57,61	0
2	OLC	A	362	14/25	0.82	0.15	38,44,49,49	0
2	OLC	E	348	12/25	0.83	0.13	42,49,52,52	0
2	OLC	E	347	25/25	0.83	0.17	26,45,53,57	0
2	OLC	C	361	12/25	0.83	0.15	24,32,37,37	0
2	OLC	A	359	25/25	0.83	0.18	28,40,54,54	0
2	OLC	A	348	10/25	0.83	0.15	40,44,49,50	0
2	OLC	E	341	25/25	0.84	0.17	21,39,49,53	0
2	OLC	A	357	10/25	0.84	0.17	26,37,44,46	0
2	OLC	C	343	8/25	0.85	0.42	56,62,66,66	0
2	OLC	B	345	25/25	0.85	0.17	33,43,52,60	0
2	OLC	D	347	8/25	0.85	0.14	28,36,41,41	0
2	OLC	A	352	10/25	0.86	0.17	38,47,51,51	0
2	OLC	A	364	12/25	0.86	0.32	48,54,56,56	0
2	OLC	B	344	10/25	0.86	0.12	42,44,53,54	0
2	OLC	B	352	16/25	0.86	0.16	32,41,46,47	0
2	OLC	E	342	8/25	0.86	0.17	40,41,43,45	0
2	OLC	B	347	14/25	0.86	0.13	30,38,47,49	0
2	OLC	D	348	8/25	0.86	0.17	37,43,44,46	0
2	OLC	C	349	10/25	0.87	0.21	36,44,52,56	0
2	OLC	B	346	25/25	0.87	0.16	29,39,54,61	0
2	OLC	A	342	8/25	0.87	0.12	48,50,58,60	0
2	OLC	C	359	25/25	0.87	0.14	30,38,57,63	0
2	OLC	C	364	12/25	0.88	0.14	37,44,47,47	0
2	OLC	A	347	8/25	0.89	0.13	25,29,36,39	0
2	OLC	C	355	10/25	0.89	0.13	33,41,50,51	0
2	OLC	C	346	10/25	0.90	0.12	34,44,54,57	0
2	OLC	A	356	25/25	0.90	0.16	22,36,53,65	0
2	OLC	A	343	8/25	0.91	0.17	32,36,42,43	0
2	OLC	D	343	8/25	0.91	0.22	39,44,48,53	0
2	OLC	A	354	8/25	0.91	0.15	28,35,39,44	0
2	OLC	B	343	8/25	0.93	0.14	30,37,44,48	0
2	OLC	C	342	8/25	0.93	0.11	26,35,46,48	0
2	OLC	D	341	5/25	0.93	0.11	36,39,44,45	0
2	OLC	A	353	8/25	0.94	0.09	32,34,43,44	0
2	OLC	A	341	8/25	0.94	0.10	28,32,41,43	0
4	SCN	E	352	3/3	0.95	0.11	20,20,21,35	0
3	K	F	350	1/1	0.95	0.18	42,42,42,42	0
2	OLC	D	344	8/25	0.95	0.12	27,31,47,51	0

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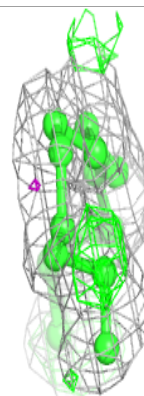
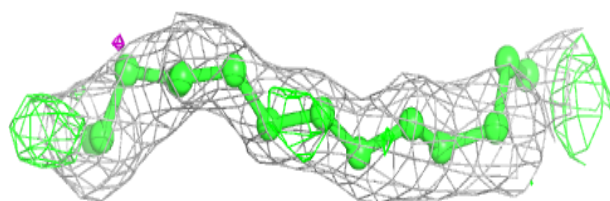
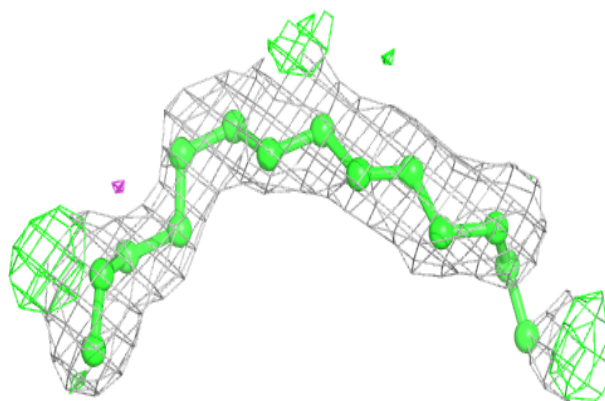
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SCN	B	358	3/3	0.95	0.08	25,25,26,37	0
3	K	B	356	1/1	0.96	0.15	38,38,38,38	0
4	SCN	E	353	3/3	0.96	0.12	40,40,44,49	0
3	K	C	367	1/1	0.96	0.06	38,38,38,38	0
4	SCN	D	354	3/3	0.96	0.06	25,25,25,36	0
4	SCN	A	369	3/3	0.96	0.08	23,23,25,32	0
4	SCN	F	352	3/3	0.97	0.09	21,21,23,34	0
3	K	B	355	1/1	0.98	0.07	34,34,34,34	0
3	K	A	368	1/1	0.98	0.07	32,32,32,32	0
3	K	E	350	1/1	0.98	0.03	26,26,26,26	0
3	K	D	353	1/1	0.98	0.08	38,38,38,38	0
3	K	E	351	1/1	0.98	0.11	33,33,33,33	0
3	K	F	349	1/1	0.99	0.08	30,30,30,30	0
3	K	D	351	1/1	0.99	0.04	29,29,29,29	0
3	K	C	366	1/1	0.99	0.05	28,28,28,28	0
3	K	A	367	1/1	0.99	0.05	27,27,27,27	0
3	K	D	352	1/1	0.99	0.09	38,38,38,38	0
3	K	F	351	1/1	0.99	0.21	44,44,44,44	0
3	K	C	368	1/1	0.99	0.11	36,36,36,36	0
3	K	B	357	1/1	0.99	0.15	41,41,41,41	0
3	K	C	365	1/1	0.99	0.04	25,25,25,25	0
3	K	A	366	1/1	1.00	0.05	25,25,25,25	0
3	K	D	350	1/1	1.00	0.04	23,23,23,23	0
3	K	E	349	1/1	1.00	0.02	23,23,23,23	0

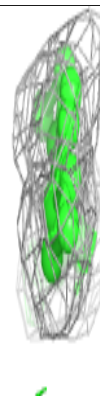
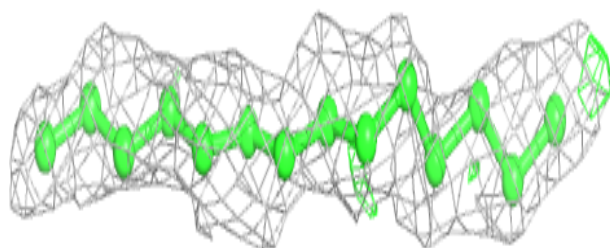
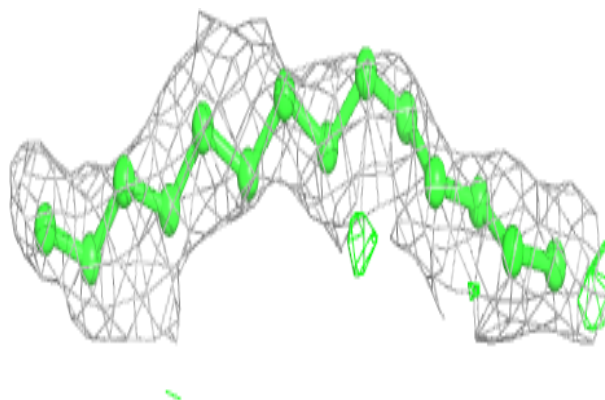
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC E 345:

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

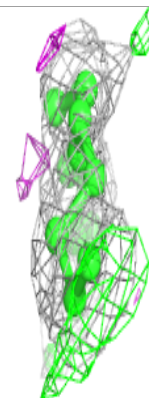
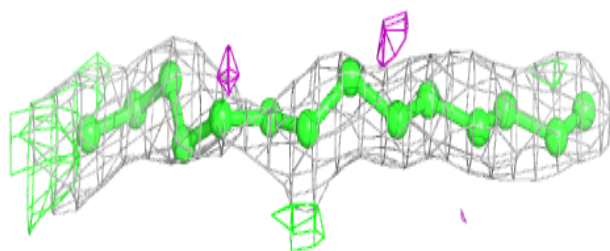
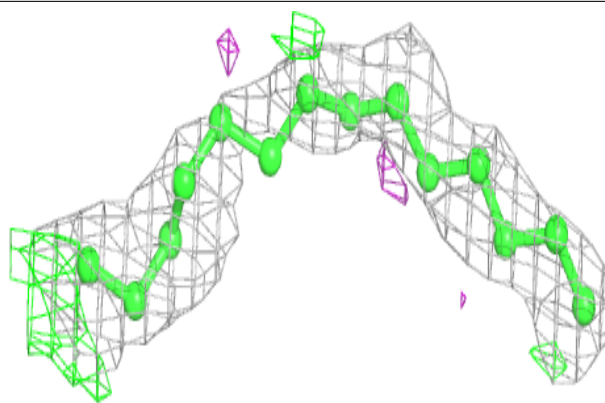
**Electron density around OLC B 348:**

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

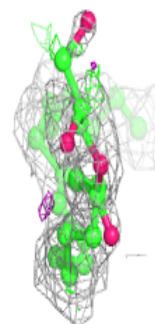
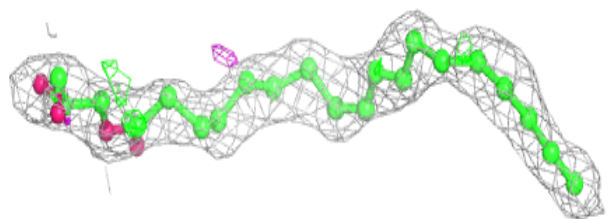
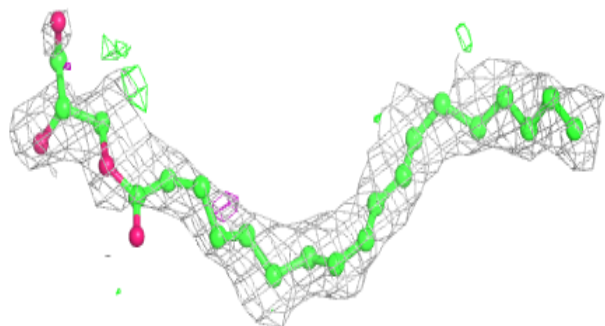


Electron density around OLC F 342:

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

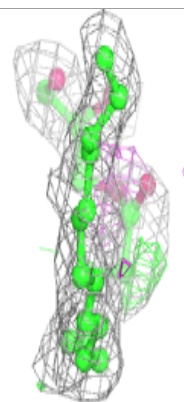
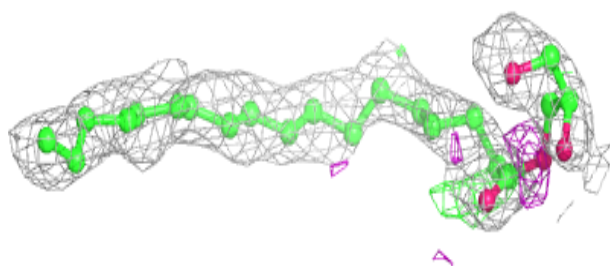
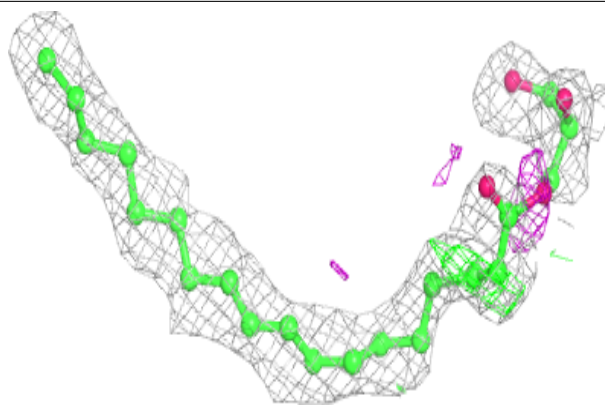
**Electron density around OLC D 342:**

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



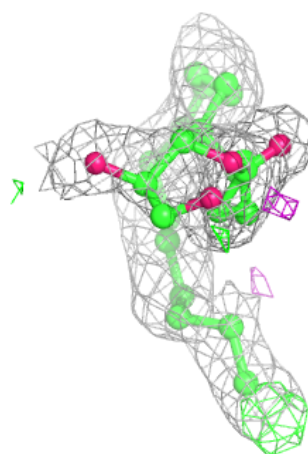
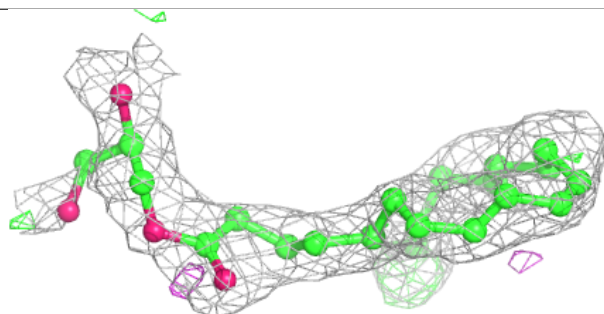
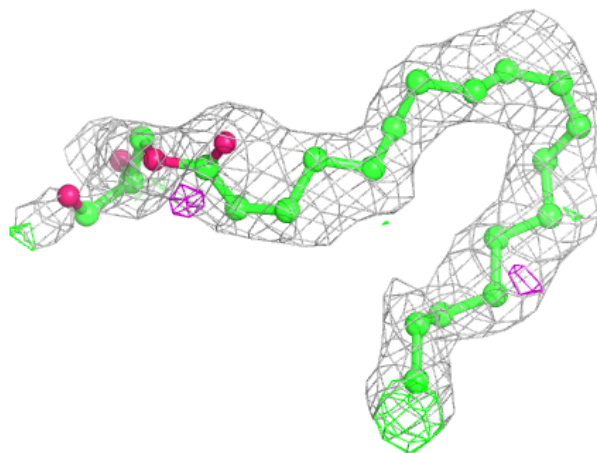
Electron density around OLC A 358:

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



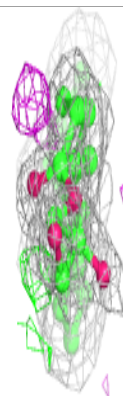
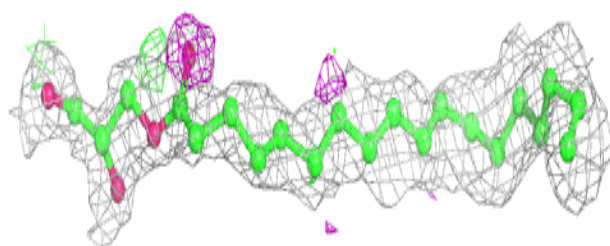
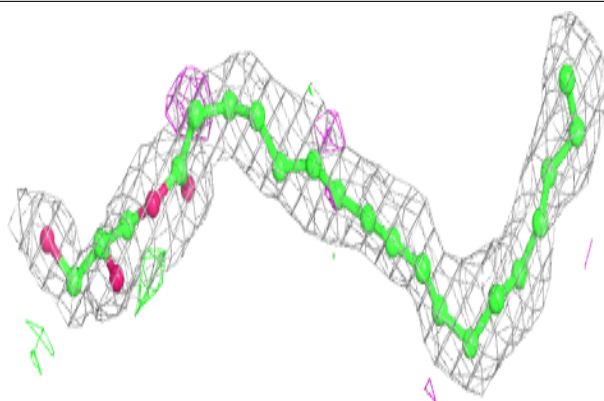
Electron density around OLC B 351:

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

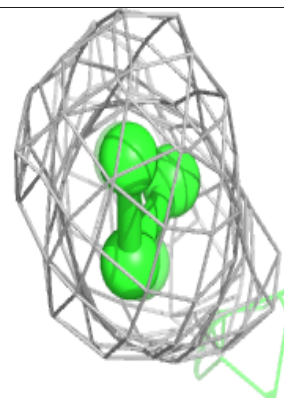
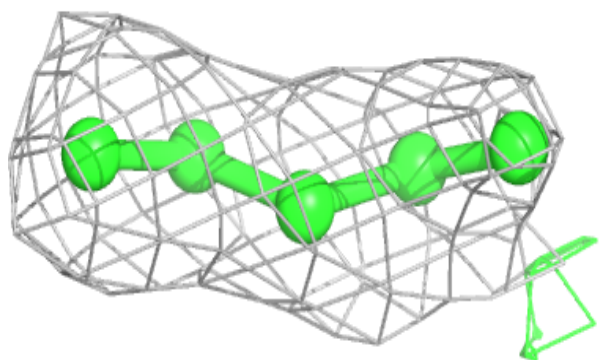
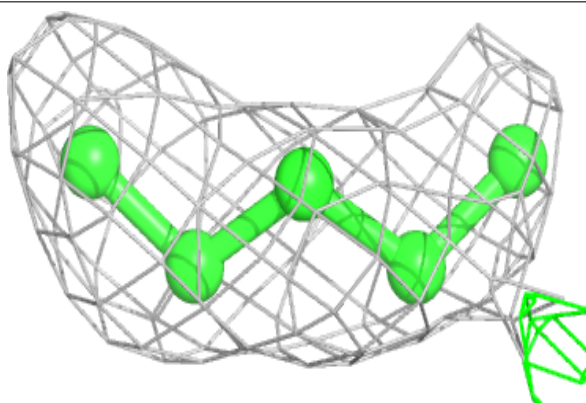


Electron density around OLC D 349:

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

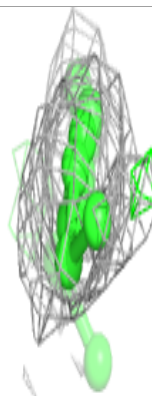
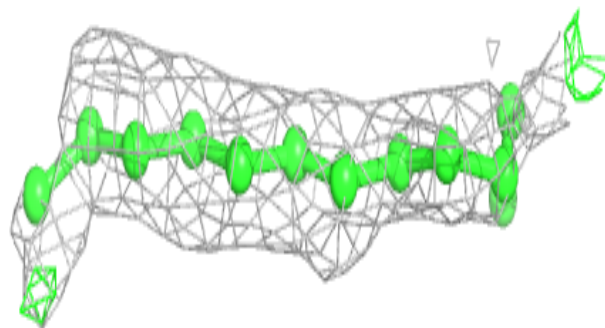
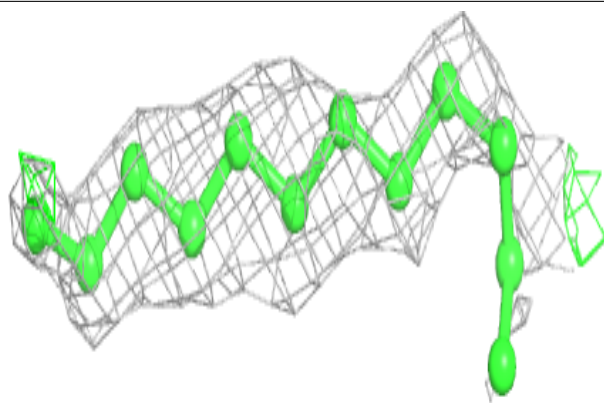
**Electron density around OLC B 341:**

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

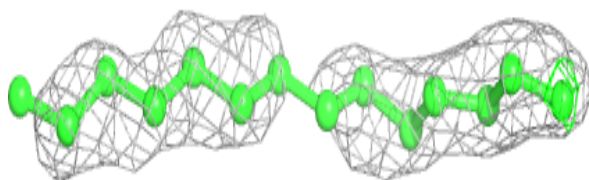
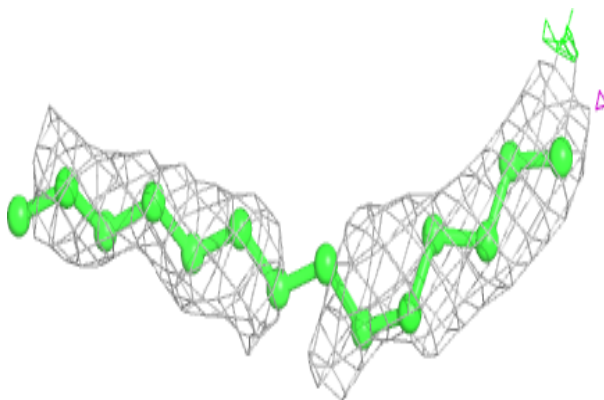


Electron density around OLC A 360:

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

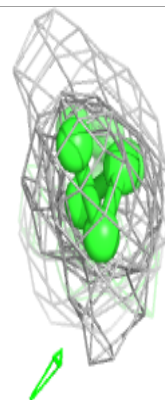
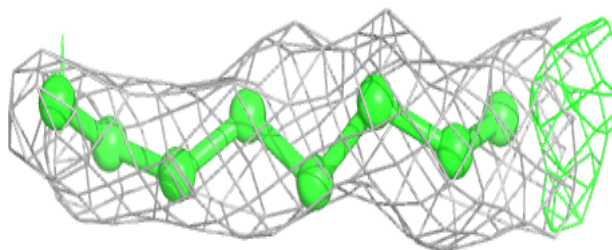
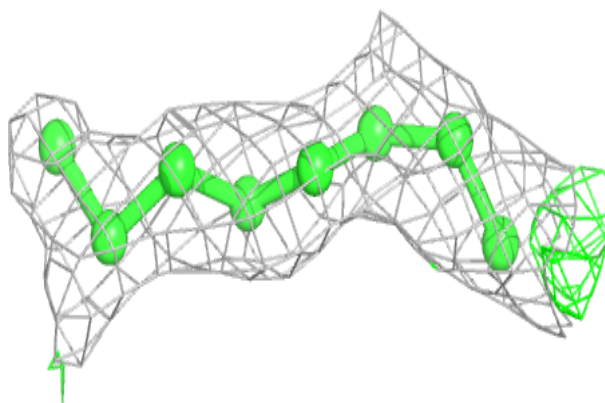
**Electron density around OLC B 342:**

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

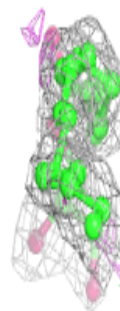
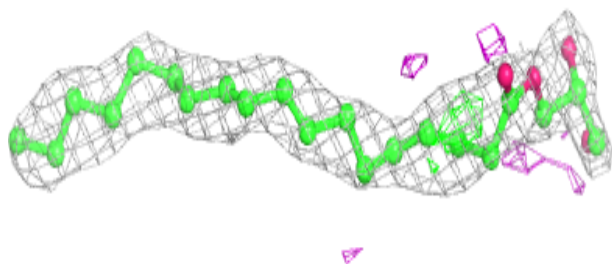
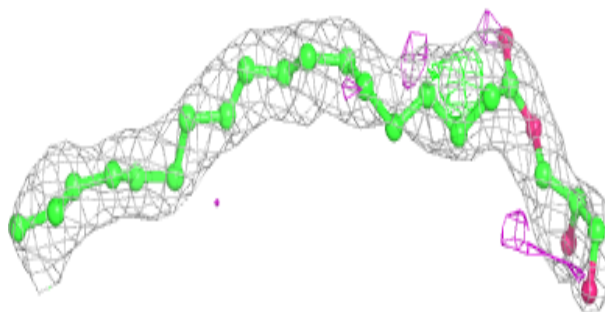


Electron density around OLC A 365:

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

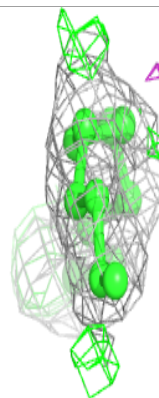
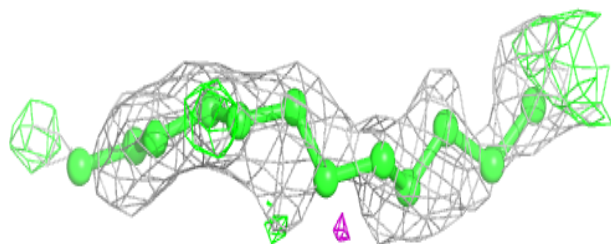
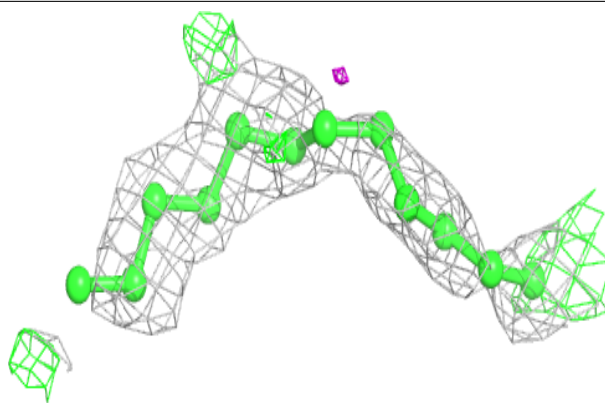
**Electron density around OLC B 350:**

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

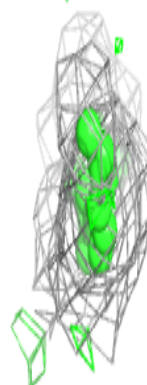
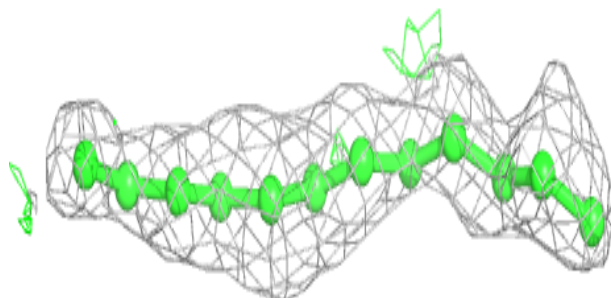
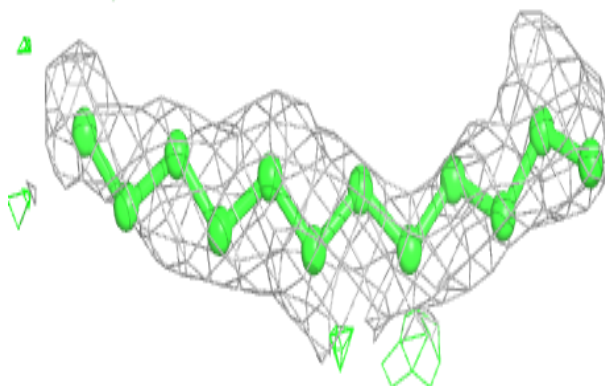


Electron density around OLC C 352:

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

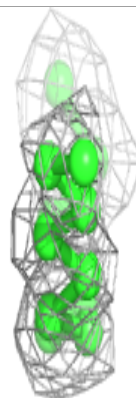
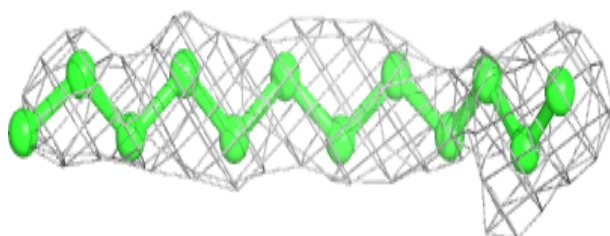
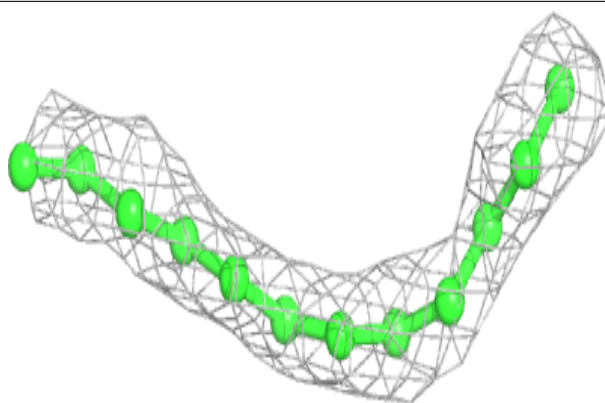
**Electron density around OLC C 348:**

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

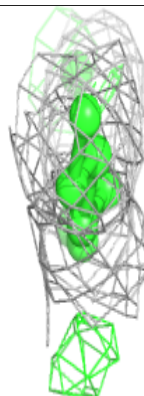
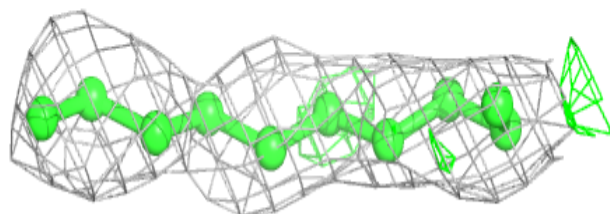
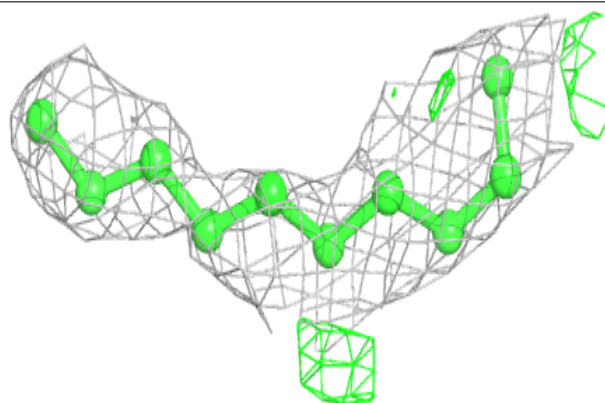


Electron density around OLC E 344:

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

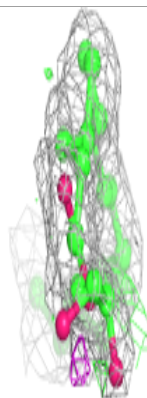
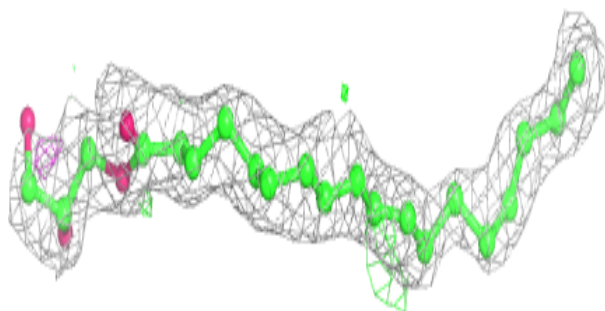
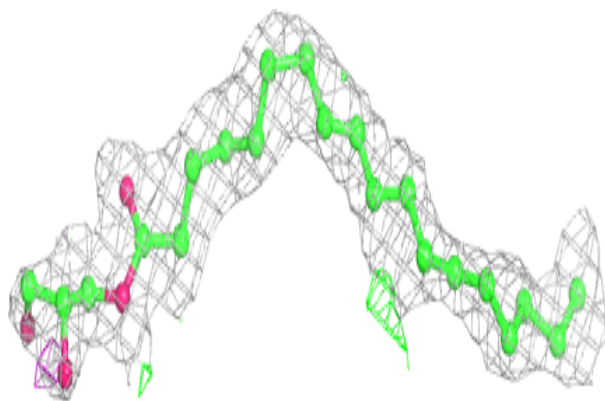
**Electron density around OLC F 344:**

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

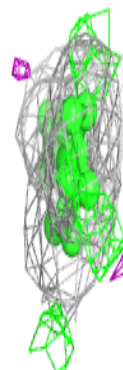
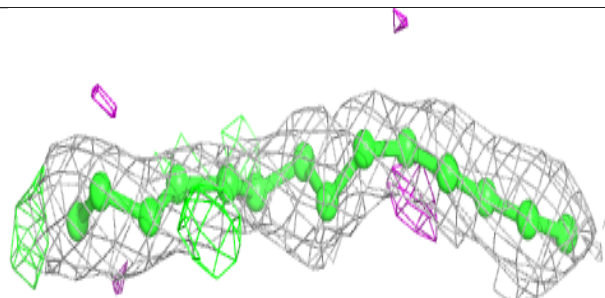
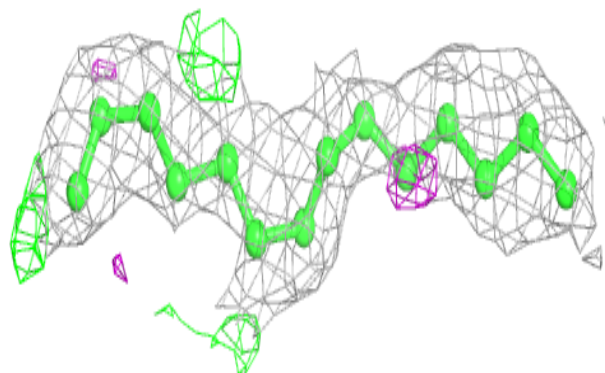


Electron density around OLC C 363:

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

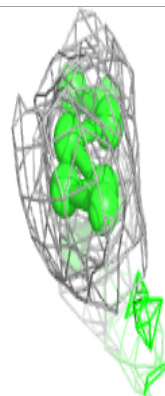
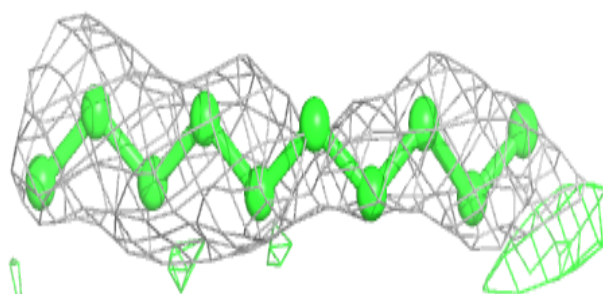
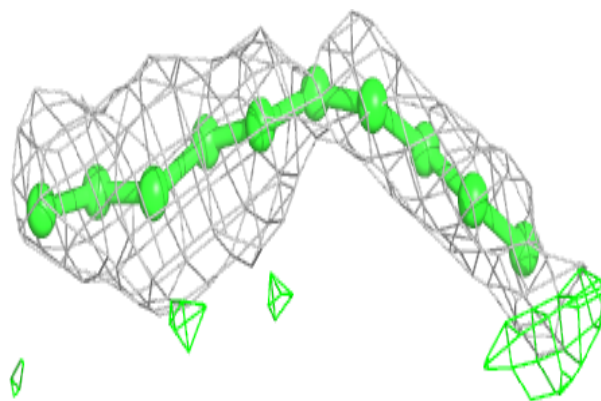
**Electron density around OLC C 357:**

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

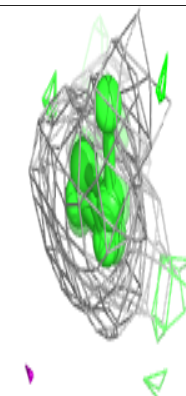
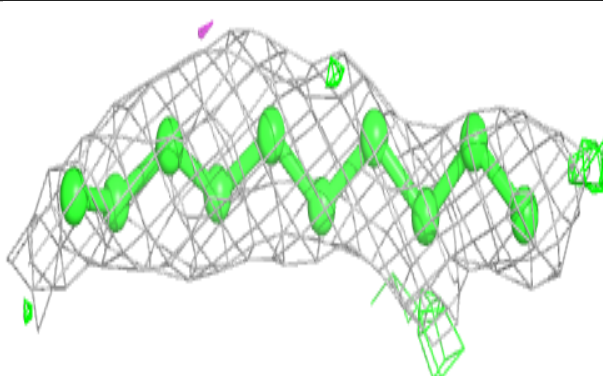
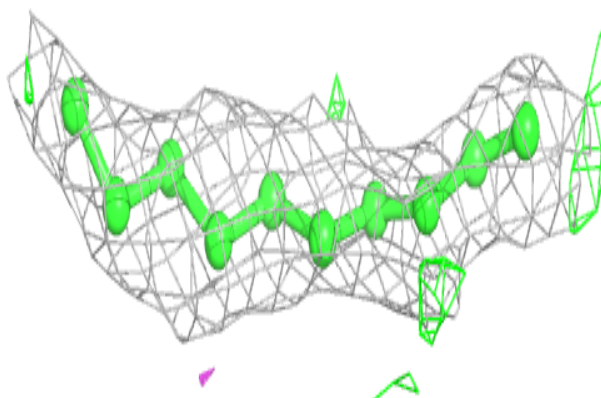


Electron density around OLC E 346:

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

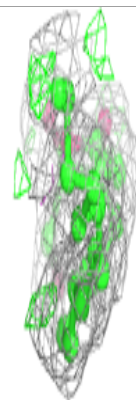
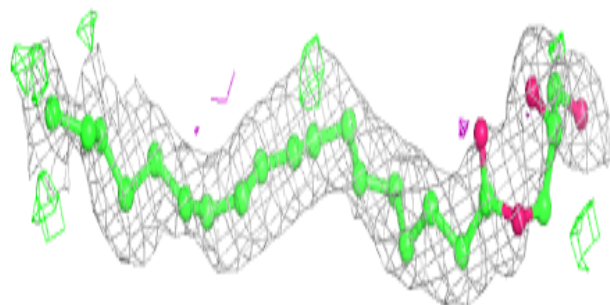
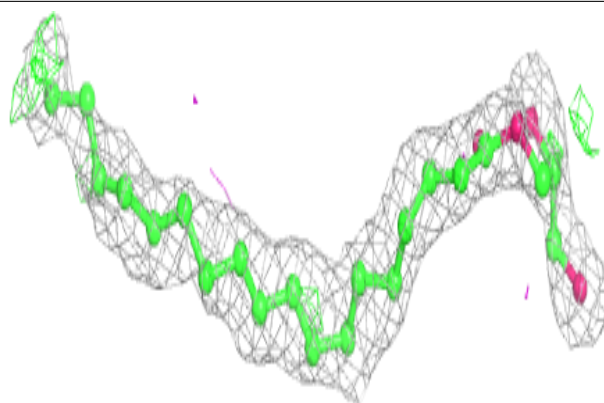
**Electron density around OLC D 345:**

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

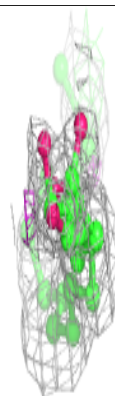
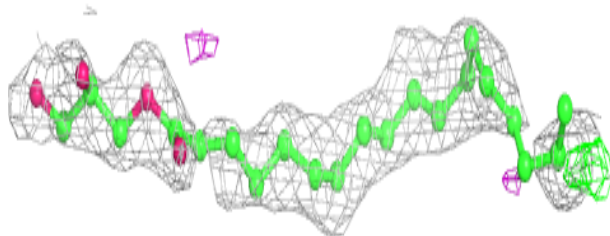
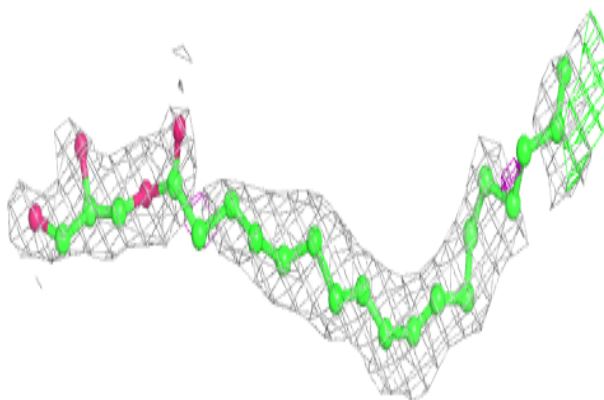


Electron density around OLC C 362:

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

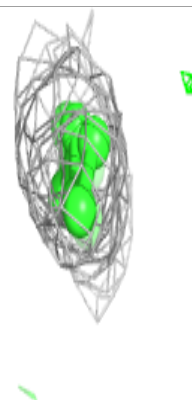
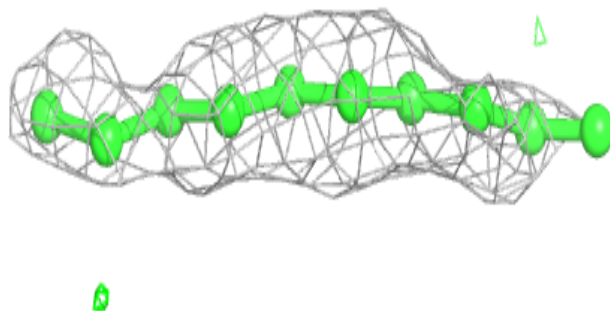
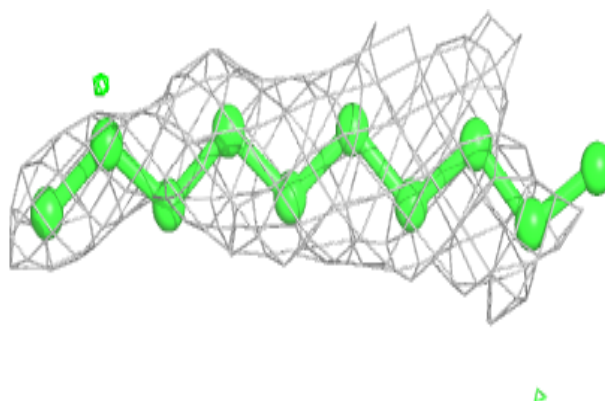
**Electron density around OLC A 361:**

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

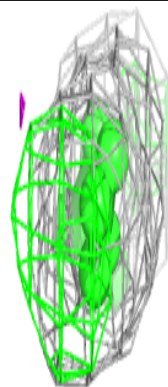
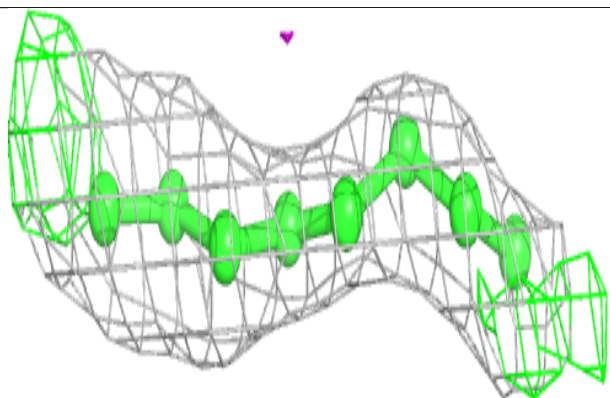
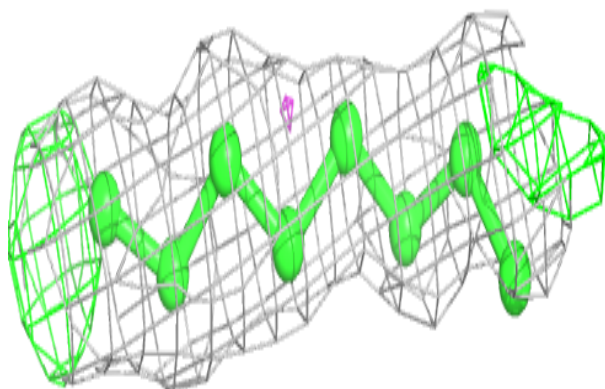


Electron density around OLC C 354:

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

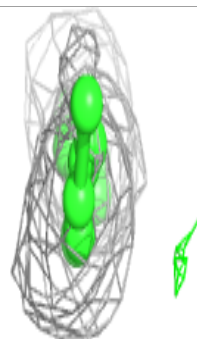
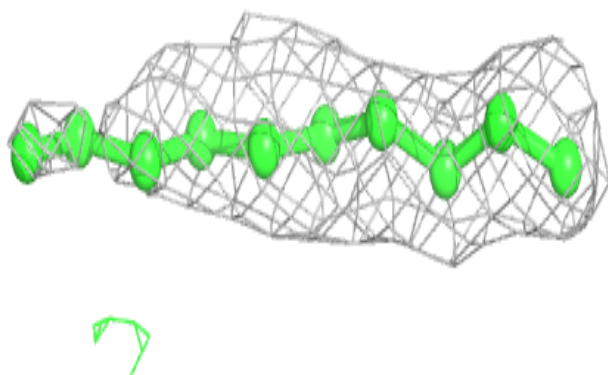
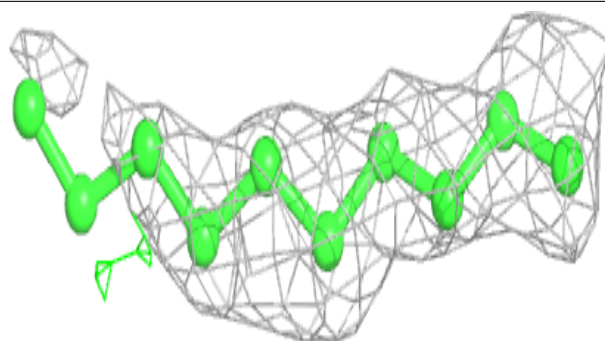
**Electron density around OLC B 354:**

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

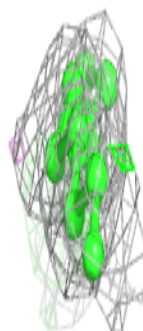
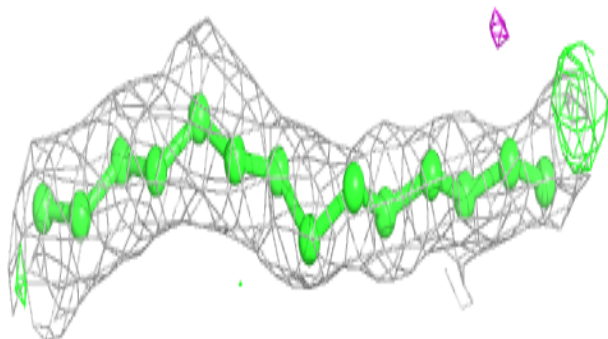
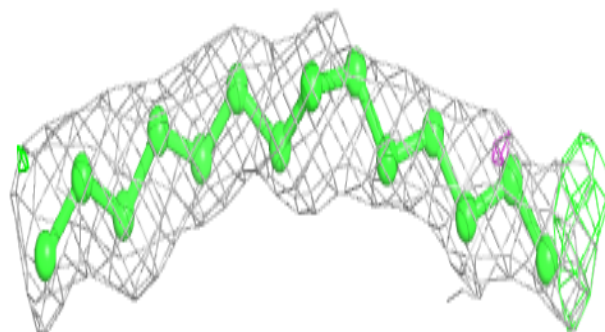


Electron density around OLC C 347:

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

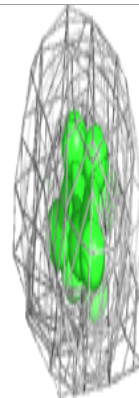
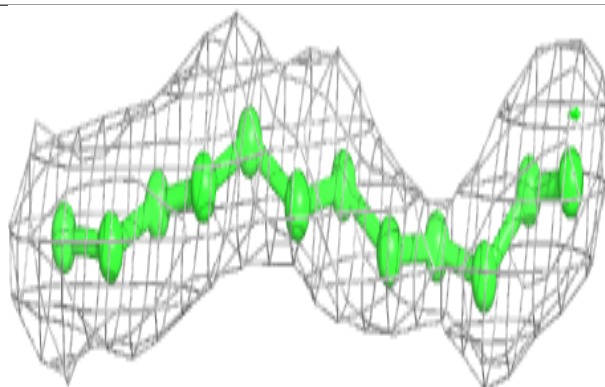
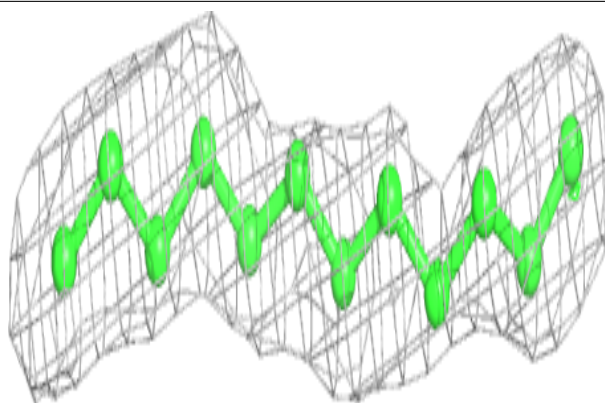
**Electron density around OLC C 350:**

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

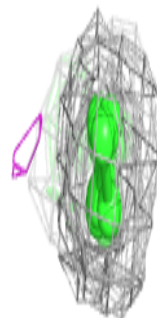
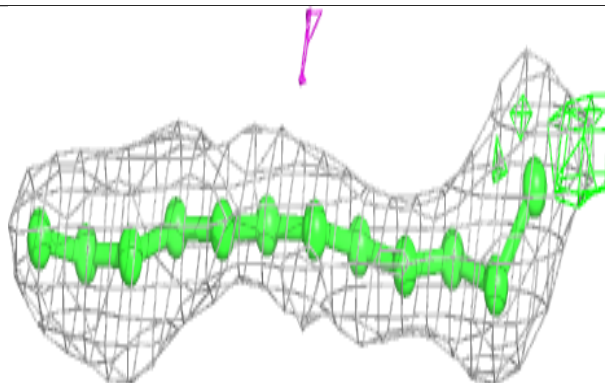
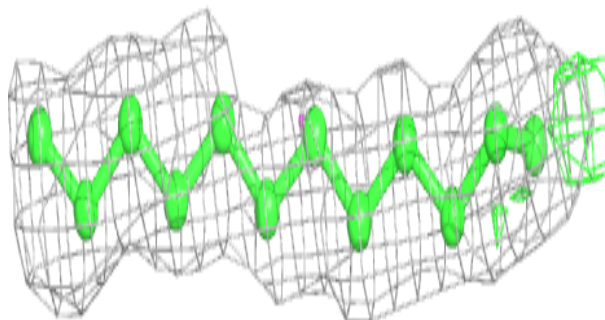


Electron density around OLC D 346:

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

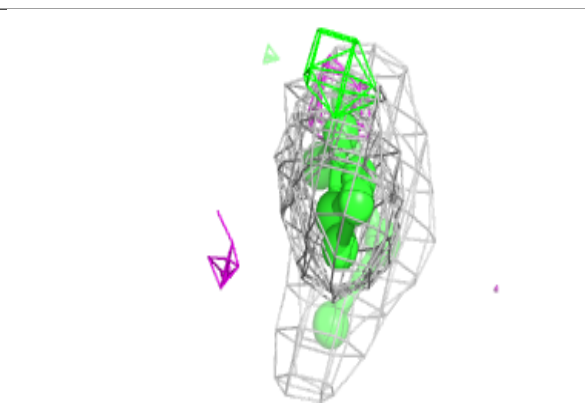
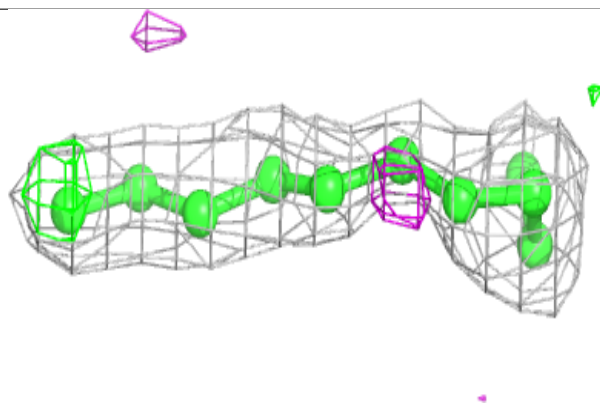
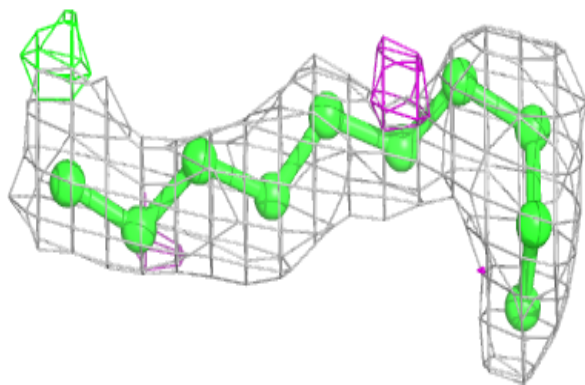
**Electron density around OLC C 345:**

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

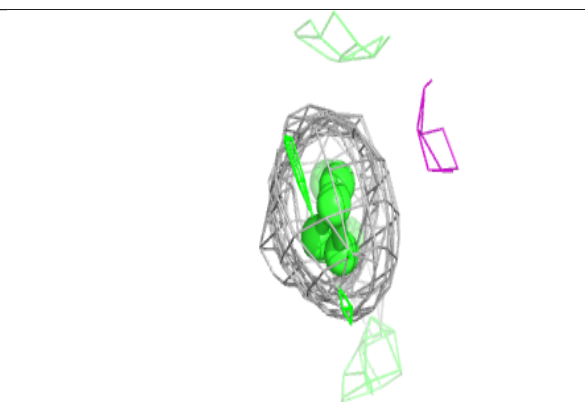
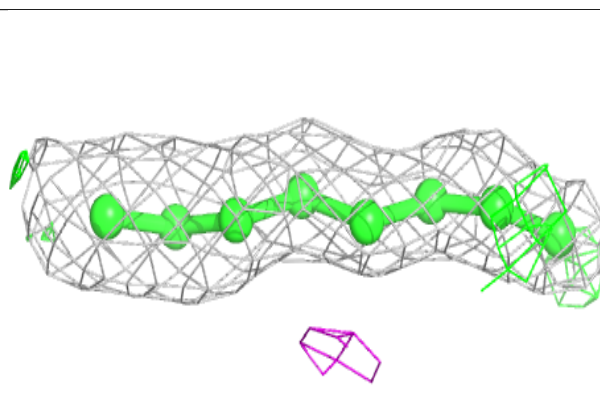
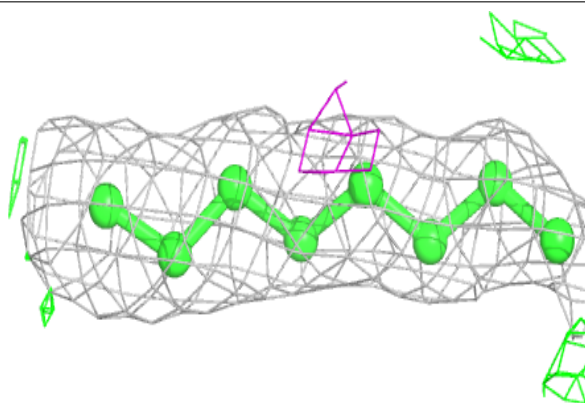


Electron density around OLC A 344:

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

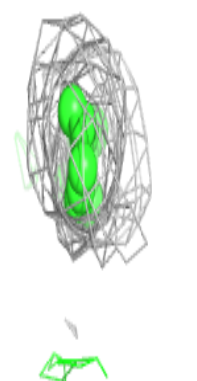
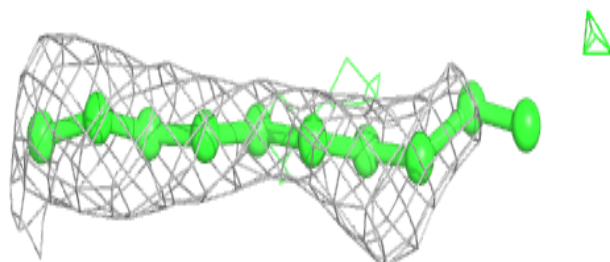
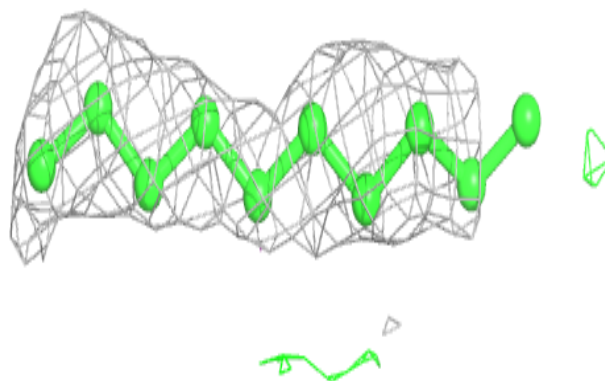
**Electron density around OLC A 345:**

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

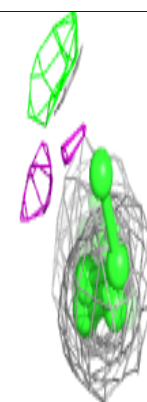
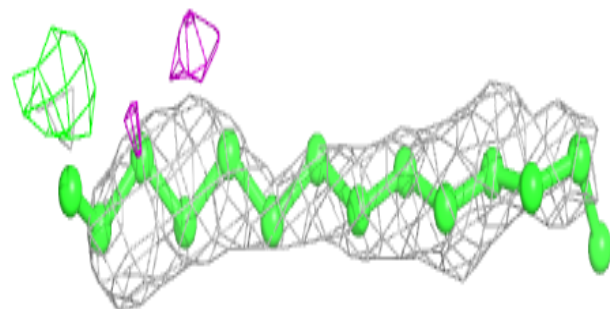
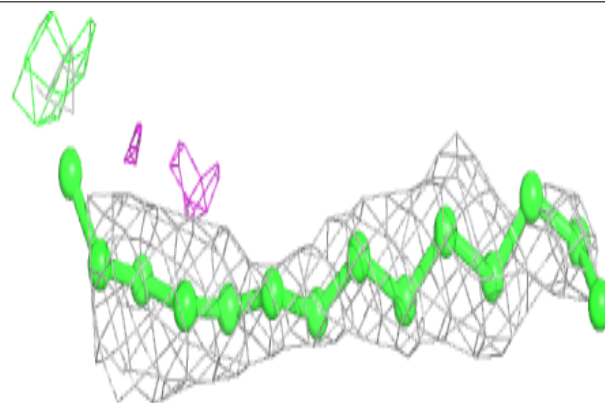


Electron density around OLC A 355:

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

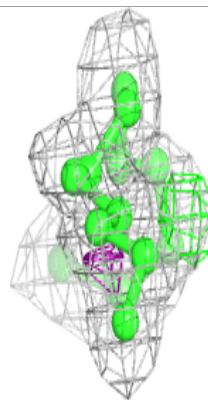
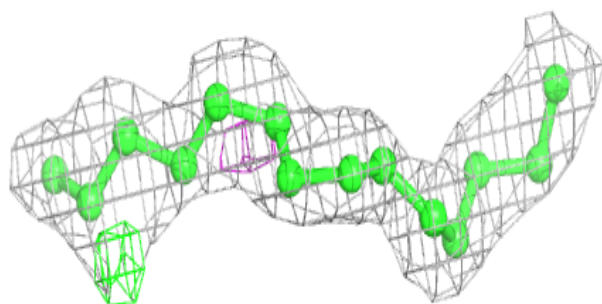
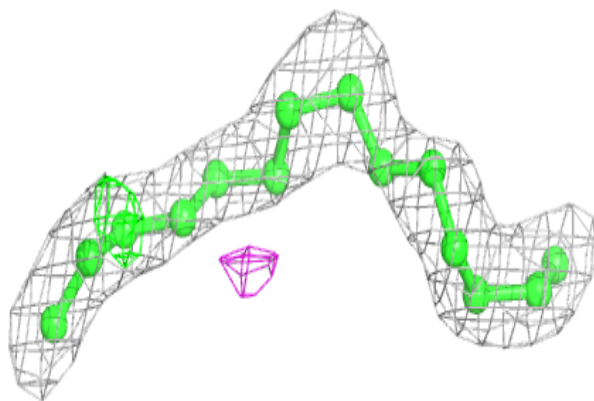
**Electron density around OLC F 347:**

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

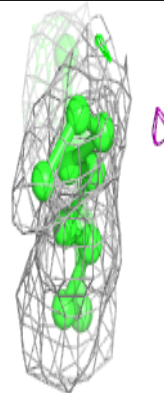
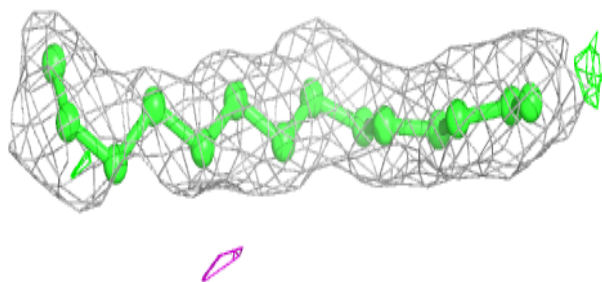
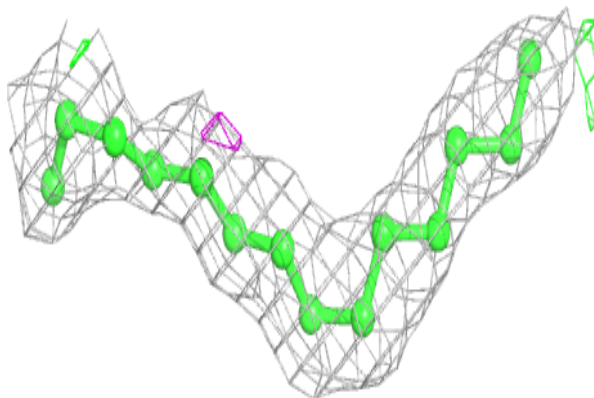


Electron density around OLC F 348:

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

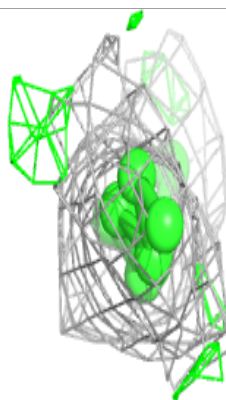
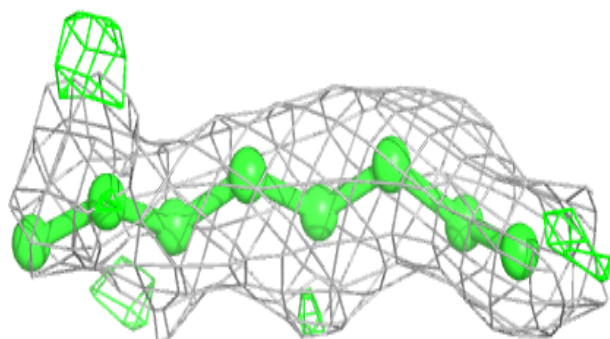
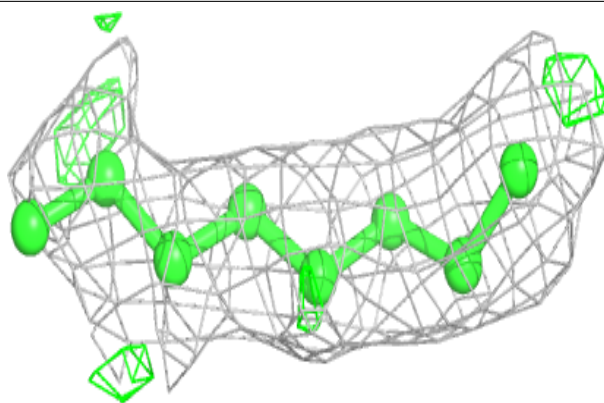
**Electron density around OLC A 350:**

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

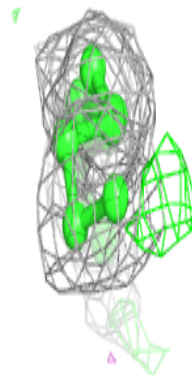
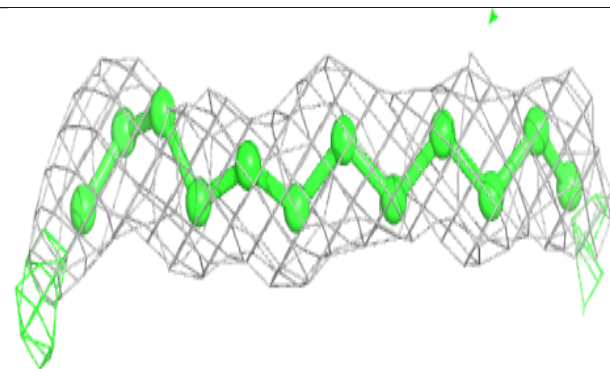
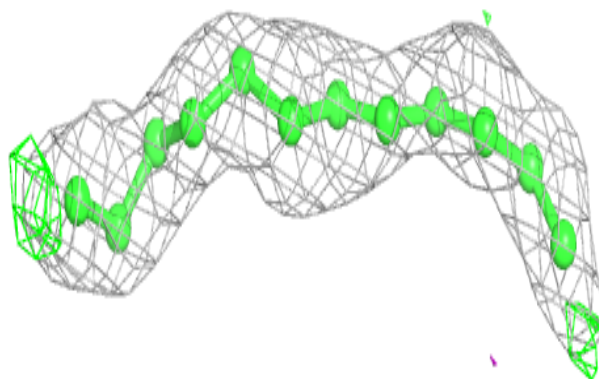


Electron density around OLC C 344:

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

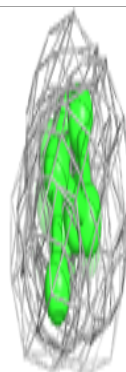
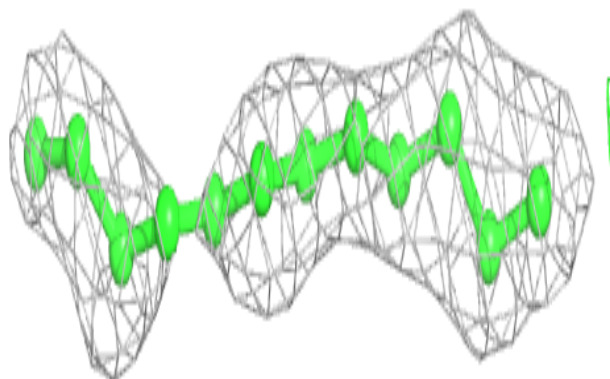
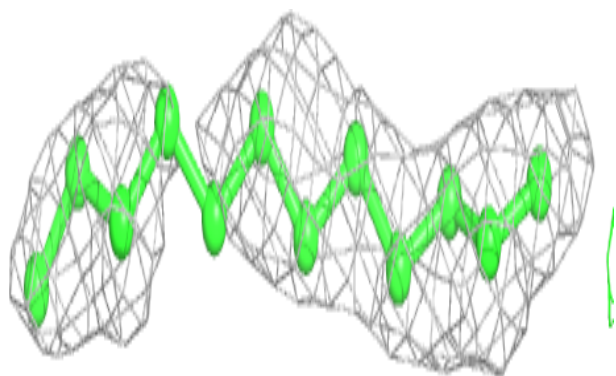
**Electron density around OLC E 343:**

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

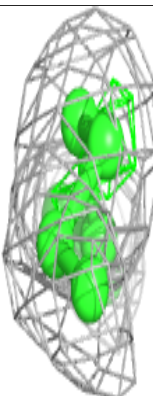
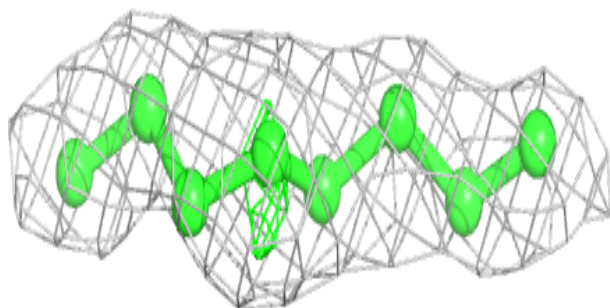
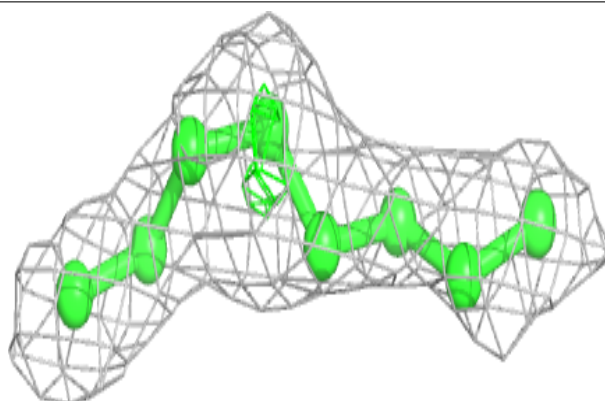


Electron density around OLC F 345:

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

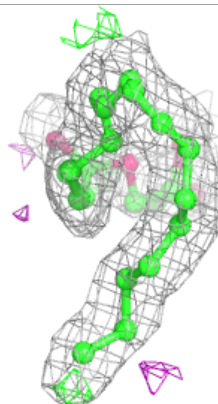
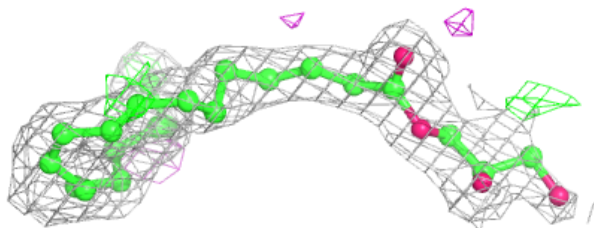
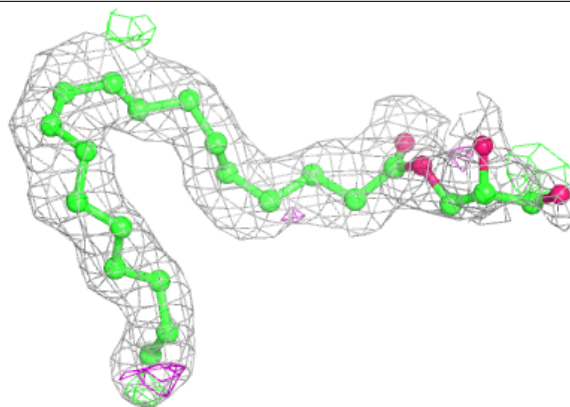
**Electron density around OLC B 353:**

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

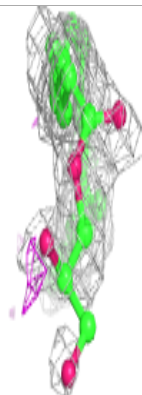
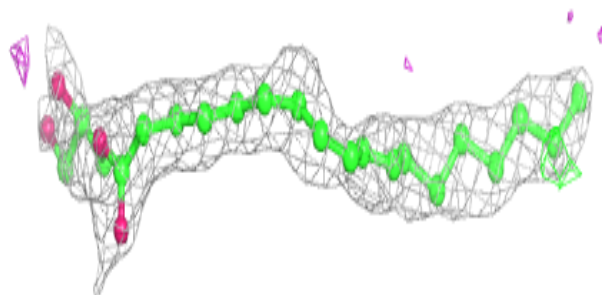
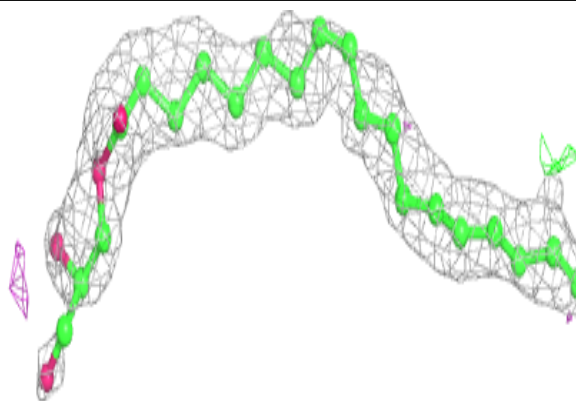


Electron density around OLC C 360:

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

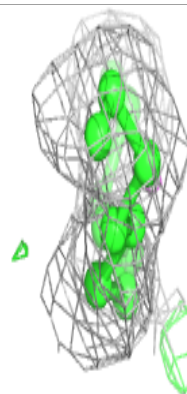
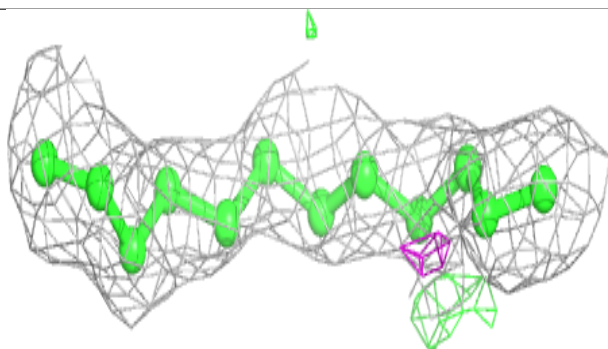
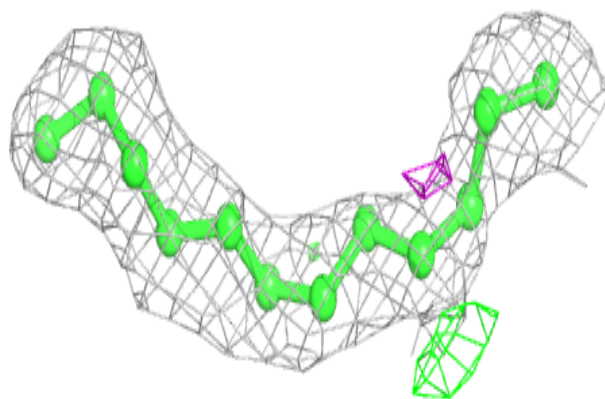
**Electron density around OLC A 349:**

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

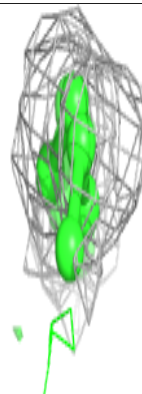
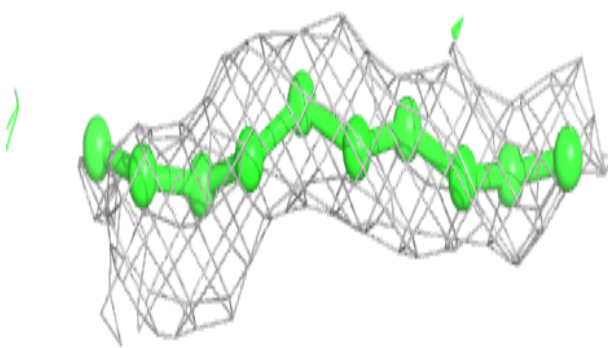
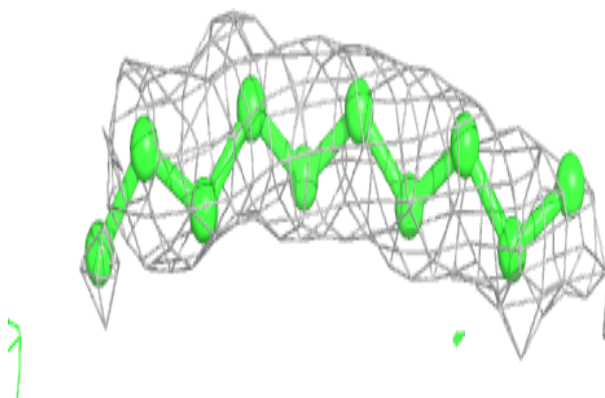


Electron density around OLC A 363:

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

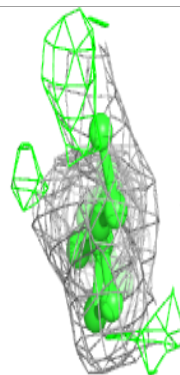
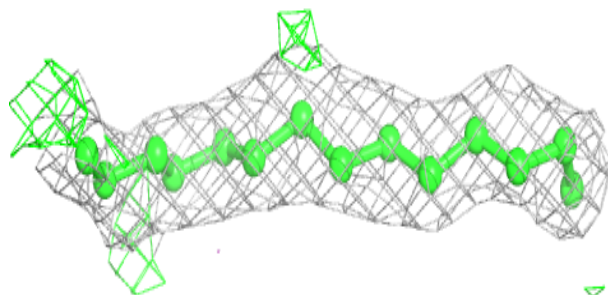
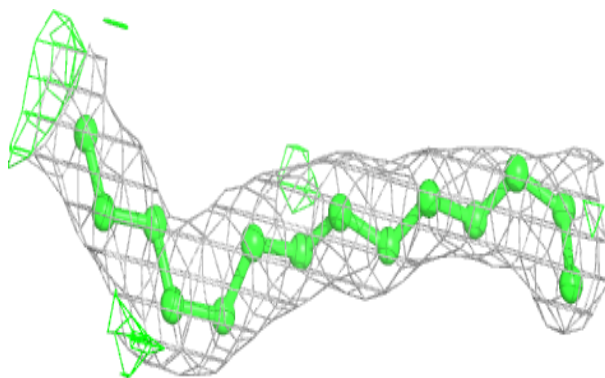
**Electron density around OLC C 353:**

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

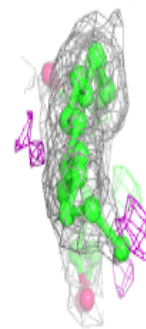
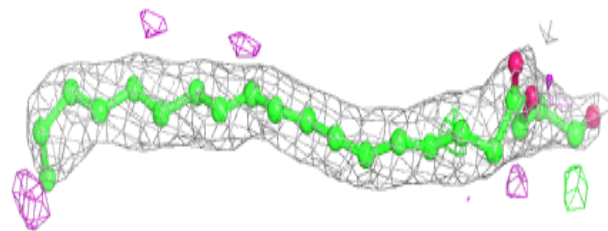
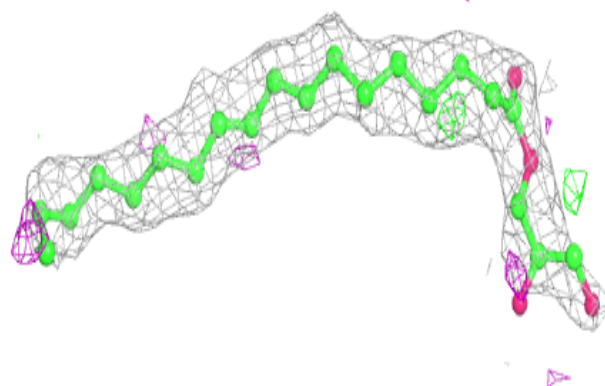


Electron density around OLC A 351:

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

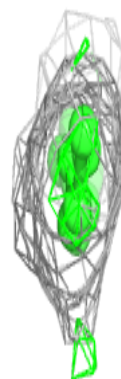
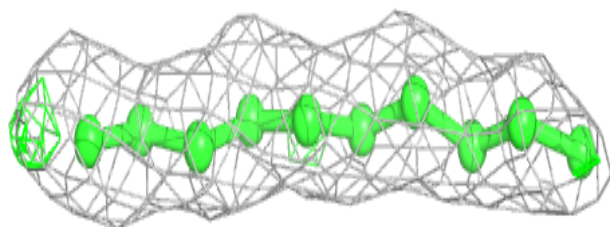
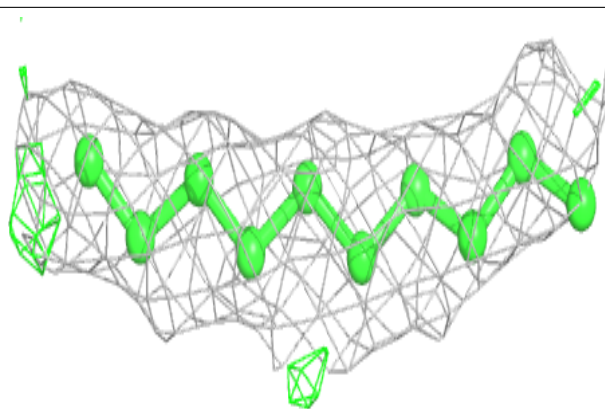
**Electron density around OLC C 358:**

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

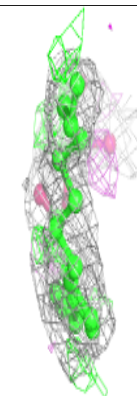
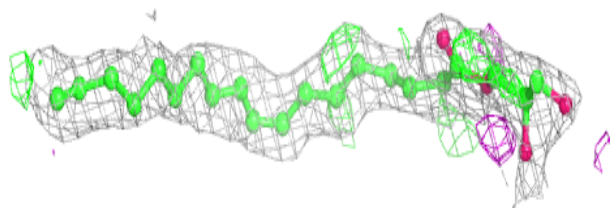
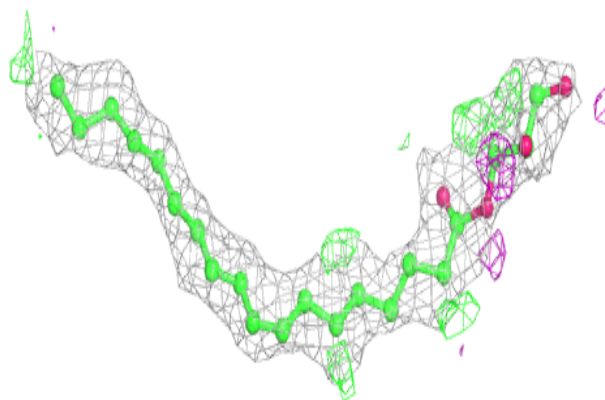


Electron density around OLC C 341:

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

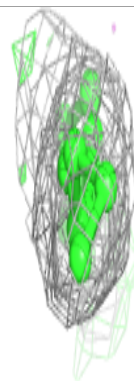
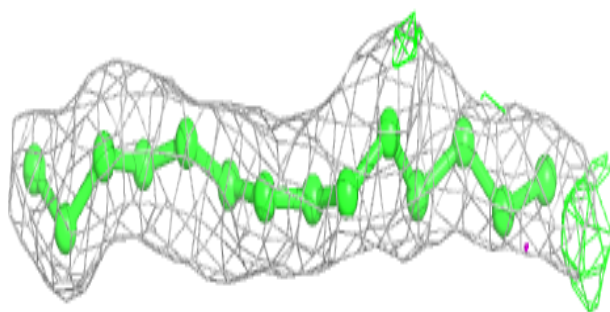
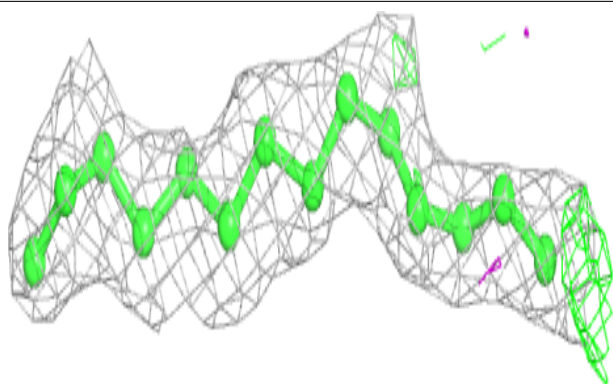
**Electron density around OLC A 346:**

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

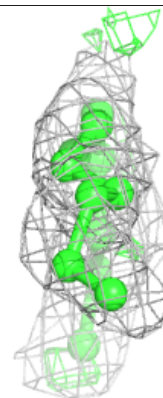
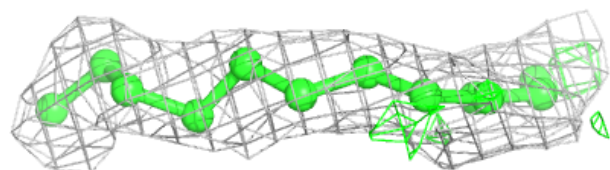
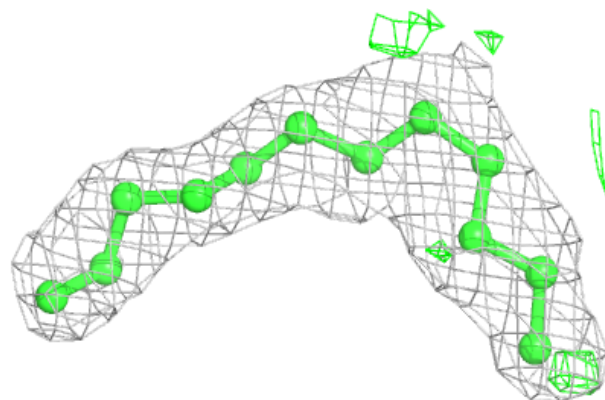


Electron density around OLC A 362:

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

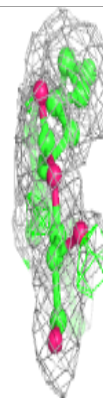
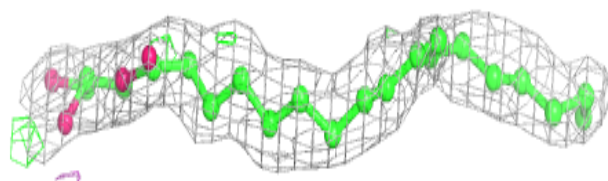
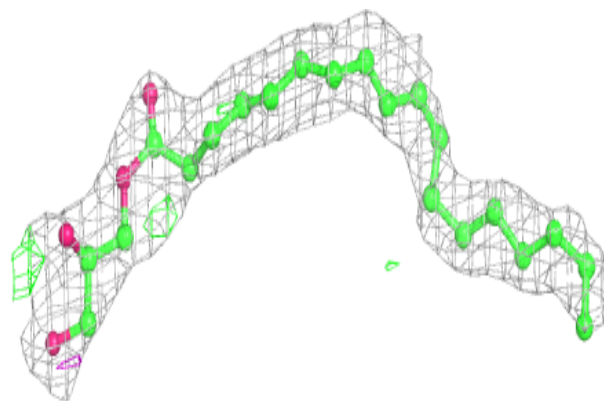
**Electron density around OLC E 348:**

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

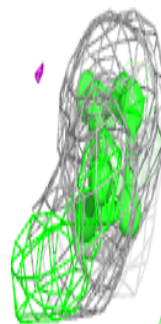
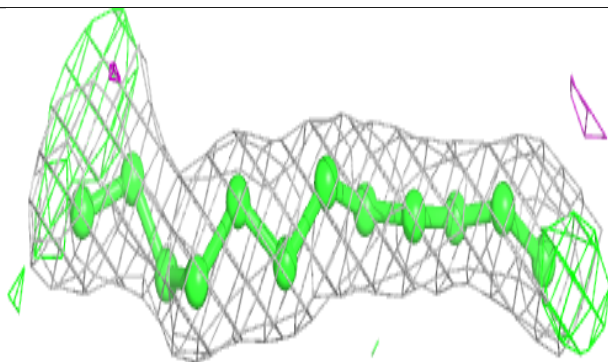
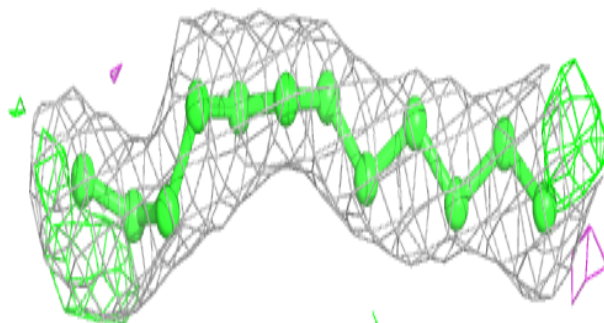


Electron density around OLC E 347:

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

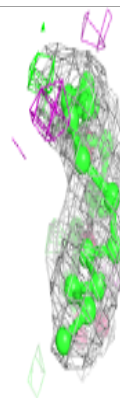
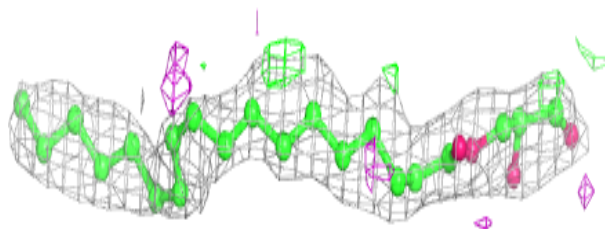
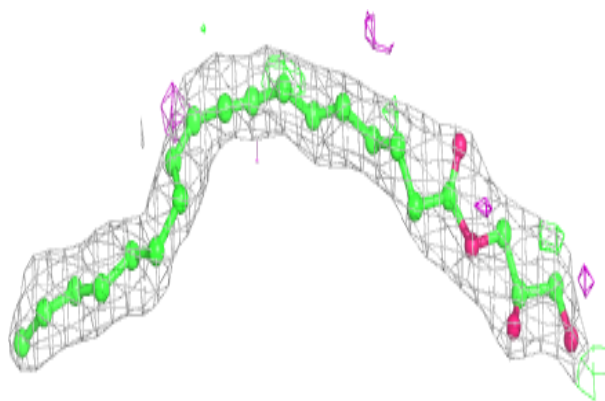
**Electron density around OLC C 361:**

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

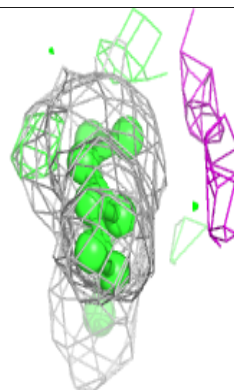
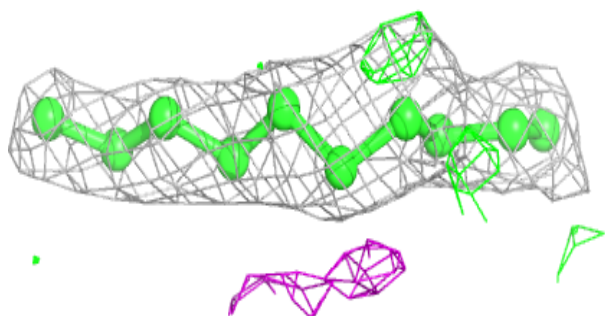
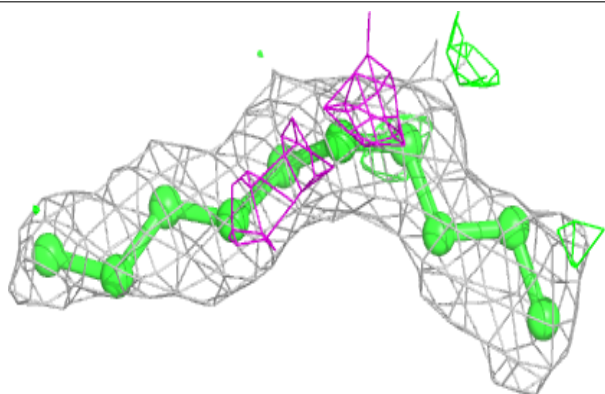


Electron density around OLC A 359:

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

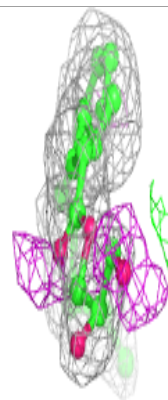
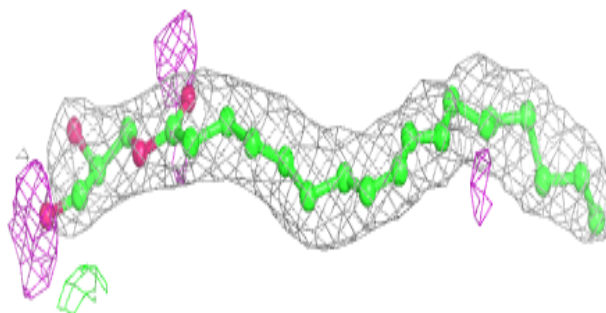
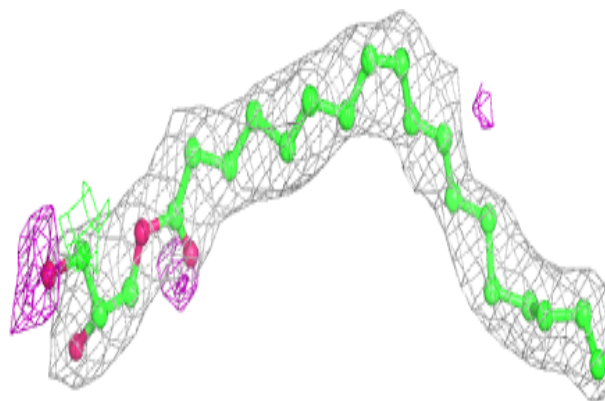
**Electron density around OLC A 348:**

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

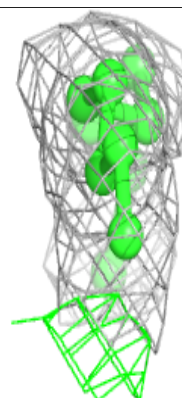
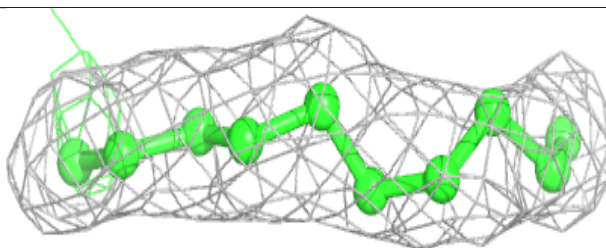
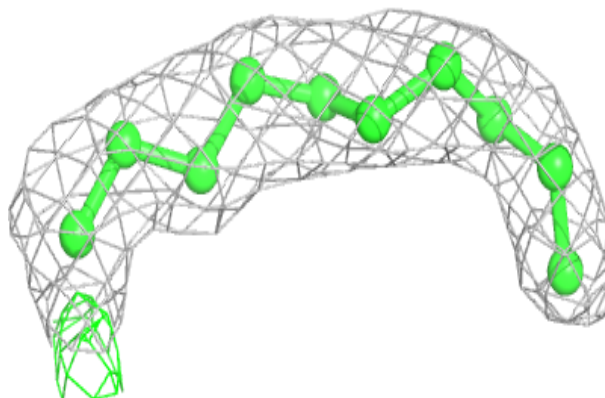


Electron density around OLC E 341:

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

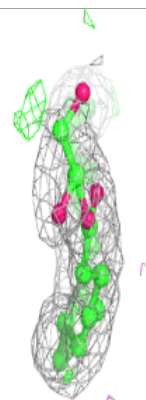
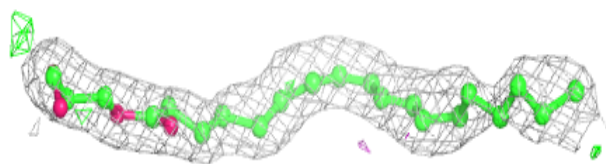
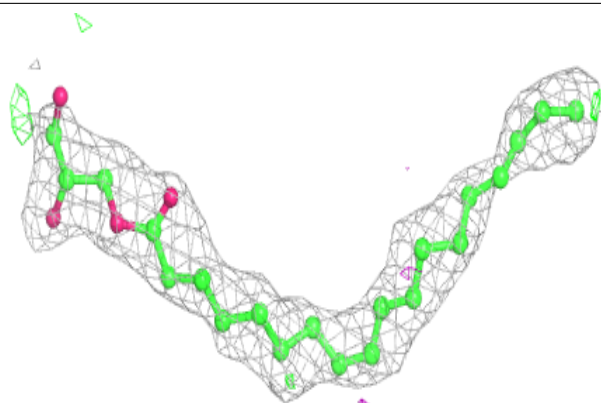
**Electron density around OLC A 357:**

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

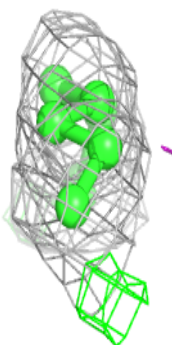
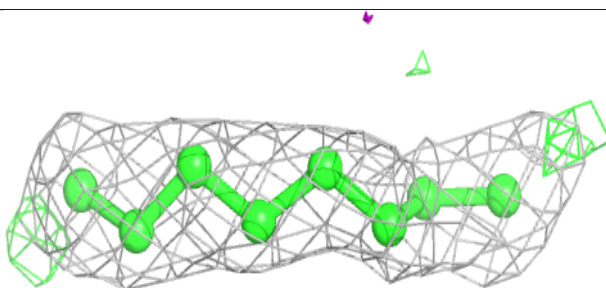
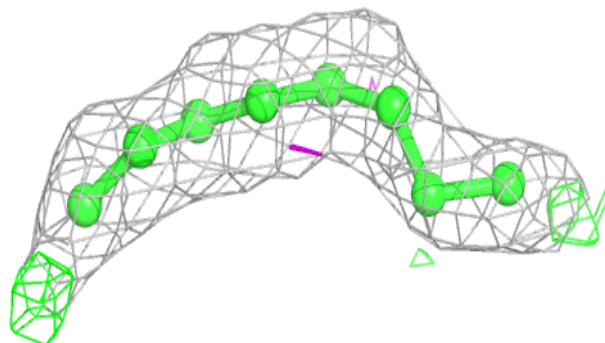


Electron density around OLC B 345:

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

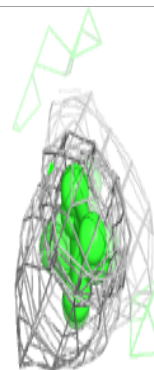
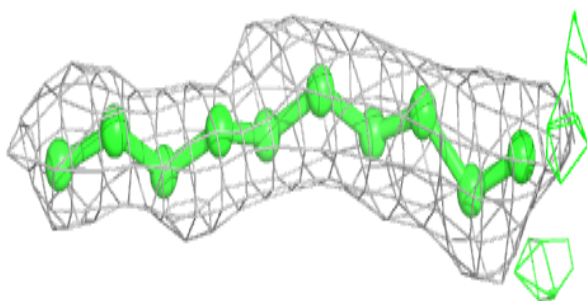
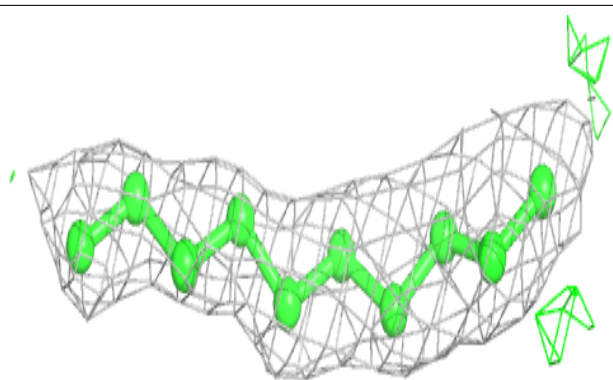
**Electron density around OLC D 347:**

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

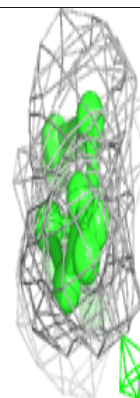
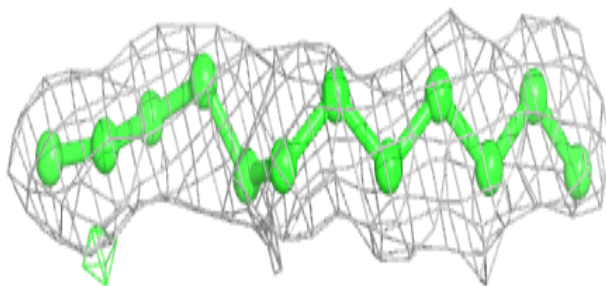
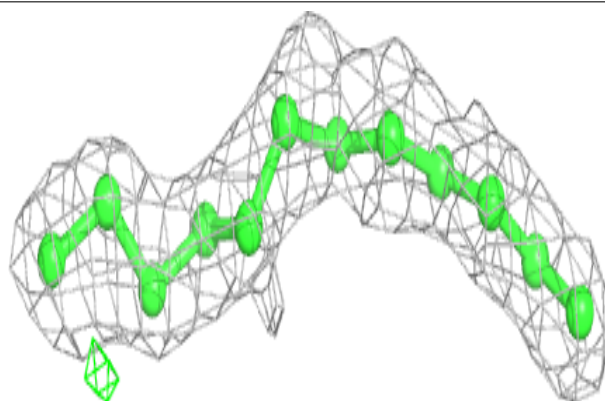


Electron density around OLC A 352:

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

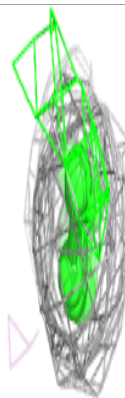
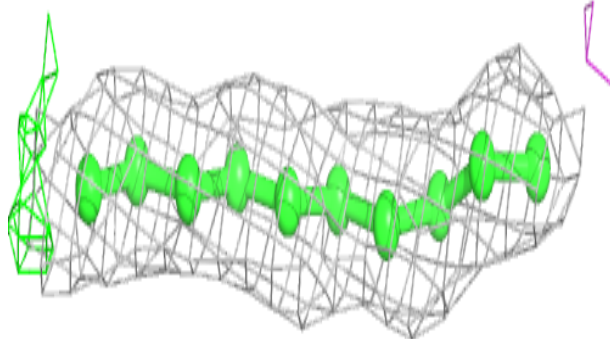
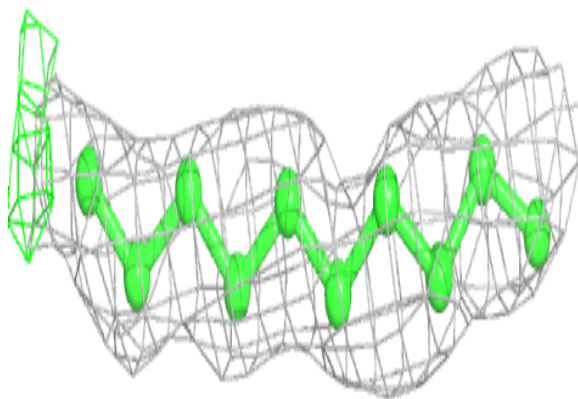
**Electron density around OLC A 364:**

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

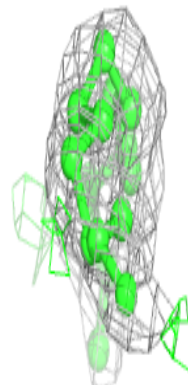
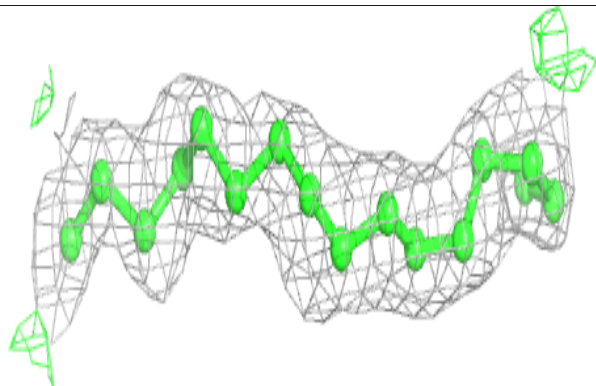
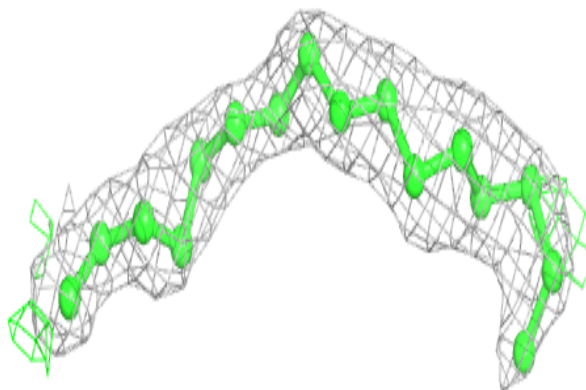


Electron density around OLC B 344:

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

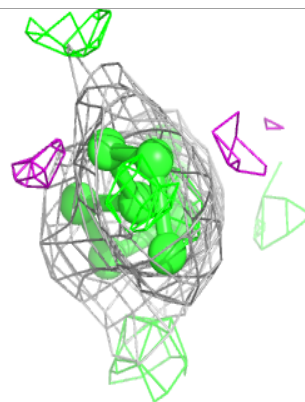
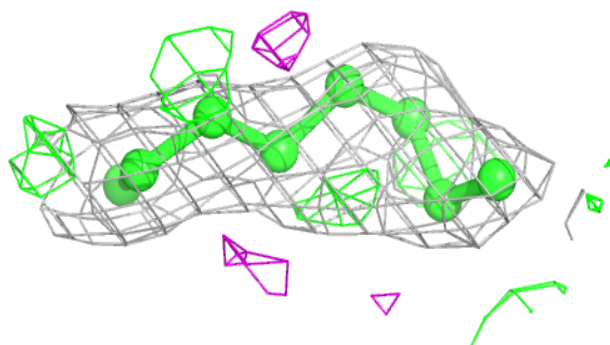
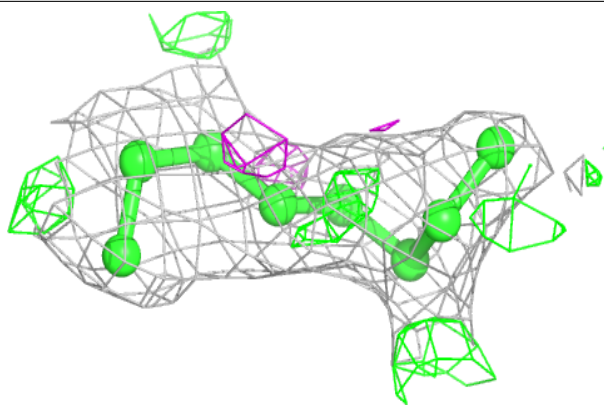
**Electron density around OLC B 352:**

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

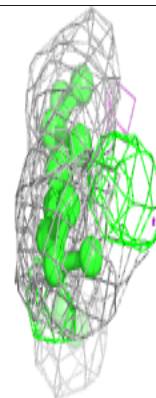
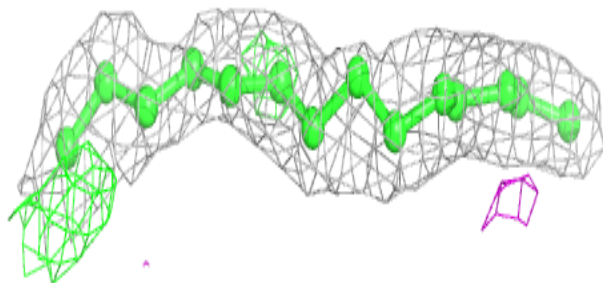
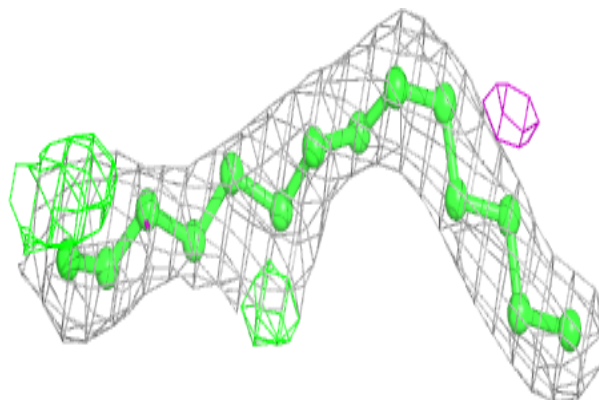


Electron density around OLC E 342:

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

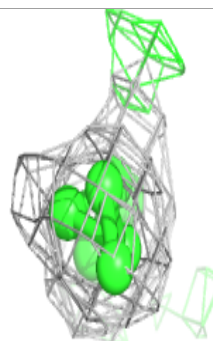
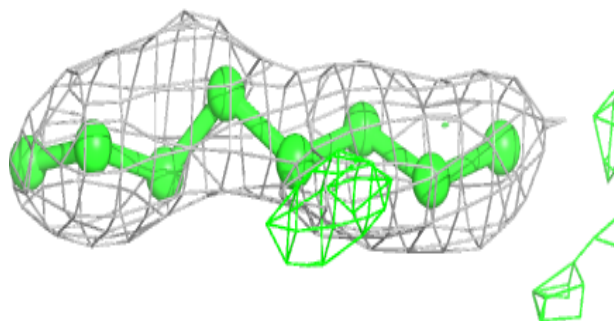
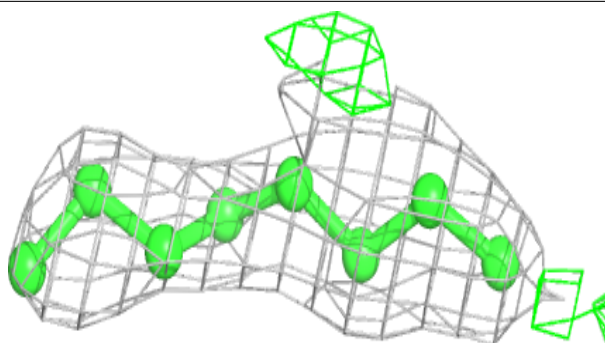
**Electron density around OLC B 347:**

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

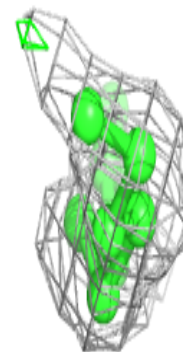
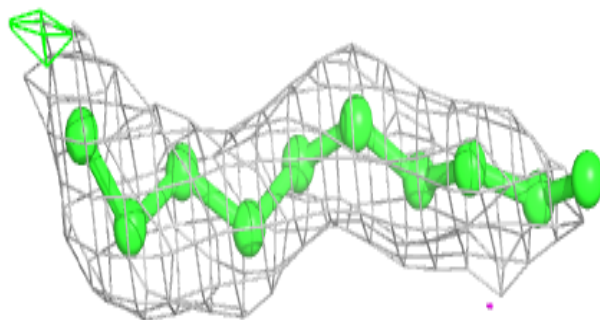
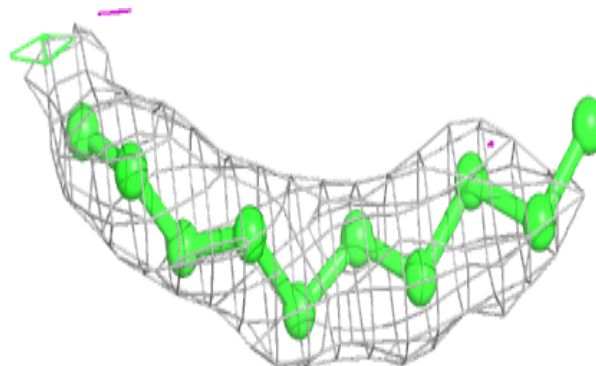


Electron density around OLC D 348:

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

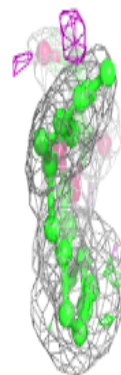
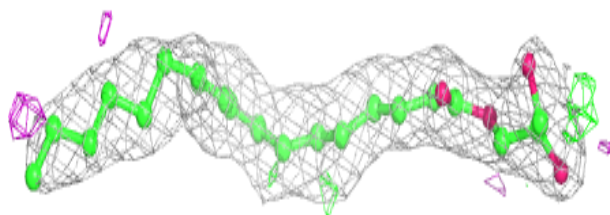
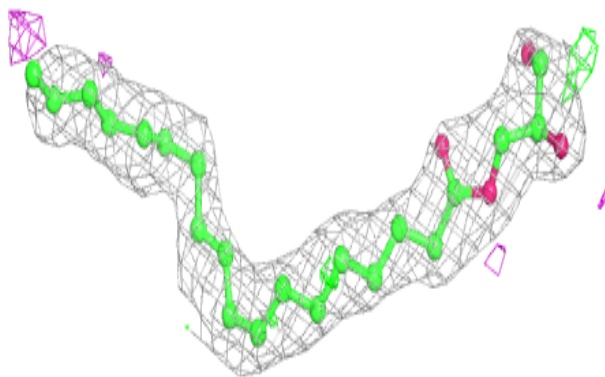
**Electron density around OLC C 349:**

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

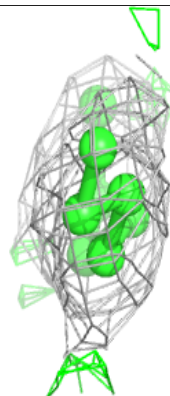
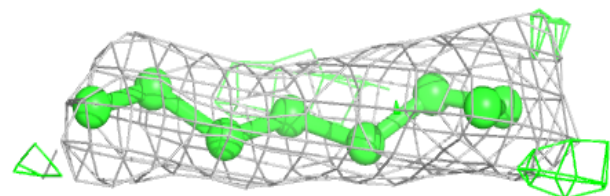
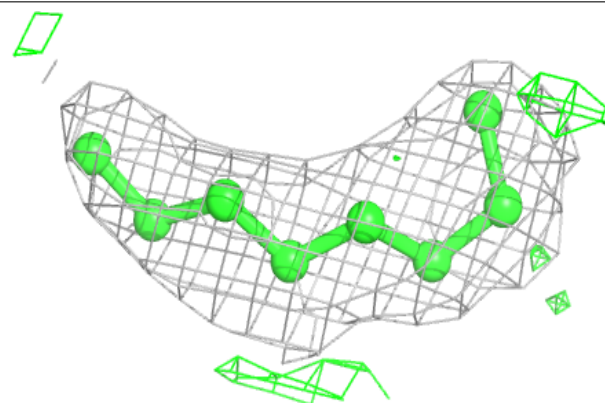


Electron density around OLC B 346:

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

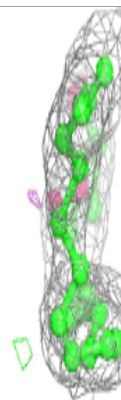
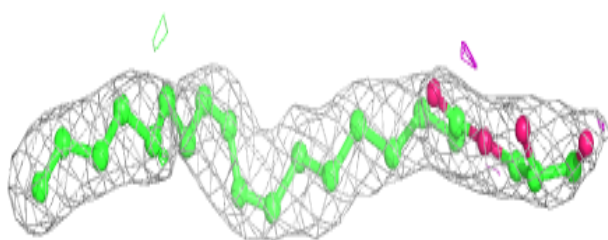
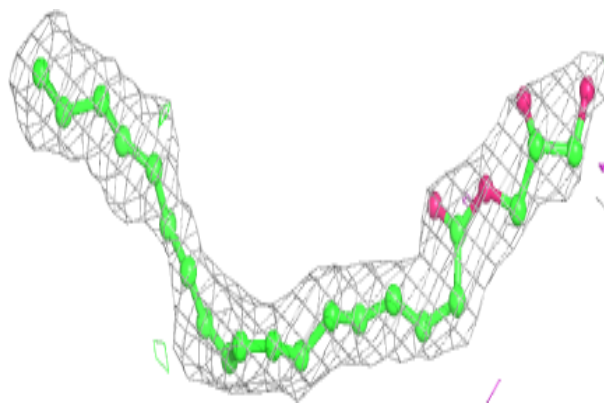
**Electron density around OLC A 342:**

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

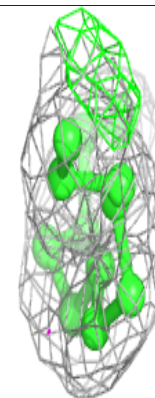
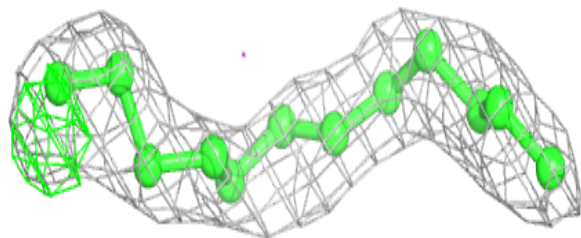
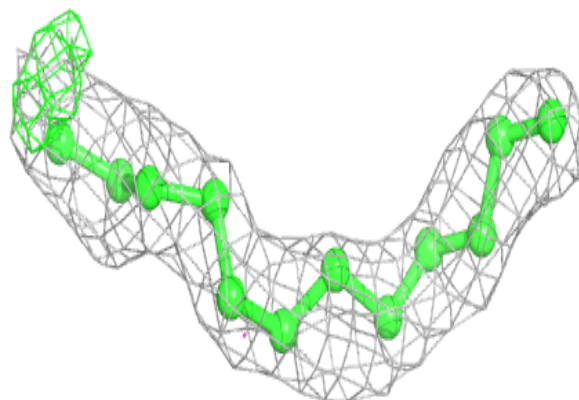


Electron density around OLC C 359:

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

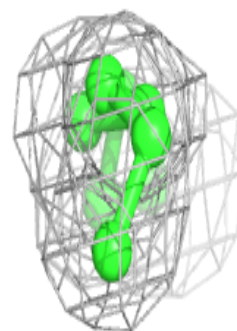
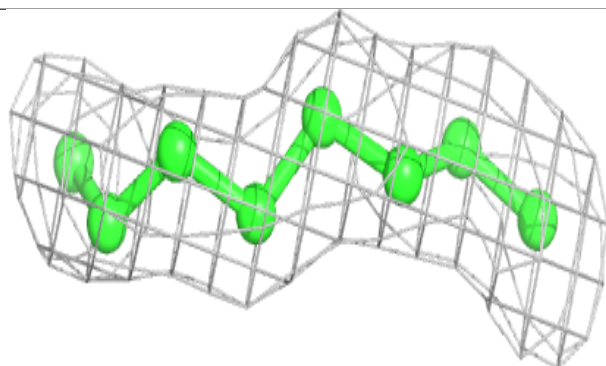
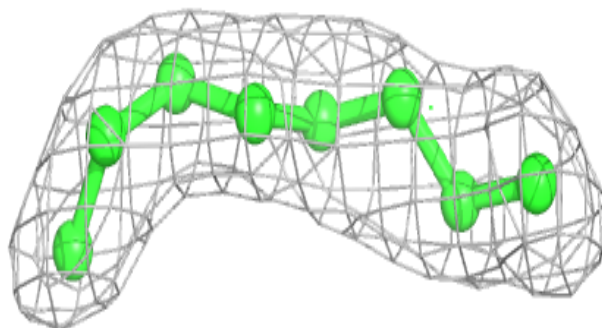
**Electron density around OLC C 364:**

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

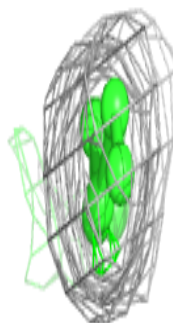
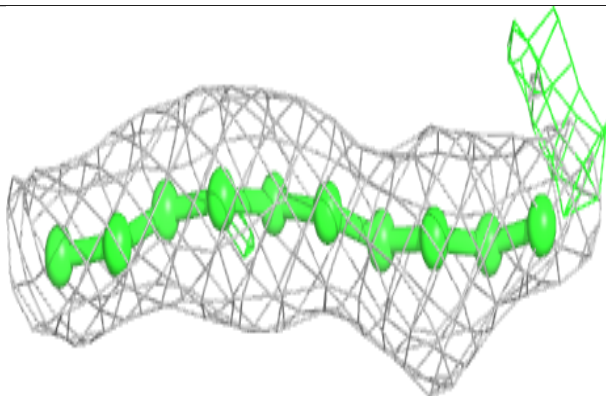
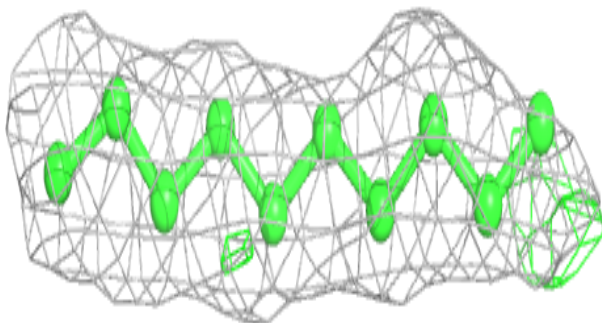


Electron density around OLC A 347:

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

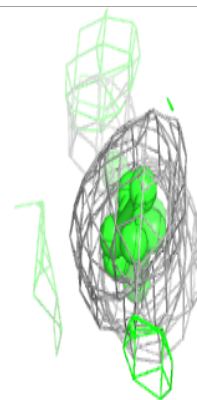
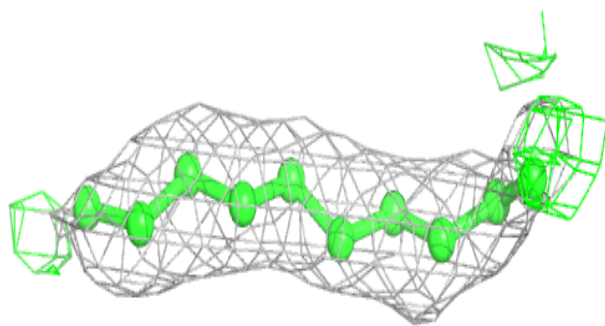
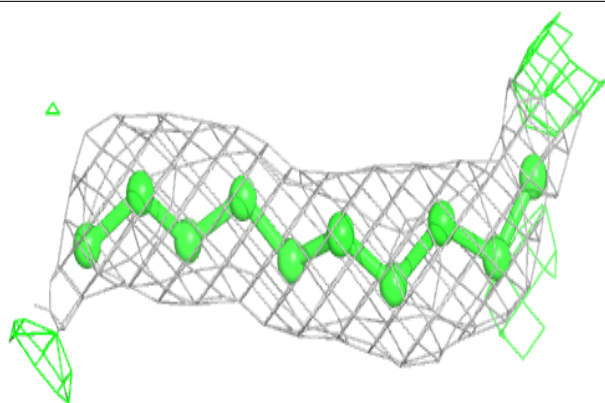
**Electron density around OLC C 355:**

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

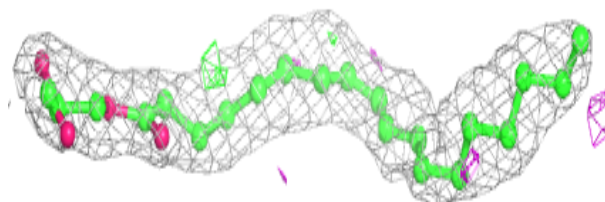
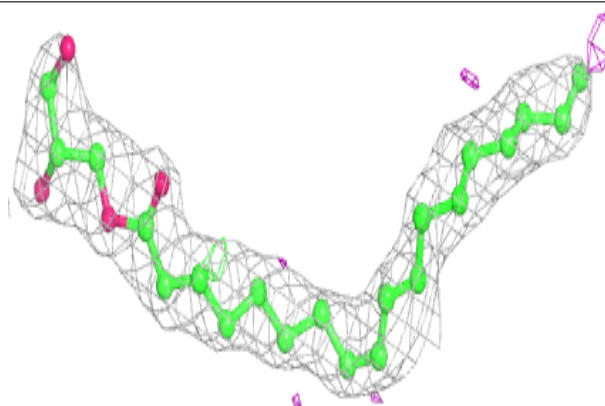


Electron density around OLC C 346:

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

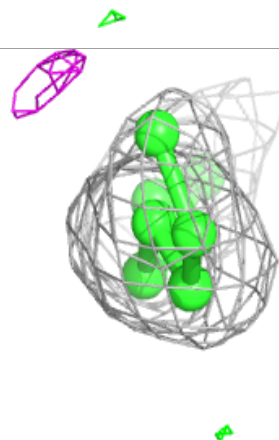
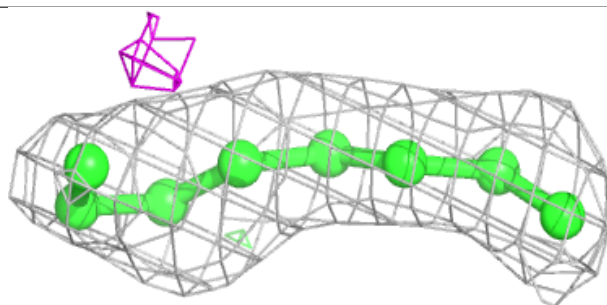
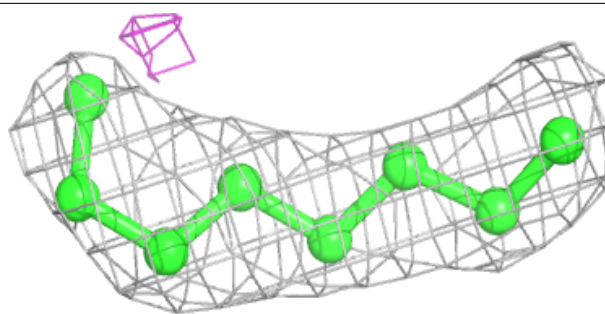
**Electron density around OLC A 356:**

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

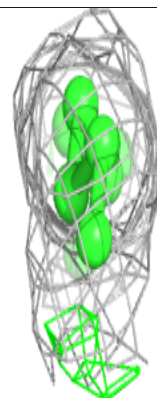
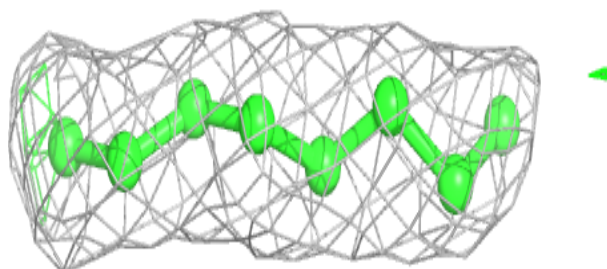
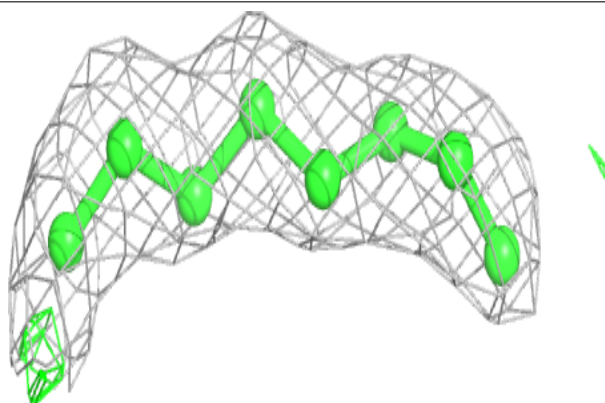


Electron density around OLC A 343:

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

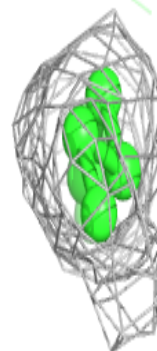
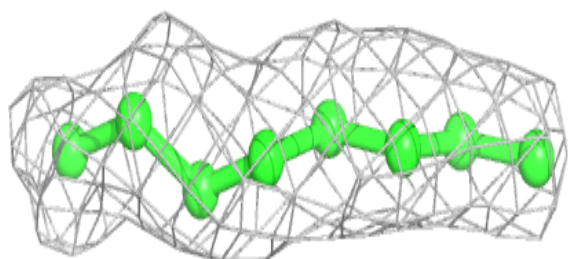
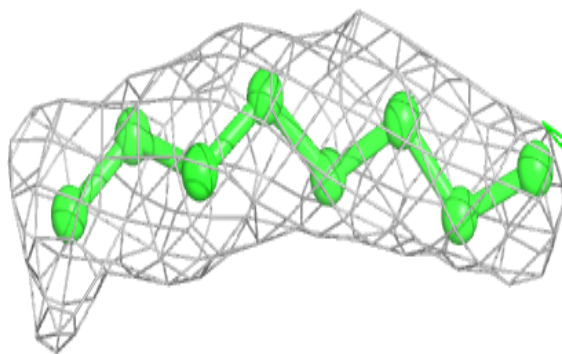
**Electron density around OLC A 354:**

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

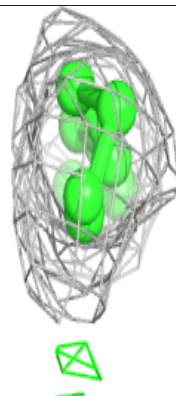
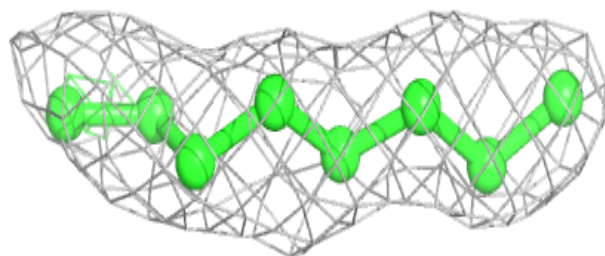
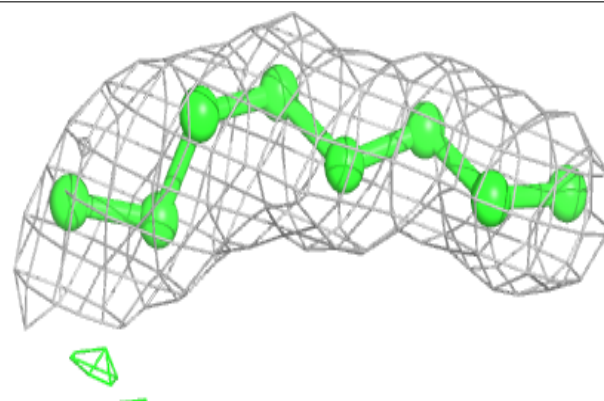


Electron density around OLC C 342:

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

**Electron density around OLC D 344:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.