



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:41 PM UTC

PDB ID : 3POX / pdb_00003pox
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 types of validation reports are described at

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

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

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

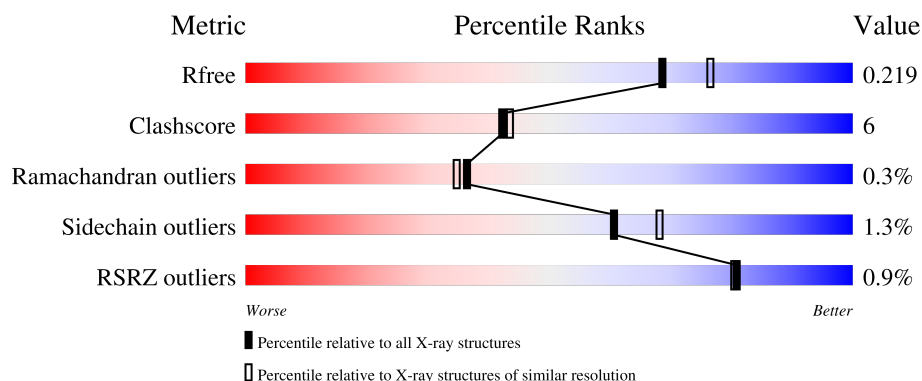
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	340	% 88% 12%
1	B	340	% 86% 14%
1	C	340	% 89% 10%
1	D	340	% 89% 11%
1	E	340	% 89% 10%

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Mol	Chain	Length	Quality of chain
1	F	340	2% 89% 10%

2 Entry composition [i](#)

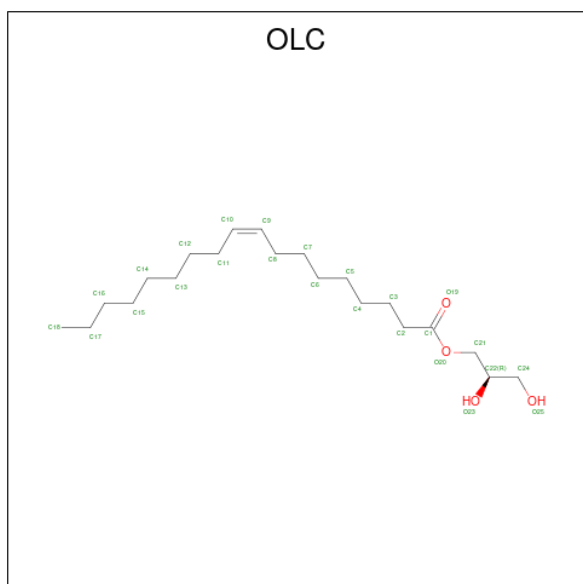
There are 5 unique types of molecules in this entry. The entry contains 18507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



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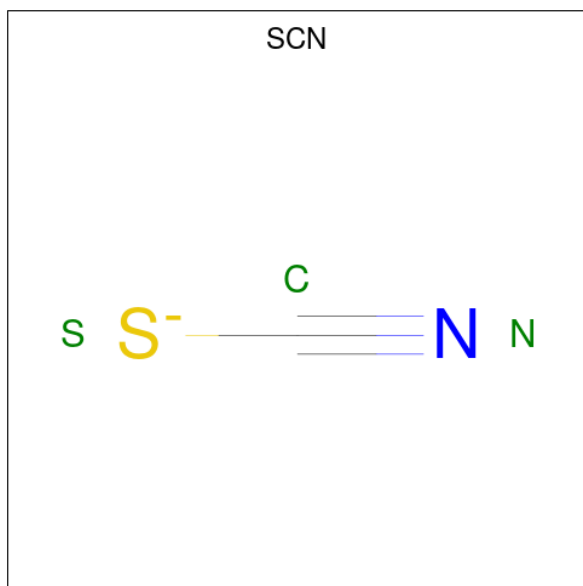
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C 8 8	0	0
2	F	1	Total C 14 14	0	0
2	F	1	Total C 14 14	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 4 is THIOCYANATE ION (CCD ID: 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

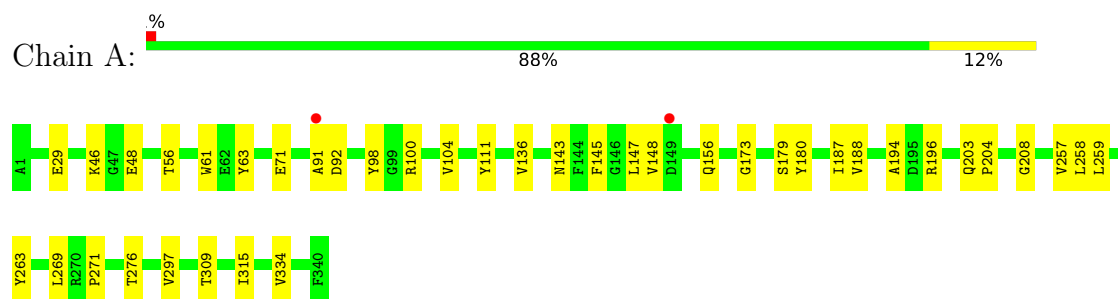
- Molecule 5 is water.

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

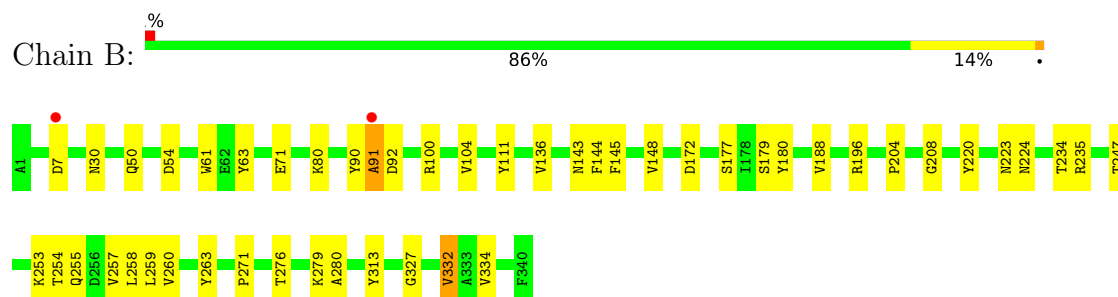
3 Residue-property plots [i](#)

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

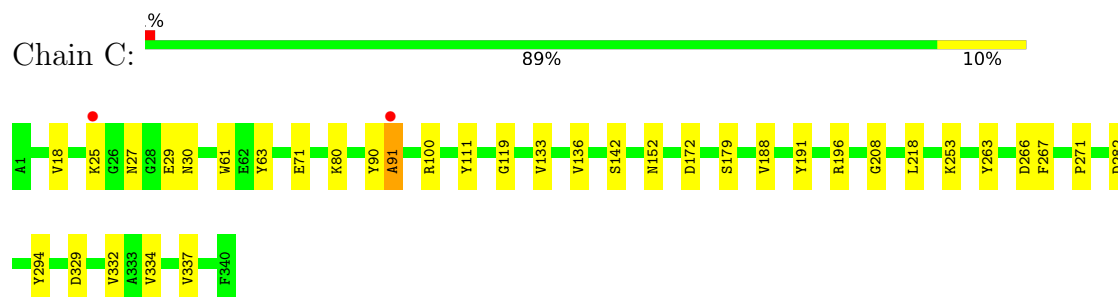
- Molecule 1: OmpF protein



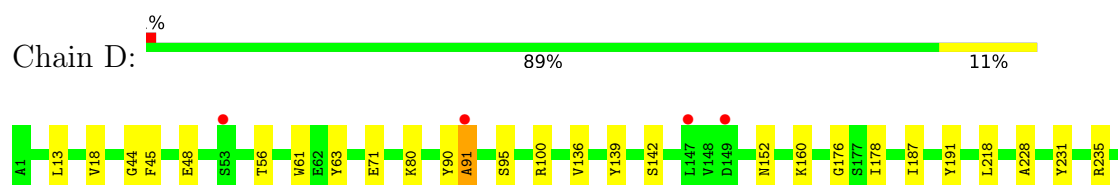
- Molecule 1: OmpF protein



- Molecule 1: OmpF protein

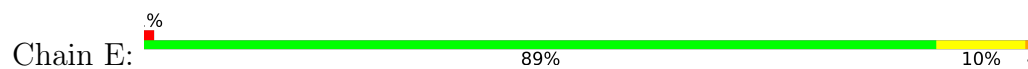


- Molecule 1: OmpF protein

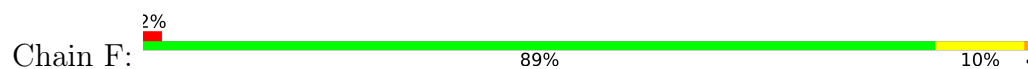




• Molecule 1: OmpF protein



• Molecule 1: OmpF protein



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) 96.5 (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 , 0.219	Depositor DCC
R_{free} test set	9833 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 , 59.4	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: SCN, K, OLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/2683	0.74	0/3628
1	B	0.44	0/2683	0.75	0/3628
1	C	0.47	0/2683	0.73	0/3628
1	D	0.48	0/2683	0.74	0/3628
1	E	0.49	0/2683	0.75	0/3628
1	F	0.43	0/2683	0.73	0/3628
All	All	0.47	0/16098	0.74	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	34	0
1	B	2627	0	2444	39	0
1	C	2627	0	2444	31	0
1	D	2627	0	2444	29	0
1	E	2627	0	2444	27	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	19	0
2	D	109	0	167	9	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	3	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	211	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 (211) 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:A:263:TYR:O	1:A:271:PRO:HD2	2.05	0.56
1:F:259:LEU:HD11	2:F:344:OLC:H7A	1.86	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:C:25:LYS:HE3	1:C:329:ASP:CG	2.33	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:71:GLU:HG3	1:C:100:ARG:NH2	2.26	0.51
1:B:313:TYR:CE2	1:B:332:VAL:HG22	2.46	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: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:B:111:TYR:OH	1:B:188:VAL:CG2	2.58	0.51
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:H8A	2:C:360:OLC:H12A	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: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:7:ASP:HB2	5:B:661:HOH:O	2.15	0.47
1:B:313:TYR:CD2	1:B:332:VAL:HG22	2.49	0.47
1:A:104:VAL:HG13	1:A:156:GLN:CD	2.40	0.46
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:E:90:TYR:O	1:E:91:ALA:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:111:TYR:CZ	1:A:188:VAL:HG23	2.51	0.45
1:D:90:TYR:O	1:D:91:ALA:C	2.60	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:48:GLU:HG3	1:D:56:THR:CG2	2.46	0.45
1:D:270:ARG:O	1:D:270:ARG:HG2	2.17	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:61:TRP:CZ2	1:B:63:TYR:HB2	2.53	0.44
1:B:220:TYR:OH	2:B:345:OLC:H21A	2.17	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:C:90:TYR:O	1:C:91:ALA:C	2.61	0.43
1:D:294:TYR:CD1	1:D:294:TYR:C	2.96	0.43
1:C:172:ASP:CG	2:C:359:OLC:H24	2.44	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:176:GLY:C	2:D:342:OLC:H12A	2.43	0.42
1:D:228:ALA:HB3	1:D:260:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ASN:O	1:E:30:ASN:CG	2.63	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:C:294:TYR:CD1	1:C:294:TYR:C	2.98	0.42
1:B:30:ASN:O	1:B:30:ASN:CG	2.63	0.42
1:D:13:LEU:HD12	1:D:44:GLY:O	2.20	0.42
1:E:71:GLU:HG3	1:F:100:ARG:NH2	2.35	0.42
1:B:143:ASN:O	1:B:144:PHE:C	2.62	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:E:25:LYS:HD3	2:E:344:OLC:H2	2.02	0.41
1:C:30:ASN:CG	1:C:30:ASN:O	2.62	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:45:PHE:CD1	1:D:45:PHE:C	2.99	0.41
1:D:191:TYR:CE1	2:D:345:OLC:H5A	2.56	0.41
1:B:90:TYR:O	1:B:91:ALA:C	2.64	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: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:48:GLU:HG2	1:A:56:THR:CG2	2.52	0.40
1:A:269:LEU:HG	1:A:271:PRO:HD3	2.03	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	36	35
1	B	338/340 (99%)	323 (96%)	14 (4%)	1 (0%)	36	35
1	C	338/340 (99%)	324 (96%)	13 (4%)	1 (0%)	36	35
1	D	338/340 (99%)	327 (97%)	10 (3%)	1 (0%)	36	35
1	E	338/340 (99%)	325 (96%)	12 (4%)	1 (0%)	36	35
1	F	338/340 (99%)	321 (95%)	16 (5%)	1 (0%)	36	35
All	All	2028/2040 (99%)	1945 (96%)	77 (4%)	6 (0%)	36	35

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%)	261 (99%)	2 (1%)	73	80
1	B	263/263 (100%)	259 (98%)	4 (2%)	57	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	263/263 (100%)	260 (99%)	3 (1%)	65	73
1	D	263/263 (100%)	260 (99%)	3 (1%)	65	73
1	E	263/263 (100%)	259 (98%)	4 (2%)	57	64
1	F	263/263 (100%)	259 (98%)	4 (2%)	57	64
All	All	1578/1578 (100%)	1558 (99%)	20 (1%)	61	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	136	VAL
1	B	80	LYS
1	B	136	VAL
1	B	260	VAL
1	B	332	VAL
1	C	133	VAL
1	C	136	VAL
1	C	332	VAL
1	D	136	VAL
1	D	243	LYS
1	D	332	VAL
1	E	46	LYS
1	E	80	LYS
1	E	136	VAL
1	E	210	LYS
1	F	56	THR
1	F	104	VAL
1	F	258	LEU
1	F	311	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	230	ASN
1	B	30	ASN
1	B	35	ASN
1	B	50	GLN
1	B	60	GLN
1	B	264	GLN

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Mol	Chain	Res	Type
1	C	230	ASN
1	C	306	ASN
1	D	9	ASN
1	D	30	ASN
1	D	50	GLN
1	D	60	GLN
1	D	230	ASN
1	D	339	GLN
1	E	60	GLN
1	E	230	ASN
1	F	30	ASN
1	F	50	GLN
1	F	203	GLN
1	F	223	ASN
1	F	230	ASN
1	F	306	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	350	-	13,13,24	1.09	1 (7%)	12,12,25	0.90	0
2	OLC	D	345	-	9,9,24	1.21	1 (11%)	8,8,25	0.98	1 (12%)
2	OLC	B	349	-	7,7,24	0.24	0	6,6,25	0.48	0
2	OLC	A	349	-	24,24,24	1.35	4 (16%)	25,25,25	1.11	2 (8%)
2	OLC	A	348	-	9,9,24	1.22	1 (11%)	8,8,25	0.91	1 (12%)
2	OLC	A	360	-	11,11,24	1.18	1 (9%)	10,10,25	1.02	1 (10%)
2	OLC	C	362	-	24,24,24	1.37	4 (16%)	25,25,25	1.41	3 (12%)
2	OLC	C	347	-	9,9,24	1.23	1 (11%)	8,8,25	1.02	1 (12%)
2	OLC	D	342	-	24,24,24	1.39	4 (16%)	25,25,25	1.06	2 (8%)
2	OLC	A	346	-	24,24,24	1.39	4 (16%)	25,25,25	1.22	3 (12%)
2	OLC	D	346	-	11,11,24	1.21	1 (9%)	10,10,25	1.15	1 (10%)
2	OLC	C	348	-	11,11,24	1.19	1 (9%)	10,10,25	1.08	1 (10%)
2	OLC	D	343	-	7,7,24	0.22	0	6,6,25	0.57	0
2	OLC	B	342	-	13,13,24	1.08	1 (7%)	12,12,25	0.88	0
2	OLC	F	341	-	7,7,24	0.25	0	6,6,25	0.48	0
2	OLC	E	346	-	9,9,24	1.22	1 (11%)	8,8,25	0.92	1 (12%)
2	OLC	C	351	-	7,7,24	0.24	0	6,6,25	0.50	0
2	OLC	A	342	-	7,7,24	0.22	0	6,6,25	0.59	0
2	OLC	A	350	-	13,13,24	1.12	1 (7%)	12,12,25	0.84	0
2	OLC	D	348	-	7,7,24	0.16	0	6,6,25	0.86	0
2	OLC	A	357	-	9,9,24	1.24	1 (11%)	8,8,25	0.86	1 (12%)
2	OLC	C	353	-	9,9,24	1.22	1 (11%)	8,8,25	0.93	1 (12%)
2	OLC	E	343	-	11,11,24	1.21	1 (9%)	10,10,25	1.01	1 (10%)
2	OLC	C	359	-	24,24,24	1.36	4 (16%)	25,25,25	1.29	3 (12%)
2	OLC	A	362	-	13,13,24	1.14	1 (7%)	12,12,25	0.94	1 (8%)
2	OLC	C	341	-	9,9,24	1.22	1 (11%)	8,8,25	0.93	1 (12%)
2	OLC	C	345	-	11,11,24	1.21	1 (9%)	10,10,25	1.04	1 (10%)
2	OLC	E	348	-	11,11,24	1.29	1 (9%)	10,10,25	1.13	1 (10%)
2	OLC	C	349	-	9,9,24	1.21	1 (11%)	8,8,25	1.06	1 (12%)
2	OLC	C	357	-	13,13,24	1.15	1 (7%)	12,12,25	0.73	0
2	OLC	F	344	-	9,9,24	1.21	1 (11%)	8,8,25	0.97	1 (12%)
2	OLC	A	363	-	11,11,24	1.29	1 (9%)	10,10,25	0.92	1 (10%)
2	OLC	A	345	-	7,7,24	0.27	0	6,6,25	0.49	0
2	OLC	C	358	-	24,24,24	1.36	4 (16%)	25,25,25	1.17	1 (4%)
2	OLC	D	349	3	24,24,24	1.31	4 (16%)	25,25,25	1.24	3 (12%)
2	OLC	A	351	-	13,13,24	1.09	1 (7%)	12,12,25	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	E	341	-	24,24,24	1.35	4 (16%)	25,25,25	1.43	3 (12%)
4	SCN	E	352	-	1,2,2	0.98	0	0,1,1	-	-
2	OLC	A	341	-	7,7,24	0.22	0	6,6,25	0.46	0
2	OLC	E	347	-	24,24,24	1.40	4 (16%)	25,25,25	1.17	2 (8%)
2	OLC	B	343	-	7,7,24	0.22	0	6,6,25	0.47	0
2	OLC	E	342	-	7,7,24	0.22	0	6,6,25	0.62	0
2	OLC	A	361	-	24,24,24	1.48	4 (16%)	25,25,25	1.37	2 (8%)
2	OLC	F	343	-	7,7,24	0.21	0	6,6,25	0.65	0
2	OLC	C	342	-	7,7,24	0.21	0	6,6,25	0.59	0
2	OLC	B	348	-	13,13,24	1.07	1 (7%)	12,12,25	0.92	1 (8%)
4	SCN	B	358	-	1,2,2	0.97	0	0,1,1	-	-
2	OLC	A	359	-	24,24,24	1.32	4 (16%)	25,25,25	1.02	2 (8%)
4	SCN	A	369	-	1,2,2	1.06	0	0,1,1	-	-
2	OLC	A	365	-	7,7,24	0.49	0	6,6,25	0.85	0
2	OLC	C	346	-	9,9,24	1.22	1 (11%)	8,8,25	1.04	1 (12%)
2	OLC	F	347	-	13,13,24	1.09	1 (7%)	12,12,25	0.86	0
2	OLC	C	356	-	7,7,24	0.27	0	6,6,25	0.41	0
2	OLC	B	344	-	9,9,24	1.24	1 (11%)	8,8,25	0.86	1 (12%)
4	SCN	E	353	-	1,2,2	1.03	0	0,1,1	-	-
2	OLC	A	343	-	7,7,24	0.22	0	6,6,25	0.58	0
2	OLC	A	347	-	7,7,24	0.23	0	6,6,25	0.52	0
2	OLC	B	353	-	7,7,24	0.36	0	6,6,25	0.46	0
2	OLC	B	345	-	24,24,24	1.38	4 (16%)	25,25,25	1.06	2 (8%)
2	OLC	B	354	-	7,7,24	0.47	0	6,6,25	0.71	0
2	OLC	B	351	-	24,24,24	1.31	4 (16%)	25,25,25	1.08	1 (4%)
2	OLC	C	361	-	11,11,24	1.23	1 (9%)	10,10,25	0.98	1 (10%)
2	OLC	C	352	-	11,11,24	1.18	1 (9%)	10,10,25	1.14	1 (10%)
2	OLC	D	341	-	4,4,24	0.27	0	3,3,25	0.35	0
2	OLC	A	356	-	24,24,24	1.37	4 (16%)	25,25,25	1.30	3 (12%)
2	OLC	C	364	-	11,11,24	1.22	1 (9%)	10,10,25	1.19	1 (10%)
2	OLC	F	346	-	7,7,24	0.22	0	6,6,25	0.66	0
4	SCN	F	352	-	1,2,2	0.89	0	0,1,1	-	-
2	OLC	C	344	-	7,7,24	0.29	0	6,6,25	0.46	0
2	OLC	A	353	-	7,7,24	0.19	0	6,6,25	0.56	0
2	OLC	F	342	-	13,13,24	1.12	1 (7%)	12,12,25	0.81	1 (8%)
2	OLC	B	352	-	15,15,24	0.99	1 (6%)	14,14,25	1.13	2 (14%)
2	OLC	A	352	-	9,9,24	1.23	1 (11%)	8,8,25	0.89	1 (12%)
4	SCN	D	354	-	1,2,2	1.11	0	0,1,1	-	-
2	OLC	D	344	-	7,7,24	0.21	0	6,6,25	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	B	341	-	4,4,24	0.21	0	3,3,25	0.46	0
2	OLC	B	350	-	24,24,24	1.37	4 (16%)	25,25,25	1.04	1 (4%)
2	OLC	E	344	-	11,11,24	1.17	1 (9%)	10,10,25	1.12	1 (10%)
2	OLC	F	345	-	11,11,24	1.18	1 (9%)	10,10,25	1.10	1 (10%)
2	OLC	A	355	-	9,9,24	1.23	1 (11%)	8,8,25	0.94	1 (12%)
2	OLC	B	346	-	24,24,24	1.38	4 (16%)	25,25,25	1.45	3 (12%)
2	OLC	C	354	-	9,9,24	1.22	1 (11%)	8,8,25	0.94	1 (12%)
2	OLC	E	345	-	13,13,24	1.11	1 (7%)	12,12,25	0.80	0
2	OLC	C	363	-	24,24,24	1.35	4 (16%)	25,25,25	1.40	2 (8%)
2	OLC	A	344	-	9,9,24	1.26	1 (11%)	8,8,25	0.90	1 (12%)
2	OLC	F	348	-	13,13,24	1.17	1 (7%)	12,12,25	0.85	0
2	OLC	B	347	-	13,13,24	1.09	1 (7%)	12,12,25	0.92	1 (8%)
2	OLC	D	347	-	7,7,24	0.32	0	6,6,25	0.52	0
2	OLC	C	343	-	7,7,24	0.21	0	6,6,25	0.54	0
2	OLC	A	354	-	7,7,24	0.24	0	6,6,25	0.54	0
2	OLC	C	360	3	24,24,24	1.41	4 (16%)	25,25,25	1.03	2 (8%)
2	OLC	A	358	-	24,24,24	1.37	4 (16%)	25,25,25	1.15	2 (8%)
2	OLC	C	355	-	9,9,24	1.21	1 (11%)	8,8,25	0.93	1 (12%)
2	OLC	A	364	-	11,11,24	1.23	1 (9%)	10,10,25	1.12	1 (10%)

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	350	-	-	3/11/11/24	-
2	OLC	D	345	-	-	1/7/7/24	-
2	OLC	B	349	-	-	0/5/5/24	-
2	OLC	A	349	-	-	11/24/24/24	-
2	OLC	A	348	-	-	5/7/7/24	-
2	OLC	A	360	-	-	2/9/9/24	-
2	OLC	C	362	-	-	15/24/24/24	-
2	OLC	C	347	-	-	2/7/7/24	-
2	OLC	D	342	-	-	11/24/24/24	-
2	OLC	A	346	-	-	7/24/24/24	-
2	OLC	D	346	-	-	4/9/9/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	348	-	-	2/9/9/24	-
2	OLC	D	343	-	-	0/5/5/24	-
2	OLC	B	342	-	-	3/11/11/24	-
2	OLC	F	341	-	-	0/5/5/24	-
2	OLC	E	346	-	-	2/7/7/24	-
2	OLC	C	351	-	-	0/5/5/24	-
2	OLC	A	342	-	-	1/5/5/24	-
2	OLC	A	350	-	-	4/11/11/24	-
2	OLC	D	348	-	-	3/5/5/24	-
2	OLC	A	357	-	-	4/7/7/24	-
2	OLC	C	353	-	-	3/7/7/24	-
2	OLC	E	343	-	-	3/9/9/24	-
2	OLC	C	359	-	-	12/24/24/24	-
2	OLC	A	362	-	-	6/11/11/24	-
2	OLC	C	341	-	-	1/7/7/24	-
2	OLC	C	345	-	-	1/9/9/24	-
2	OLC	E	348	-	-	6/9/9/24	-
2	OLC	C	349	-	-	4/7/7/24	-
2	OLC	C	357	-	-	2/11/11/24	-
2	OLC	F	344	-	-	1/7/7/24	-
2	OLC	A	363	-	-	6/9/9/24	-
2	OLC	A	345	-	-	1/5/5/24	-
2	OLC	C	358	-	-	8/24/24/24	-
2	OLC	D	349	3	-	14/24/24/24	-
2	OLC	A	351	-	-	1/11/11/24	-
2	OLC	E	341	-	-	11/24/24/24	-
2	OLC	A	341	-	-	0/5/5/24	-
2	OLC	E	347	-	-	7/24/24/24	-
2	OLC	B	343	-	-	0/5/5/24	-
2	OLC	E	342	-	-	2/5/5/24	-
2	OLC	A	361	-	-	15/24/24/24	-
2	OLC	F	343	-	-	0/5/5/24	-
2	OLC	C	342	-	-	2/5/5/24	-
2	OLC	B	348	-	-	3/11/11/24	-
2	OLC	A	359	-	-	9/24/24/24	-
2	OLC	A	365	-	-	3/5/5/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	C	346	-	-	3/7/7/24	-
2	OLC	F	347	-	-	4/11/11/24	-
2	OLC	C	356	-	-	0/5/5/24	-
2	OLC	B	344	-	-	2/7/7/24	-
2	OLC	A	343	-	-	2/5/5/24	-
2	OLC	A	347	-	-	3/5/5/24	-
2	OLC	B	353	-	-	1/5/5/24	-
2	OLC	B	345	-	-	9/24/24/24	-
2	OLC	B	354	-	-	2/5/5/24	-
2	OLC	B	351	-	-	16/24/24/24	-
2	OLC	C	361	-	-	4/9/9/24	-
2	OLC	C	352	-	-	6/9/9/24	-
2	OLC	D	341	-	-	0/2/2/24	-
2	OLC	A	356	-	-	5/24/24/24	-
2	OLC	C	364	-	-	5/9/9/24	-
2	OLC	F	346	-	-	0/5/5/24	-
2	OLC	C	344	-	-	1/5/5/24	-
2	OLC	A	353	-	-	0/5/5/24	-
2	OLC	F	342	-	-	4/11/11/24	-
2	OLC	B	352	-	-	9/13/13/24	-
2	OLC	A	352	-	-	3/7/7/24	-
2	OLC	D	344	-	-	2/5/5/24	-
2	OLC	B	341	-	-	1/2/2/24	-
2	OLC	B	350	-	-	18/24/24/24	-
2	OLC	E	344	-	-	4/9/9/24	-
2	OLC	F	345	-	-	4/9/9/24	-
2	OLC	A	355	-	-	2/7/7/24	-
2	OLC	B	346	-	-	9/24/24/24	-
2	OLC	C	354	-	-	1/7/7/24	-
2	OLC	E	345	-	-	7/11/11/24	-
2	OLC	C	363	-	-	12/24/24/24	-
2	OLC	A	344	-	-	0/7/7/24	-
2	OLC	F	348	-	-	6/11/11/24	-
2	OLC	B	347	-	-	1/11/11/24	-
2	OLC	D	347	-	-	3/5/5/24	-
2	OLC	C	343	-	-	0/5/5/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	354	-	-	4/5/5/24	-
2	OLC	C	360	3	-	16/24/24/24	-
2	OLC	A	358	-	-	16/24/24/24	-
2	OLC	C	355	-	-	1/7/7/24	-
2	OLC	A	364	-	-	6/9/9/24	-

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	OLC	O20-C1	4.90	1.47	1.33
2	C	360	OLC	O20-C1	4.67	1.47	1.33
2	E	347	OLC	O20-C1	4.57	1.46	1.33
2	D	342	OLC	O20-C1	4.51	1.46	1.33
2	B	346	OLC	O20-C1	4.46	1.46	1.33
2	A	346	OLC	O20-C1	4.41	1.46	1.33
2	A	356	OLC	O20-C1	4.39	1.46	1.33
2	B	345	OLC	O20-C1	4.37	1.46	1.33
2	C	362	OLC	O20-C1	4.27	1.45	1.33
2	C	363	OLC	O20-C1	4.23	1.45	1.33
2	A	358	OLC	O20-C1	4.23	1.45	1.33
2	B	350	OLC	O20-C1	4.20	1.45	1.33
2	A	359	OLC	O20-C1	4.12	1.45	1.33
2	A	349	OLC	O20-C1	4.12	1.45	1.33
2	C	359	OLC	O20-C1	4.10	1.45	1.33
2	E	341	OLC	O20-C1	4.09	1.45	1.33
2	C	358	OLC	O20-C1	4.09	1.45	1.33
2	A	363	OLC	C9-C10	4.06	1.54	1.31
2	E	348	OLC	C9-C10	4.02	1.54	1.31
2	F	348	OLC	C9-C10	4.00	1.54	1.31
2	C	361	OLC	C9-C10	3.97	1.54	1.31
2	C	357	OLC	C9-C10	3.93	1.54	1.31
2	B	351	OLC	O20-C1	3.92	1.44	1.33
2	C	364	OLC	C9-C10	3.90	1.53	1.31
2	A	362	OLC	C9-C10	3.88	1.53	1.31
2	D	346	OLC	C9-C10	3.87	1.53	1.31
2	A	364	OLC	C9-C10	3.86	1.53	1.31
2	F	342	OLC	C9-C10	3.85	1.53	1.31
2	E	343	OLC	C9-C10	3.84	1.53	1.31
2	A	350	OLC	C9-C10	3.83	1.53	1.31
2	E	345	OLC	C9-C10	3.82	1.53	1.31
2	C	345	OLC	C9-C10	3.80	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	347	OLC	C9-C10	3.80	1.53	1.31
2	F	347	OLC	C9-C10	3.79	1.53	1.31
2	C	348	OLC	C9-C10	3.78	1.53	1.31
2	D	349	OLC	O20-C1	3.78	1.44	1.33
2	A	360	OLC	C9-C10	3.77	1.53	1.31
2	C	350	OLC	C9-C10	3.77	1.53	1.31
2	A	351	OLC	C9-C10	3.77	1.53	1.31
2	B	342	OLC	C9-C10	3.76	1.53	1.31
2	F	345	OLC	C9-C10	3.75	1.53	1.31
2	C	352	OLC	C9-C10	3.74	1.53	1.31
2	E	344	OLC	C9-C10	3.74	1.53	1.31
2	B	348	OLC	C9-C10	3.72	1.52	1.31
2	A	344	OLC	C10-C9	3.64	1.52	1.29
2	B	352	OLC	C9-C10	3.62	1.52	1.31
2	A	357	OLC	C10-C9	3.59	1.52	1.29
2	B	344	OLC	C10-C9	3.55	1.52	1.29
2	A	348	OLC	C10-C9	3.55	1.52	1.29
2	A	355	OLC	C10-C9	3.54	1.52	1.29
2	A	352	OLC	C10-C9	3.54	1.52	1.29
2	C	349	OLC	C10-C9	3.53	1.51	1.29
2	C	354	OLC	C10-C9	3.53	1.51	1.29
2	E	346	OLC	C10-C9	3.53	1.51	1.29
2	C	346	OLC	C10-C9	3.52	1.51	1.29
2	C	347	OLC	C10-C9	3.52	1.51	1.29
2	C	355	OLC	C10-C9	3.52	1.51	1.29
2	C	353	OLC	C10-C9	3.52	1.51	1.29
2	C	341	OLC	C10-C9	3.51	1.51	1.29
2	D	345	OLC	C10-C9	3.51	1.51	1.29
2	F	344	OLC	C10-C9	3.50	1.51	1.29
2	C	358	OLC	C11-C10	-3.13	1.32	1.50
2	E	341	OLC	C11-C10	-3.10	1.33	1.50
2	B	350	OLC	C8-C9	-3.09	1.33	1.50
2	B	350	OLC	C11-C10	-3.09	1.33	1.50
2	E	341	OLC	C8-C9	-3.08	1.33	1.50
2	D	349	OLC	C9-C10	3.06	1.49	1.31
2	C	359	OLC	C11-C10	-3.04	1.33	1.50
2	A	356	OLC	C11-C10	-3.04	1.33	1.50
2	A	349	OLC	C11-C10	-3.04	1.33	1.50
2	A	346	OLC	C11-C10	-3.04	1.33	1.50
2	C	358	OLC	C8-C9	-3.02	1.33	1.50
2	E	347	OLC	C8-C9	-3.01	1.33	1.50
2	B	345	OLC	C11-C10	-3.00	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	358	OLC	C11-C10	-3.00	1.33	1.50
2	B	346	OLC	C11-C10	-3.00	1.33	1.50
2	A	358	OLC	C8-C9	-3.00	1.33	1.50
2	C	359	OLC	C8-C9	-2.97	1.33	1.50
2	B	346	OLC	C8-C9	-2.96	1.33	1.50
2	A	349	OLC	C8-C9	-2.96	1.33	1.50
2	C	363	OLC	C8-C9	-2.93	1.33	1.50
2	A	346	OLC	C8-C9	-2.93	1.34	1.50
2	B	345	OLC	C8-C9	-2.92	1.34	1.50
2	A	361	OLC	C11-C10	-2.92	1.34	1.50
2	A	356	OLC	C8-C9	-2.91	1.34	1.50
2	C	362	OLC	C11-C10	-2.90	1.34	1.50
2	D	342	OLC	C8-C9	-2.88	1.34	1.50
2	C	363	OLC	C11-C10	-2.87	1.34	1.50
2	C	362	OLC	C8-C9	-2.84	1.34	1.50
2	D	342	OLC	C11-C10	-2.83	1.34	1.50
2	E	347	OLC	C11-C10	-2.83	1.34	1.50
2	C	360	OLC	C9-C10	2.81	1.47	1.31
2	C	360	OLC	C8-C9	-2.80	1.34	1.50
2	A	361	OLC	C8-C9	-2.79	1.34	1.50
2	C	360	OLC	C11-C10	-2.78	1.34	1.50
2	A	359	OLC	C11-C10	-2.78	1.34	1.50
2	B	351	OLC	C8-C9	-2.78	1.34	1.50
2	A	361	OLC	C9-C10	2.77	1.47	1.31
2	B	351	OLC	C9-C10	2.76	1.47	1.31
2	A	359	OLC	C8-C9	-2.76	1.34	1.50
2	C	362	OLC	C9-C10	2.75	1.47	1.31
2	B	351	OLC	C11-C10	-2.68	1.35	1.50
2	D	342	OLC	C9-C10	2.66	1.46	1.31
2	A	346	OLC	C9-C10	2.65	1.46	1.31
2	A	359	OLC	C9-C10	2.62	1.46	1.31
2	C	359	OLC	C9-C10	2.60	1.46	1.31
2	D	349	OLC	C8-C9	-2.60	1.35	1.50
2	A	349	OLC	C9-C10	2.60	1.46	1.31
2	A	358	OLC	C9-C10	2.60	1.46	1.31
2	E	347	OLC	C9-C10	2.58	1.46	1.31
2	B	345	OLC	C9-C10	2.57	1.46	1.31
2	D	349	OLC	C11-C10	-2.56	1.36	1.50
2	E	341	OLC	C9-C10	2.55	1.46	1.31
2	B	350	OLC	C9-C10	2.54	1.46	1.31
2	C	363	OLC	C9-C10	2.50	1.45	1.31
2	C	358	OLC	C9-C10	2.49	1.45	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	356	OLC	C9-C10	2.48	1.45	1.31
2	B	346	OLC	C9-C10	2.47	1.45	1.31

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	OLC	O20-C1-C2	4.76	126.35	111.83
2	C	362	OLC	O20-C1-C2	4.24	124.75	111.83
2	E	341	OLC	O20-C1-C2	4.21	124.68	111.83
2	B	346	OLC	O20-C1-C2	4.13	124.42	111.83
2	C	363	OLC	O20-C1-C2	3.94	123.85	111.83
2	A	356	OLC	O20-C1-C2	3.93	123.83	111.83
2	A	358	OLC	O20-C1-C2	3.68	123.07	111.83
2	C	359	OLC	O20-C1-C2	3.66	123.00	111.83
2	D	349	OLC	O20-C1-C2	3.66	123.00	111.83
2	E	347	OLC	O20-C1-C2	3.66	122.99	111.83
2	C	362	OLC	O20-C1-O19	-3.63	114.55	123.63
2	A	361	OLC	O20-C1-O19	-3.50	114.87	123.63
2	A	346	OLC	O20-C1-C2	3.38	122.13	111.83
2	C	363	OLC	O20-C1-O19	-3.31	115.34	123.63
2	B	345	OLC	O20-C1-C2	3.27	121.80	111.83
2	D	349	OLC	O20-C1-O19	-3.18	115.67	123.63
2	A	349	OLC	O20-C1-C2	3.14	121.41	111.83
2	E	348	OLC	C11-C10-C9	-3.10	107.76	126.42
2	A	359	OLC	O20-C1-C2	3.07	121.19	111.83
2	E	341	OLC	C3-C2-C1	-3.06	102.47	113.69
2	C	360	OLC	O20-C1-C2	3.06	121.16	111.83
2	D	342	OLC	O20-C1-C2	3.04	121.11	111.83
2	C	352	OLC	C11-C10-C9	-2.93	108.80	126.42
2	B	351	OLC	O20-C1-C2	2.80	120.37	111.83
2	B	346	OLC	O20-C1-O19	-2.78	116.68	123.63
2	C	364	OLC	C11-C10-C9	-2.77	109.76	126.42
2	C	358	OLC	O20-C1-C2	2.72	120.14	111.83
2	A	364	OLC	C11-C10-C9	-2.69	110.26	126.42
2	C	359	OLC	O20-C1-O19	-2.68	116.92	123.63
2	A	356	OLC	O20-C1-O19	-2.67	116.95	123.63
2	C	345	OLC	C11-C10-C9	-2.66	110.42	126.42
2	D	346	OLC	C11-C10-C9	-2.64	110.55	126.42
2	C	348	OLC	C11-C10-C9	-2.61	110.73	126.42
2	F	345	OLC	C11-C10-C9	-2.58	110.89	126.42
2	A	349	OLC	O20-C1-O19	-2.57	117.21	123.63
2	E	341	OLC	O20-C1-O19	-2.56	117.23	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	344	OLC	C11-C10-C9	-2.44	111.73	126.42
2	A	362	OLC	C8-C9-C10	-2.36	107.15	124.83
2	C	359	OLC	C21-O20-C1	2.36	125.73	117.12
2	A	358	OLC	O20-C1-O19	-2.34	117.78	123.63
2	A	346	OLC	O20-C1-O19	-2.31	117.84	123.63
2	D	349	OLC	C12-C11-C10	2.30	125.51	112.60
2	A	360	OLC	C11-C10-C9	-2.30	112.59	126.42
2	C	349	OLC	C8-C9-C10	-2.27	110.08	126.65
2	A	359	OLC	O20-C1-O19	-2.25	118.00	123.63
2	D	345	OLC	C8-C9-C10	-2.24	110.29	126.65
2	B	347	OLC	C8-C9-C10	-2.22	108.17	124.83
2	C	346	OLC	C8-C9-C10	-2.21	110.56	126.65
2	B	350	OLC	O20-C1-C2	2.19	118.50	111.83
2	E	343	OLC	C11-C10-C9	-2.18	113.29	126.42
2	E	347	OLC	O20-C1-O19	-2.16	118.23	123.63
2	A	355	OLC	C8-C9-C10	-2.15	110.94	126.65
2	E	346	OLC	C8-C9-C10	-2.15	110.99	126.65
2	B	348	OLC	C11-C10-C9	-2.14	108.81	124.83
2	A	344	OLC	C8-C9-C10	-2.14	111.06	126.65
2	A	356	OLC	C3-C2-C1	-2.13	105.91	113.69
2	C	362	OLC	C3-C2-C1	-2.12	105.91	113.69
2	C	355	OLC	C8-C9-C10	-2.12	111.16	126.65
2	C	353	OLC	C8-C9-C10	-2.11	111.24	126.65
2	F	344	OLC	C8-C9-C10	-2.10	111.35	126.65
2	A	348	OLC	C8-C9-C10	-2.10	111.35	126.65
2	F	342	OLC	C8-C9-C10	-2.10	109.13	124.83
2	B	352	OLC	C11-C10-C9	-2.09	109.20	124.83
2	A	363	OLC	C11-C10-C9	-2.08	113.88	126.42
2	D	342	OLC	O20-C1-O19	-2.08	118.42	123.63
2	B	346	OLC	C3-C2-C1	-2.07	106.10	113.69
2	C	354	OLC	C8-C9-C10	-2.07	111.55	126.65
2	C	360	OLC	O20-C1-O19	-2.07	118.46	123.63
2	B	345	OLC	O20-C1-O19	-2.06	118.48	123.63
2	C	347	OLC	C8-C9-C10	-2.05	111.66	126.65
2	B	352	OLC	C8-C9-C10	-2.05	109.47	124.83
2	A	357	OLC	C8-C9-C10	-2.05	111.70	126.65
2	B	344	OLC	C8-C9-C10	-2.05	111.72	126.65
2	A	346	OLC	C3-C2-C1	-2.03	106.26	113.69
2	A	352	OLC	C8-C9-C10	-2.03	111.87	126.65
2	C	361	OLC	C11-C10-C9	-2.02	114.24	126.42
2	C	341	OLC	C8-C9-C10	-2.01	111.97	126.65

There are no chirality outliers.

All (393) 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	A	358	OLC	O20-C21-C22-C24
2	A	358	OLC	O20-C21-C22-O23
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	B	351	OLC	C21-C22-C24-O25
2	C	358	OLC	C2-C1-O20-C21
2	C	358	OLC	O19-C1-O20-C21
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	C	360	OLC	O20-C21-C22-C24
2	C	360	OLC	O20-C21-C22-O23
2	C	360	OLC	O19-C1-O20-C21
2	C	362	OLC	O20-C21-C22-C24
2	C	362	OLC	O20-C21-C22-O23
2	D	342	OLC	C2-C1-O20-C21
2	D	342	OLC	O19-C1-O20-C21
2	D	349	OLC	O23-C22-C24-O25
2	E	347	OLC	C2-C1-O20-C21
2	E	347	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	A	358	OLC	C2-C1-O20-C21
2	B	351	OLC	C2-C1-O20-C21
2	C	362	OLC	C2-C1-O20-C21
2	A	361	OLC	O19-C1-O20-C21
2	A	363	OLC	C11-C10-C9-C8
2	C	360	OLC	C11-C10-C9-C8
2	C	362	OLC	O19-C1-O20-C21
2	B	346	OLC	O20-C21-C22-O23
2	A	359	OLC	C11-C12-C13-C14
2	A	361	OLC	C2-C1-O20-C21
2	A	361	OLC	C11-C10-C9-C8
2	B	351	OLC	C11-C10-C9-C8
2	B	352	OLC	C11-C10-C9-C8
2	C	361	OLC	C11-C10-C9-C8
2	A	349	OLC	C2-C1-O20-C21
2	E	341	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
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	F	344	OLC	C7-C8-C9-C10
2	C	358	OLC	C1-C2-C3-C4
2	D	349	OLC	C1-C2-C3-C4
2	E	347	OLC	C1-C2-C3-C4
2	B	350	OLC	C11-C10-C9-C8
2	A	359	OLC	C1-C2-C3-C4
2	A	343	OLC	C1-C2-C3-C4
2	C	358	OLC	C11-C10-C9-C8
2	B	350	OLC	C21-C22-C24-O25
2	C	359	OLC	C21-C22-C24-O25
2	D	342	OLC	C21-C22-C24-O25
2	D	349	OLC	C21-C22-C24-O25
2	C	363	OLC	C5-C6-C7-C8
2	A	361	OLC	C5-C6-C7-C8
2	A	359	OLC	C11-C10-C9-C8
2	C	364	OLC	C11-C10-C9-C8
2	F	345	OLC	C11-C10-C9-C8
2	A	364	OLC	C5-C6-C7-C8
2	B	350	OLC	O23-C22-C24-O25
2	B	351	OLC	O23-C22-C24-O25
2	A	358	OLC	C1-C2-C3-C4
2	E	347	OLC	C6-C7-C8-C9
2	B	351	OLC	C14-C15-C16-C17
2	C	363	OLC	C2-C3-C4-C5
2	A	358	OLC	C2-C3-C4-C5
2	C	349	OLC	C4-C5-C6-C7
2	C	363	OLC	C3-C4-C5-C6
2	C	364	OLC	C2-C3-C4-C5
2	D	347	OLC	C4-C5-C6-C7
2	A	349	OLC	C11-C12-C13-C14
2	A	364	OLC	C2-C3-C4-C5
2	A	361	OLC	C14-C15-C16-C17
2	B	352	OLC	C4-C5-C6-C7
2	B	352	OLC	C12-C13-C14-C15
2	A	356	OLC	C11-C12-C13-C14
2	A	356	OLC	C2-C3-C4-C5
2	C	352	OLC	C4-C5-C6-C7
2	A	349	OLC	C1-C2-C3-C4
2	A	362	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	D	348	OLC	C3-C4-C5-C6
2	A	358	OLC	C6-C7-C8-C9
2	C	360	OLC	C6-C7-C8-C9
2	C	359	OLC	C11-C10-C9-C8
2	C	362	OLC	C3-C4-C5-C6
2	C	363	OLC	C1-C2-C3-C4
2	D	349	OLC	C2-C1-O20-C21
2	C	359	OLC	O20-C21-C22-C24
2	D	349	OLC	C2-C3-C4-C5
2	A	361	OLC	C2-C3-C4-C5
2	B	352	OLC	C2-C3-C4-C5
2	C	357	OLC	C4-C5-C6-C7
2	C	349	OLC	C3-C4-C5-C6
2	C	362	OLC	C2-C3-C4-C5
2	D	342	OLC	C5-C6-C7-C8
2	E	348	OLC	C4-C5-C6-C7
2	A	364	OLC	C9-C10-C11-C12
2	E	343	OLC	C9-C10-C11-C12
2	E	344	OLC	C9-C10-C11-C12
2	A	347	OLC	C2-C3-C4-C5
2	A	363	OLC	C2-C3-C4-C5
2	C	361	OLC	C4-C5-C6-C7
2	E	348	OLC	C2-C3-C4-C5
2	B	352	OLC	C1-C2-C3-C4
2	A	346	OLC	C14-C15-C16-C17
2	A	358	OLC	C4-C5-C6-C7
2	A	363	OLC	C5-C6-C7-C8
2	E	345	OLC	C2-C3-C4-C5
2	C	350	OLC	C6-C7-C8-C9
2	C	363	OLC	C10-C11-C12-C13
2	A	361	OLC	C12-C13-C14-C15
2	A	346	OLC	C3-C4-C5-C6
2	A	357	OLC	C3-C4-C5-C6
2	A	346	OLC	C1-C2-C3-C4
2	B	351	OLC	C4-C5-C6-C7
2	C	362	OLC	C14-C15-C16-C17
2	C	342	OLC	C2-C3-C4-C5
2	A	361	OLC	C10-C11-C12-C13
2	B	351	OLC	C10-C11-C12-C13
2	C	352	OLC	C6-C7-C8-C9
2	C	360	OLC	C10-C11-C12-C13
2	A	348	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	C	363	OLC	C4-C5-C6-C7
2	A	351	OLC	C9-C10-C11-C12
2	A	361	OLC	C3-C4-C5-C6
2	C	361	OLC	C5-C6-C7-C8
2	D	348	OLC	C2-C3-C4-C5
2	B	348	OLC	C4-C5-C6-C7
2	D	342	OLC	C2-C3-C4-C5
2	A	361	OLC	C4-C5-C6-C7
2	C	363	OLC	C11-C12-C13-C14
2	F	348	OLC	C10-C11-C12-C13
2	D	349	OLC	O19-C1-O20-C21
2	B	351	OLC	C5-C6-C7-C8
2	B	345	OLC	C2-C1-O20-C21
2	D	346	OLC	C11-C10-C9-C8
2	B	350	OLC	C6-C7-C8-C9
2	B	351	OLC	C6-C7-C8-C9
2	B	352	OLC	C10-C11-C12-C13
2	A	342	OLC	C5-C6-C7-C8
2	A	354	OLC	C4-C5-C6-C7
2	C	362	OLC	C11-C12-C13-C14
2	C	360	OLC	C5-C6-C7-C8
2	A	357	OLC	C6-C7-C8-C9
2	F	342	OLC	C6-C7-C8-C9
2	E	344	OLC	C3-C4-C5-C6
2	F	345	OLC	C2-C3-C4-C5
2	A	364	OLC	C4-C5-C6-C7
2	B	345	OLC	C11-C12-C13-C14
2	E	341	OLC	C13-C14-C15-C16
2	C	360	OLC	C14-C15-C16-C17
2	A	357	OLC	C4-C5-C6-C7
2	A	354	OLC	C1-C2-C3-C4
2	B	351	OLC	C11-C12-C13-C14
2	C	362	OLC	C12-C13-C14-C15
2	C	360	OLC	C11-C12-C13-C14
2	A	358	OLC	C14-C15-C16-C17
2	A	347	OLC	C5-C6-C7-C8
2	E	345	OLC	C1-C2-C3-C4
2	E	345	OLC	C10-C11-C12-C13
2	E	348	OLC	C1-C2-C3-C4
2	C	352	OLC	C3-C4-C5-C6
2	B	351	OLC	C15-C16-C17-C18
2	A	360	OLC	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
2	A	359	OLC	O23-C22-C24-O25
2	A	365	OLC	C5-C6-C7-C8
2	D	342	OLC	C13-C14-C15-C16
2	B	345	OLC	C4-C5-C6-C7
2	A	350	OLC	C11-C12-C13-C14
2	A	365	OLC	C1-C2-C3-C4
2	F	348	OLC	C11-C12-C13-C14
2	B	345	OLC	O19-C1-O20-C21
2	B	345	OLC	C15-C16-C17-C18
2	B	350	OLC	C5-C6-C7-C8
2	A	354	OLC	C3-C4-C5-C6
2	E	345	OLC	C11-C12-C13-C14
2	C	359	OLC	C14-C15-C16-C17
2	A	348	OLC	C4-C5-C6-C7
2	B	351	OLC	C3-C4-C5-C6
2	B	351	OLC	C2-C3-C4-C5
2	F	342	OLC	C5-C6-C7-C8
2	E	341	OLC	C2-C3-C4-C5
2	A	359	OLC	C2-C3-C4-C5
2	D	349	OLC	C11-C12-C13-C14
2	C	350	OLC	C4-C5-C6-C7
2	E	346	OLC	C3-C4-C5-C6
2	B	352	OLC	C13-C14-C15-C16
2	C	360	OLC	C15-C16-C17-C18
2	B	345	OLC	C12-C13-C14-C15
2	C	357	OLC	C7-C8-C9-C10
2	B	350	OLC	C1-C2-C3-C4
2	B	350	OLC	O20-C21-C22-C24
2	C	347	OLC	C7-C8-C9-C10
2	B	346	OLC	C6-C7-C8-C9
2	A	363	OLC	C9-C10-C11-C12
2	C	364	OLC	C9-C10-C11-C12
2	D	346	OLC	C9-C10-C11-C12
2	C	359	OLC	O23-C22-C24-O25
2	A	365	OLC	C3-C4-C5-C6
2	A	361	OLC	C15-C16-C17-C18
2	C	360	OLC	C12-C13-C14-C15
2	A	363	OLC	C1-C2-C3-C4
2	E	341	OLC	C4-C5-C6-C7
2	A	362	OLC	C11-C12-C13-C14
2	F	348	OLC	C1-C2-C3-C4
2	B	345	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	C	362	OLC	C10-C11-C12-C13
2	B	346	OLC	C11-C12-C13-C14
2	C	352	OLC	C2-C3-C4-C5
2	C	344	OLC	C5-C6-C7-C8
2	D	347	OLC	C5-C6-C7-C8
2	B	352	OLC	C11-C12-C13-C14
2	E	348	OLC	C3-C4-C5-C6
2	A	362	OLC	C5-C6-C7-C8
2	A	361	OLC	C1-C2-C3-C4
2	A	356	OLC	C4-C5-C6-C7
2	D	346	OLC	C3-C4-C5-C6
2	A	359	OLC	C6-C7-C8-C9
2	C	359	OLC	C6-C7-C8-C9
2	C	349	OLC	C7-C8-C9-C10
2	C	353	OLC	C3-C4-C5-C6
2	A	349	OLC	C5-C6-C7-C8
2	A	346	OLC	C15-C16-C17-C18
2	B	353	OLC	C4-C5-C6-C7
2	C	358	OLC	C5-C6-C7-C8
2	C	364	OLC	C3-C4-C5-C6
2	D	349	OLC	C13-C14-C15-C16
2	A	346	OLC	C10-C11-C12-C13
2	C	364	OLC	C6-C7-C8-C9
2	C	363	OLC	C12-C13-C14-C15
2	A	356	OLC	C9-C10-C11-C12
2	A	358	OLC	C7-C8-C9-C10
2	B	350	OLC	C7-C8-C9-C10
2	C	360	OLC	C7-C8-C9-C10
2	C	362	OLC	C9-C10-C11-C12
2	D	342	OLC	C9-C10-C11-C12
2	C	360	OLC	C3-C4-C5-C6
2	E	341	OLC	C15-C16-C17-C18
2	F	348	OLC	C6-C7-C8-C9
2	D	342	OLC	C1-C2-C3-C4
2	F	347	OLC	C11-C12-C13-C14
2	A	352	OLC	C7-C8-C9-C10
2	B	344	OLC	C7-C8-C9-C10
2	C	354	OLC	C7-C8-C9-C10
2	A	346	OLC	C9-C10-C11-C12
2	A	349	OLC	C9-C10-C11-C12
2	A	358	OLC	C9-C10-C11-C12
2	A	359	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	361	OLC	C7-C8-C9-C10
2	B	342	OLC	C7-C8-C9-C10
2	B	345	OLC	C9-C10-C11-C12
2	B	350	OLC	C9-C10-C11-C12
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	E	341	OLC	C9-C10-C11-C12
2	E	347	OLC	C7-C8-C9-C10
2	B	354	OLC	C1-C2-C3-C4
2	A	358	OLC	C15-C16-C17-C18
2	B	346	OLC	C9-C10-C11-C12
2	B	351	OLC	C7-C8-C9-C10
2	C	350	OLC	C9-C10-C11-C12
2	C	362	OLC	C7-C8-C9-C10
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	361	OLC	C9-C10-C11-C12
2	B	346	OLC	C21-C22-C24-O25
2	A	364	OLC	C3-C4-C5-C6
2	D	349	OLC	C9-C10-C11-C12
2	D	349	OLC	C7-C8-C9-C10
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	348	OLC	C9-C10-C11-C12
2	C	352	OLC	C9-C10-C11-C12
2	E	348	OLC	C9-C10-C11-C12
2	F	345	OLC	C9-C10-C11-C12
2	A	350	OLC	C5-C6-C7-C8
2	B	354	OLC	C2-C3-C4-C5
2	E	342	OLC	C1-C2-C3-C4
2	C	347	OLC	C5-C6-C7-C8
2	C	358	OLC	C15-C16-C17-C18
2	D	344	OLC	C5-C6-C7-C8
2	A	362	OLC	C10-C11-C12-C13
2	E	348	OLC	C7-C8-C9-C10
2	E	343	OLC	C1-C2-C3-C4
2	B	350	OLC	C2-C3-C4-C5

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

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Mol	Chain	Res	Type	Atoms
2	C	360	OLC	C13-C14-C15-C16
2	A	360	OLC	C7-C8-C9-C10
2	E	344	OLC	C4-C5-C6-C7
2	C	363	OLC	C14-C15-C16-C17
2	F	342	OLC	C4-C5-C6-C7
2	B	346	OLC	O19-C1-O20-C21
2	B	350	OLC	O20-C21-C22-O23
2	C	362	OLC	C13-C14-C15-C16
2	A	349	OLC	O20-C1-C2-C3
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	C	362	OLC	C6-C7-C8-C9
2	C	342	OLC	C3-C4-C5-C6
2	A	350	OLC	C9-C10-C11-C12
2	A	364	OLC	C7-C8-C9-C10
2	C	345	OLC	C7-C8-C9-C10
2	A	362	OLC	C9-C10-C11-C12
2	B	347	OLC	C9-C10-C11-C12
2	F	347	OLC	C9-C10-C11-C12
2	E	342	OLC	C5-C6-C7-C8
2	D	349	OLC	C4-C5-C6-C7
2	A	362	OLC	C7-C8-C9-C10
2	C	360	OLC	C4-C5-C6-C7
2	A	358	OLC	O20-C1-C2-C3
2	E	347	OLC	C2-C3-C4-C5
2	A	352	OLC	C4-C5-C6-C7
2	E	347	OLC	C11-C12-C13-C14
2	C	353	OLC	C7-C8-C9-C10
2	E	345	OLC	C4-C5-C6-C7
2	A	359	OLC	C12-C13-C14-C15
2	C	361	OLC	C9-C10-C11-C12
2	F	348	OLC	C4-C5-C6-C7
2	A	354	OLC	C2-C3-C4-C5
2	A	358	OLC	O19-C1-C2-C3
2	F	347	OLC	C7-C8-C9-C10
2	B	346	OLC	C2-C1-O20-C21
2	A	352	OLC	C2-C3-C4-C5
2	B	350	OLC	O20-C1-C2-C3
2	A	345	OLC	C5-C6-C7-C8
2	A	346	OLC	C7-C8-C9-C10
2	A	349	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	359	OLC	C9-C10-C11-C12
2	B	345	OLC	C7-C8-C9-C10
2	D	342	OLC	C7-C8-C9-C10
2	E	341	OLC	C7-C8-C9-C10
2	B	341	OLC	C2-C3-C4-C5
2	E	343	OLC	C2-C3-C4-C5
2	A	349	OLC	O19-C1-C2-C3
2	A	356	OLC	C7-C8-C9-C10
2	E	345	OLC	C7-C8-C9-C10
2	B	350	OLC	C11-C12-C13-C14
2	B	350	OLC	O19-C1-C2-C3
2	B	351	OLC	C9-C10-C11-C12
2	C	348	OLC	C7-C8-C9-C10
2	C	359	OLC	C9-C10-C11-C12
2	C	359	OLC	C7-C8-C9-C10

There are no ring outliers.

44 monomers are involved in 83 short contacts:

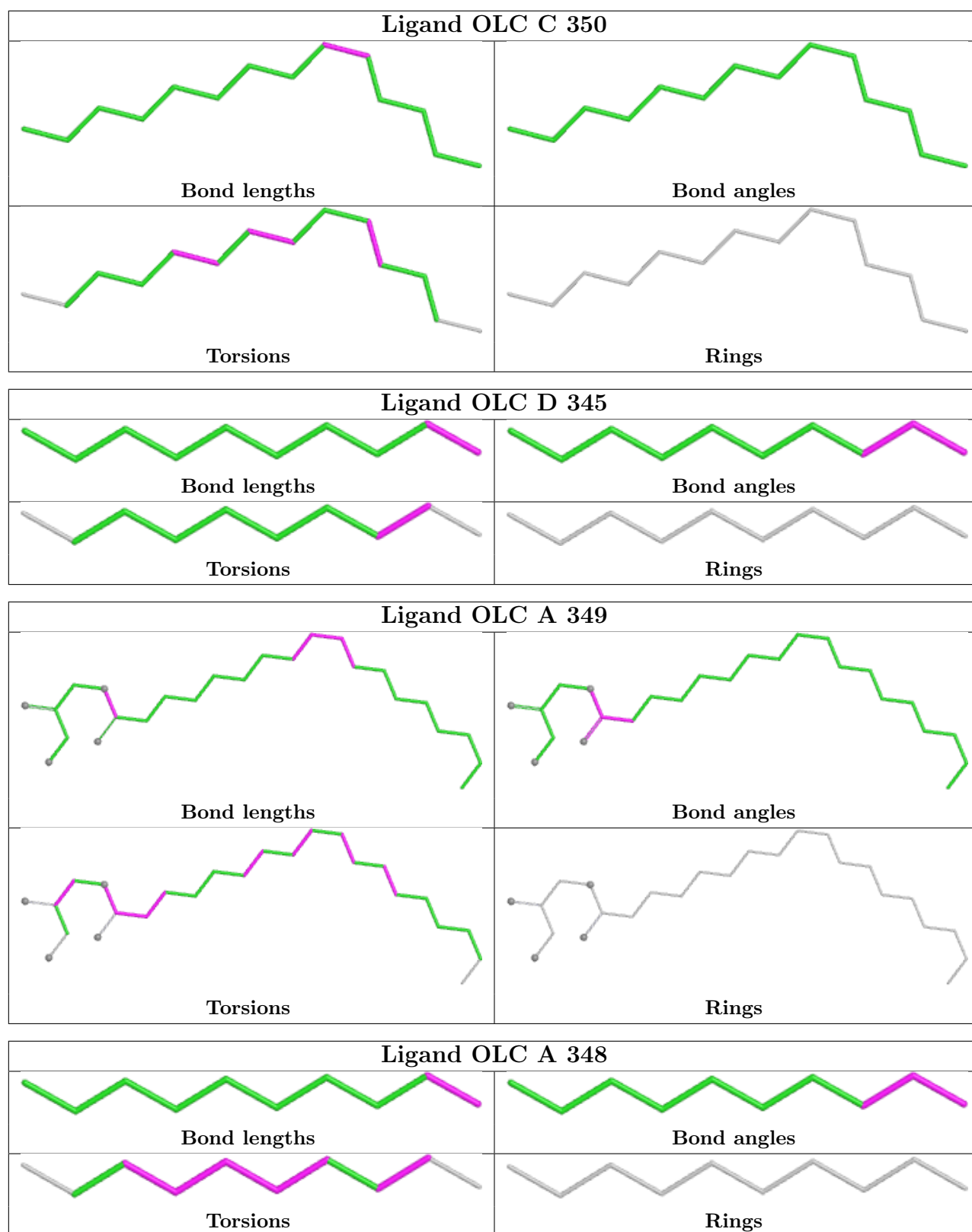
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	345	OLC	1	0
2	A	349	OLC	3	0
2	A	360	OLC	4	0
2	C	362	OLC	2	0
2	C	347	OLC	2	0
2	D	342	OLC	5	0
2	D	346	OLC	1	0
2	C	348	OLC	2	0
2	F	341	OLC	1	0
2	E	346	OLC	2	0
2	D	348	OLC	1	0
2	C	353	OLC	1	0
2	E	343	OLC	1	0
2	C	359	OLC	4	0
2	A	362	OLC	1	0
2	E	348	OLC	6	0
2	C	349	OLC	3	0
2	F	344	OLC	1	0
2	A	345	OLC	1	0
2	C	358	OLC	2	0
2	D	349	OLC	1	0
2	E	341	OLC	1	0

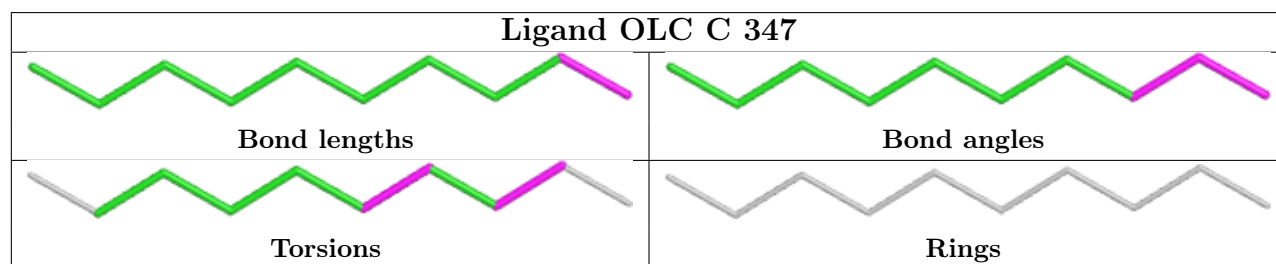
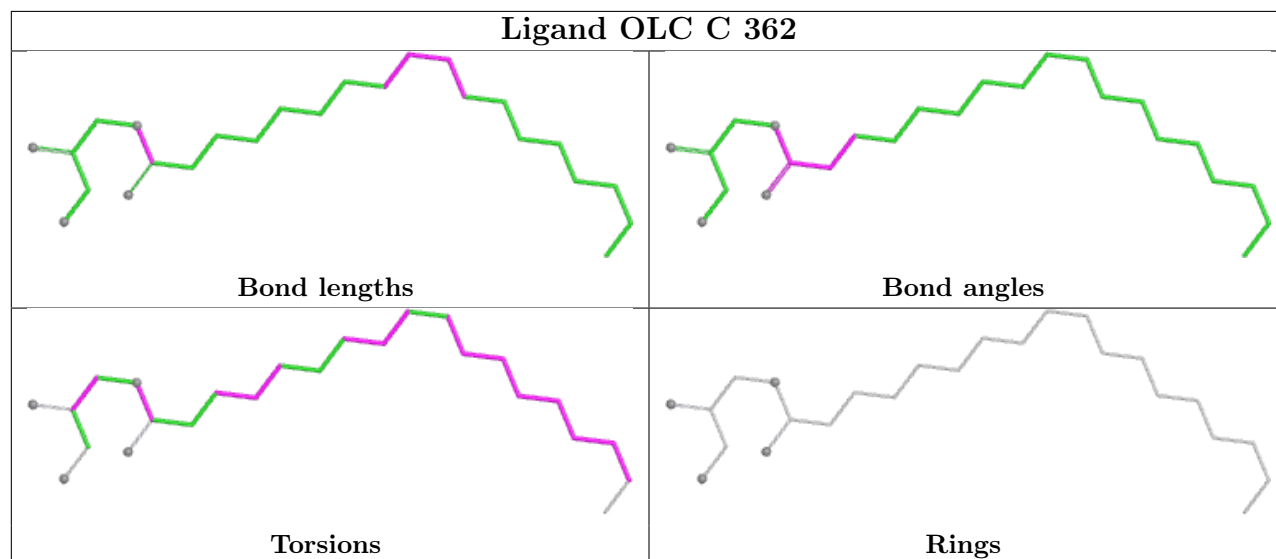
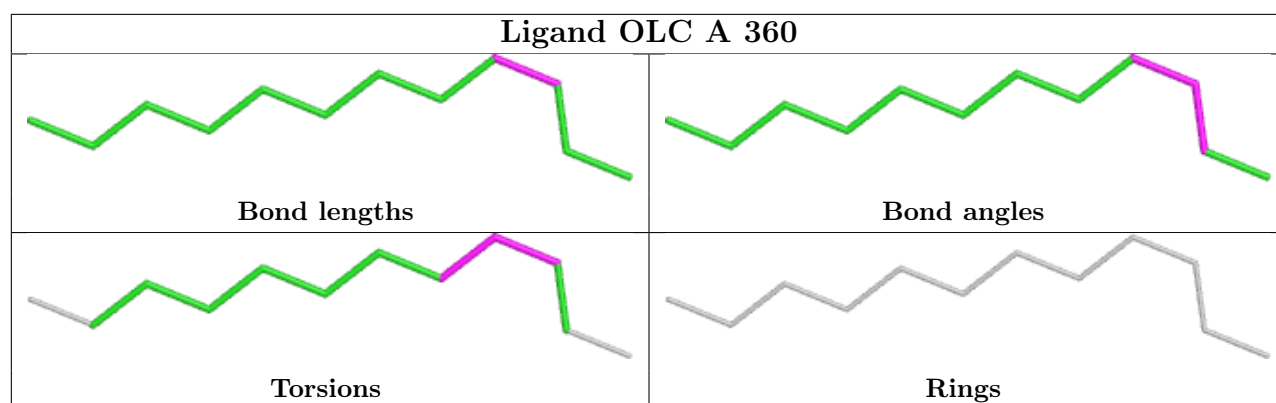
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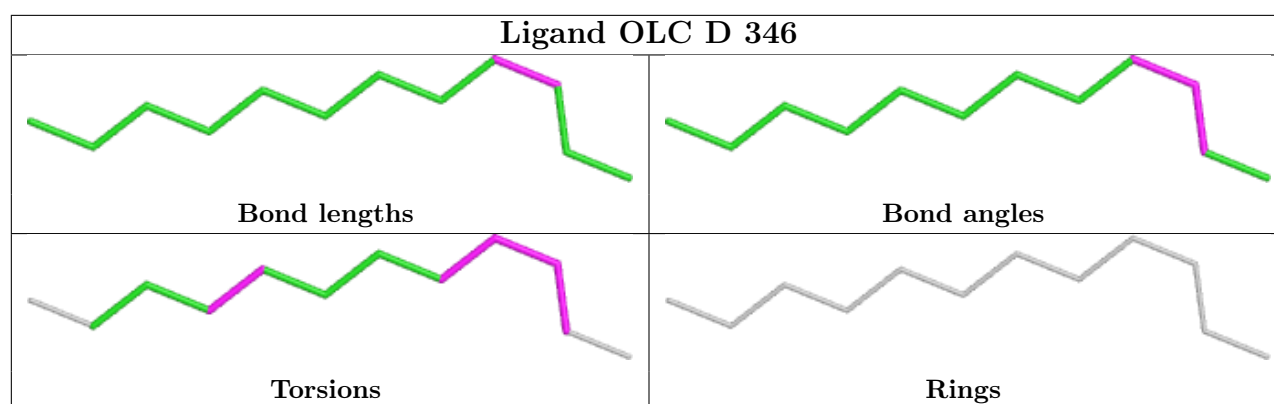
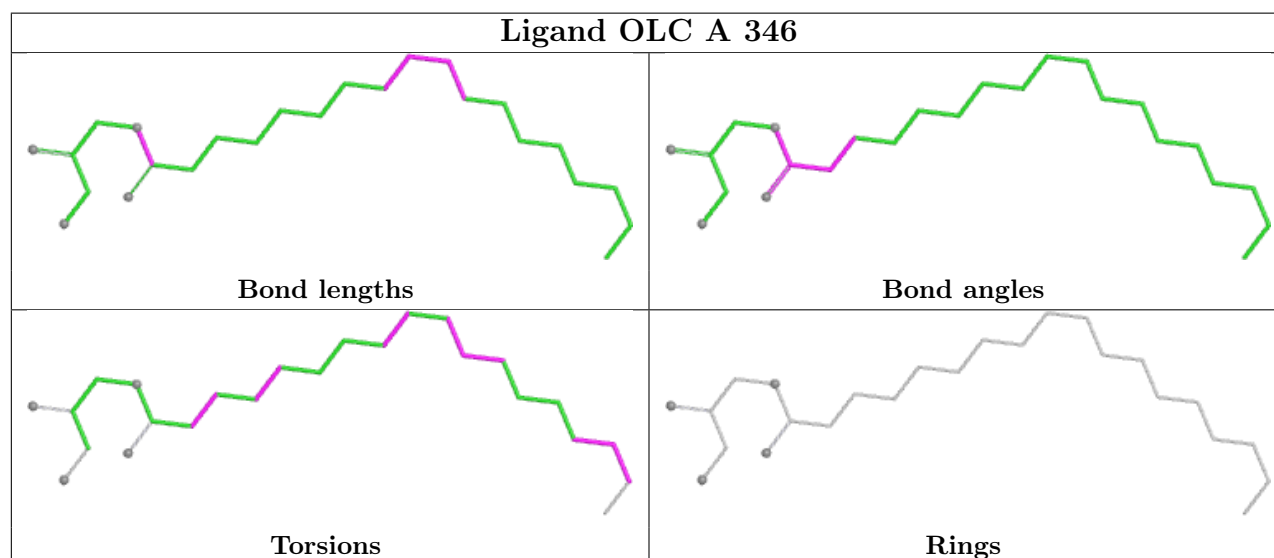
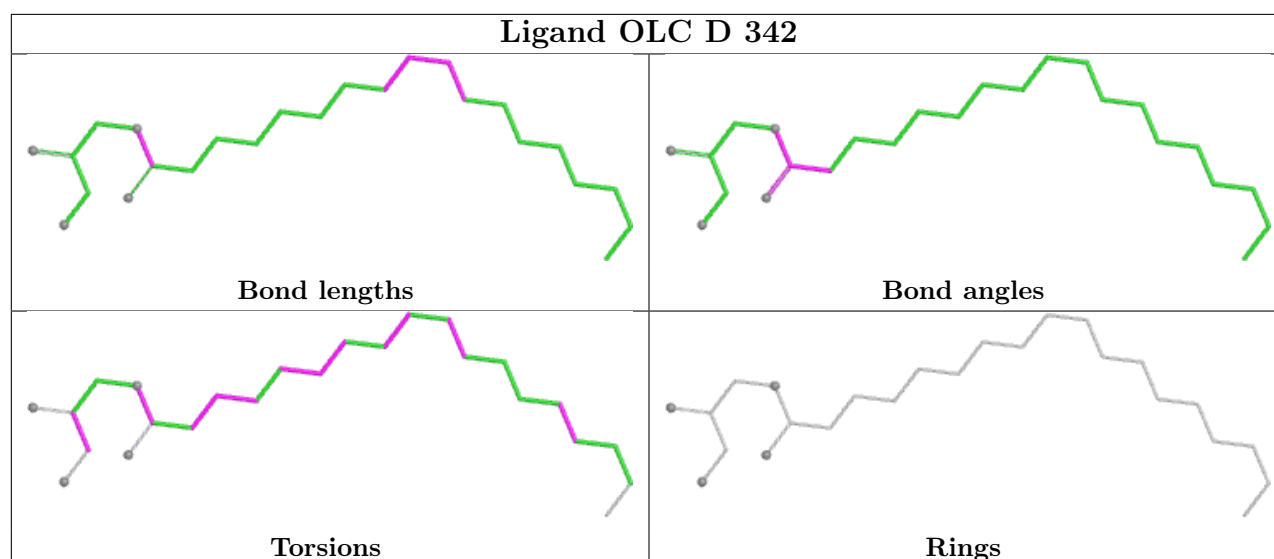
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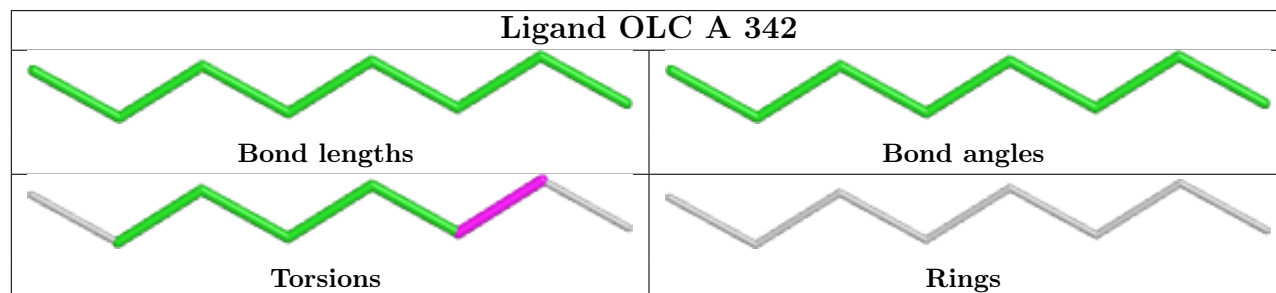
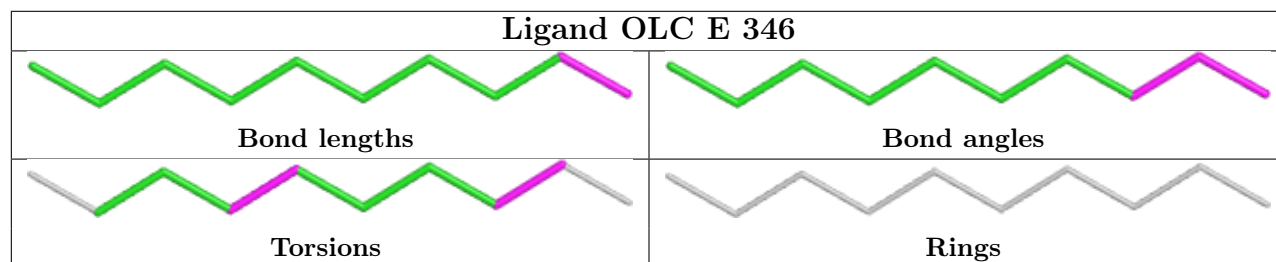
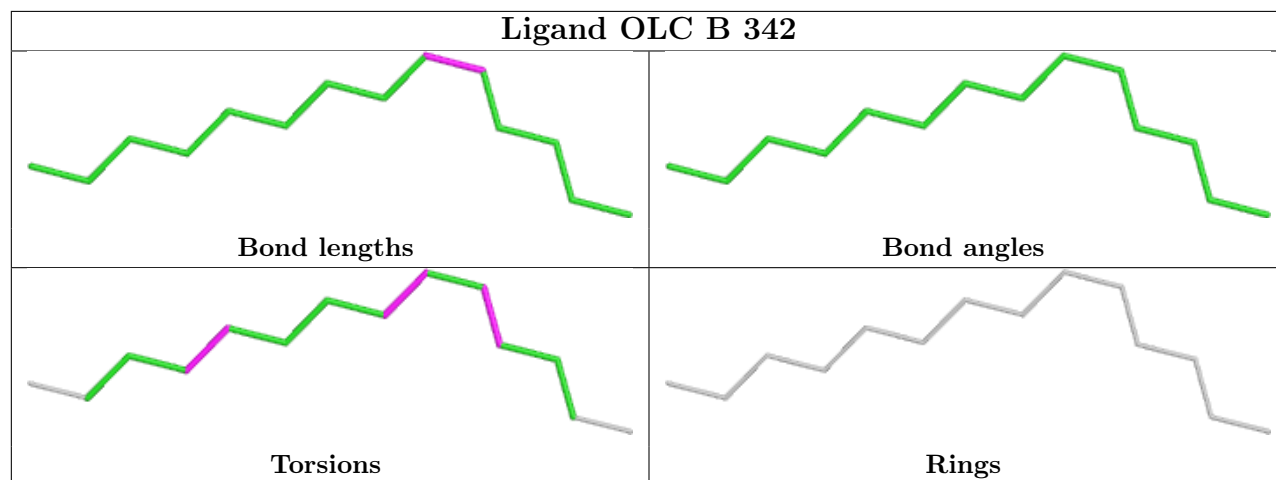
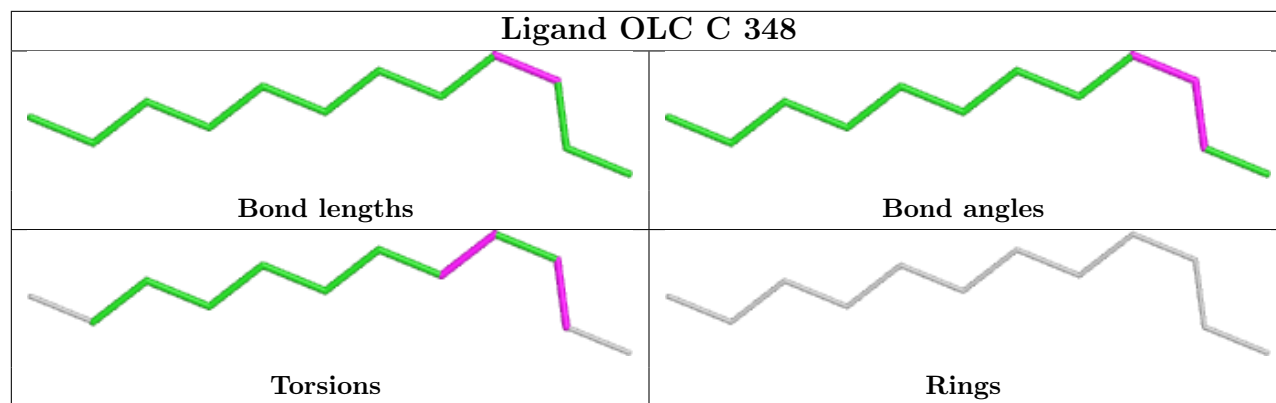
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	341	OLC	2	0
2	E	347	OLC	11	0
2	E	342	OLC	1	0
2	A	361	OLC	8	0
2	F	343	OLC	1	0
2	A	359	OLC	3	0
2	A	365	OLC	5	0
2	F	347	OLC	3	0
2	B	344	OLC	1	0
2	A	343	OLC	1	0
2	B	345	OLC	2	0
2	B	351	OLC	2	0
2	C	352	OLC	3	0
2	A	356	OLC	2	0
2	A	353	OLC	1	0
2	F	342	OLC	3	0
2	B	350	OLC	1	0
2	E	344	OLC	3	0
2	F	345	OLC	1	0
2	C	363	OLC	4	0
2	A	344	OLC	1	0
2	C	360	OLC	2	0

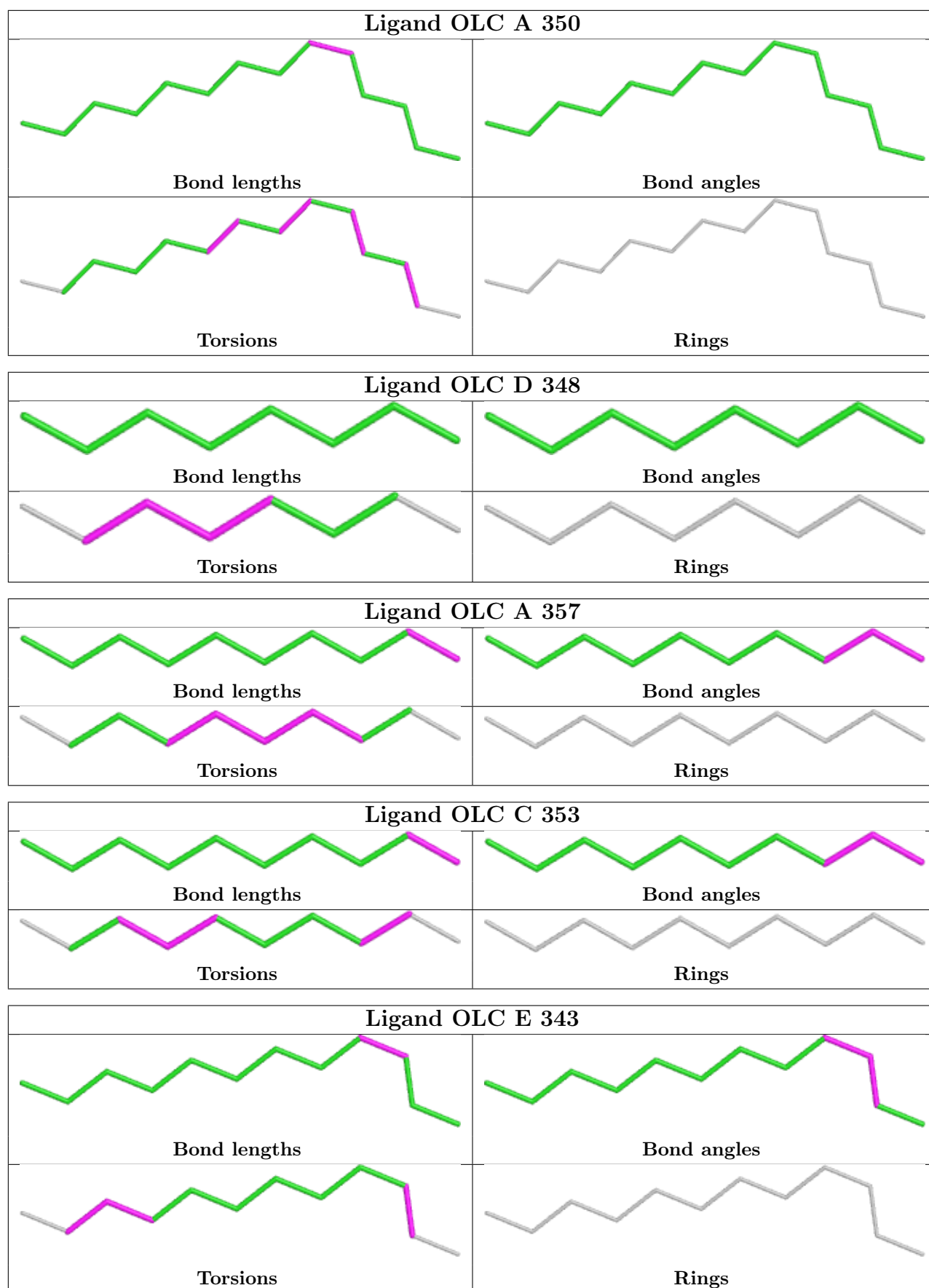
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

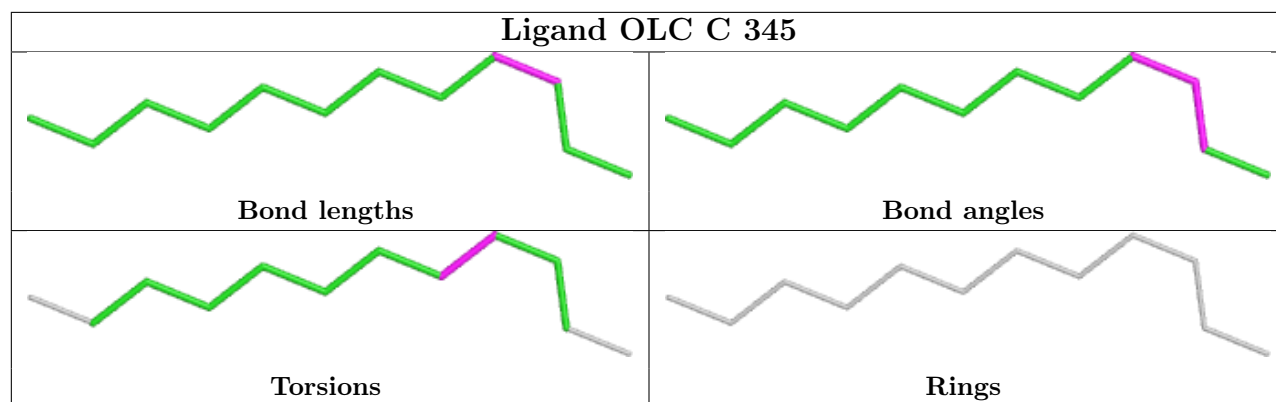
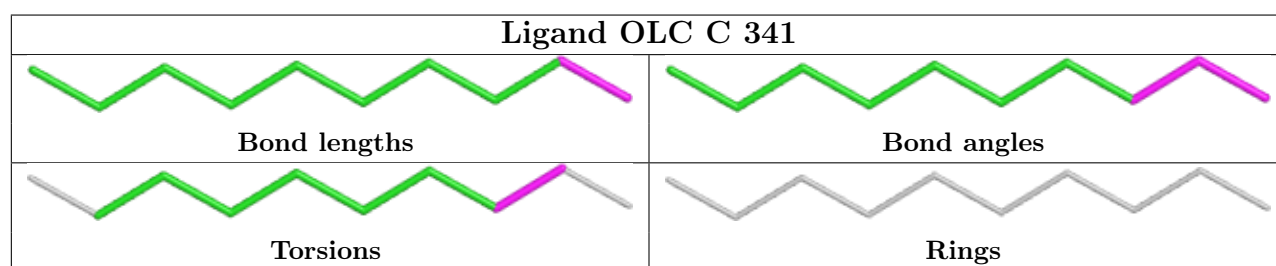
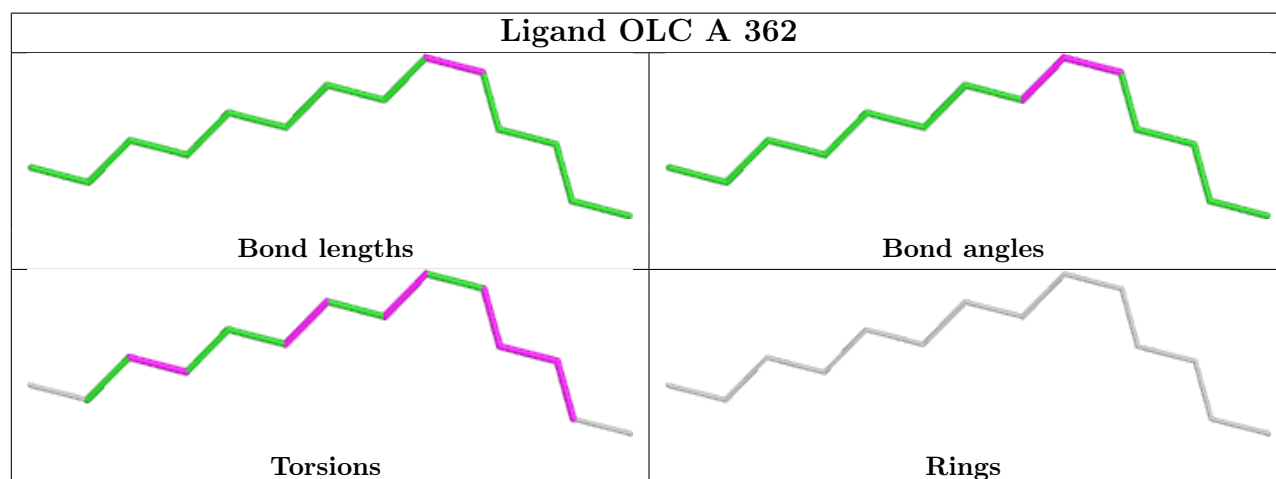
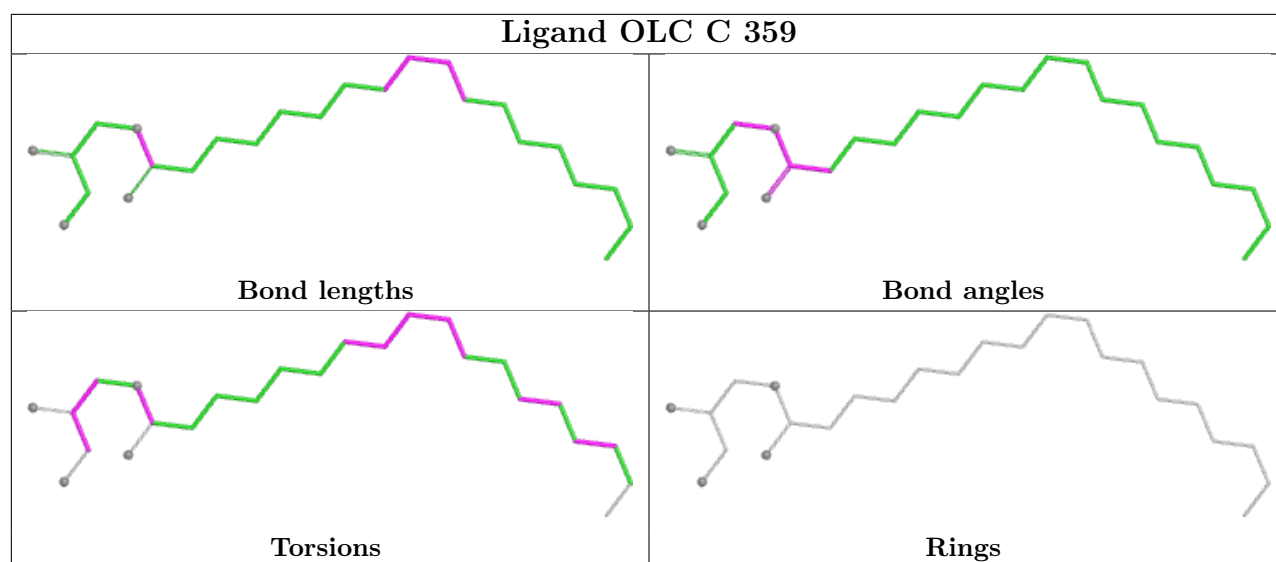


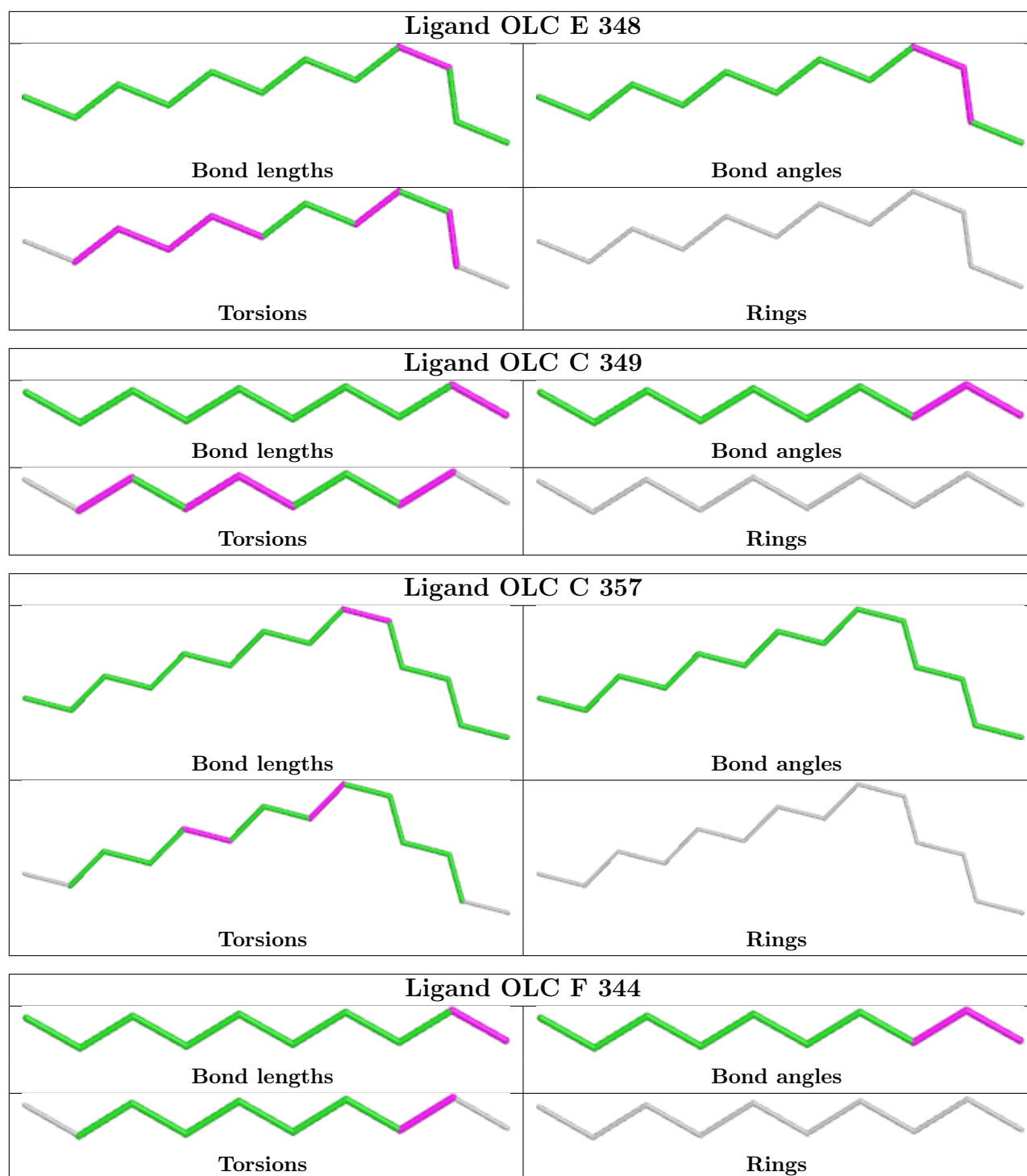


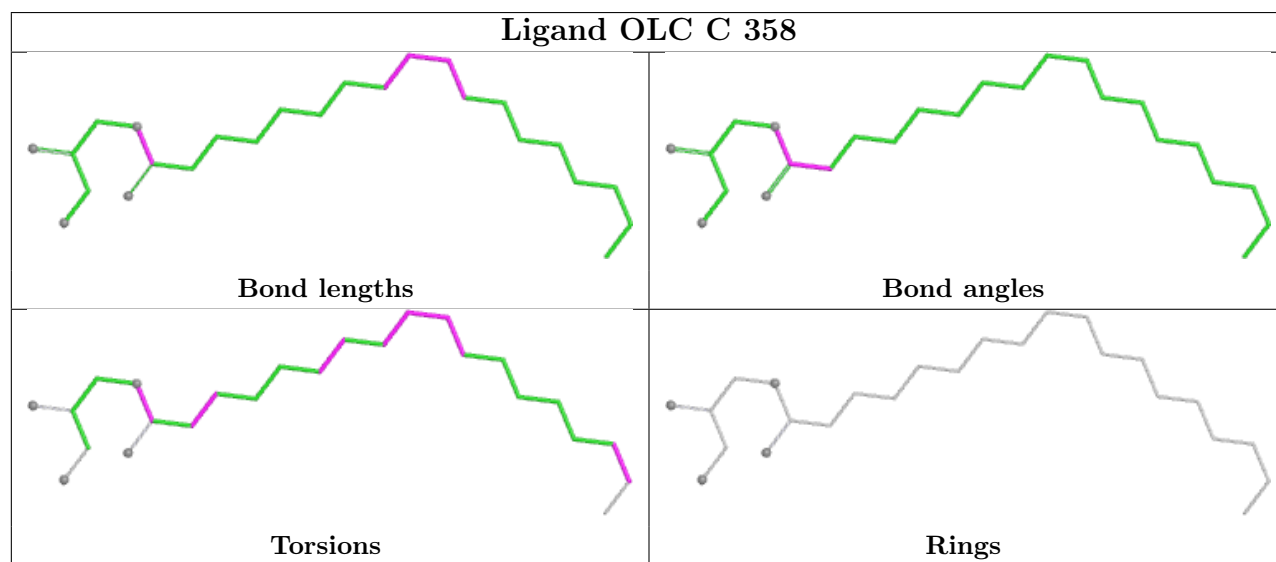
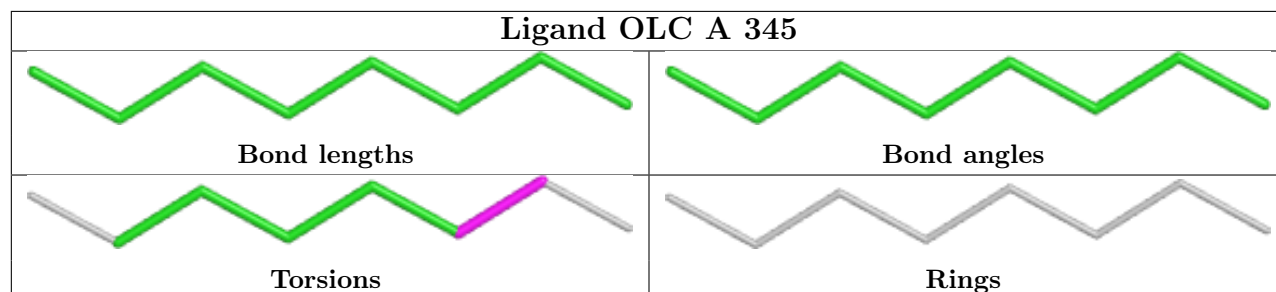
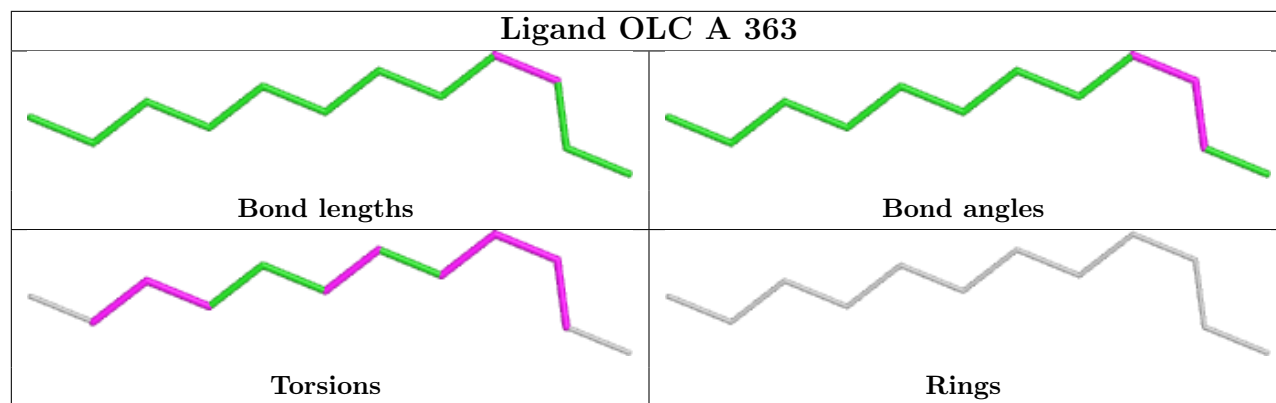


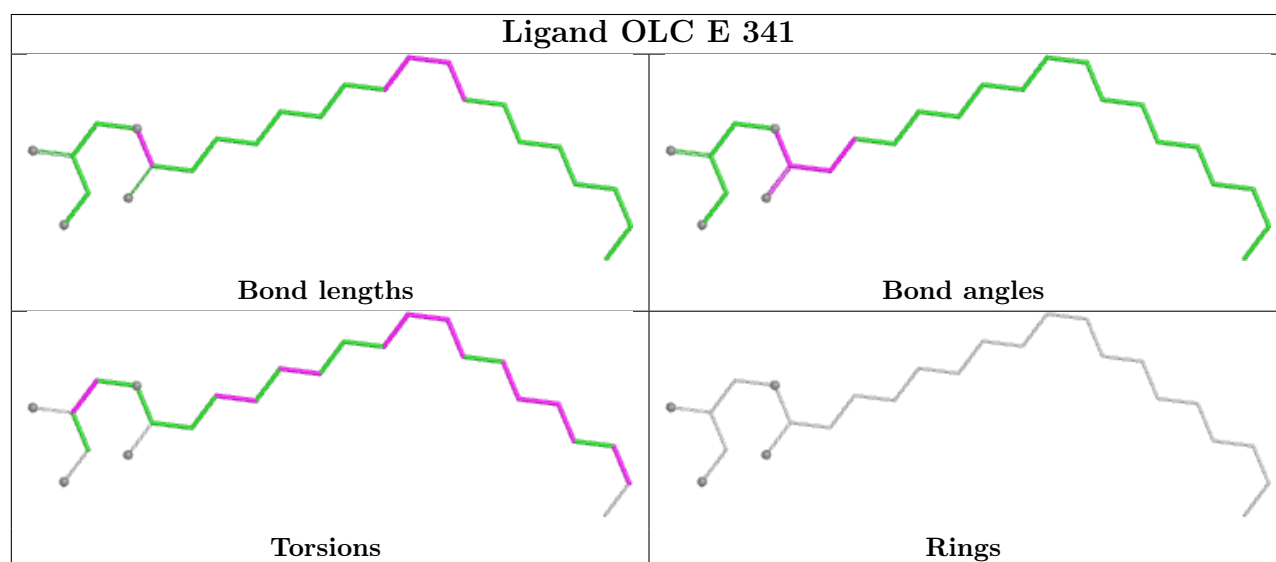
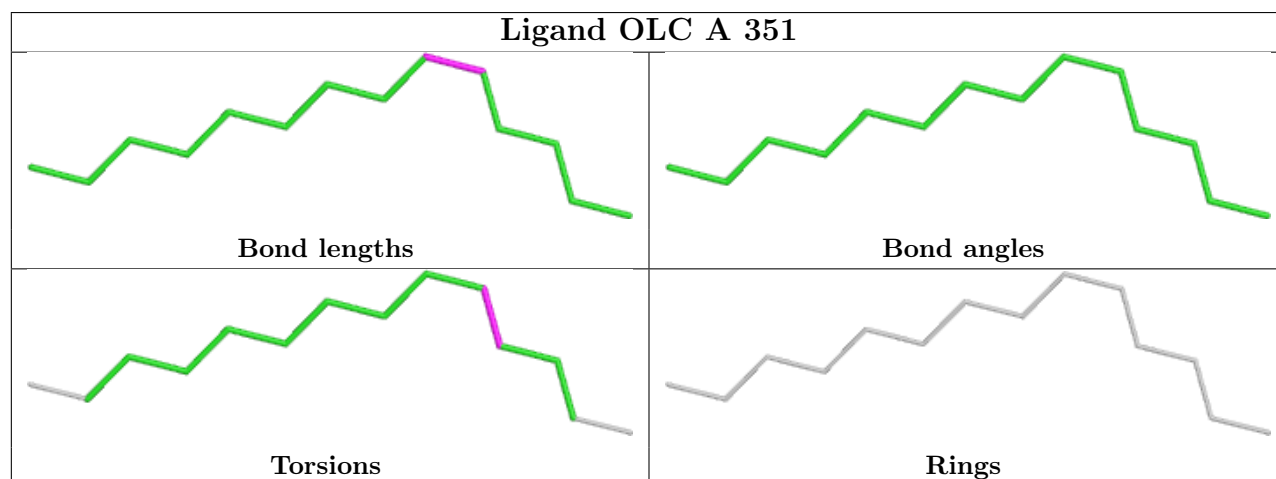
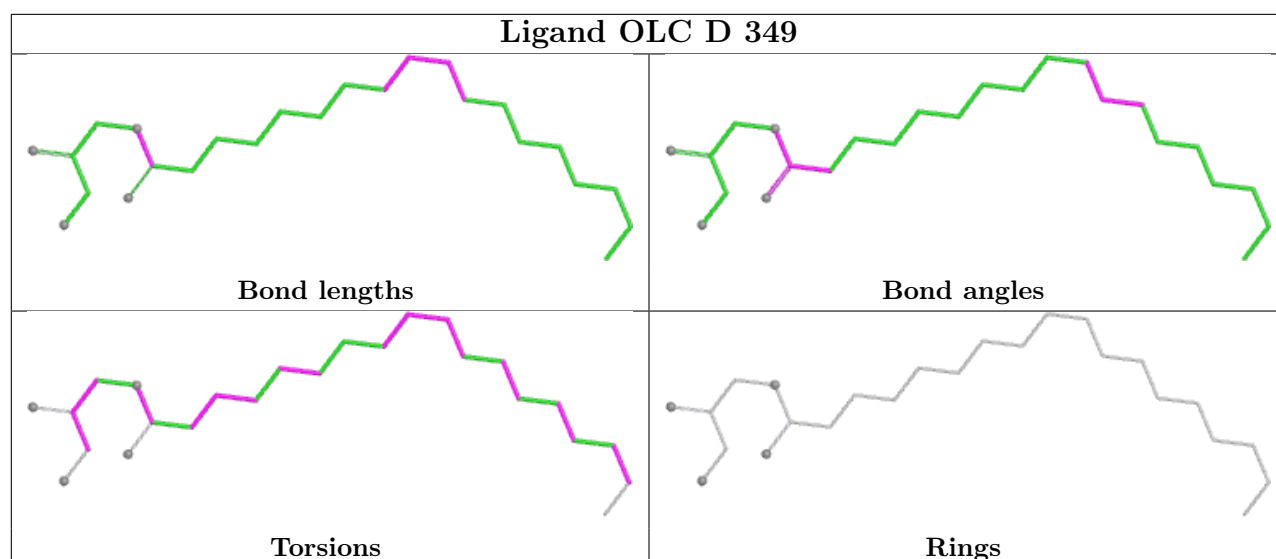


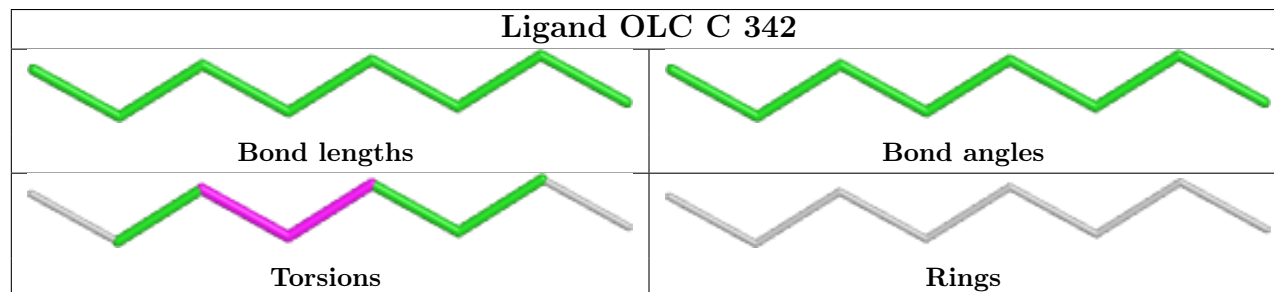
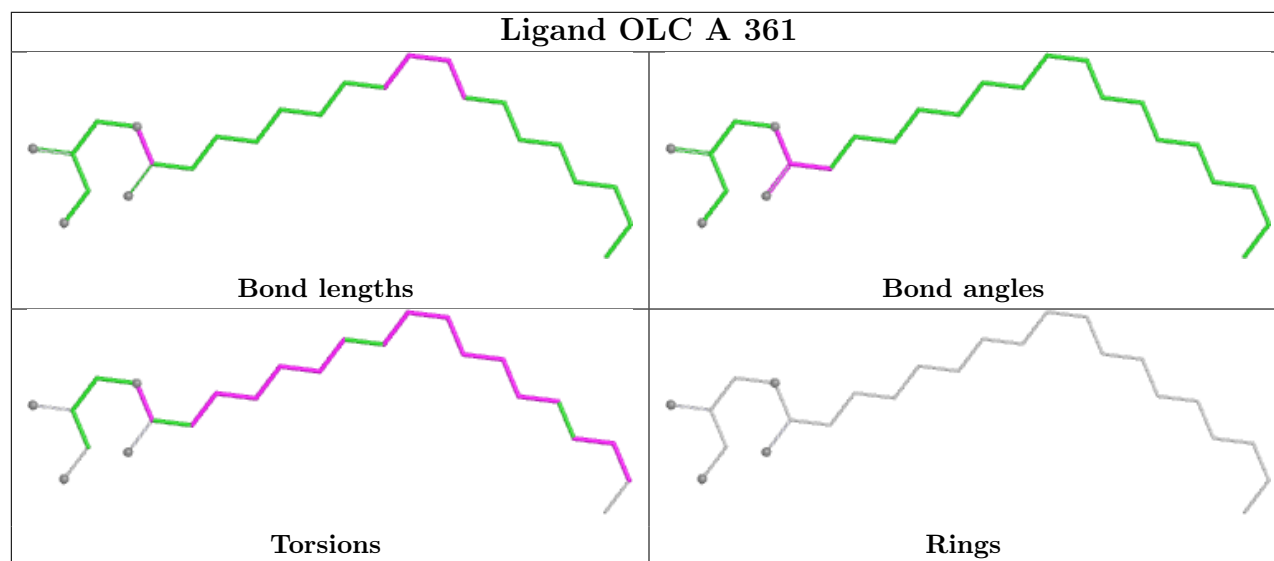
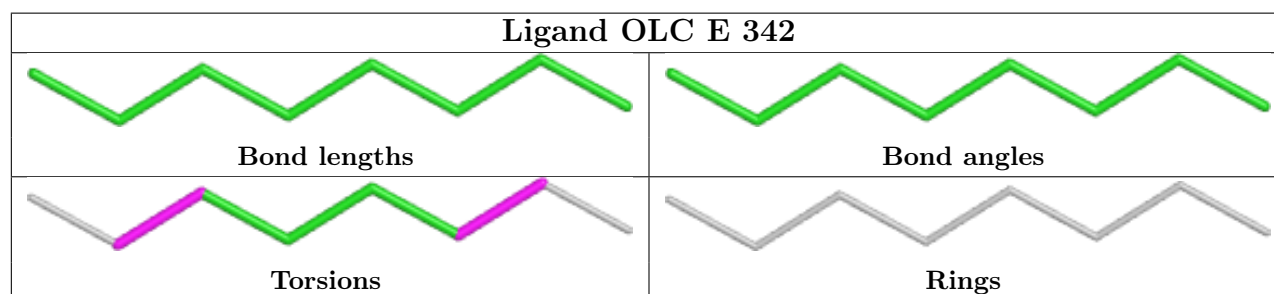
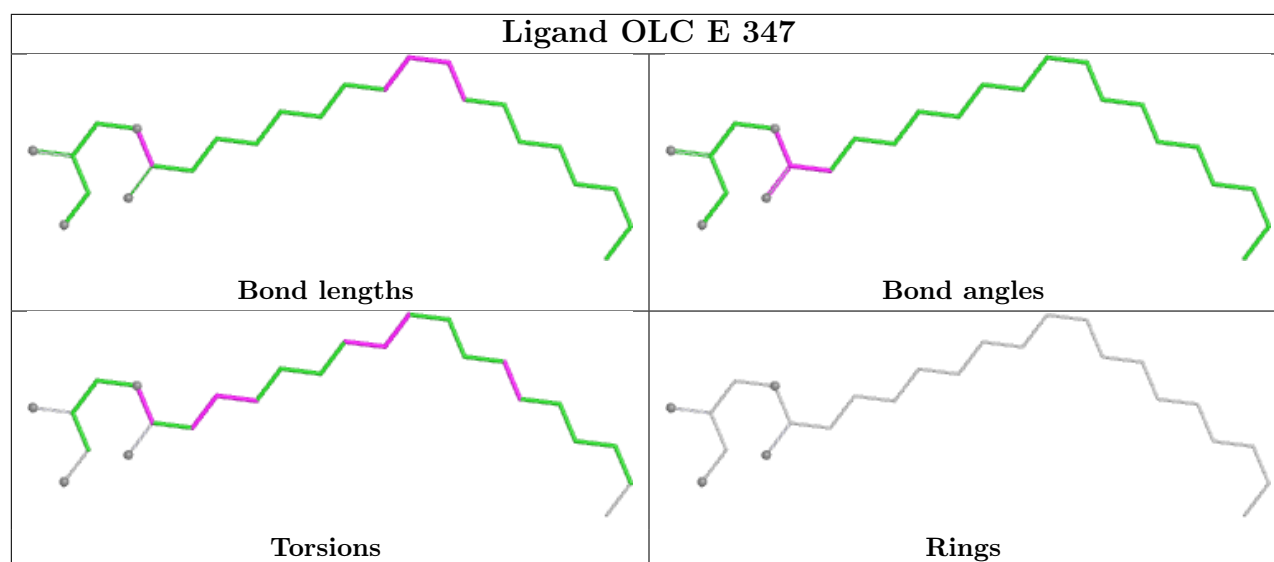


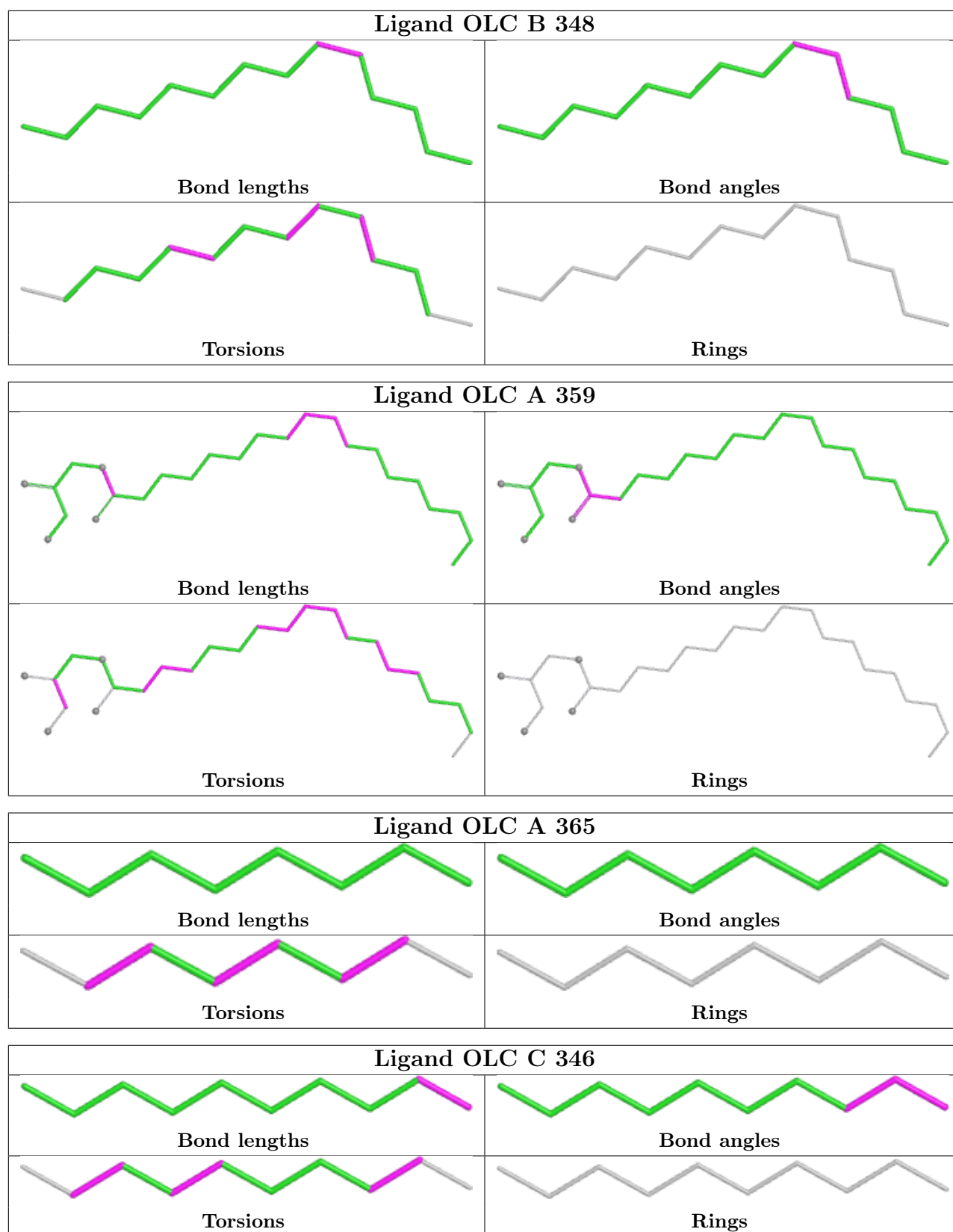


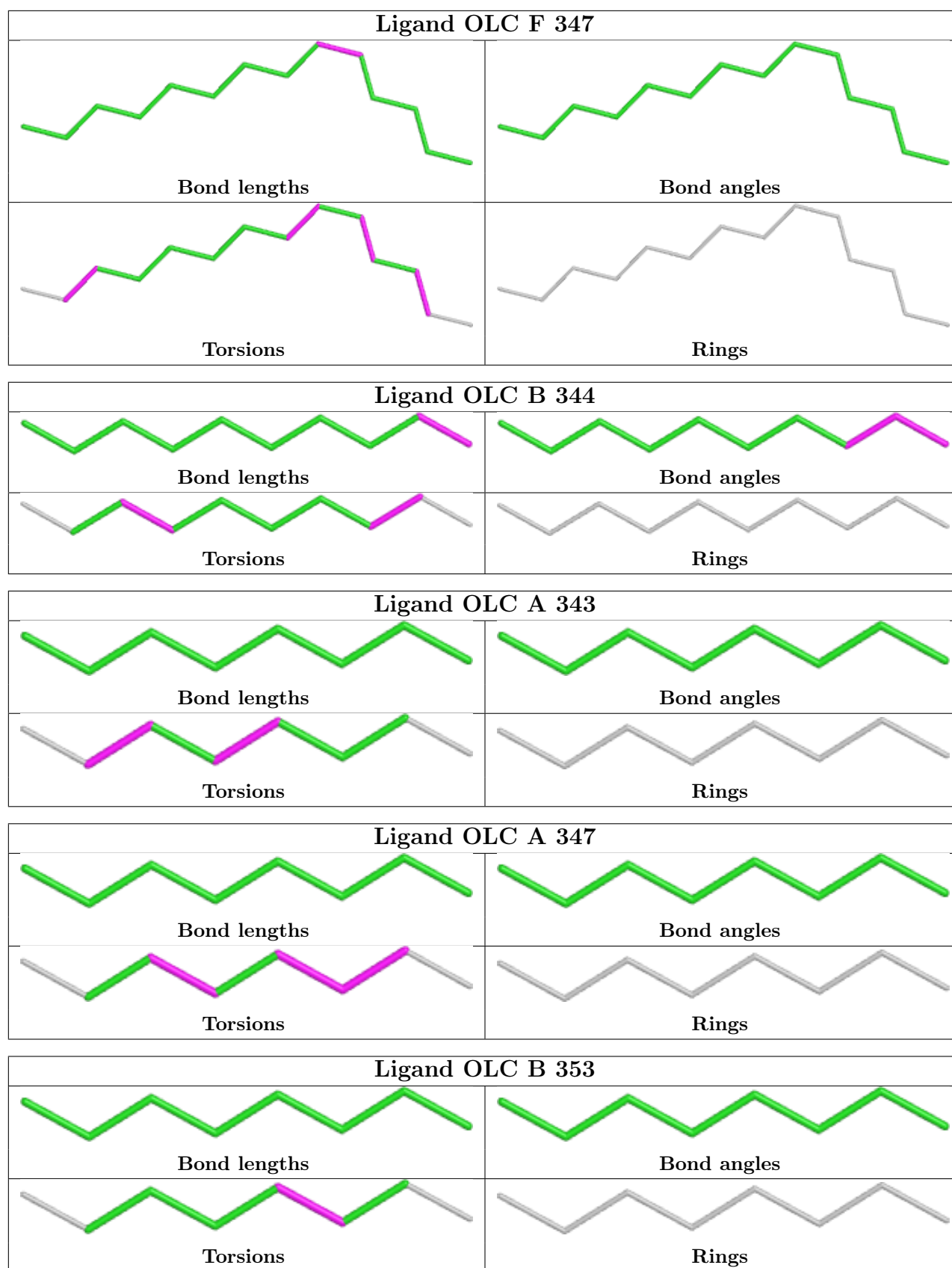


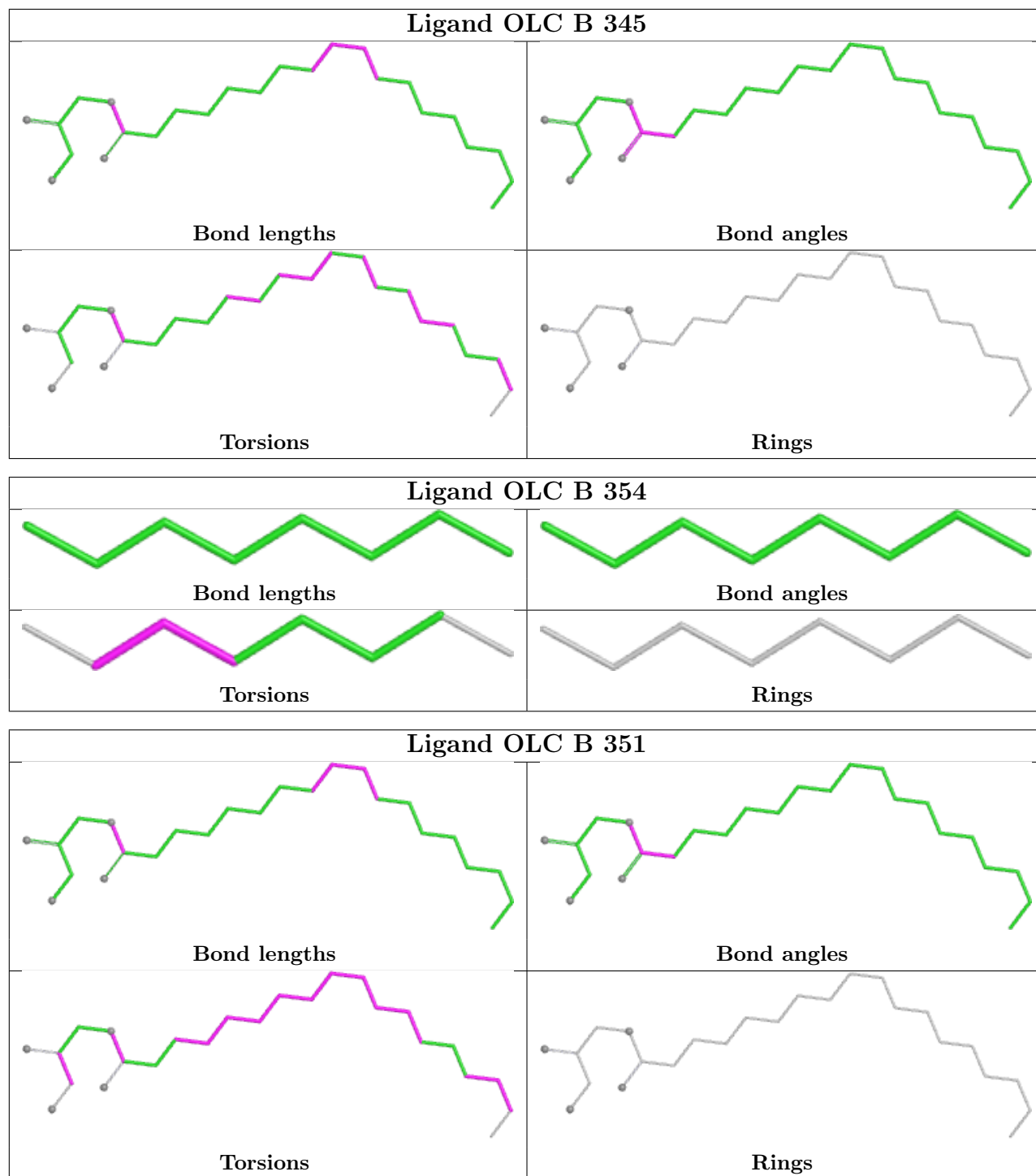


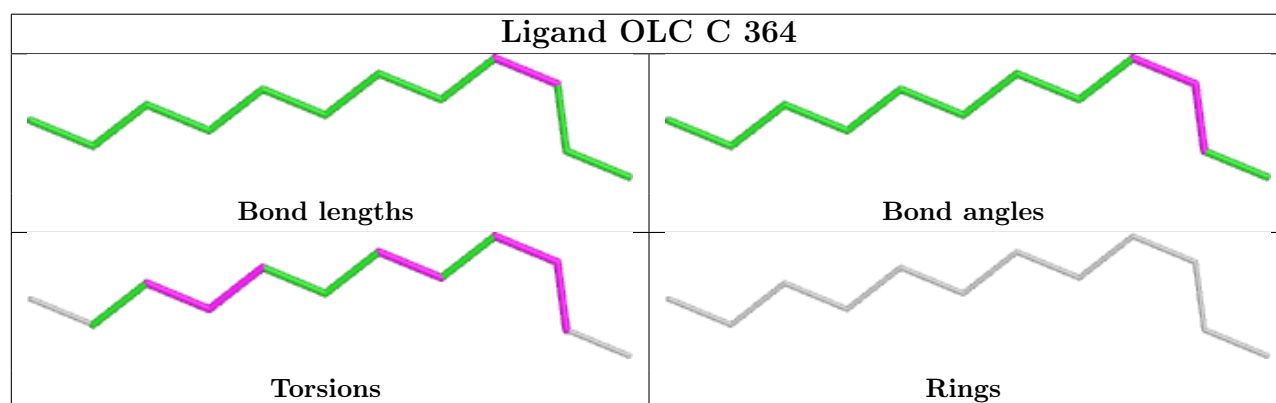
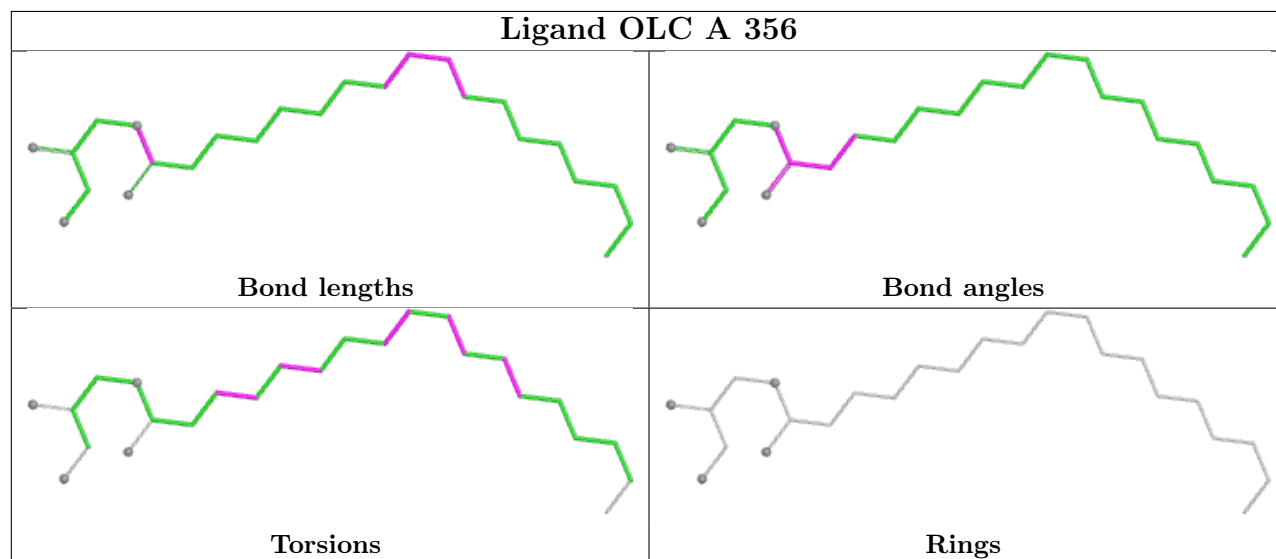
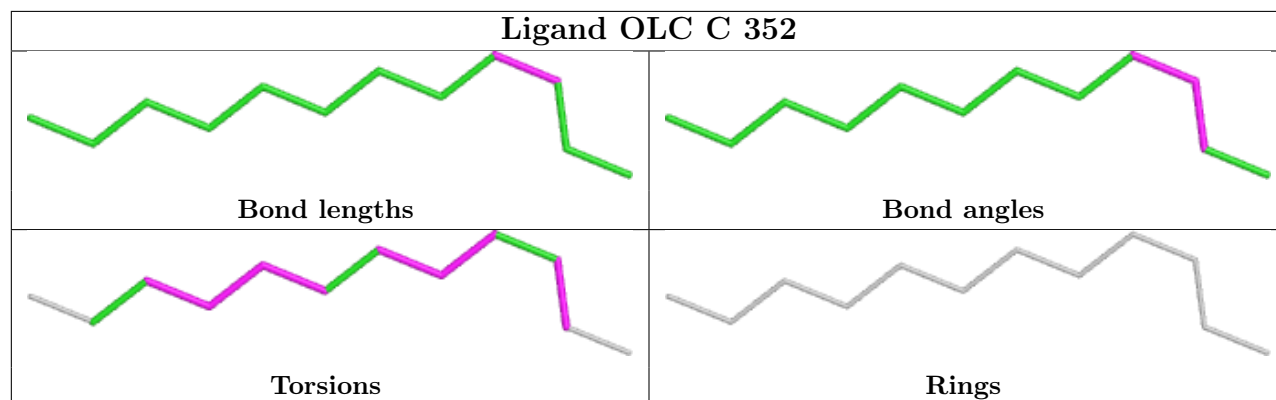
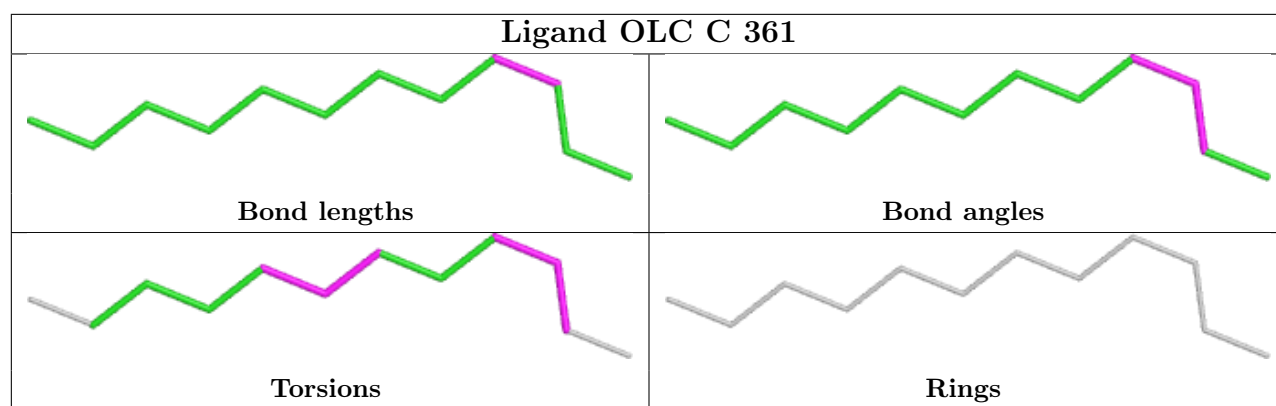


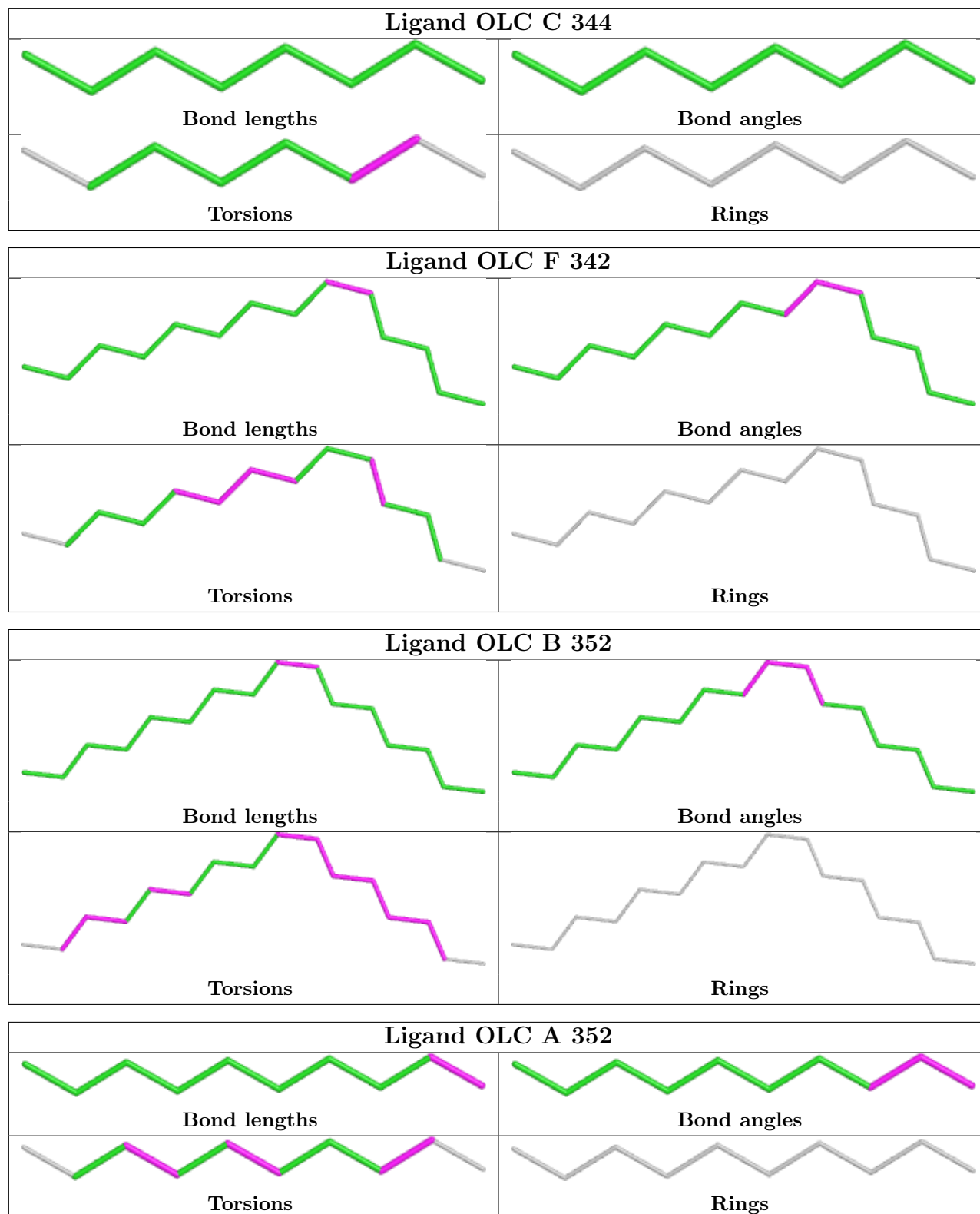


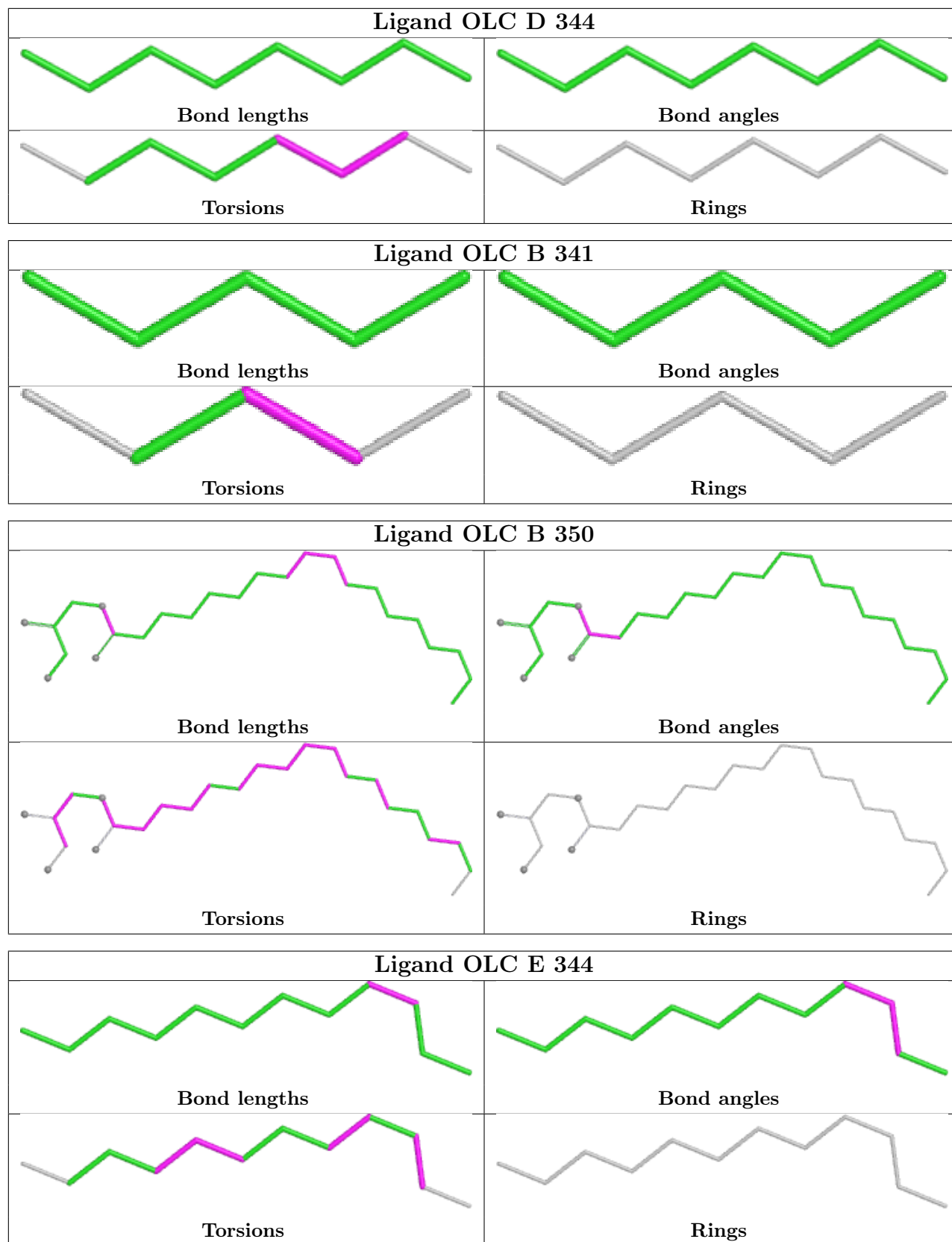


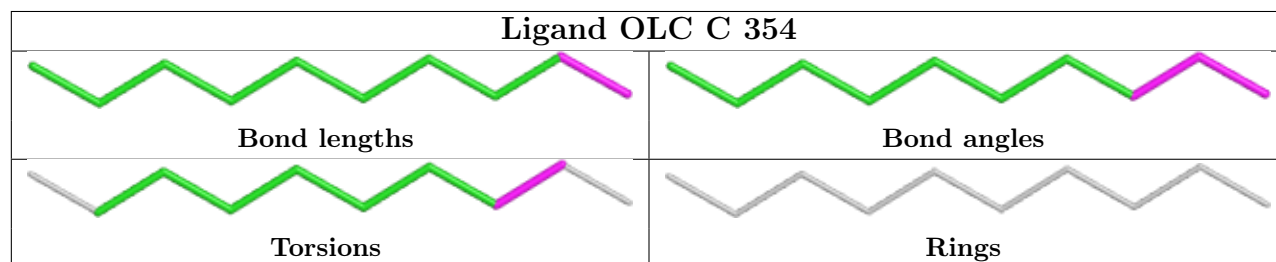
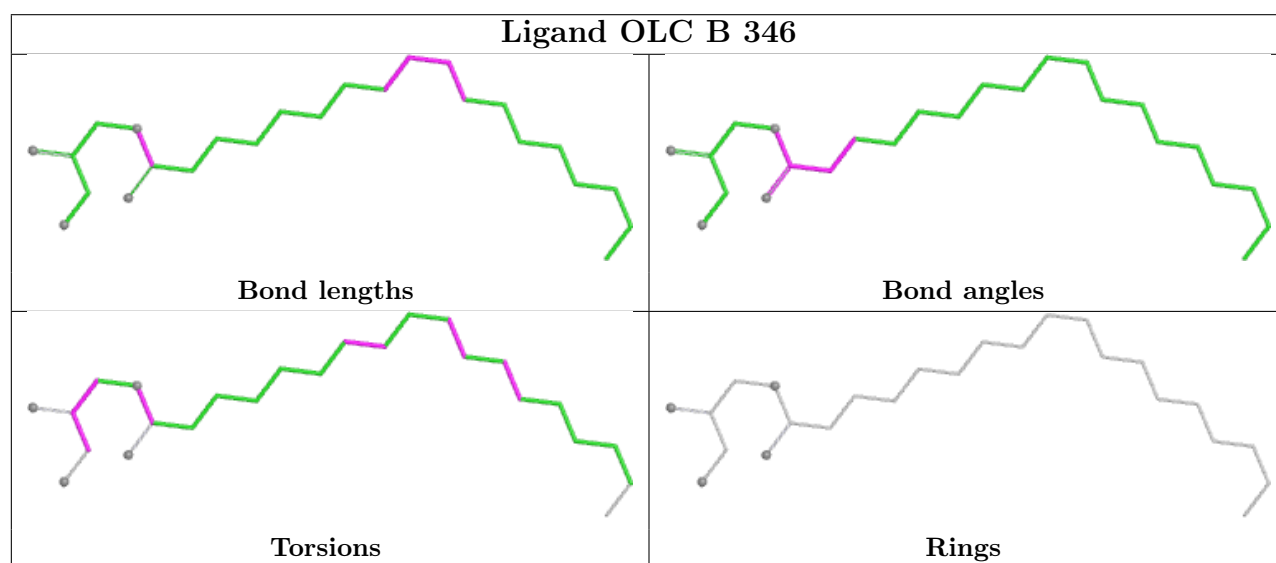
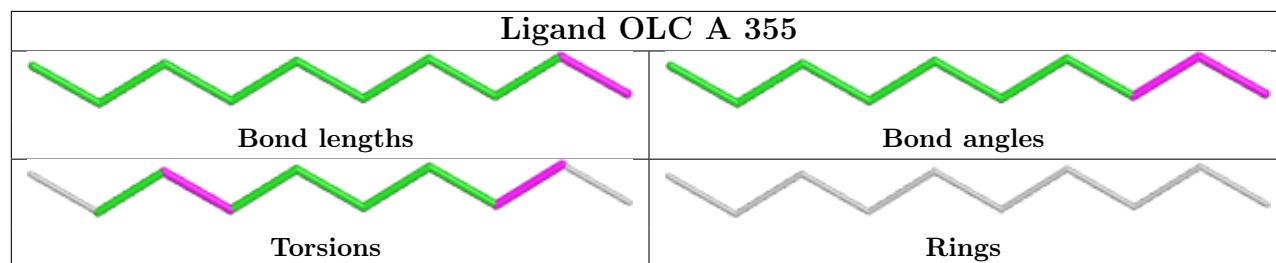
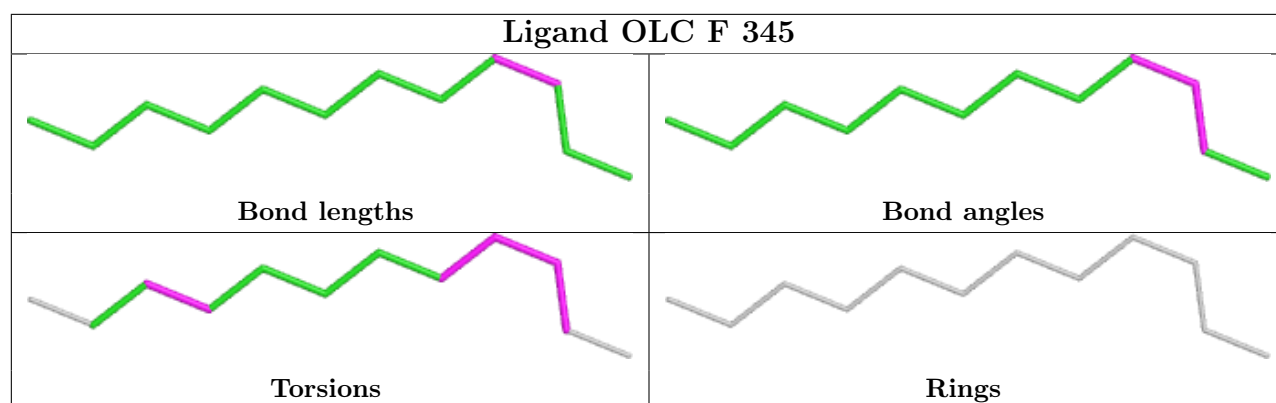


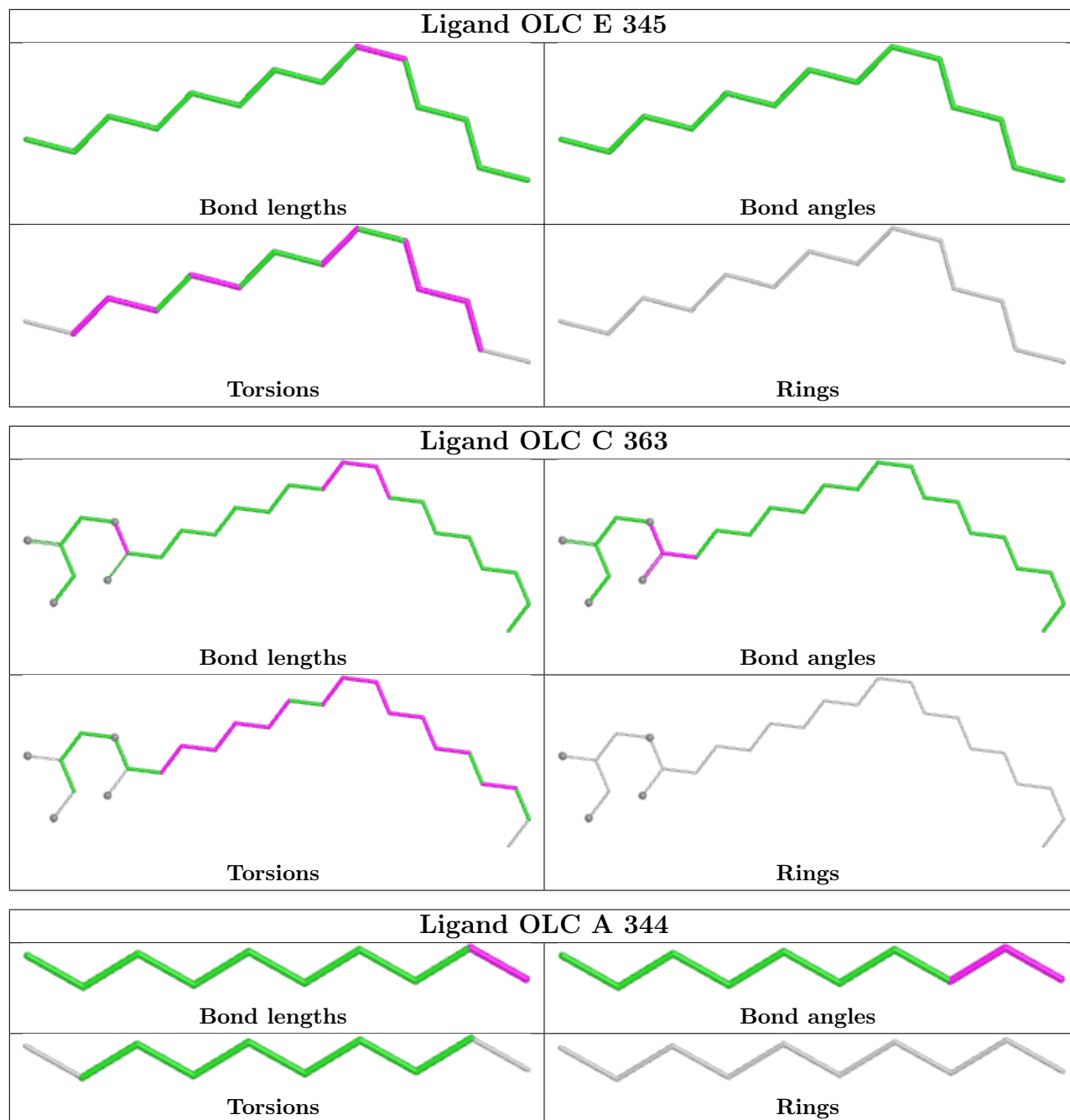


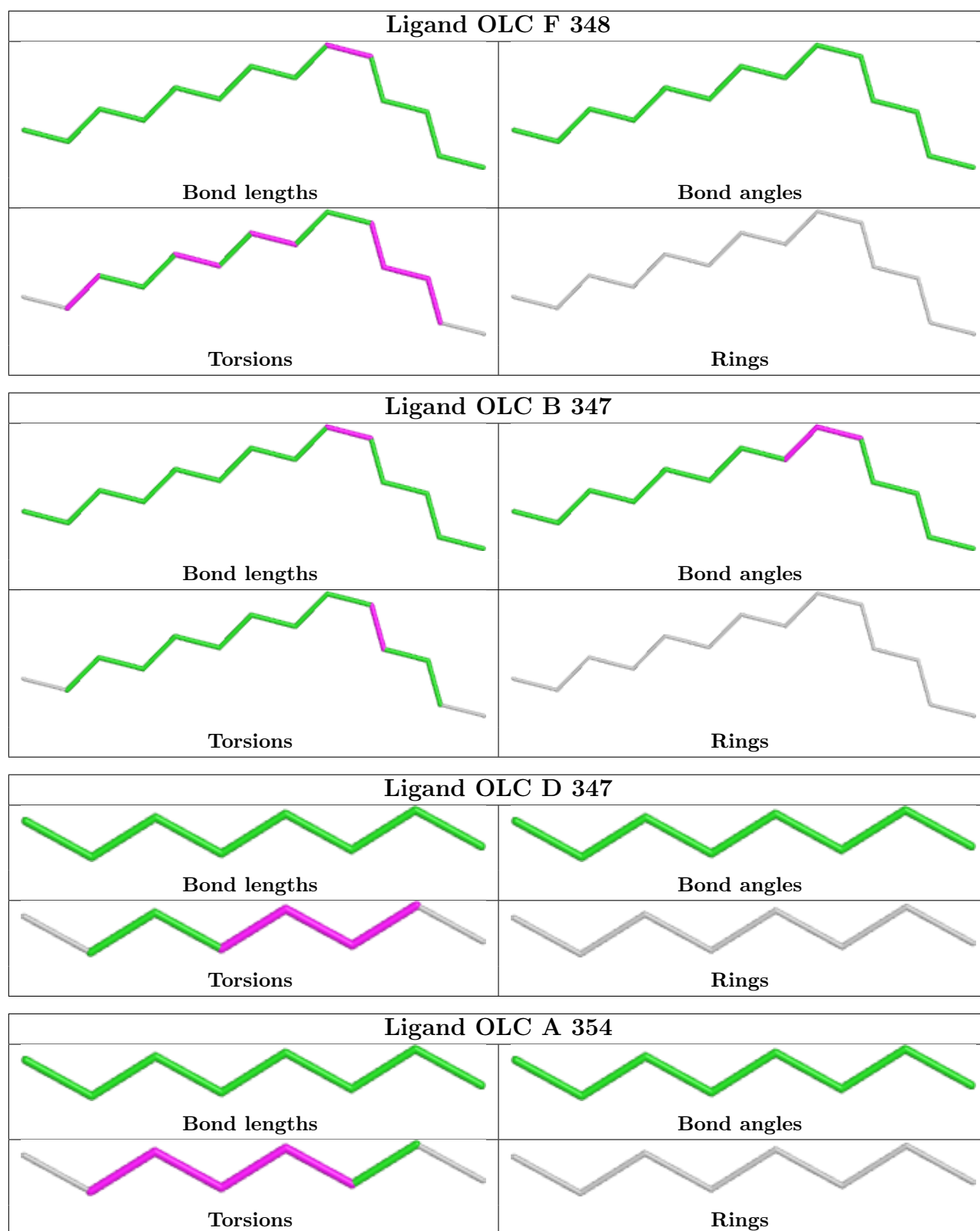


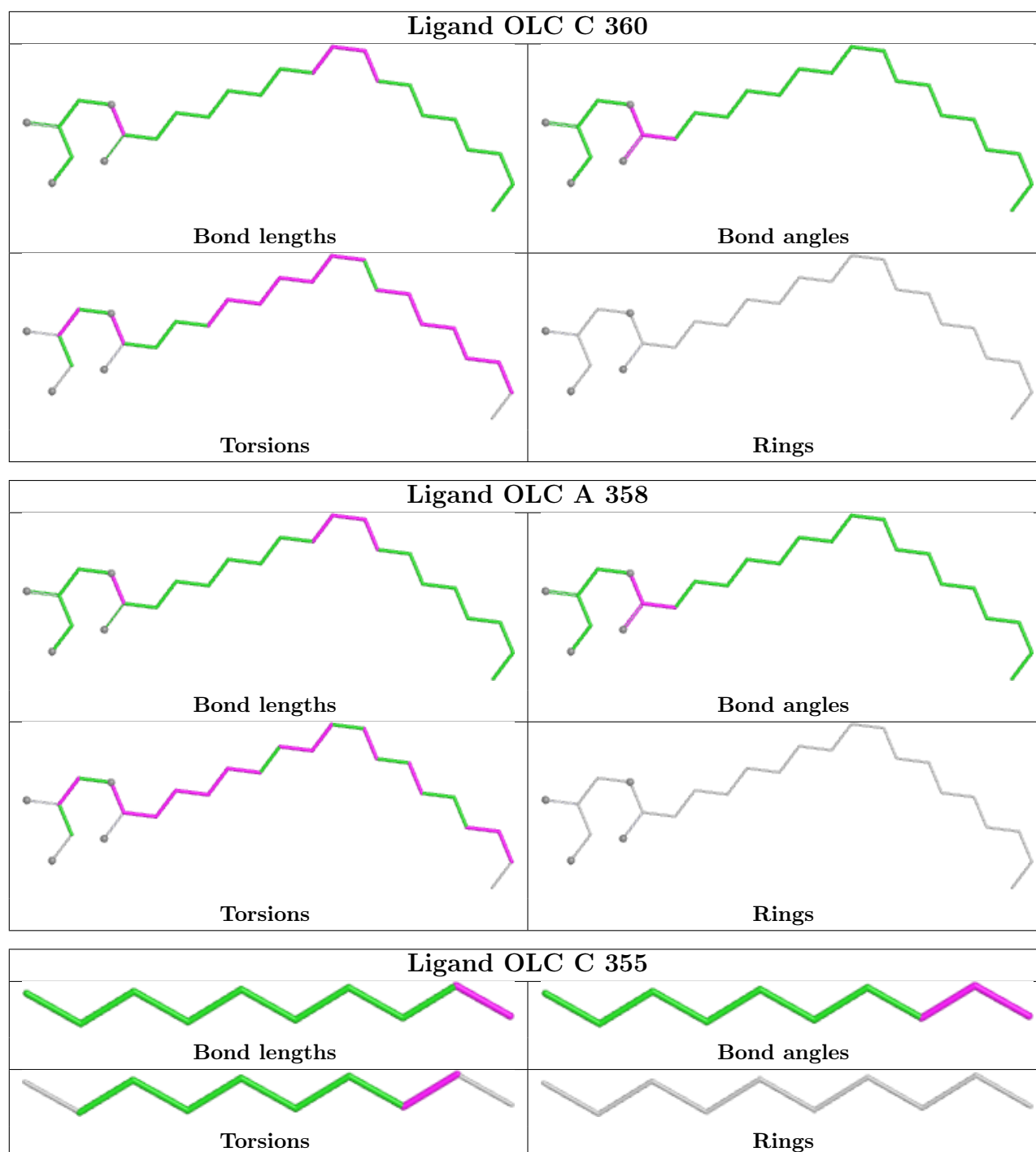


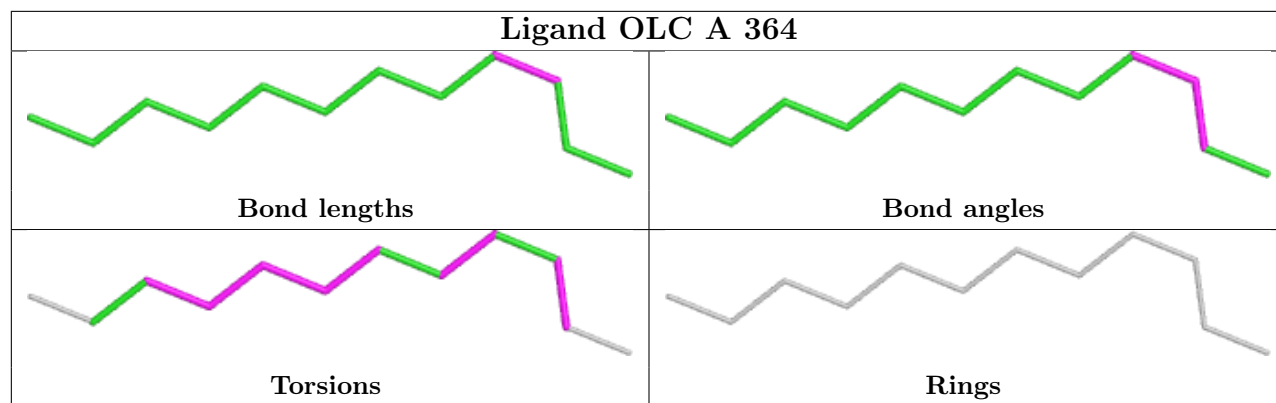












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/340 (100%)	-0.43	2 (0%) 85 85	11, 19, 38, 53	0
1	B	340/340 (100%)	-0.19	2 (0%) 85 85	14, 25, 46, 59	0
1	C	340/340 (100%)	-0.32	2 (0%) 85 85	13, 22, 40, 53	0
1	D	340/340 (100%)	-0.37	4 (1%) 76 76	12, 21, 42, 56	0
1	E	340/340 (100%)	-0.41	3 (0%) 81 80	11, 20, 38, 51	0
1	F	340/340 (100%)	-0.10	6 (1%) 67 67	13, 27, 49, 65	0
All	All	2040/2040 (100%)	-0.31	19 (0%) 81 80	11, 22, 44, 65	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	ALA	4.1
1	D	91	ALA	3.9
1	E	91	ALA	3.4
1	A	91	ALA	3.2
1	F	182	TYR	3.1
1	D	53	SER	2.6
1	B	91	ALA	2.6
1	F	91	ALA	2.6
1	F	147	LEU	2.5
1	D	149	ASP	2.4
1	D	147	LEU	2.4
1	F	8	GLY	2.4
1	B	7	ASP	2.2
1	E	185	PHE	2.1
1	C	25	LYS	2.1
1	A	149	ASP	2.1
1	E	8	GLY	2.1
1	F	148	VAL	2.1
1	F	7	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	F	342	14/25	0.59	0.24	50,52,58,59	0
2	OLC	C	352	12/25	0.61	0.23	51,56,59,59	0
2	OLC	F	344	10/25	0.63	0.21	49,57,62,63	0
2	OLC	C	354	10/25	0.65	0.18	60,64,67,67	0
2	OLC	B	348	14/25	0.66	0.19	50,58,61,61	0
2	OLC	C	351	8/25	0.66	0.24	53,56,60,60	0
2	OLC	C	348	12/25	0.68	0.20	50,55,59,59	0
2	OLC	A	365	8/25	0.68	0.15	44,48,60,60	0
2	OLC	A	358	25/25	0.69	0.21	49,55,61,64	0
2	OLC	A	360	12/25	0.69	0.20	49,54,68,68	0
2	OLC	E	345	14/25	0.72	0.18	32,50,57,59	0
2	OLC	C	353	10/25	0.72	0.20	54,56,62,63	0
2	OLC	B	354	8/25	0.72	0.17	36,48,60,64	0
2	OLC	C	347	10/25	0.73	0.17	49,50,62,63	0
2	OLC	F	347	14/25	0.73	0.20	49,60,63,64	0
2	OLC	C	357	14/25	0.74	0.17	28,46,50,51	0
2	OLC	C	363	25/25	0.74	0.17	38,46,56,66	0
2	OLC	B	341	5/25	0.74	0.19	42,44,47,47	0
2	OLC	A	352	10/25	0.75	0.16	38,47,51,51	0
2	OLC	C	356	8/25	0.75	0.20	35,50,58,59	0
2	OLC	E	346	10/25	0.76	0.16	58,60,62,62	0
2	OLC	E	348	12/25	0.76	0.15	42,49,52,52	0
2	OLC	A	361	25/25	0.76	0.18	40,53,64,67	0
2	OLC	D	342	25/25	0.76	0.17	45,51,70,75	0
2	OLC	B	342	14/25	0.76	0.20	51,56,62,64	0
2	OLC	F	348	14/25	0.76	0.17	36,43,50,50	0
2	OLC	B	347	14/25	0.77	0.15	30,38,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	D	345	10/25	0.77	0.17	39,45,49,51	0
2	OLC	D	349	25/25	0.77	0.14	39,49,54,55	0
2	OLC	A	362	14/25	0.77	0.11	38,44,49,49	0
2	OLC	A	355	10/25	0.77	0.20	40,51,66,66	0
2	OLC	E	342	8/25	0.78	0.17	40,41,43,45	0
2	OLC	E	343	12/25	0.78	0.15	40,48,52,54	0
2	OLC	A	351	14/25	0.78	0.16	42,50,56,56	0
2	OLC	A	364	12/25	0.78	0.14	48,54,56,56	0
2	OLC	A	344	10/25	0.78	0.14	29,42,49,49	0
2	OLC	C	364	12/25	0.78	0.16	37,44,47,47	0
2	OLC	B	353	8/25	0.78	0.18	35,41,49,50	0
2	OLC	A	346	25/25	0.78	0.15	35,44,57,61	0
2	OLC	C	343	8/25	0.78	0.15	56,62,66,66	0
2	OLC	C	344	8/25	0.79	0.16	40,44,53,55	0
2	OLC	D	347	8/25	0.79	0.17	28,36,41,41	0
2	OLC	B	351	25/25	0.79	0.15	37,46,61,68	0
2	OLC	A	348	10/25	0.79	0.14	40,44,49,50	0
2	OLC	C	362	25/25	0.80	0.16	27,41,58,60	0
2	OLC	F	341	8/25	0.80	0.17	40,44,48,52	0
2	OLC	B	344	10/25	0.81	0.12	42,44,53,54	0
2	OLC	C	345	12/25	0.81	0.16	37,43,49,49	0
2	OLC	B	349	8/25	0.81	0.13	43,45,49,50	0
2	OLC	C	361	12/25	0.82	0.12	24,32,37,37	0
2	OLC	B	350	25/25	0.82	0.15	34,49,60,71	0
2	OLC	D	343	8/25	0.82	0.14	39,44,48,53	0
2	OLC	C	350	14/25	0.82	0.15	37,49,53,55	0
2	OLC	D	348	8/25	0.83	0.16	37,43,44,46	0
2	OLC	C	349	10/25	0.83	0.15	36,44,52,56	0
2	OLC	A	342	8/25	0.83	0.16	48,50,58,60	0
2	OLC	A	363	12/25	0.84	0.13	31,39,47,48	0
2	OLC	E	344	12/25	0.84	0.13	29,54,59,59	0
2	OLC	F	343	8/25	0.84	0.16	48,55,61,61	0
2	OLC	B	345	25/25	0.84	0.14	33,43,52,60	0
2	OLC	F	346	8/25	0.84	0.15	40,45,50,51	0
2	OLC	C	355	10/25	0.84	0.13	33,41,50,51	0
2	OLC	D	346	12/25	0.84	0.14	32,36,41,43	0
2	OLC	C	346	10/25	0.85	0.12	34,44,54,57	0
2	OLC	A	349	25/25	0.85	0.13	36,42,56,63	0
2	OLC	F	345	12/25	0.85	0.15	37,46,57,57	0
2	OLC	A	359	25/25	0.85	0.14	28,40,54,54	0
2	OLC	C	360	25/25	0.85	0.12	23,40,72,74	0
2	OLC	D	341	5/25	0.85	0.15	36,39,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLC	B	352	16/25	0.86	0.12	32,41,46,47	0
2	OLC	E	341	25/25	0.86	0.12	21,39,49,53	0
2	OLC	E	347	25/25	0.86	0.13	26,45,53,57	0
2	OLC	B	343	8/25	0.86	0.13	30,37,44,48	0
2	OLC	A	350	14/25	0.86	0.13	31,35,46,47	0
2	OLC	C	358	25/25	0.86	0.14	31,39,63,66	0
2	OLC	A	343	8/25	0.87	0.11	32,36,42,43	0
2	OLC	A	356	25/25	0.87	0.12	22,36,53,65	0
2	OLC	A	345	8/25	0.87	0.11	35,44,47,49	0
2	OLC	B	346	25/25	0.87	0.13	29,39,54,61	0
2	OLC	C	342	8/25	0.87	0.13	26,35,46,48	0
2	OLC	C	341	10/25	0.88	0.11	36,40,55,59	0
2	OLC	A	354	8/25	0.88	0.12	28,35,39,44	0
2	OLC	D	344	8/25	0.88	0.12	27,31,47,51	0
2	OLC	A	357	10/25	0.88	0.12	26,37,44,46	0
2	OLC	A	347	8/25	0.89	0.10	25,29,36,39	0
2	OLC	A	341	8/25	0.89	0.10	28,32,41,43	0
2	OLC	C	359	25/25	0.89	0.12	30,38,57,63	0
2	OLC	A	353	8/25	0.91	0.10	32,34,43,44	0
3	K	B	356	1/1	0.95	0.10	38,38,38,38	0
3	K	C	367	1/1	0.95	0.07	38,38,38,38	0
3	K	F	350	1/1	0.95	0.15	42,42,42,42	0
4	SCN	E	352	3/3	0.95	0.08	20,20,21,35	0
4	SCN	F	352	3/3	0.95	0.08	21,21,23,34	0
4	SCN	A	369	3/3	0.96	0.07	23,23,25,32	0
4	SCN	B	358	3/3	0.96	0.07	25,25,26,37	0
4	SCN	D	354	3/3	0.97	0.06	25,25,25,36	0
3	K	B	355	1/1	0.97	0.08	34,34,34,34	0
3	K	B	357	1/1	0.97	0.13	41,41,41,41	0
3	K	F	351	1/1	0.98	0.16	44,44,44,44	0
3	K	C	368	1/1	0.98	0.08	36,36,36,36	0
3	K	D	353	1/1	0.98	0.07	38,38,38,38	0
3	K	E	351	1/1	0.98	0.09	33,33,33,33	0
3	K	F	349	1/1	0.98	0.09	30,30,30,30	0
4	SCN	E	353	3/3	0.98	0.10	40,40,44,49	0
3	K	A	368	1/1	0.98	0.07	32,32,32,32	0
3	K	A	366	1/1	0.99	0.02	25,25,25,25	0
3	K	A	367	1/1	0.99	0.05	27,27,27,27	0
3	K	D	350	1/1	0.99	0.07	23,23,23,23	0
3	K	D	351	1/1	0.99	0.06	29,29,29,29	0
3	K	D	352	1/1	0.99	0.09	38,38,38,38	0
3	K	C	365	1/1	0.99	0.03	25,25,25,25	0

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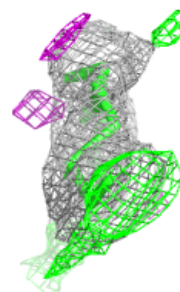
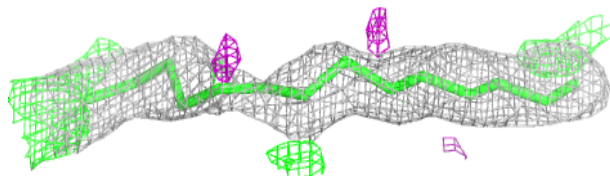
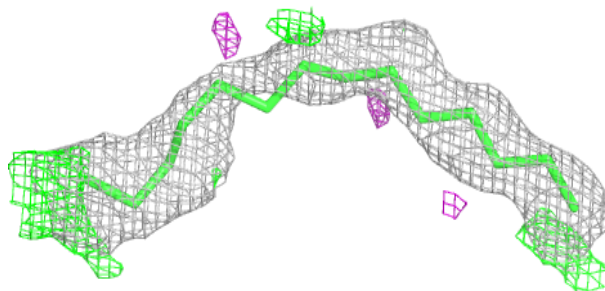
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	E	349	1/1	0.99	0.04	23,23,23,23	0
3	K	E	350	1/1	0.99	0.05	26,26,26,26	0
3	K	C	366	1/1	0.99	0.05	28,28,28,28	0

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.

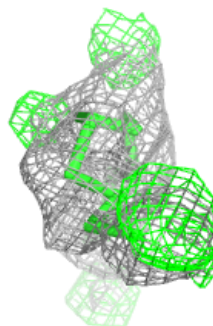
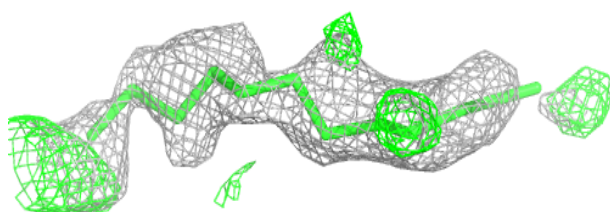
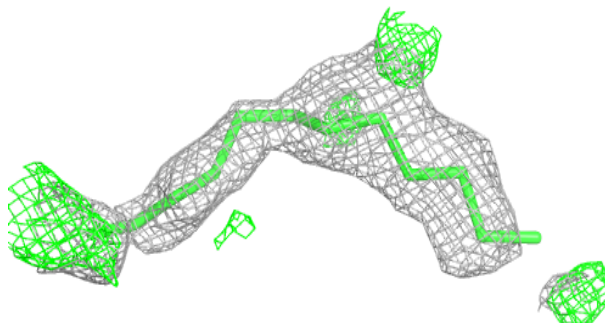
Electron density around OLC F 342:

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

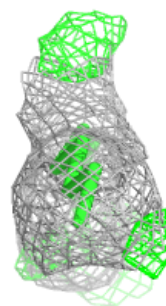
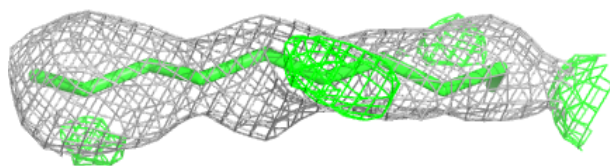
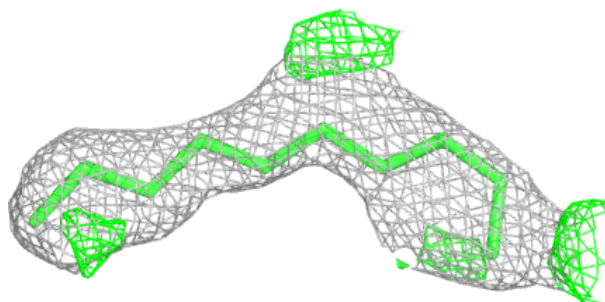


Electron density around OLC C 352:

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

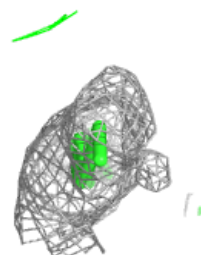
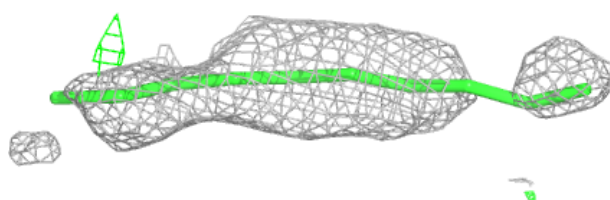
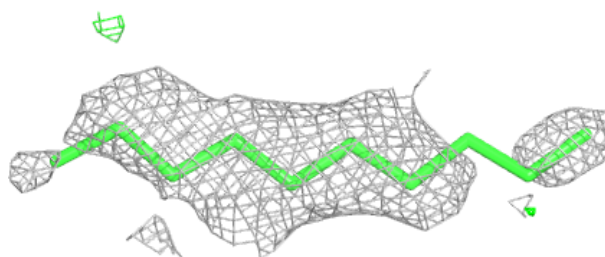
**Electron density around OLC F 344:**

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

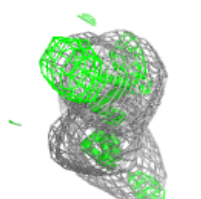
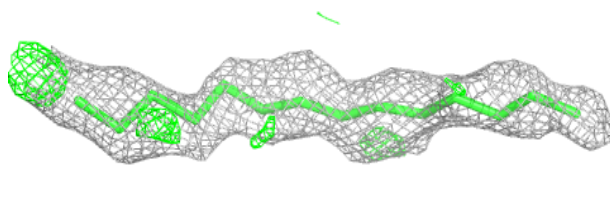
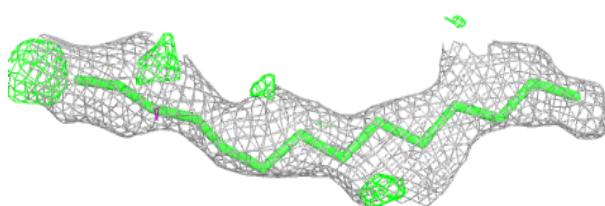


Electron density around OLC C 354:

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

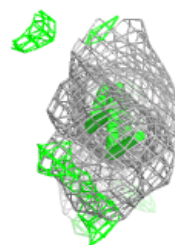
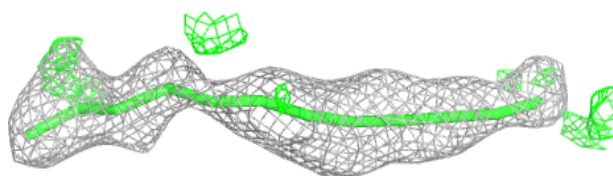
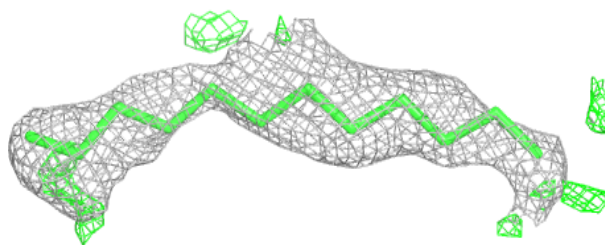
**Electron density around OLC B 348:**

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

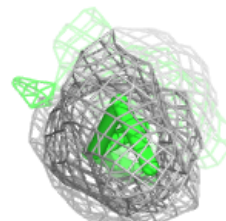
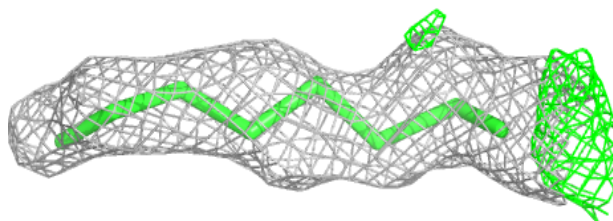
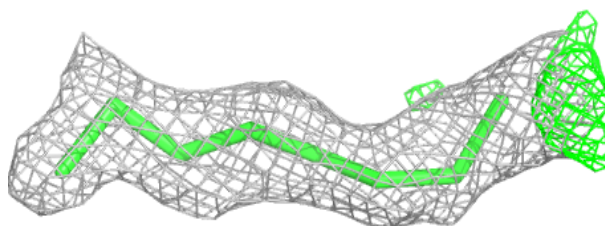


Electron density around OLC C 348:

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

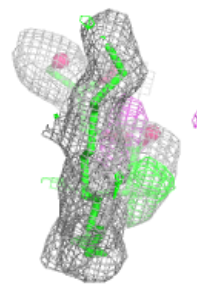
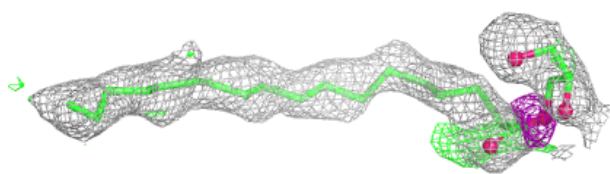
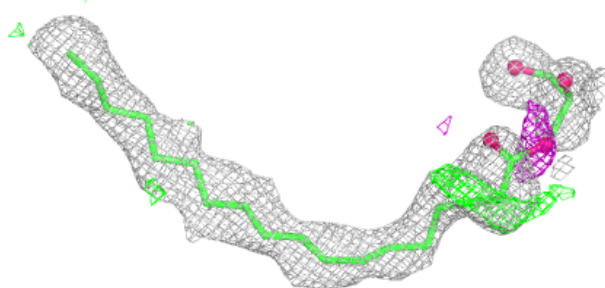
**Electron density around OLC A 365:**

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

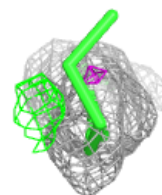
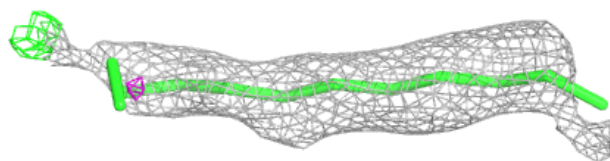
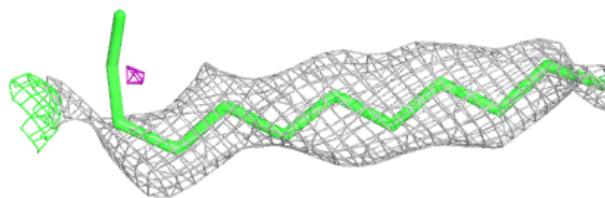


Electron density around OLC A 358:

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

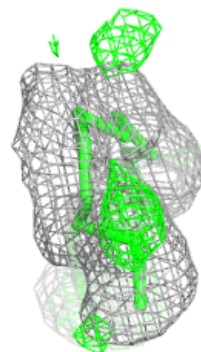
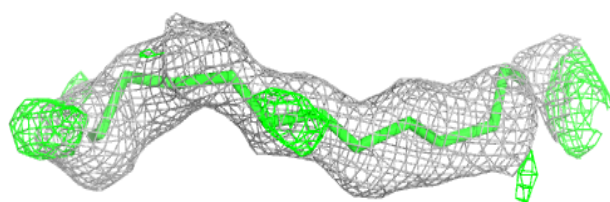
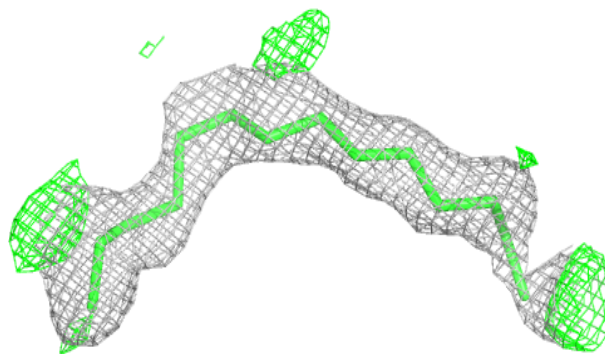
**Electron density around OLC A 360:**

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

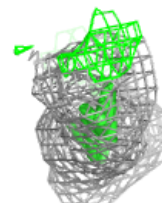
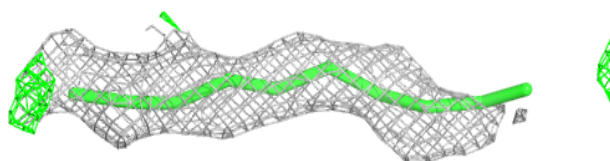
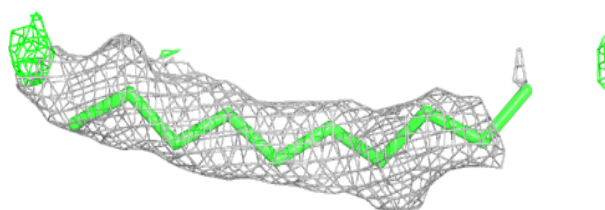


Electron density around OLC E 345:

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

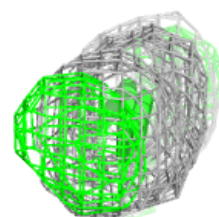
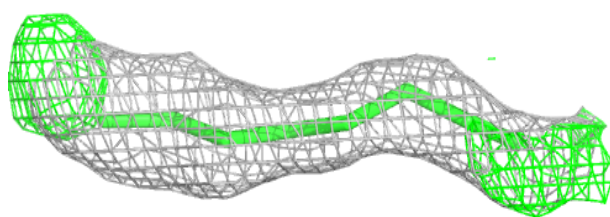
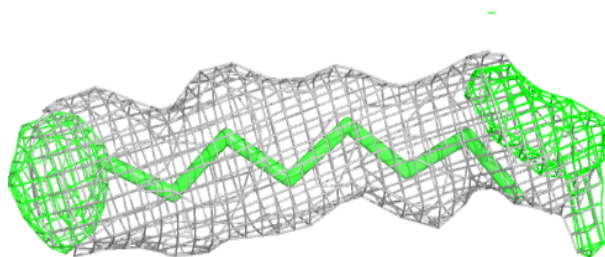
**Electron density around OLC C 353:**

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

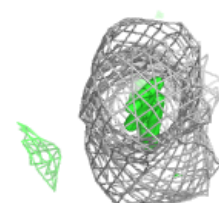
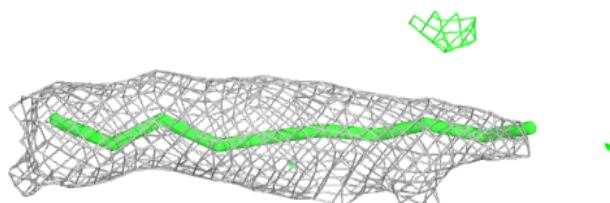
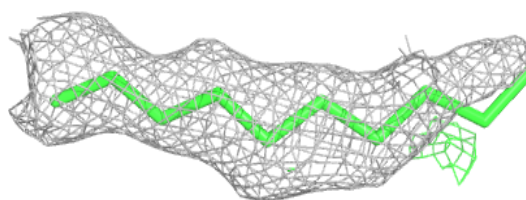


Electron density around OLC B 354:

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

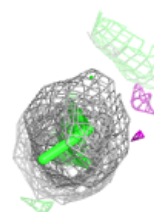
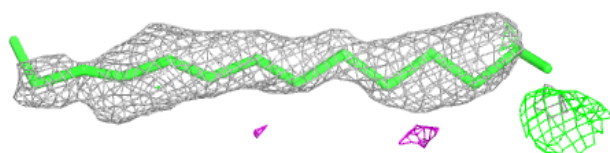
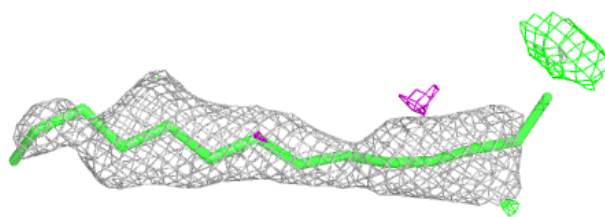
**Electron density around OLC C 347:**

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

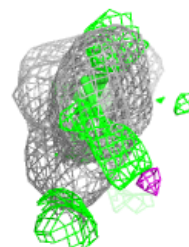
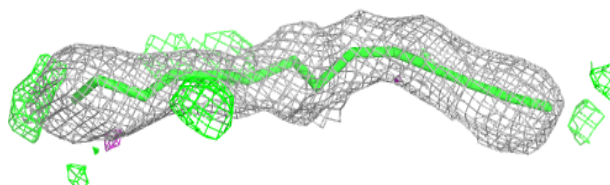
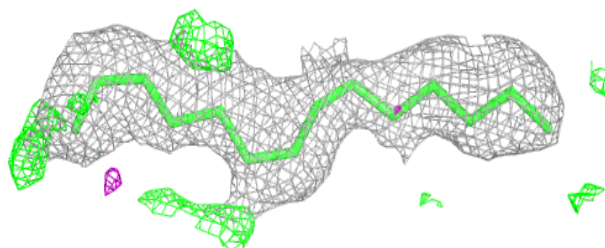


Electron density around OLC F 347:

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

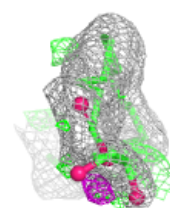
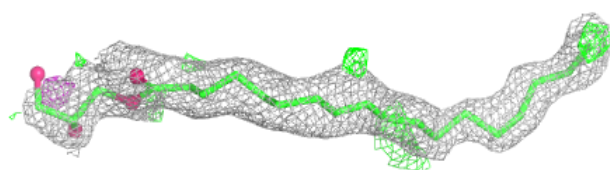
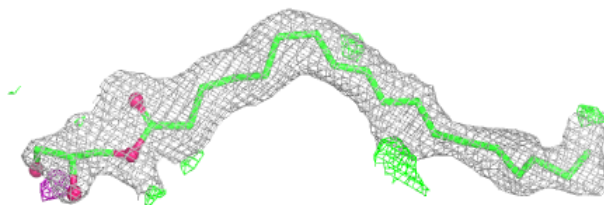
**Electron density around OLC C 357:**

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

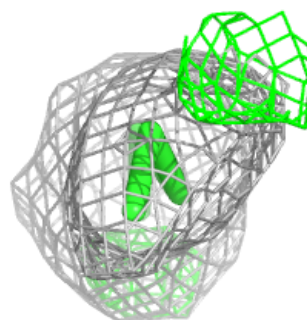
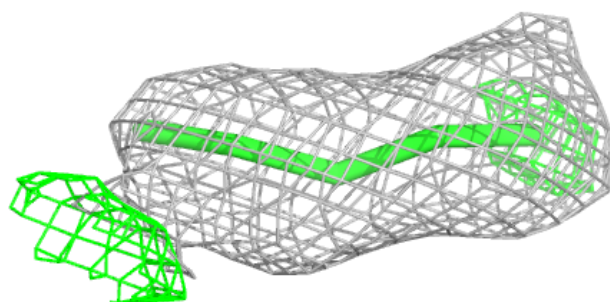
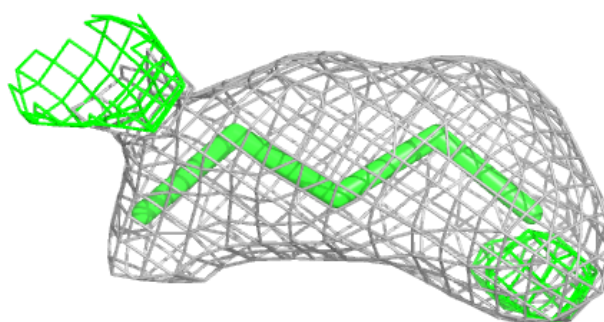


Electron density around OLC C 363:

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

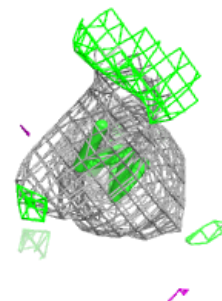
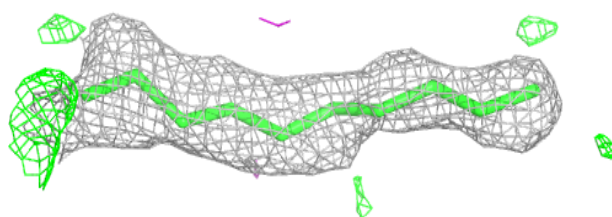
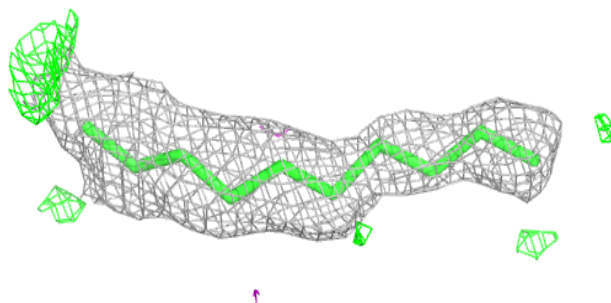
**Electron density around OLC B 341:**

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

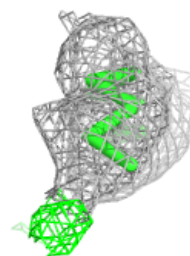
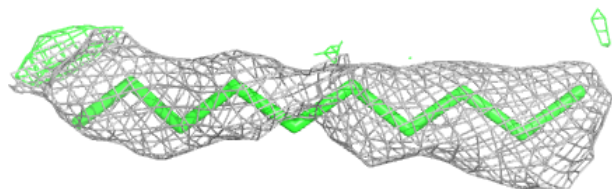
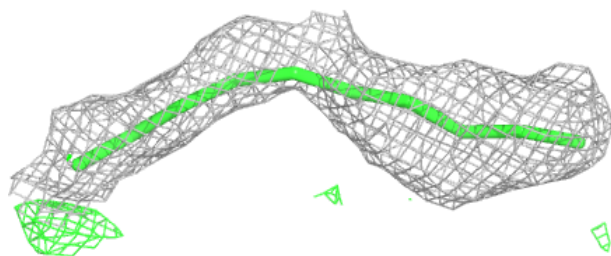


Electron density around OLC A 352:

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

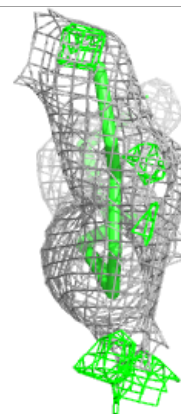
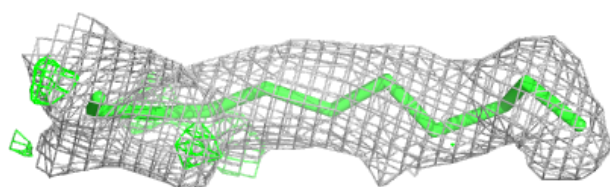
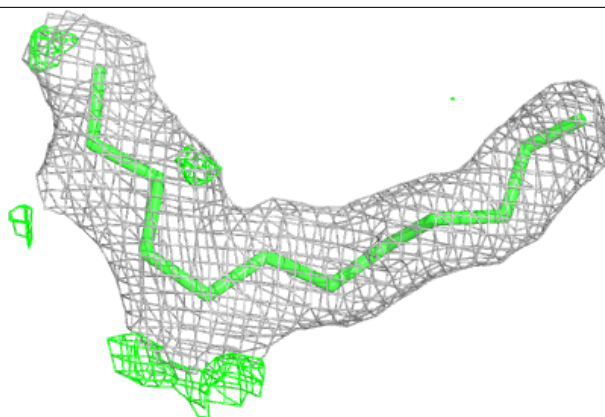
**Electron density around OLC E 346:**

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

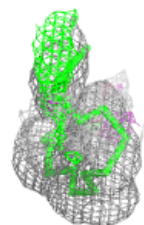
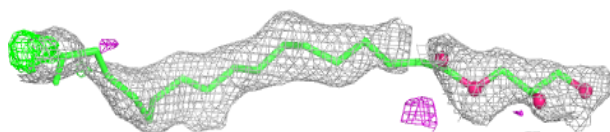
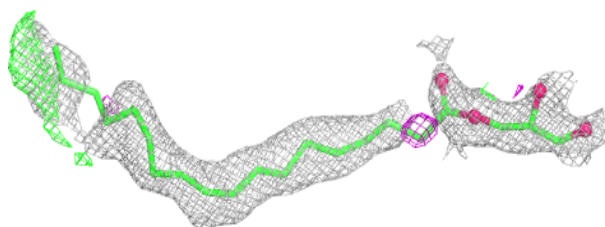


Electron density around OLC E 348:

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

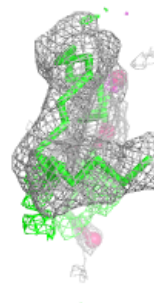
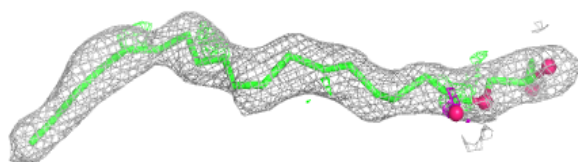
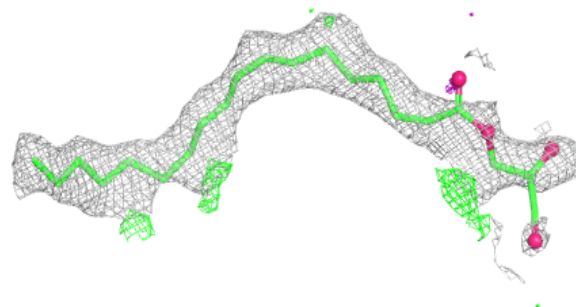
**Electron density around OLC A 361:**

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

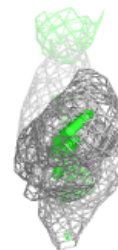
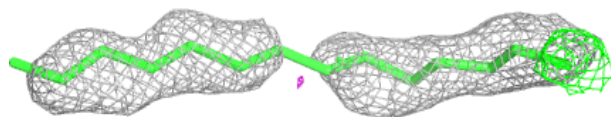
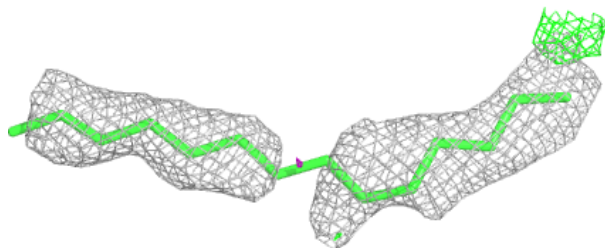


Electron density around OLC D 342:

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

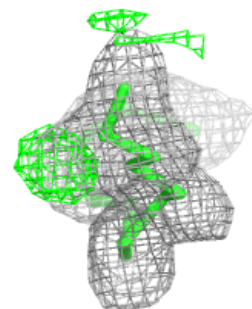
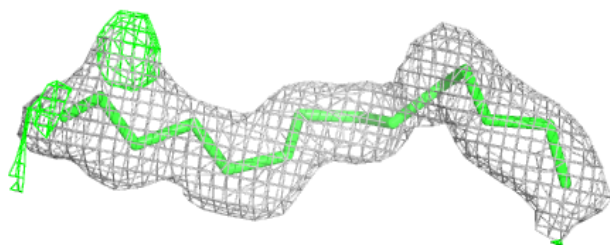
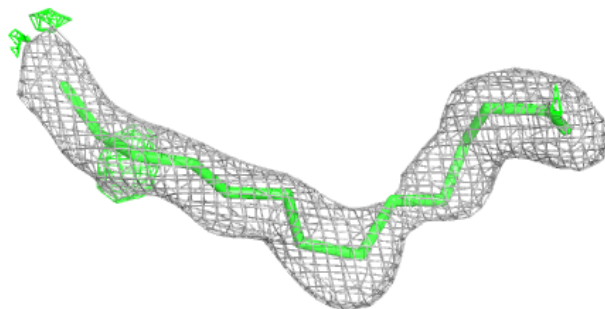
**Electron density around OLC B 342:**

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

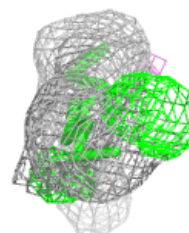
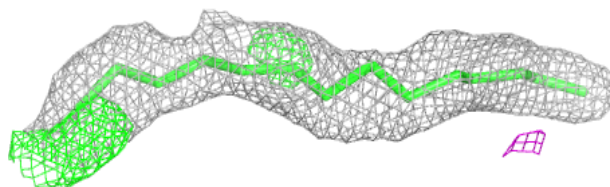
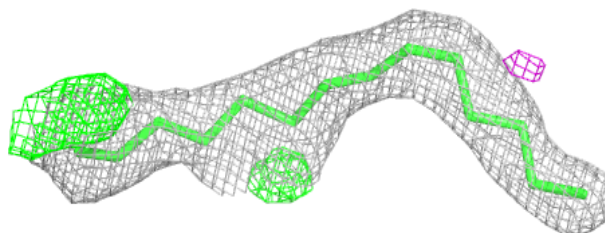


Electron density around OLC F 348:

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

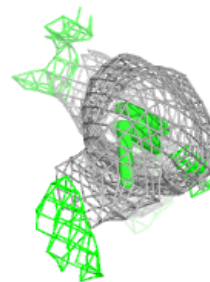
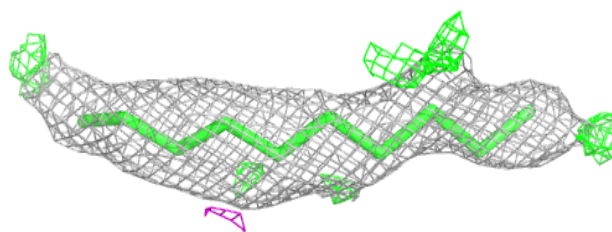
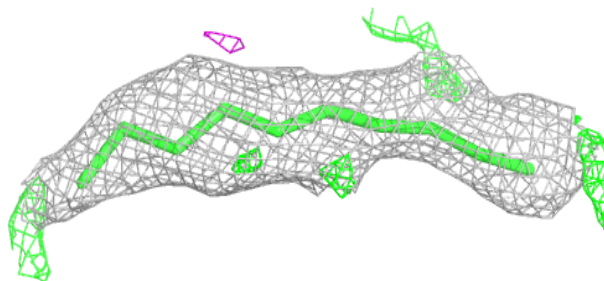
**Electron density around OLC B 347:**

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

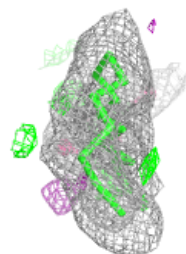
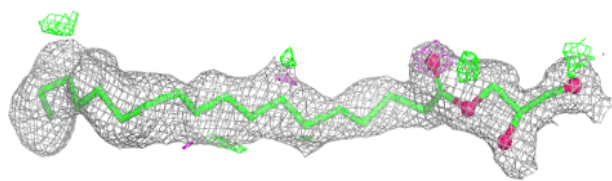
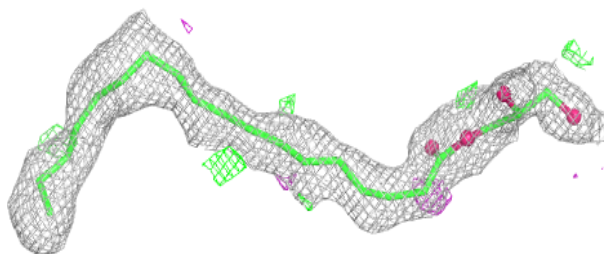


Electron density around OLC D 345:

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

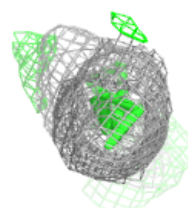
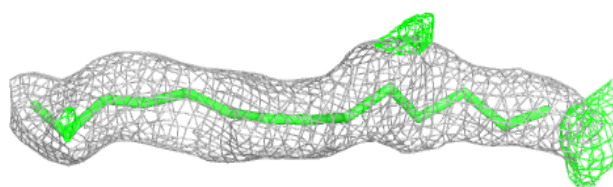
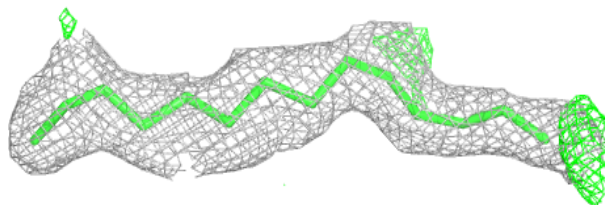
**Electron density around OLC D 349:**

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

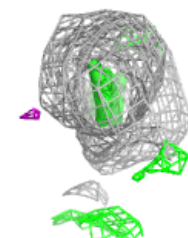
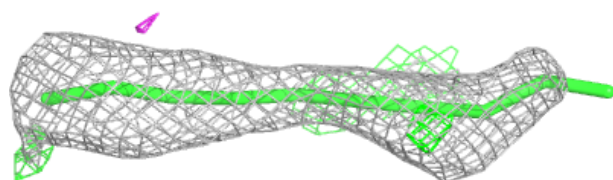
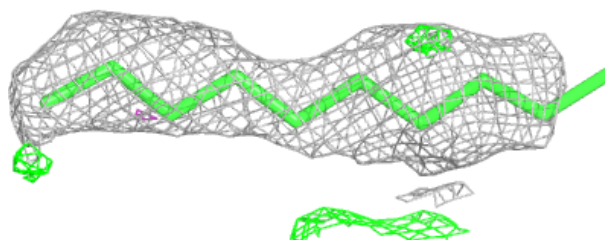


Electron density around OLC A 362:

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

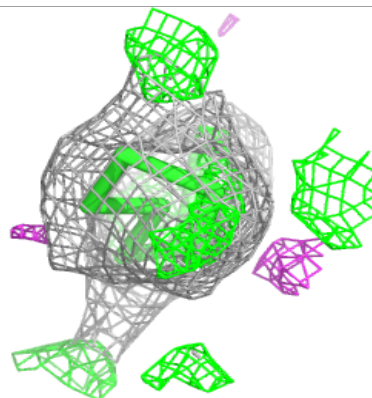
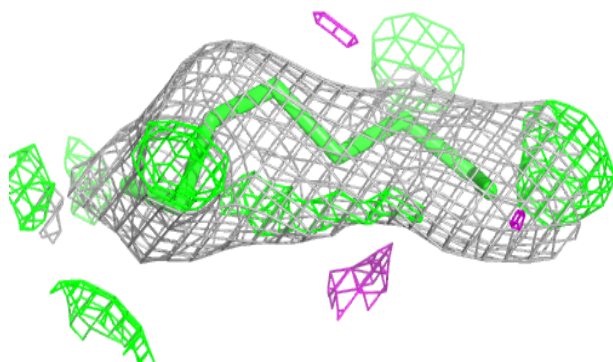
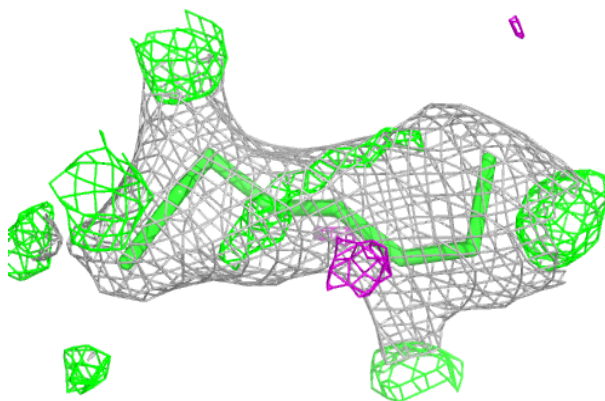
**Electron density around OLC A 355:**

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

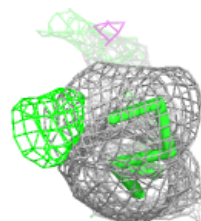
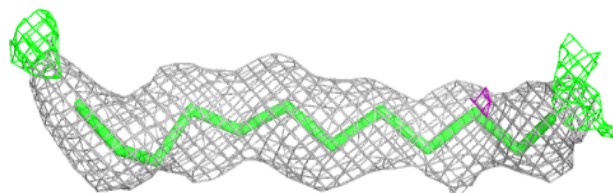
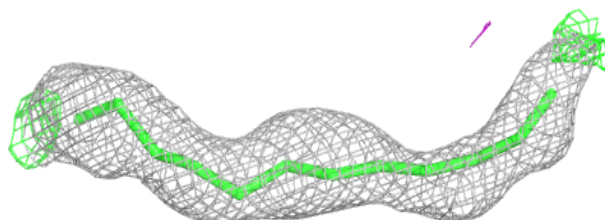


Electron density around OLC E 342:

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

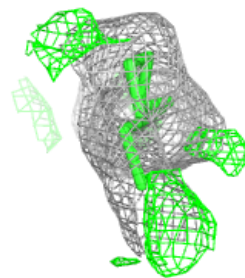
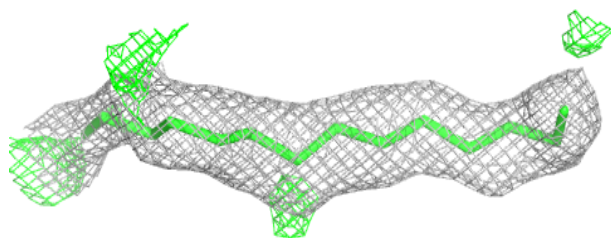
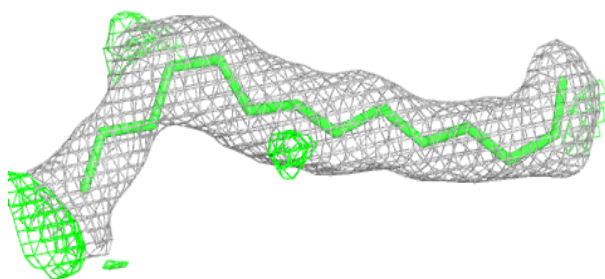
**Electron density around OLC E 343:**

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

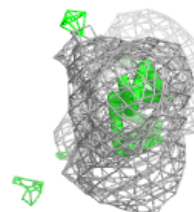
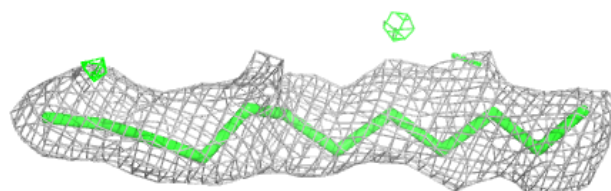
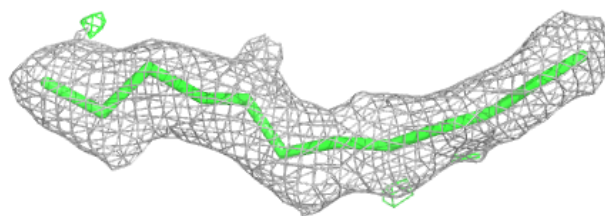


Electron density around OLC A 351:

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

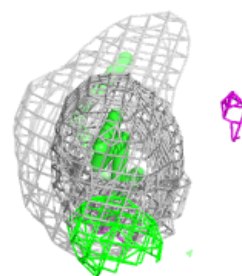
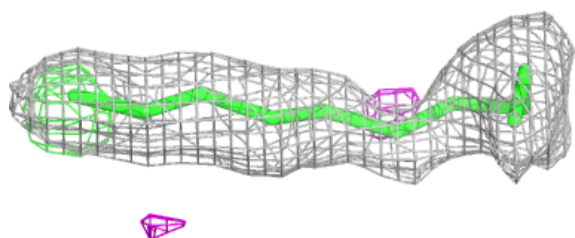
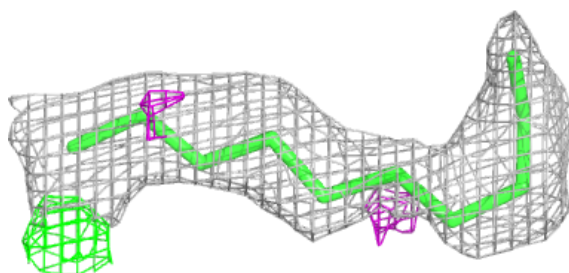
**Electron density around OLC A 364:**

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

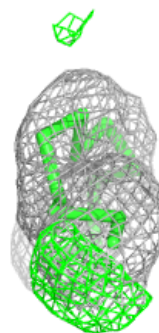
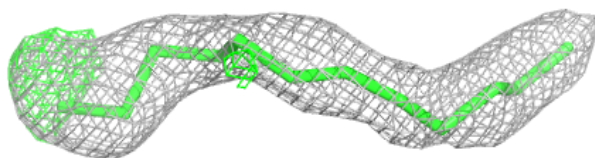
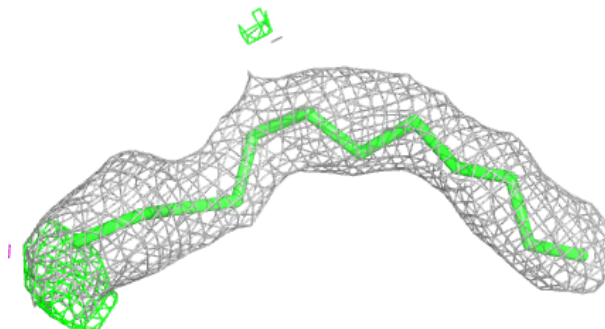


Electron density around OLC A 344:

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

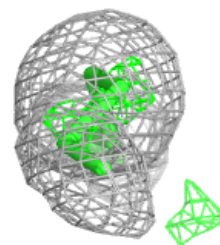
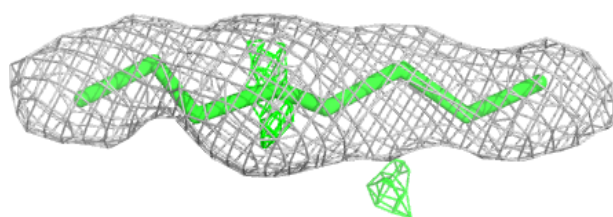
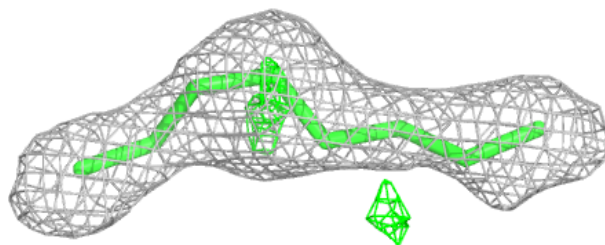
**Electron density around OLC C 364:**

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

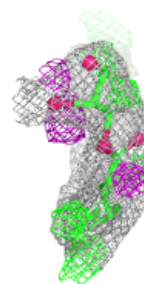
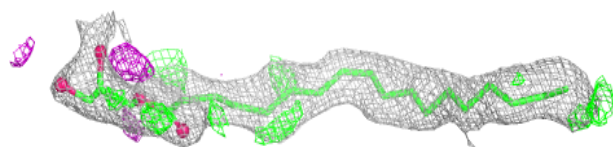
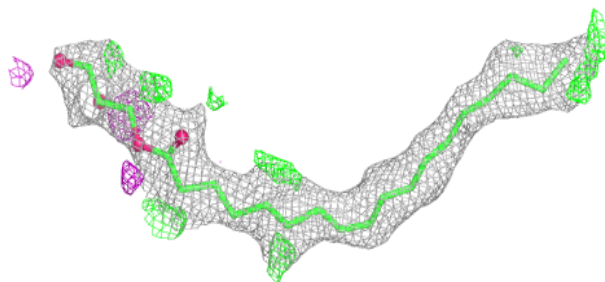


Electron density around OLC B 353:

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

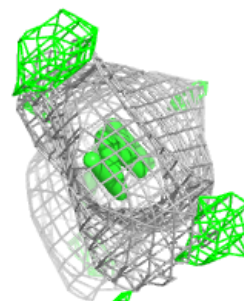
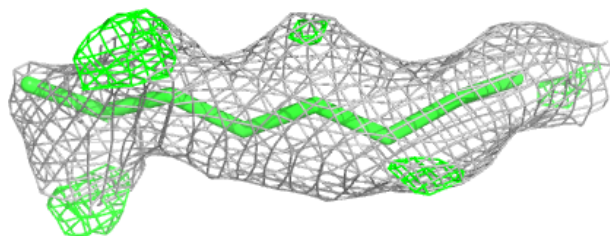
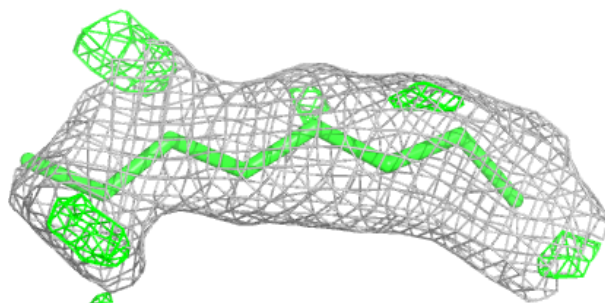
**Electron density around OLC A 346:**

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

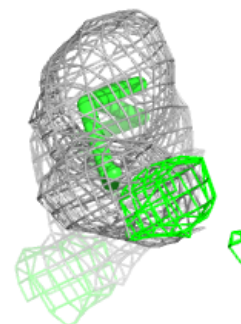
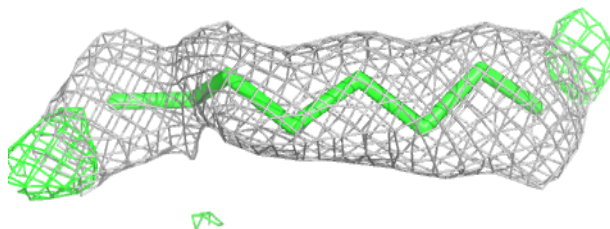
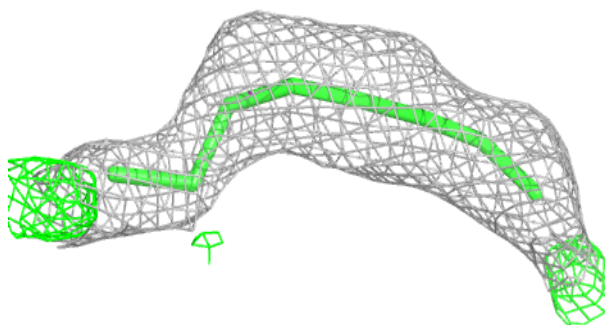


Electron density around OLC C 344:

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

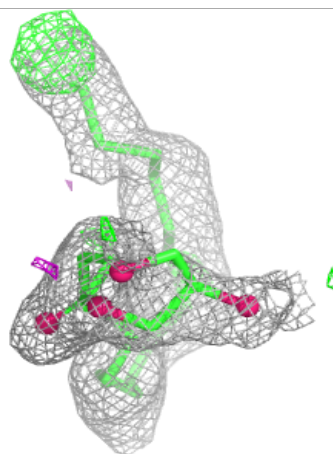
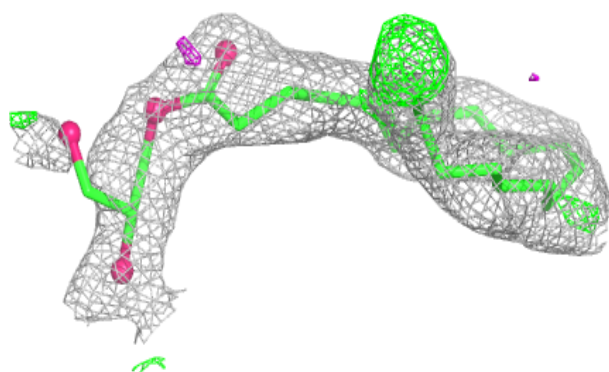
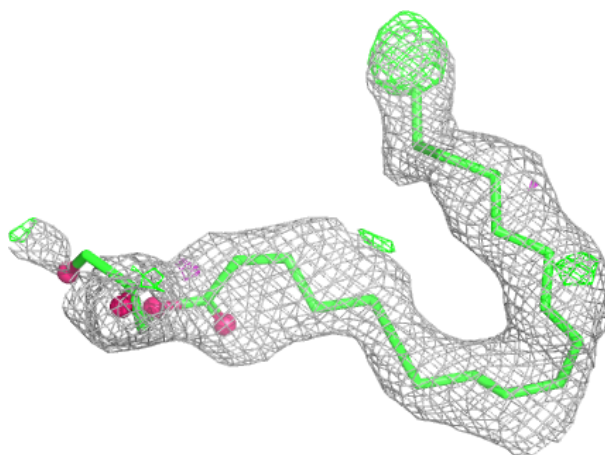
**Electron density around OLC D 347:**

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



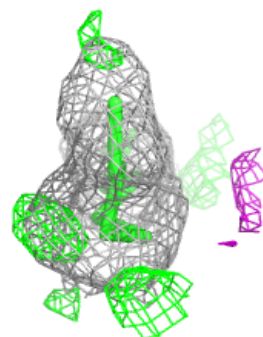
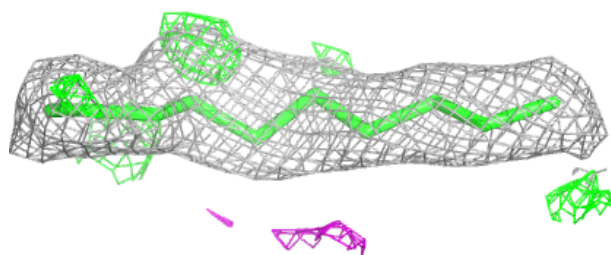
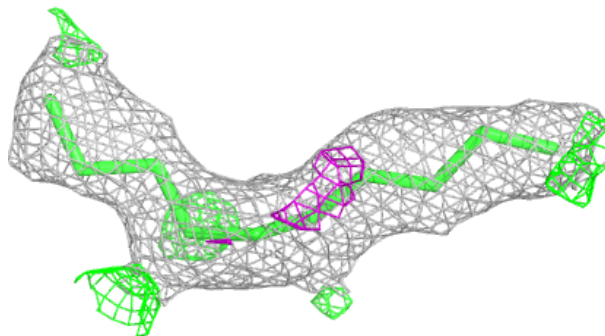
Electron density around OLC B 351:

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

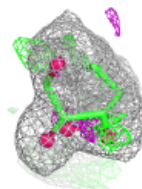
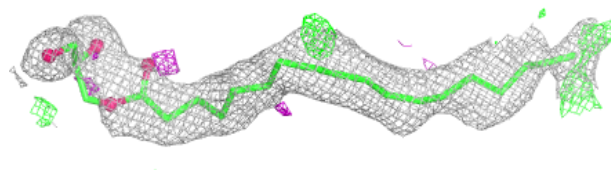
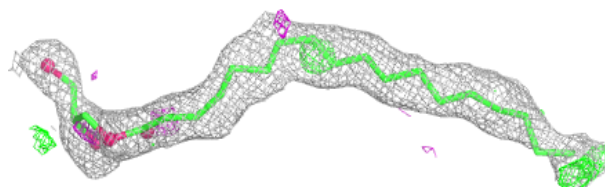


Electron density around OLC A 348:

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

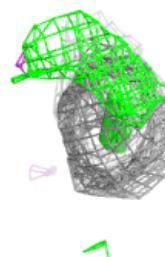
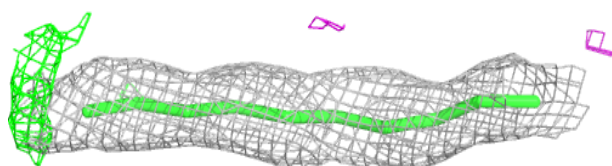
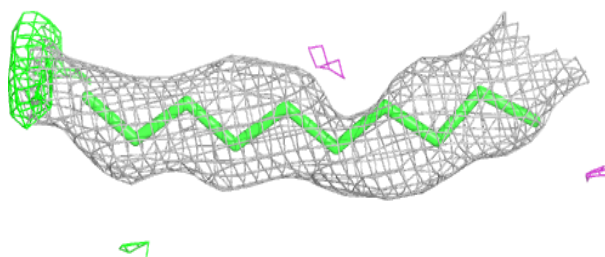
**Electron density around OLC C 362:**

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

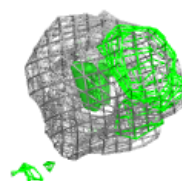
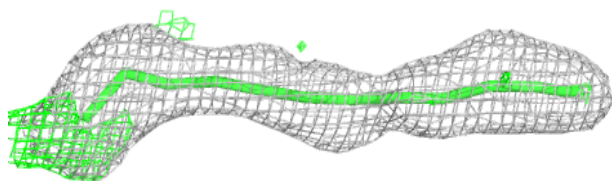
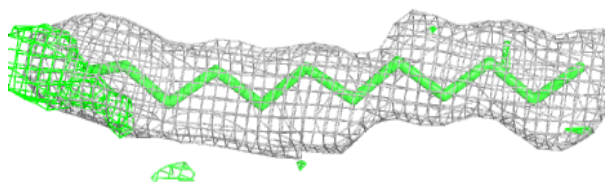


Electron density around OLC B 344:

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

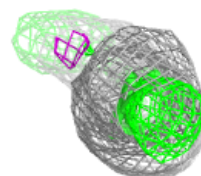
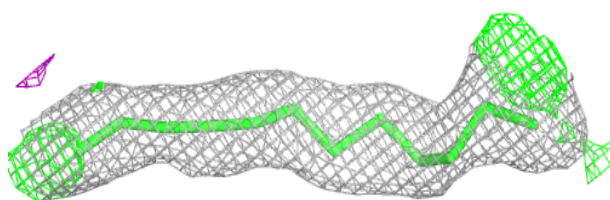
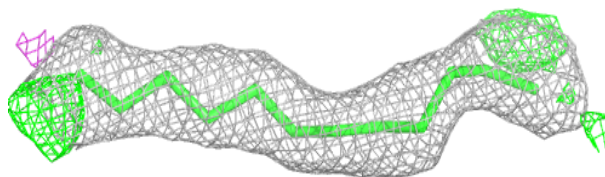
**Electron density around OLC C 345:**

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

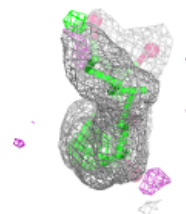
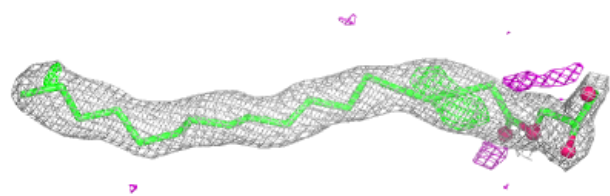
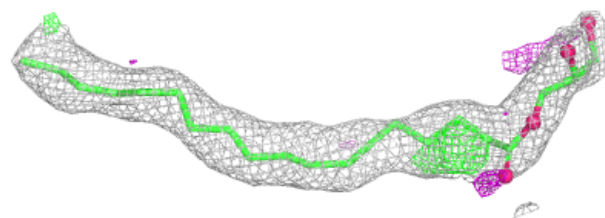


Electron density around OLC C 361:

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

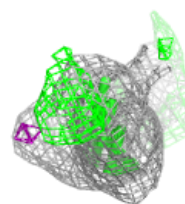
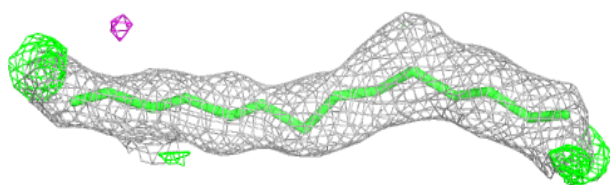
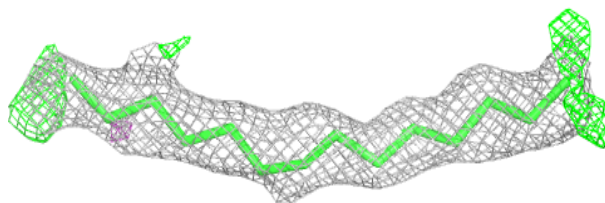
**Electron density around OLC B 350:**

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

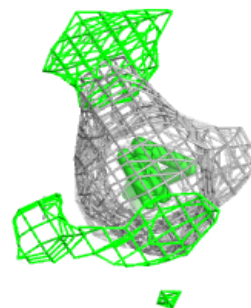
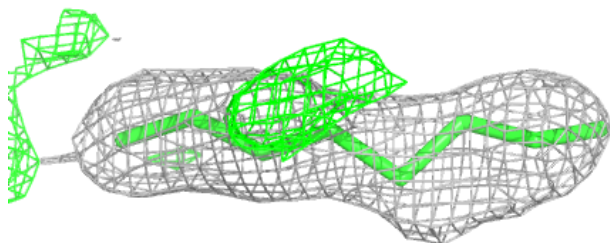
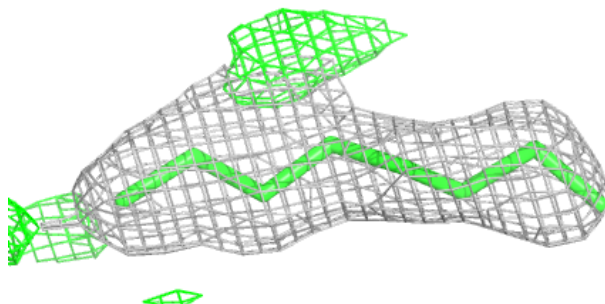


Electron density around OLC C 350:

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

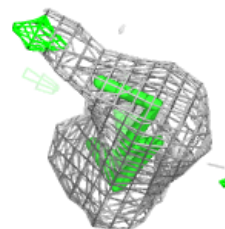
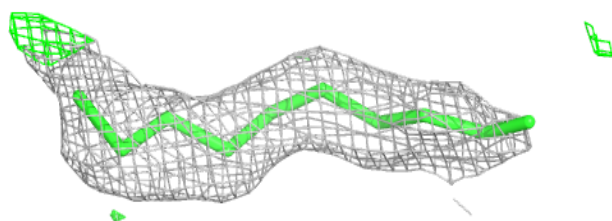
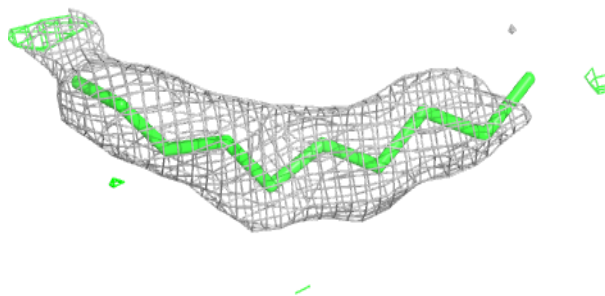
**Electron density around OLC D 348:**

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

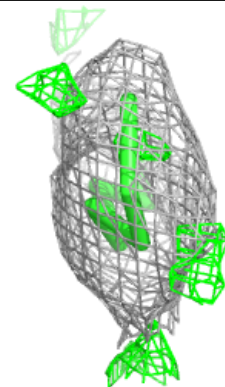
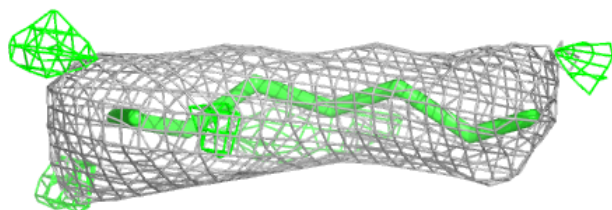
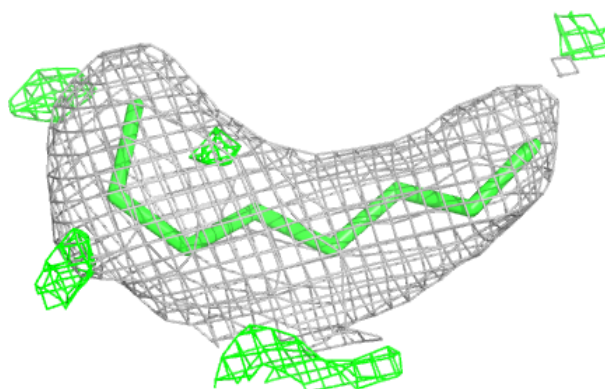


Electron density around OLC C 349:

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

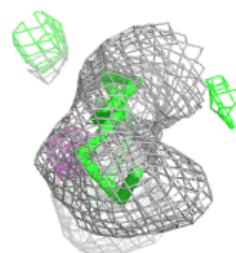
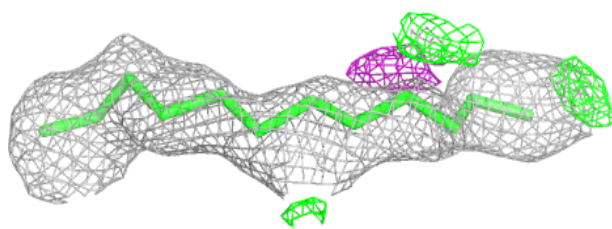
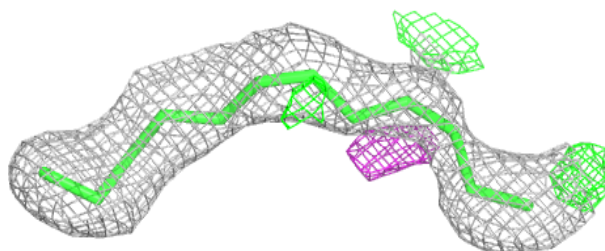
**Electron density around OLC A 342:**

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

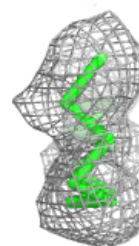
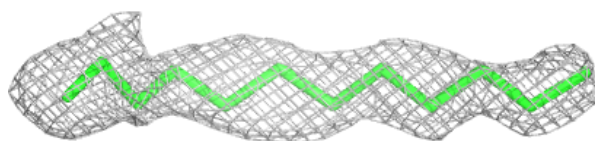
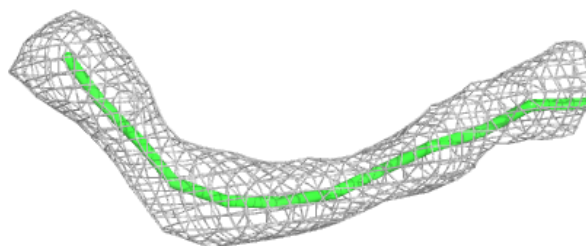


Electron density around OLC A 363:

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

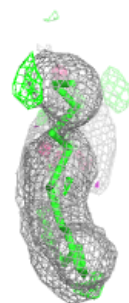
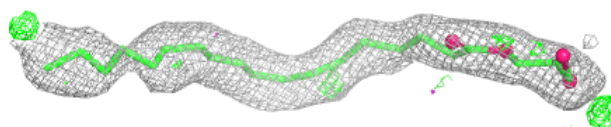
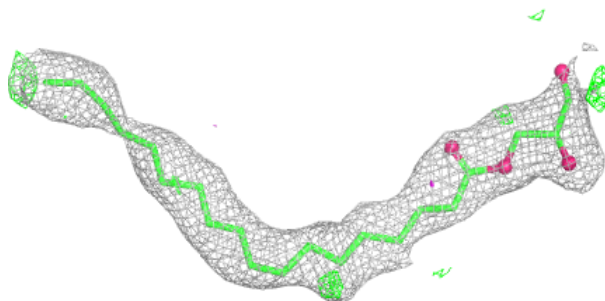
**Electron density around OLC E 344:**

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

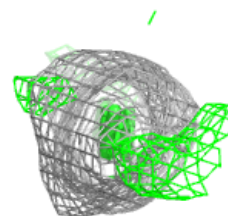
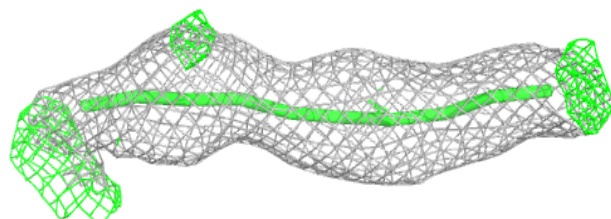
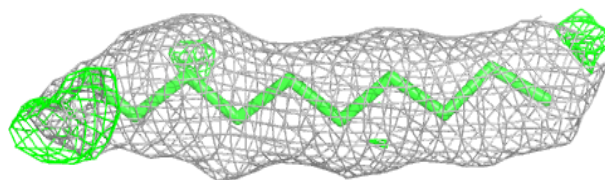


Electron density around OLC B 345:

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

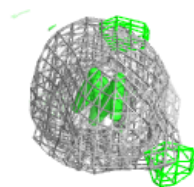
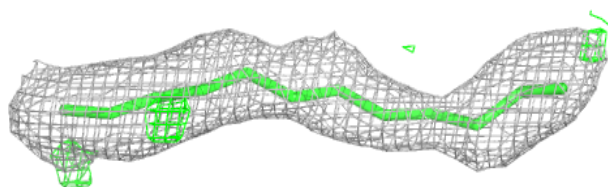
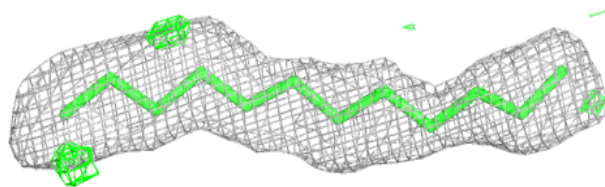
**Electron density around OLC C 355:**

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

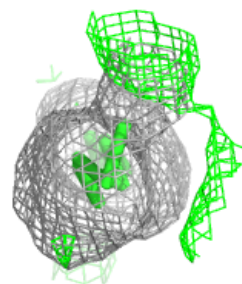
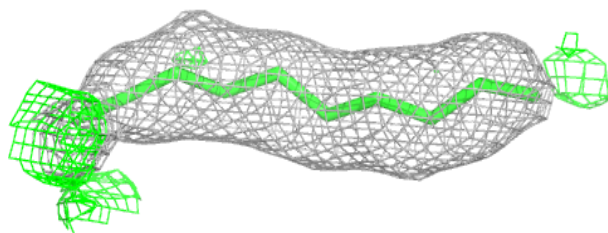
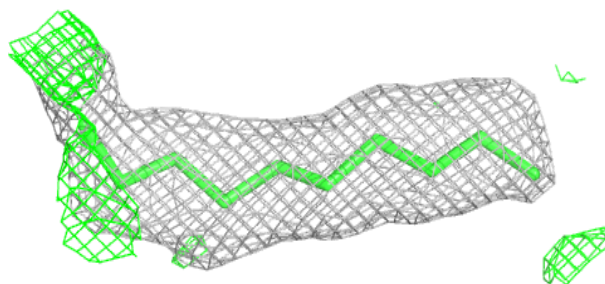


Electron density around OLC D 346:

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

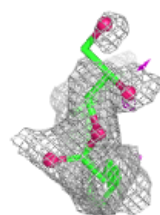
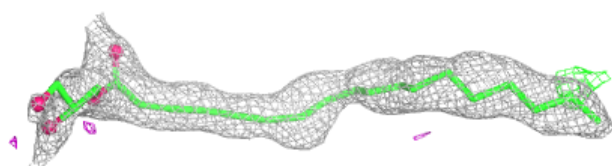
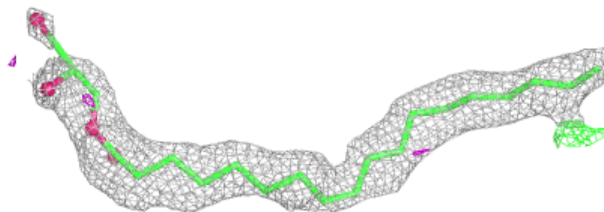
**Electron density around OLC C 346:**

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

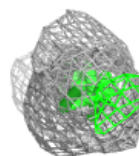
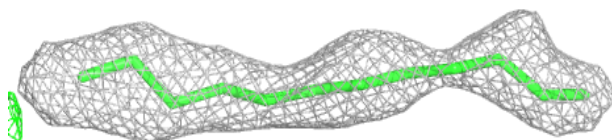
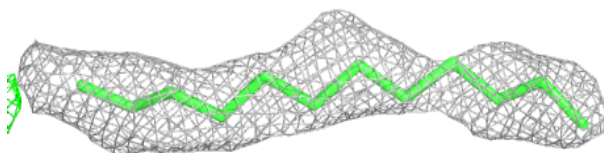


Electron density around OLC A 349:

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

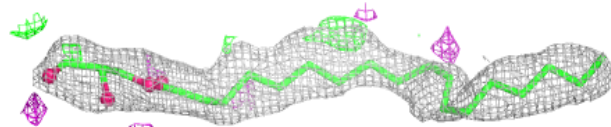
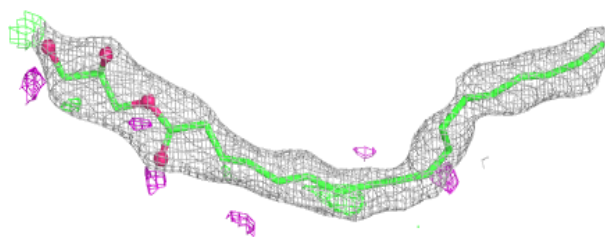
**Electron density around OLC F 345:**

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

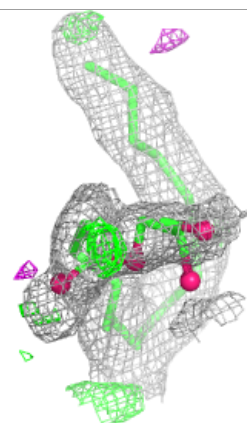
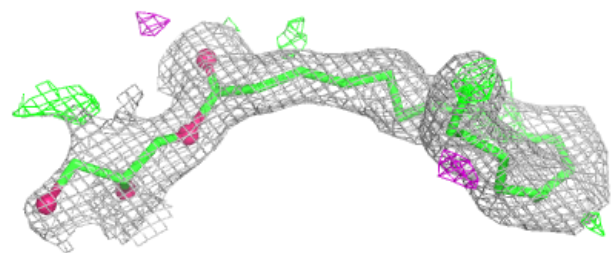
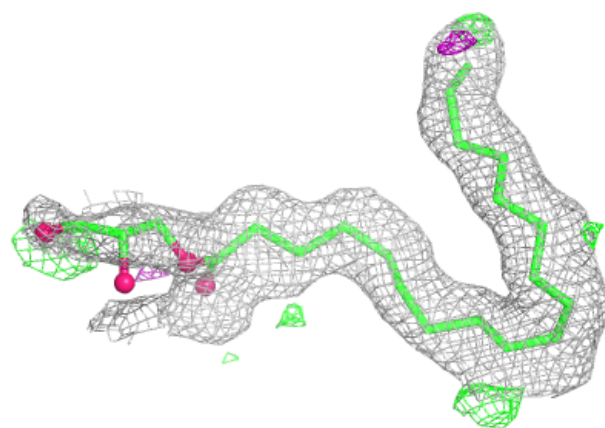


Electron density around OLC A 359:

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

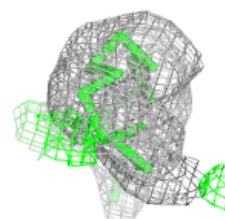
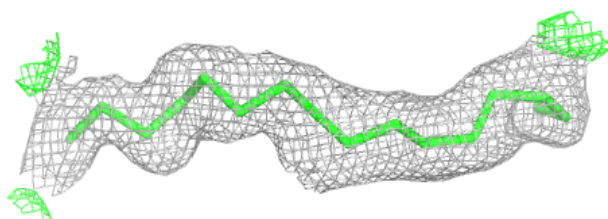
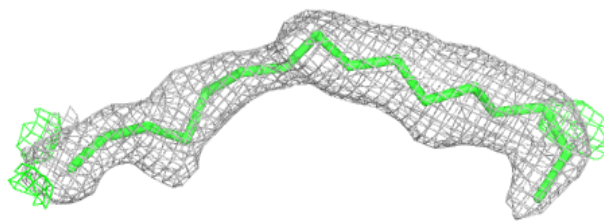
**Electron density around OLC C 360:**

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

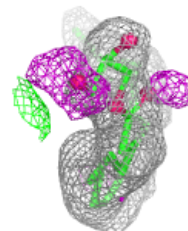
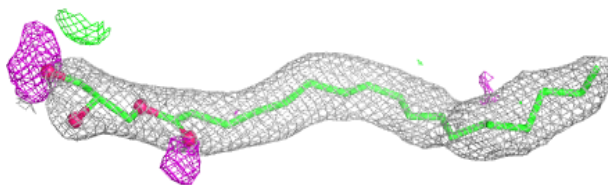
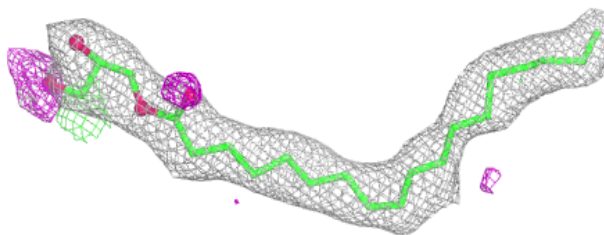


Electron density around OLC B 352:

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

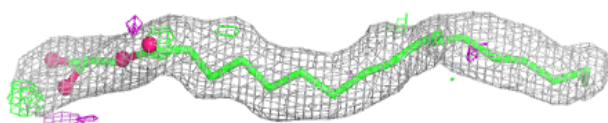
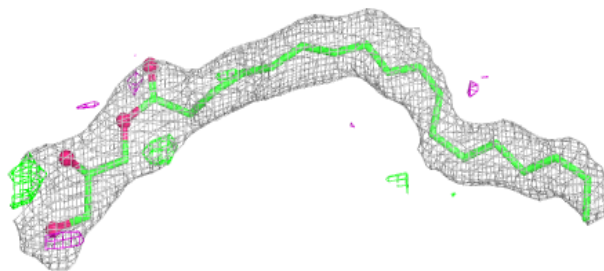
**Electron density around OLC E 341:**

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

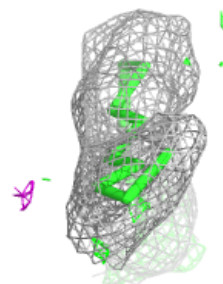
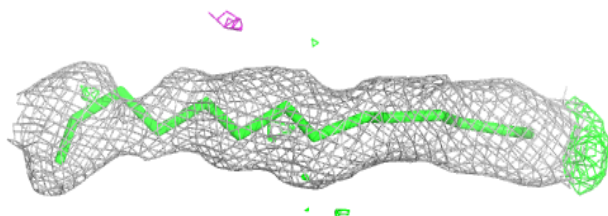
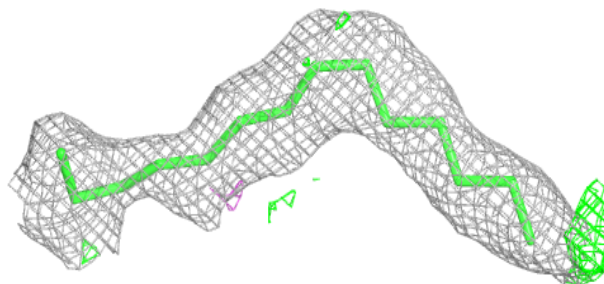


Electron density around OLC E 347:

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

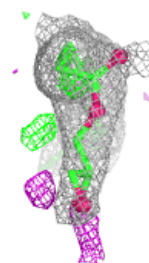
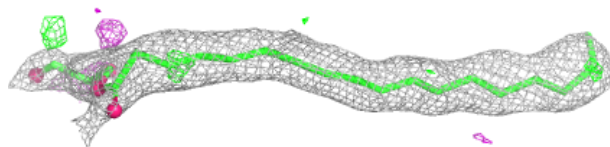
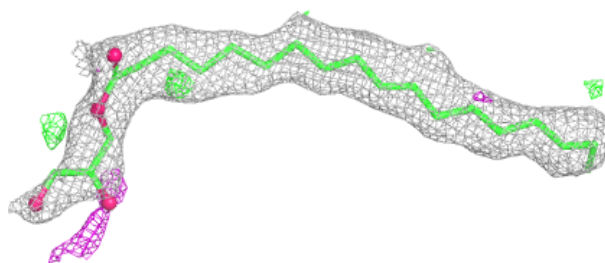
**Electron density around OLC A 350:**

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

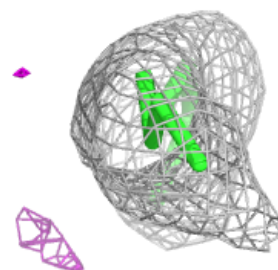
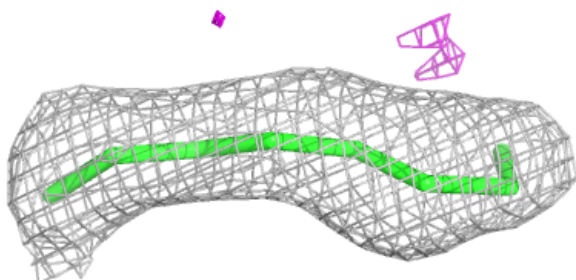
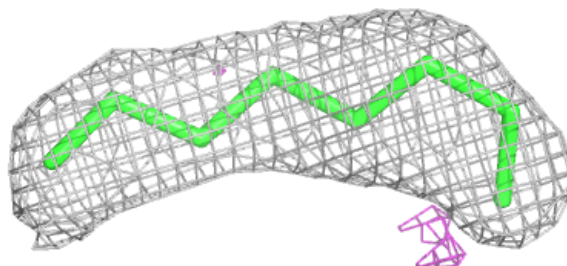


Electron density around OLC C 358:

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

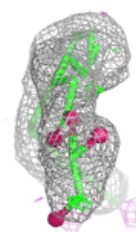
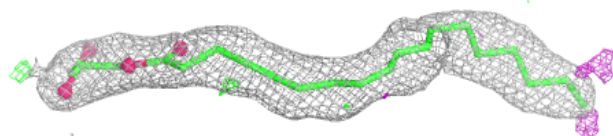
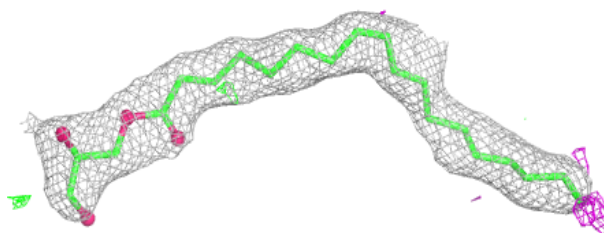
**Electron density around OLC A 343:**

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

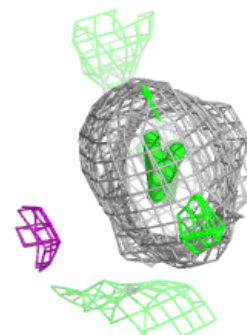
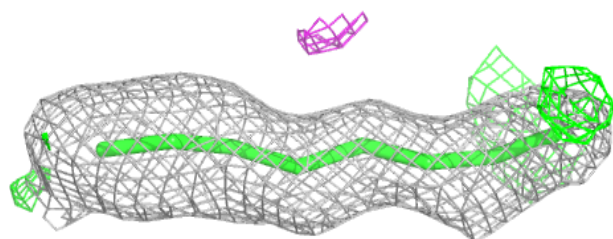
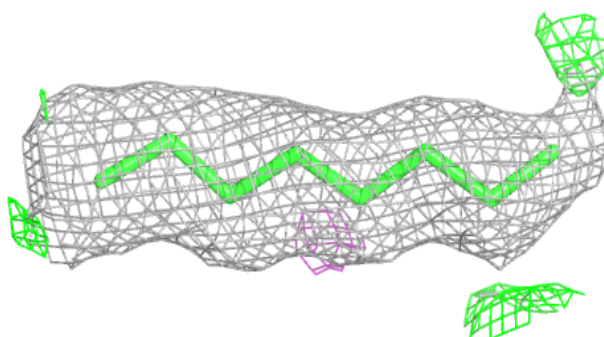


Electron density around OLC A 356:

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

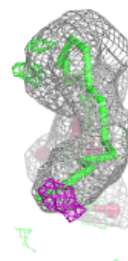
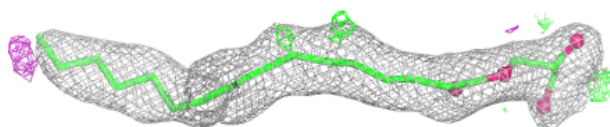
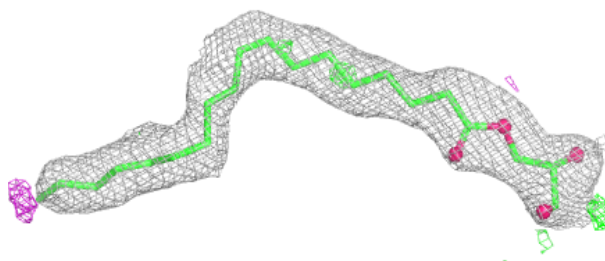
**Electron density around OLC A 345:**

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

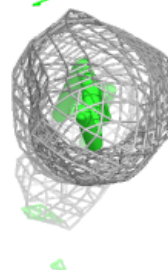
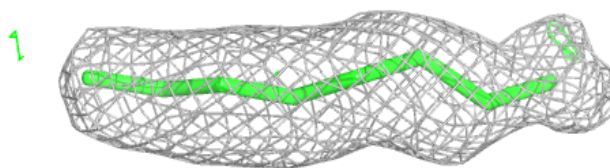
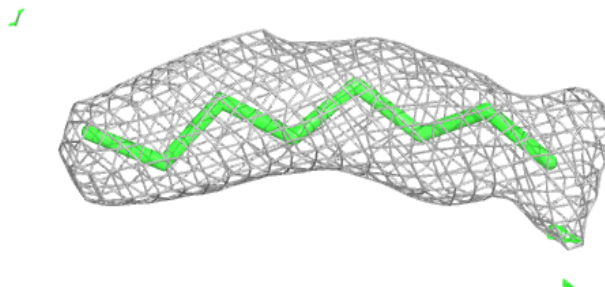


Electron density around OLC B 346:

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

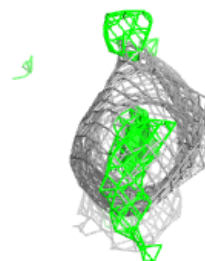
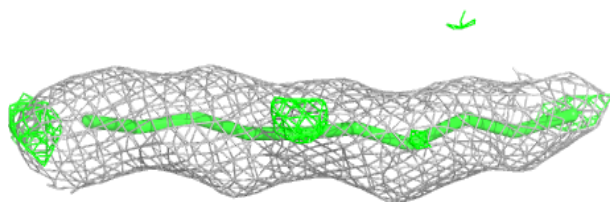
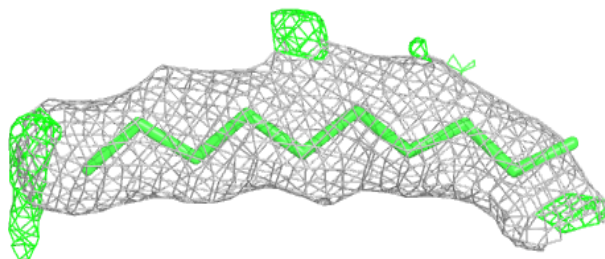
**Electron density around OLC C 342:**

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

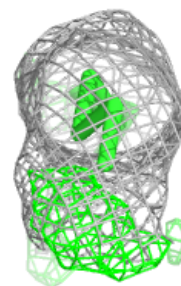
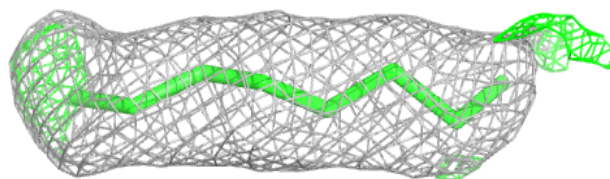
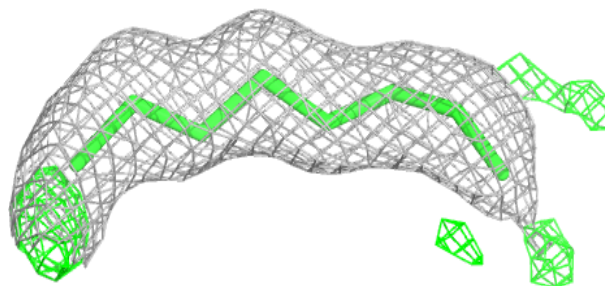


Electron density around OLC C 341:

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

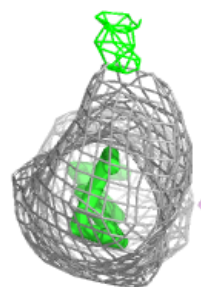
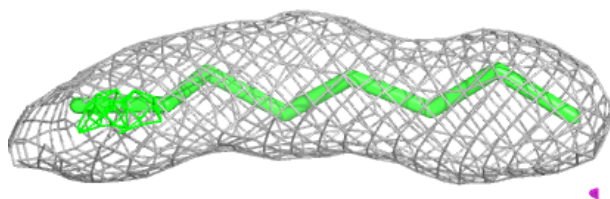
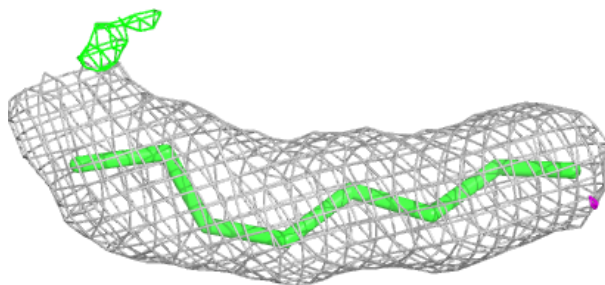
**Electron density around OLC A 354:**

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

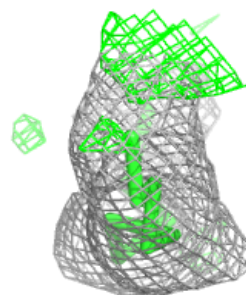
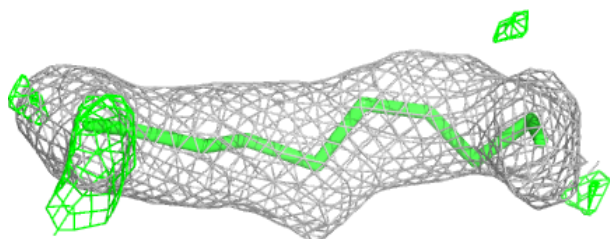
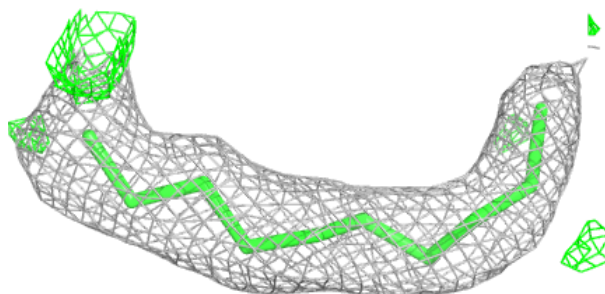


Electron density around OLC D 344:

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

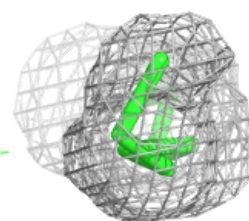
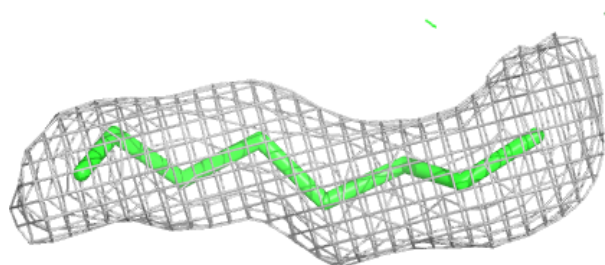
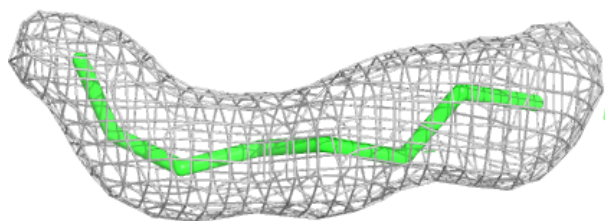
**Electron density around OLC A 357:**

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

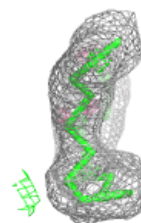
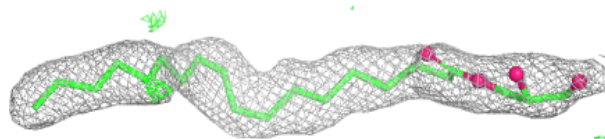
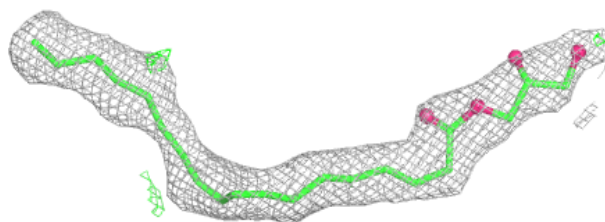


Electron density around OLC A 347:

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

**Electron density around OLC C 359:**

$2mF_o-DF_c$ (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.