



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:48 PM UTC

PDB ID : 10LE / pdb_000010le
Title : X-ray structure of the Bacteroides fragilis Nramp/MntH divalent transition metal transporter WT in an inward-open, manganese-bound state
Authors : Ray, S.; Gaudet, R.
Deposited on : 2026-01-26
Resolution : 2.40 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

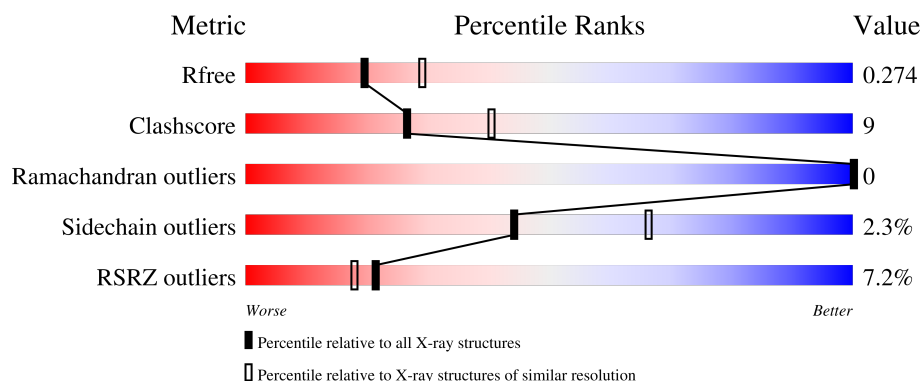
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	416	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	416	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6483 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 Divalent metal cation transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2787	1857	424	491	15			
1	B	370	Total	C	N	O	S	0	0	0
			2786	1855	424	492	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP A0A0K6BUR1
A	3	HIS	-	expression tag	UNP A0A0K6BUR1
A	4	HIS	-	expression tag	UNP A0A0K6BUR1
A	5	HIS	-	expression tag	UNP A0A0K6BUR1
A	6	HIS	-	expression tag	UNP A0A0K6BUR1
A	7	HIS	-	expression tag	UNP A0A0K6BUR1
A	8	HIS	-	expression tag	UNP A0A0K6BUR1
A	9	HIS	-	expression tag	UNP A0A0K6BUR1
A	10	HIS	-	expression tag	UNP A0A0K6BUR1
A	11	ALA	-	expression tag	UNP A0A0K6BUR1
A	12	HIS	-	expression tag	UNP A0A0K6BUR1
A	13	MET	-	expression tag	UNP A0A0K6BUR1
B	2	MET	-	initiating methionine	UNP A0A0K6BUR1
B	3	HIS	-	expression tag	UNP A0A0K6BUR1
B	4	HIS	-	expression tag	UNP A0A0K6BUR1
B	5	HIS	-	expression tag	UNP A0A0K6BUR1
B	6	HIS	-	expression tag	UNP A0A0K6BUR1
B	7	HIS	-	expression tag	UNP A0A0K6BUR1
B	8	HIS	-	expression tag	UNP A0A0K6BUR1
B	9	HIS	-	expression tag	UNP A0A0K6BUR1
B	10	HIS	-	expression tag	UNP A0A0K6BUR1
B	11	ALA	-	expression tag	UNP A0A0K6BUR1
B	12	HIS	-	expression tag	UNP A0A0K6BUR1
B	13	MET	-	expression tag	UNP A0A0K6BUR1

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2 | A | 1 | Total Mn
1 1 | 0 | 0 |
| 2 | B | 1 | Total Mn
1 1 | 0 | 0 |

- # OLC
-
- The image displays the chemical structure of 1-octadec-7-en-1-ol, a long-chain monounsaturated alcohol. The molecule consists of an 18-carbon chain. A double bond is located between carbons 7 and 8, and a hydroxyl group is attached to carbon 1. The carbons are labeled C1 through C18, and the oxygens are labeled O00 and O01. The hydroxyl group is shown in red, with the oxygen atom labeled O01 and the hydrogen atom labeled H01. The carbon chain is shown in a zig-zag conformation, with the double bond between C7 and C8. The hydroxyl group is attached to C1, and the oxygen atom is labeled O01. The carbon chain is labeled C1 through C18, and the oxygen atoms are labeled O00 and O01.
- CCCCC/C=C\CCCCO

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 24 20 4	0	0
3	A	1	Total C O 11 7 4	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C O 22 18 4	0	0
3	A	1	Total C 12 12	0	0
3	A	1	Total C 14 14	0	0
3	A	1	Total C 17 17	0	0
3	A	1	Total C 9 9	0	0



WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 8 8	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C O 16 12 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 13 13	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 7 7	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 17 17	0	0
3	A	1	Total C 18 18	0	0

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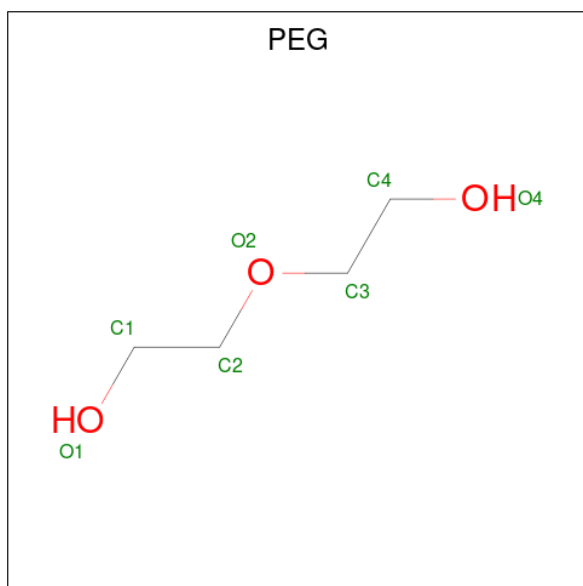
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 18 14 4	0	0
3	B	1	Total C O 23 19 4	0	0
3	B	1	Total C 15 15	0	0
3	B	1	Total C O 14 10 4	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 14 14	0	0
3	B	1	Total C 5 5	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 20 16 4	0	0
3	B	1	Total C 13 13	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C O 25 21 4	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C O 25 21 4	0	0
3	B	1	Total C O 11 7 4	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C O 13 9 4	0	0
3	B	1	Total C 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C 10 10	0	0
3	B	1	Total C O 25 21 4	0	0
3	B	1	Total C 15 15	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 17 17	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 4 2	0	0
4	B	1	Total C O 4 3 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total 52	O 52	0	0
5	B	52	Total 52	O 52	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	68.85Å 101.91Å 118.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.84 – 2.40 46.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.84-2.40) 99.7 (46.84-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.238 , 0.275 0.238 , 0.274	Depositor DCC
R_{free} test set	2000 reflections (5.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6483	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1082e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, OLC, MN

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	0.09	0/2845	0.23	0/3876
1	B	0.09	0/2844	0.24	0/3875
All	All	0.09	0/5689	0.24	0/7751

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

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	2787	0	2907	52	0
1	B	2786	0	2900	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	413	0	675	38	0
3	B	381	0	599	41	0
4	A	6	0	7	0	0
4	B	4	0	2	0	0
5	A	52	0	0	0	0
5	B	52	0	0	0	0
All	All	6483	0	7090	125	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 9.

All (125) 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:159:ILE:HG23	1:B:302:MET:HB3	1.70	0.73
1:A:191:PRO:HG3	3:A:519:OLC:H17	1.68	0.72
1:A:336:VAL:HG12	3:B:514:OLC:H5	1.73	0.69
1:A:340:LEU:HB2	3:B:514:OLC:H11	1.76	0.66
1:B:190:THR:HG22	3:B:510:OLC:H8A	1.76	0.66
1:A:339:ILE:HB	3:B:514:OLC:H9	1.78	0.65
1:A:159:ILE:HG23	1:A:302:MET:HB3	1.78	0.65
1:A:68:ILE:HG12	1:A:249:MET:HG3	1.80	0.64
1:B:346:LEU:HA	1:B:349:ILE:HD12	1.80	0.63
3:B:522:OLC:H8	3:B:524:OLC:H13A	1.81	0.62
1:A:168:LEU:HD22	3:A:502:OLC:H13	1.80	0.62
1:A:247:PHE:HB2	3:A:509:OLC:H17A	1.82	0.62
1:B:406:ILE:HG23	3:B:519:OLC:H8A	1.82	0.61
1:A:348:LEU:HD13	1:B:348:LEU:HG	1.82	0.61
1:B:68:ILE:HG12	1:B:249:MET:HG3	1.83	0.61
1:A:357:LYS:HG2	3:A:524:OLC:H2A	1.82	0.60
1:B:103:GLY:HA3	3:B:514:OLC:H13	1.84	0.59
3:A:511:OLC:H14A	3:A:520:OLC:H7A	1.84	0.58
1:A:95:LYS:HE3	3:A:514:OLC:H24A	1.87	0.57
1:A:295:VAL:HG22	3:A:504:OLC:H10	1.87	0.56
1:A:244:ASP:HA	3:A:509:OLC:H18A	1.87	0.56
1:B:136:ALA:HB1	1:B:349:ILE:HD13	1.88	0.55
1:B:193:ILE:H	3:B:524:OLC:H9	1.70	0.55
1:A:348:LEU:HD11	1:B:351:PHE:HB2	1.88	0.55
3:B:522:OLC:H11	3:B:524:OLC:H15A	1.89	0.55
3:A:509:OLC:H18B	3:A:509:OLC:H12A	1.88	0.55
1:A:148:PHE:CE1	3:B:514:OLC:H2	2.41	0.55
1:A:72:HIS:CD2	1:A:242:LEU:HB2	2.41	0.54
1:B:97:VAL:HG11	3:B:504:OLC:H11A	1.89	0.54
1:B:378:VAL:HG22	1:B:400:LEU:HB3	1.90	0.54
3:B:519:OLC:H9	3:B:524:OLC:H18	1.90	0.53
1:B:93:THR:HG22	3:B:504:OLC:H7	1.90	0.52
1:B:104:THR:HG22	3:B:514:OLC:H18	1.90	0.52
1:B:399:VAL:HG21	3:B:529:OLC:H13	1.91	0.52
1:A:242:LEU:HD21	3:A:526:OLC:H4A	1.92	0.52
1:B:357:LYS:HE3	3:B:503:OLC:H3A	1.92	0.52
3:B:527:OLC:H12	3:B:528:OLC:H14A	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:MET:HE3	1:B:367:SER:HB3	1.91	0.51
1:B:288:LEU:C	3:B:505:OLC:H2A	2.36	0.51
1:A:156:GLU:O	1:A:160:ILE:HG12	2.10	0.51
1:B:128:LEU:HD21	3:B:507:OLC:H8	1.92	0.51
1:B:118:LEU:HD11	1:B:355:PRO:HB3	1.92	0.51
1:A:152:TYR:HB2	1:A:309:ILE:HD13	1.93	0.50
1:A:147:LEU:HD21	1:A:309:ILE:HG23	1.92	0.50
1:A:175:PHE:HE2	3:A:530:OLC:H14	1.77	0.50
1:A:148:PHE:HE1	3:B:514:OLC:H2	1.76	0.50
1:B:178:ASP:HB2	3:B:502:OLC:H22	1.93	0.49
1:B:247:PHE:HB2	3:B:527:OLC:H18B	1.94	0.49
1:A:374:VAL:O	1:A:378:VAL:HG23	2.13	0.49
1:B:374:VAL:O	1:B:378:VAL:HG23	2.12	0.49
1:B:191:PRO:HG2	3:B:522:OLC:H18	1.94	0.49
1:A:136:ALA:HB1	1:A:349:ILE:HD13	1.94	0.49
1:B:395:TRP:HE1	3:B:529:OLC:H12A	1.78	0.49
1:B:186:GLU:HB2	3:B:510:OLC:H21A	1.95	0.49
1:B:289:GLY:HA3	3:B:505:OLC:H4A	1.95	0.49
1:A:58:TRP:HB2	3:A:519:OLC:H17A	1.95	0.48
1:A:247:PHE:H	3:A:509:OLC:H18	1.79	0.48
1:B:36:PHE:HD1	1:B:160:ILE:HG23	1.79	0.48
1:A:181:TRP:CG	3:A:508:OLC:H3	2.49	0.48
1:A:199:LEU:HD21	3:A:524:OLC:H3A	1.96	0.47
1:B:192:ALA:HA	3:B:524:OLC:H9	1.95	0.47
1:A:57:LEU:HB3	1:A:188:TRP:CD1	2.50	0.47
1:A:357:LYS:HZ2	3:A:524:OLC:H24	1.80	0.47
1:A:172:TYR:HB2	3:A:502:OLC:H8	1.96	0.46
3:A:511:OLC:H14	3:A:512:OLC:H7	1.96	0.46
3:A:512:OLC:H8A	3:A:520:OLC:H10	1.97	0.46
3:A:509:OLC:H17A	3:A:522:OLC:H16A	1.97	0.46
1:B:143:VAL:HG11	1:B:308:THR:HG22	1.98	0.46
1:A:378:VAL:HG22	1:A:400:LEU:HB3	1.97	0.46
1:B:147:LEU:HD21	1:B:309:ILE:HG23	1.98	0.46
1:B:112:THR:O	1:B:116:GLU:HG2	2.16	0.45
1:B:284:LEU:HB3	1:B:288:LEU:HD12	1.98	0.45
1:A:112:THR:O	1:A:116:GLU:HG2	2.15	0.45
1:A:351:PHE:CG	1:B:348:LEU:HD21	2.52	0.45
1:B:64:THR:O	1:B:68:ILE:HG13	2.16	0.45
1:B:395:TRP:NE1	3:B:529:OLC:H12A	2.31	0.45
1:A:202:MET:HE3	1:A:367:SER:HB3	1.99	0.45
3:B:520:OLC:H14	3:B:520:OLC:H11	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:HG23	1:A:179:ILE:HG13	1.97	0.44
1:A:211:PRO:HB3	1:A:370:LEU:HD13	2.00	0.44
3:A:524:OLC:H2	3:A:524:OLC:H5A	1.75	0.44
1:B:339:ILE:HB	3:B:520:OLC:H12	1.98	0.44
1:A:127:LEU:HD13	3:A:515:OLC:H11A	1.99	0.44
3:A:529:OLC:H15A	1:B:104:THR:HB	1.99	0.44
3:B:514:OLC:H12	3:B:514:OLC:H15	1.49	0.44
1:B:169:SER:HB3	1:B:287:LEU:HD22	1.99	0.44
1:A:76:HIS:CD2	3:A:503:OLC:H21	2.52	0.44
1:B:156:GLU:O	1:B:160:ILE:HG13	2.18	0.44
1:B:242:LEU:HD21	3:B:529:OLC:H6A	2.00	0.43
1:A:245:THR:HG22	1:A:249:MET:HG2	2.00	0.43
3:B:514:OLC:H5A	3:B:514:OLC:H8	1.80	0.43
3:A:502:OLC:H10	3:A:502:OLC:H7	1.72	0.43
3:A:529:OLC:H18A	3:A:529:OLC:H15	1.87	0.43
1:B:57:LEU:HB3	1:B:188:TRP:CD1	2.54	0.43
3:A:511:OLC:H18A	3:A:511:OLC:H15	1.76	0.43
1:B:110:ILE:HD13	1:B:344:ILE:HG21	1.99	0.43
1:A:194:PRO:HG3	3:A:511:OLC:H3	2.00	0.43
1:A:101:ILE:HD11	3:A:507:OLC:H16	1.99	0.43
1:B:325:GLU:HG3	1:B:326:SER:H	1.83	0.42
1:B:170:PHE:HD1	1:B:262:LEU:HD12	1.84	0.42
1:B:186:GLU:HG3	3:B:510:OLC:H3	2.00	0.42
1:B:375:PHE:HB3	3:B:504:OLC:H14A	2.01	0.42
3:B:522:OLC:H4	3:B:523:OLC:H14A	2.01	0.42
1:B:354:ASP:HB3	1:B:357:LYS:HB2	2.02	0.42
3:A:529:OLC:H18	1:B:365:VAL:HG13	2.02	0.42
1:A:63:SER:HA	1:A:66:MET:HE2	2.02	0.41
3:A:525:OLC:H11A	3:A:525:OLC:H14A	1.85	0.41
3:B:515:OLC:H16	3:B:515:OLC:H13	1.68	0.41
1:A:350:PHE:CZ	3:A:529:OLC:H6	2.56	0.41
1:A:67:LEU:O	1:A:71:GLN:HB2	2.21	0.41
3:A:512:OLC:H6	3:A:520:OLC:H9	2.02	0.41
1:A:143:VAL:HG11	1:A:308:THR:HG22	2.01	0.41
3:A:507:OLC:H9	3:A:507:OLC:H12A	1.78	0.41
3:B:504:OLC:H8A	3:B:504:OLC:H5	1.65	0.41
1:A:170:PHE:HD1	1:A:262:LEU:HD12	1.86	0.41
1:A:160:ILE:HD11	1:A:306:SER:OG	2.21	0.41
1:A:114:LEU:HG	1:A:348:LEU:HD23	2.03	0.40
3:A:526:OLC:H5	3:A:526:OLC:H11	2.03	0.40
3:B:514:OLC:H3	3:B:514:OLC:H6	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:TRP:HE1	3:A:526:OLC:C9	2.34	0.40
1:B:193:ILE:HB	3:B:521:OLC:H2	2.02	0.40
3:B:522:OLC:H12	3:B:522:OLC:H15A	1.79	0.40
1:A:73:ASN:HB2	3:A:503:OLC:H3A	2.02	0.40
1:A:376:LEU:HA	3:A:507:OLC:H13	2.04	0.40
1:B:58:TRP:CD2	1:B:191:PRO:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/416 (88%)	359 (99%)	5 (1%)	0	100	100
1	B	364/416 (88%)	361 (99%)	3 (1%)	0	100	100
All	All	728/832 (88%)	720 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/350 (87%)	296 (98%)	7 (2%)	44	66
1	B	303/350 (87%)	296 (98%)	7 (2%)	44	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	606/700 (87%)	592 (98%)	14 (2%)	44 66

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ILE
1	A	164	SER
1	A	219	GLU
1	A	244	ASP
1	A	349	ILE
1	A	364	MET
1	A	378	VAL
1	B	106	VAL
1	B	132	ILE
1	B	159	ILE
1	B	164	SER
1	B	188	TRP
1	B	273	GLN
1	B	378	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	B	73	ASN
1	B	217	HIS
1	B	377	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 61 ligands modelled in this entry, 2 are monoatomic - leaving 59 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	$\# Z > 2$
3	OLC	A	503	-	10,10,24	0.48	0	11,11,25	0.48	0
3	OLC	B	505	-	13,13,24	0.41	0	14,14,25	0.44	0
3	OLC	B	526	-	6,6,24	0.28	0	5,5,25	0.09	0
3	OLC	B	529	-	16,16,24	0.24	0	15,15,25	0.28	0
3	OLC	A	528	-	15,15,24	0.24	0	14,14,25	0.24	0
3	OLC	B	509	-	9,9,24	0.45	0	10,10,25	0.55	0
3	OLC	A	512	-	12,12,24	0.24	0	11,11,25	0.26	0
3	OLC	A	527	-	6,6,24	0.25	0	5,5,25	0.20	0
3	OLC	B	520	-	10,10,24	0.26	0	9,9,25	0.24	0
3	OLC	A	525	-	12,12,24	0.24	0	11,11,25	0.32	0
3	OLC	B	517	-	10,10,24	0.48	0	11,11,25	0.50	0
3	OLC	B	522	-	16,16,24	0.23	0	15,15,25	0.23	0
3	OLC	B	527	-	11,11,24	0.28	0	10,10,25	0.36	0
3	OLC	B	503	-	22,22,24	0.36	0	23,23,25	0.40	0
3	OLC	B	528	-	10,10,24	0.29	0	9,9,25	0.19	0
3	OLC	B	512	-	5,5,24	0.27	0	4,4,25	0.16	0
3	OLC	A	513	-	9,9,24	0.27	0	8,8,25	0.27	0
3	OLC	B	519	-	11,11,24	0.31	0	10,10,25	0.23	0
3	OLC	A	510	-	7,7,24	0.28	0	6,6,25	0.12	0
3	OLC	A	511	-	24,24,24	0.36	0	25,25,25	0.42	0
3	OLC	B	518	-	5,5,24	0.29	0	4,4,25	0.13	0
3	OLC	B	508	-	4,4,24	0.22	0	3,3,25	0.26	0
3	OLC	B	515	-	8,8,24	0.24	0	7,7,25	0.15	0
3	OLC	A	521	-	8,8,24	0.24	0	7,7,25	0.17	0
3	OLC	B	524	-	24,24,24	0.34	0	25,25,25	0.41	0
3	OLC	A	526	-	17,17,24	0.23	0	16,16,25	0.23	0
4	PEG	A	531	-	5,5,6	0.32	0	4,4,5	0.21	0
3	OLC	B	516	-	24,24,24	0.33	0	25,25,25	0.50	0
3	OLC	A	502	-	23,23,24	0.34	0	24,24,25	0.43	0
3	OLC	A	506	-	11,11,24	0.29	0	10,10,25	0.25	0
3	OLC	B	506	-	10,10,24	0.27	0	9,9,25	0.19	0
3	OLC	B	514	-	24,24,24	0.34	0	25,25,25	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OLC	B	513	-	5,5,24	0.27	0	4,4,25	0.19	0
3	OLC	A	505	-	21,21,24	0.36	0	22,22,25	0.40	0
3	OLC	A	523	-	4,4,24	0.29	0	3,3,25	0.23	0
3	OLC	B	523	-	9,9,24	0.34	0	8,8,25	0.18	0
4	PEG	B	530	-	3,3,6	0.33	0	2,2,5	0.06	0
3	OLC	A	509	-	8,8,24	0.22	0	7,7,25	0.20	0
3	OLC	B	511	-	12,12,24	0.24	0	11,11,25	0.28	0
3	OLC	A	530	-	17,17,24	0.21	0	16,16,25	0.28	0
3	OLC	A	522	-	8,8,24	0.23	0	7,7,25	0.21	0
3	OLC	B	525	-	14,14,24	0.23	0	13,13,25	0.25	0
3	OLC	A	518	-	3,3,24	0.34	0	2,2,25	0.54	0
3	OLC	A	515	-	24,24,24	0.34	0	25,25,25	0.40	0
3	OLC	B	507	-	13,13,24	0.22	0	12,12,25	0.28	0
3	OLC	B	510	-	19,19,24	0.38	0	20,20,25	0.39	0
3	OLC	B	521	-	12,12,24	0.42	0	13,13,25	0.46	0
3	OLC	A	524	-	24,24,24	0.34	0	25,25,25	0.35	0
3	OLC	A	516	-	8,8,24	0.19	0	7,7,25	0.26	0
3	OLC	A	519	-	4,4,24	0.27	0	3,3,25	0.23	0
3	OLC	B	504	-	14,14,24	0.23	0	13,13,25	0.28	0
3	OLC	A	529	-	16,16,24	0.23	0	15,15,25	0.26	0
3	OLC	A	504	-	15,15,24	0.24	0	14,14,25	0.26	0
3	OLC	A	514	-	15,15,24	0.39	0	16,16,25	0.44	0
3	OLC	A	520	-	24,24,24	0.34	0	25,25,25	0.35	0
3	OLC	A	517	-	10,10,24	0.26	0	9,9,25	0.20	0
3	OLC	B	502	-	17,17,24	0.41	0	18,18,25	0.54	0
3	OLC	A	507	-	13,13,24	0.23	0	12,12,25	0.27	0
3	OLC	A	508	-	16,16,24	0.23	0	15,15,25	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	503	-	-	1/10/10/24	-
3	OLC	B	505	-	-	7/13/13/24	-
3	OLC	B	526	-	-	3/4/4/24	-
3	OLC	B	529	-	-	5/14/14/24	-
3	OLC	A	528	-	-	7/13/13/24	-
3	OLC	B	509	-	-	4/9/9/24	-
3	OLC	A	512	-	-	4/10/10/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	527	-	-	1/4/4/24	-
3	OLC	B	520	-	-	4/8/8/24	-
3	OLC	A	525	-	-	2/10/10/24	-
3	OLC	B	517	-	-	4/10/10/24	-
3	OLC	B	522	-	-	8/14/14/24	-
3	OLC	B	527	-	-	6/9/9/24	-
3	OLC	B	503	-	-	6/22/22/24	-
3	OLC	B	528	-	-	4/8/8/24	-
3	OLC	B	512	-	-	2/3/3/24	-
3	OLC	A	513	-	-	4/7/7/24	-
3	OLC	B	519	-	-	3/9/9/24	-
3	OLC	A	510	-	-	2/5/5/24	-
3	OLC	A	511	-	-	10/24/24/24	-
3	OLC	B	518	-	-	2/3/3/24	-
3	OLC	B	508	-	-	1/2/2/24	-
3	OLC	B	515	-	-	4/6/6/24	-
3	OLC	A	521	-	-	2/6/6/24	-
3	OLC	B	524	-	-	12/24/24/24	-
3	OLC	A	526	-	-	6/15/15/24	-
4	PEG	A	531	-	-	1/3/3/4	-
3	OLC	B	516	-	-	13/24/24/24	-
3	OLC	A	502	-	-	6/23/23/24	-
3	OLC	A	506	-	-	1/9/9/24	-
3	OLC	B	506	-	-	1/8/8/24	-
3	OLC	B	514	-	-	17/24/24/24	-
3	OLC	B	513	-	-	3/3/3/24	-
3	OLC	A	505	-	-	6/21/21/24	-
3	OLC	A	523	-	-	1/2/2/24	-
3	OLC	B	523	-	-	5/7/7/24	-
4	PEG	B	530	-	-	0/0/1/4	-
3	OLC	A	509	-	-	4/6/6/24	-
3	OLC	B	511	-	-	3/10/10/24	-
3	OLC	A	530	-	-	9/15/15/24	-
3	OLC	A	522	-	-	3/6/6/24	-
3	OLC	B	525	-	-	3/12/12/24	-
3	OLC	A	518	-	-	0/1/1/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	515	-	-	13/24/24/24	-
3	OLC	B	507	-	-	1/11/11/24	-
3	OLC	B	510	-	-	7/19/19/24	-
3	OLC	B	521	-	-	6/12/12/24	-
3	OLC	A	524	-	-	12/24/24/24	-
3	OLC	A	516	-	-	3/6/6/24	-
3	OLC	A	519	-	-	0/2/2/24	-
3	OLC	B	504	-	-	7/12/12/24	-
3	OLC	A	529	-	-	5/14/14/24	-
3	OLC	A	504	-	-	6/13/13/24	-
3	OLC	A	514	-	-	10/15/15/24	-
3	OLC	A	520	-	-	17/24/24/24	-
3	OLC	A	517	-	-	3/8/8/24	-
3	OLC	B	502	-	-	13/17/17/24	-
3	OLC	A	507	-	-	4/11/11/24	-
3	OLC	A	508	-	-	1/14/14/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (298) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	511	OLC	O20-C21-C22-C24
3	A	514	OLC	C21-C22-C24-O25
3	A	515	OLC	C21-C22-C24-O25
3	A	515	OLC	O20-C21-C22-C24
3	A	515	OLC	O20-C21-C22-O23
3	A	524	OLC	C21-C22-C24-O25
3	A	524	OLC	O20-C21-C22-O23
3	B	502	OLC	C21-C22-C24-O25
3	B	505	OLC	O20-C21-C22-C24
3	B	509	OLC	O20-C21-C22-C24
3	B	514	OLC	C21-C22-C24-O25
3	B	514	OLC	O20-C21-C22-O23
3	B	516	OLC	C21-C22-C24-O25
3	B	516	OLC	O20-C21-C22-O23
3	A	514	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
3	A	520	OLC	O19-C1-O20-C21
3	A	524	OLC	O19-C1-O20-C21
3	B	510	OLC	O19-C1-O20-C21
3	B	517	OLC	O19-C1-O20-C21
3	A	514	OLC	C2-C1-O20-C21
3	A	524	OLC	C2-C1-O20-C21
3	B	514	OLC	C2-C1-O20-C21
3	B	517	OLC	C2-C1-O20-C21
3	A	515	OLC	C2-C1-O20-C21
3	A	520	OLC	C2-C1-O20-C21
3	B	503	OLC	C2-C1-O20-C21
3	B	510	OLC	C2-C1-O20-C21
3	A	515	OLC	O19-C1-O20-C21
3	B	514	OLC	O19-C1-O20-C21
3	A	511	OLC	O20-C21-C22-O23
3	B	505	OLC	O20-C21-C22-O23
3	B	509	OLC	O20-C21-C22-O23
3	B	510	OLC	O20-C21-C22-O23
3	B	503	OLC	O19-C1-O20-C21
3	B	514	OLC	C14-C15-C16-C17
3	B	509	OLC	C2-C1-O20-C21
3	B	514	OLC	C12-C13-C14-C15
3	B	509	OLC	O19-C1-O20-C21
3	A	520	OLC	O20-C21-C22-C24
3	B	521	OLC	O20-C21-C22-C24
3	B	524	OLC	O20-C21-C22-C24
3	B	515	OLC	C11-C12-C13-C14
3	B	521	OLC	O20-C21-C22-O23
3	B	524	OLC	O20-C21-C22-O23
3	A	502	OLC	C1-C2-C3-C4
3	A	527	OLC	C4-C5-C6-C7
3	B	522	OLC	C12-C13-C14-C15
3	B	510	OLC	C3-C4-C5-C6
3	B	510	OLC	C5-C6-C7-C8
3	B	502	OLC	C3-C4-C5-C6
3	A	520	OLC	C10-C11-C12-C13
3	A	520	OLC	O20-C21-C22-O23
3	B	502	OLC	O20-C21-C22-O23
3	B	505	OLC	C2-C1-O20-C21
3	B	514	OLC	C5-C6-C7-C8
3	B	502	OLC	O20-C21-C22-C24
3	B	514	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
3	B	516	OLC	O20-C21-C22-C24
3	B	503	OLC	C3-C4-C5-C6
3	B	505	OLC	O19-C1-O20-C21
3	A	504	OLC	C4-C5-C6-C7
3	A	510	OLC	C12-C13-C14-C15
3	A	529	OLC	C13-C14-C15-C16
3	B	502	OLC	C4-C5-C6-C7
3	B	504	OLC	C13-C14-C15-C16
3	A	524	OLC	C4-C5-C6-C7
3	B	527	OLC	C11-C12-C13-C14
3	A	528	OLC	C5-C6-C7-C8
3	B	514	OLC	C2-C3-C4-C5
3	B	528	OLC	C11-C12-C13-C14
3	A	514	OLC	O23-C22-C24-O25
3	A	515	OLC	O23-C22-C24-O25
3	B	502	OLC	O23-C22-C24-O25
3	B	516	OLC	O23-C22-C24-O25
3	A	514	OLC	C1-C2-C3-C4
3	B	520	OLC	C13-C14-C15-C16
3	A	515	OLC	C4-C5-C6-C7
3	B	505	OLC	C3-C4-C5-C6
3	A	511	OLC	C3-C4-C5-C6
3	B	514	OLC	C11-C12-C13-C14
3	A	503	OLC	C1-C2-C3-C4
3	B	514	OLC	C3-C4-C5-C6
3	A	526	OLC	C12-C13-C14-C15
3	A	530	OLC	C4-C5-C6-C7
3	A	514	OLC	O20-C21-C22-O23
3	A	504	OLC	C13-C14-C15-C16
3	B	525	OLC	C5-C6-C7-C8
3	A	526	OLC	C3-C4-C5-C6
3	B	516	OLC	C14-C15-C16-C17
3	A	513	OLC	C3-C4-C5-C6
3	B	524	OLC	C5-C6-C7-C8
3	B	529	OLC	C10-C11-C12-C13
3	A	509	OLC	C15-C16-C17-C18
3	A	511	OLC	C2-C3-C4-C5
3	A	517	OLC	C11-C12-C13-C14
3	A	511	OLC	C14-C15-C16-C17
3	B	529	OLC	C14-C15-C16-C17
3	A	521	OLC	C15-C16-C17-C18
3	A	526	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	B	519	OLC	C7-C8-C9-C10
3	B	527	OLC	C7-C8-C9-C10
3	A	524	OLC	C2-C3-C4-C5
3	A	504	OLC	C10-C11-C12-C13
3	A	517	OLC	C10-C11-C12-C13
3	B	502	OLC	C6-C7-C8-C9
3	B	506	OLC	C10-C11-C12-C13
3	B	529	OLC	C6-C7-C8-C9
3	A	511	OLC	C15-C16-C17-C18
3	B	524	OLC	C15-C16-C17-C18
3	B	518	OLC	C14-C15-C16-C17
3	A	502	OLC	C4-C5-C6-C7
3	B	522	OLC	C3-C4-C5-C6
3	B	516	OLC	C11-C12-C13-C14
3	B	521	OLC	C2-C3-C4-C5
3	B	526	OLC	C14-C15-C16-C17
3	A	514	OLC	C5-C6-C7-C8
3	A	512	OLC	C12-C13-C14-C15
3	A	513	OLC	C5-C6-C7-C8
3	B	522	OLC	C5-C6-C7-C8
3	B	523	OLC	C11-C12-C13-C14
3	B	527	OLC	C14-C15-C16-C17
3	A	520	OLC	C1-C2-C3-C4
3	A	528	OLC	C13-C14-C15-C16
3	A	502	OLC	C6-C7-C8-C9
3	A	520	OLC	C2-C3-C4-C5
3	A	516	OLC	C4-C5-C6-C7
3	B	523	OLC	C12-C13-C14-C15
3	A	504	OLC	C12-C13-C14-C15
3	A	520	OLC	C14-C15-C16-C17
3	B	528	OLC	C13-C14-C15-C16
3	B	529	OLC	C3-C4-C5-C6
3	A	524	OLC	O23-C22-C24-O25
3	B	514	OLC	O23-C22-C24-O25
3	B	511	OLC	C13-C14-C15-C16
3	B	516	OLC	C9-C10-C11-C12
3	A	502	OLC	C11-C12-C13-C14
3	A	511	OLC	C10-C11-C12-C13
3	A	511	OLC	C6-C7-C8-C9
3	A	513	OLC	C6-C7-C8-C9
3	A	524	OLC	C6-C7-C8-C9
3	B	516	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	B	524	OLC	C2-C3-C4-C5
3	B	515	OLC	C13-C14-C15-C16
3	B	525	OLC	C14-C15-C16-C17
3	A	529	OLC	C9-C10-C11-C12
3	A	505	OLC	C10-C11-C12-C13
3	A	515	OLC	C10-C11-C12-C13
3	B	514	OLC	C10-C11-C12-C13
3	A	528	OLC	C4-C5-C6-C7
3	B	521	OLC	C3-C4-C5-C6
3	B	510	OLC	C1-C2-C3-C4
3	A	506	OLC	C10-C11-C12-C13
3	B	504	OLC	C6-C7-C8-C9
3	B	520	OLC	C10-C11-C12-C13
3	B	524	OLC	C10-C11-C12-C13
3	B	504	OLC	C5-C6-C7-C8
3	B	522	OLC	C13-C14-C15-C16
3	A	509	OLC	C12-C13-C14-C15
3	A	514	OLC	C4-C5-C6-C7
3	B	522	OLC	C15-C16-C17-C18
3	B	528	OLC	C15-C16-C17-C18
3	A	511	OLC	C9-C10-C11-C12
3	B	526	OLC	C15-C16-C17-C18
3	A	515	OLC	C15-C16-C17-C18
3	B	514	OLC	C13-C14-C15-C16
3	A	530	OLC	C15-C16-C17-C18
3	B	504	OLC	C12-C13-C14-C15
3	A	512	OLC	C13-C14-C15-C16
3	A	512	OLC	C5-C6-C7-C8
3	B	528	OLC	C14-C15-C16-C17
3	B	519	OLC	C14-C15-C16-C17
3	A	504	OLC	C3-C4-C5-C6
3	B	525	OLC	C15-C16-C17-C18
3	A	530	OLC	C1-C2-C3-C4
3	B	504	OLC	C3-C4-C5-C6
3	A	507	OLC	C5-C6-C7-C8
3	B	508	OLC	C2-C3-C4-C5
3	B	514	OLC	C15-C16-C17-C18
3	A	528	OLC	C15-C16-C17-C18
3	B	523	OLC	C15-C16-C17-C18
3	B	524	OLC	C14-C15-C16-C17
3	A	520	OLC	C12-C13-C14-C15
3	B	524	OLC	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	A	522	OLC	C11-C12-C13-C14
3	B	512	OLC	C15-C16-C17-C18
3	A	512	OLC	C11-C12-C13-C14
3	B	502	OLC	C2-C3-C4-C5
3	A	520	OLC	C5-C6-C7-C8
3	A	526	OLC	C15-C16-C17-C18
3	B	516	OLC	C12-C13-C14-C15
3	A	514	OLC	C2-C3-C4-C5
3	A	516	OLC	C1-C2-C3-C4
3	B	513	OLC	C13-C14-C15-C16
3	A	526	OLC	C14-C15-C16-C17
3	A	516	OLC	C3-C4-C5-C6
3	A	524	OLC	O20-C21-C22-C24
3	B	515	OLC	C15-C16-C17-C18
3	A	525	OLC	C12-C13-C14-C15
3	B	513	OLC	C15-C16-C17-C18
3	A	505	OLC	C2-C3-C4-C5
3	B	524	OLC	O23-C22-C24-O25
3	A	507	OLC	C11-C12-C13-C14
3	A	520	OLC	C13-C14-C15-C16
3	B	515	OLC	C12-C13-C14-C15
3	B	524	OLC	C11-C12-C13-C14
3	B	510	OLC	C10-C11-C12-C13
3	A	505	OLC	C1-C2-C3-C4
3	B	514	OLC	O20-C1-C2-C3
3	B	523	OLC	C10-C11-C12-C13
3	B	527	OLC	C10-C11-C12-C13
3	A	510	OLC	C13-C14-C15-C16
3	A	507	OLC	C10-C11-C12-C13
3	A	514	OLC	O20-C21-C22-C24
3	B	527	OLC	C12-C13-C14-C15
3	B	502	OLC	C1-C2-C3-C4
3	A	520	OLC	C15-C16-C17-C18
3	A	529	OLC	C5-C6-C7-C8
3	A	529	OLC	C15-C16-C17-C18
3	A	509	OLC	C13-C14-C15-C16
3	A	524	OLC	C7-C8-C9-C10
3	B	523	OLC	C13-C14-C15-C16
3	A	530	OLC	C11-C12-C13-C14
3	A	515	OLC	C6-C7-C8-C9
3	B	517	OLC	C1-C2-C3-C4
3	B	505	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	523	OLC	C13-C14-C15-C16
3	B	505	OLC	C4-C5-C6-C7
3	B	522	OLC	C14-C15-C16-C17
3	A	530	OLC	C13-C14-C15-C16
3	A	522	OLC	C13-C14-C15-C16
3	B	503	OLC	C4-C5-C6-C7
3	A	530	OLC	C12-C13-C14-C15
3	A	530	OLC	C2-C3-C4-C5
3	B	513	OLC	C14-C15-C16-C17
3	A	520	OLC	C3-C4-C5-C6
3	B	524	OLC	C4-C5-C6-C7
3	A	509	OLC	C14-C15-C16-C17
3	B	526	OLC	C13-C14-C15-C16
3	B	520	OLC	C11-C12-C13-C14
3	B	522	OLC	C4-C5-C6-C7
3	B	516	OLC	C15-C16-C17-C18
3	B	520	OLC	C12-C13-C14-C15
3	A	526	OLC	C2-C3-C4-C5
3	A	530	OLC	C7-C8-C9-C10
3	B	516	OLC	C5-C6-C7-C8
3	B	524	OLC	C7-C8-C9-C10
3	B	512	OLC	C13-C14-C15-C16
3	B	502	OLC	C5-C6-C7-C8
3	A	508	OLC	C2-C3-C4-C5
3	B	502	OLC	C7-C8-C9-C10
3	B	502	OLC	C2-C1-O20-C21
3	A	528	OLC	C14-C15-C16-C17
3	A	517	OLC	C15-C16-C17-C18
3	A	502	OLC	C2-C1-O20-C21
3	A	528	OLC	C12-C13-C14-C15
3	B	502	OLC	O19-C1-O20-C21
3	B	516	OLC	C13-C14-C15-C16
3	A	528	OLC	C3-C4-C5-C6
3	A	520	OLC	C7-C8-C9-C10
3	B	516	OLC	O20-C1-C2-C3
3	A	502	OLC	O19-C1-O20-C21
3	A	520	OLC	C11-C12-C13-C14
3	B	511	OLC	C10-C11-C12-C13
3	A	505	OLC	C7-C8-C9-C10
3	A	513	OLC	C7-C8-C9-C10
3	A	524	OLC	C15-C16-C17-C18
3	A	529	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	B	504	OLC	C14-C15-C16-C17
4	A	531	PEG	C1-C2-O2-C3
3	A	522	OLC	C12-C13-C14-C15
3	B	527	OLC	C15-C16-C17-C18
3	B	504	OLC	C7-C8-C9-C10
3	A	504	OLC	C5-C6-C7-C8
3	B	507	OLC	C2-C3-C4-C5
3	B	503	OLC	O20-C1-C2-C3
3	B	519	OLC	C9-C10-C11-C12
3	A	505	OLC	O20-C1-C2-C3
3	A	530	OLC	C14-C15-C16-C17
3	B	514	OLC	O19-C1-C2-C3
3	A	521	OLC	C10-C11-C12-C13
3	A	525	OLC	C11-C12-C13-C14
3	B	511	OLC	C12-C13-C14-C15
3	A	524	OLC	C10-C11-C12-C13
3	A	515	OLC	C11-C12-C13-C14
3	B	521	OLC	O20-C1-C2-C3
3	A	520	OLC	O20-C1-C2-C3
3	A	511	OLC	C1-C2-C3-C4
3	B	522	OLC	C6-C7-C8-C9
3	A	515	OLC	C14-C15-C16-C17
3	A	505	OLC	O19-C1-C2-C3
3	B	518	OLC	C15-C16-C17-C18
3	A	520	OLC	O19-C1-C2-C3
3	B	521	OLC	O19-C1-C2-C3
3	B	517	OLC	O20-C21-C22-O23
3	B	503	OLC	O19-C1-C2-C3
3	A	515	OLC	C1-C2-C3-C4
3	A	507	OLC	C7-C8-C9-C10
3	B	529	OLC	C9-C10-C11-C12

There are no ring outliers.

35 monomers are involved in 79 short contacts:

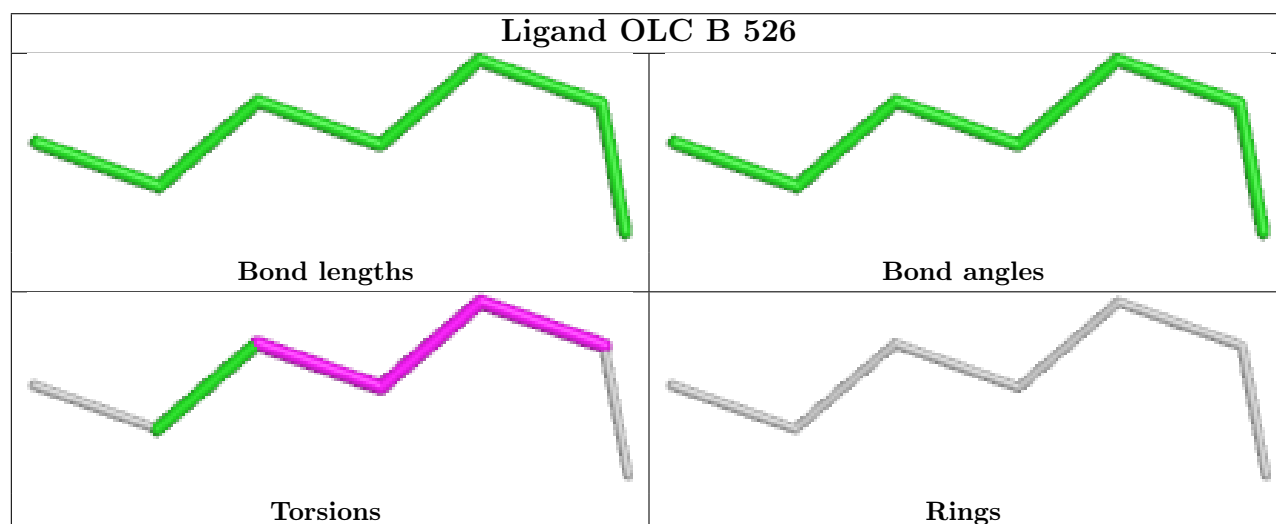
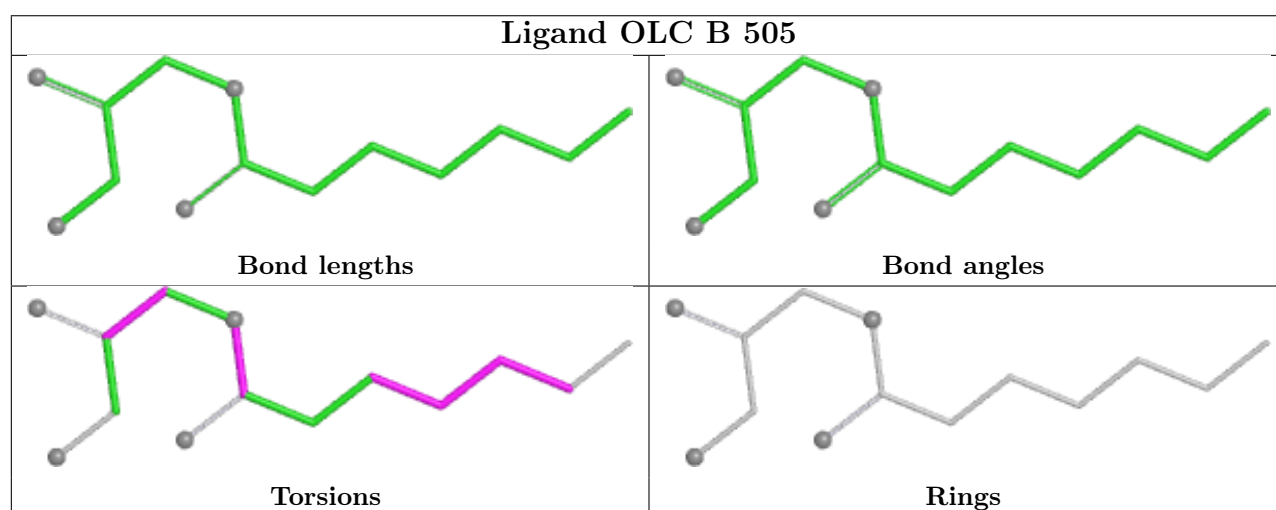
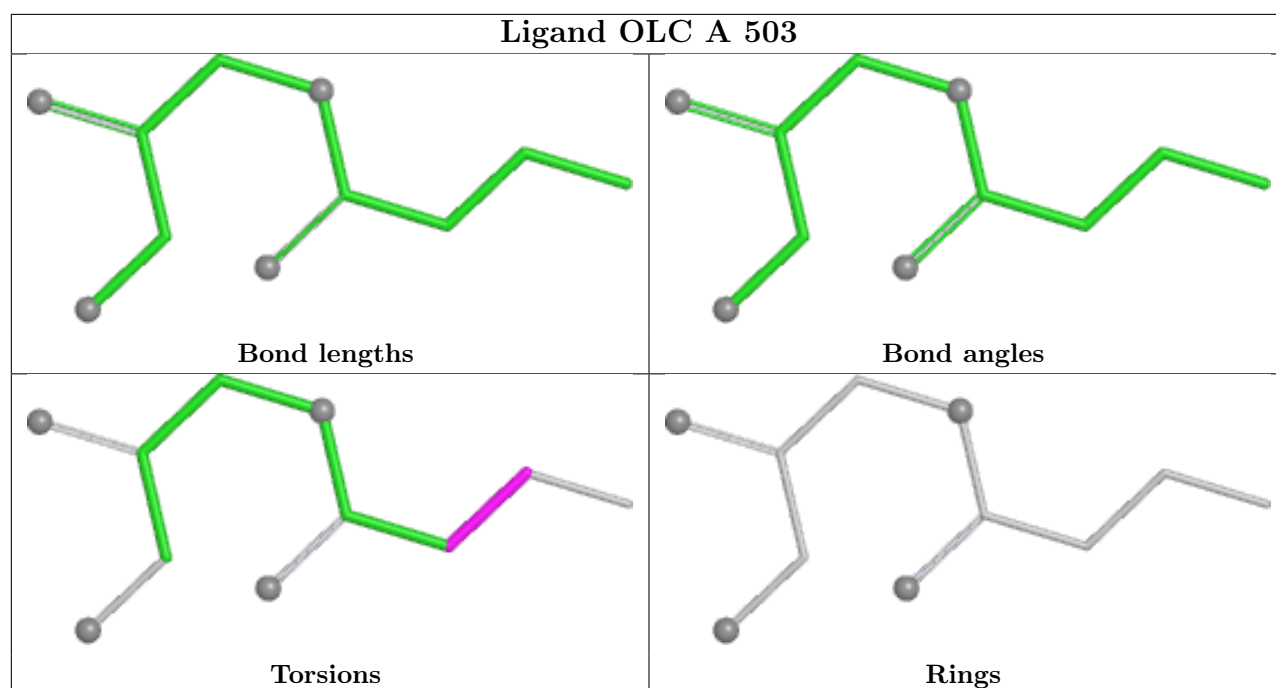
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	OLC	2	0
3	B	505	OLC	2	0
3	B	529	OLC	4	0
3	A	512	OLC	3	0
3	B	520	OLC	2	0
3	A	525	OLC	1	0

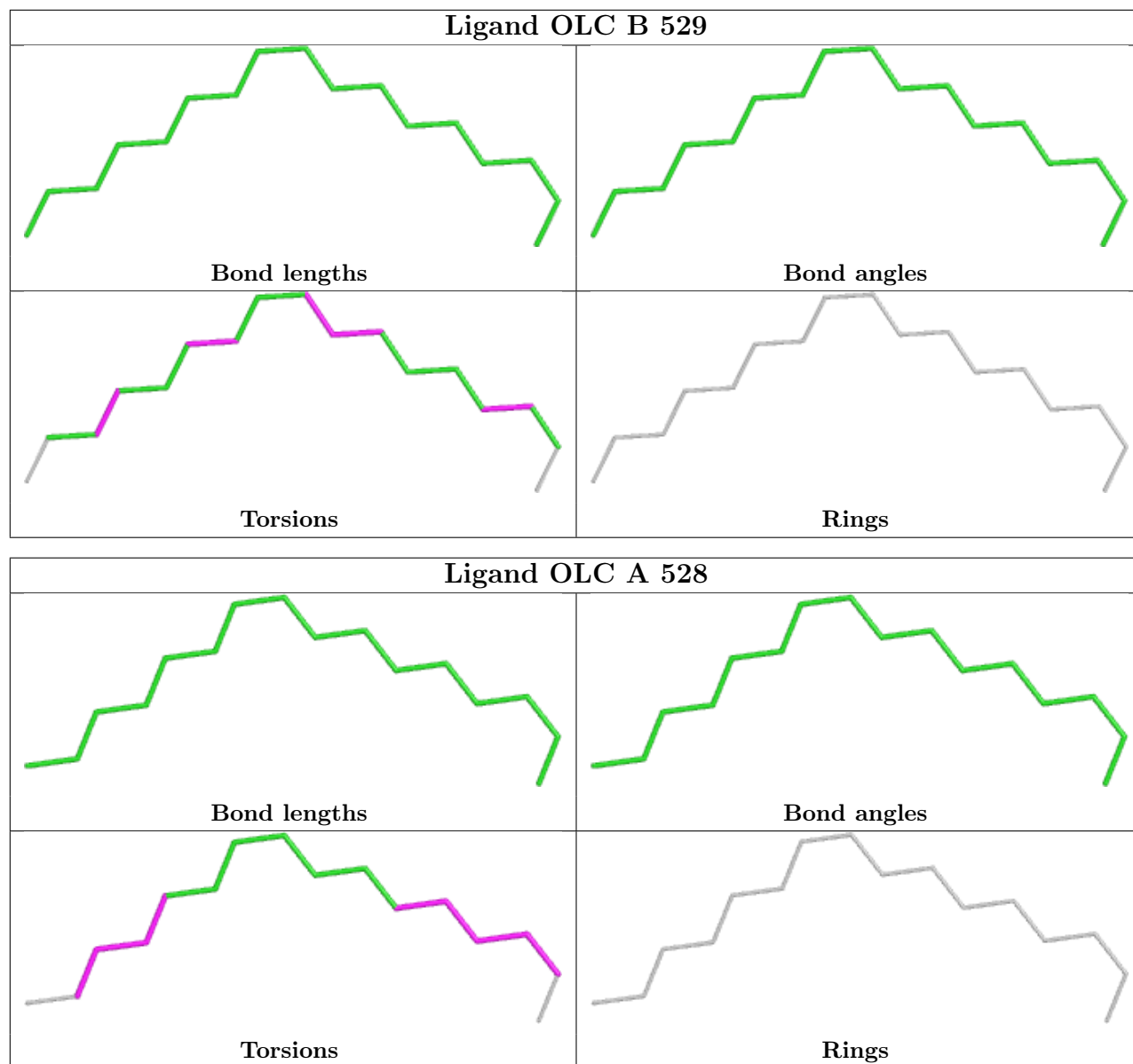
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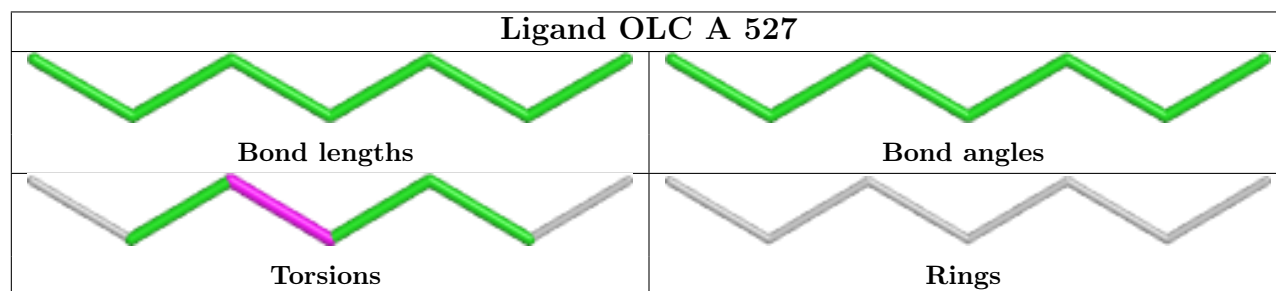
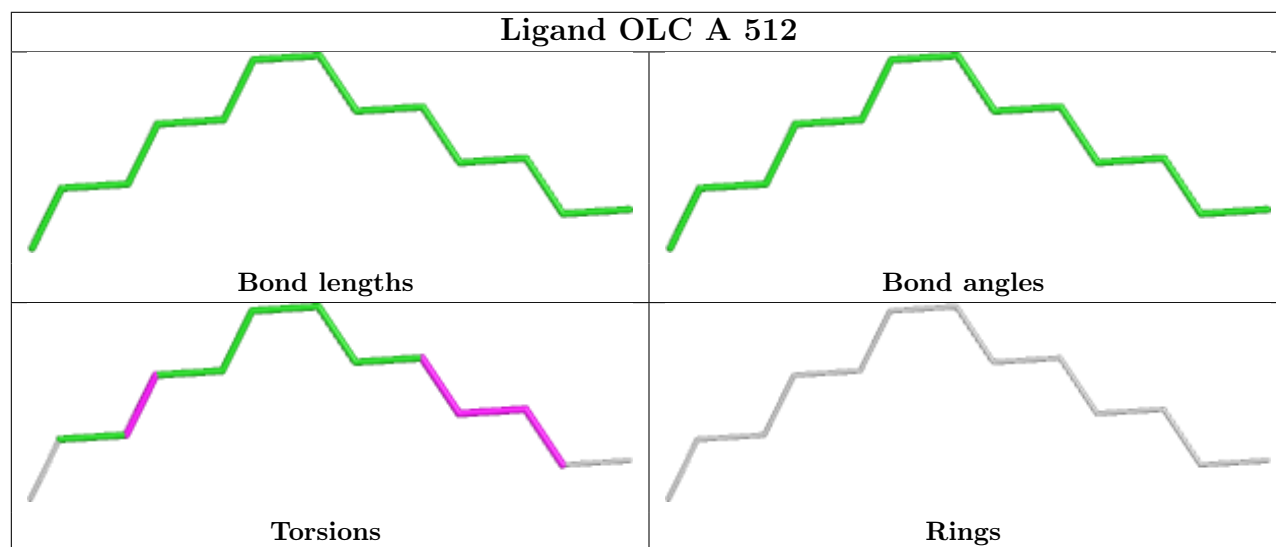
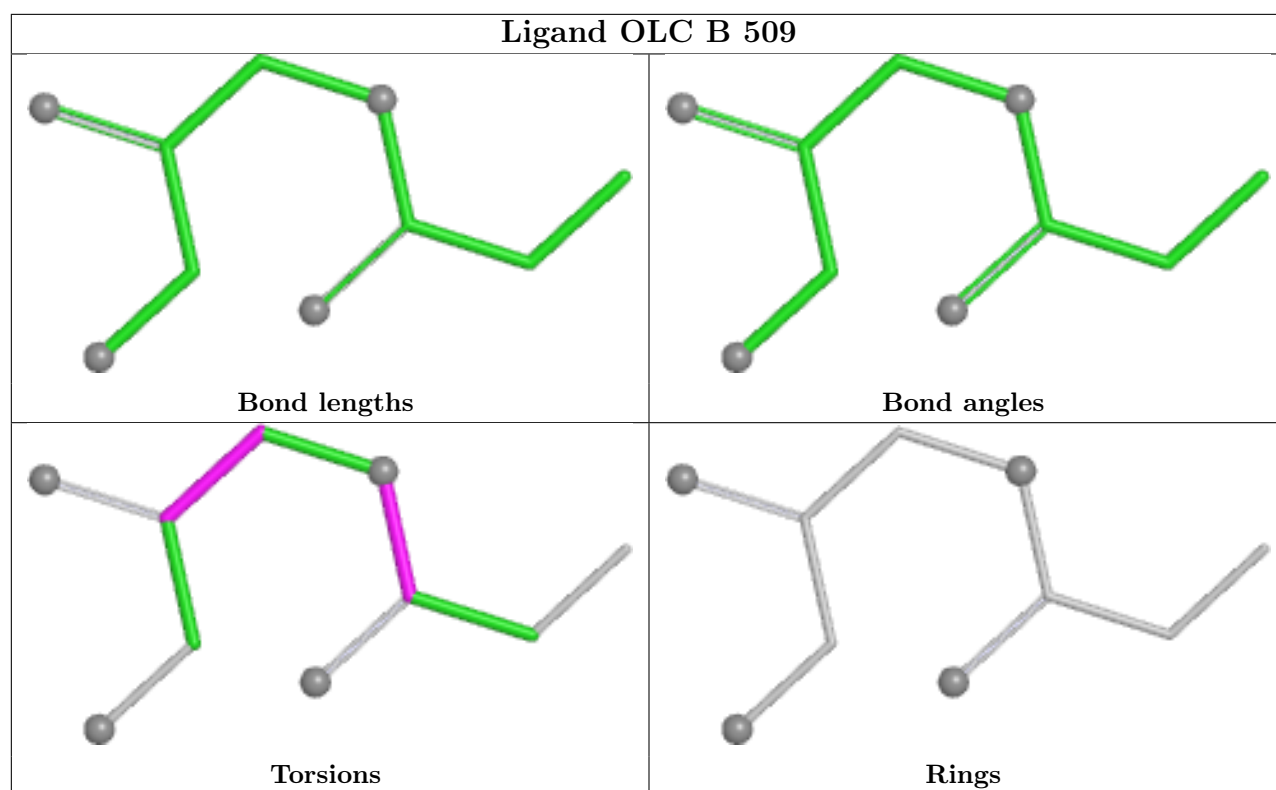
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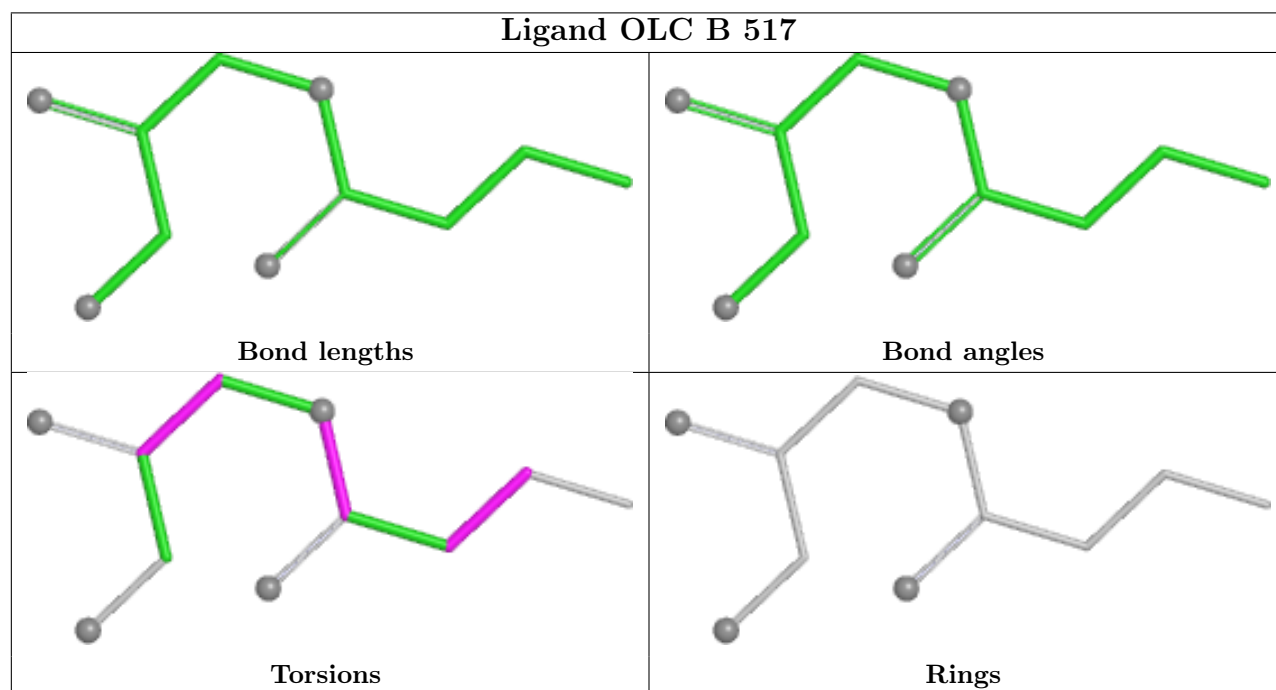
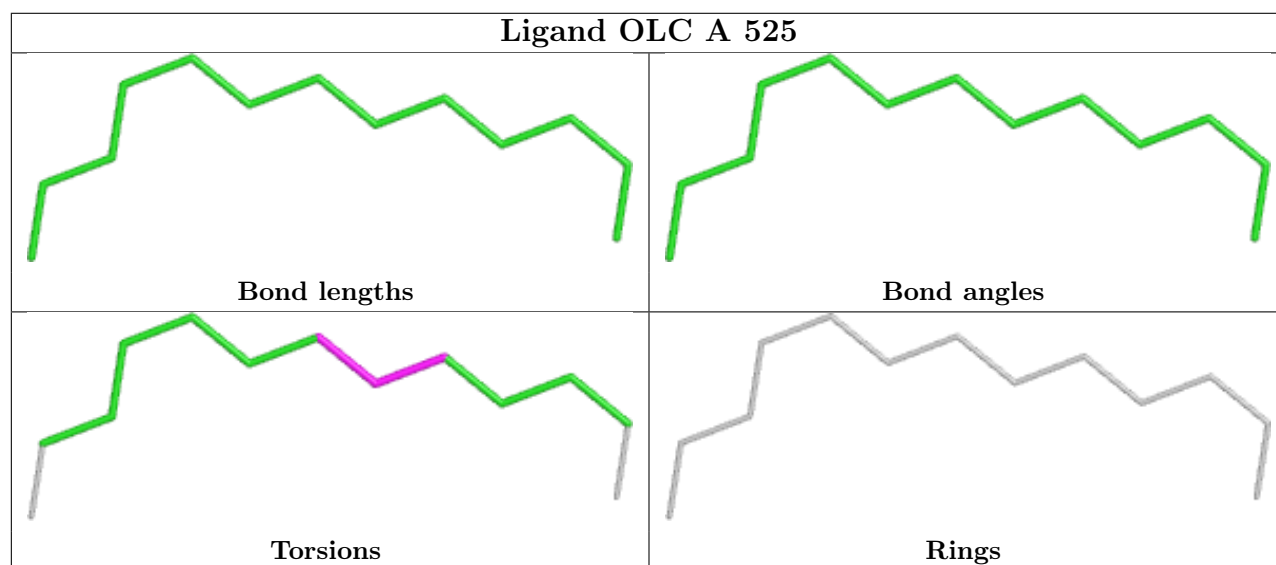
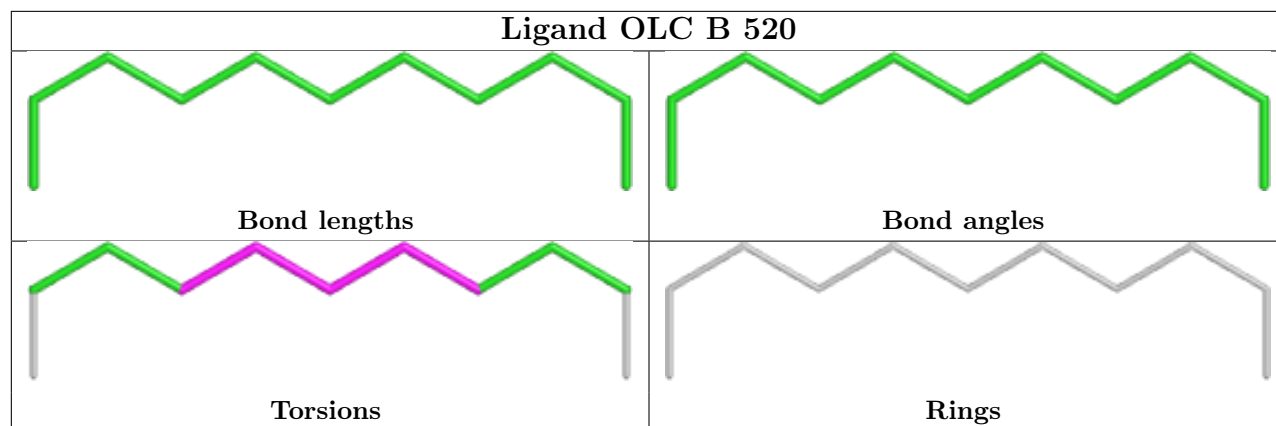
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	522	OLC	5	0
3	B	527	OLC	2	0
3	B	503	OLC	1	0
3	B	528	OLC	1	0
3	B	519	OLC	2	0
3	A	511	OLC	4	0
3	B	515	OLC	1	0
3	B	524	OLC	5	0
3	A	526	OLC	3	0
3	A	502	OLC	3	0
3	B	514	OLC	10	0
3	B	523	OLC	1	0
3	A	509	OLC	5	0
3	A	530	OLC	1	0
3	A	522	OLC	1	0
3	A	515	OLC	1	0
3	B	507	OLC	1	0
3	B	510	OLC	3	0
3	B	521	OLC	1	0
3	A	524	OLC	4	0
3	A	519	OLC	2	0
3	B	504	OLC	4	0
3	A	529	OLC	4	0
3	A	504	OLC	1	0
3	A	514	OLC	1	0
3	A	520	OLC	3	0
3	B	502	OLC	1	0
3	A	507	OLC	3	0
3	A	508	OLC	1	0

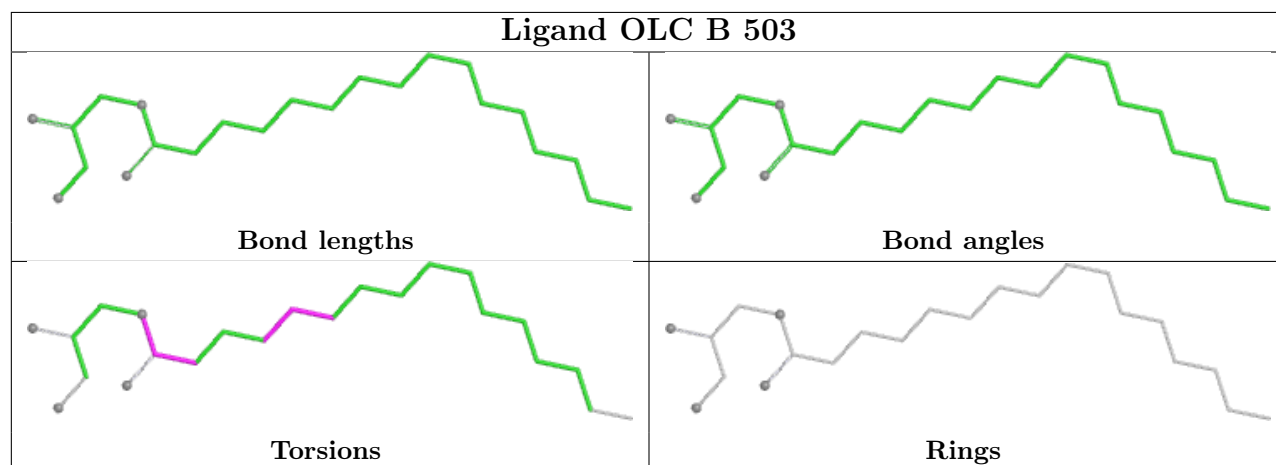
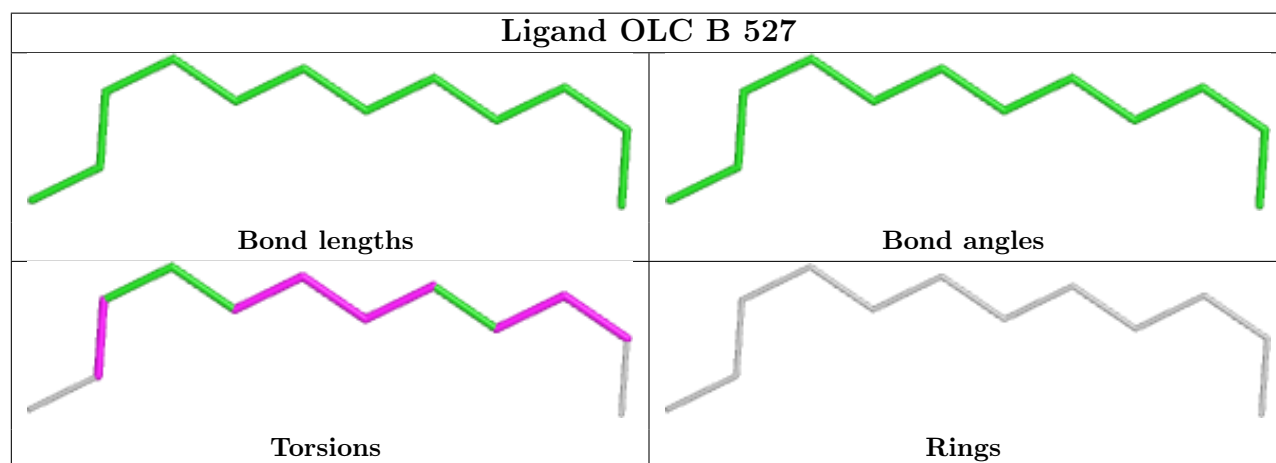
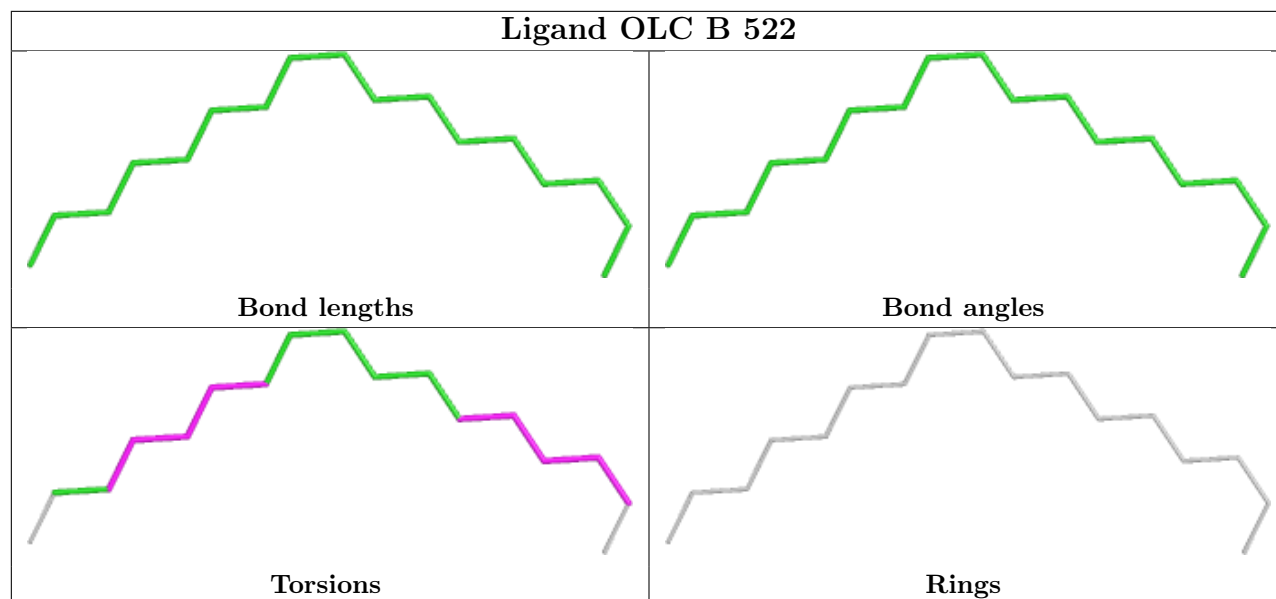
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

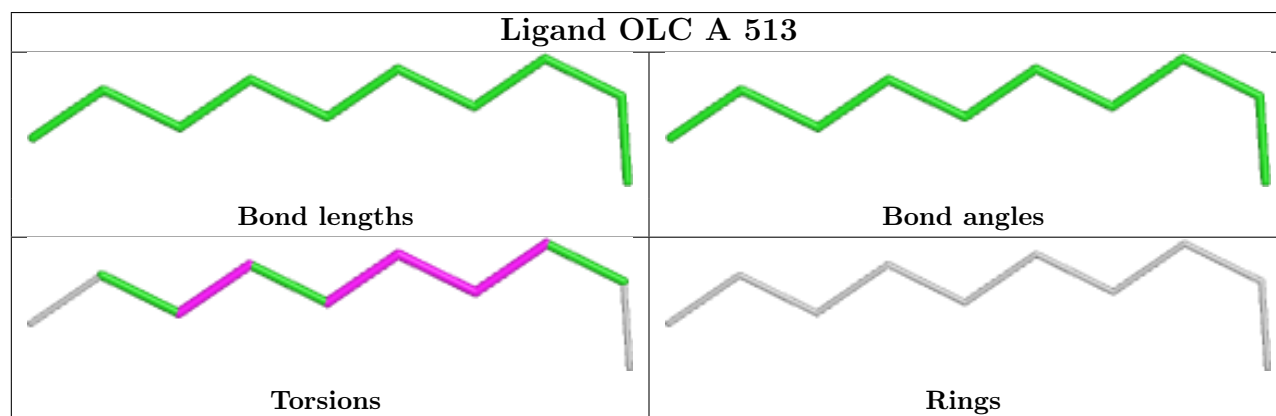
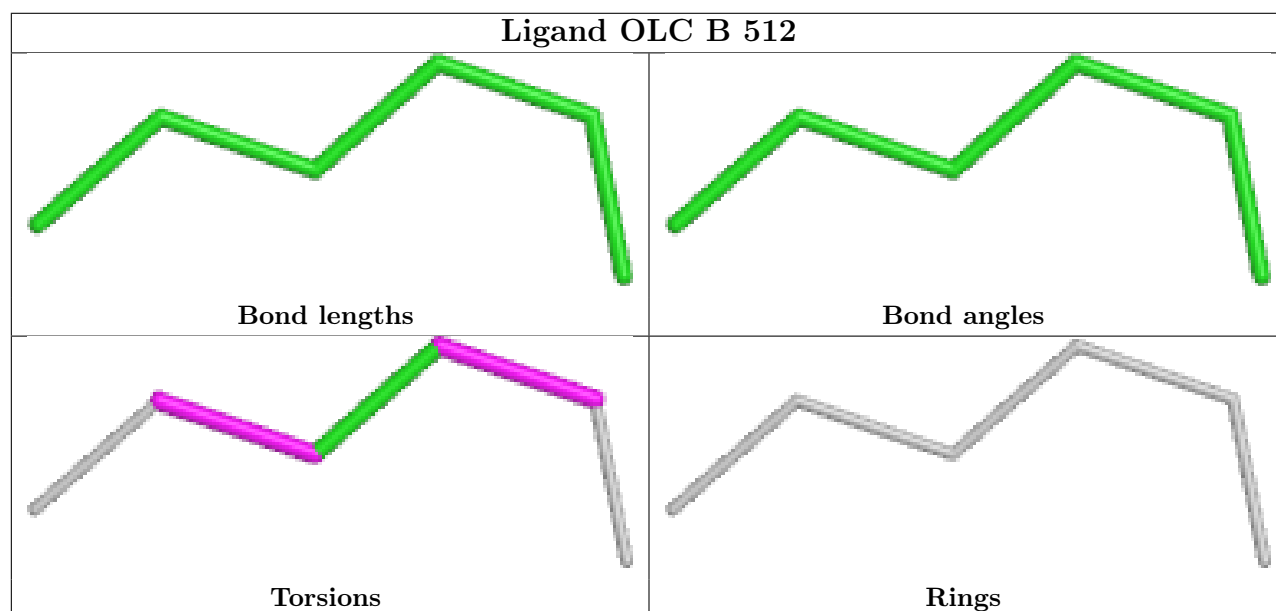
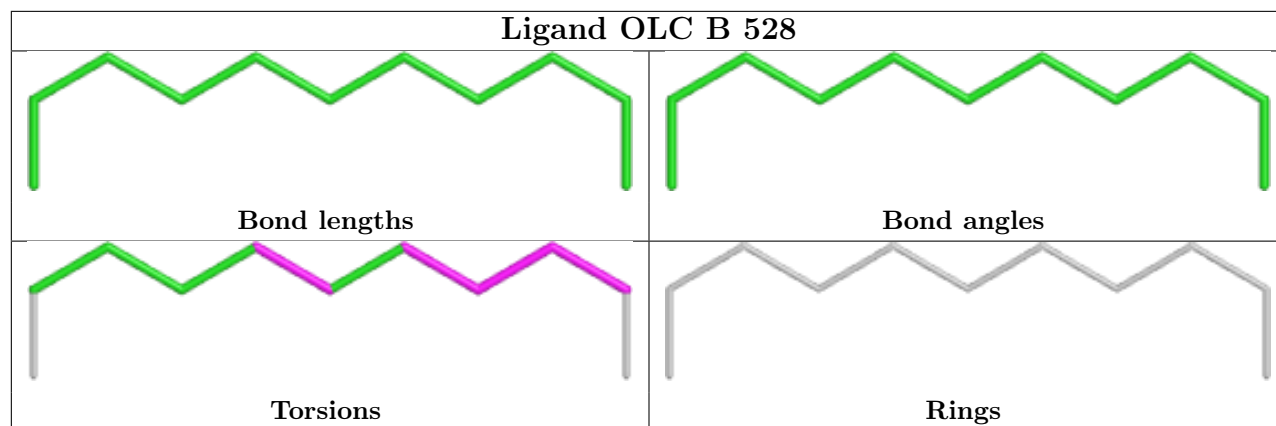


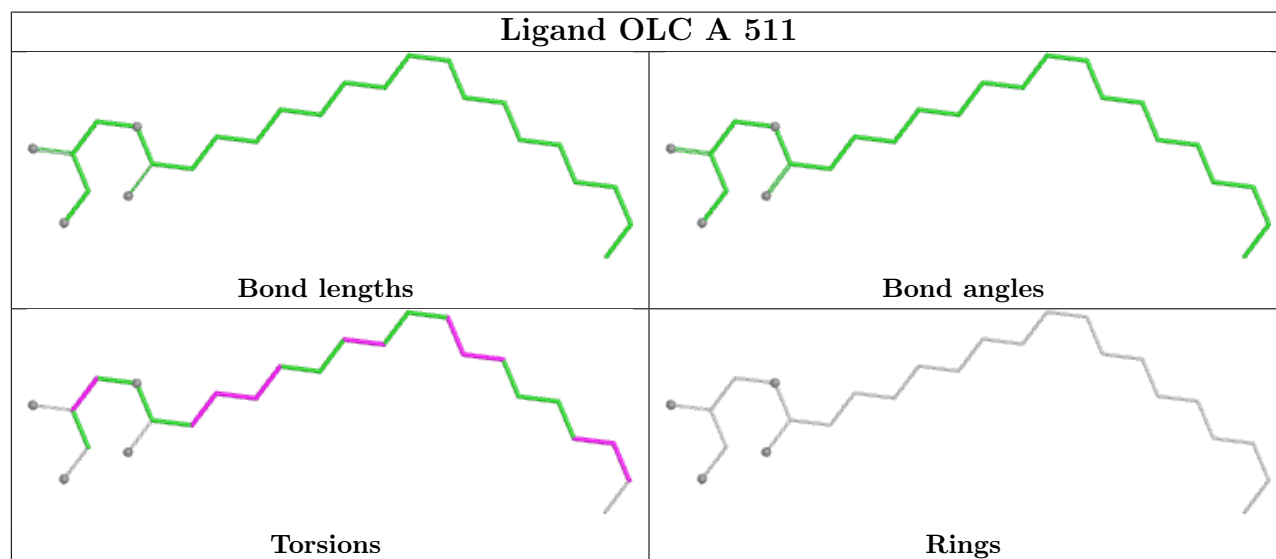
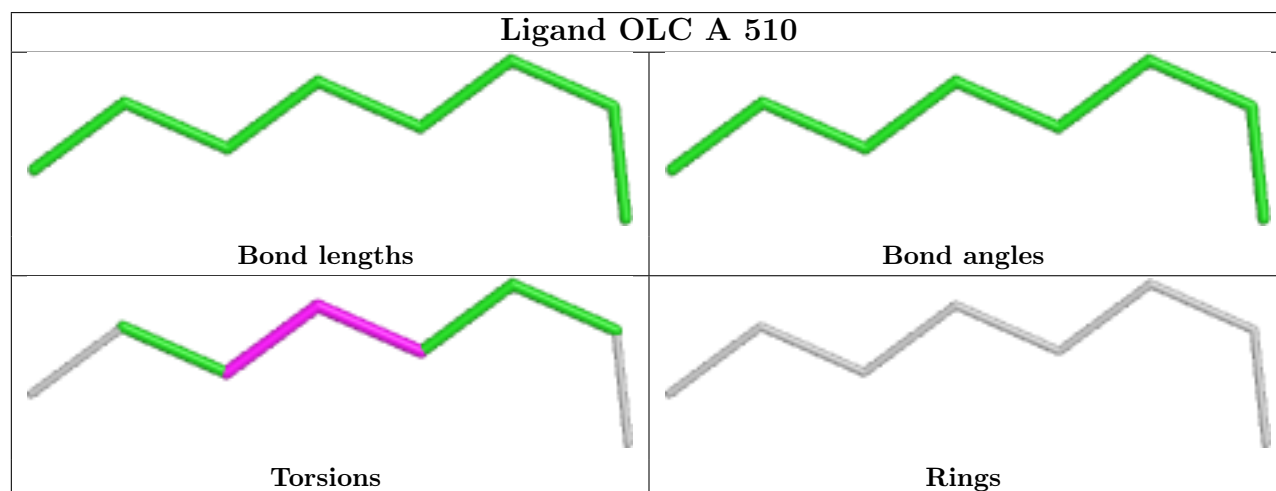
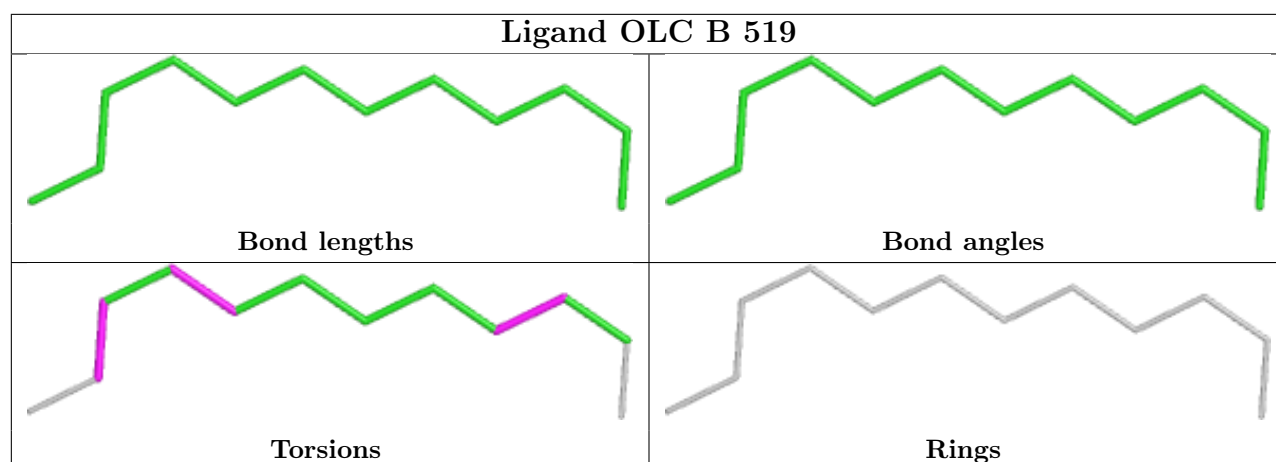


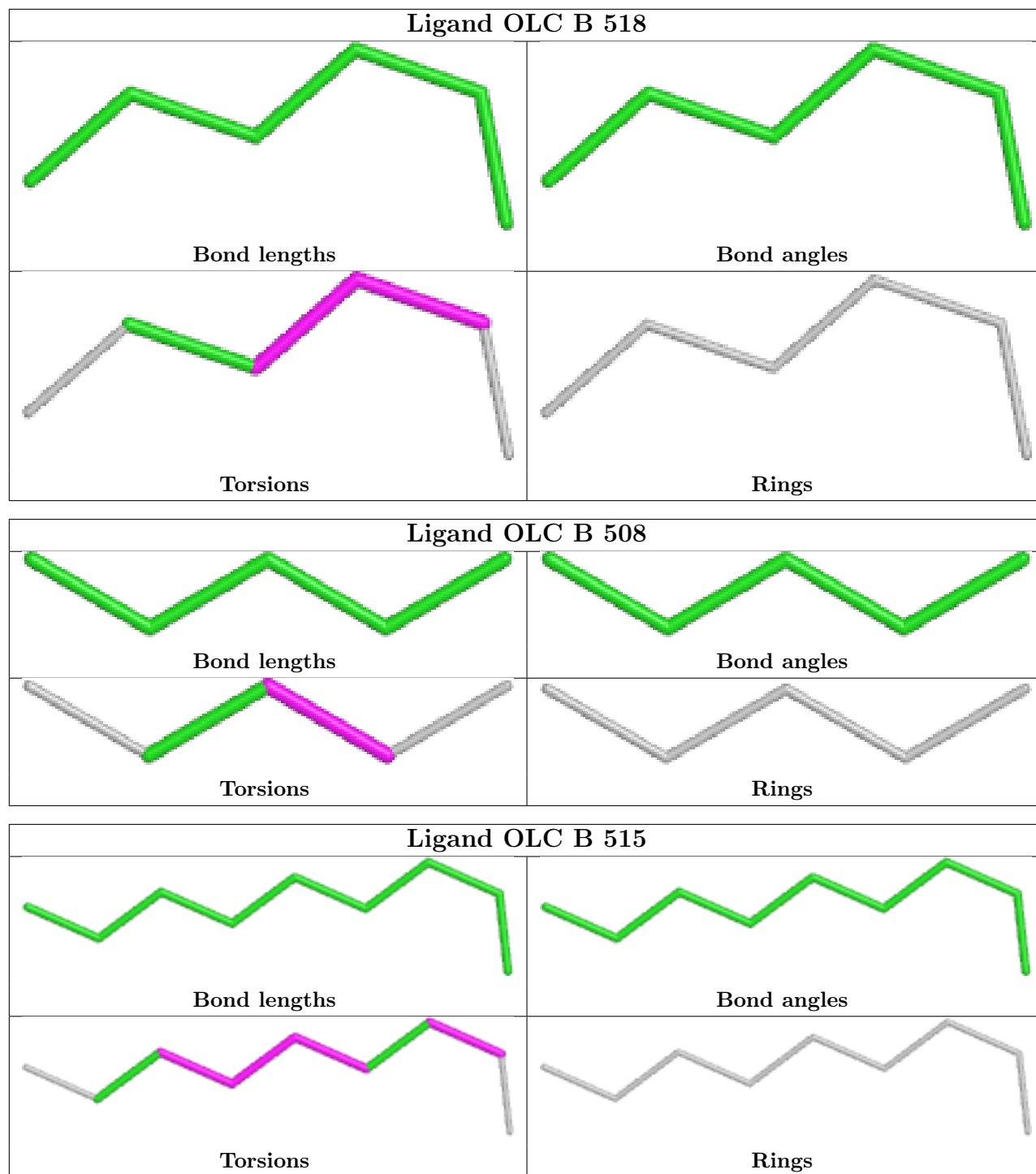


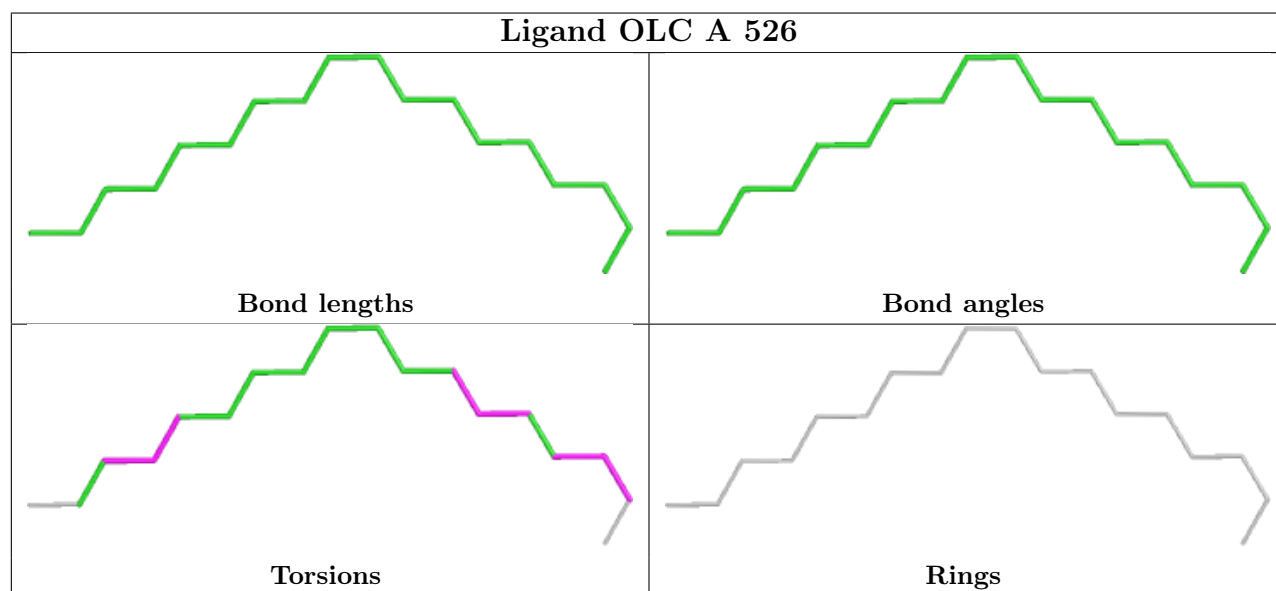
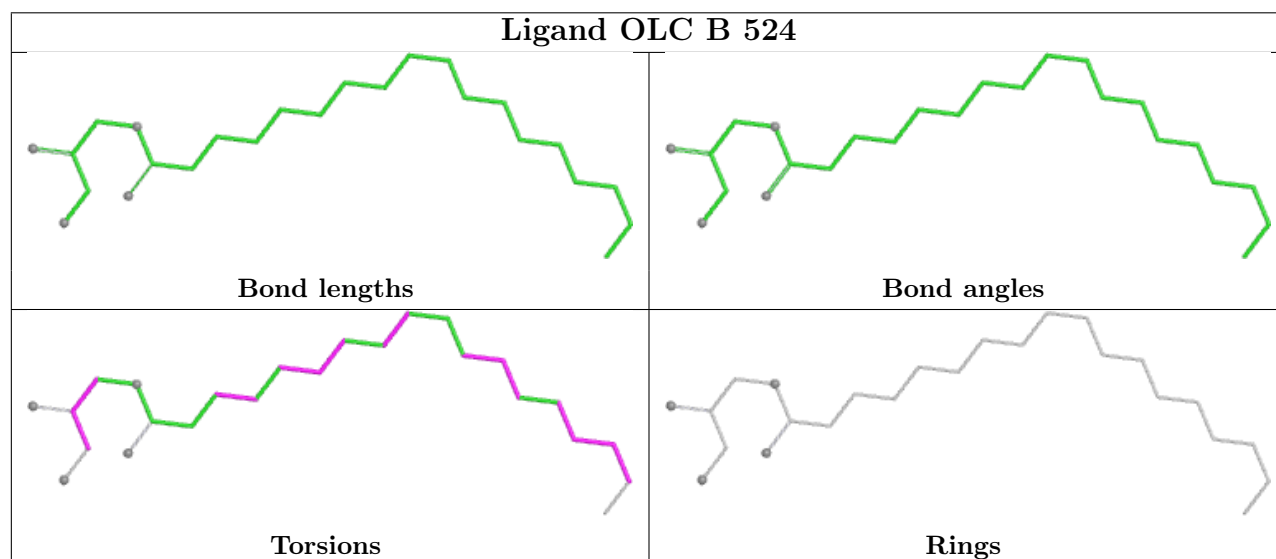
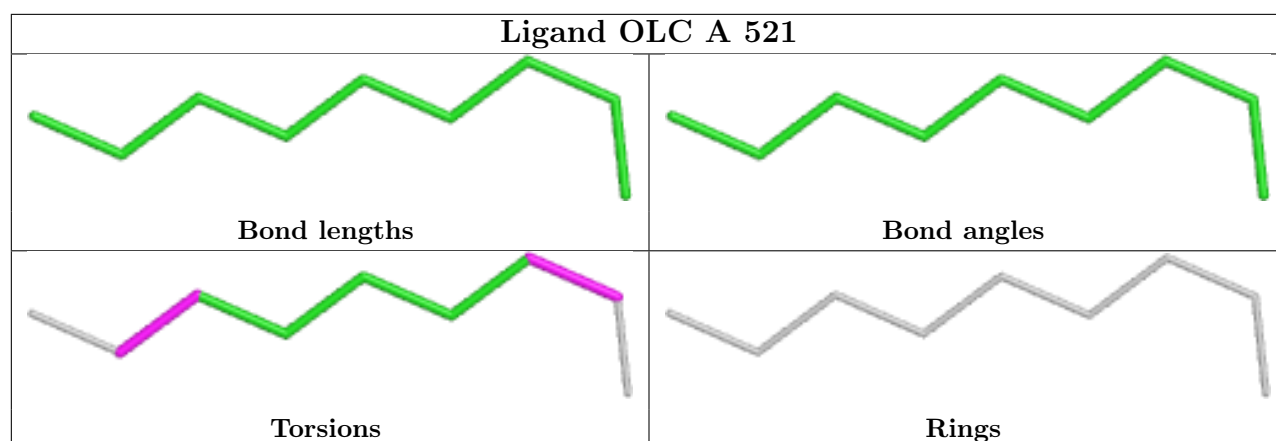


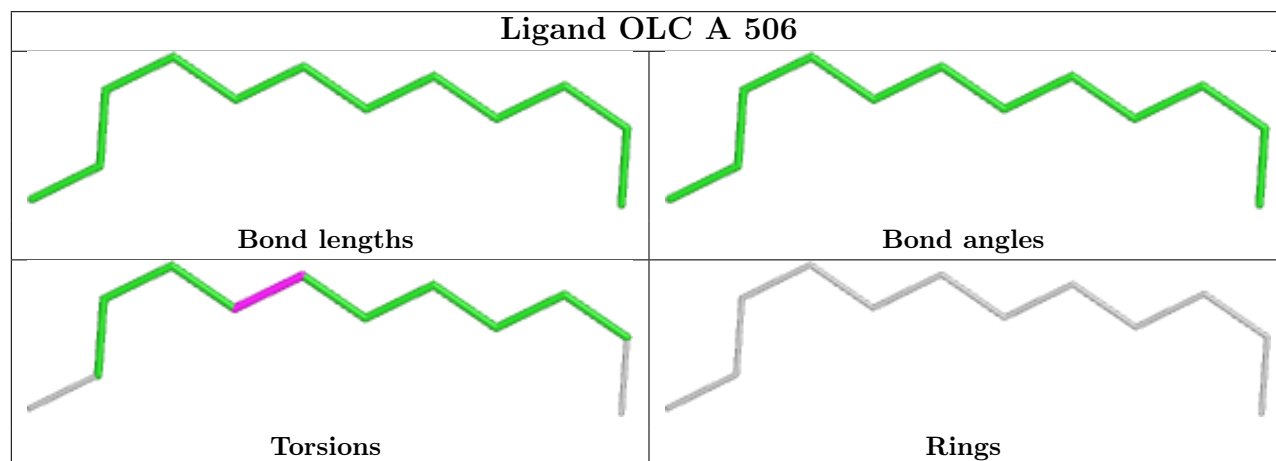
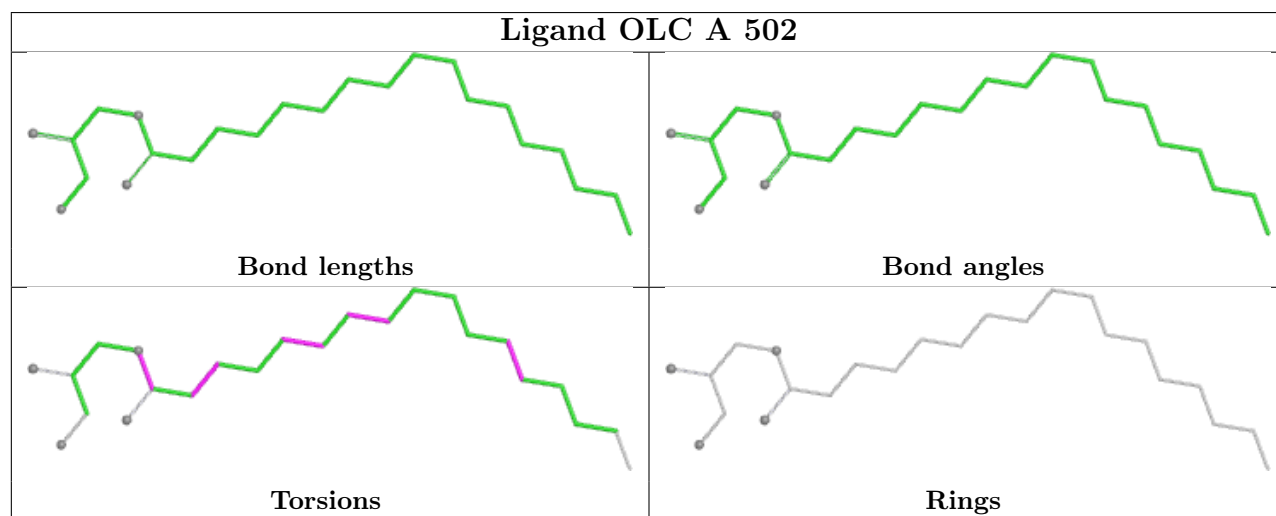
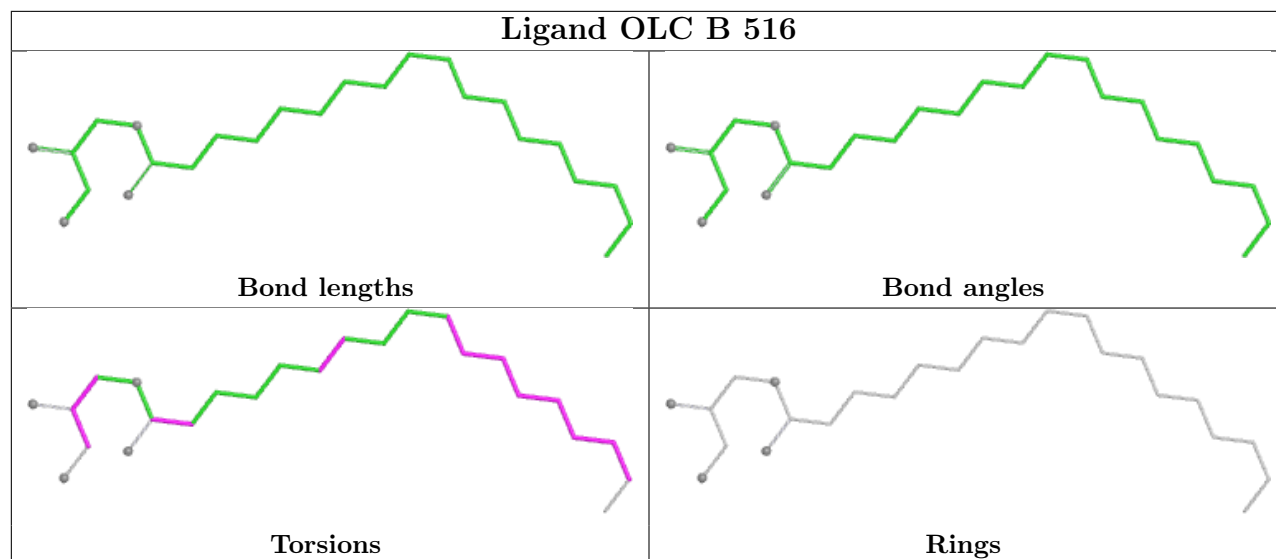


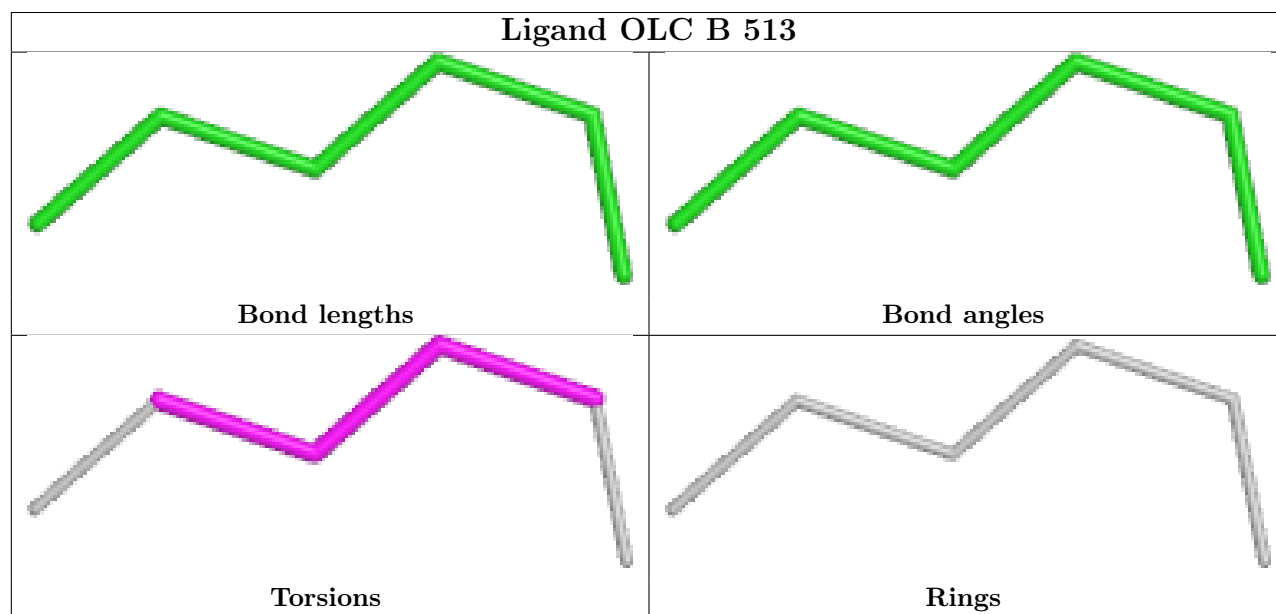
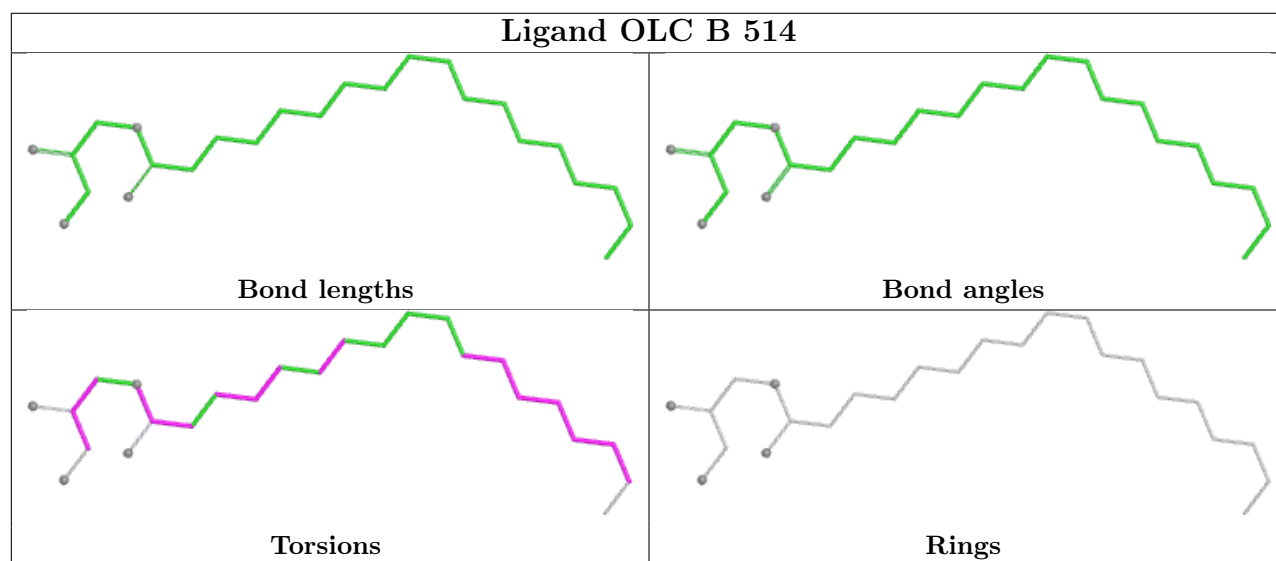
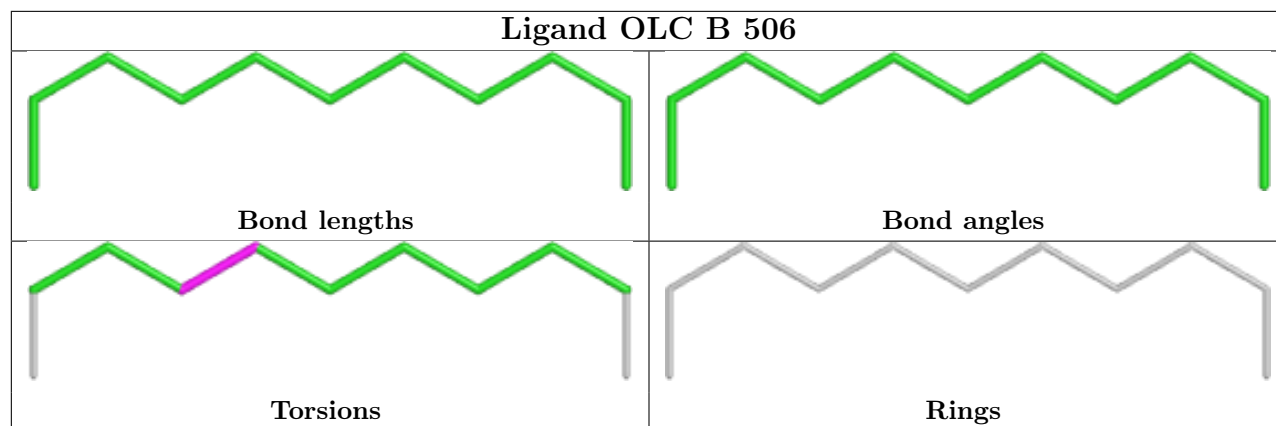


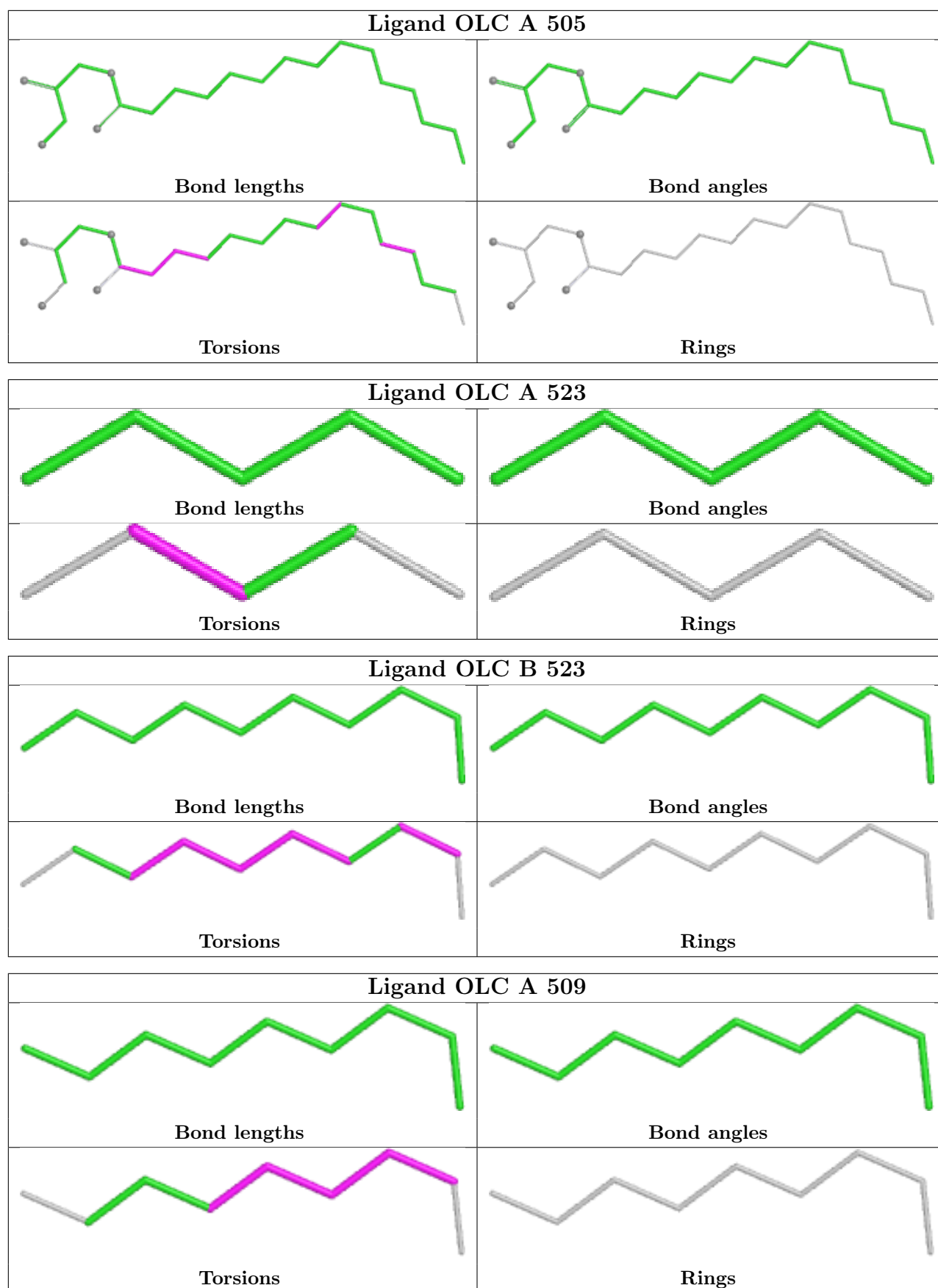


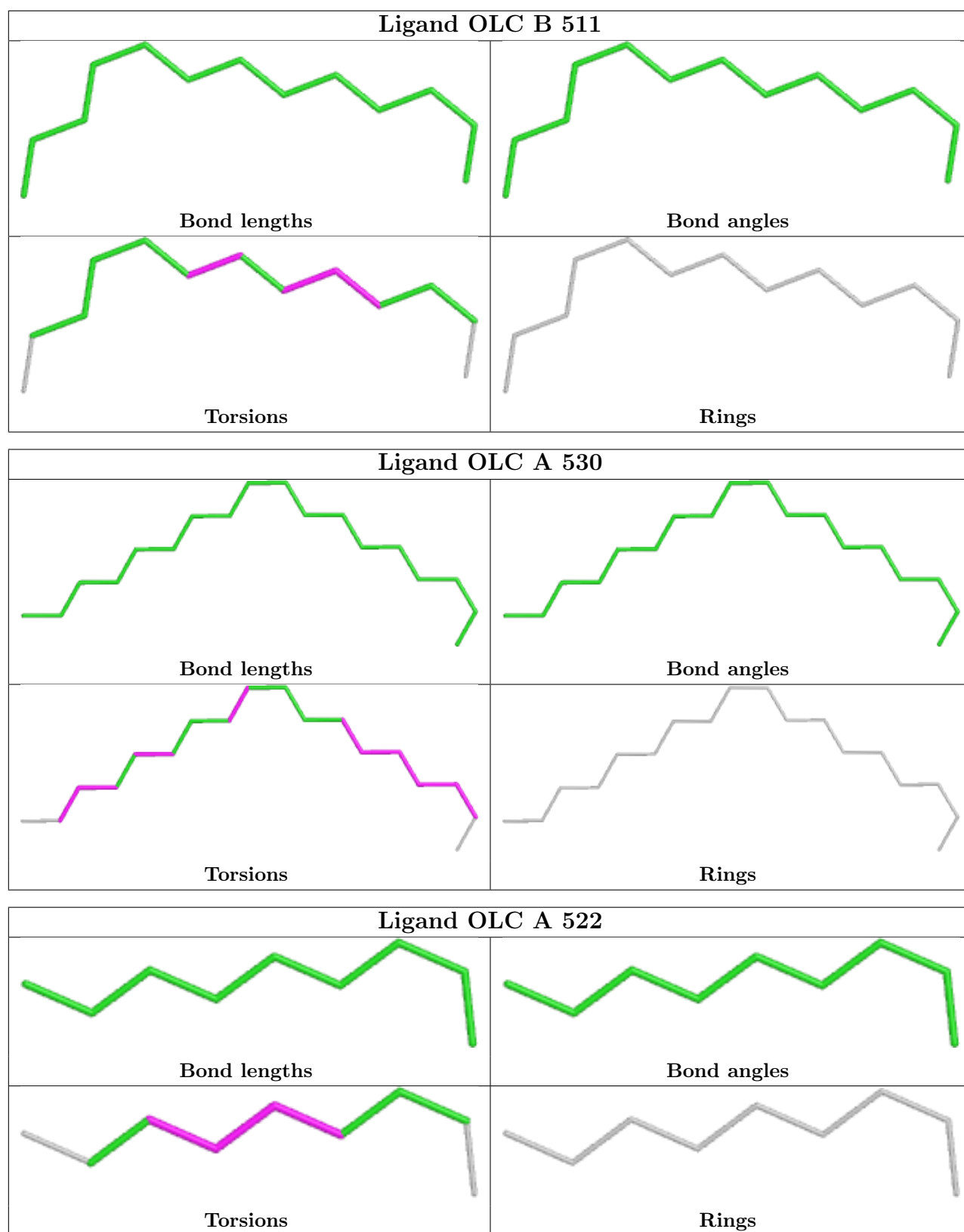


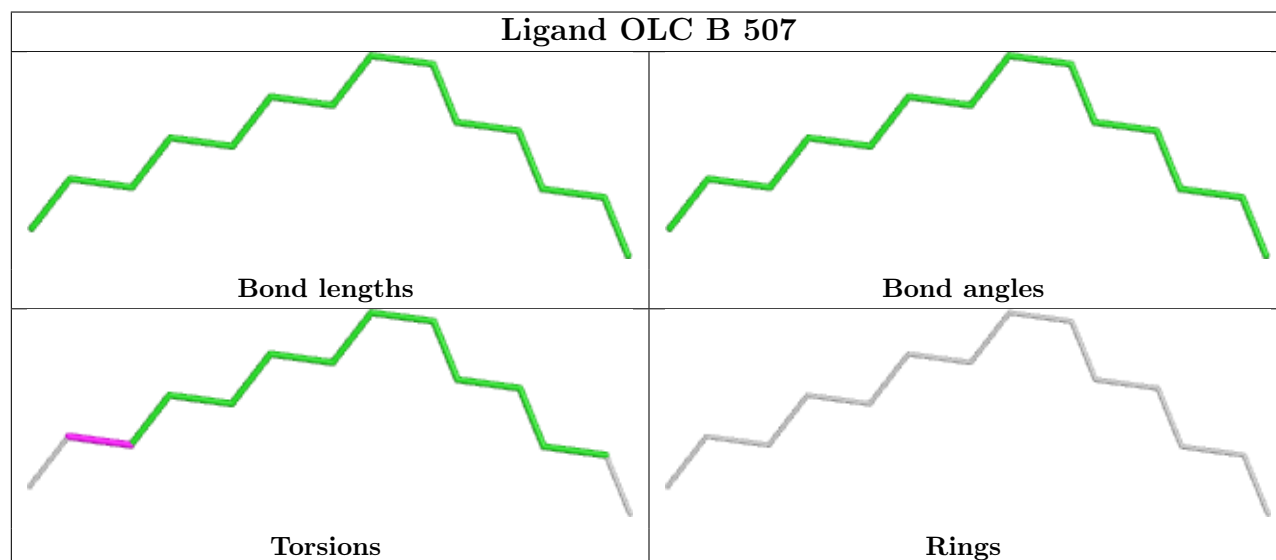
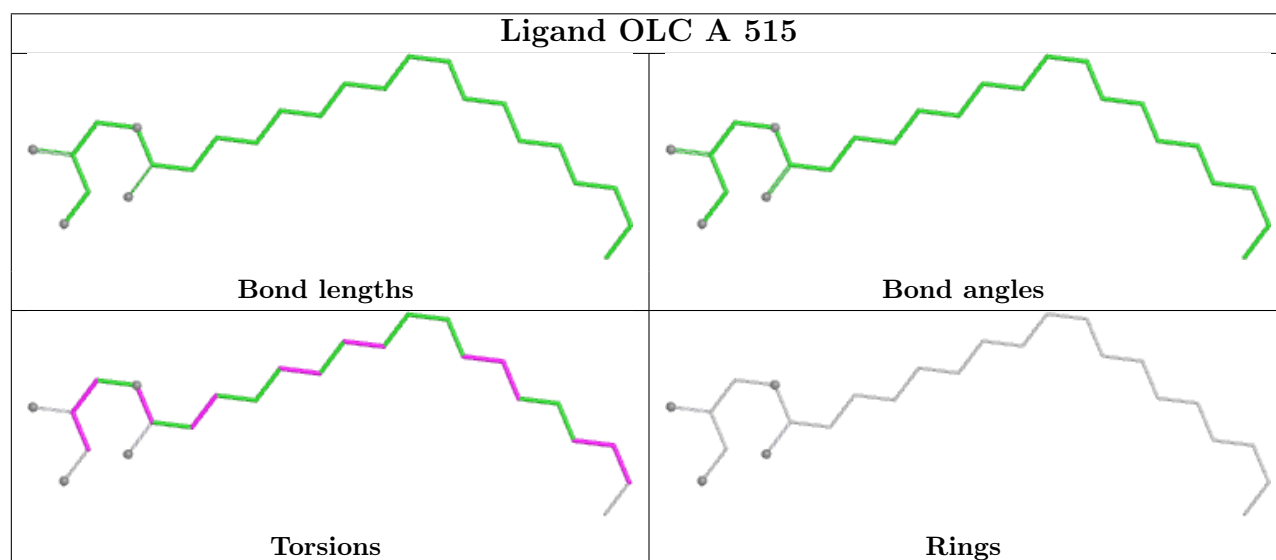
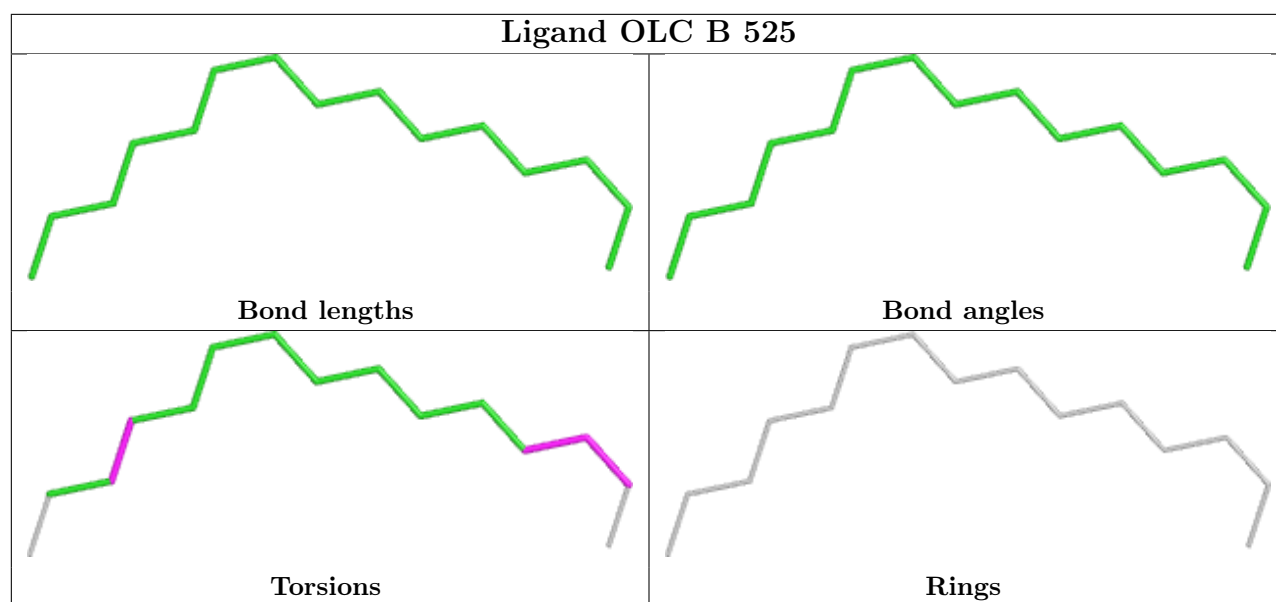


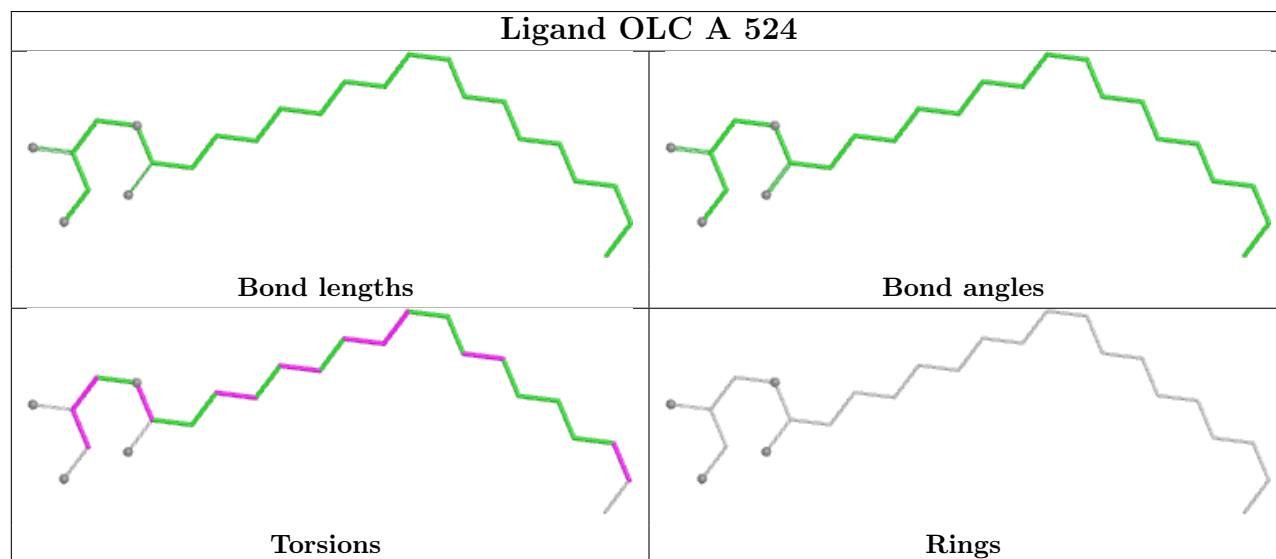
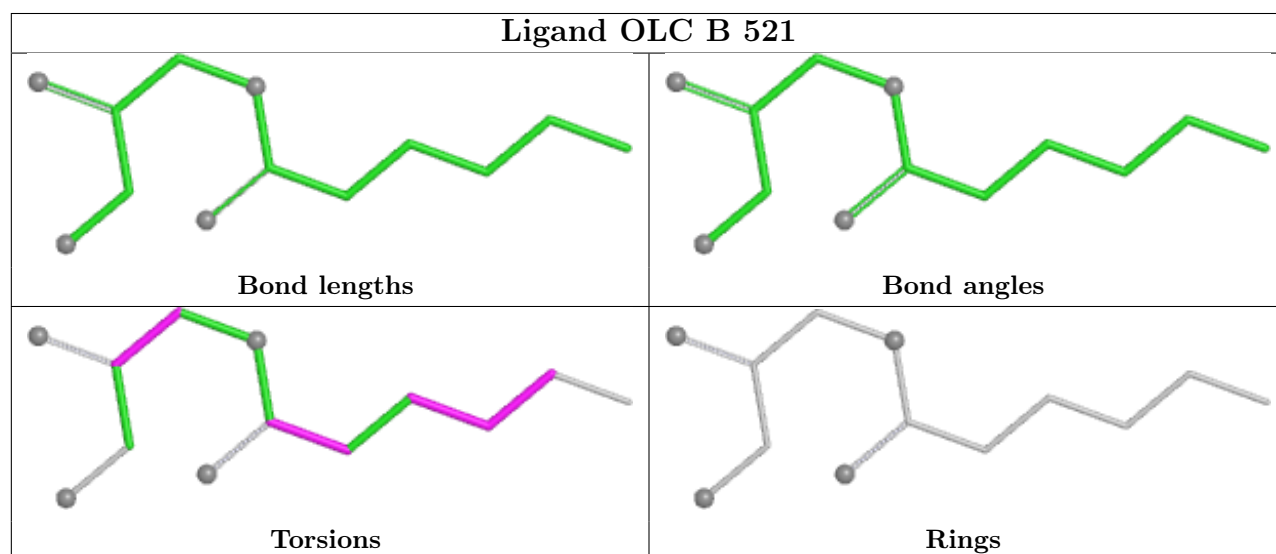
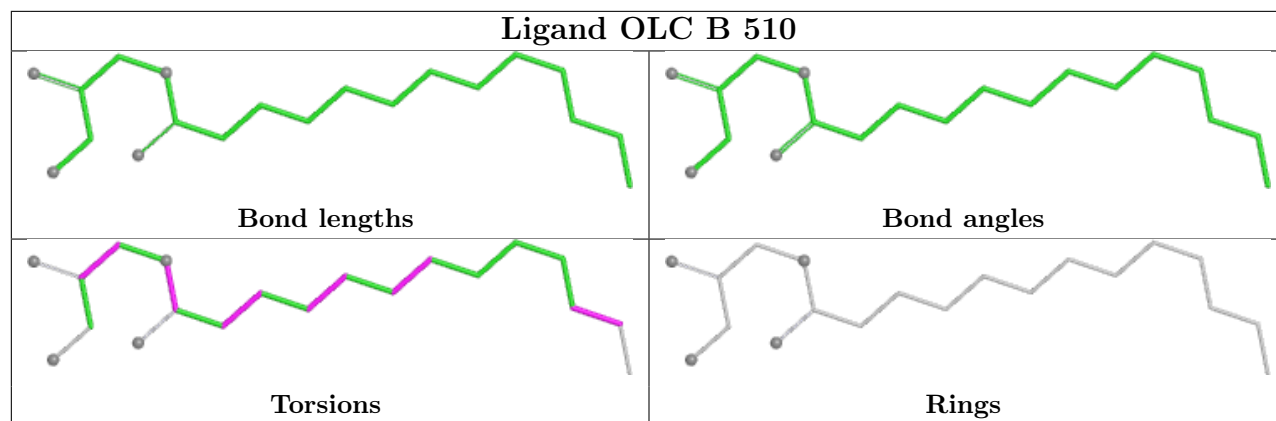


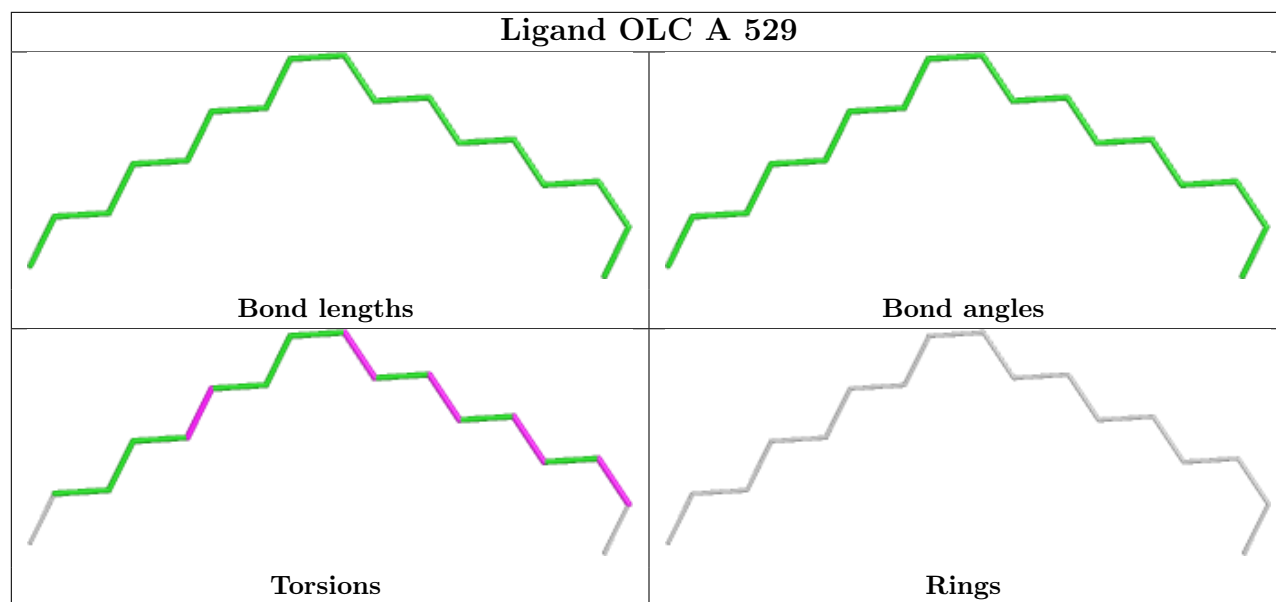
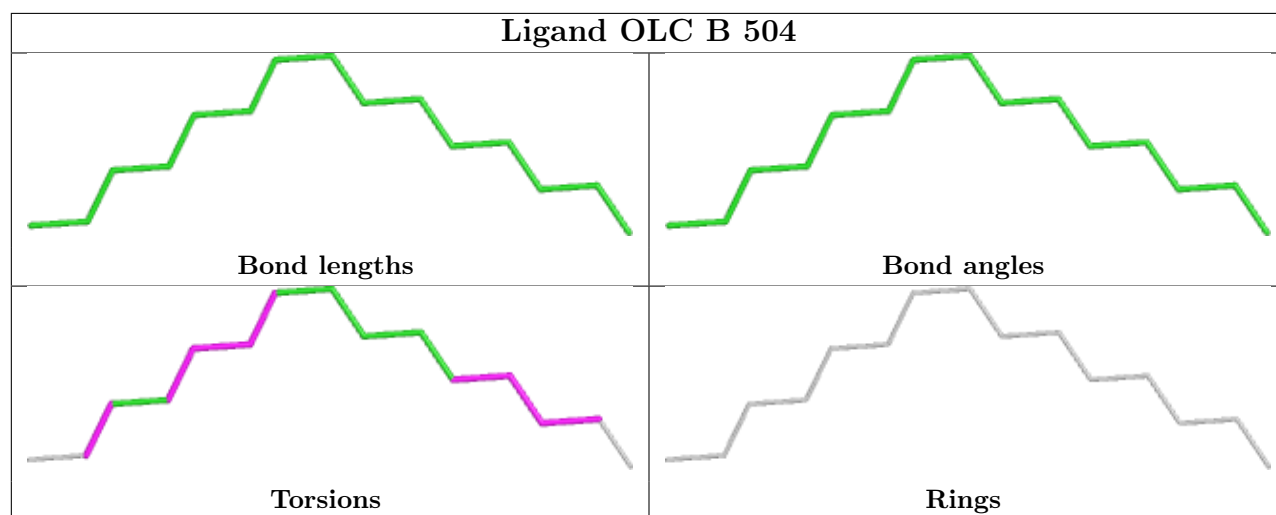
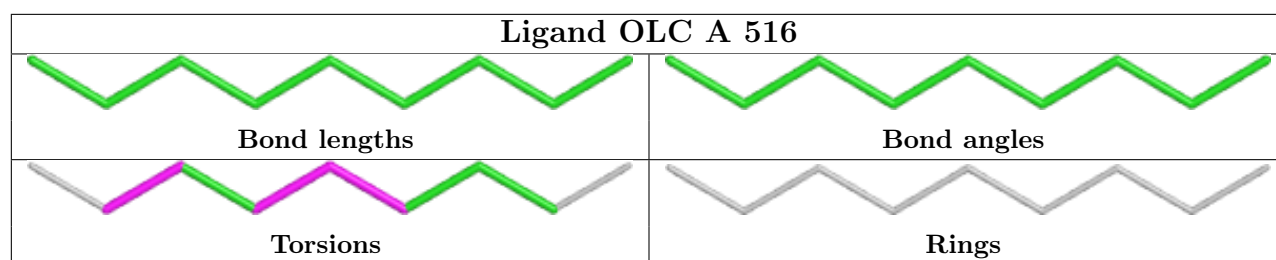


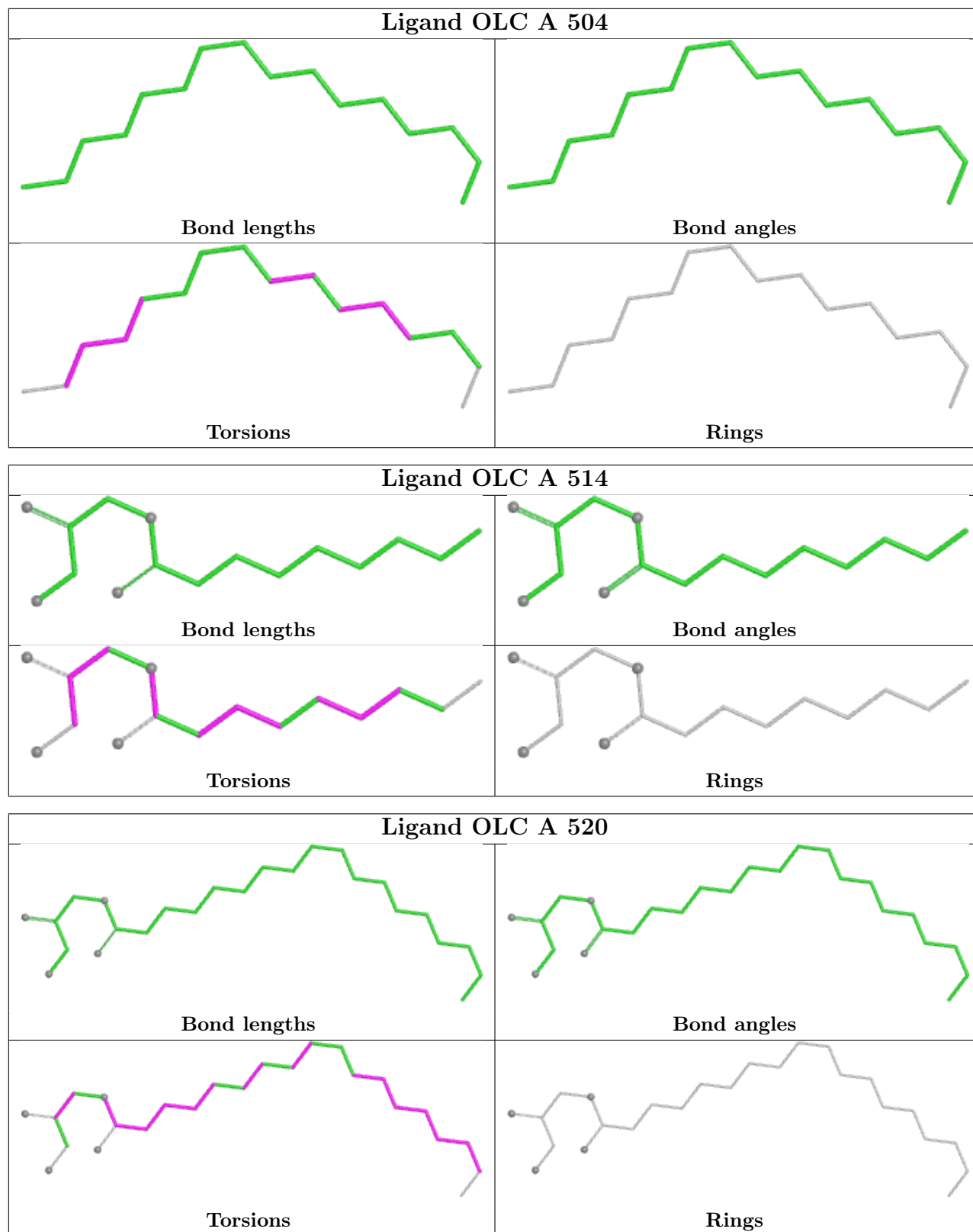


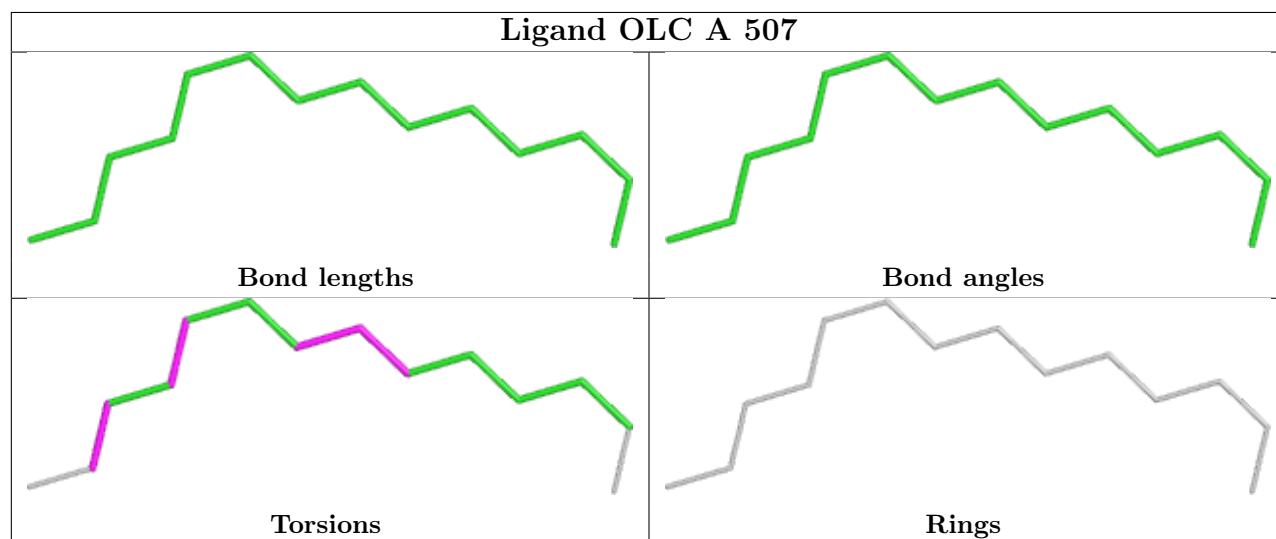
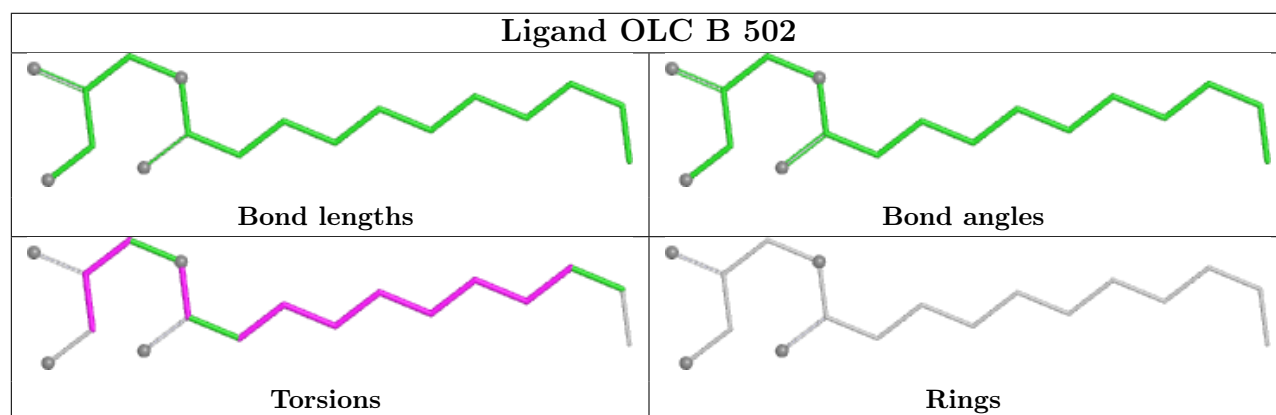
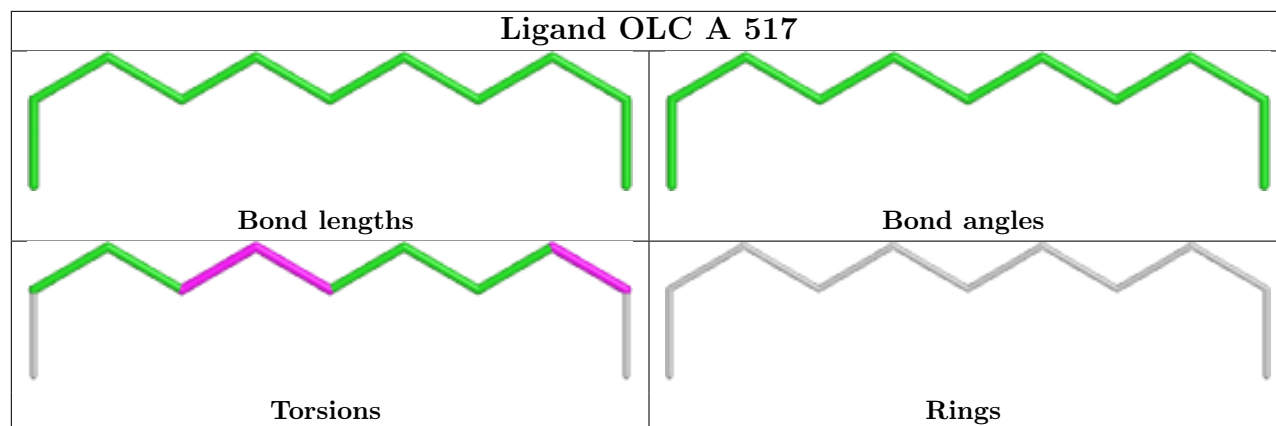


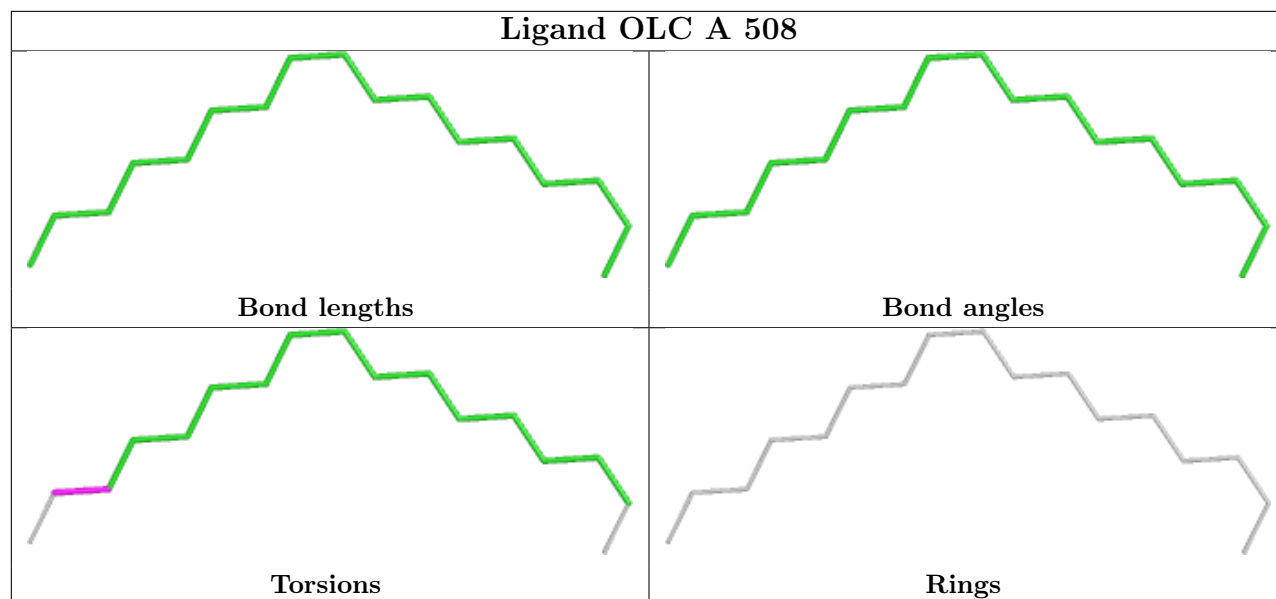












5.7 Other polymers [i](#)

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	370/416 (88%)	0.47	31 (8%) 17 14	25, 38, 82, 340	0
1	B	370/416 (88%)	0.32	22 (5%) 28 24	25, 35, 75, 311	0
All	All	740/832 (88%)	0.39	53 (7%) 21 18	25, 36, 79, 340	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	VAL	7.0
1	A	32	VAL	6.8
1	B	31	LEU	5.6
1	B	33	THR	5.4
1	A	240	TYR	4.5
1	B	326	SER	4.3
1	A	33	THR	4.1
1	B	34	VAL	4.0
1	B	30	LEU	3.9
1	A	324	GLY	3.9
1	A	31	LEU	3.8
1	A	34	VAL	3.8
1	A	29	GLY	3.8
1	A	221	ILE	3.6
1	A	220	VAL	3.3
1	B	220	VAL	3.2
1	A	325	GLU	3.1
1	A	416	PHE	3.0
1	A	233	SER	3.0
1	A	178	ASP	2.9
1	B	334	SER	2.9
1	B	353	GLY	2.7
1	B	35	GLY	2.7
1	A	417	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	234	ILE	2.7
1	B	219	GLU	2.7
1	A	30	LEU	2.6
1	B	416	PHE	2.6
1	A	323	PHE	2.6
1	B	385	LYS	2.6
1	B	221	ILE	2.6
1	B	240	TYR	2.6
1	A	247	PHE	2.5
1	A	149	THR	2.5
1	B	150	ASN	2.4
1	A	237	VAL	2.4
1	B	233	SER	2.4
1	A	271	GLY	2.3
1	A	244	ASP	2.3
1	A	159	ILE	2.3
1	B	314	ALA	2.3
1	A	335	GLN	2.2
1	A	270	SER	2.2
1	B	417	SER	2.2
1	A	218	SER	2.2
1	A	239	LYS	2.2
1	B	218	SER	2.1
1	B	237	VAL	2.1
1	A	35	GLY	2.1
1	A	236	LYS	2.1
1	A	385	LYS	2.0
1	B	79	ILE	2.0
1	A	150	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLC	B	518	6/25	0.44	0.34	60,87,95,97	0
3	OLC	B	509	10/25	0.46	0.21	66,82,87,90	0
3	OLC	A	527	7/25	0.52	0.26	54,67,70,71	0
3	OLC	B	502	18/25	0.56	0.20	47,63,72,75	0
3	OLC	A	528	16/25	0.58	0.25	43,61,69,73	0
3	OLC	A	514	16/25	0.61	0.24	51,66,80,83	0
3	OLC	A	516	9/25	0.61	0.24	72,85,93,93	0
3	OLC	A	521	9/25	0.61	0.25	66,81,95,97	0
3	OLC	A	509	9/25	0.61	0.23	49,55,66,68	0
3	OLC	B	527	12/25	0.64	0.23	55,61,67,72	0
3	OLC	B	512	6/25	0.67	0.20	55,62,69,73	0
3	OLC	B	524	25/25	0.68	0.20	30,49,61,67	0
3	OLC	B	513	6/25	0.68	0.23	60,71,73,79	0
3	OLC	B	523	10/25	0.70	0.21	47,56,59,60	0
3	OLC	B	514	25/25	0.70	0.20	40,62,79,90	0
3	OLC	A	530	18/25	0.70	0.18	40,50,58,60	0
3	OLC	A	529	17/25	0.71	0.22	35,55,69,72	0
3	OLC	A	518	4/25	0.72	0.36	43,48,56,57	0
3	OLC	A	524	25/25	0.72	0.20	36,56,75,85	0
3	OLC	B	522	17/25	0.72	0.23	37,54,64,68	0
3	OLC	A	526	18/25	0.73	0.20	36,55,69,69	0
3	OLC	B	521	13/25	0.73	0.17	52,63,74,77	0
3	OLC	A	520	25/25	0.74	0.18	50,62,78,86	0
3	OLC	B	503	23/25	0.74	0.19	37,50,72,80	0
3	OLC	B	529	17/25	0.74	0.21	38,54,62,68	0
3	OLC	A	502	24/25	0.75	0.19	41,62,68,74	0
3	OLC	B	510	20/25	0.75	0.17	47,58,71,74	0
3	OLC	A	525	13/25	0.76	0.18	38,50,55,60	0
3	OLC	A	504	16/25	0.76	0.16	29,45,54,70	0
3	OLC	A	511	25/25	0.76	0.17	36,46,60,67	0
3	OLC	A	523	5/25	0.76	0.18	48,55,58,59	0
3	OLC	A	512	13/25	0.76	0.22	38,56,71,87	0
3	OLC	A	505	22/25	0.77	0.16	36,53,63,75	0
3	OLC	A	508	17/25	0.77	0.16	31,42,55,60	0
3	OLC	B	506	11/25	0.77	0.21	44,59,88,88	0
3	OLC	A	515	25/25	0.78	0.15	39,56,78,82	0
3	OLC	B	528	11/25	0.78	0.18	48,55,60,61	0

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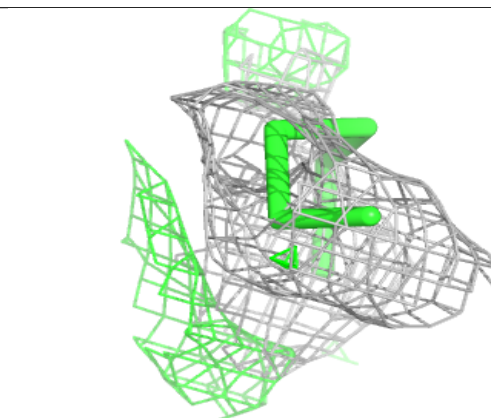
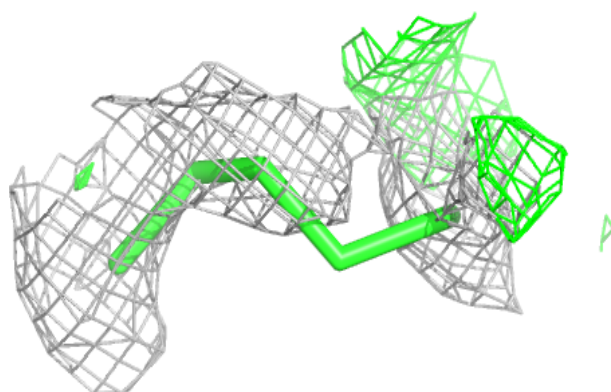
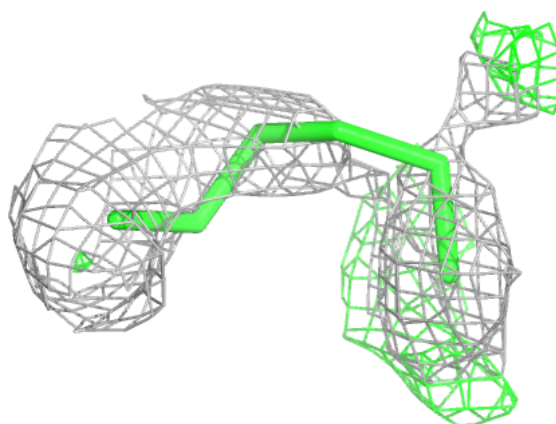
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	OLC	B	511	13/25	0.78	0.20	53,65,84,88	0
3	OLC	B	516	25/25	0.79	0.15	32,52,65,66	0
3	OLC	B	505	14/25	0.80	0.17	30,45,63,69	0
3	OLC	A	510	8/25	0.80	0.18	35,48,55,56	0
3	OLC	B	526	7/25	0.80	0.15	39,43,52,52	0
3	OLC	B	520	11/25	0.80	0.17	36,47,62,64	0
3	OLC	A	522	9/25	0.80	0.16	36,49,52,56	0
3	OLC	A	507	14/25	0.80	0.18	36,48,60,64	0
4	PEG	A	531	6/7	0.80	0.21	51,58,67,68	0
3	OLC	A	519	5/25	0.81	0.20	39,49,51,51	0
3	OLC	B	515	9/25	0.81	0.17	41,45,61,67	0
3	OLC	A	517	11/25	0.81	0.18	39,46,59,64	0
3	OLC	B	517	11/25	0.81	0.15	39,50,62,74	0
3	OLC	A	513	10/25	0.81	0.17	47,53,59,61	0
3	OLC	B	504	15/25	0.82	0.15	26,38,53,53	0
3	OLC	B	519	12/25	0.82	0.14	39,44,54,55	0
3	OLC	A	503	11/25	0.82	0.12	47,54,60,61	0
3	OLC	B	525	15/25	0.83	0.14	33,43,58,60	0
3	OLC	A	506	12/25	0.84	0.13	38,44,51,51	0
4	PEG	B	530	4/7	0.85	0.13	33,33,43,51	0
3	OLC	B	507	14/25	0.87	0.14	40,48,58,62	0
3	OLC	B	508	5/25	0.88	0.12	37,41,45,46	0
2	MN	B	501	1/1	0.95	0.12	71,71,71,71	1
2	MN	A	501	1/1	0.96	0.10	68,68,68,68	1

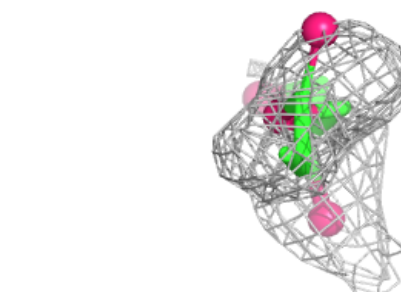
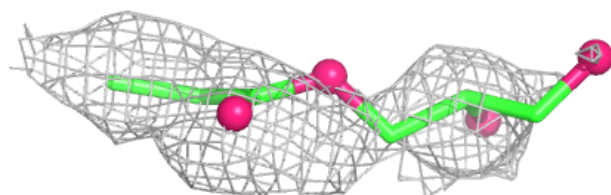
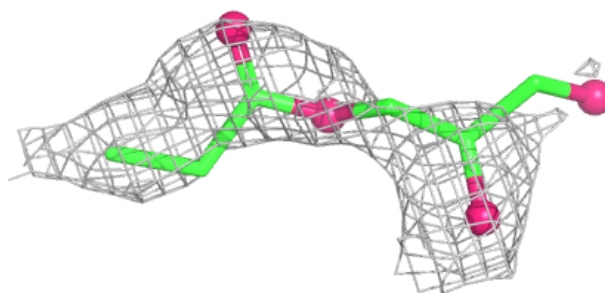
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC B 518:

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

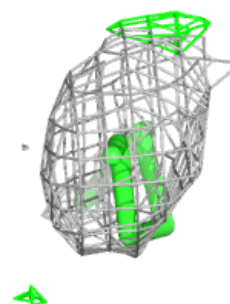
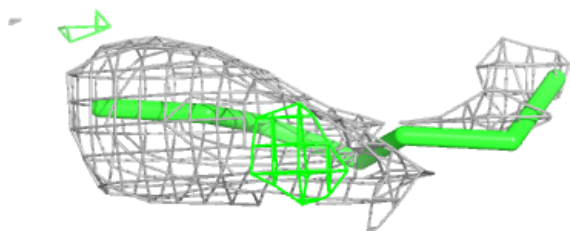
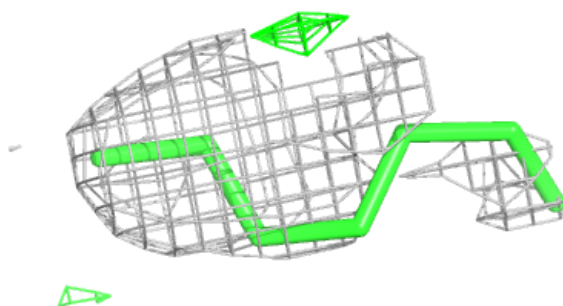
**Electron density around OLC B 509:**

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

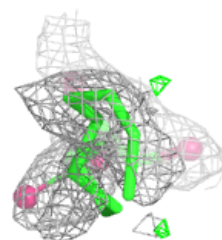
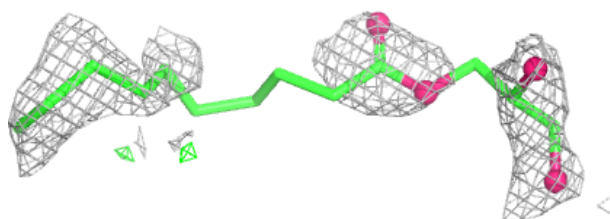
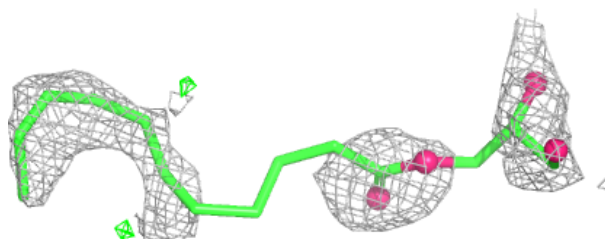


Electron density around OLC A 527:

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

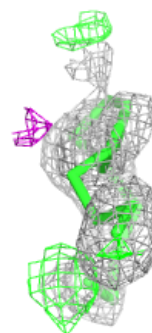
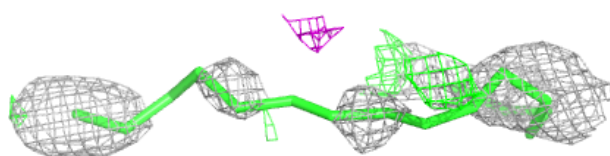
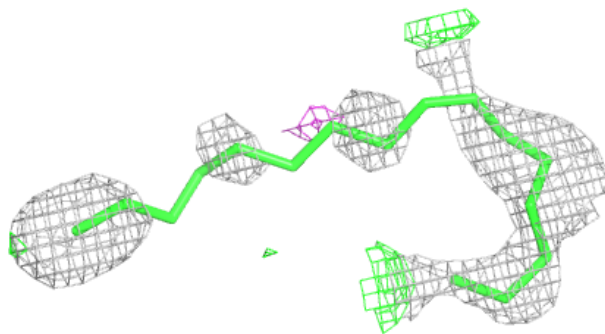
**Electron density around OLC B 502:**

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

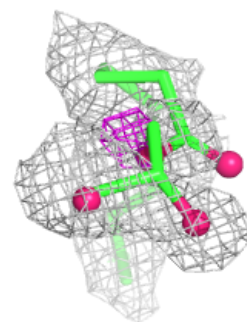
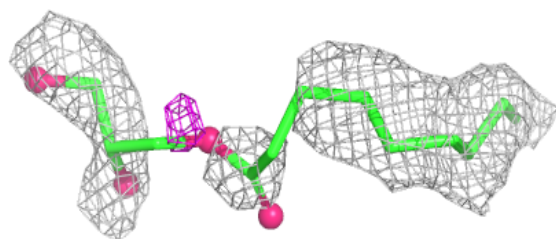
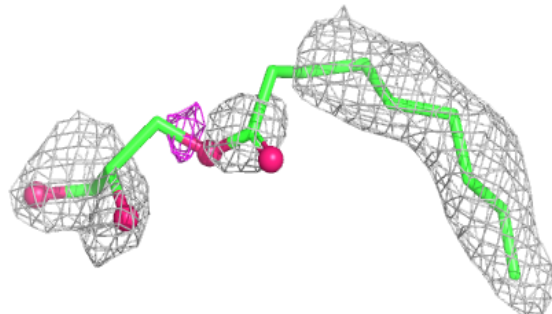


Electron density around OLC A 528:

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

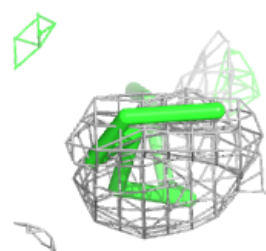
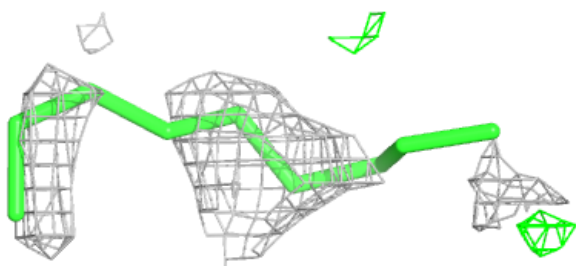
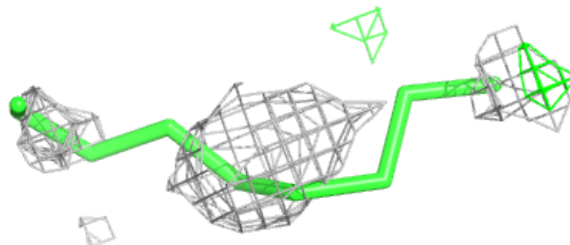
**Electron density around OLC A 514:**

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

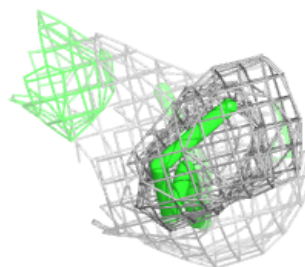
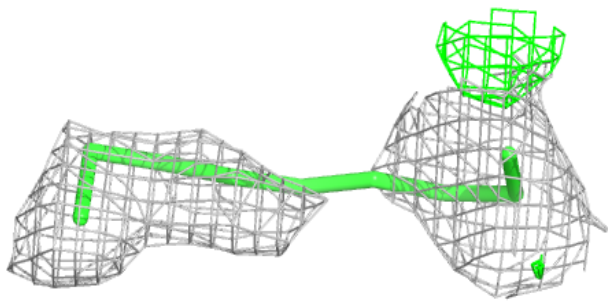
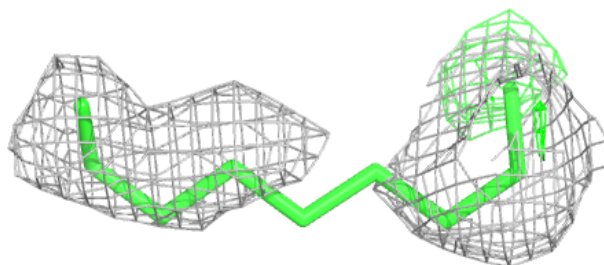


Electron density around OLC A 516:

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

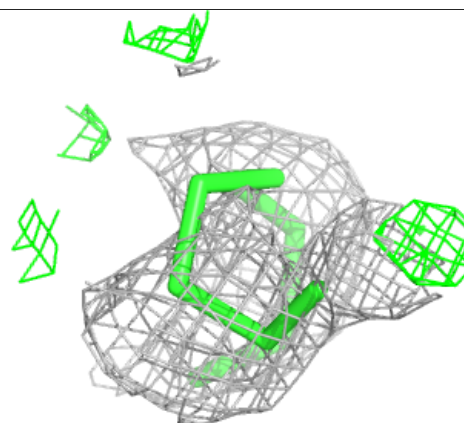
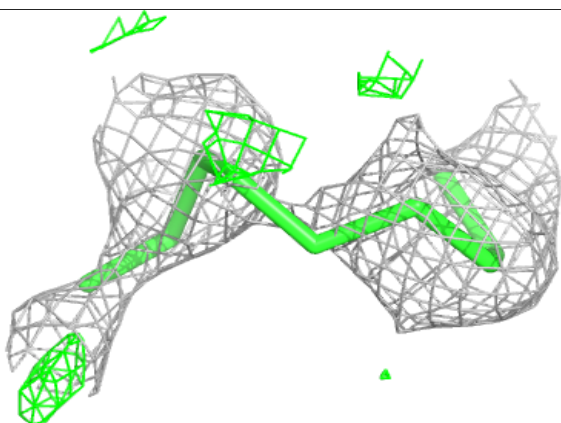
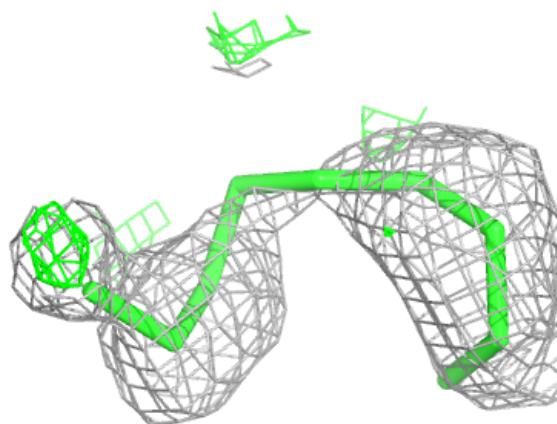
**Electron density around OLC A 521:**

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

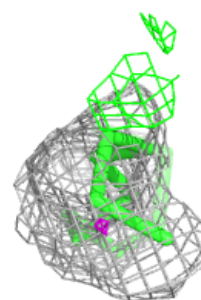
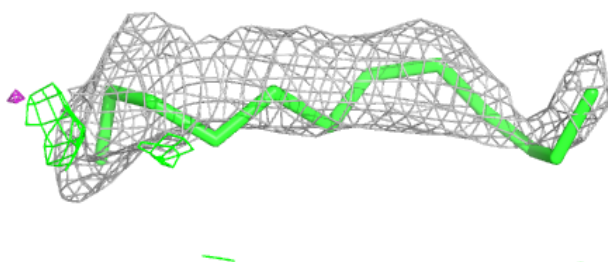
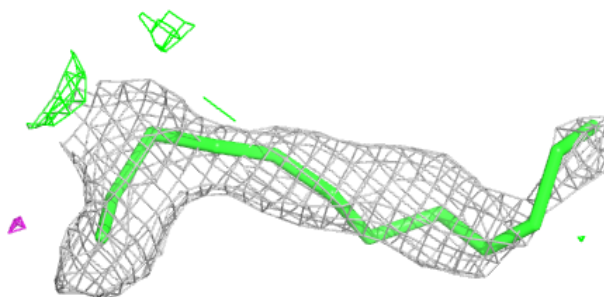


Electron density around OLC A 509:

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

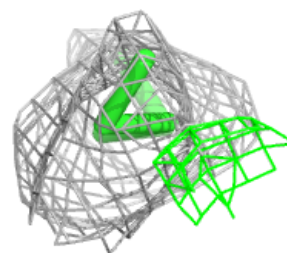
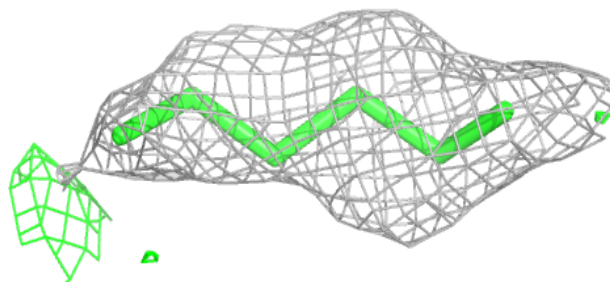
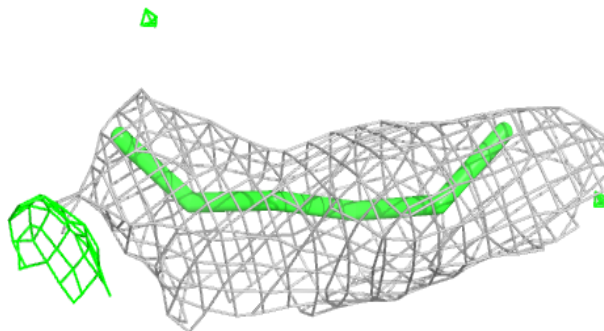
**Electron density around OLC B 527:**

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

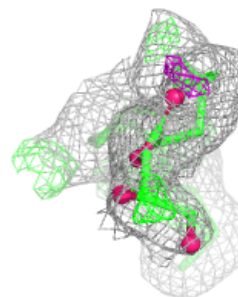
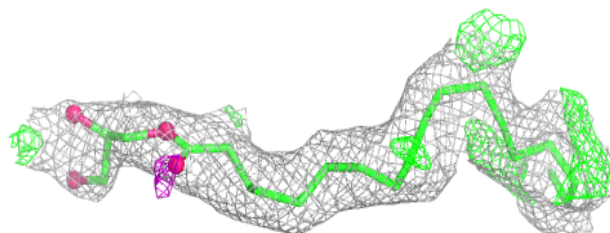
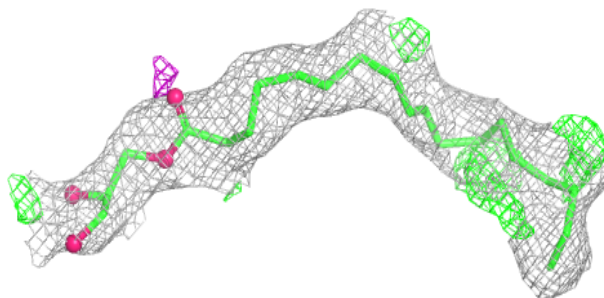


Electron density around OLC B 512:

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

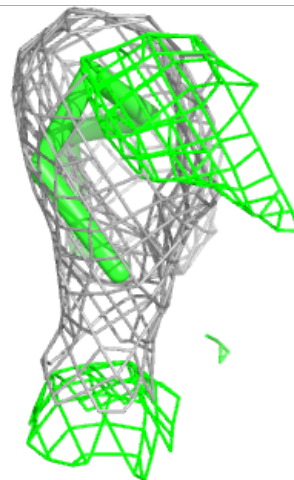
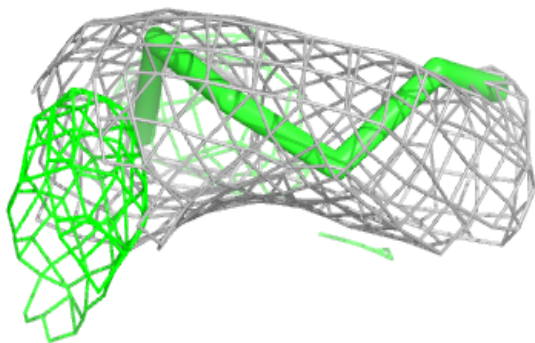
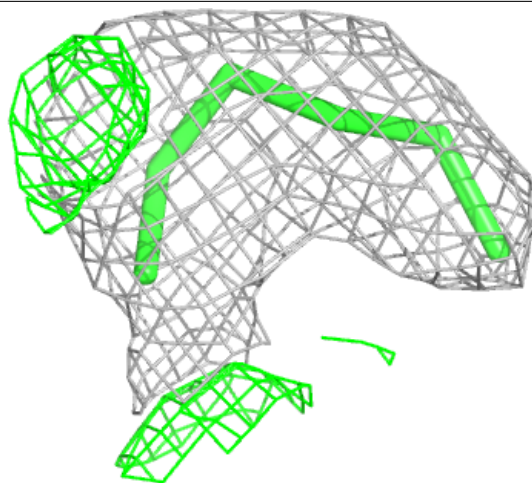
**Electron density around OLC B 524:**

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



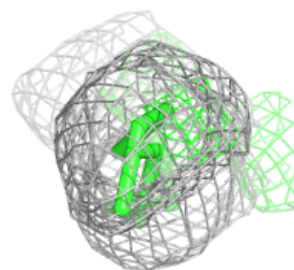
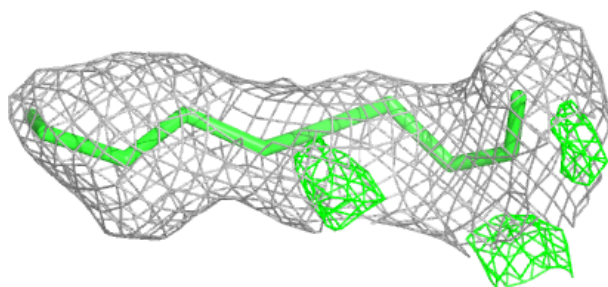
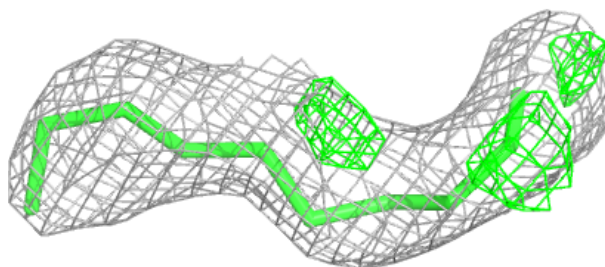
Electron density around OLC B 513:

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

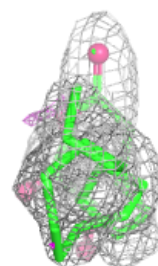
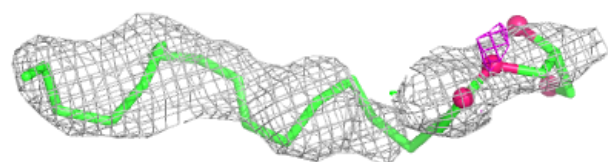
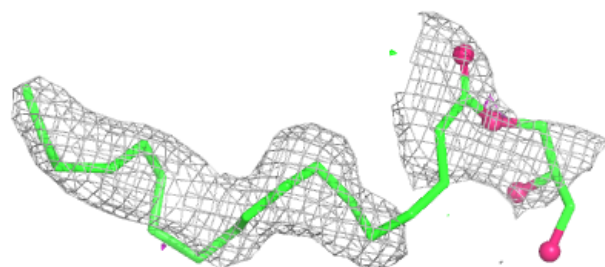


Electron density around OLC B 523:

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

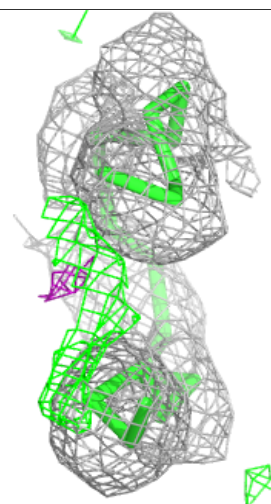
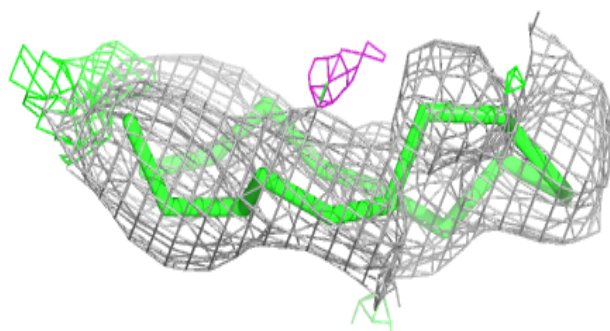
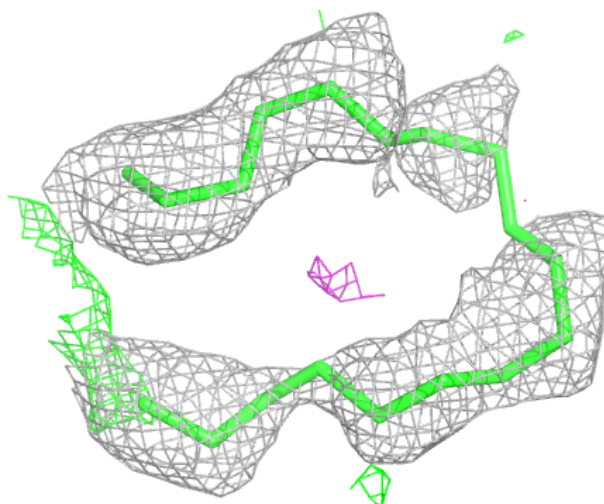
**Electron density around OLC B 514:**

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



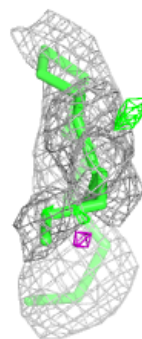
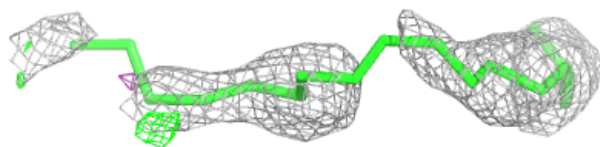
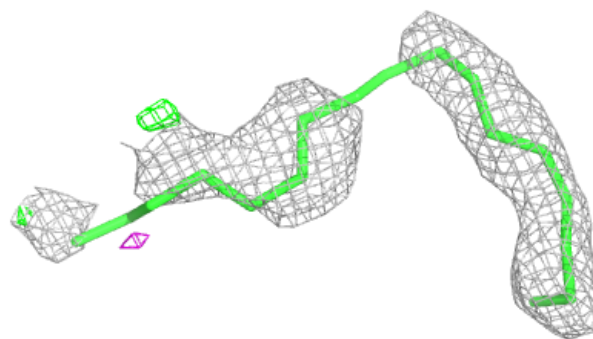
Electron density around OLC A 530:

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

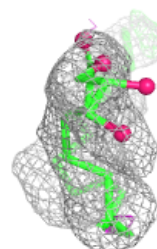
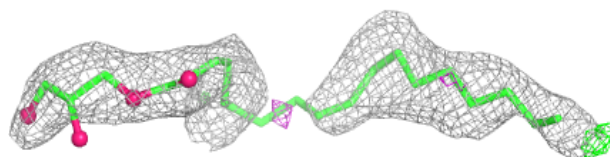
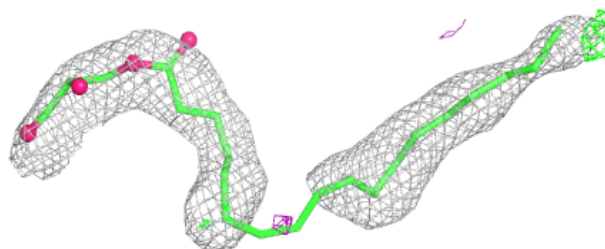


Electron density around OLC A 529:

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

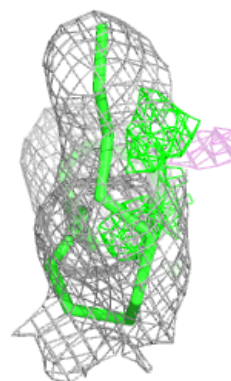
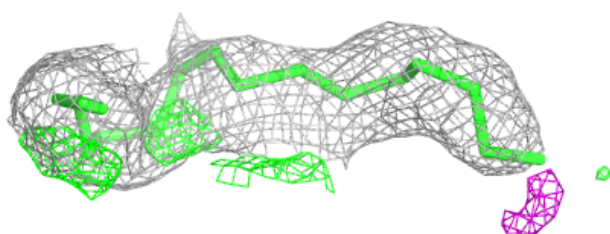
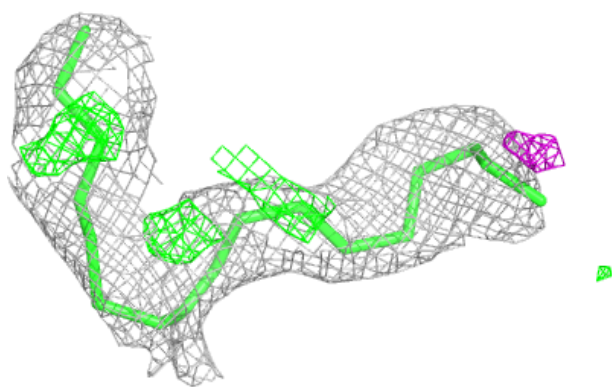
**Electron density around OLC A 524:**

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

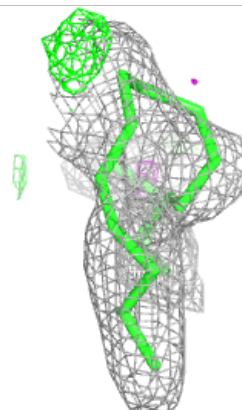
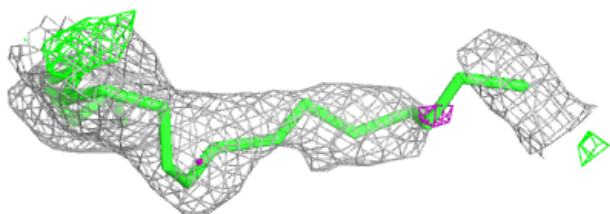
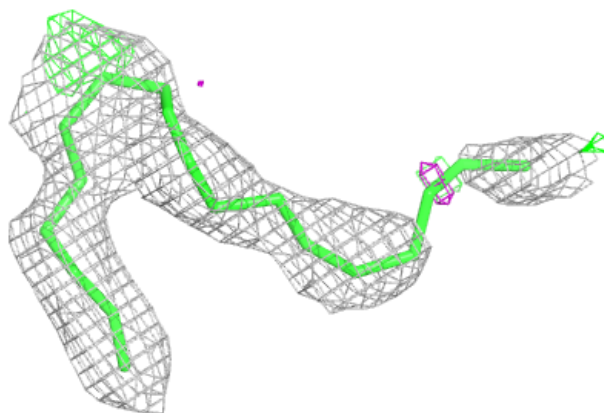


Electron density around OLC B 522:

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

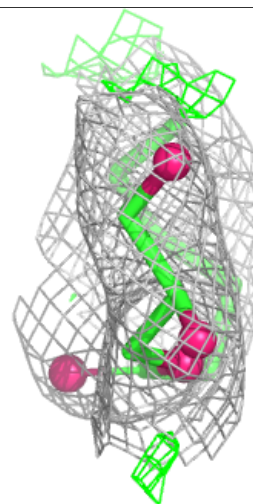
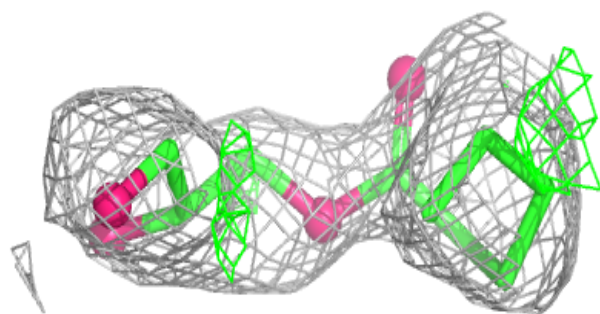
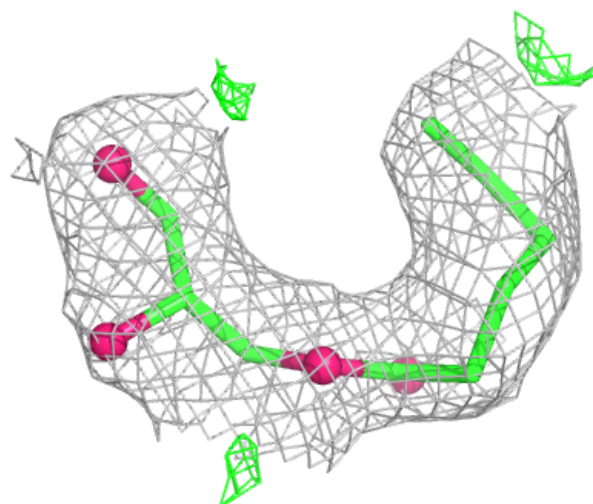
**Electron density around OLC A 526:**

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



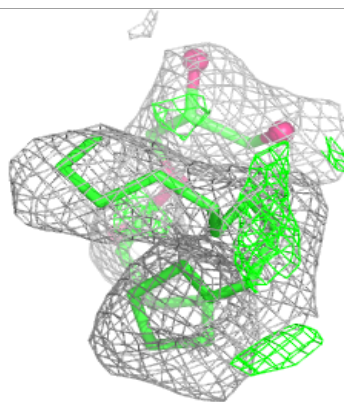
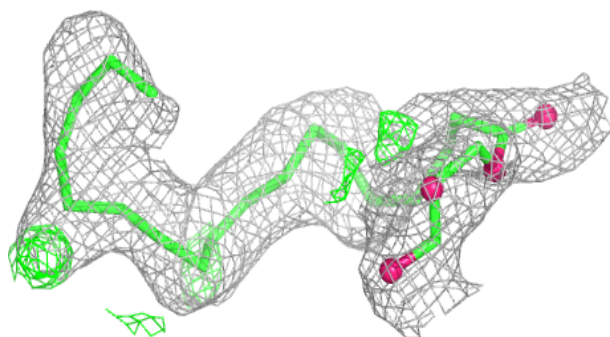
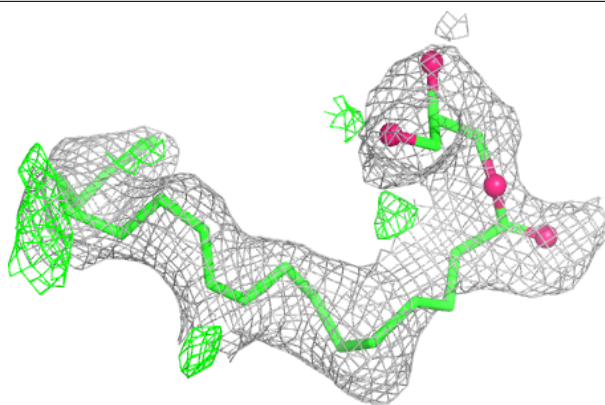
Electron density around OLC B 521:

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

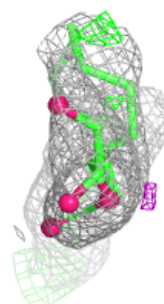
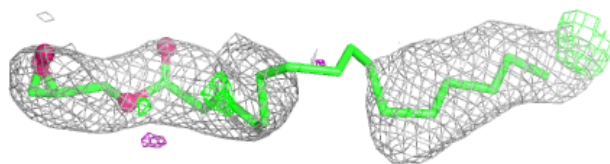
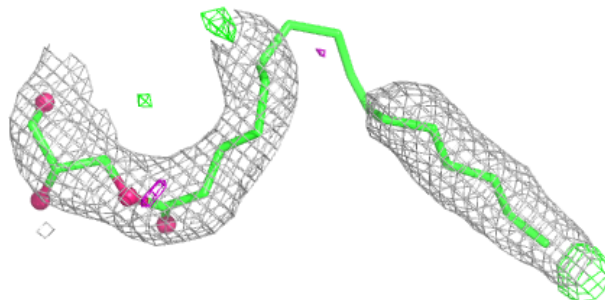


Electron density around OLC A 520:

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

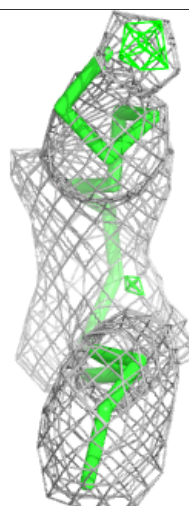
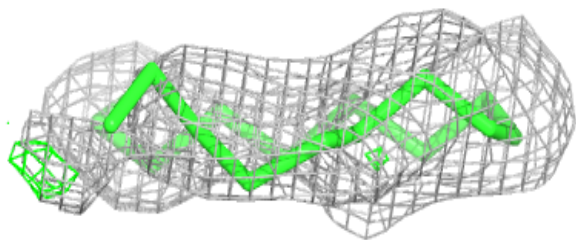
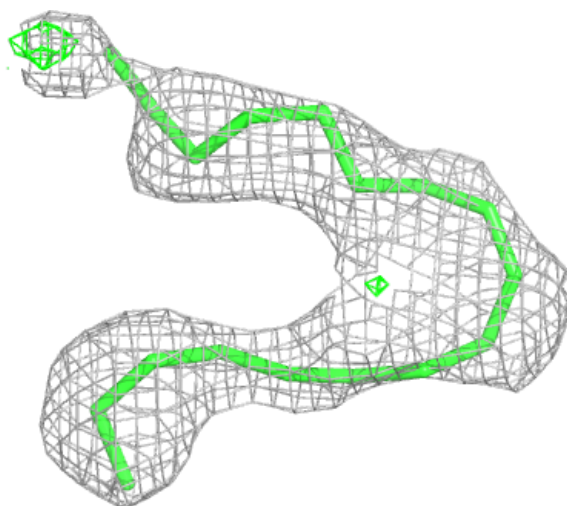
**Electron density around OLC B 503:**

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



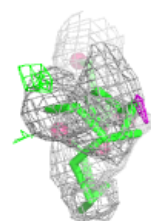
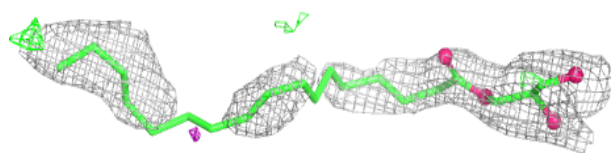
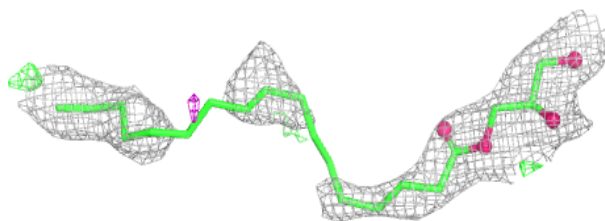
Electron density around OLC B 529:

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

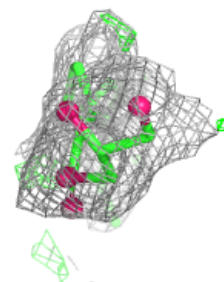
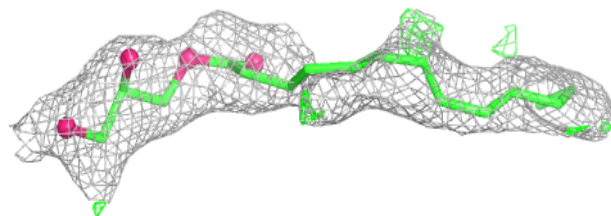
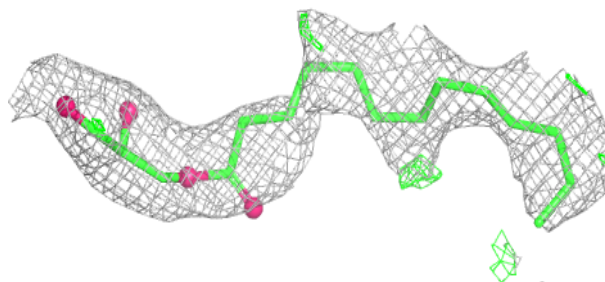


Electron density around OLC A 502:

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

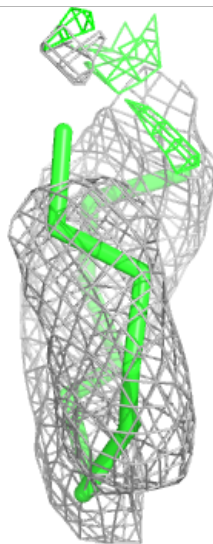
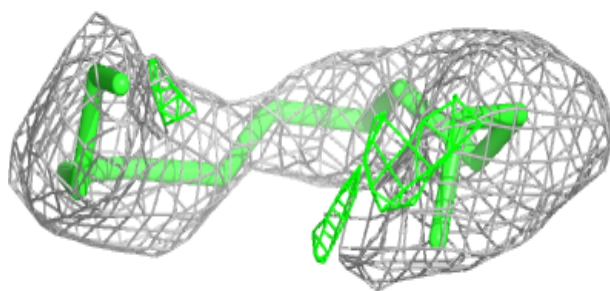
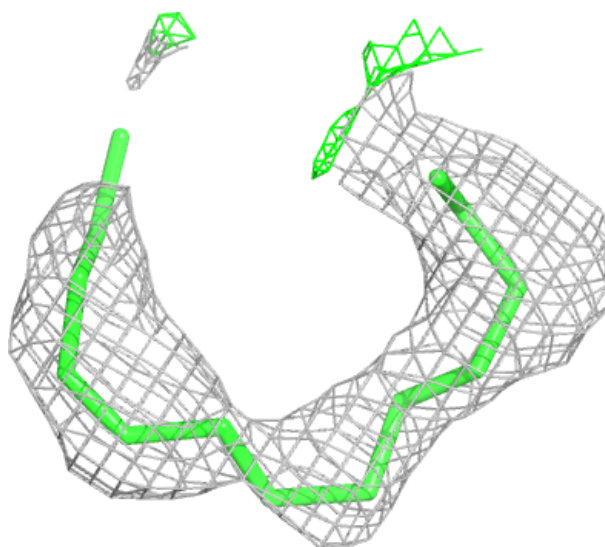
**Electron density around OLC B 510:**

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



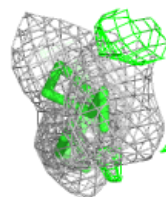
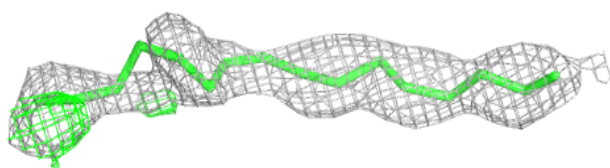
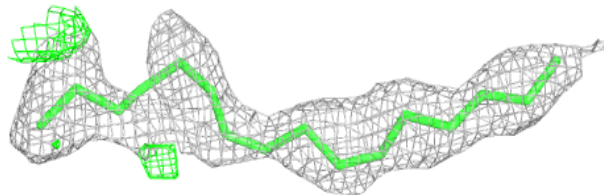
Electron density around OLC A 525:

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

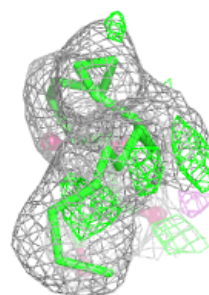
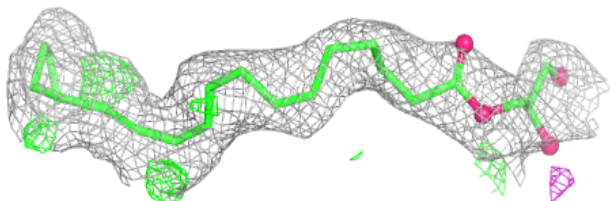
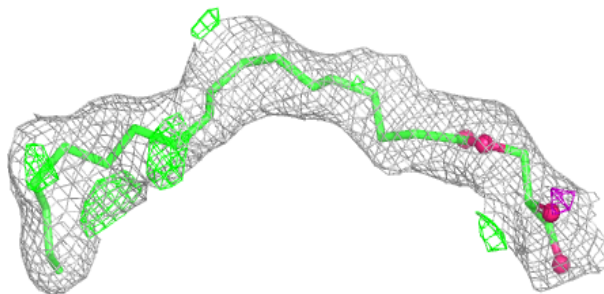


Electron density around OLC A 504:

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

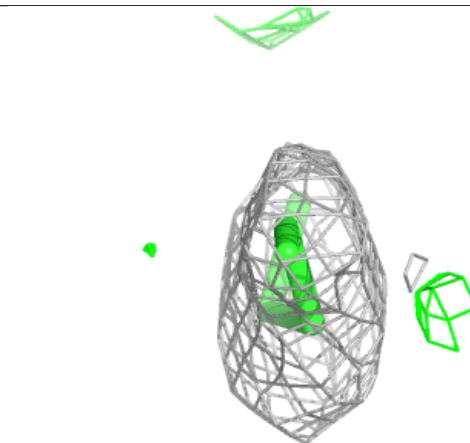
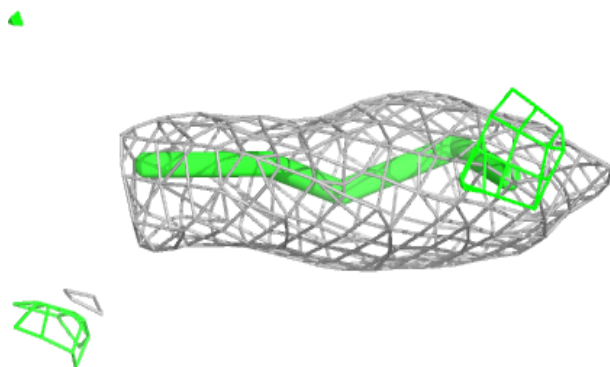
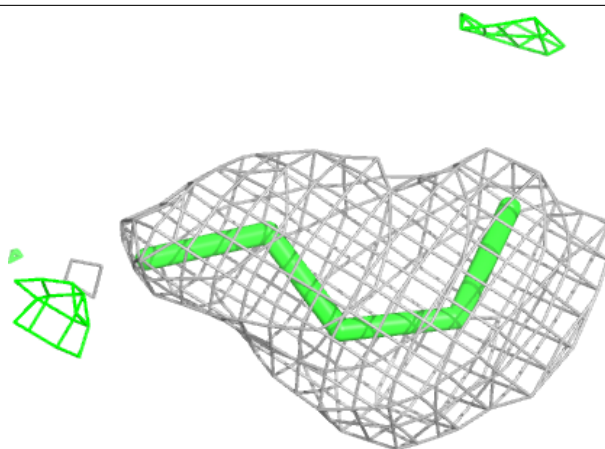
**Electron density around OLC A 511:**

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

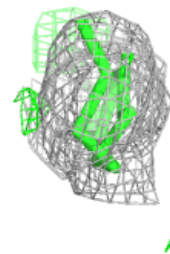
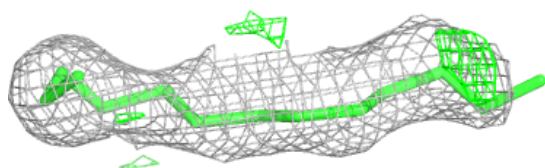
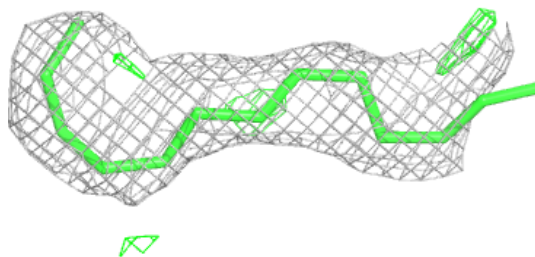


Electron density around OLC A 523:

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

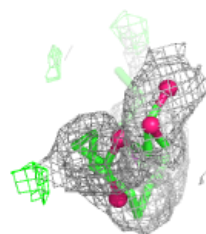
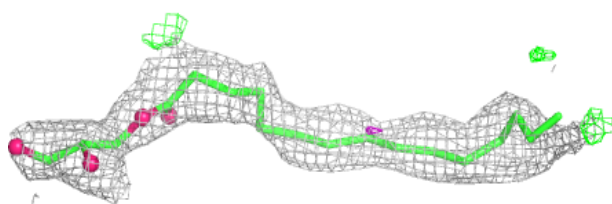
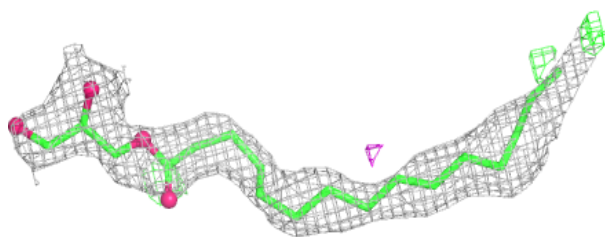
**Electron density around OLC A 512:**

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

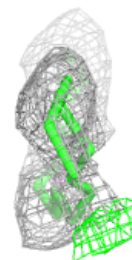
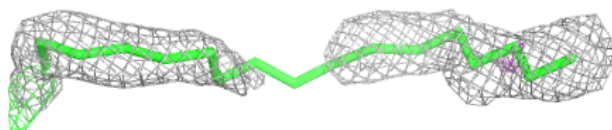
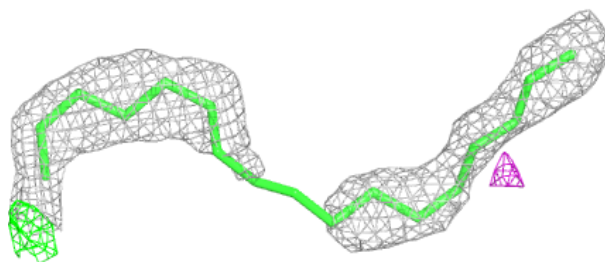


Electron density around OLC A 505:

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

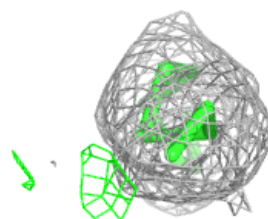
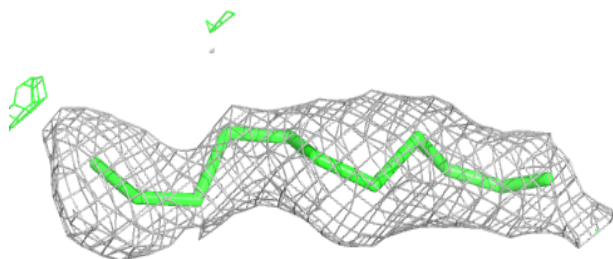
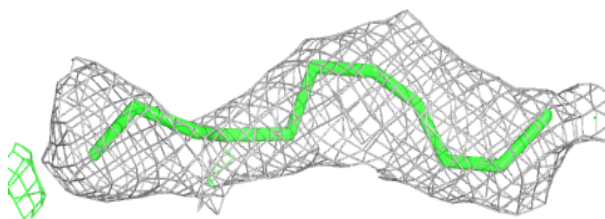
**Electron density around OLC A 508:**

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

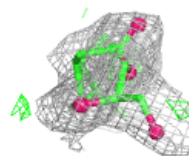
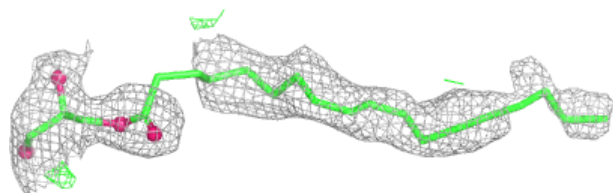
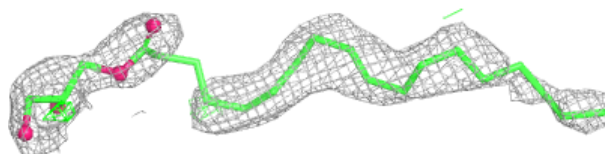


Electron density around OLC B 506:

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

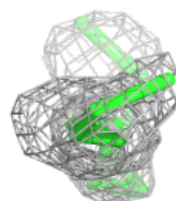
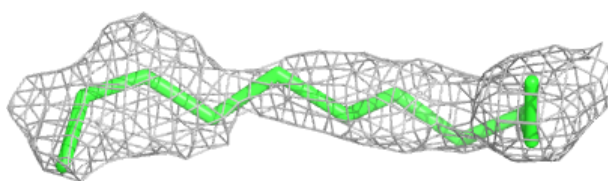
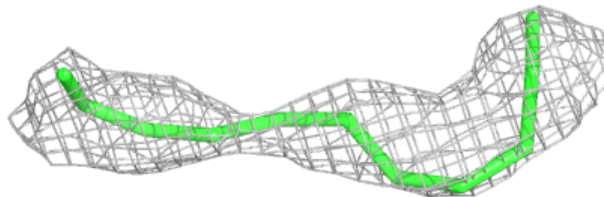
**Electron density around OLC A 515:**

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

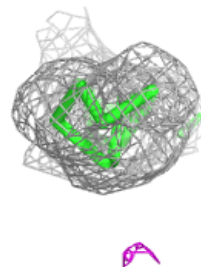
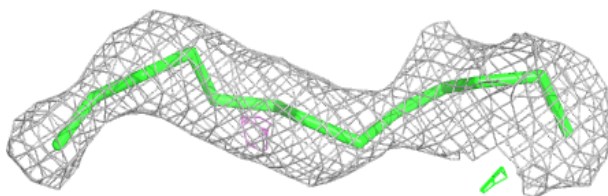
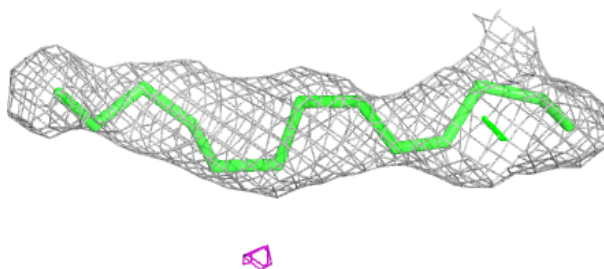


Electron density around OLC B 528:

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

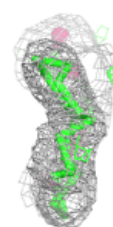
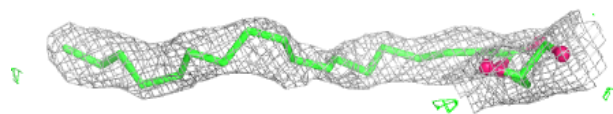
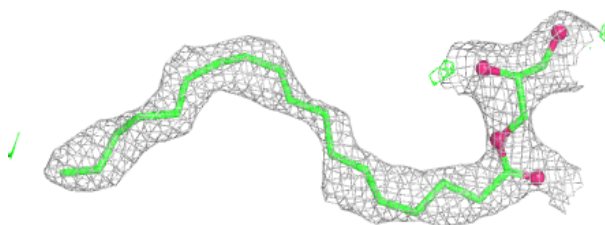
**Electron density around OLC B 511:**

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



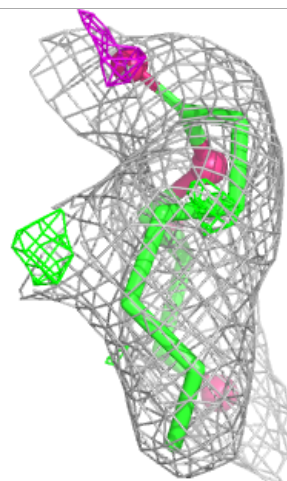
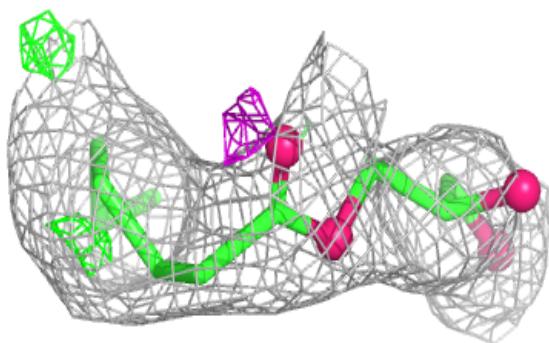
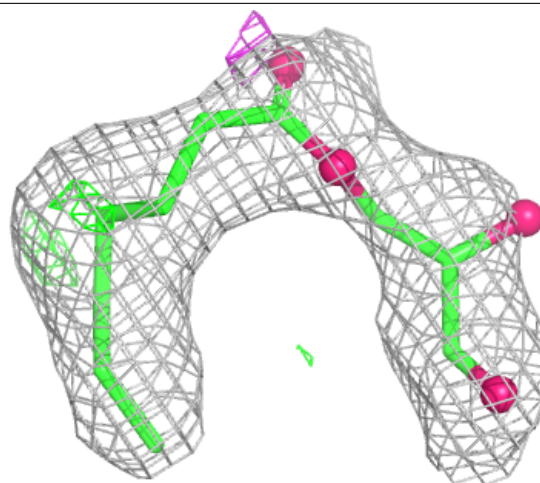
Electron density around OLC B 516:

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



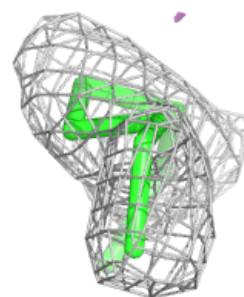
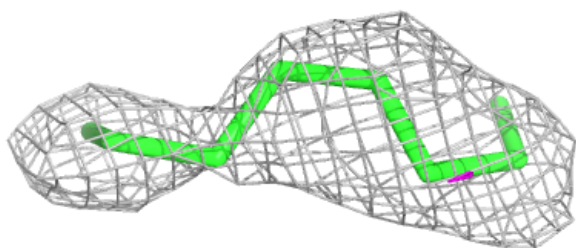
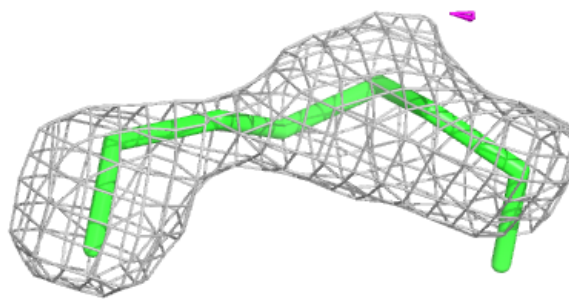
Electron density around OLC B 505:

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

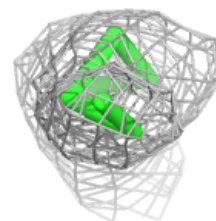
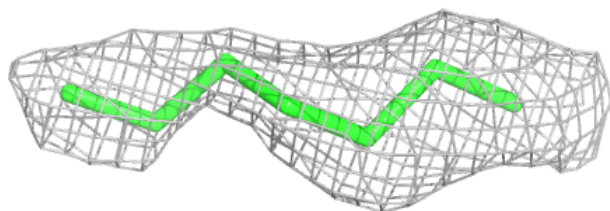
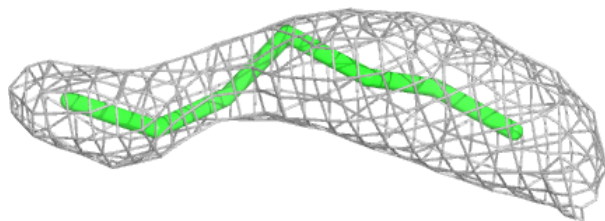


Electron density around OLC A 510:

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

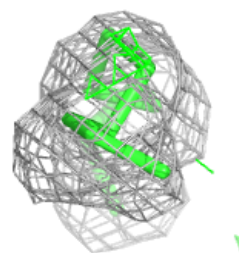
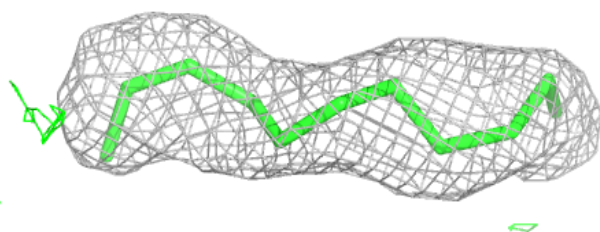
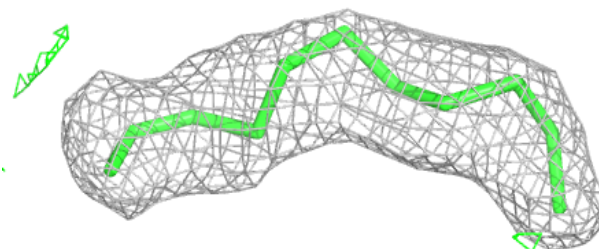
**Electron density around OLC B 526:**

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

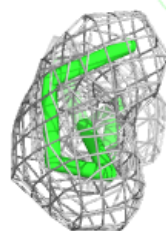
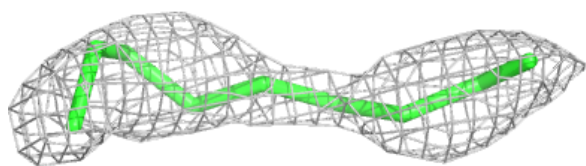
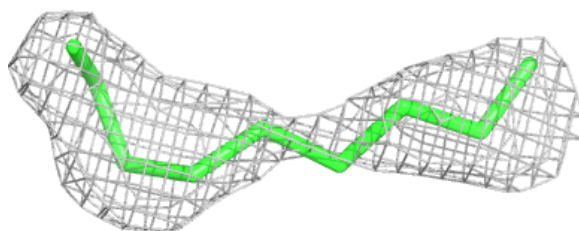


Electron density around OLC B 520:

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

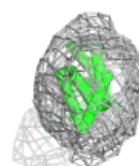
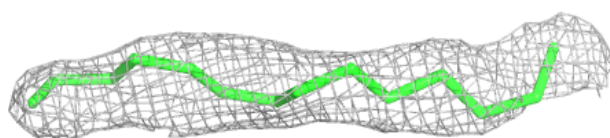
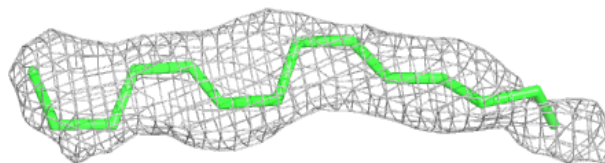
**Electron density around OLC A 522:**

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

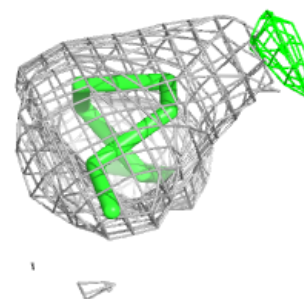
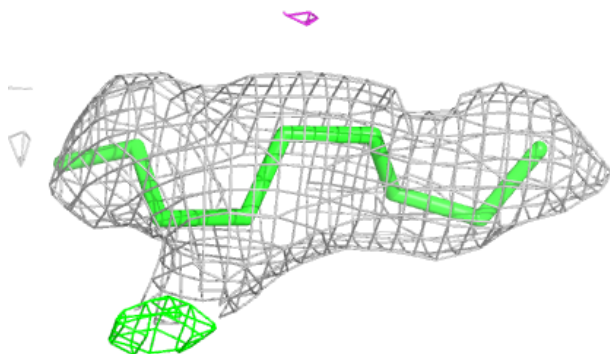
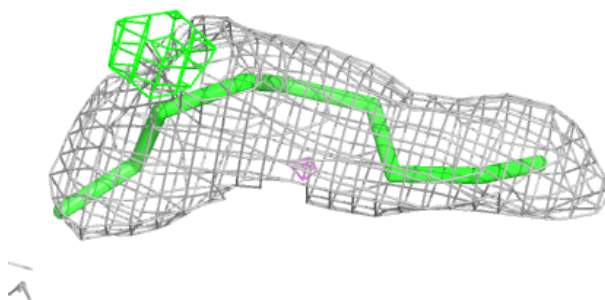


Electron density around OLC A 507:

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

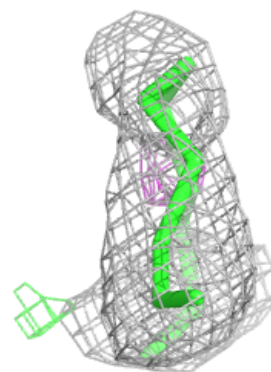
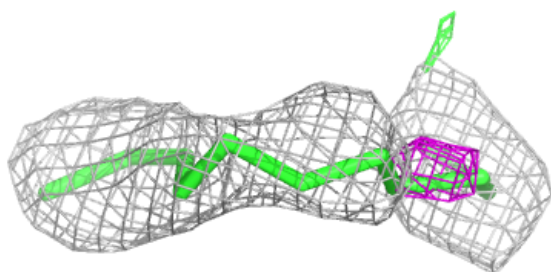
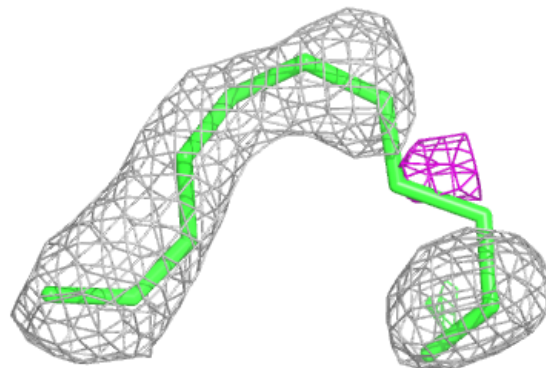
**Electron density around OLC B 515:**

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

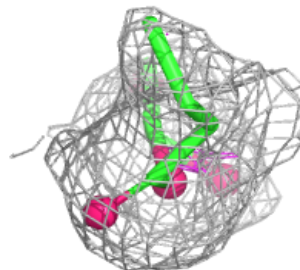
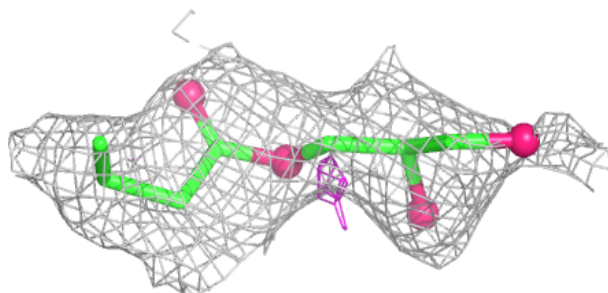
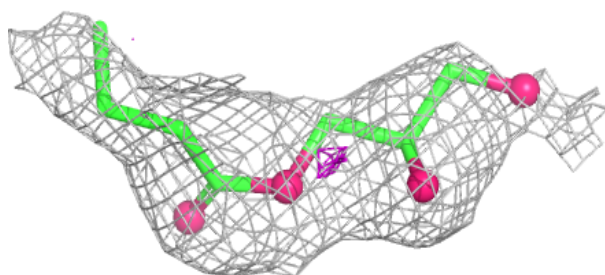


Electron density around OLC A 517:

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

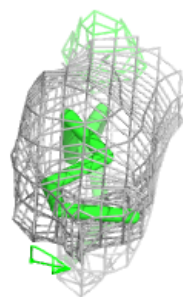
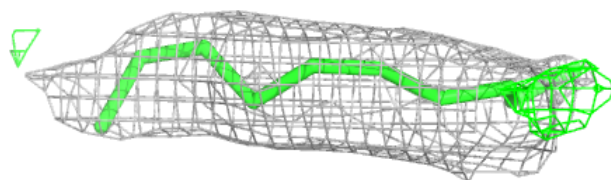
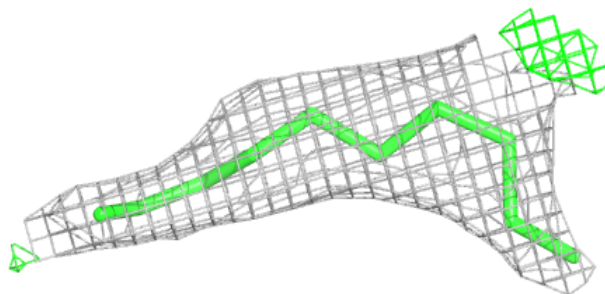
**Electron density around OLC B 517:**

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

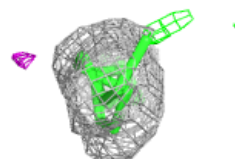
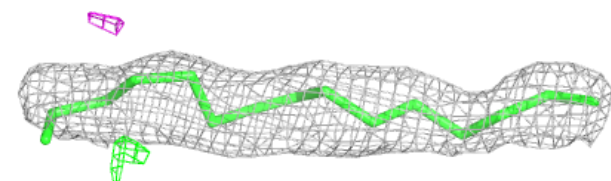
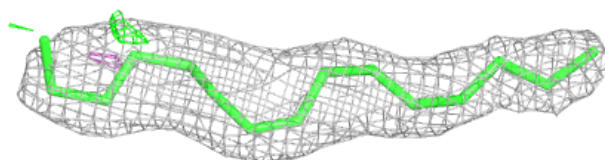


Electron density around OLC A 513:

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

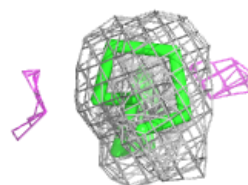
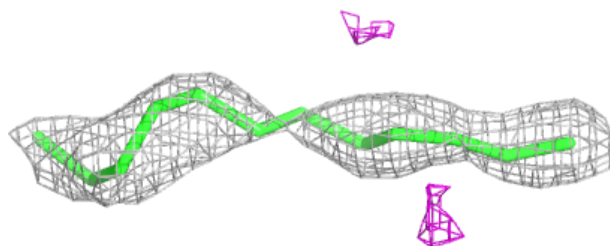
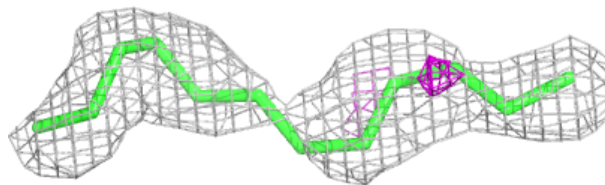
**Electron density around OLC B 504:**

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

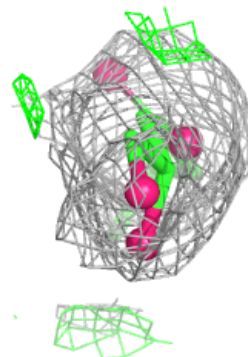
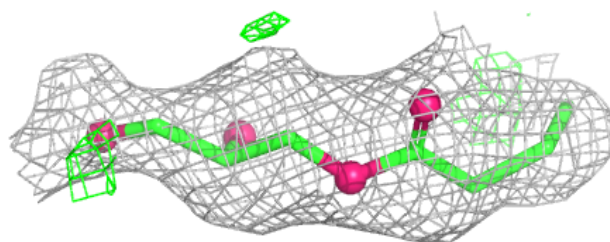
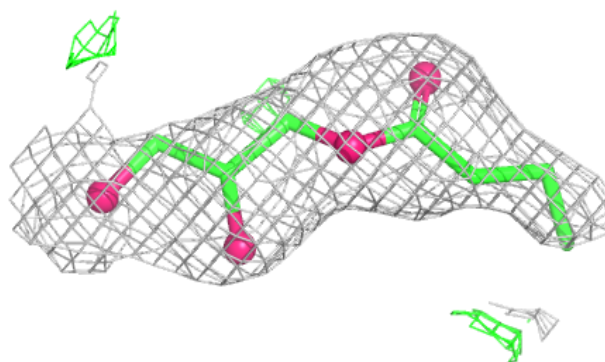


Electron density around OLC B 519:

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

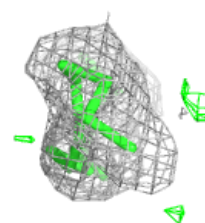
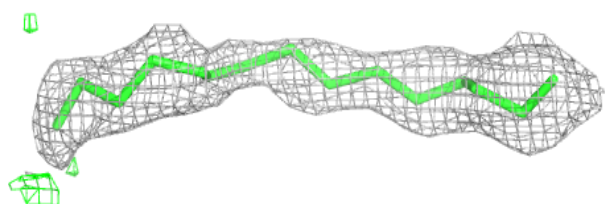
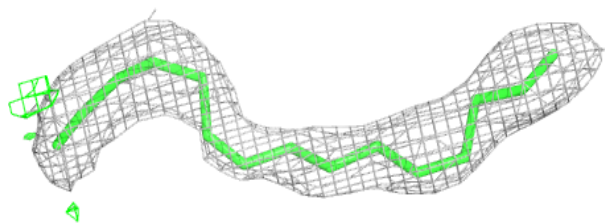
**Electron density around OLC A 503:**

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

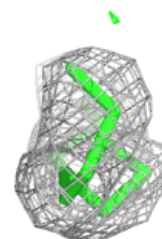
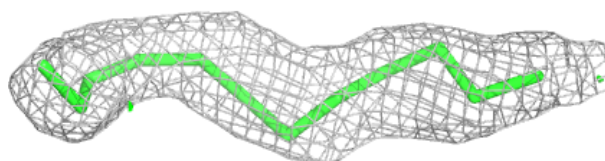
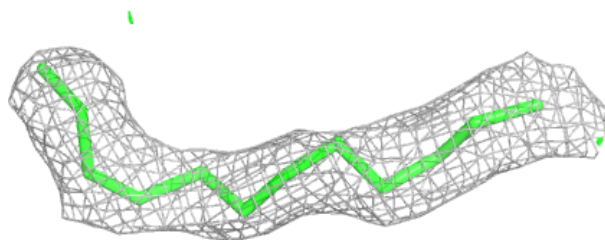


Electron density around OLC B 525:

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

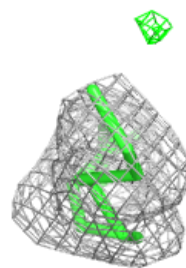
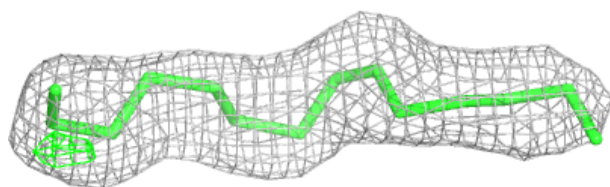
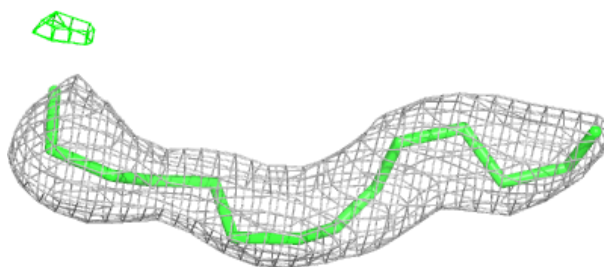
**Electron density around OLC A 506:**

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

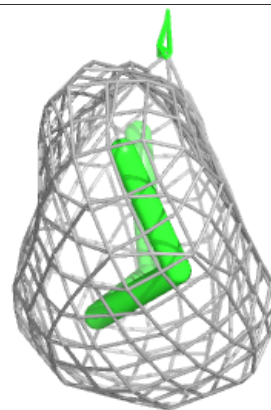
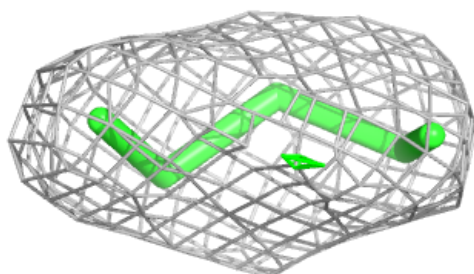
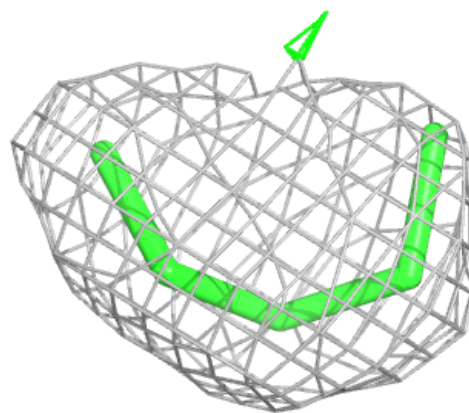


Electron density around OLC B 507:

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

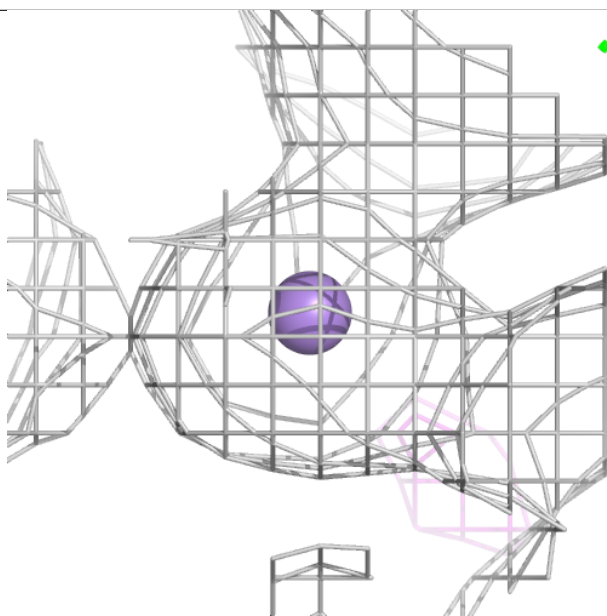
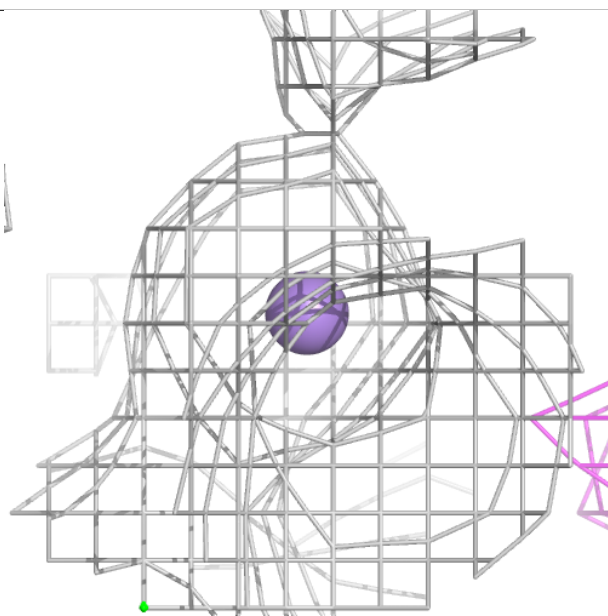
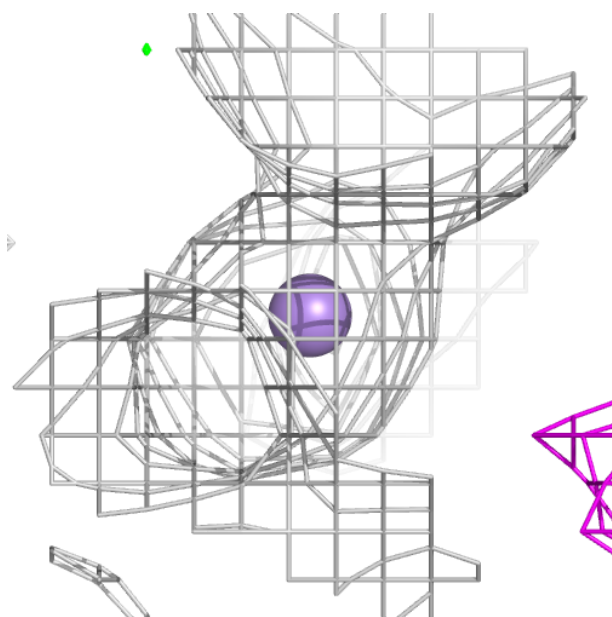
**Electron density around OLC B 508:**

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



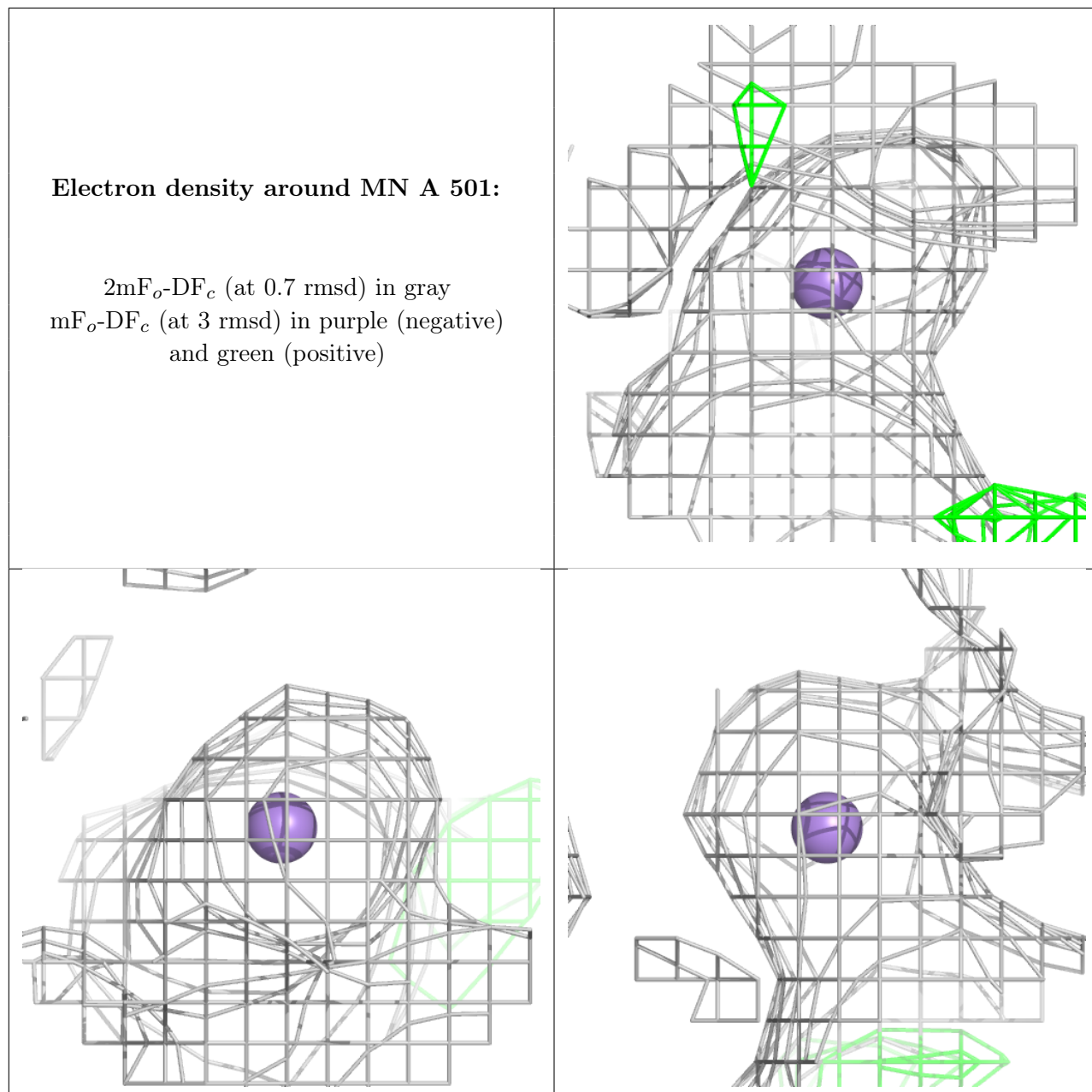
Electron density around MN B 501:

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



Electron density around MN A 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.