



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:33 AM UTC

PDB ID : 10KY / pdb_000010ky
Title : X-ray structure of the Bacteroides fragilis Nramp/MntH divalent transition metal transporter WT in an inward-open, state
Authors : Ray, S.; Gaudet, R.
Deposited on : 2026-01-26
Resolution : 2.48 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

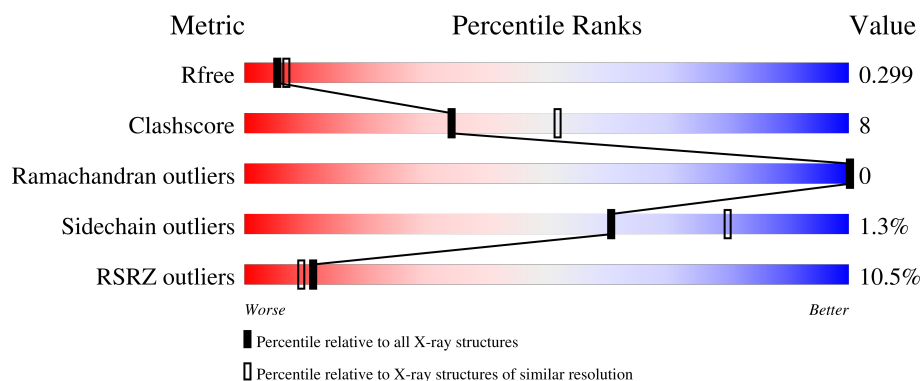
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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>10%</div> <div>76%</div> <div>13%</div> <div>10%</div> </div>
1	B	416	<div> <div>9%</div> <div>76%</div> <div>14%</div> <div>10%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6507 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.

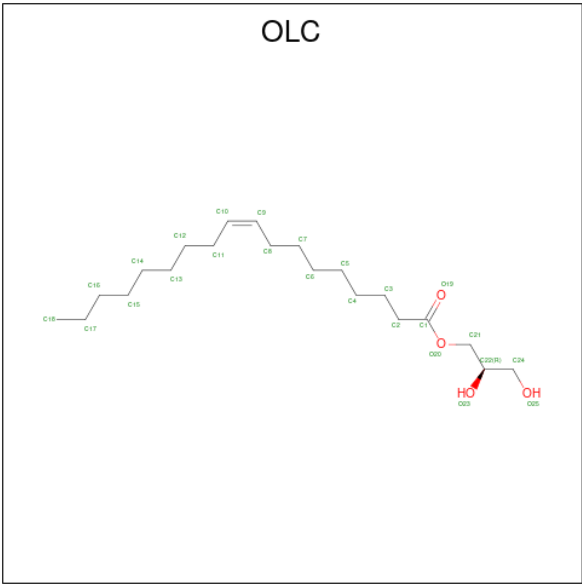
- Molecule 1 is a protein called Divalent metal cation transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2831	1883	433	500	15			
1	B	375	Total	C	N	O	S	0	0	0
			2832	1883	433	501	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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	20	4		
2	A	1	Total	C	O	0	0
			16	12	4		
2	A	1	Total	C		0	0
			16	16			
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C		0	0
			10	10			
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			23	19	4		
2	A	1	Total	C		0	0
			13	13			
2	A	1	Total	C		0	0
			16	16			
2	A	1	Total	C		0	0
			11	11			
2	A	1	Total	C		0	0
			13	13			

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 16 12 4	0	0
2	B	1	Total C O 13 9 4	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 15 15	0	0
2	B	1	Total C O 13 9 4	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 13 13	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 18 18	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 8 8	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

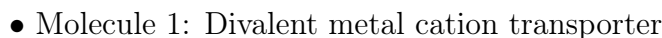


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	19	Total	O	0	0
			19	19		

- Molecule 1: Divalent metal cation transporter



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	69.12Å 102.27Å 119.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.14 – 2.48 45.14 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.14-2.48) 99.6 (45.14-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.48Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.259 , 0.298 0.260 , 0.299	Depositor DCC
R_{free} test set	2000 reflections (6.51%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6507	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.22 % 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 7.6996e-05. 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: OLC, PEG

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	0.08	0/2893	0.21	0/3941
1	B	0.08	0/2894	0.21	0/3944
All	All	0.08	0/5787	0.21	0/7885

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	2831	0	2945	42	0
1	B	2832	0	2936	40	0
2	A	421	0	665	30	0
2	B	363	0	558	26	0
3	A	12	0	14	1	0
3	B	6	0	7	1	0
4	A	23	0	0	0	0
4	B	19	0	0	0	0
All	All	6507	0	7125	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (103) 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	0.72
1:A:159:ILE:HG23	1:A:302:MET:HB3	1.71	0.72
3:A:522:PEG:H31	1:B:353:GLY:HA3	1.72	0.69
1:B:194:PRO:HG3	2:B:519:OLC:H4	1.75	0.69
2:A:519:OLC:H11A	2:A:520:OLC:H6A	1.76	0.68
1:A:375:PHE:HB3	2:A:509:OLC:H11	1.76	0.67
1:B:375:PHE:HB3	2:B:506:OLC:H14A	1.78	0.65
1:B:357:LYS:HG2	2:B:504:OLC:H21A	1.79	0.64
1:A:379:GLY:HA2	2:A:508:OLC:H6A	1.78	0.64
1:B:247:PHE:HB2	2:B:509:OLC:H12A	1.80	0.62
1:B:69:ILE:HG23	2:B:505:OLC:H4A	1.81	0.61
1:B:34:VAL:HG13	1:B:251:ILE:HG21	1.82	0.60
1:A:328:HIS:HB2	1:A:331:ASP:HB2	1.83	0.60
1:A:69:ILE:HA	2:A:504:OLC:H4	1.86	0.57
1:A:189:VAL:HG21	2:A:516:OLC:H13A	1.85	0.57
1:B:289:GLY:HA3	2:B:510:OLC:H6A	1.86	0.57
2:A:508:OLC:H9	2:A:509:OLC:H7A	1.86	0.56
1:A:68:ILE:HG12	1:A:249:MET:HG3	1.88	0.55
2:A:508:OLC:H12A	2:A:509:OLC:H11A	1.89	0.55
1:B:383:SER:HB2	2:B:507:OLC:H4	1.89	0.55
1:A:344:ILE:HD13	1:B:344:ILE:HD13	1.89	0.55
1:B:378:VAL:HG22	1:B:400:LEU:HB3	1.90	0.54
1:A:353:GLY:HA3	3:B:524:PEG:H31	1.89	0.54
1:B:395:TRP:CE2	2:B:511:OLC:H3	2.43	0.54
1:A:374:VAL:O	1:A:378:VAL:HG23	2.08	0.53
2:B:519:OLC:H14	2:B:520:OLC:H11	1.90	0.53
1:B:282:SER:HA	1:B:285:GLU:HB2	1.92	0.52
2:B:519:OLC:H17	2:B:521:OLC:H10	1.92	0.52
1:A:92:TYR:HD1	1:A:385:LYS:HE2	1.73	0.51
1:A:348:LEU:HD21	1:B:351:PHE:CG	2.45	0.51
1:B:379:GLY:HA2	2:B:507:OLC:H5A	1.93	0.51
2:A:504:OLC:H18	2:A:513:OLC:H14A	1.91	0.51
1:A:282:SER:HA	1:A:285:GLU:HB2	1.93	0.51
1:B:170:PHE:HD1	1:B:262:LEU:HD12	1.75	0.51
1:B:374:VAL:O	1:B:378:VAL:HG23	2.10	0.51
1:A:357:LYS:HE3	2:A:524:OLC:H24A	1.93	0.50
1:B:57:LEU:HB3	1:B:188:TRP:CD1	2.47	0.49
1:A:346:LEU:HA	1:A:349:ILE:HD12	1.94	0.49
1:A:378:VAL:HG22	1:A:400:LEU:HB3	1.95	0.49
1:B:382:SER:HA	1:B:391:VAL:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:TRP:CE2	2:B:517:OLC:H6	2.47	0.49
1:A:63:SER:HA	1:A:66:MET:HE2	1.95	0.48
1:B:147:LEU:HD21	1:B:309:ILE:HG23	1.95	0.48
1:A:189:VAL:HG11	2:A:516:OLC:H11	1.96	0.48
1:A:411:ASN:HB3	2:A:518:OLC:H13A	1.95	0.47
2:A:516:OLC:H14A	2:A:516:OLC:H17	1.62	0.47
1:A:72:HIS:HE2	1:A:238:LEU:HB3	1.79	0.47
2:A:519:OLC:H8A	2:A:519:OLC:H18B	1.96	0.47
2:A:521:OLC:H13	2:A:525:OLC:H16A	1.96	0.47
1:B:68:ILE:HG12	1:B:249:MET:HG3	1.95	0.47
1:A:42:TRP:HA	1:A:259:MET:HE1	1.96	0.47
2:A:519:OLC:H6	2:A:520:OLC:H4A	1.97	0.46
2:A:521:OLC:H16A	2:A:525:OLC:H11	1.96	0.46
2:A:514:OLC:H10	2:A:514:OLC:H7A	1.79	0.46
1:B:336:VAL:HA	1:B:339:ILE:HG22	1.98	0.46
1:A:351:PHE:CG	1:B:348:LEU:HD21	2.51	0.46
1:A:395:TRP:CD1	2:A:511:OLC:H16A	2.51	0.46
1:A:112:THR:O	1:A:116:GLU:HG2	2.15	0.45
1:A:156:GLU:O	1:A:160:ILE:HG12	2.16	0.45
1:A:114:LEU:HG	1:A:348:LEU:HD22	1.97	0.45
1:A:72:HIS:ND1	2:A:504:OLC:H3	2.31	0.45
1:A:346:LEU:HD23	2:A:521:OLC:H15A	1.99	0.45
1:B:112:THR:O	1:B:116:GLU:HG2	2.16	0.45
2:A:525:OLC:H5	2:B:504:OLC:H11A	1.99	0.45
1:A:147:LEU:HD21	1:A:309:ILE:HG23	1.98	0.45
1:B:395:TRP:CD1	2:B:511:OLC:H21A	2.52	0.45
2:A:501:OLC:H9	2:A:510:OLC:H7	1.98	0.44
2:A:524:OLC:H11A	2:B:517:OLC:H7	1.99	0.44
2:B:514:OLC:H9	2:B:514:OLC:H6A	1.82	0.44
1:B:312:GLY:O	1:B:338:VAL:HG22	2.18	0.44
1:A:348:LEU:HG	1:B:348:LEU:HG	1.99	0.44
1:B:73:ASN:ND2	1:B:377:GLN:HG2	2.33	0.44
2:B:504:OLC:H5	2:B:504:OLC:H2A	1.81	0.43
2:A:519:OLC:H13	2:A:520:OLC:H10	2.01	0.43
1:A:30:LEU:O	1:A:34:VAL:HG13	2.19	0.43
1:A:57:LEU:HB3	1:A:188:TRP:CD1	2.54	0.43
1:A:395:TRP:CE2	2:A:511:OLC:H12	2.53	0.43
2:B:519:OLC:H18B	2:B:519:OLC:H15A	1.91	0.43
1:A:298:LEU:HG	1:A:302:MET:HE3	2.01	0.42
2:B:521:OLC:H12	2:B:521:OLC:H15	1.96	0.42
1:A:69:ILE:HG12	2:A:504:OLC:H7A	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:HA3	2:B:501:OLC:H8	2.01	0.42
1:B:152:TYR:HB2	1:B:309:ILE:HD13	2.01	0.42
1:A:148:PHE:HZ	1:A:339:ILE:HB	1.84	0.42
1:B:198:MET:O	1:B:202:MET:HG2	2.19	0.42
2:B:503:OLC:H18A	2:B:503:OLC:H15	1.89	0.42
1:A:136:ALA:HB1	1:A:349:ILE:HD13	2.02	0.41
1:B:42:TRP:HA	1:B:259:MET:HE1	2.01	0.41
2:A:514:OLC:H15A	2:B:517:OLC:H13	2.02	0.41
1:B:114:LEU:HG	1:B:348:LEU:HD22	2.01	0.41
2:A:524:OLC:H7A	2:A:524:OLC:H10	1.76	0.41
1:B:94:PRO:HD3	2:B:506:OLC:H21A	2.03	0.41
2:B:510:OLC:H6A	2:B:510:OLC:H3A	1.72	0.41
1:B:55:SER:OG	2:B:519:OLC:H3A	2.20	0.41
1:B:192:ALA:HA	2:B:519:OLC:H12A	2.02	0.41
1:A:104:THR:HB	2:A:517:OLC:H9	2.03	0.41
1:B:148:PHE:HZ	1:B:339:ILE:HB	1.85	0.40
1:A:73:ASN:HD22	1:A:377:GLN:HG2	1.87	0.40
1:B:245:THR:HG22	1:B:249:MET:HG2	2.02	0.40
1:B:332:SER:HA	1:B:335:GLN:HG2	2.02	0.40
1:A:284:LEU:HB3	1:A:288:LEU:HD12	2.04	0.40
2:A:504:OLC:H4A	2:A:515:OLC:H12A	2.04	0.40
1:A:143:VAL:HG11	1:A:308:THR:HG22	2.02	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	370/416 (89%)	366 (99%)	4 (1%)	0	100	100
1	B	371/416 (89%)	364 (98%)	7 (2%)	0	100	100
All	All	741/832 (89%)	730 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/350 (88%)	307 (99%)	2 (1%)	78	90
1	B	308/350 (88%)	302 (98%)	6 (2%)	50	73
All	All	617/700 (88%)	609 (99%)	8 (1%)	61	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	298	LEU
1	B	34	VAL
1	B	79	ILE
1	B	84	CYS
1	B	93	THR
1	B	219	GLU
1	B	329	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	150	ASN
1	A	335	GLN
1	A	377	GLN
1	A	392	ASN
1	B	72	HIS
1	B	328	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

50 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OLC	A	518	-	6,6,24	0.26	0	5,5,25	0.14	0
2	OLC	A	510	-	15,15,24	0.23	0	14,14,25	0.25	0
2	OLC	A	503	-	15,15,24	0.22	0	14,14,25	0.27	0
3	PEG	A	523	-	5,5,6	0.32	0	4,4,5	0.21	0
2	OLC	B	512	-	9,9,24	0.31	0	8,8,25	0.28	0
2	OLC	B	504	-	20,20,24	0.37	0	21,21,25	0.44	0
3	PEG	A	522	-	5,5,6	0.31	0	4,4,5	0.18	0
2	OLC	B	503	-	24,24,24	0.34	0	25,25,25	0.42	0
2	OLC	B	502	-	19,19,24	0.37	0	20,20,25	0.37	0
2	OLC	A	502	-	15,15,24	0.39	0	16,16,25	0.47	0
2	OLC	A	501	-	23,23,24	0.34	0	24,24,25	0.36	0
2	OLC	B	508	-	12,12,24	0.24	0	11,11,25	0.30	0
2	OLC	A	505	-	9,9,24	0.27	0	8,8,25	0.22	0
2	OLC	A	521	-	12,12,24	0.25	0	11,11,25	0.24	0
2	OLC	A	524	-	19,19,24	0.37	0	20,20,25	0.42	0
2	OLC	B	513	-	7,7,24	0.26	0	6,6,25	0.20	0
2	OLC	A	506	-	24,24,24	0.35	0	25,25,25	0.42	0
2	OLC	A	516	-	10,10,24	0.27	0	9,9,25	0.21	0
2	OLC	A	515	-	8,8,24	0.23	0	7,7,25	0.17	0
2	OLC	A	517	-	7,7,24	0.26	0	6,6,25	0.26	0
2	OLC	A	509	-	12,12,24	0.23	0	11,11,25	0.29	0
2	OLC	A	512	-	12,12,24	0.24	0	11,11,25	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	B	517	-	15,15,24	0.23	0	14,14,25	0.27	0
2	OLC	B	515	-	12,12,24	0.42	0	13,13,25	0.58	0
2	OLC	B	510	-	15,15,24	0.39	0	16,16,25	0.41	0
2	OLC	B	518	-	12,12,24	0.25	0	11,11,25	0.27	0
2	OLC	B	501	-	11,11,24	0.30	0	10,10,25	0.26	0
2	OLC	B	506	-	21,21,24	0.35	0	22,22,25	0.41	0
2	OLC	B	514	-	14,14,24	0.24	0	13,13,25	0.26	0
2	OLC	A	511	-	10,10,24	0.27	0	9,9,25	0.18	0
3	PEG	B	524	-	5,5,6	0.32	0	4,4,5	0.20	0
2	OLC	A	526	-	20,20,24	0.36	0	21,21,25	0.41	0
2	OLC	A	504	-	24,24,24	0.35	0	25,25,25	0.35	0
2	OLC	B	509	-	16,16,24	0.22	0	15,15,25	0.26	0
2	OLC	A	507	-	24,24,24	0.34	0	25,25,25	0.38	0
2	OLC	A	525	-	14,14,24	0.23	0	13,13,25	0.27	0
2	OLC	A	520	-	24,24,24	0.34	0	25,25,25	0.43	0
2	OLC	B	523	-	7,7,24	0.27	0	6,6,25	0.17	0
2	OLC	A	513	-	24,24,24	0.33	0	25,25,25	0.44	0
2	OLC	A	519	-	24,24,24	0.34	0	25,25,25	0.37	0
2	OLC	B	505	-	18,18,24	0.40	0	19,19,25	0.41	0
2	OLC	B	522	-	6,6,24	0.27	0	5,5,25	0.12	0
2	OLC	A	514	-	24,24,24	0.33	0	25,25,25	0.41	0
2	OLC	B	511	-	12,12,24	0.43	0	13,13,25	0.54	0
2	OLC	B	520	-	24,24,24	0.35	0	25,25,25	0.39	0
2	OLC	B	516	-	4,4,24	0.27	0	3,3,25	0.28	0
2	OLC	B	507	-	21,21,24	0.36	0	22,22,25	0.40	0
2	OLC	B	521	-	17,17,24	0.22	0	16,16,25	0.26	0
2	OLC	A	508	-	22,22,24	0.33	0	23,23,25	0.49	0
2	OLC	B	519	-	24,24,24	0.33	0	25,25,25	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	518	-	-	4/4/4/24	-
2	OLC	A	510	-	-	3/13/13/24	-
2	OLC	A	503	-	-	7/13/13/24	-
3	PEG	A	523	-	-	1/3/3/4	-
2	OLC	B	512	-	-	1/7/7/24	-
2	OLC	B	504	-	-	9/20/20/24	-
3	PEG	A	522	-	-	1/3/3/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	503	-	-	12/24/24/24	-
2	OLC	B	502	-	-	7/19/19/24	-
2	OLC	A	502	-	-	7/15/15/24	-
2	OLC	A	501	-	-	10/23/23/24	-
2	OLC	B	508	-	-	4/10/10/24	-
2	OLC	A	505	-	-	3/7/7/24	-
2	OLC	A	521	-	-	3/10/10/24	-
2	OLC	A	524	-	-	10/19/19/24	-
2	OLC	B	513	-	-	3/5/5/24	-
2	OLC	A	506	-	-	4/24/24/24	-
2	OLC	A	516	-	-	4/8/8/24	-
2	OLC	A	515	-	-	2/6/6/24	-
2	OLC	A	517	-	-	3/5/5/24	-
2	OLC	A	509	-	-	5/10/10/24	-
2	OLC	A	512	-	-	4/10/10/24	-
2	OLC	B	517	-	-	4/13/13/24	-
2	OLC	B	515	-	-	1/12/12/24	-
2	OLC	B	510	-	-	7/15/15/24	-
2	OLC	B	518	-	-	4/10/10/24	-
2	OLC	B	501	-	-	1/9/9/24	-
2	OLC	B	506	-	-	8/21/21/24	-
2	OLC	B	514	-	-	6/12/12/24	-
2	OLC	A	511	-	-	2/8/8/24	-
3	PEG	B	524	-	-	1/3/3/4	-
2	OLC	A	526	-	-	5/20/20/24	-
2	OLC	A	504	-	-	9/24/24/24	-
2	OLC	B	509	-	-	7/14/14/24	-
2	OLC	A	507	-	-	3/24/24/24	-
2	OLC	A	525	-	-	4/12/12/24	-
2	OLC	A	520	-	-	10/24/24/24	-
2	OLC	B	523	-	-	3/5/5/24	-
2	OLC	A	513	-	-	8/24/24/24	-
2	OLC	A	519	-	-	11/24/24/24	-
2	OLC	B	505	-	-	5/18/18/24	-
2	OLC	B	522	-	-	1/4/4/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	514	-	-	12/24/24/24	-
2	OLC	B	511	-	-	4/12/12/24	-
2	OLC	B	520	-	-	9/24/24/24	-
2	OLC	B	516	-	-	0/2/2/24	-
2	OLC	B	507	-	-	7/21/21/24	-
2	OLC	B	521	-	-	8/15/15/24	-
2	OLC	A	508	-	-	15/22/22/24	-
2	OLC	B	519	-	-	8/24/24/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (270) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	508	OLC	C2-C1-O20-C21
2	A	508	OLC	O19-C1-O20-C21
2	A	514	OLC	O20-C21-C22-C24
2	A	514	OLC	O20-C21-C22-O23
2	A	517	OLC	C10-C11-C12-C13
2	A	520	OLC	O20-C21-C22-C24
2	A	520	OLC	O20-C21-C22-O23
2	A	521	OLC	C6-C7-C8-C9
2	B	502	OLC	O20-C21-C22-C24
2	B	504	OLC	O20-C21-C22-C24
2	B	504	OLC	O20-C21-C22-O23
2	B	515	OLC	O20-C21-C22-O23
2	B	519	OLC	C21-C22-C24-O25
2	B	519	OLC	O23-C22-C24-O25
2	A	524	OLC	O19-C1-O20-C21
2	B	510	OLC	O19-C1-O20-C21
2	B	506	OLC	O19-C1-O20-C21
2	B	511	OLC	O19-C1-O20-C21
2	A	524	OLC	C2-C1-O20-C21
2	B	506	OLC	C2-C1-O20-C21
2	B	510	OLC	C2-C1-O20-C21
2	A	519	OLC	O19-C1-O20-C21
2	A	513	OLC	C2-C1-O20-C21
2	B	504	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	B	511	OLC	C2-C1-O20-C21
2	A	514	OLC	O19-C1-O20-C21
2	A	501	OLC	C2-C1-O20-C21
2	A	519	OLC	C2-C1-O20-C21
2	A	513	OLC	O19-C1-O20-C21
2	B	504	OLC	C6-C7-C8-C9
2	A	514	OLC	C2-C1-O20-C21
2	B	504	OLC	O19-C1-O20-C21
2	A	515	OLC	C12-C13-C14-C15
2	A	501	OLC	O19-C1-O20-C21
2	B	510	OLC	O20-C21-C22-C24
2	B	504	OLC	C1-C2-C3-C4
2	A	524	OLC	C1-C2-C3-C4
2	B	505	OLC	C1-C2-C3-C4
2	B	507	OLC	C1-C2-C3-C4
2	A	519	OLC	C1-C2-C3-C4
2	A	511	OLC	C11-C12-C13-C14
2	A	504	OLC	C4-C5-C6-C7
2	A	516	OLC	C14-C15-C16-C17
2	B	520	OLC	O20-C21-C22-O23
2	A	514	OLC	C1-C2-C3-C4
2	A	506	OLC	C4-C5-C6-C7
2	B	520	OLC	O20-C21-C22-C24
2	B	502	OLC	C2-C3-C4-C5
2	B	507	OLC	C4-C5-C6-C7
2	B	505	OLC	C3-C4-C5-C6
2	A	508	OLC	C21-C22-C24-O25
2	A	514	OLC	C21-C22-C24-O25
2	B	506	OLC	C21-C22-C24-O25
2	B	506	OLC	C6-C7-C8-C9
2	A	510	OLC	C12-C13-C14-C15
2	B	521	OLC	C12-C13-C14-C15
2	B	510	OLC	C3-C4-C5-C6
2	B	520	OLC	C11-C12-C13-C14
2	A	502	OLC	C2-C3-C4-C5
2	B	510	OLC	C2-C3-C4-C5
2	B	521	OLC	C5-C6-C7-C8
2	A	501	OLC	C11-C12-C13-C14
2	A	506	OLC	C14-C15-C16-C17
2	A	508	OLC	C3-C4-C5-C6
2	B	501	OLC	C14-C15-C16-C17
2	B	517	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	A	520	OLC	C4-C5-C6-C7
2	B	503	OLC	C3-C4-C5-C6
2	B	503	OLC	C13-C14-C15-C16
2	A	508	OLC	O23-C22-C24-O25
2	A	510	OLC	C4-C5-C6-C7
2	A	526	OLC	C2-C3-C4-C5
2	B	517	OLC	C5-C6-C7-C8
2	A	504	OLC	C1-C2-C3-C4
2	A	514	OLC	C2-C3-C4-C5
2	B	508	OLC	C5-C6-C7-C8
2	B	502	OLC	C5-C6-C7-C8
2	B	503	OLC	C12-C13-C14-C15
2	A	501	OLC	C1-C2-C3-C4
2	B	511	OLC	C1-C2-C3-C4
2	A	508	OLC	C2-C3-C4-C5
2	B	509	OLC	C11-C12-C13-C14
2	A	513	OLC	C3-C4-C5-C6
2	B	511	OLC	C2-C3-C4-C5
2	A	520	OLC	C2-C3-C4-C5
2	B	513	OLC	C12-C13-C14-C15
2	B	509	OLC	C3-C4-C5-C6
2	B	503	OLC	C1-C2-C3-C4
2	A	524	OLC	C6-C7-C8-C9
2	B	514	OLC	C6-C7-C8-C9
2	A	526	OLC	C2-C1-O20-C21
2	B	520	OLC	C1-C2-C3-C4
2	A	504	OLC	C5-C6-C7-C8
2	A	503	OLC	C11-C12-C13-C14
2	B	514	OLC	C14-C15-C16-C17
2	B	504	OLC	C5-C6-C7-C8
2	A	504	OLC	C2-C1-O20-C21
2	A	507	OLC	C2-C3-C4-C5
2	A	505	OLC	C11-C12-C13-C14
2	B	512	OLC	C12-C13-C14-C15
2	B	503	OLC	C14-C15-C16-C17
2	B	521	OLC	C2-C3-C4-C5
2	B	521	OLC	C4-C5-C6-C7
2	A	508	OLC	C10-C11-C12-C13
2	B	519	OLC	C10-C11-C12-C13
2	B	520	OLC	C5-C6-C7-C8
2	B	503	OLC	C2-C3-C4-C5
2	B	509	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	525	OLC	C5-C6-C7-C8
2	B	514	OLC	C5-C6-C7-C8
2	A	505	OLC	C12-C13-C14-C15
2	A	503	OLC	C10-C11-C12-C13
2	B	518	OLC	C6-C7-C8-C9
2	B	521	OLC	C6-C7-C8-C9
2	A	520	OLC	C12-C13-C14-C15
2	A	514	OLC	C5-C6-C7-C8
2	B	517	OLC	C11-C12-C13-C14
2	B	510	OLC	C4-C5-C6-C7
2	A	508	OLC	C12-C13-C14-C15
2	A	516	OLC	C12-C13-C14-C15
2	B	504	OLC	C4-C5-C6-C7
2	B	509	OLC	C4-C5-C6-C7
2	A	520	OLC	C3-C4-C5-C6
2	B	518	OLC	C11-C12-C13-C14
2	A	515	OLC	C10-C11-C12-C13
2	A	514	OLC	O23-C22-C24-O25
2	A	519	OLC	O23-C22-C24-O25
2	B	503	OLC	C5-C6-C7-C8
2	B	506	OLC	C3-C4-C5-C6
2	A	503	OLC	C6-C7-C8-C9
2	A	504	OLC	C6-C7-C8-C9
2	A	514	OLC	C6-C7-C8-C9
2	A	526	OLC	O19-C1-O20-C21
2	B	517	OLC	C12-C13-C14-C15
2	A	504	OLC	O19-C1-O20-C21
2	A	508	OLC	C11-C12-C13-C14
2	B	520	OLC	C4-C5-C6-C7
2	A	504	OLC	C2-C3-C4-C5
2	A	509	OLC	C10-C11-C12-C13
2	B	507	OLC	C6-C7-C8-C9
2	B	521	OLC	C13-C14-C15-C16
2	A	504	OLC	C3-C4-C5-C6
2	A	509	OLC	C3-C4-C5-C6
2	A	508	OLC	C1-C2-C3-C4
2	A	506	OLC	C6-C7-C8-C9
2	A	503	OLC	C13-C14-C15-C16
2	A	513	OLC	C14-C15-C16-C17
2	A	516	OLC	C13-C14-C15-C16
2	A	505	OLC	C14-C15-C16-C17
2	B	502	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	504	OLC	C12-C13-C14-C15
2	A	503	OLC	C2-C3-C4-C5
2	A	519	OLC	C14-C15-C16-C17
2	A	521	OLC	C10-C11-C12-C13
2	A	520	OLC	C2-C1-O20-C21
2	B	508	OLC	C2-C3-C4-C5
2	A	520	OLC	C13-C14-C15-C16
2	A	514	OLC	C12-C13-C14-C15
2	A	519	OLC	C3-C4-C5-C6
2	A	516	OLC	C15-C16-C17-C18
2	B	506	OLC	O20-C21-C22-C24
2	B	502	OLC	C3-C4-C5-C6
2	A	512	OLC	C10-C11-C12-C13
2	A	518	OLC	C14-C15-C16-C17
2	B	520	OLC	C13-C14-C15-C16
2	A	518	OLC	C15-C16-C17-C18
2	A	512	OLC	C11-C12-C13-C14
2	A	508	OLC	C7-C8-C9-C10
2	A	524	OLC	C4-C5-C6-C7
2	A	514	OLC	C4-C5-C6-C7
2	B	514	OLC	C15-C16-C17-C18
2	B	520	OLC	C10-C11-C12-C13
2	B	505	OLC	C2-C3-C4-C5
2	B	521	OLC	C3-C4-C5-C6
2	A	508	OLC	C5-C6-C7-C8
2	B	506	OLC	C5-C6-C7-C8
2	B	513	OLC	C14-C15-C16-C17
2	A	502	OLC	C6-C7-C8-C9
2	B	503	OLC	C11-C12-C13-C14
2	A	520	OLC	O19-C1-O20-C21
2	A	506	OLC	C11-C12-C13-C14
2	B	503	OLC	C7-C8-C9-C10
2	A	503	OLC	C14-C15-C16-C17
2	A	513	OLC	C2-C3-C4-C5
2	B	503	OLC	C15-C16-C17-C18
2	A	521	OLC	C14-C15-C16-C17
2	B	502	OLC	O20-C21-C22-O23
2	A	501	OLC	C10-C11-C12-C13
2	B	520	OLC	C3-C4-C5-C6
2	A	502	OLC	C5-C6-C7-C8
2	B	518	OLC	C13-C14-C15-C16
2	A	501	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	509	OLC	C6-C7-C8-C9
2	B	502	OLC	C6-C7-C8-C9
2	B	519	OLC	C13-C14-C15-C16
3	A	522	PEG	C4-C3-O2-C2
2	A	501	OLC	O20-C21-C22-C24
2	A	524	OLC	C5-C6-C7-C8
2	A	513	OLC	C6-C7-C8-C9
2	B	503	OLC	O20-C21-C22-C24
2	A	518	OLC	C12-C13-C14-C15
3	B	524	PEG	C4-C3-O2-C2
2	A	518	OLC	C13-C14-C15-C16
2	B	519	OLC	C15-C16-C17-C18
2	A	512	OLC	C13-C14-C15-C16
2	A	524	OLC	C2-C3-C4-C5
2	B	514	OLC	C13-C14-C15-C16
2	A	513	OLC	O20-C21-C22-O23
2	B	519	OLC	C2-C3-C4-C5
2	A	524	OLC	C9-C10-C11-C12
2	B	506	OLC	C2-C3-C4-C5
2	A	517	OLC	C6-C7-C8-C9
2	A	524	OLC	C10-C11-C12-C13
2	A	519	OLC	C2-C3-C4-C5
3	A	523	PEG	C1-C2-O2-C3
2	A	509	OLC	C5-C6-C7-C8
2	A	519	OLC	C21-C22-C24-O25
2	A	501	OLC	C14-C15-C16-C17
2	A	510	OLC	C15-C16-C17-C18
2	A	519	OLC	C11-C12-C13-C14
2	A	519	OLC	C4-C5-C6-C7
2	A	503	OLC	C4-C5-C6-C7
2	B	505	OLC	C6-C7-C8-C9
2	B	504	OLC	C2-C3-C4-C5
2	A	508	OLC	O20-C21-C22-O23
2	B	523	OLC	C11-C12-C13-C14
2	A	507	OLC	C11-C12-C13-C14
2	A	526	OLC	C4-C5-C6-C7
2	B	505	OLC	O20-C1-C2-C3
2	A	509	OLC	C9-C10-C11-C12
2	A	519	OLC	C7-C8-C9-C10
2	B	510	OLC	O20-C21-C22-O23
2	B	503	OLC	C10-C11-C12-C13
2	B	523	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	B	507	OLC	O20-C1-C2-C3
2	A	525	OLC	C13-C14-C15-C16
2	B	519	OLC	C11-C12-C13-C14
2	A	512	OLC	C14-C15-C16-C17
2	A	513	OLC	C1-C2-C3-C4
2	B	522	OLC	C12-C13-C14-C15
2	A	517	OLC	C9-C10-C11-C12
2	A	526	OLC	C9-C10-C11-C12
2	B	514	OLC	C11-C12-C13-C14
2	B	509	OLC	C6-C7-C8-C9
2	B	507	OLC	C5-C6-C7-C8
2	B	507	OLC	C12-C13-C14-C15
2	B	518	OLC	C7-C8-C9-C10
2	B	509	OLC	C2-C3-C4-C5
2	B	508	OLC	C4-C5-C6-C7
2	A	511	OLC	C14-C15-C16-C17
2	A	508	OLC	O20-C21-C22-C24
2	B	521	OLC	C9-C10-C11-C12
2	B	509	OLC	C15-C16-C17-C18
2	B	523	OLC	C14-C15-C16-C17
2	A	525	OLC	C15-C16-C17-C18
2	A	507	OLC	C12-C13-C14-C15
2	A	502	OLC	O20-C1-C2-C3
2	B	519	OLC	C12-C13-C14-C15
2	B	513	OLC	C13-C14-C15-C16
2	B	507	OLC	C3-C4-C5-C6
2	A	520	OLC	C11-C12-C13-C14
2	A	524	OLC	C7-C8-C9-C10
2	A	508	OLC	C6-C7-C8-C9
2	A	502	OLC	C3-C4-C5-C6
2	A	525	OLC	C12-C13-C14-C15
2	A	502	OLC	O19-C1-C2-C3
2	A	502	OLC	C1-C2-C3-C4
2	A	501	OLC	O20-C1-C2-C3
2	A	501	OLC	C2-C3-C4-C5
2	B	508	OLC	C3-C4-C5-C6

There are no ring outliers.

33 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	518	OLC	1	0

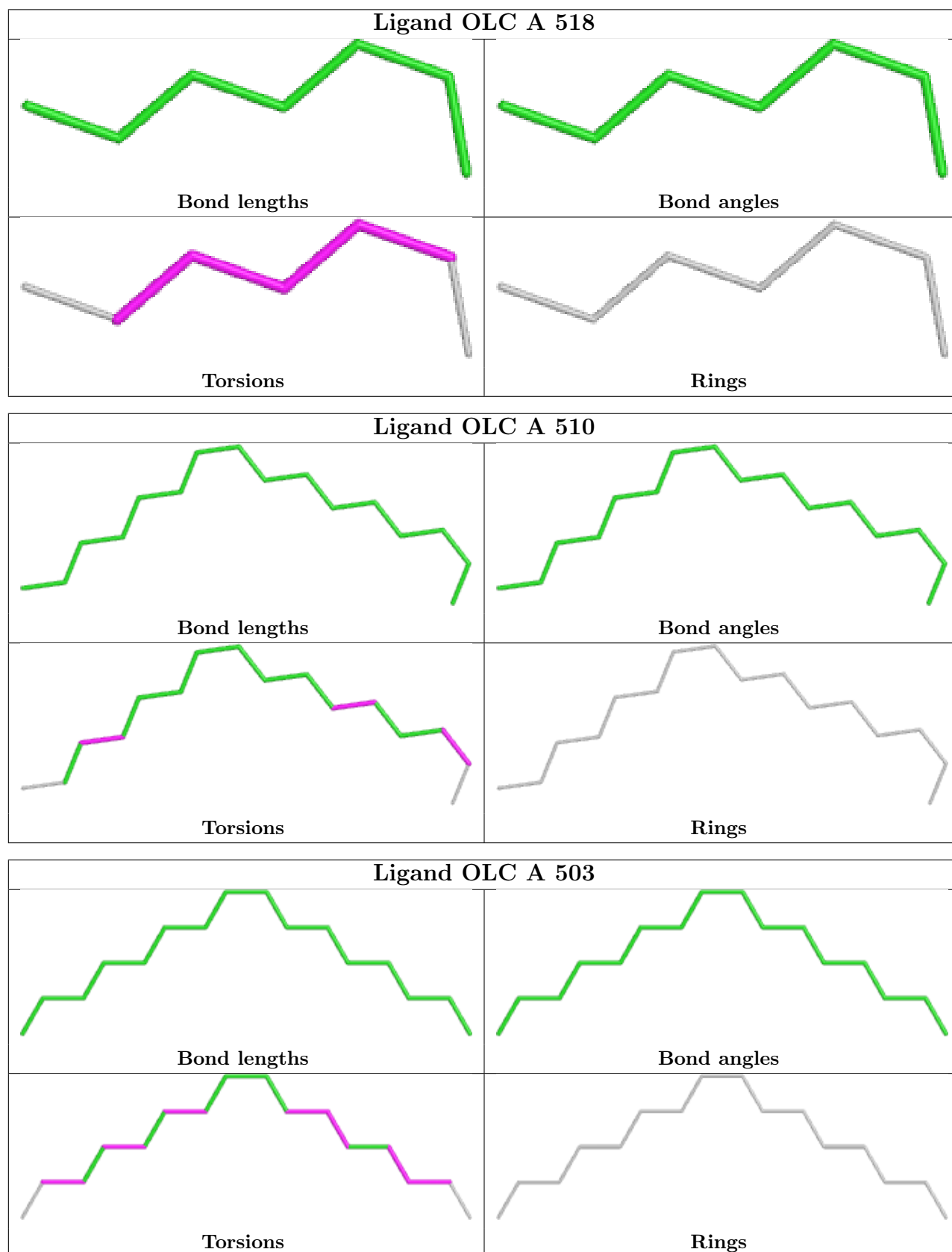
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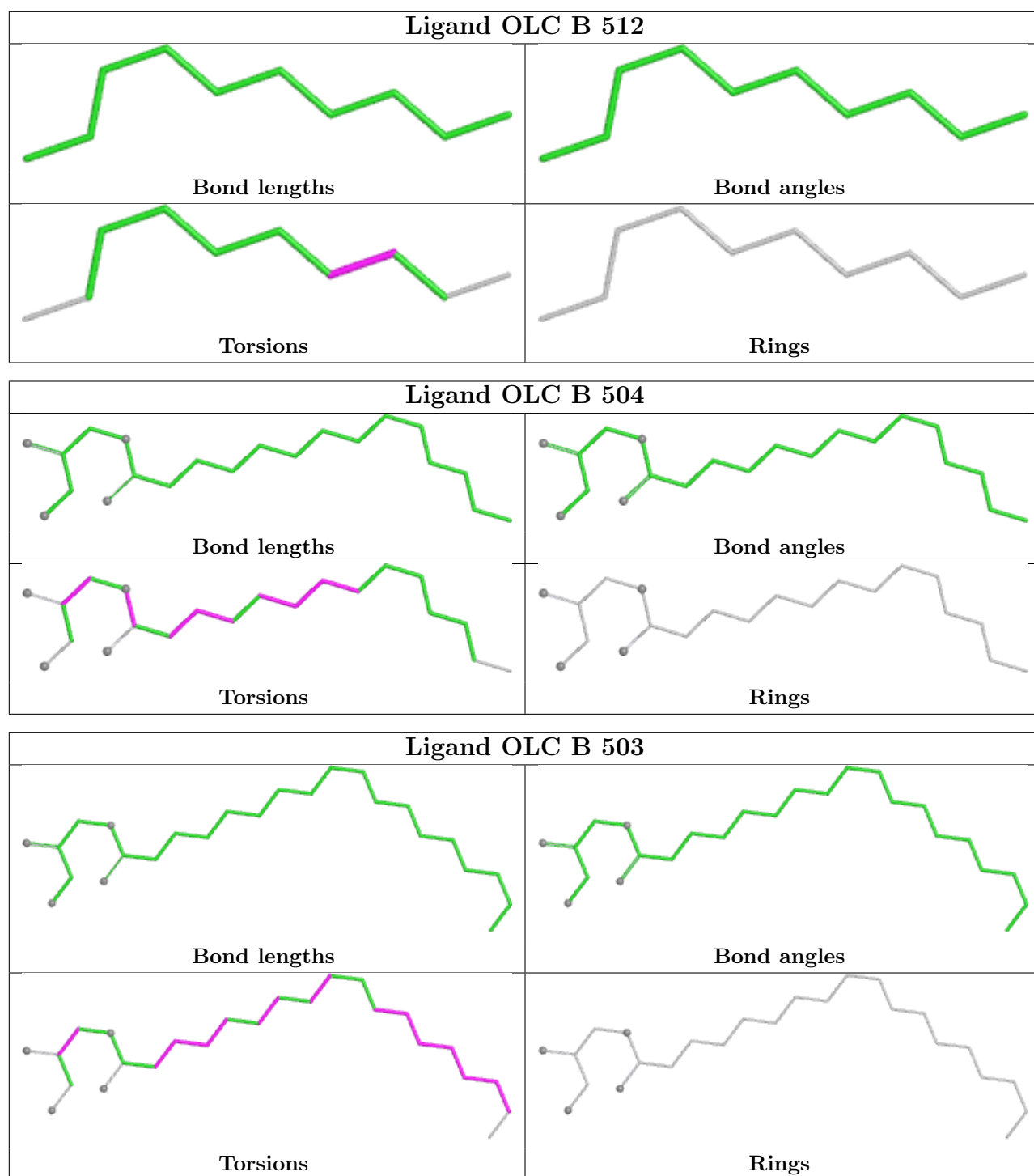
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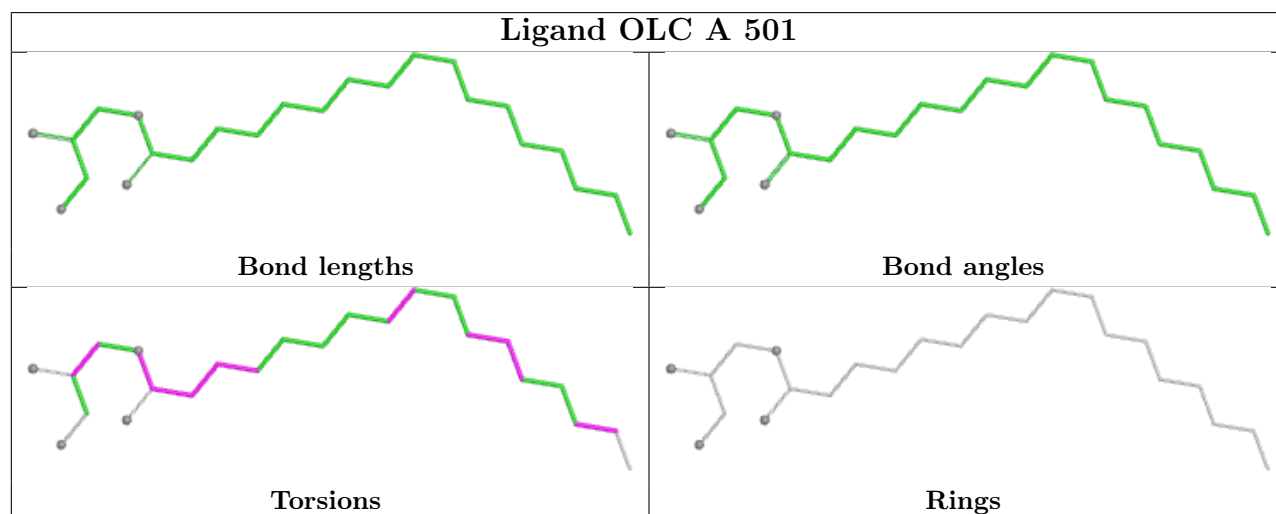
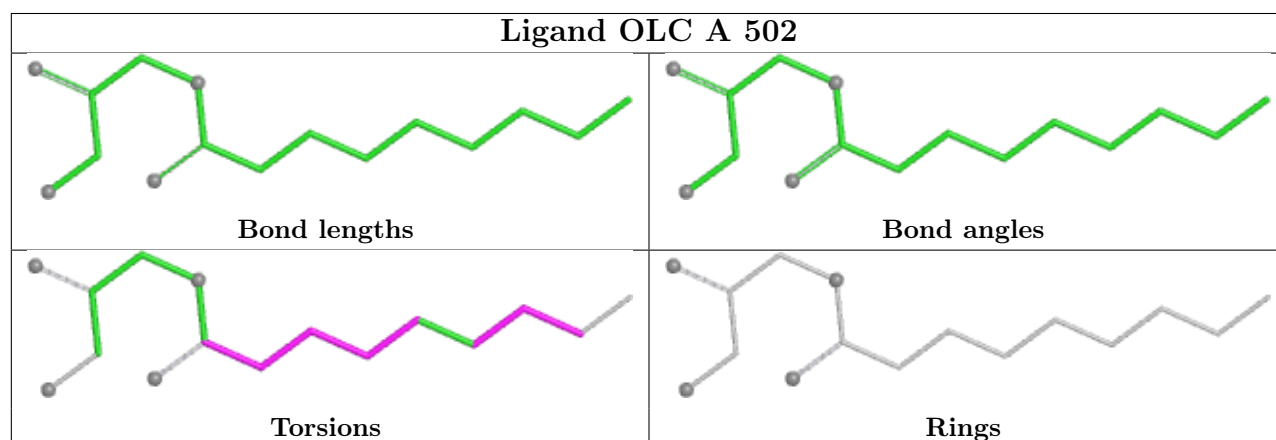
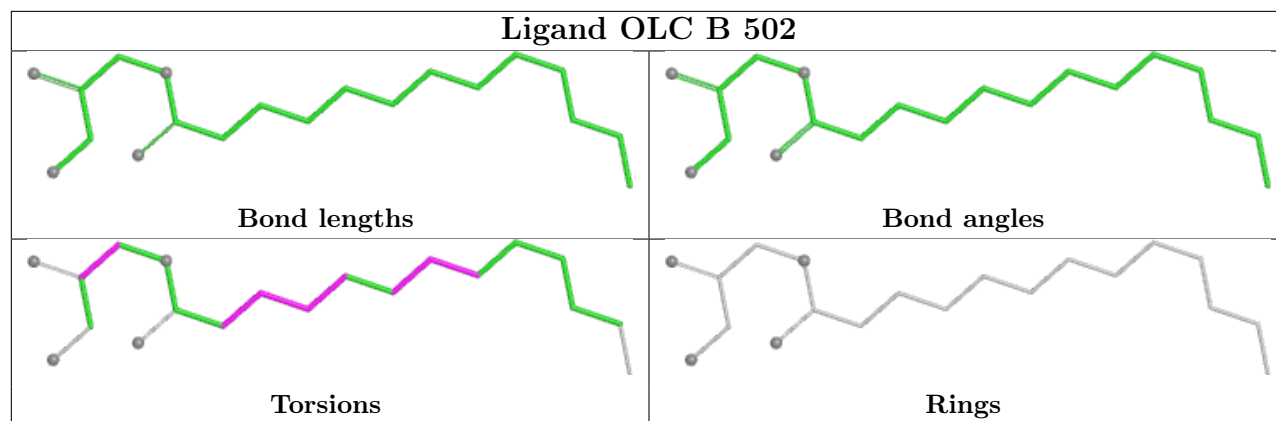
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	510	OLC	1	0
2	B	504	OLC	3	0
3	A	522	PEG	1	0
2	B	503	OLC	1	0
2	A	501	OLC	1	0
2	A	521	OLC	3	0
2	A	524	OLC	3	0
2	A	516	OLC	3	0
2	A	515	OLC	1	0
2	A	517	OLC	1	0
2	A	509	OLC	3	0
2	B	517	OLC	3	0
2	B	510	OLC	2	0
2	B	501	OLC	1	0
2	B	506	OLC	2	0
2	B	514	OLC	1	0
2	A	511	OLC	2	0
3	B	524	PEG	1	0
2	A	504	OLC	5	0
2	B	509	OLC	1	0
2	A	525	OLC	3	0
2	A	520	OLC	3	0
2	A	513	OLC	1	0
2	A	519	OLC	4	0
2	B	505	OLC	1	0
2	A	514	OLC	2	0
2	B	511	OLC	2	0
2	B	520	OLC	1	0
2	B	507	OLC	2	0
2	B	521	OLC	2	0
2	A	508	OLC	3	0
2	B	519	OLC	6	0

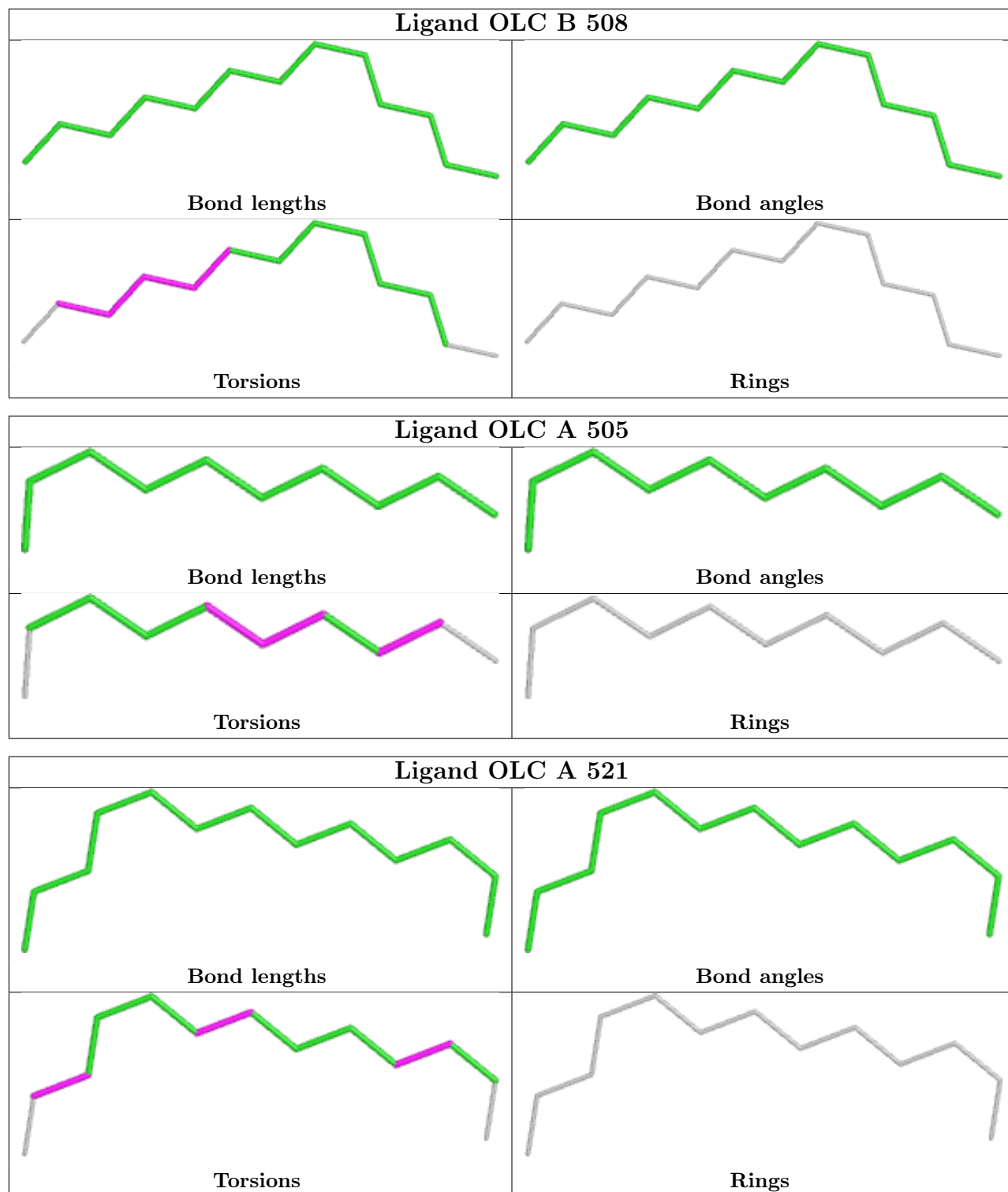
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

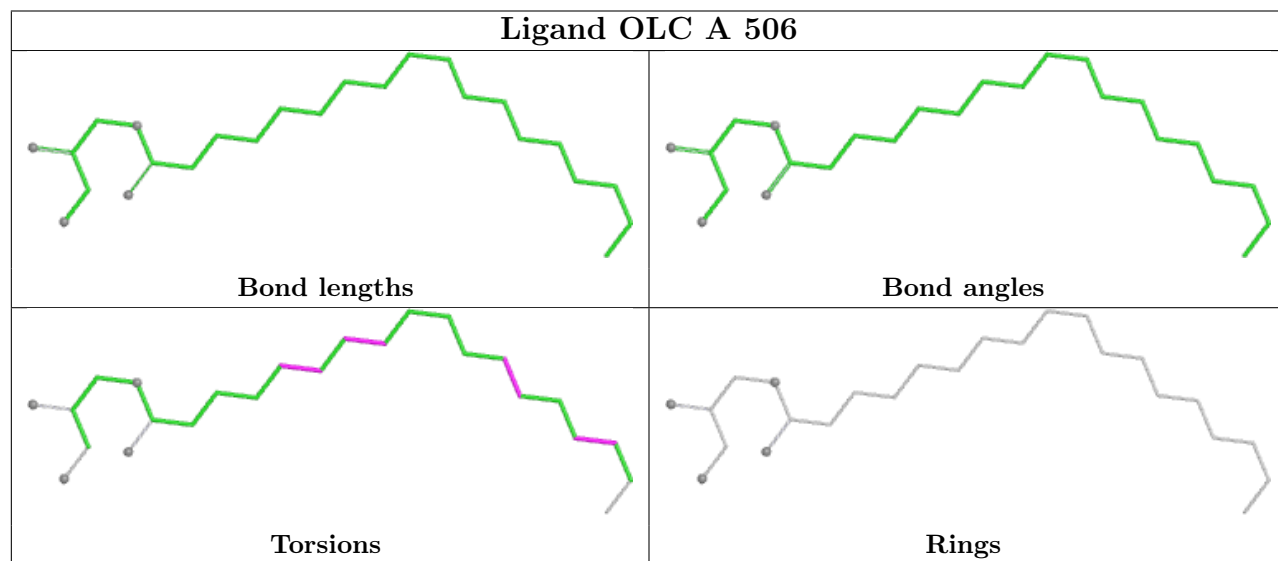
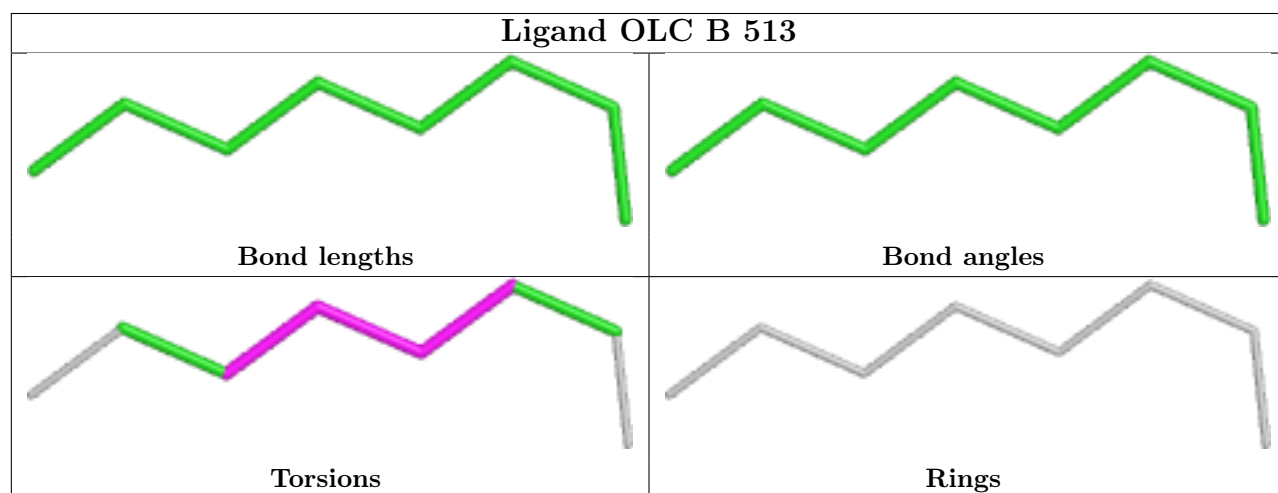
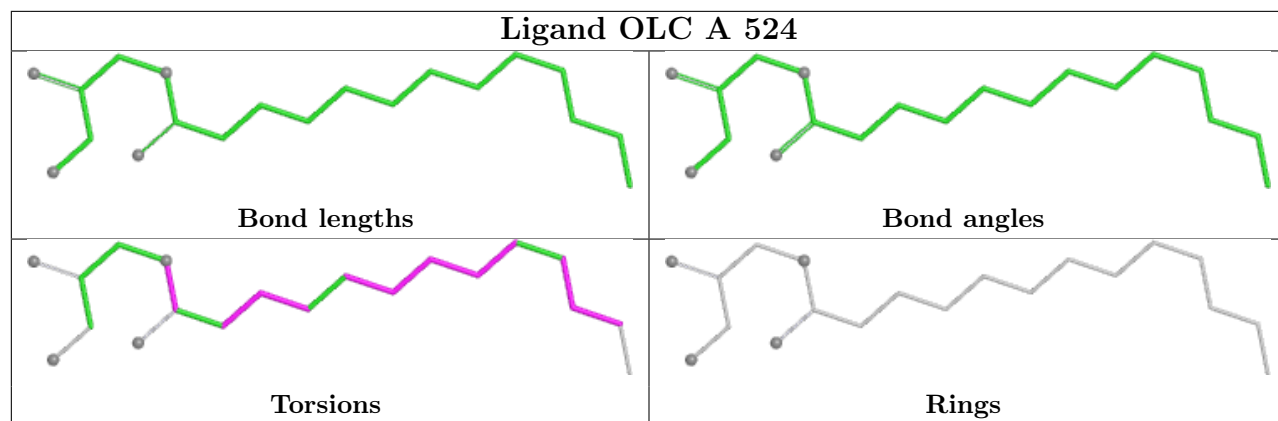
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

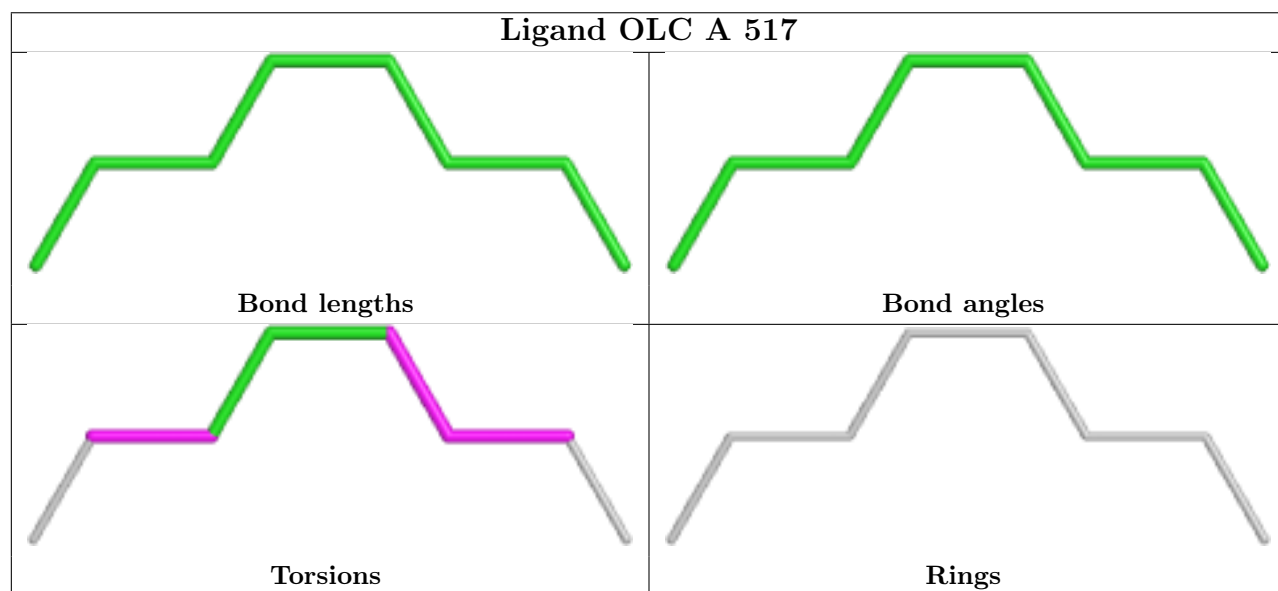
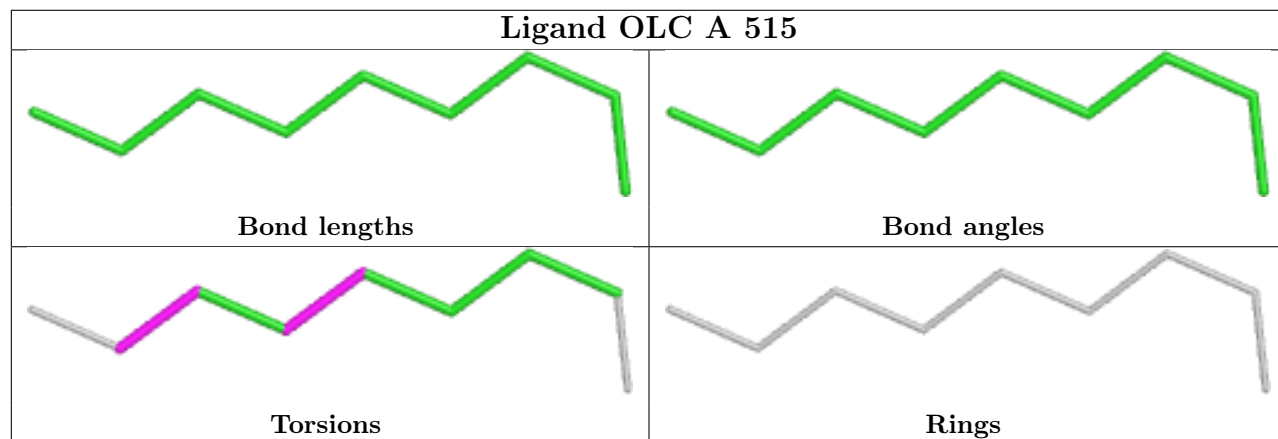
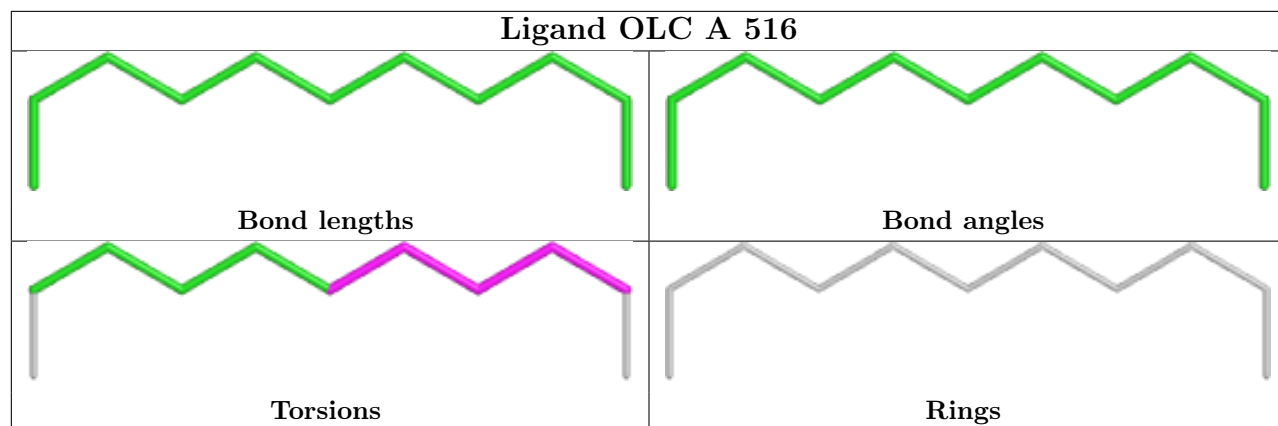


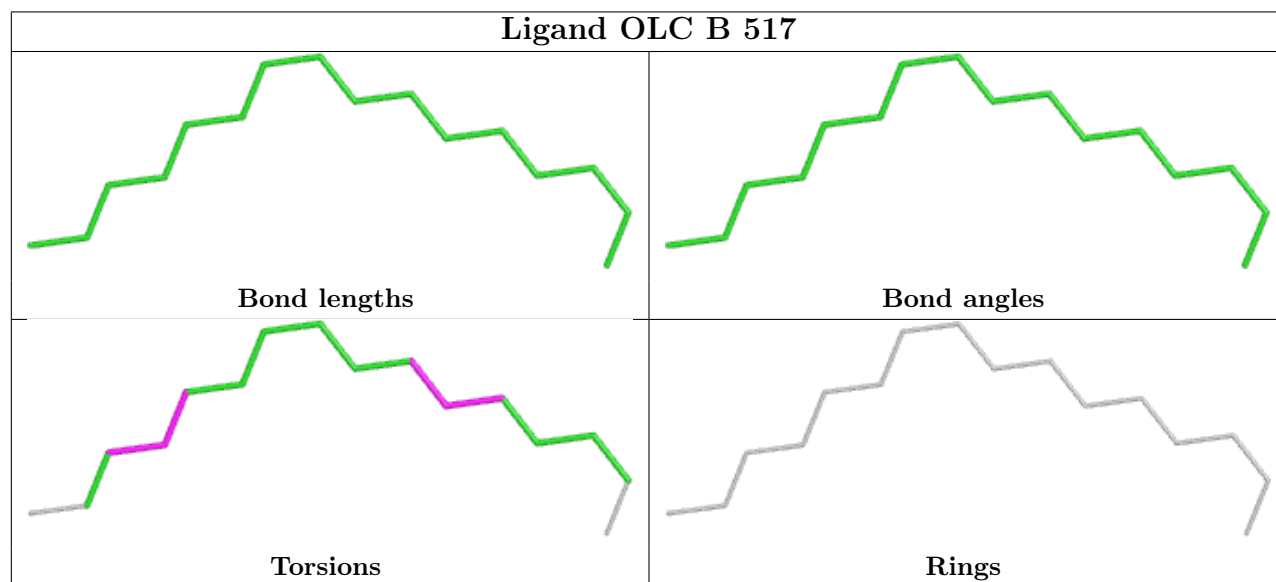
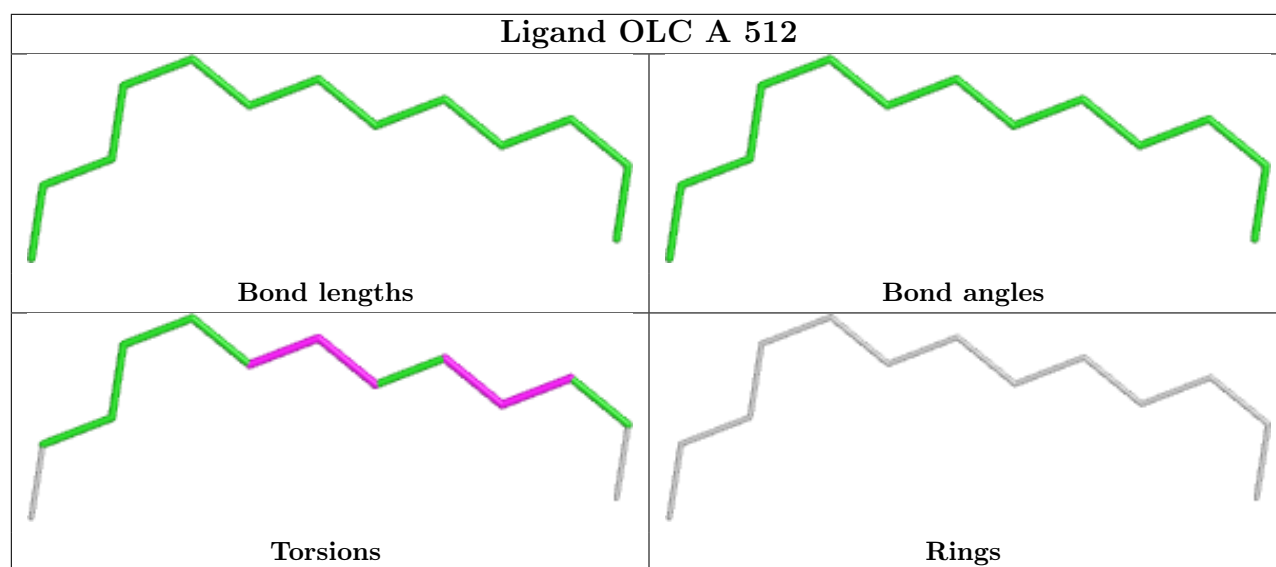
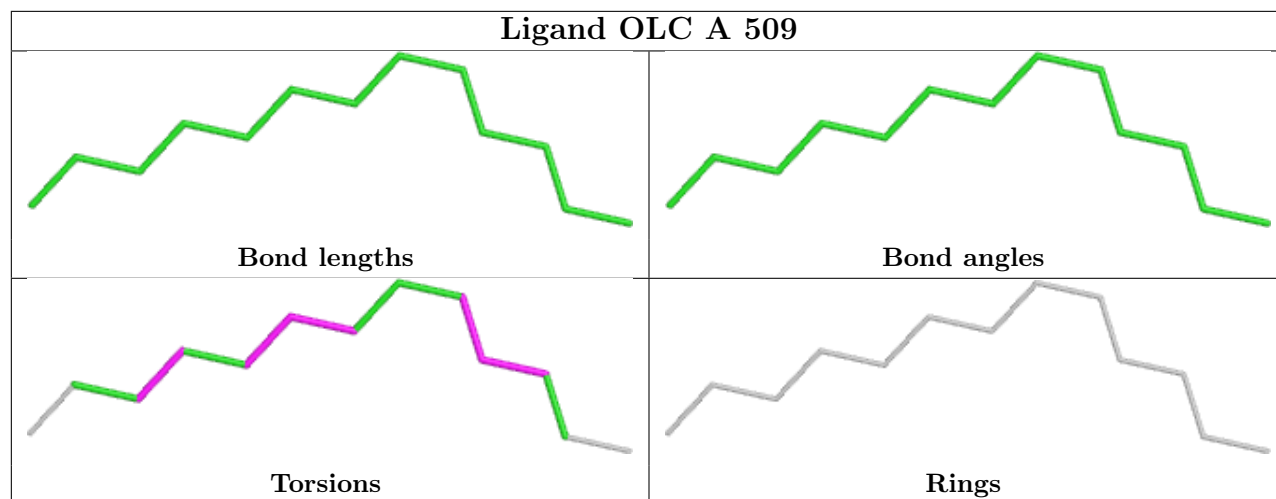


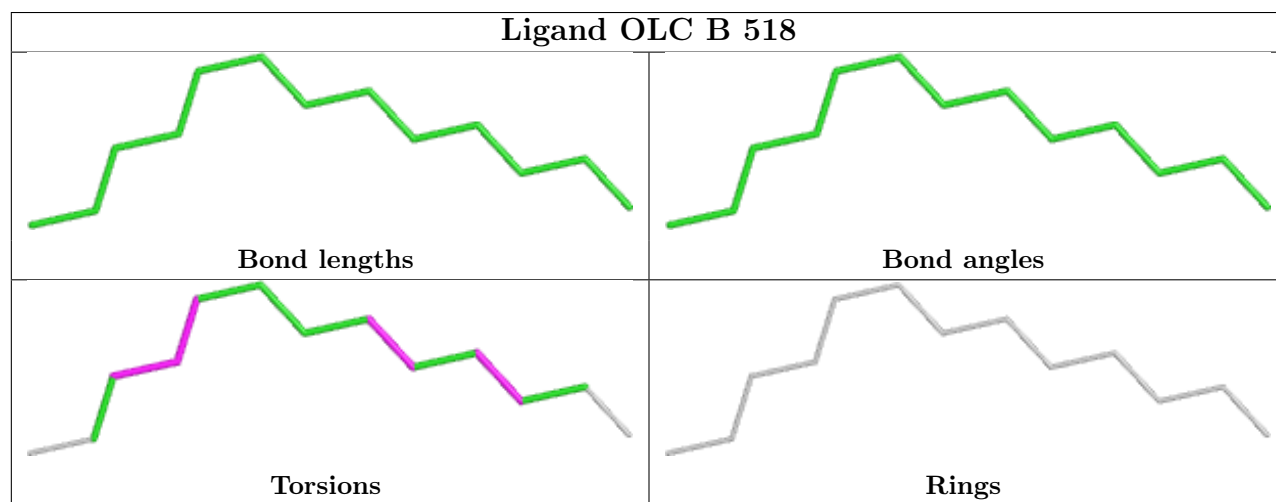
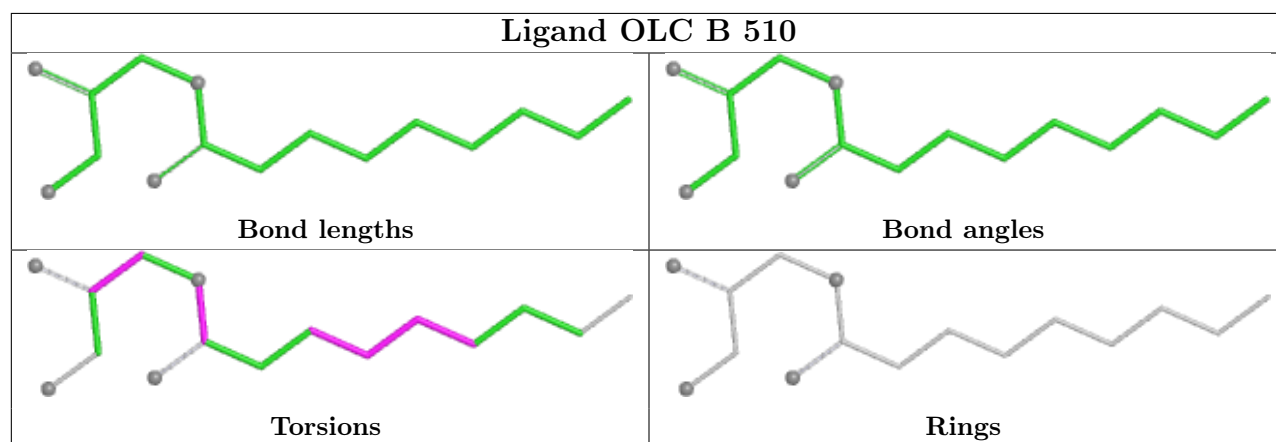
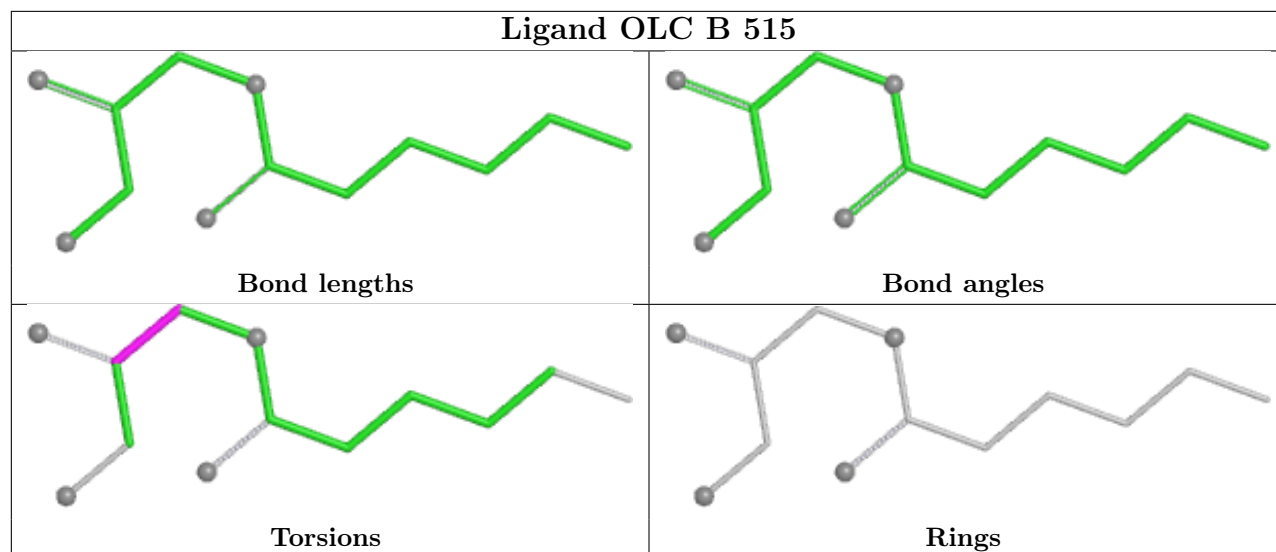


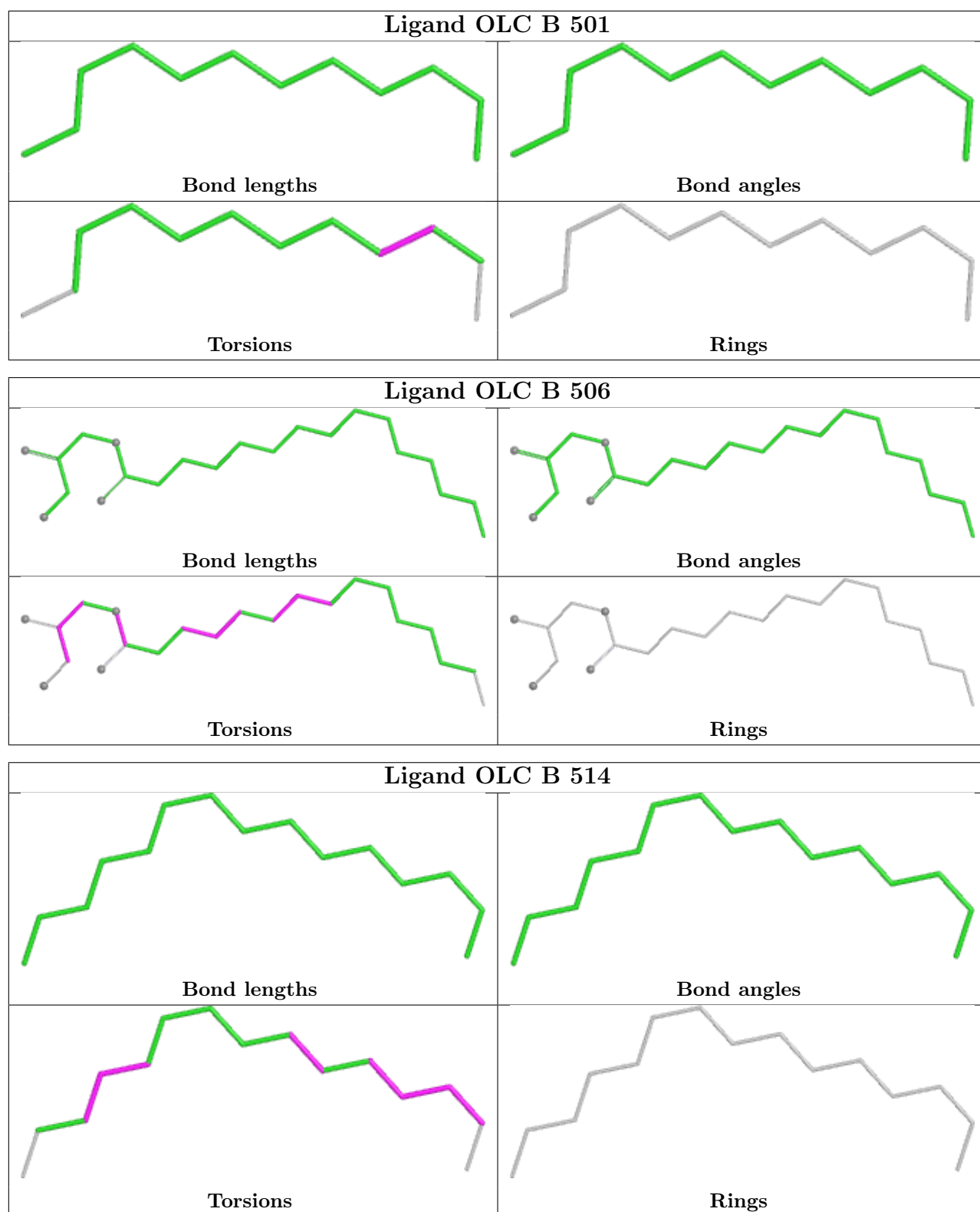


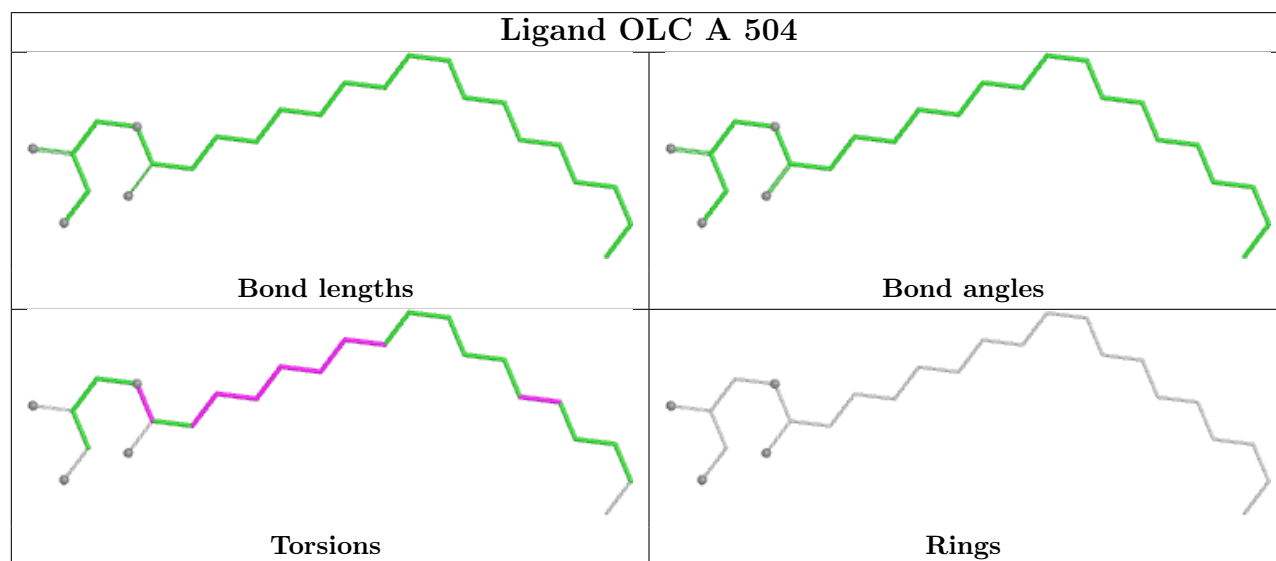
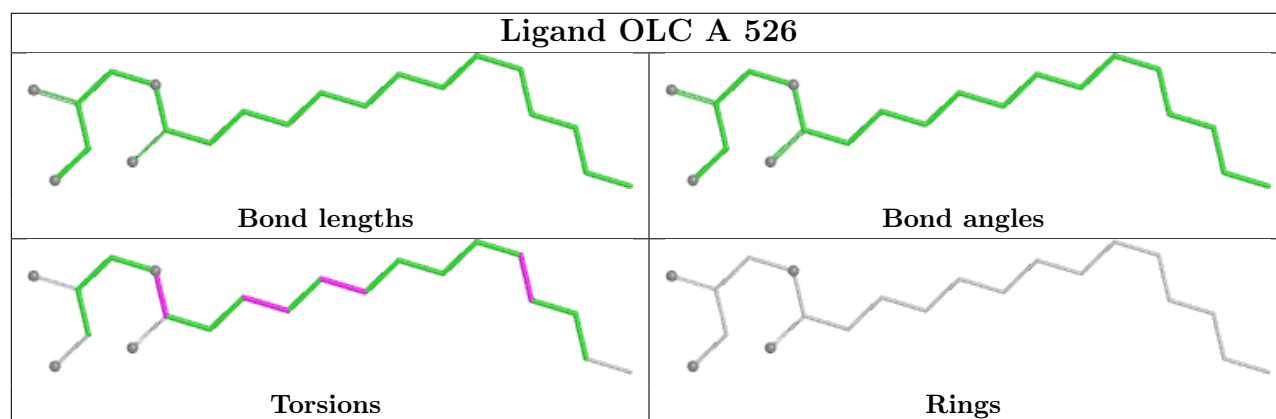
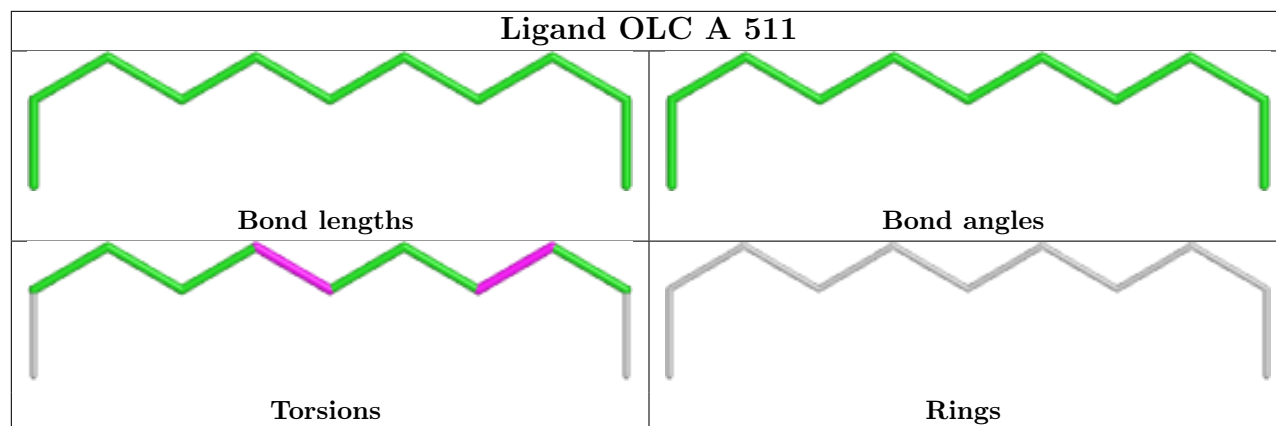


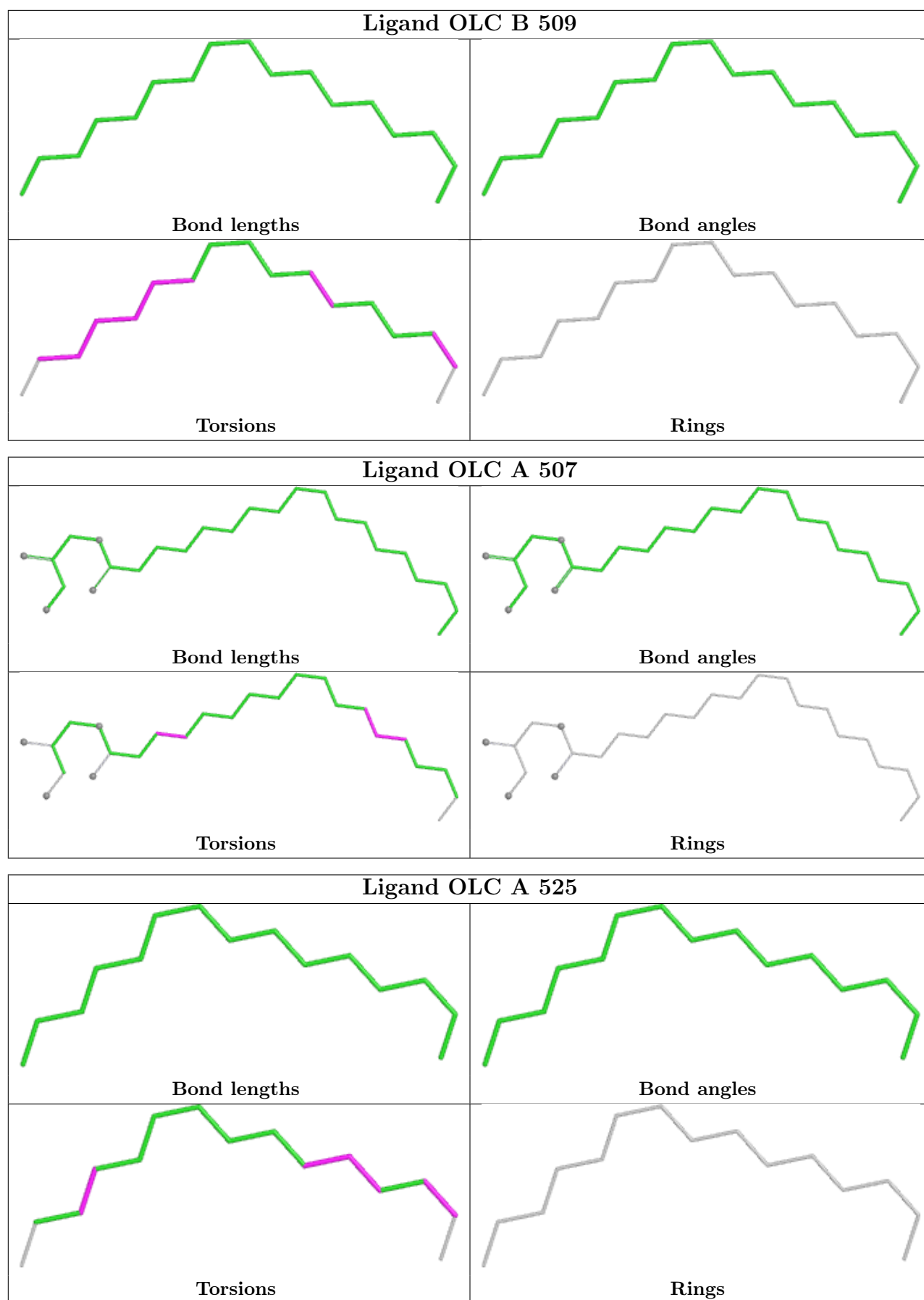


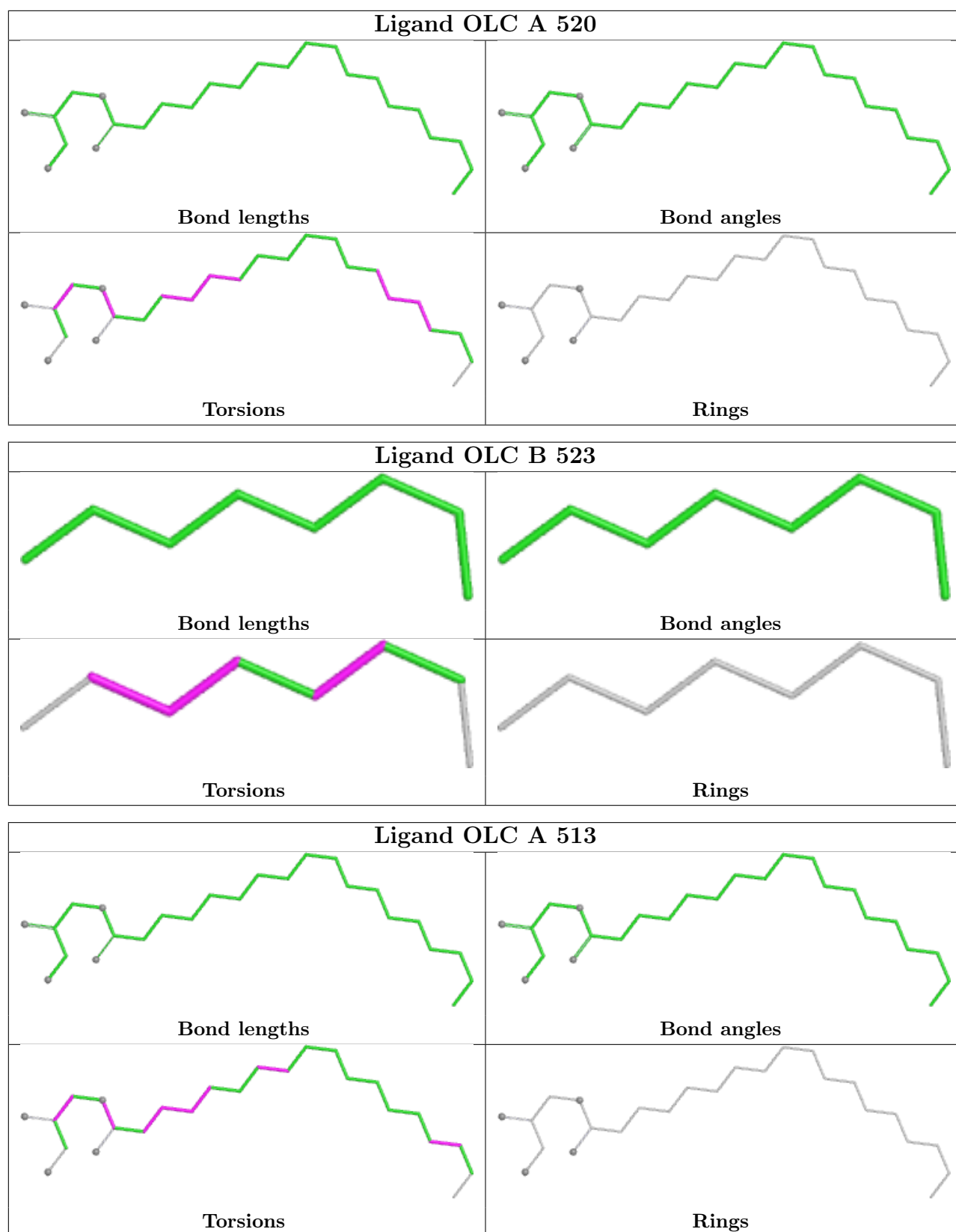


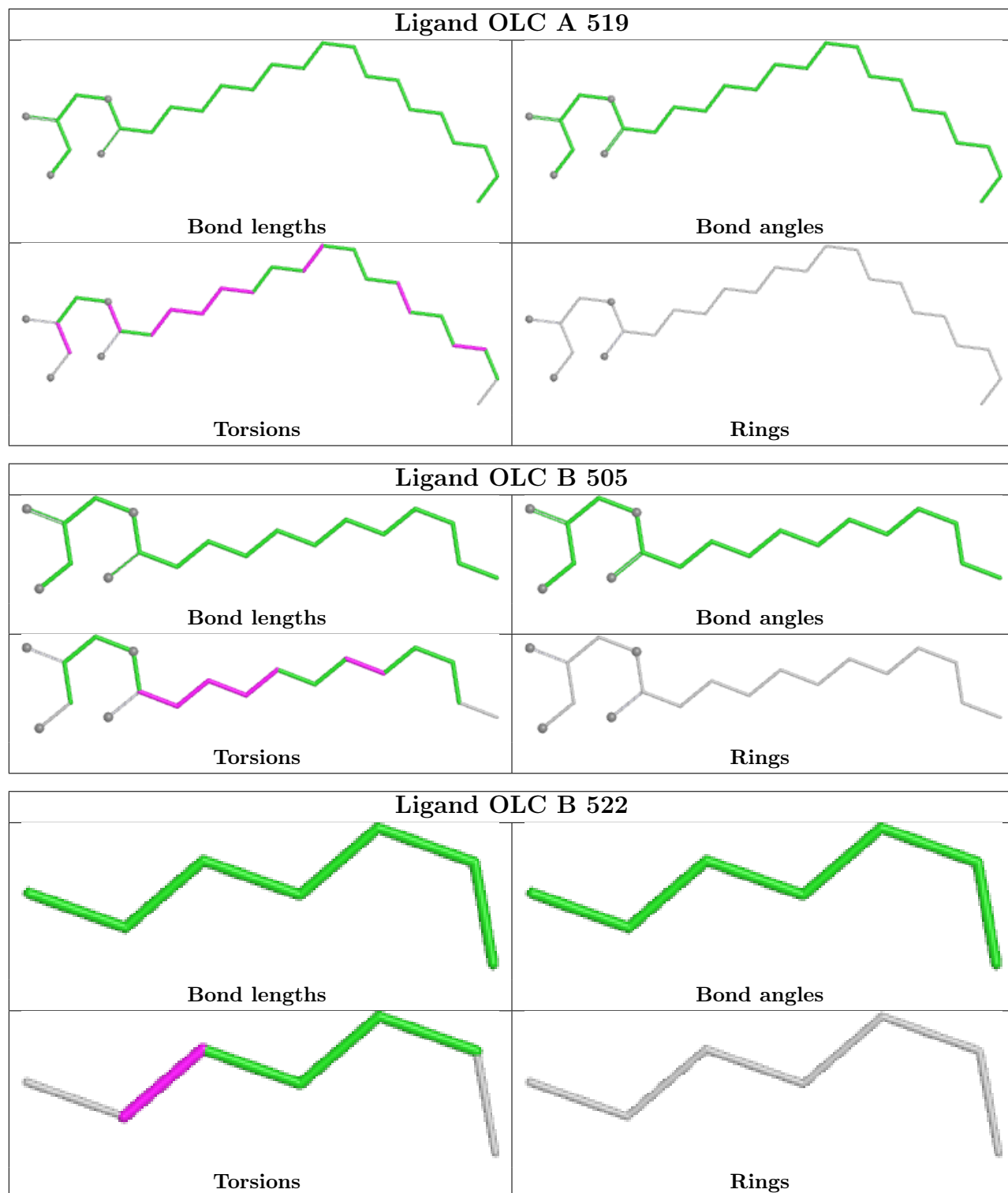


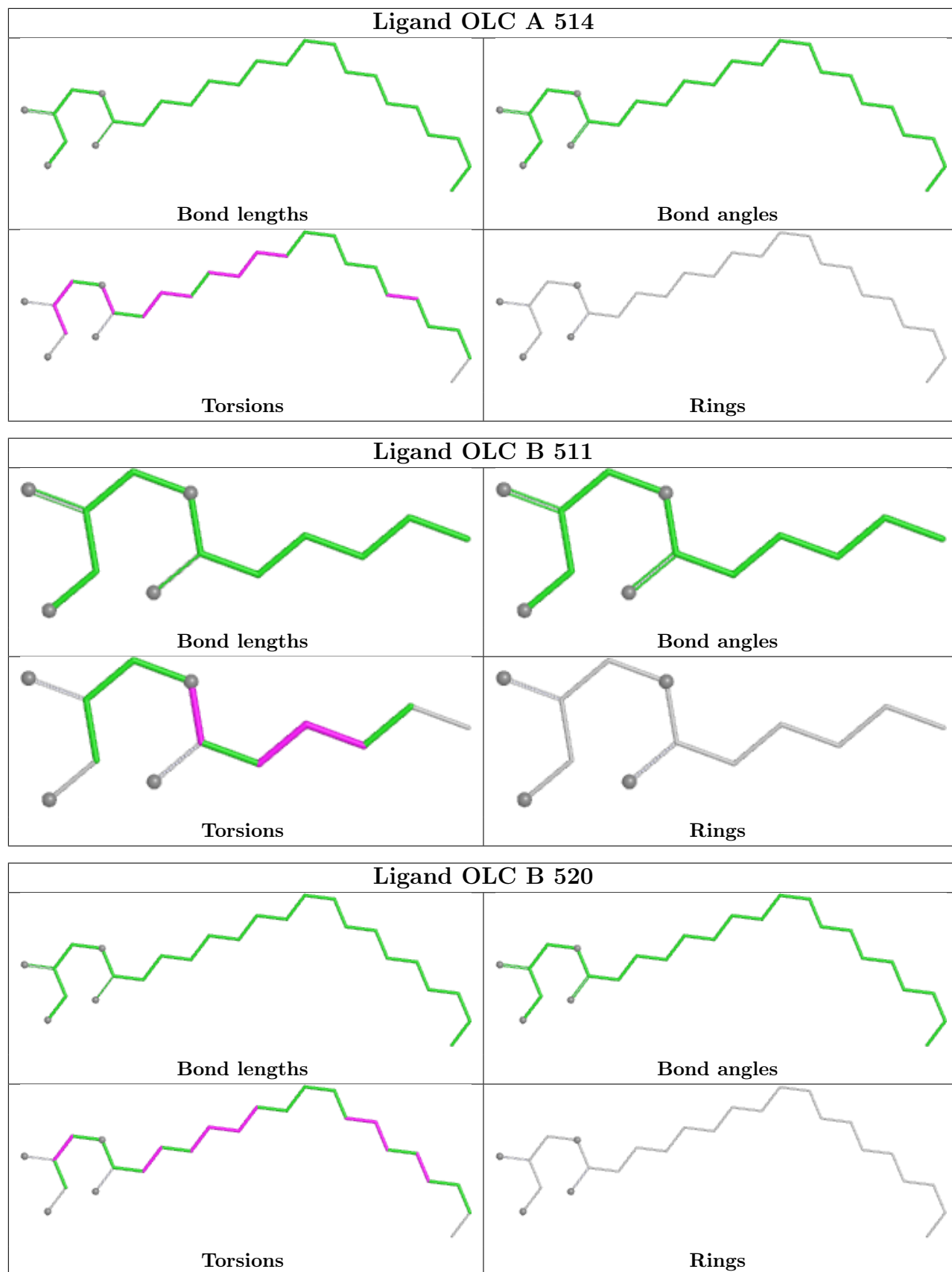


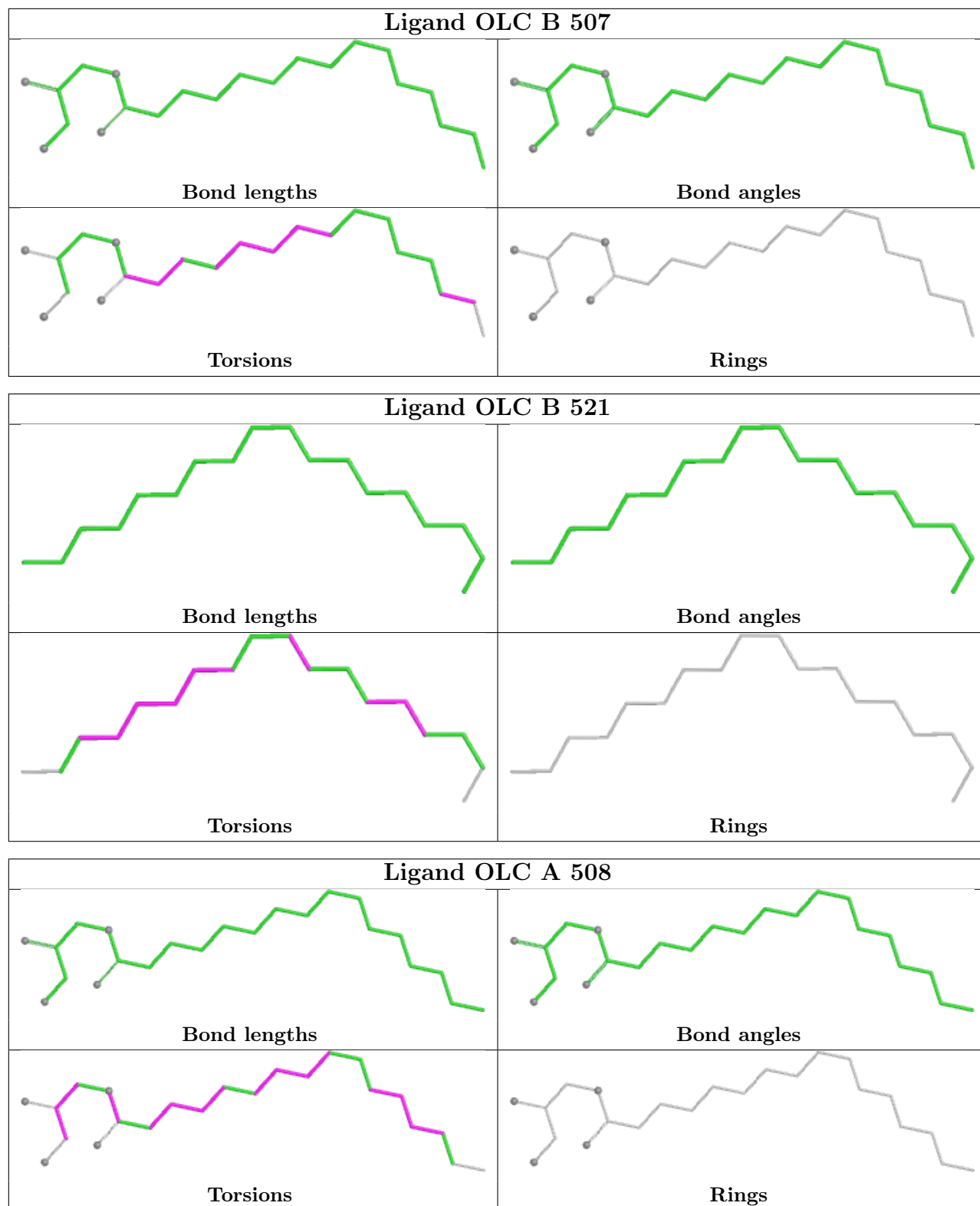


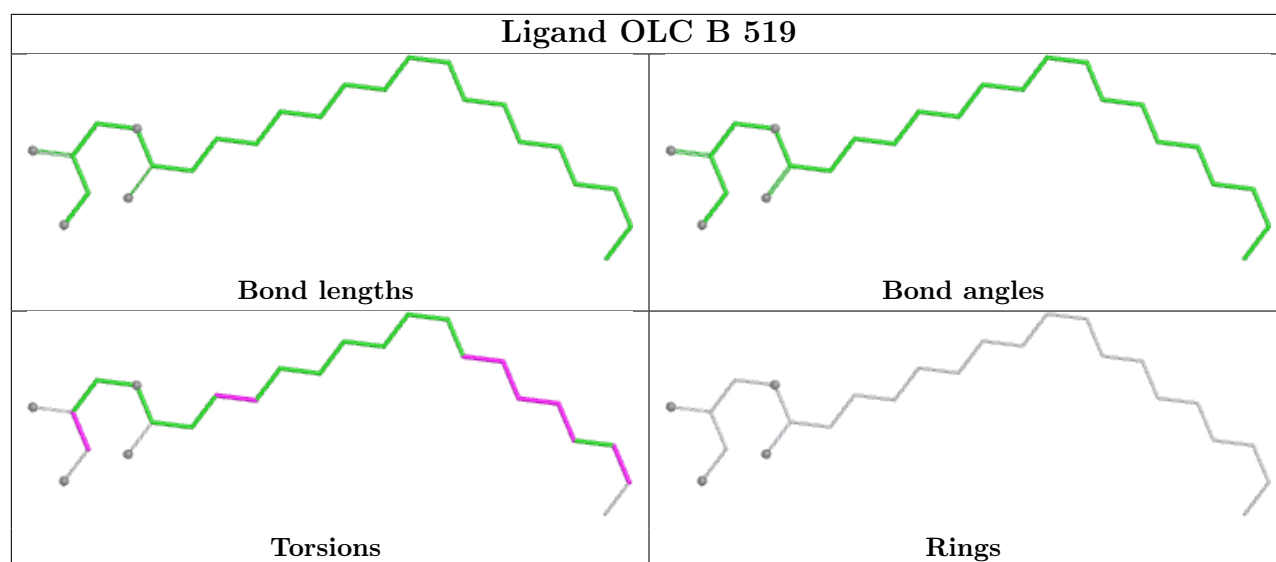












5.7 Other polymers [i](#)

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	374/416 (89%)	0.73	41 (10%) 10 8	35, 50, 116, 327	0
1	B	375/416 (90%)	0.74	38 (10%) 12 10	37, 51, 122, 335	0
All	All	749/832 (90%)	0.74	79 (10%) 11 9	35, 51, 119, 335	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	VAL	5.7
1	A	34	VAL	5.7
1	A	148	PHE	4.9
1	A	32	VAL	4.7
1	B	148	PHE	4.6
1	B	30	LEU	4.4
1	B	31	LEU	4.2
1	A	329	ILE	4.2
1	B	33	THR	4.1
1	A	33	THR	3.9
1	B	339	ILE	3.8
1	B	34	VAL	3.6
1	A	31	LEU	3.6
1	A	35	GLY	3.6
1	B	234	ILE	3.5
1	A	323	PHE	3.5
1	B	327	TYR	3.5
1	B	272	ILE	3.4
1	A	244	ASP	3.3
1	B	324	GLY	3.2
1	B	330	LYS	3.2
1	B	239	LYS	3.0
1	A	84	CYS	3.0
1	A	36	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	321	GLY	2.9
1	A	37	ILE	2.9
1	A	237	VAL	2.9
1	A	339	ILE	2.9
1	A	269	LYS	2.9
1	A	152	TYR	2.8
1	B	152	TYR	2.8
1	A	322	ILE	2.8
1	B	319	PHE	2.8
1	A	150	ASN	2.7
1	A	417	SER	2.7
1	B	329	ILE	2.7
1	A	30	LEU	2.6
1	A	327	TYR	2.6
1	A	29	GLY	2.6
1	A	146	MET	2.6
1	B	238	LEU	2.6
1	A	80	VAL	2.6
1	B	390	TYR	2.6
1	B	323	PHE	2.5
1	A	219	GLU	2.5
1	B	271	GLY	2.5
1	B	321	GLY	2.5
1	B	240	TYR	2.4
1	A	88	ALA	2.4
1	B	244	ASP	2.4
1	A	235	LYS	2.4
1	A	179	ILE	2.3
1	B	83	LEU	2.3
1	B	326	SER	2.3
1	A	271	GLY	2.3
1	A	79	ILE	2.3
1	A	385	LYS	2.3
1	A	324	GLY	2.3
1	A	76	HIS	2.2
1	B	241	GLU	2.2
1	B	416	PHE	2.2
1	B	237	VAL	2.2
1	B	35	GLY	2.2
1	B	217	HIS	2.2
1	B	149	THR	2.2
1	B	29	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	386	VAL	2.1
1	A	241	GLU	2.1
1	A	390	TYR	2.1
1	B	78	GLY	2.1
1	B	266	THR	2.1
1	A	239	LYS	2.1
1	B	218	SER	2.1
1	A	243	PHE	2.0
1	B	325	GLU	2.0
1	B	236	LYS	2.0
1	A	326	SER	2.0
1	B	282	SER	2.0
1	A	83	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	A	516	11/25	0.52	0.25	56,62,71,72	0
2	OLC	A	519	25/25	0.52	0.22	57,68,80,81	0
2	OLC	B	502	20/25	0.58	0.20	78,91,102,107	0
2	OLC	A	520	25/25	0.59	0.19	51,73,81,88	0
2	OLC	B	506	22/25	0.65	0.19	50,72,84,87	0
3	PEG	A	522	6/7	0.65	0.30	53,58,64,65	0
2	OLC	B	519	25/25	0.66	0.19	45,59,70,74	0
2	OLC	B	520	25/25	0.67	0.18	60,73,82,93	0
2	OLC	B	509	17/25	0.68	0.20	56,79,85,88	0
2	OLC	B	517	16/25	0.69	0.23	66,73,78,80	0

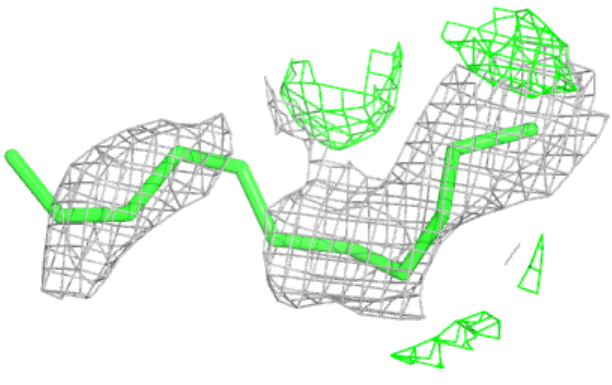
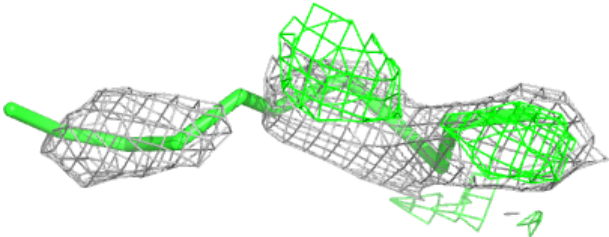
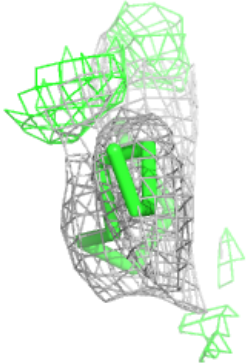
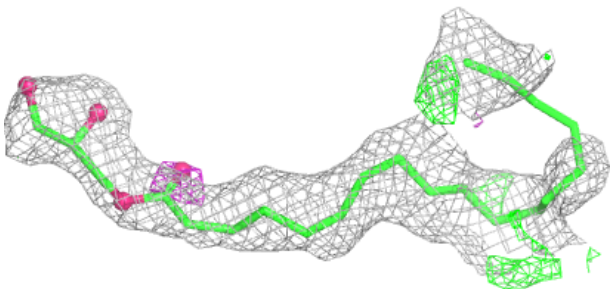
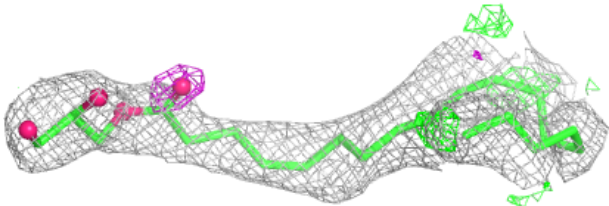
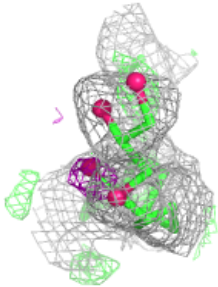
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	A	513	25/25	0.69	0.18	42,70,87,91	0
2	OLC	A	515	9/25	0.69	0.25	55,62,66,67	0
2	OLC	B	516	5/25	0.69	0.26	64,69,71,73	0
2	OLC	A	525	15/25	0.70	0.22	53,72,77,78	0
2	OLC	B	507	22/25	0.70	0.19	52,74,88,89	0
2	OLC	A	504	25/25	0.71	0.20	41,64,71,75	0
2	OLC	A	526	21/25	0.71	0.19	65,86,94,102	0
2	OLC	B	518	13/25	0.71	0.21	56,61,70,79	0
2	OLC	B	504	21/25	0.72	0.20	51,61,72,75	0
2	OLC	A	506	25/25	0.72	0.18	49,60,70,80	0
2	OLC	A	511	11/25	0.73	0.24	51,61,67,70	0
2	OLC	B	503	25/25	0.73	0.19	59,70,76,84	0
2	OLC	A	502	16/25	0.73	0.17	64,73,83,84	0
2	OLC	B	521	18/25	0.74	0.20	45,70,76,79	0
2	OLC	B	508	13/25	0.74	0.21	48,61,73,74	0
2	OLC	B	512	10/25	0.75	0.17	49,62,68,96	0
2	OLC	B	515	13/25	0.75	0.16	56,66,77,80	0
2	OLC	B	523	8/25	0.75	0.20	51,54,65,74	0
2	OLC	A	524	20/25	0.75	0.17	53,61,74,76	0
2	OLC	A	510	16/25	0.76	0.17	48,67,77,79	0
2	OLC	A	501	24/25	0.76	0.18	61,73,75,78	0
2	OLC	A	509	13/25	0.76	0.21	48,59,74,78	0
3	PEG	B	524	6/7	0.76	0.22	50,53,55,62	0
2	OLC	A	521	13/25	0.77	0.22	60,69,78,80	0
2	OLC	A	508	23/25	0.77	0.15	61,71,95,98	0
2	OLC	A	514	25/25	0.77	0.18	56,73,87,90	0
2	OLC	B	510	16/25	0.77	0.17	46,56,66,66	0
2	OLC	A	507	25/25	0.77	0.15	44,58,71,74	0
2	OLC	A	503	16/25	0.78	0.19	54,60,77,96	0
2	OLC	B	514	15/25	0.78	0.18	42,55,64,65	0
2	OLC	A	512	13/25	0.78	0.20	64,67,76,79	0
3	PEG	A	523	6/7	0.79	0.18	66,72,75,78	0
2	OLC	B	505	19/25	0.80	0.15	61,68,75,77	0
2	OLC	B	522	7/25	0.80	0.20	56,60,63,63	0
2	OLC	A	517	8/25	0.83	0.15	51,61,65,67	0
2	OLC	B	511	13/25	0.83	0.15	71,76,83,84	0
2	OLC	A	518	7/25	0.85	0.17	50,57,63,67	0
2	OLC	B	513	8/25	0.85	0.16	52,60,63,66	0
2	OLC	B	501	12/25	0.85	0.20	59,68,78,80	0
2	OLC	A	505	10/25	0.89	0.12	43,46,50,55	0

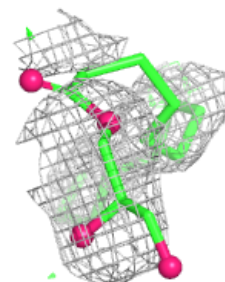
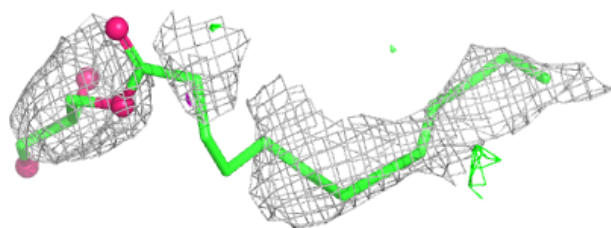
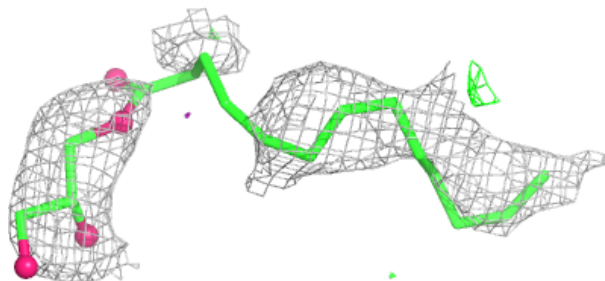
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

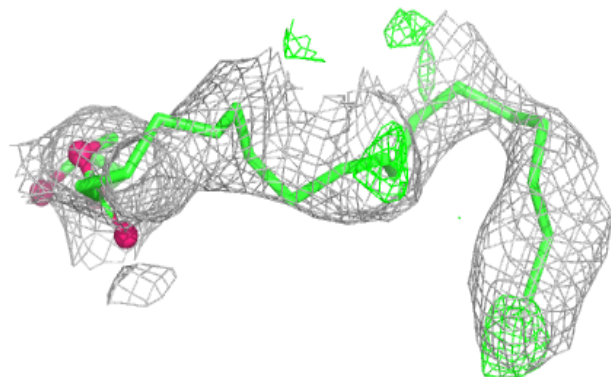
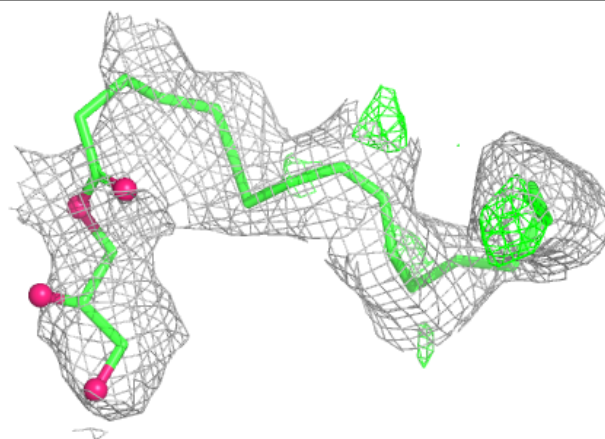
<p>Electron density around OLC A 516:</p> <p>$2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)</p>	
	
<p>Electron density around OLC A 519:</p> <p>$2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)</p>	
	

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)

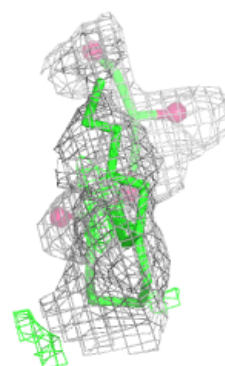
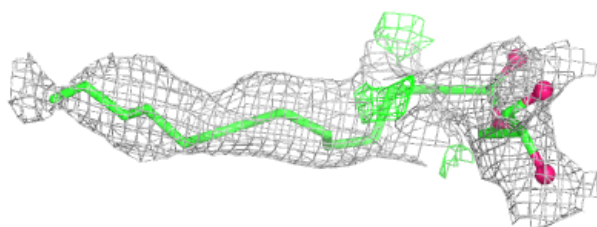
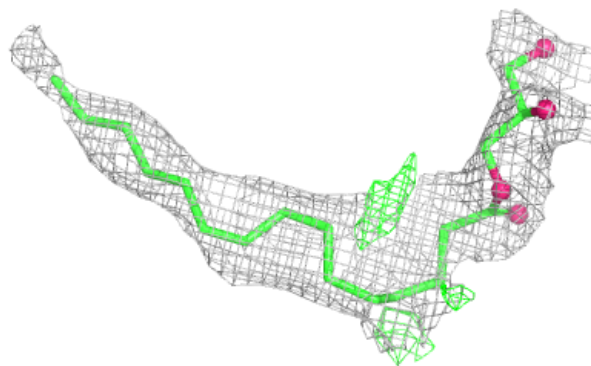
**Electron density around OLC A 520:**

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

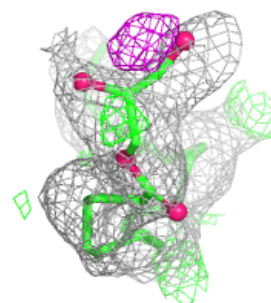
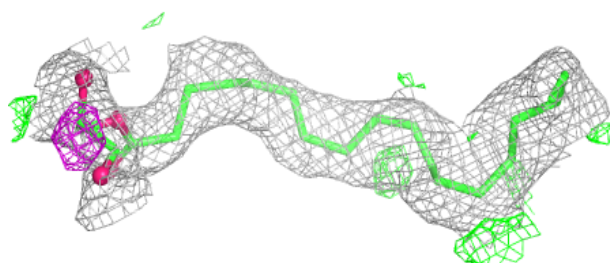
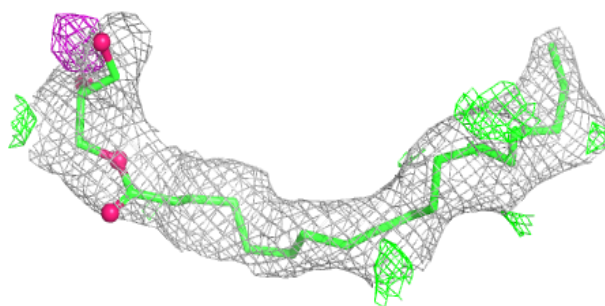


Electron density around OLC B 506:

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

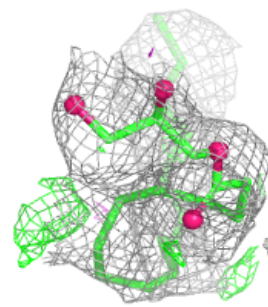
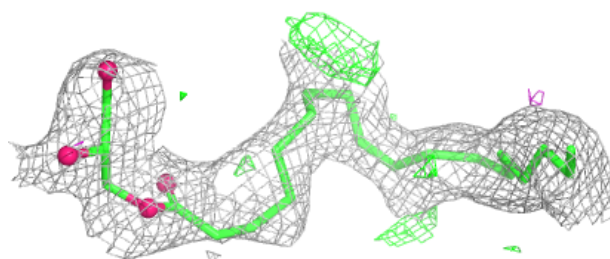
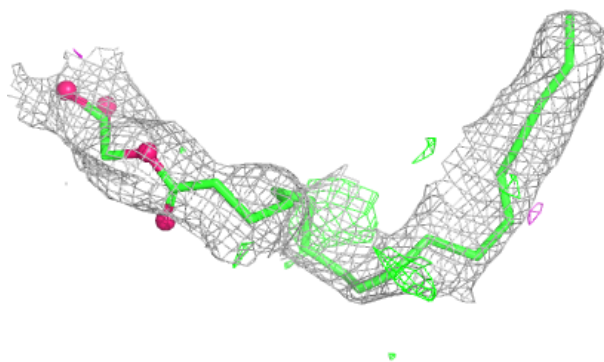
**Electron density around OLC B 519:**

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

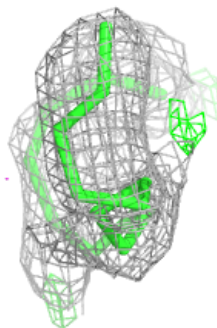
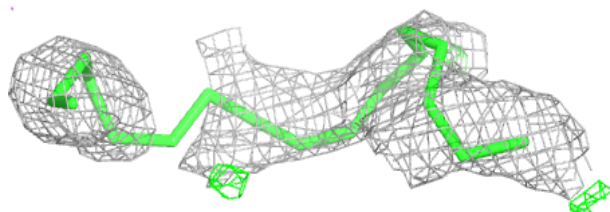
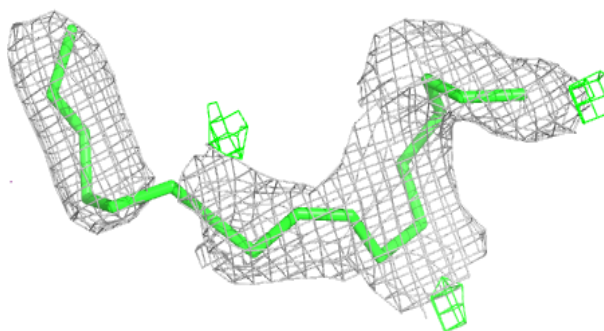


Electron density around OLC B 520:

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

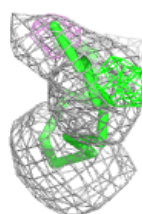
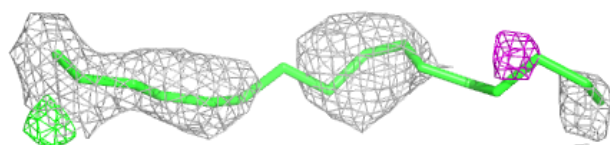
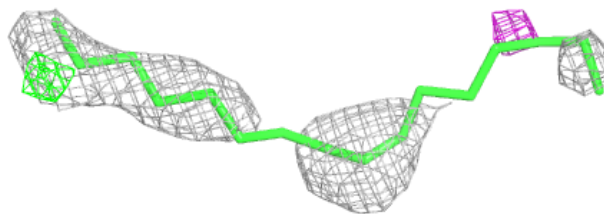
**Electron density around OLC B 509:**

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

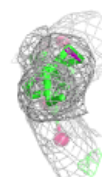
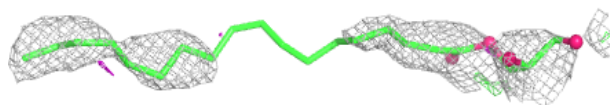
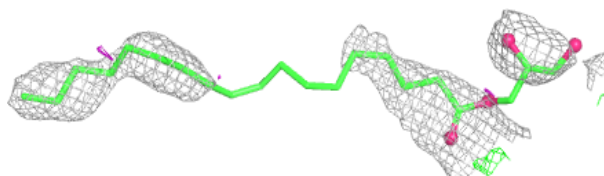


Electron density around OLC B 517:

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

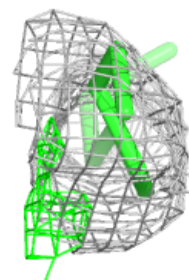
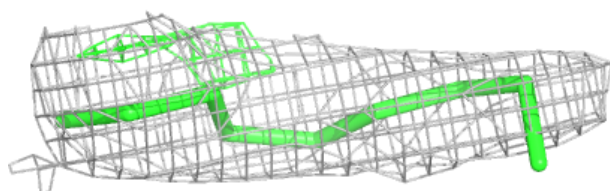
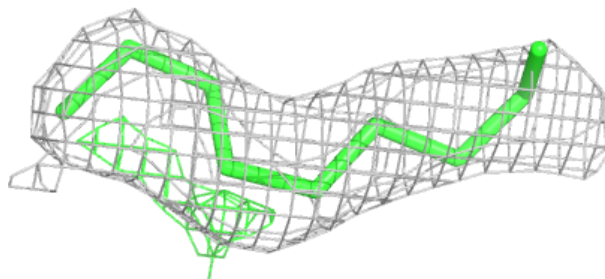
**Electron density around OLC A 513:**

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

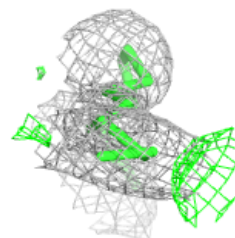
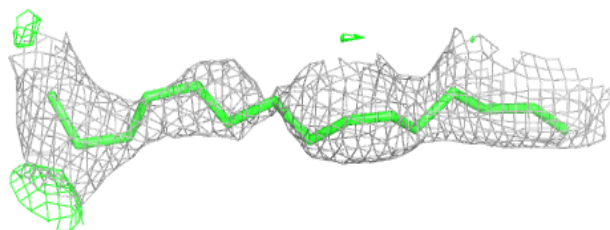
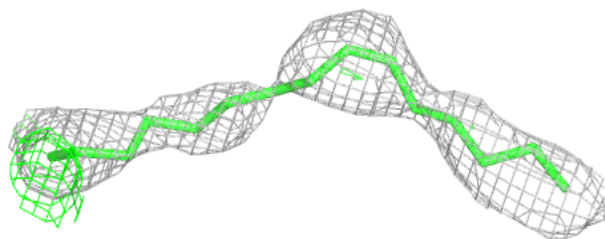


Electron density around OLC A 515:

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

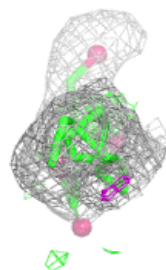
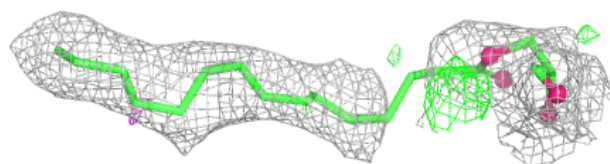
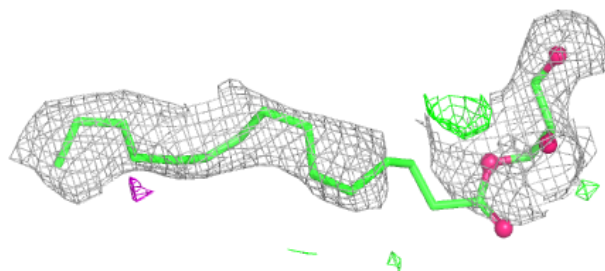
**Electron density around OLC A 525:**

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

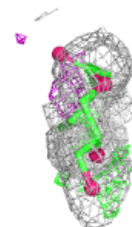
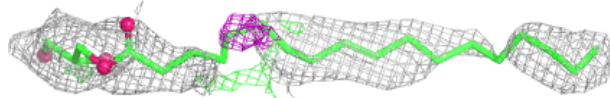
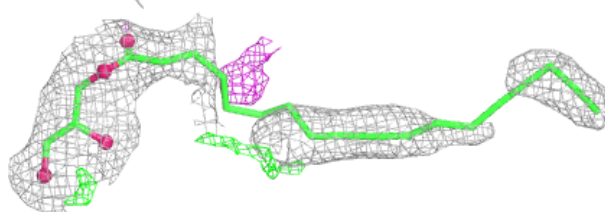


Electron density around OLC B 507:

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

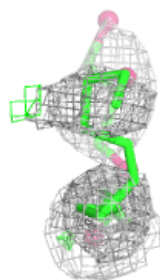
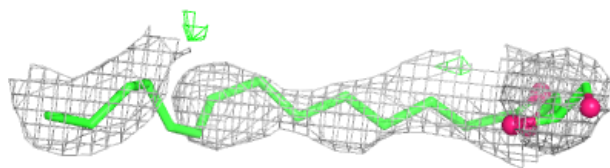
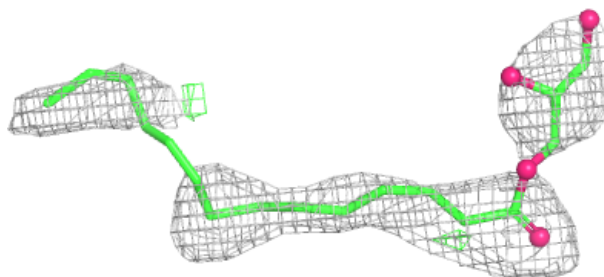
**Electron density around OLC A 504:**

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

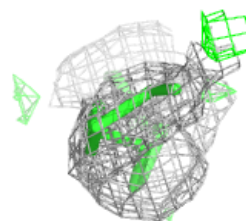
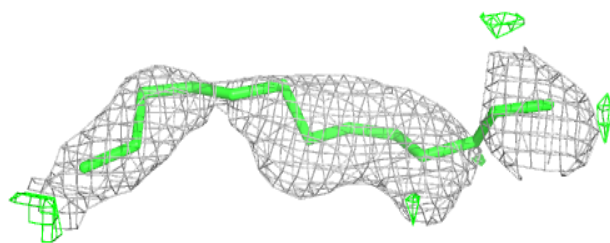
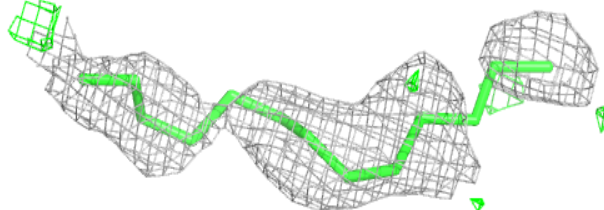


Electron density around OLC A 526:

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

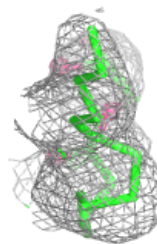
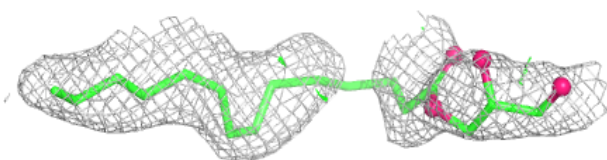
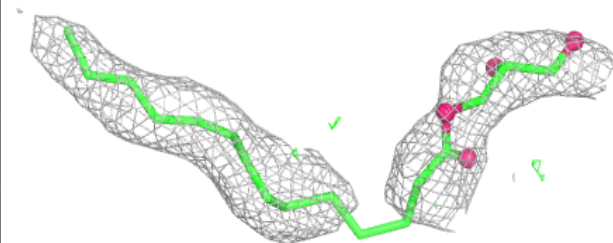
**Electron density around OLC B 518:**

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

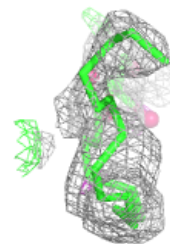
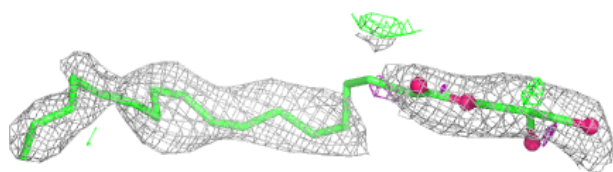
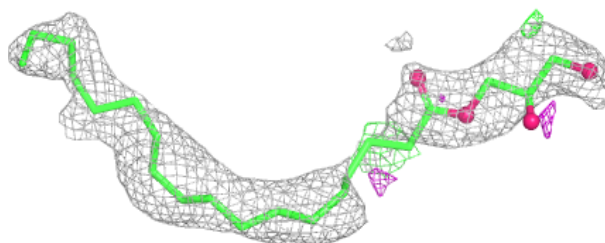


Electron density around OLC B 504:

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

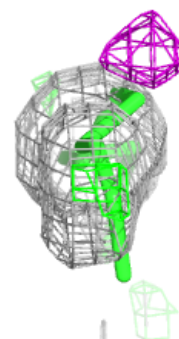
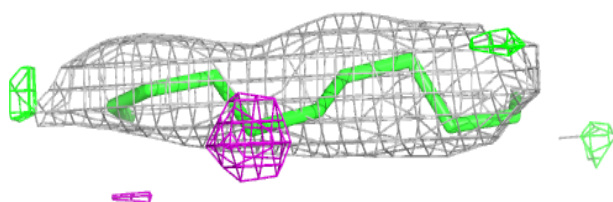
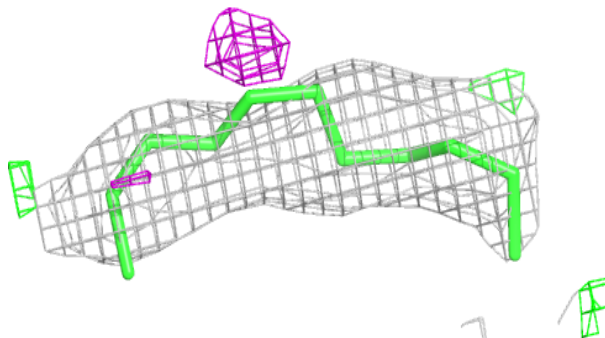
**Electron density around OLC A 506:**

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

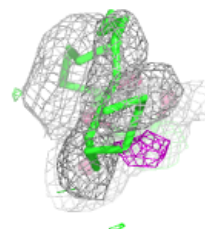
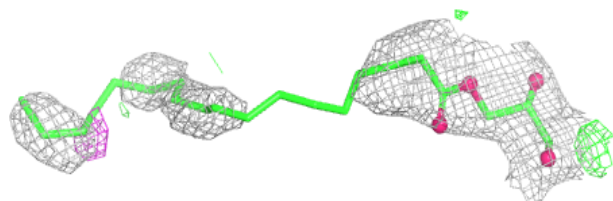
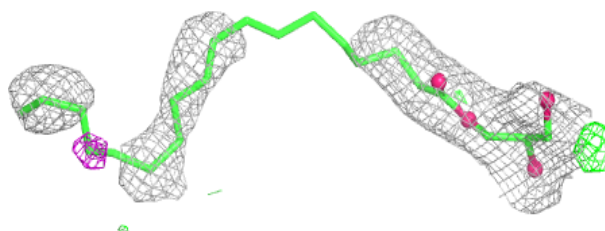


Electron density around OLC A 511:

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

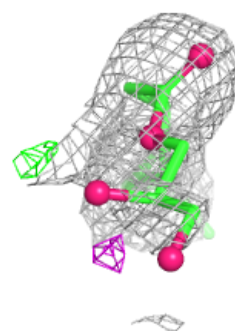
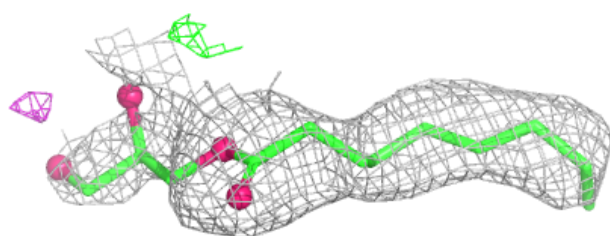
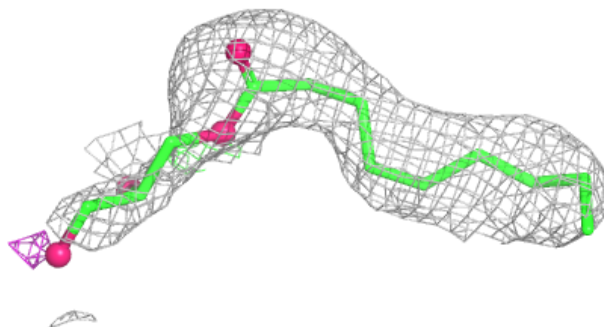
**Electron density around OLC B 503:**

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

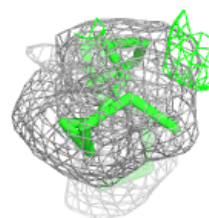
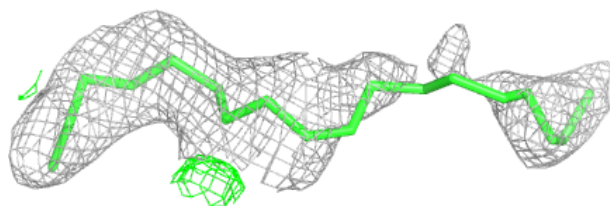
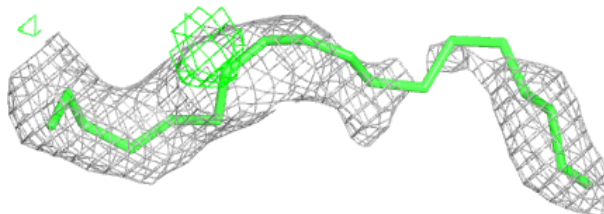


Electron density around OLC A 502:

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

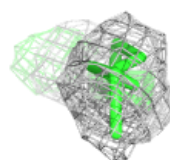
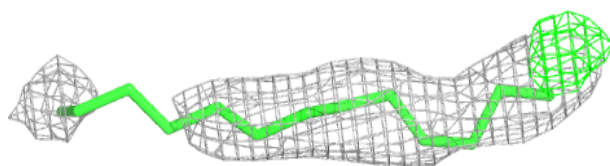
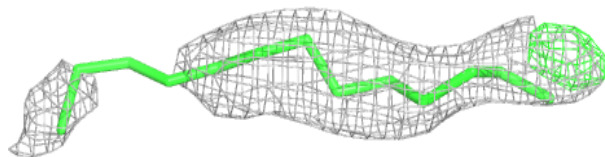
**Electron density around OLC B 521:**

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

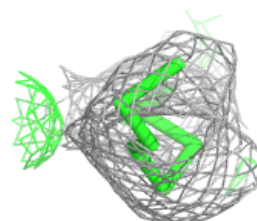
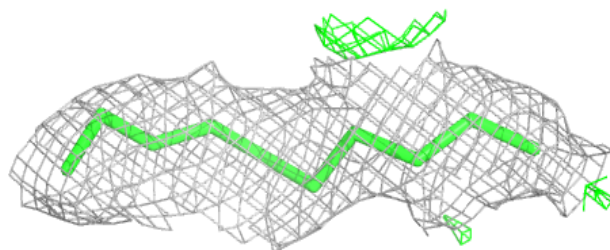
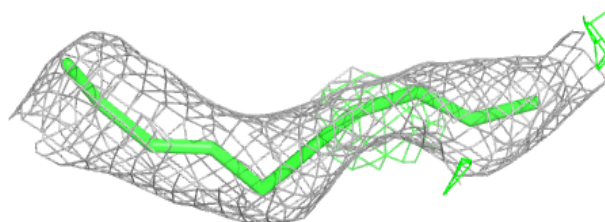


Electron density around OLC B 508:

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

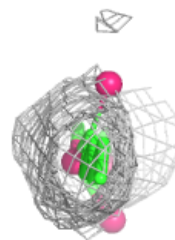
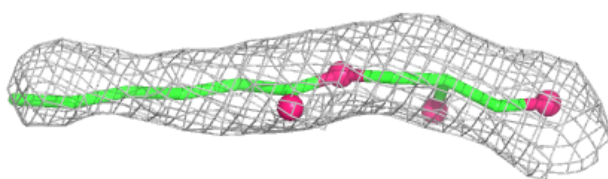
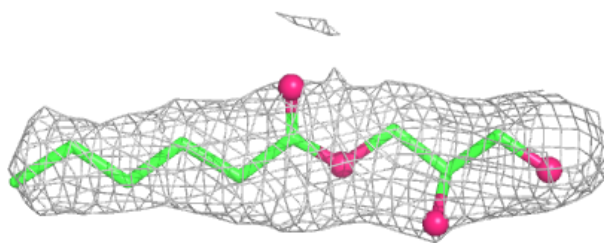
**Electron density around OLC B 512:**

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

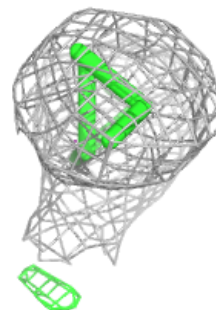
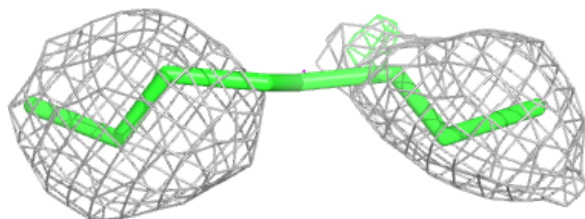
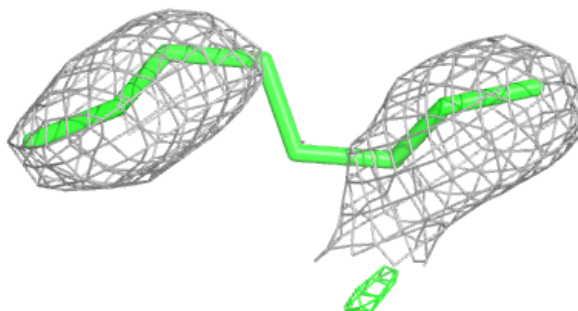


Electron density around OLC B 515:

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

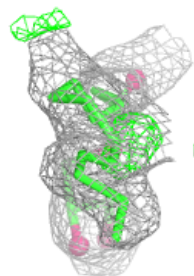
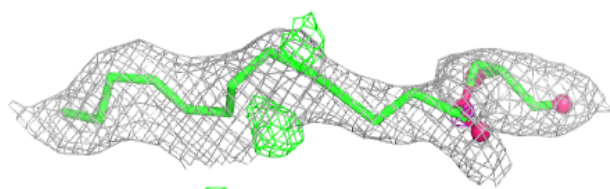
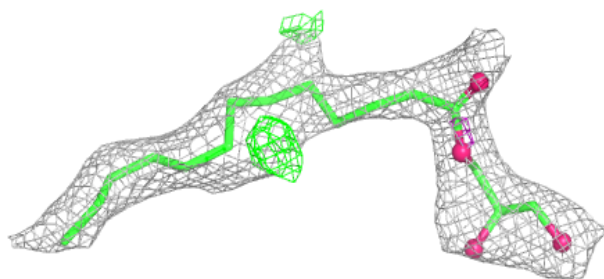
**Electron density around OLC B 523:**

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

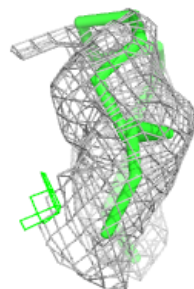
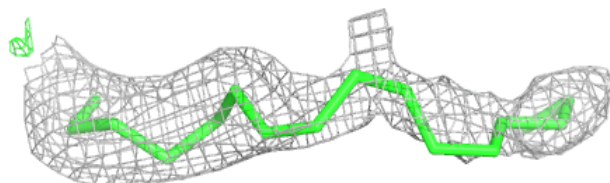
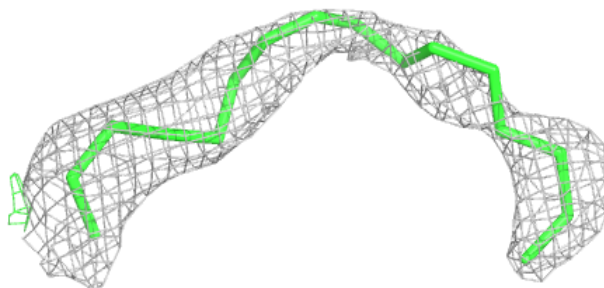


Electron density around OLC A 524:

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

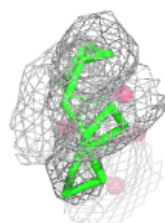
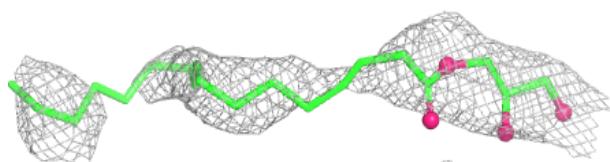
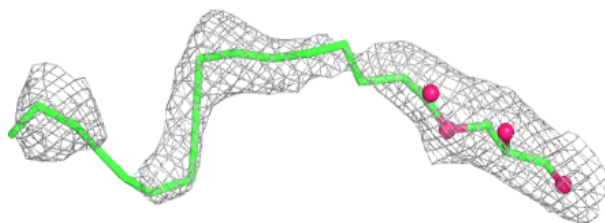
**Electron density around OLC A 510:**

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

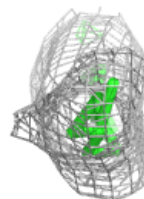
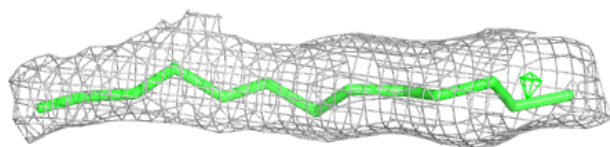
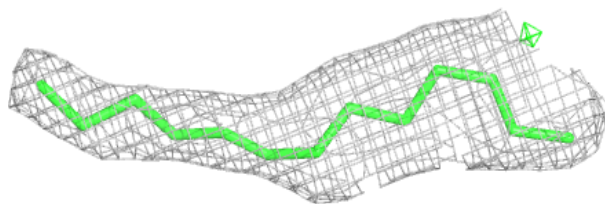


Electron density around OLC A 501:

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

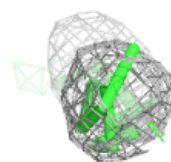
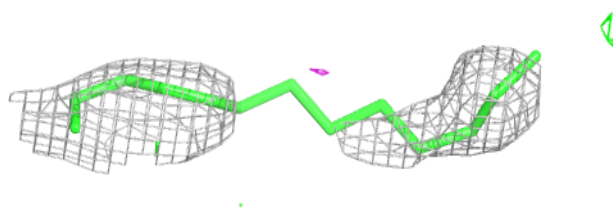
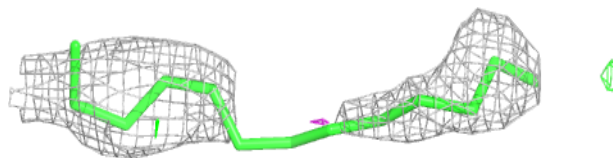
**Electron density around OLC A 509:**

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

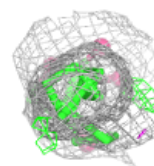
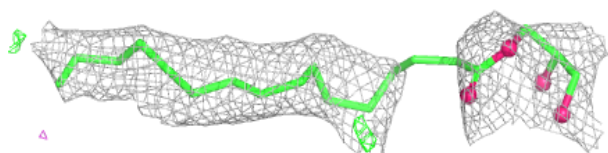
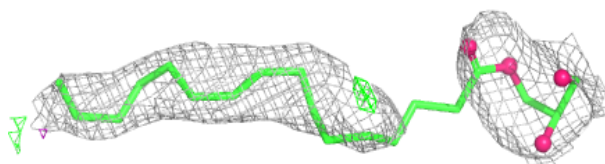


Electron density around OLC A 521:

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

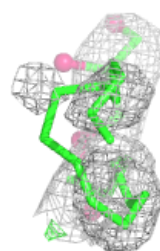
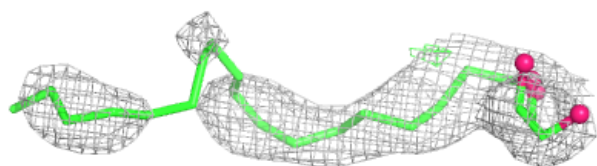
**Electron density around OLC A 508:**

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

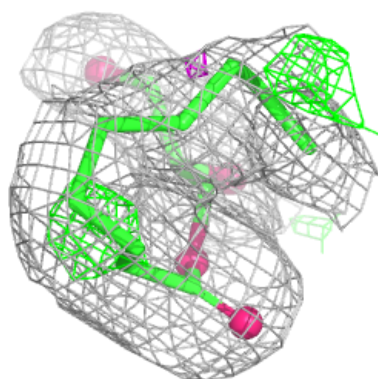
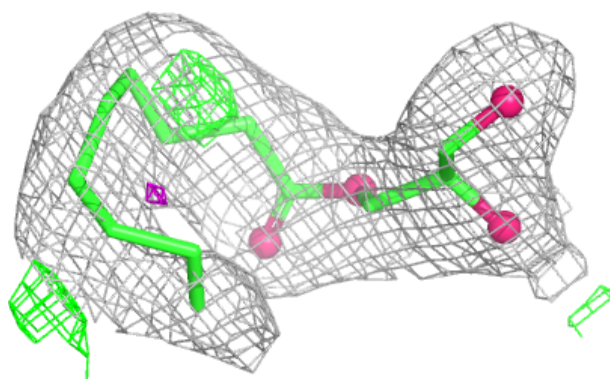
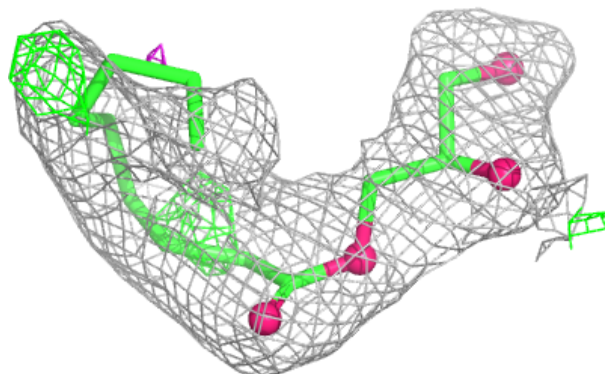


Electron density around OLC A 514:

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

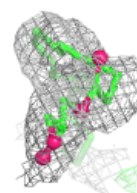
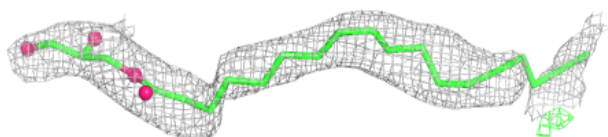
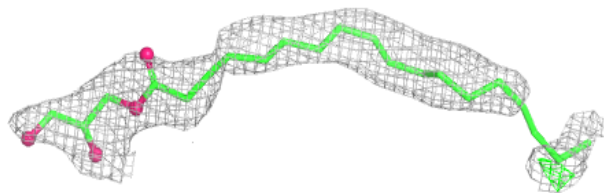
**Electron density around OLC B 510:**

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

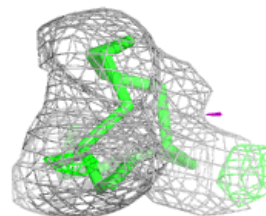
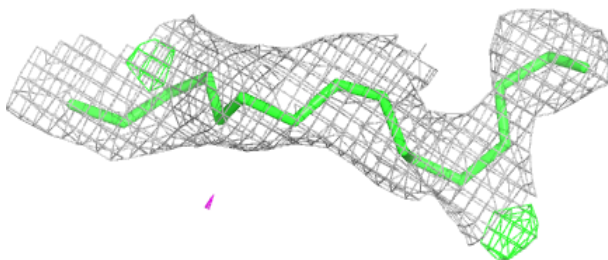
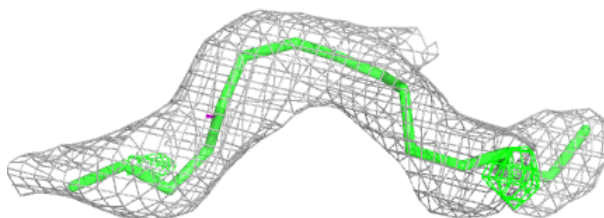


Electron density around OLC A 507:

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

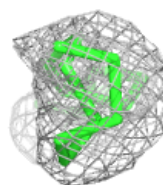
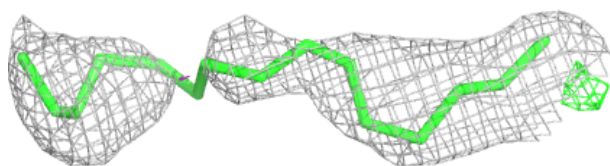
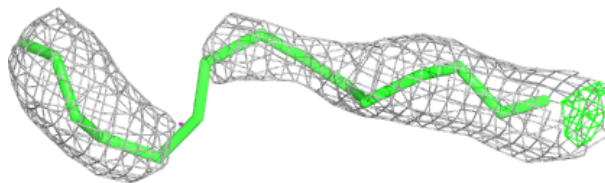
**Electron density around OLC A 503:**

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

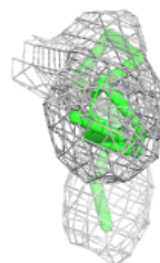
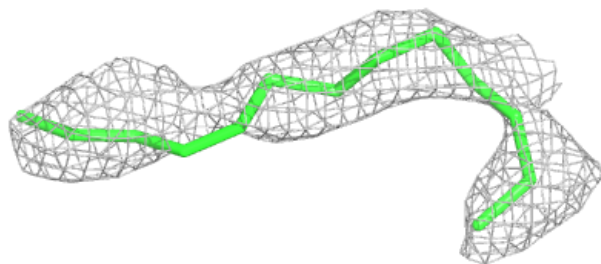


Electron density around OLC B 514:

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

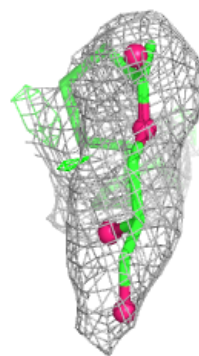
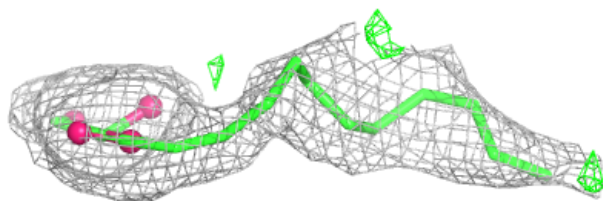
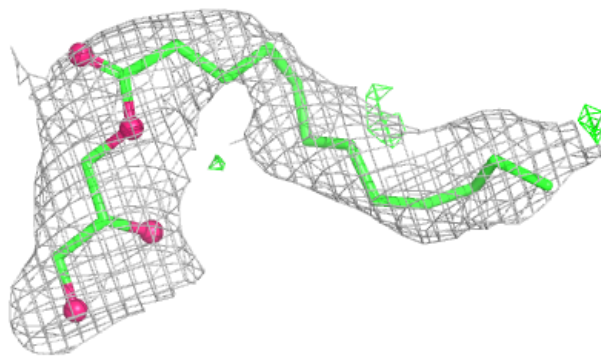
**Electron density around OLC A 512:**

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

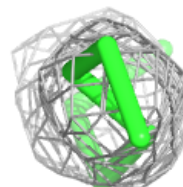
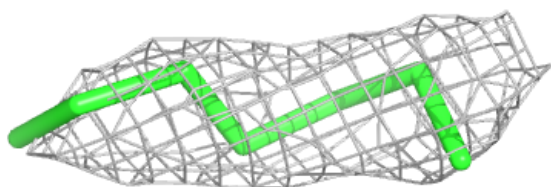
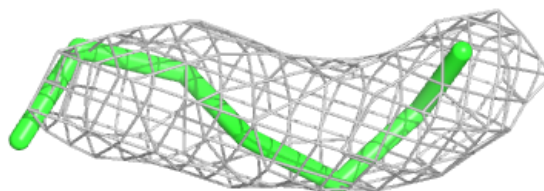


Electron density around OLC B 505:

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

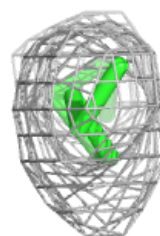
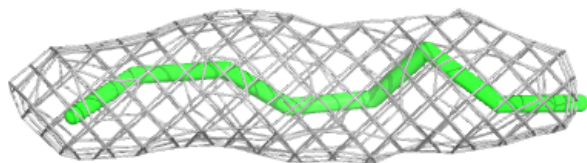
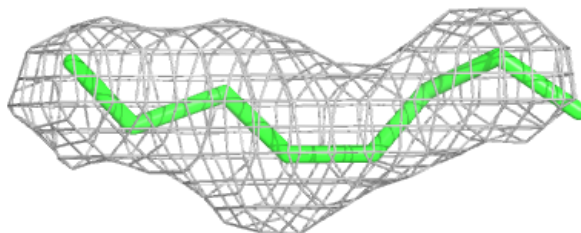
**Electron density around OLC B 522:**

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

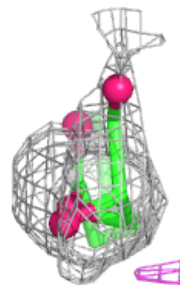
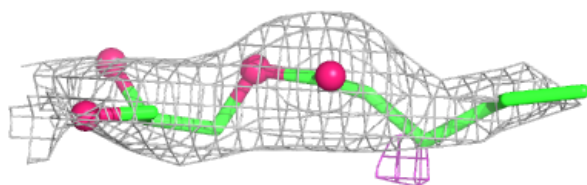
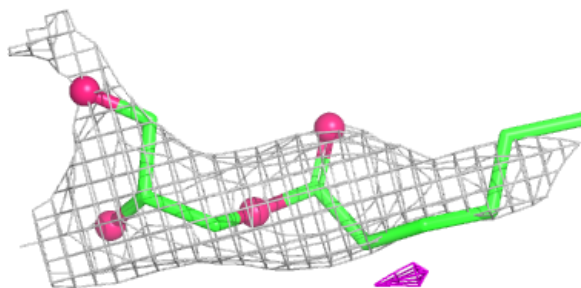


Electron density around OLC A 517:

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

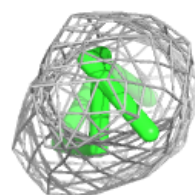
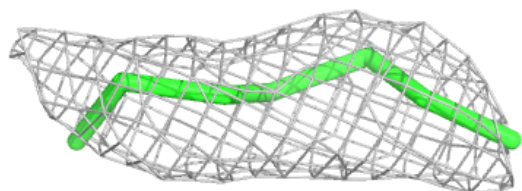
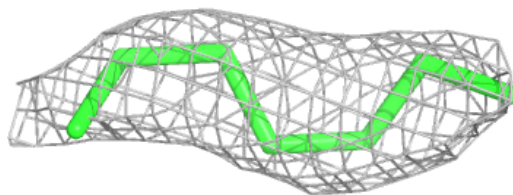
**Electron density around OLC B 511:**

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

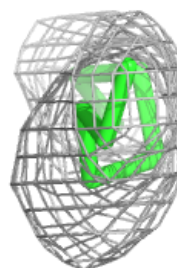
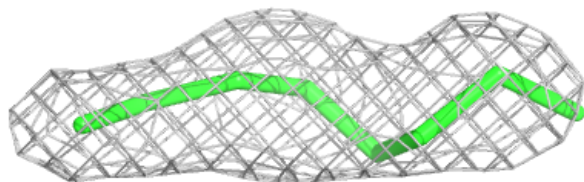
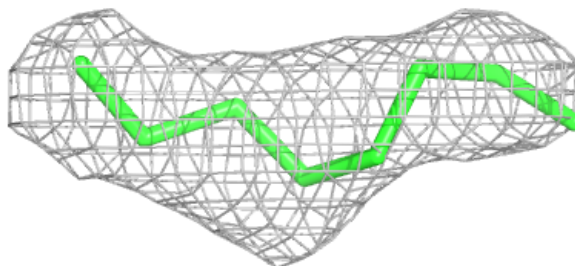


Electron density around OLC A 518:

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

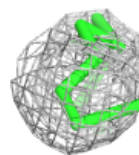
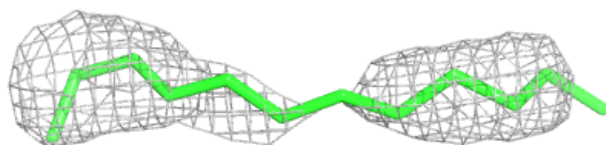
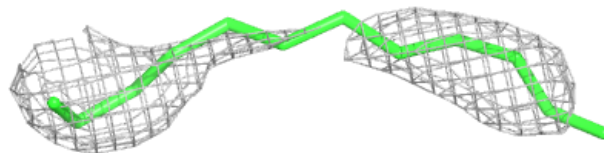
**Electron density around OLC B 513:**

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

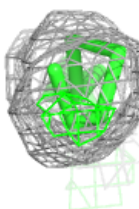
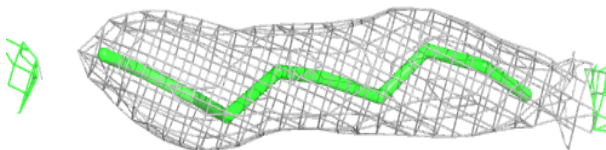
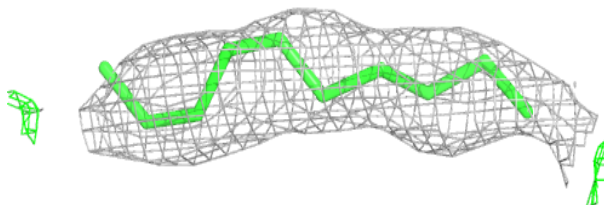


Electron density around OLC B 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.