



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:13 PM UTC

PDB ID : 6NC9 / pdb_00006nc9
Title : Lipid II flippase MurJ, outward-facing conformation
Authors : Kuk, A.C.Y.; Lee, S.-Y.
Deposited on : 2018-12-11
Resolution : 1.80 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

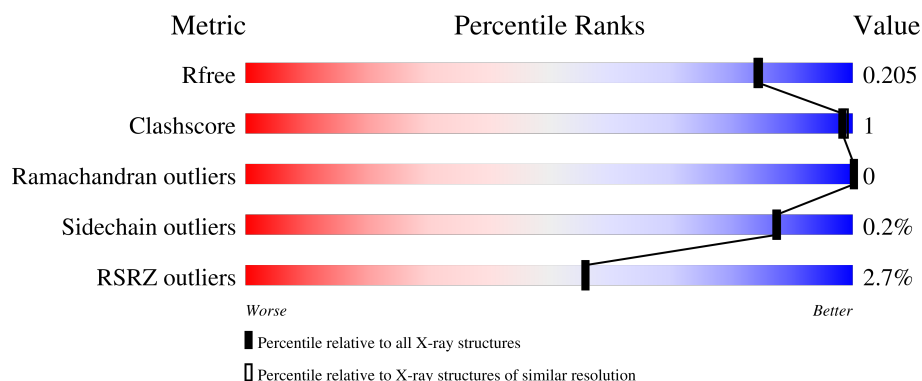
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

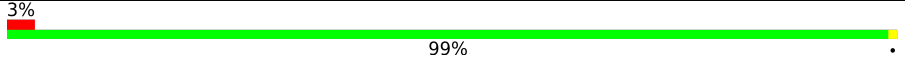
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	475	

2 Entry composition [i](#)

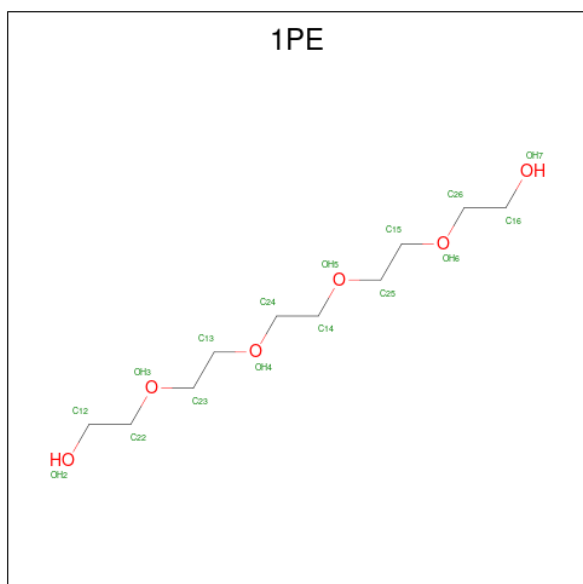
There are 6 unique types of molecules in this entry. The entry contains 8487 atoms, of which 4262 are hydrogens and 0 are deuteriums.

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 Lipid II flippase MurJ.

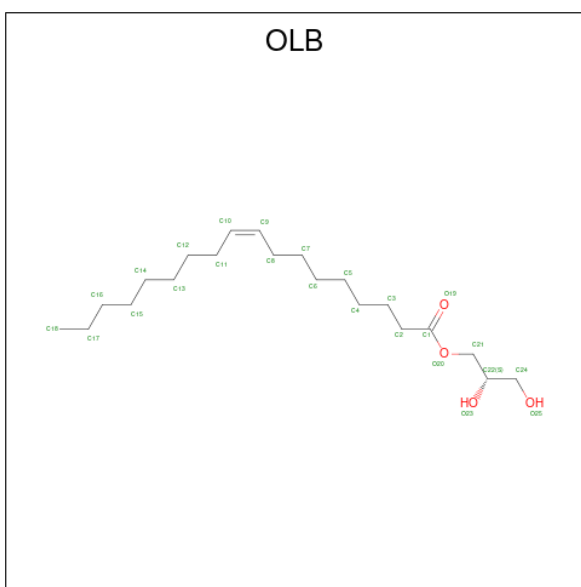
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	475	Total	C	H	N	O	S	0	0	0
			7628	2566	3853	556	644	9			

- Molecule 2 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 3 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLB) (formula: $C_{21}H_{40}O_4$).

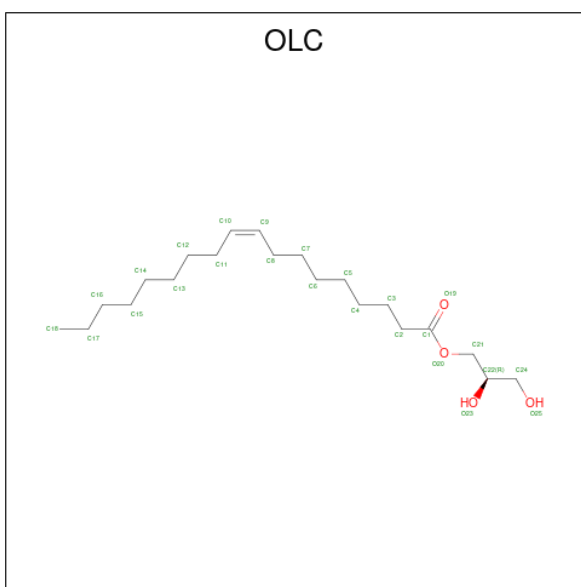


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			54	18	32	4		
3	A	1	Total	C	H	O	0	0
			45	15	26	4		
3	A	1	Total	C	H	O	0	0
			48	17	28	3		
3	A	1	Total	C	H	O	0	0
			42	14	24	4		
3	A	1	Total	C	H	O	0	0
			45	15	26	4		
3	A	1	Total	C	H	O	0	0
			54	18	32	4		
3	A	1	Total	C	H	O	0	0
			54	18	32	4		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			51	17	30	4		
5	A	1	Total	C	H	O	0	0
			30	11	17	2		
5	A	1	Total	C	H	O	0	0
			35	11	20	4		
5	A	1	Total	C	H	O	0	0
			54	18	32	4		
5	A	1	Total	C	H	O	0	0
			32	10	18	4		
5	A	1	Total	C	H	O	0	0
			35	11	20	4		
5	A	1	Total	C	H	O	0	0
			20	7	10	3		
5	A	1	Total	C	H	O	0	0
			65	21	40	4		

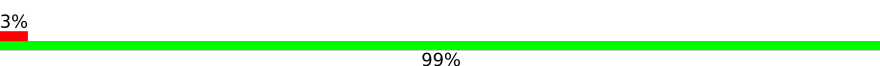
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total	O	0	0
			156	156		

3 Residue-property plots [i](#)

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

- Molecule 1: Lipid II flippase MurJ

Chain A:  3% 99%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.58Å 57.44Å 86.41Å 90.00° 100.72° 90.00°	Depositor
Resolution (Å)	84.90 – 1.80 84.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	88.5 (84.90-1.80) 85.0 (84.90-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.80Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.180 , 0.200 0.184 , 0.205	Depositor DCC
R_{free} test set	2556 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8487	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OLC, 1PE, OLB

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	0.14	0/3883	0.33	0/5282

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	3775	3853	3833	5	0
2	A	16	22	22	0	0
3	A	142	200	193	2	0
4	A	1	0	0	0	0
5	A	135	187	179	0	0
6	A	156	0	0	0	0
All	All	4225	4262	4227	5	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 1.

All (5) 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:A:464:ASP:OD1	1:A:467:ARG:NH1	2.44	0.50
1:A:362:THR:HB	1:A:363:PRO:HD3	2.00	0.43
1:A:335:ILE:HD11	3:A:503:OLB:H22	2.02	0.42
1:A:34:VAL:O	1:A:34:VAL:CG2	2.66	0.42
1:A:464:ASP:H	3:A:504:OLB:C22	2.34	0.41

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	473/475 (100%)	469 (99%)	4 (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	408/428 (95%)	407 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	229	GLN
1	A	288	ASN

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 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	OLB	A	508	-	21,21,24	0.87	1 (4%)	22,22,25	0.83	1 (4%)
5	OLC	A	514	-	13,13,24	1.06	2 (15%)	14,14,25	0.89	1 (7%)
5	OLC	A	516	-	9,9,24	1.16	1 (11%)	9,9,25	1.05	1 (11%)
3	OLB	A	507	-	21,21,24	0.85	2 (9%)	22,22,25	0.91	0
3	OLB	A	504	-	19,19,24	0.81	1 (5%)	19,19,25	0.92	1 (5%)
5	OLC	A	517	-	24,24,24	0.80	2 (8%)	25,25,25	0.93	1 (4%)
5	OLC	A	510	-	20,20,24	0.89	2 (10%)	21,21,25	0.83	0
2	1PE	A	501	-	15,15,15	0.54	0	14,14,14	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLC	A	515	-	14,14,24	1.03	1 (7%)	15,15,25	0.87	1 (6%)
3	OLB	A	506	-	18,18,24	0.93	2 (11%)	19,19,25	0.96	1 (5%)
3	OLB	A	503	-	18,18,24	0.94	2 (11%)	19,19,25	0.94	1 (5%)
5	OLC	A	512	-	14,14,24	1.03	2 (14%)	15,15,25	1.03	1 (6%)
5	OLC	A	511	-	12,12,24	1.97	2 (16%)	12,12,25	1.07	0
3	OLB	A	502	-	21,21,24	0.86	1 (4%)	22,22,25	0.87	1 (4%)
5	OLC	A	513	-	21,21,24	0.85	2 (9%)	22,22,25	1.05	1 (4%)
3	OLB	A	505	-	17,17,24	0.96	2 (11%)	18,18,25	0.98	1 (5%)

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	OLB	A	508	-	-	11/21/21/24	-
5	OLC	A	514	-	-	3/13/13/24	-
5	OLC	A	516	-	-	1/8/8/24	-
3	OLB	A	507	-	-	4/21/21/24	-
3	OLB	A	504	-	-	6/18/18/24	-
5	OLC	A	517	-	-	9/24/24/24	-
5	OLC	A	510	-	-	4/20/20/24	-
2	1PE	A	501	-	-	2/13/13/13	-
5	OLC	A	515	-	-	4/14/14/24	-
3	OLB	A	506	-	-	6/18/18/24	-
3	OLB	A	503	-	-	8/18/18/24	-
5	OLC	A	512	-	-	6/14/14/24	-
5	OLC	A	511	-	-	3/10/10/24	-
3	OLB	A	502	-	-	4/21/21/24	-
5	OLC	A	513	-	-	7/21/21/24	-
3	OLB	A	505	-	-	8/17/17/24	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	511	OLC	O19-C1	5.59	1.40	1.22
5	A	511	OLC	O20-C1	-3.55	1.19	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	OLB	O20-C1	2.53	1.40	1.33
3	A	502	OLB	O20-C1	2.52	1.40	1.33
3	A	503	OLB	O20-C1	2.51	1.40	1.33
5	A	515	OLC	O20-C1	2.49	1.40	1.33
5	A	514	OLC	O20-C1	2.44	1.40	1.33
5	A	516	OLC	O20-C1	2.41	1.40	1.33
5	A	512	OLC	O20-C1	2.41	1.40	1.33
3	A	506	OLB	O20-C1	2.38	1.40	1.33
3	A	505	OLB	O20-C1	2.37	1.40	1.33
5	A	513	OLC	O20-C1	2.37	1.40	1.33
5	A	510	OLC	O20-C21	-2.35	1.39	1.45
5	A	517	OLC	O20-C21	-2.34	1.39	1.45
5	A	510	OLC	O20-C1	2.32	1.40	1.33
3	A	507	OLB	O20-C1	2.29	1.40	1.33
3	A	507	OLB	O20-C21	-2.29	1.40	1.45
3	A	504	OLB	O20-C1	2.26	1.39	1.33
5	A	517	OLC	O20-C1	2.21	1.39	1.33
5	A	512	OLC	O20-C21	-2.20	1.40	1.45
3	A	506	OLB	O20-C21	-2.15	1.40	1.45
5	A	514	OLC	O20-C21	-2.15	1.40	1.45
3	A	505	OLB	O20-C21	-2.15	1.40	1.45
5	A	513	OLC	O20-C21	-2.14	1.40	1.45
3	A	503	OLB	O20-C21	-2.06	1.40	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	513	OLC	O20-C1-C2	2.99	120.94	111.83
5	A	512	OLC	O20-C1-C2	2.60	119.78	111.83
3	A	508	OLB	O20-C1-C2	2.49	119.43	111.83
3	A	505	OLB	O20-C1-C2	2.48	119.39	111.83
3	A	506	OLB	O20-C1-C2	2.44	119.28	111.83
3	A	503	OLB	O20-C1-C2	2.42	119.21	111.83
5	A	517	OLC	O20-C1-C2	2.35	119.00	111.83
5	A	516	OLC	O20-C1-C2	2.34	118.97	111.83
3	A	502	OLB	O20-C1-C2	2.29	118.83	111.83
5	A	515	OLC	O20-C1-C2	2.26	118.74	111.83
3	A	504	OLB	C3-C2-C1	-2.19	105.66	113.69
5	A	514	OLC	O20-C1-C2	2.01	117.96	111.83

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	OLB	C21-C22-C24-O25
5	A	517	OLC	O20-C21-C22-C24
3	A	504	OLB	O20-C21-C22-C24
3	A	508	OLB	O20-C21-C22-C24
5	A	514	OLC	O20-C21-C22-C24
3	A	508	OLB	O20-C21-C22-O23
5	A	514	OLC	O20-C21-C22-O23
5	A	517	OLC	O20-C21-C22-O23
3	A	503	OLB	C1-C2-C3-C4
3	A	508	OLB	C1-C2-C3-C4
5	A	512	OLC	C1-C2-C3-C4
3	A	505	OLB	O20-C21-C22-O23
3	A	506	OLB	O20-C21-C22-O23
5	A	512	OLC	O20-C21-C22-O23
5	A	513	OLC	C1-C2-C3-C4
3	A	505	OLB	O20-C21-C22-C24
3	A	506	OLB	O20-C21-C22-C24
5	A	512	OLC	O20-C21-C22-C24
3	A	505	OLB	C21-C22-C24-O25
5	A	517	OLC	C21-C22-C24-O25
5	A	511	OLC	C3-C4-C5-C6
5	A	511	OLC	C2-C3-C4-C5
5	A	512	OLC	C4-C5-C6-C7
3	A	508	OLB	C4-C5-C6-C7
2	A	501	1PE	OH7-C16-C26-OH6
3	A	503	OLB	C4-C5-C6-C7
5	A	513	OLC	C3-C4-C5-C6
5	A	511	OLC	C4-C5-C6-C7
3	A	503	OLB	C9-C10-C11-C12
3	A	504	OLB	C3-C4-C5-C6
3	A	504	OLB	C2-C3-C4-C5
3	A	505	OLB	C5-C6-C7-C8
5	A	510	OLC	C3-C4-C5-C6
3	A	508	OLB	C5-C6-C7-C8
3	A	505	OLB	O23-C22-C24-O25
3	A	506	OLB	O23-C22-C24-O25
3	A	503	OLB	C6-C7-C8-C9
3	A	508	OLB	C6-C7-C8-C9
5	A	515	OLC	C2-C3-C4-C5
5	A	517	OLC	C3-C4-C5-C6
3	A	505	OLB	C3-C4-C5-C6
3	A	504	OLB	C6-C7-C8-C9
3	A	508	OLB	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
5	A	515	OLC	C3-C4-C5-C6
5	A	513	OLC	C2-C3-C4-C5
3	A	507	OLB	C3-C4-C5-C6
3	A	502	OLB	C11-C12-C13-C14
5	A	516	OLC	C2-C3-C4-C5
5	A	513	OLC	C4-C5-C6-C7
5	A	517	OLC	C11-C12-C13-C14
5	A	510	OLC	C2-C3-C4-C5
3	A	502	OLB	C1-C2-C3-C4
3	A	508	OLB	C2-C3-C4-C5
3	A	503	OLB	C21-C22-C24-O25
5	A	517	OLC	C4-C5-C6-C7
3	A	504	OLB	C4-C5-C6-C7
5	A	517	OLC	C2-C3-C4-C5
3	A	507	OLB	C9-C10-C11-C12
5	A	513	OLC	C9-C10-C11-C12
5	A	517	OLC	O23-C22-C24-O25
3	A	504	OLB	C9-C10-C11-C12
5	A	510	OLC	C7-C8-C9-C10
5	A	515	OLC	C4-C5-C6-C7
3	A	506	OLB	C9-C10-C11-C12
3	A	508	OLB	C9-C10-C11-C12
3	A	502	OLB	C12-C13-C14-C15
5	A	515	OLC	C1-C2-C3-C4
3	A	503	OLB	C2-C3-C4-C5
5	A	514	OLC	C3-C4-C5-C6
3	A	508	OLB	C7-C8-C9-C10
3	A	505	OLB	C4-C5-C6-C7
2	A	501	1PE	C25-C15-OH6-C26
3	A	508	OLB	C11-C12-C13-C14
5	A	517	OLC	C15-C16-C17-C18
3	A	505	OLB	C7-C8-C9-C10
3	A	502	OLB	C10-C11-C12-C13
5	A	513	OLC	C7-C8-C9-C10
3	A	503	OLB	C7-C8-C9-C10
5	A	513	OLC	C6-C7-C8-C9
3	A	506	OLB	C7-C8-C9-C10
5	A	510	OLC	C9-C10-C11-C12
5	A	512	OLC	O20-C1-C2-C3
3	A	507	OLB	C5-C6-C7-C8
3	A	503	OLB	O20-C1-C2-C3
5	A	512	OLC	O19-C1-C2-C3

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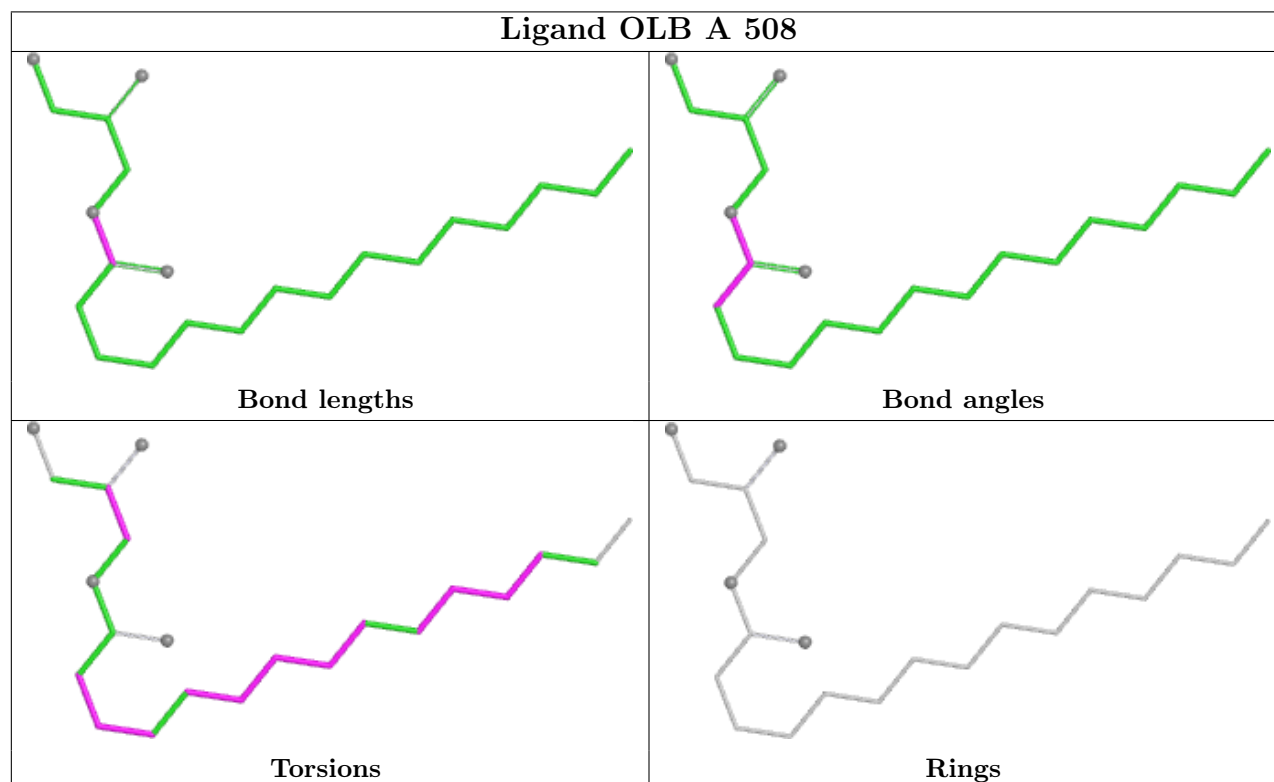
Mol	Chain	Res	Type	Atoms
3	A	507	OLB	C4-C5-C6-C7

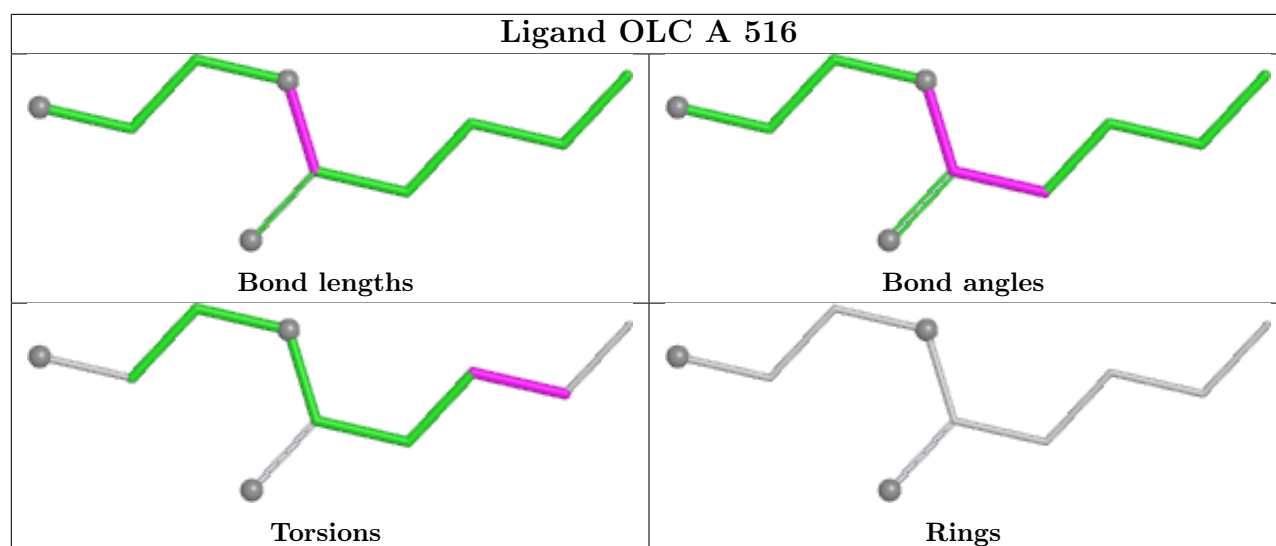
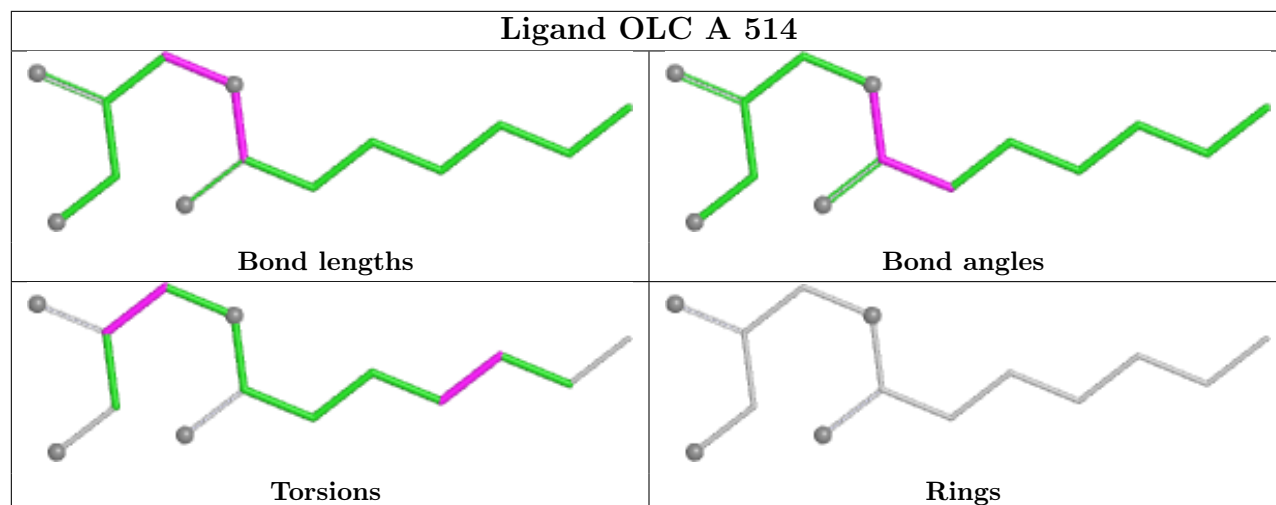
There are no ring outliers.

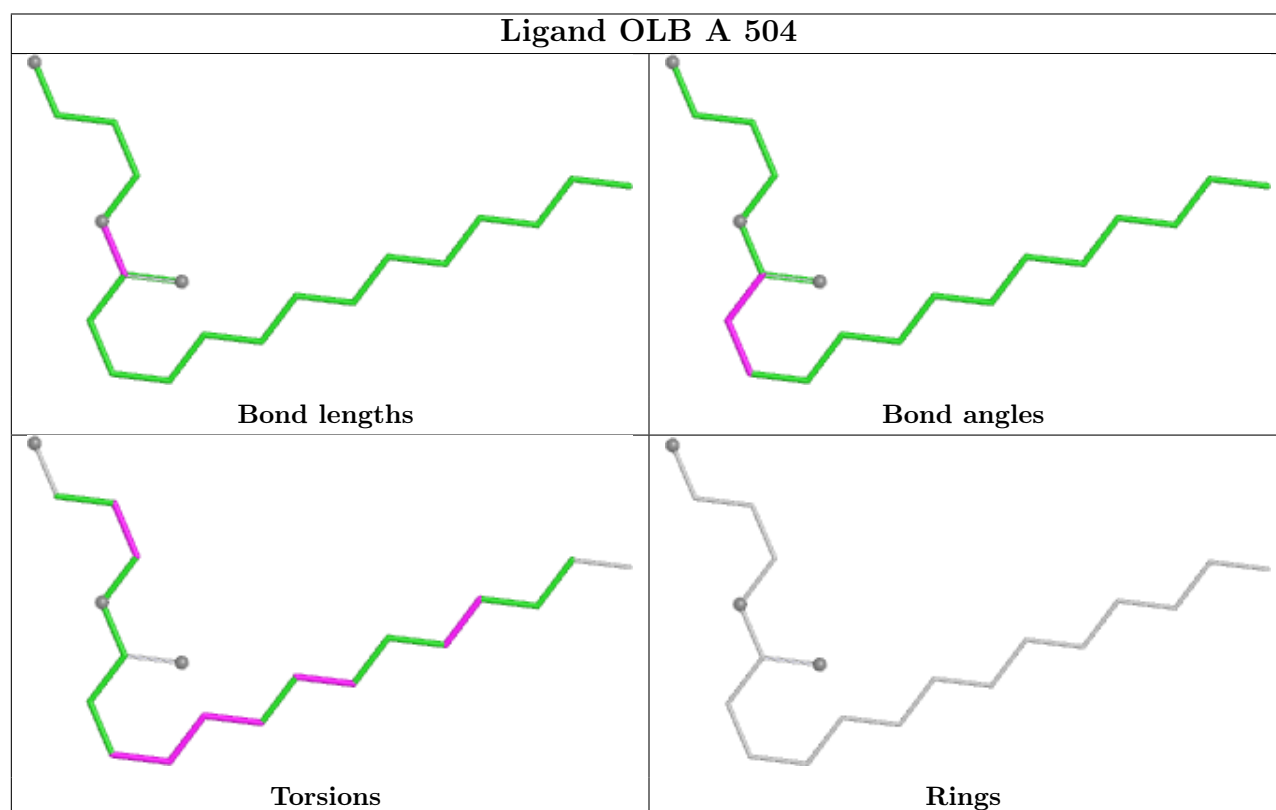
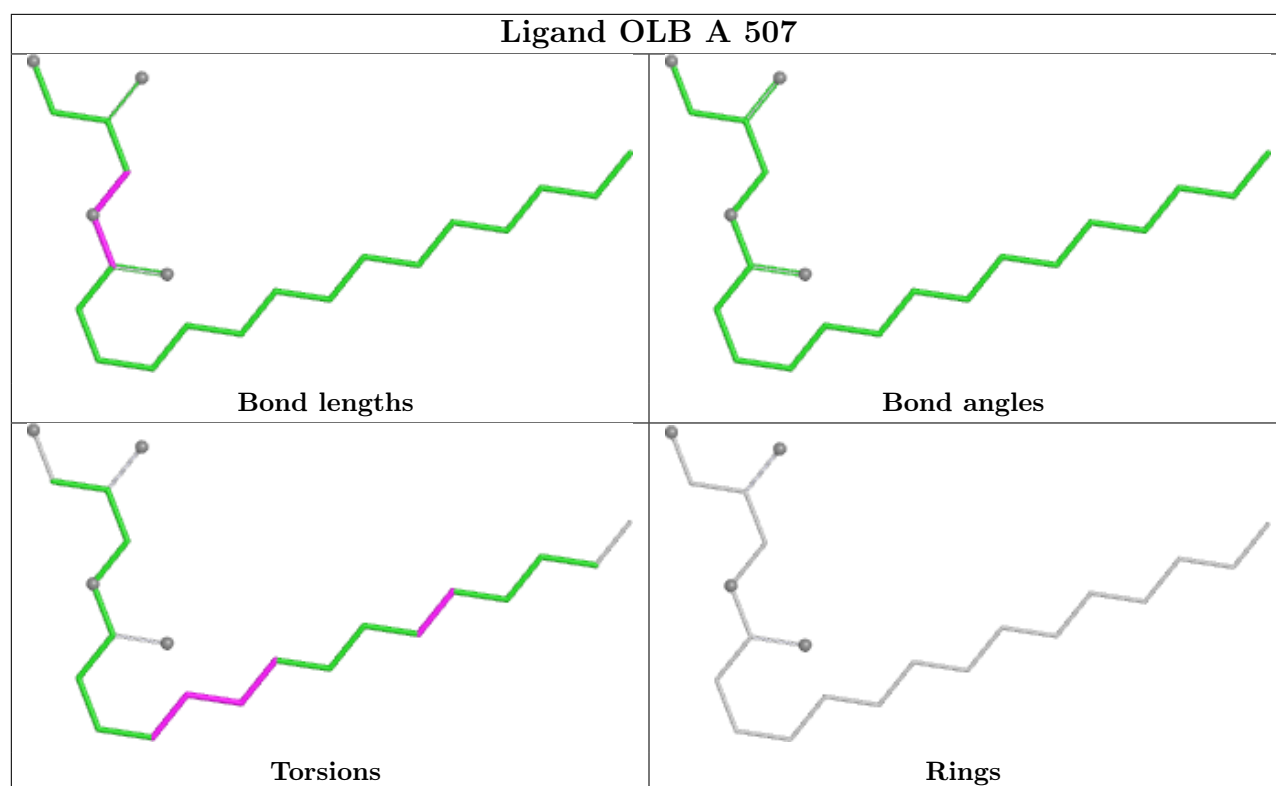
2 monomers are involved in 2 short contacts:

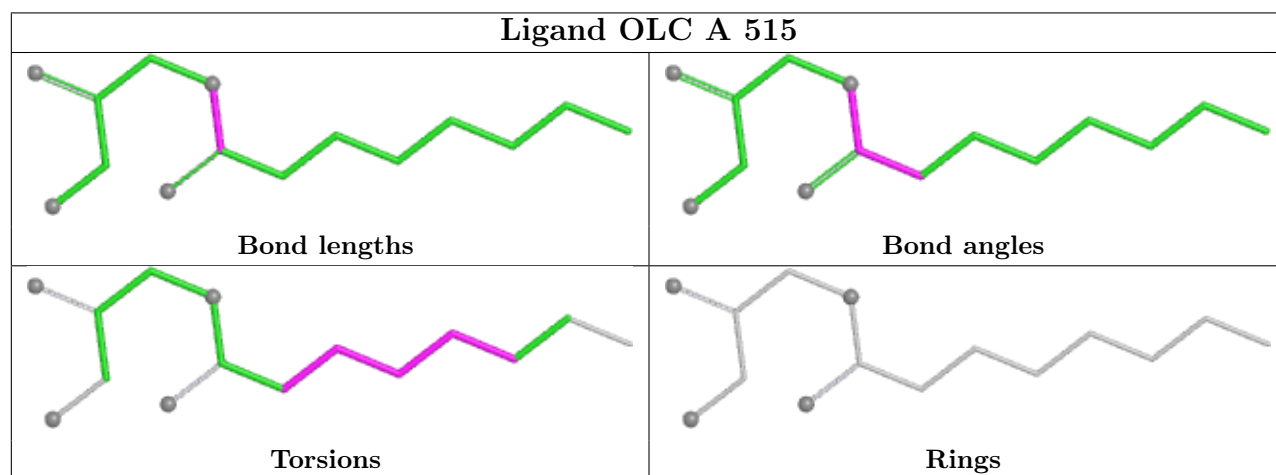
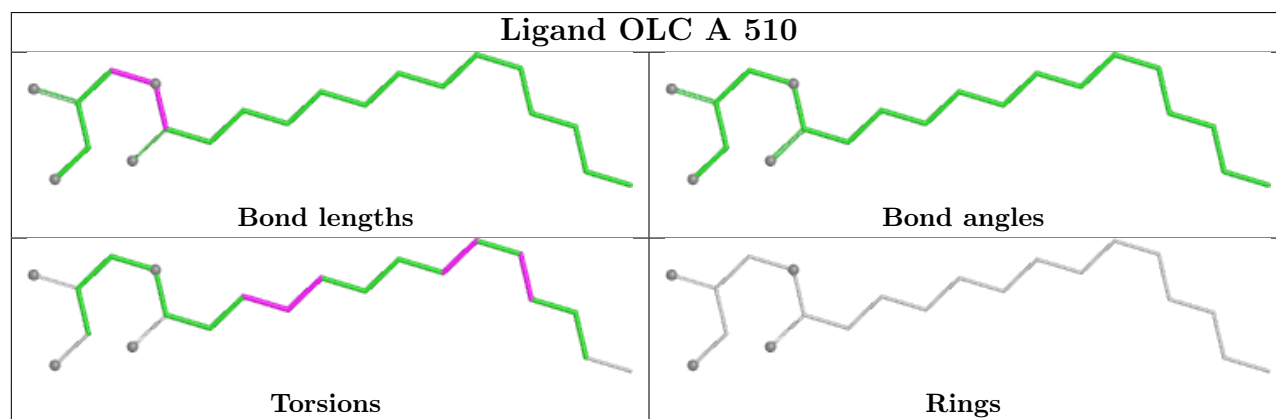
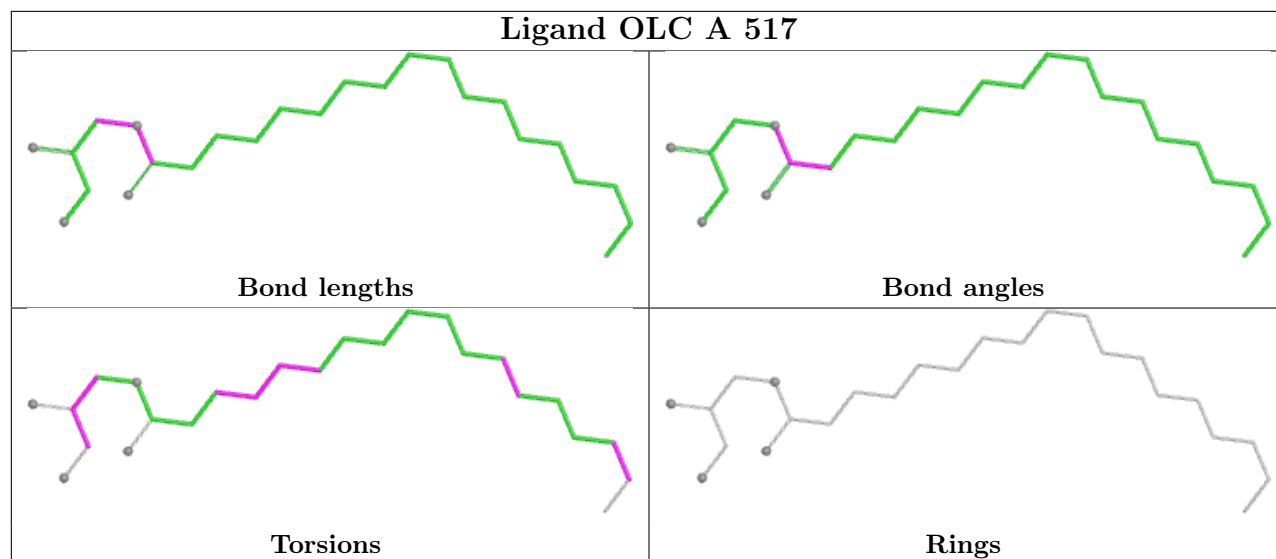
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	OLB	1	0
3	A	503	OLB	1	0

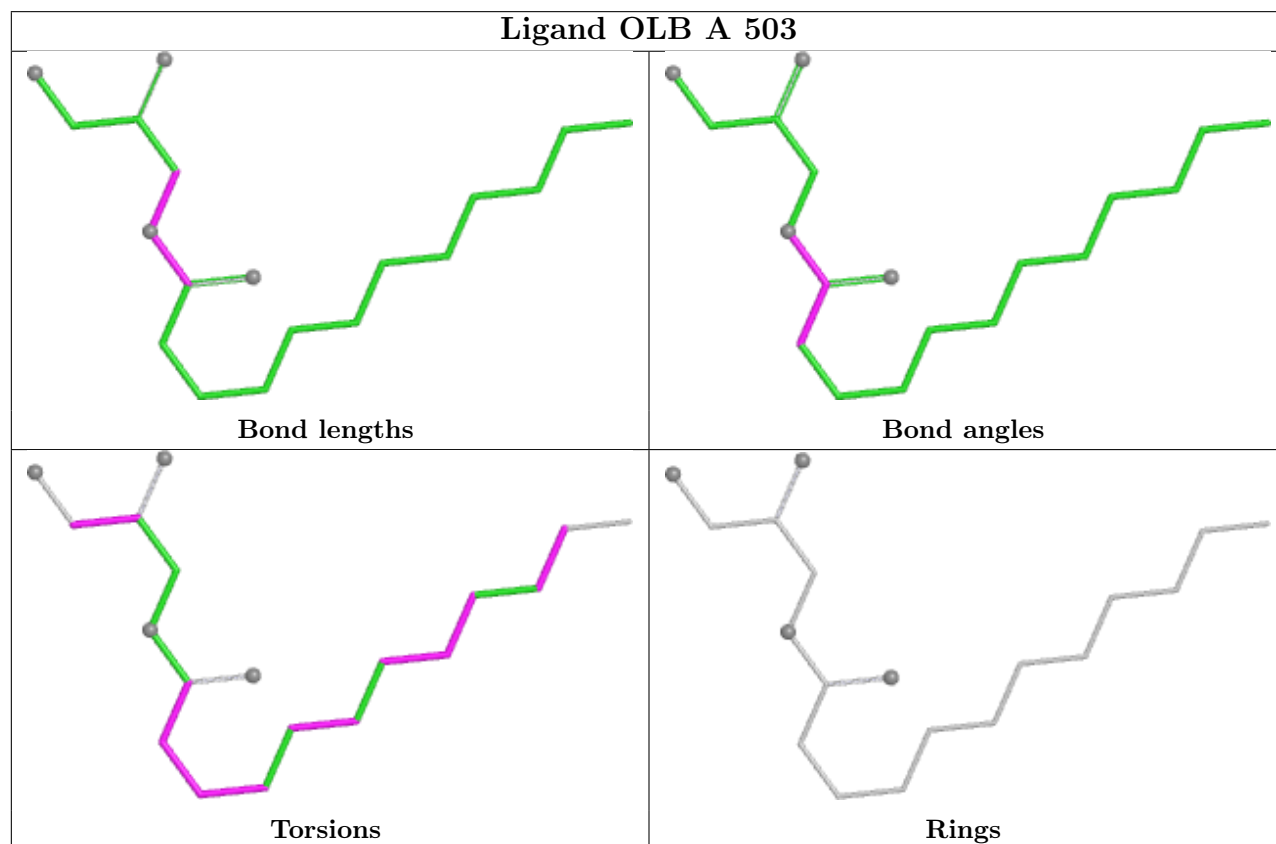
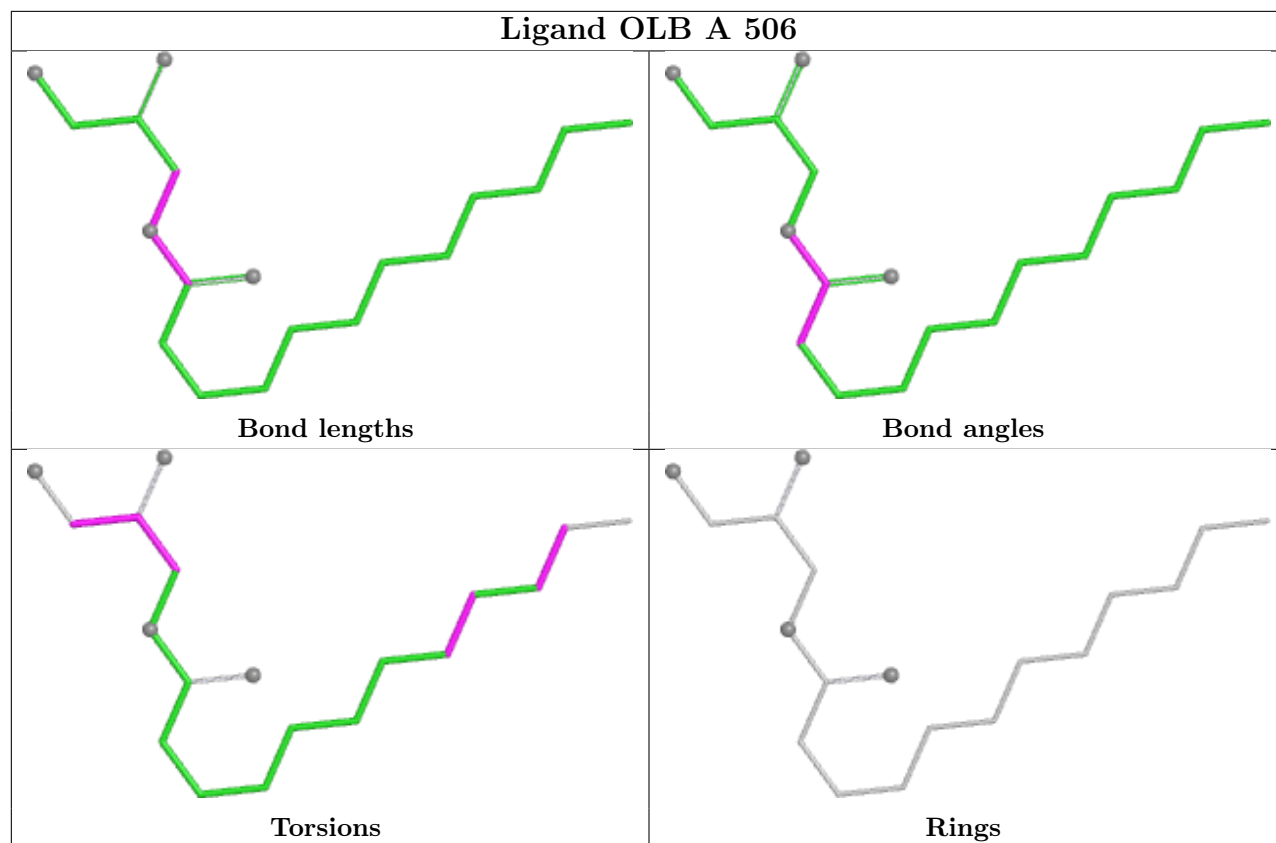
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

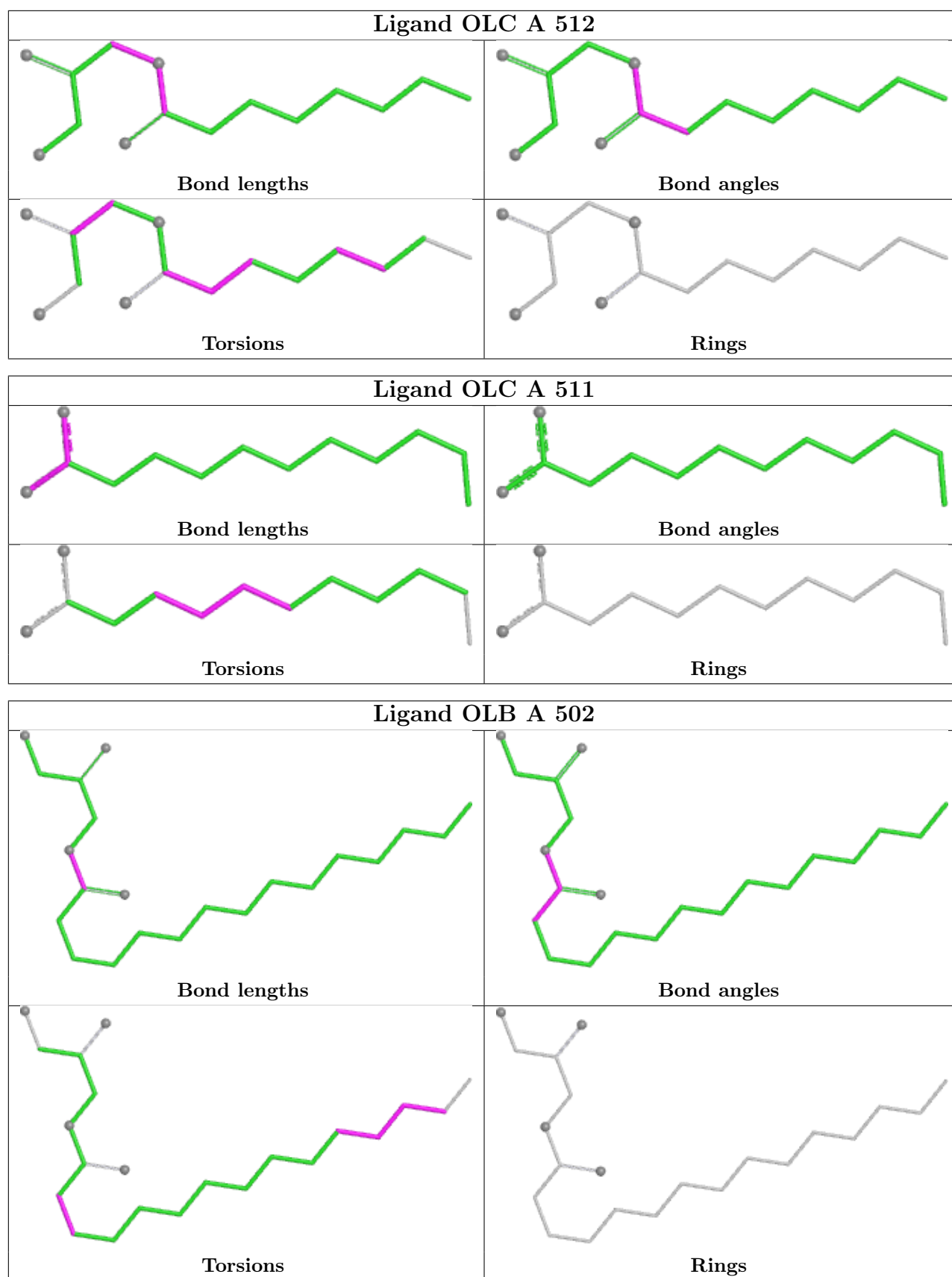


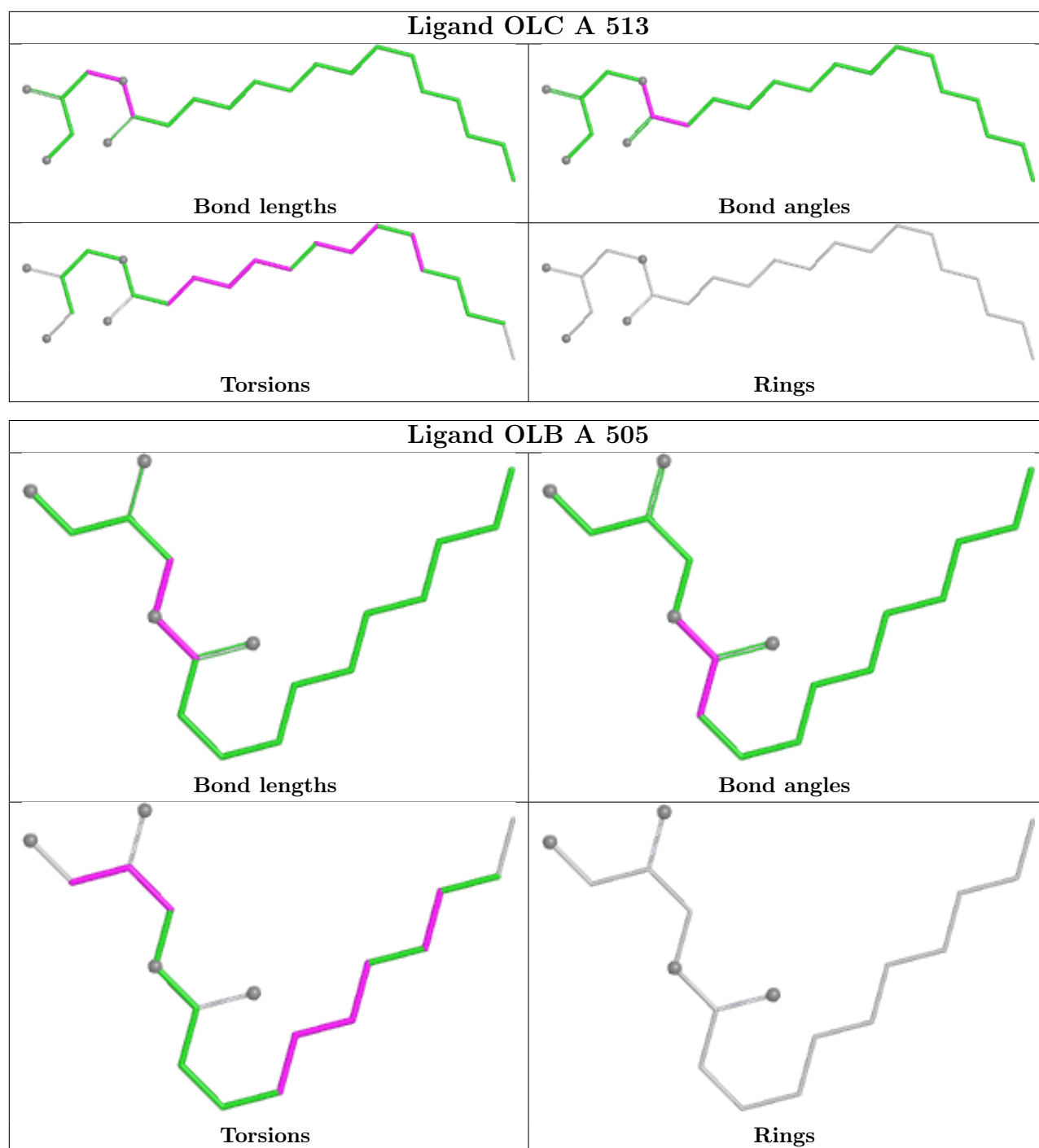












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	475/475 (100%)	-0.09	13 (2%) 56 56	9, 20, 41, 69	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	LYS	6.3
1	A	427	MET	4.8
1	A	34	VAL	3.9
1	A	1	MET	3.8
1	A	108	LEU	3.2
1	A	474	LYS	3.0
1	A	473	ARG	2.9
1	A	247	ILE	2.8
1	A	244	LYS	2.5
1	A	193	PHE	2.3
1	A	471	TYR	2.2
1	A	319	HIS	2.1
1	A	316	PHE	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 ⓘ

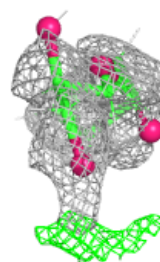
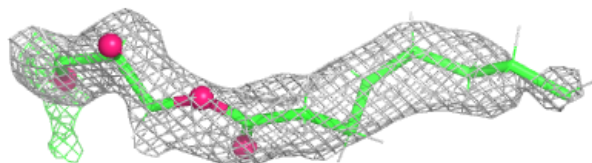
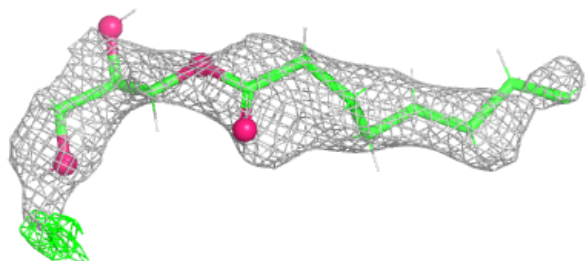
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	OLC	A	515	15/25	0.71	0.21	43,59,71,72	0
5	OLC	A	512	15/25	0.76	0.20	46,56,63,65	0
3	OLB	A	505	18/25	0.76	0.20	47,56,67,68	0
3	OLB	A	503	19/25	0.78	0.20	33,50,61,63	0
5	OLC	A	513	22/25	0.78	0.21	44,54,64,66	0
5	OLC	A	514	14/25	0.78	0.19	49,59,66,67	0
5	OLC	A	511	13/25	0.78	0.19	48,59,66,67	0
3	OLB	A	502	22/25	0.79	0.19	40,53,66,67	0
5	OLC	A	517	25/25	0.80	0.19	45,56,65,66	0
2	1PE	A	501	16/16	0.82	0.14	39,49,71,72	0
5	OLC	A	516	10/25	0.82	0.19	44,53,59,63	0
3	OLB	A	506	19/25	0.82	0.17	35,46,59,62	0
3	OLB	A	504	20/25	0.83	0.17	28,52,65,66	0
5	OLC	A	510	21/25	0.84	0.19	40,53,65,69	0
3	OLB	A	507	22/25	0.86	0.17	33,48,69,69	0
3	OLB	A	508	22/25	0.86	0.17	17,49,59,60	0
4	NA	A	509	1/1	0.99	0.05	17,17,17,17	0

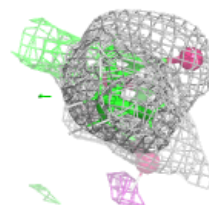
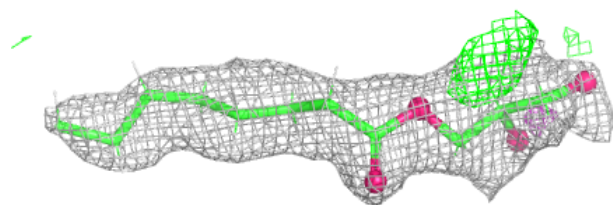
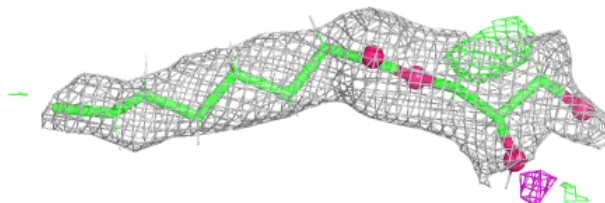
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC 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)

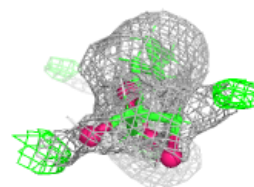
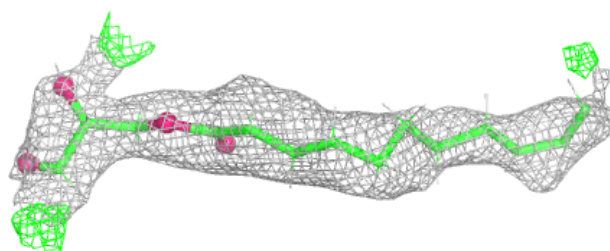
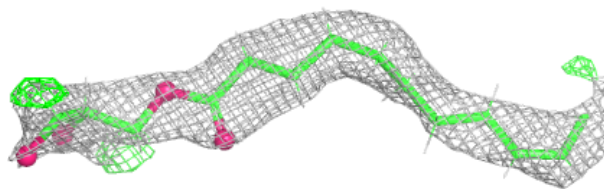
**Electron density around OLC A 512:**

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

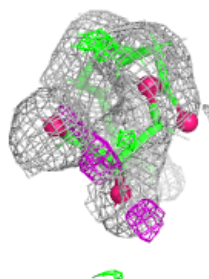
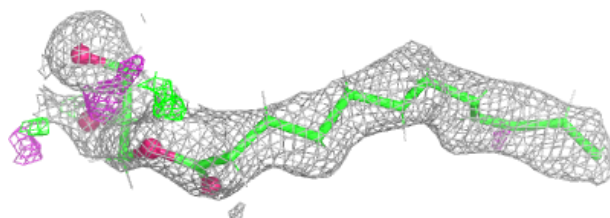
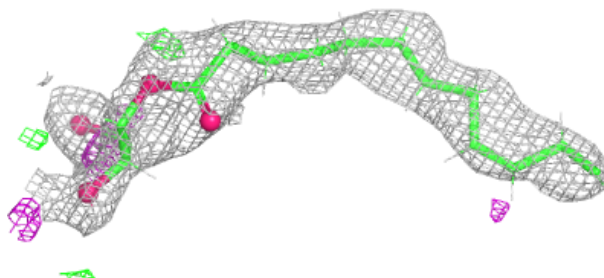


Electron density around OLB A 505:

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

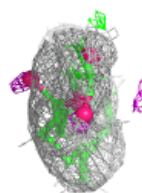
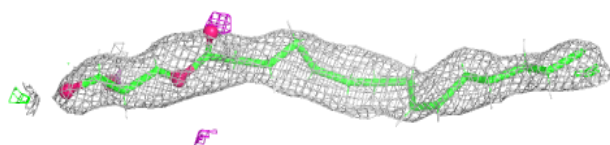
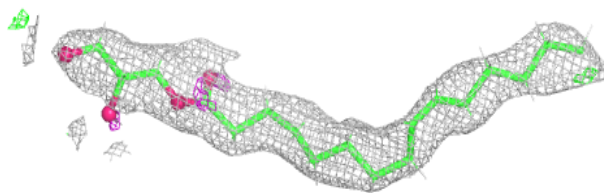
**Electron density around OLB A 503:**

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

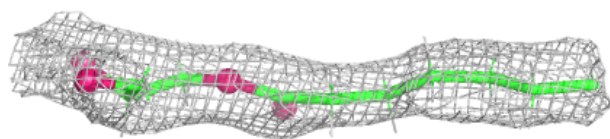


Electron density around OLC A 513:

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

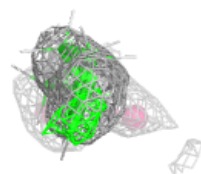
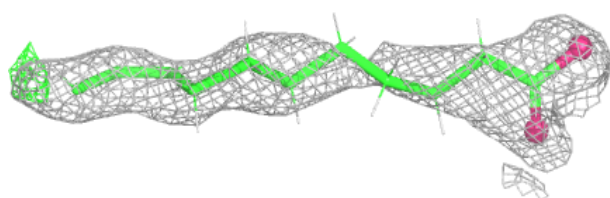
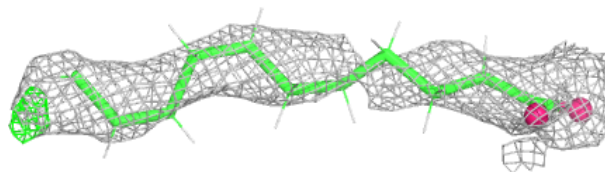
**Electron density around OLC A 514:**

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

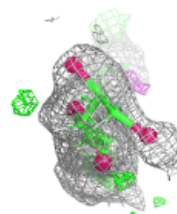
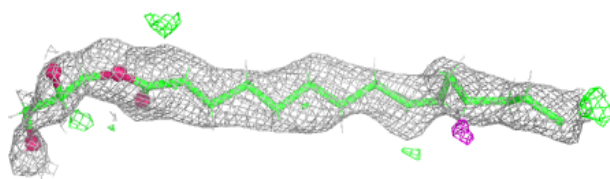
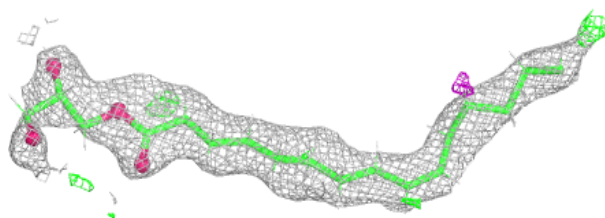


Electron density around OLC A 511:

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

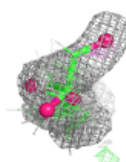
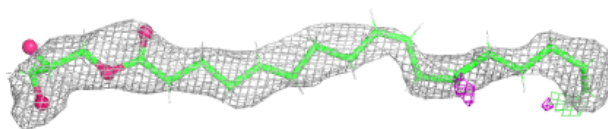
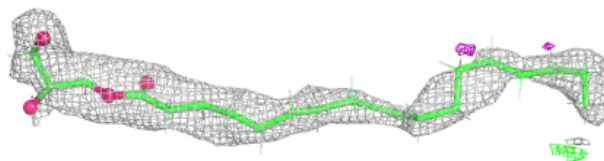
**Electron density around OLB A 502:**

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

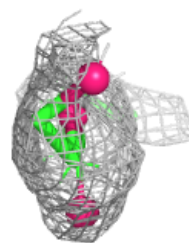
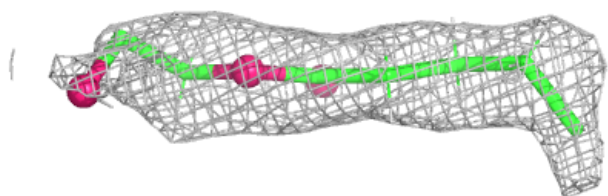
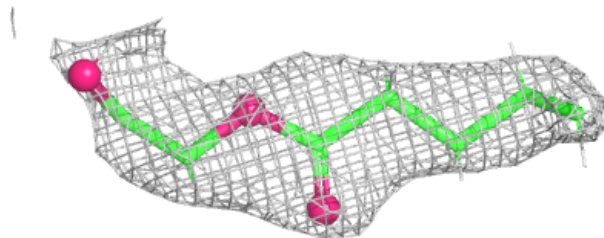


Electron density around OLC A 517:

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

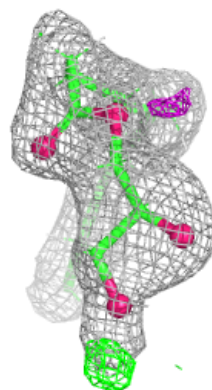
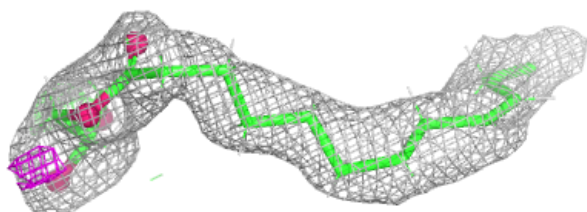
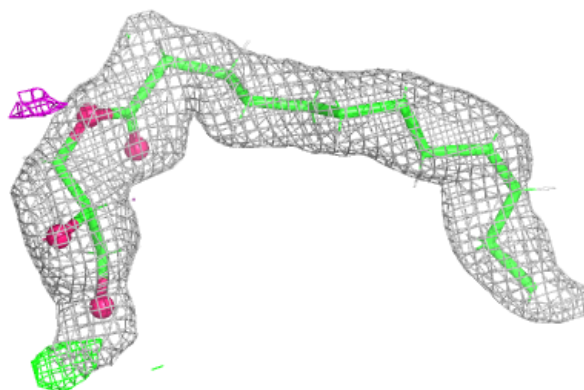
**Electron density around OLC A 516:**

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

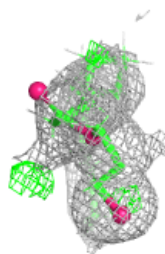
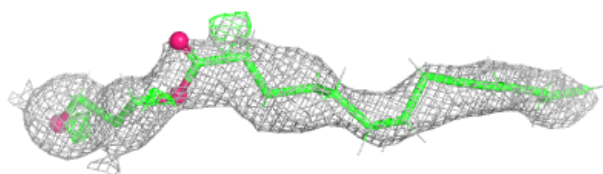
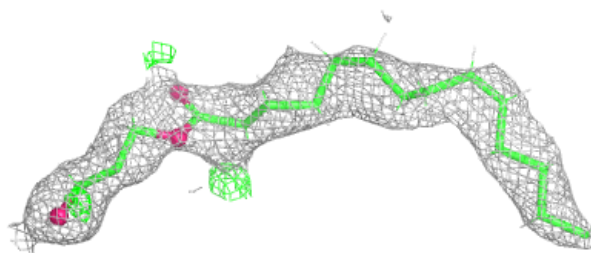


Electron density around OLB A 506:

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

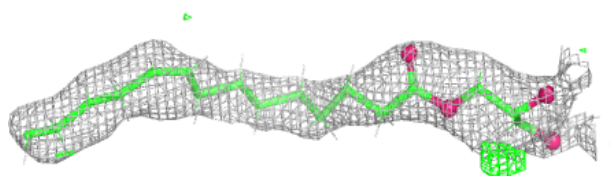
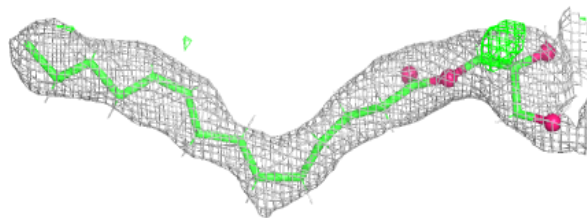
**Electron density around OLB A 504:**

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

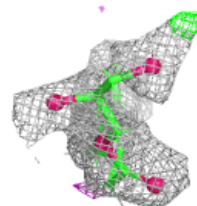
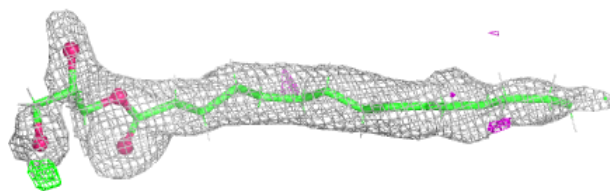
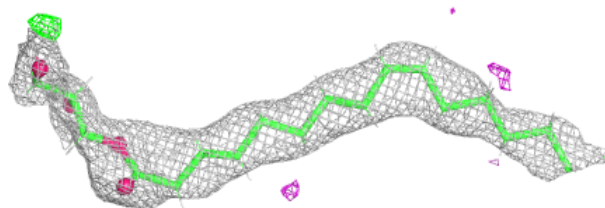


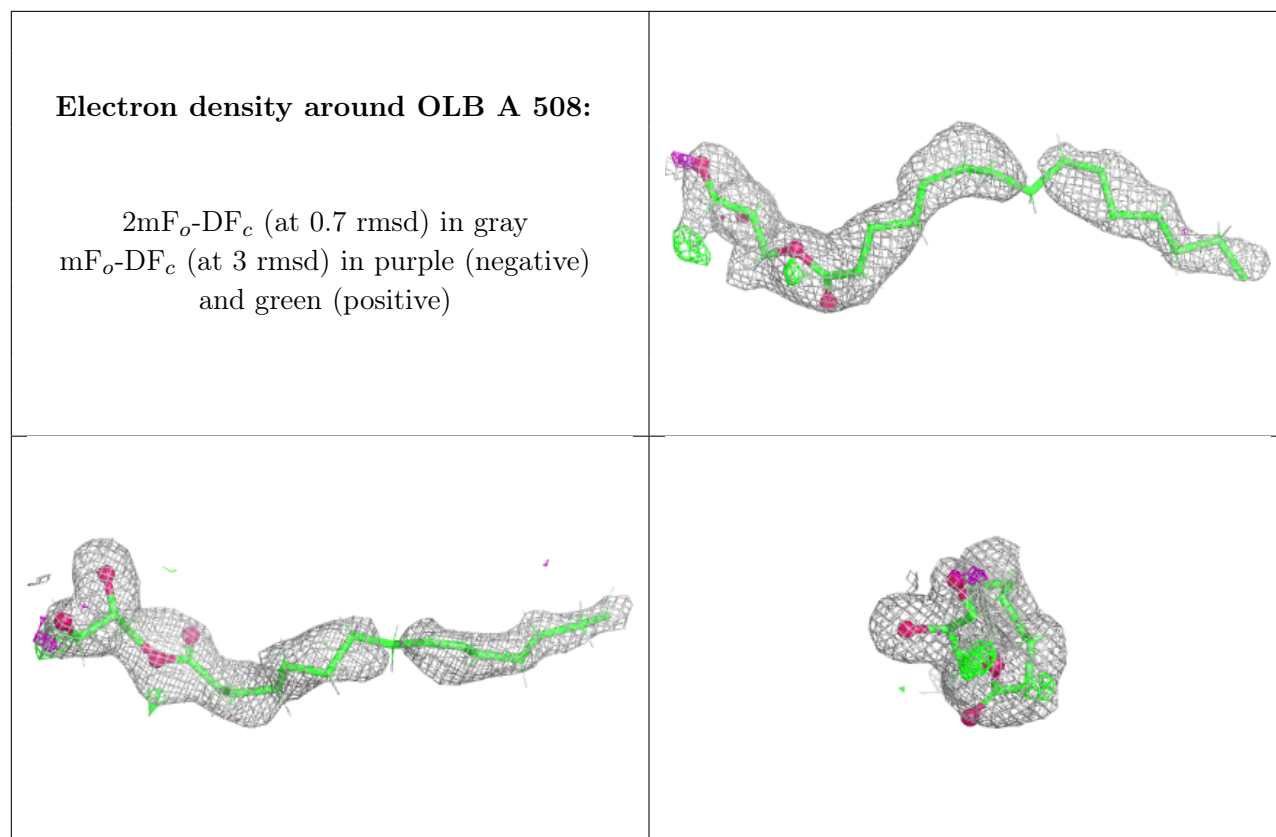
Electron density around OLC A 510:

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

**Electron density around OLB 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.