



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:06 PM UTC

PDB ID : 8E6I / pdb_00008e6i
Title : X-ray structure of the Deinococcus radiodurans Nramp/MntH divalent transition metal transporter M230A mutant in an inward-open, manganese-bound state
Authors : Ray, S.; Gaudet, R.
Deposited on : 2022-08-22
Resolution : 2.52 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

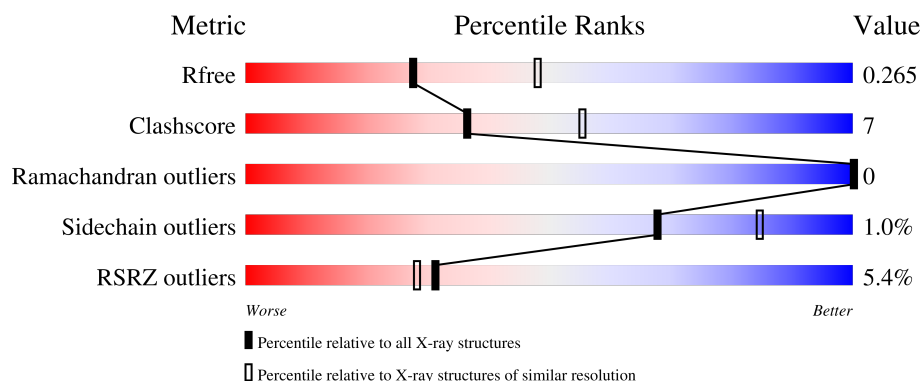
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	414	5% 81% 13% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3451 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 MntH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	2	0
			2934	1935	486	497	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP Q9RTP8
A	24	HIS	-	expression tag	UNP Q9RTP8
A	25	HIS	-	expression tag	UNP Q9RTP8
A	26	HIS	-	expression tag	UNP Q9RTP8
A	27	HIS	-	expression tag	UNP Q9RTP8
A	28	HIS	-	expression tag	UNP Q9RTP8
A	29	HIS	-	expression tag	UNP Q9RTP8
A	30	HIS	-	expression tag	UNP Q9RTP8
A	31	HIS	-	expression tag	UNP Q9RTP8
A	230	ALA	MET	engineered mutation	UNP Q9RTP8

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



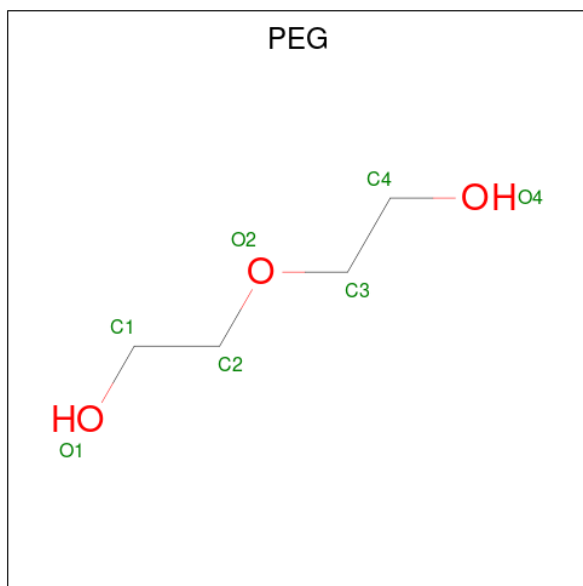
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	18	4		
4	A	1	Total	C	O	0	0
			22	18	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C		0	0
			18	18			
4	A	1	Total	C	O	0	0
			18	14	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C		0	0
			17	17			
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C	O	0	0
			16	12	4		
4	A	1	Total	C	O	0	0
			25	21	4		
4	A	1	Total	C		0	0
			14	14			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 17 17	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 23 19 4	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C O 12 8 4	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 3 1	0	0

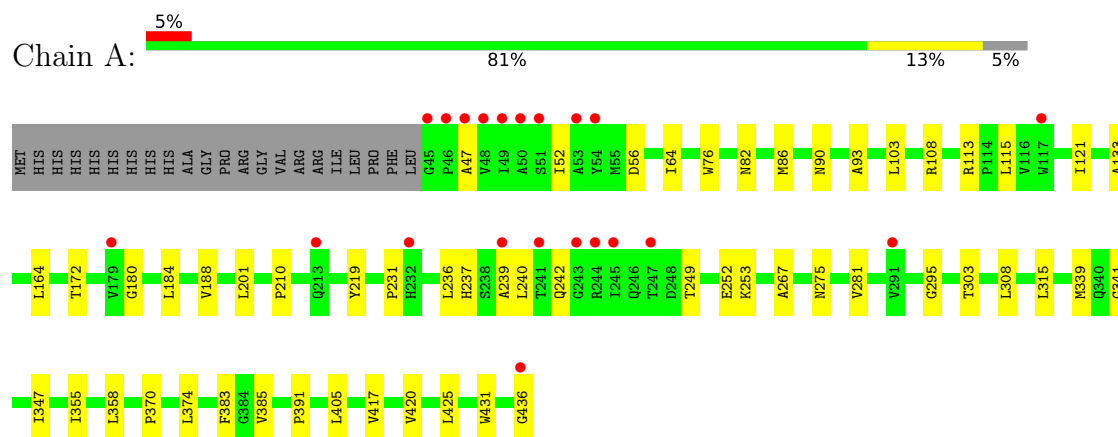
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	69	Total	O	0	0
			69	69		

3 Residue-property plots

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: Divalent metal cation transporter MntH



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	58.67Å 71.35Å 98.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.32 – 2.52 45.32 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.32-2.52) 99.9 (45.32-2.52)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.266 0.224 , 0.265	Depositor DCC
R_{free} test set	1455 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3451	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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: CL, OLC, PEG, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.09	0/3003	0.22	0/4111

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	2934	0	3058	36	0
2	A	2	0	0	0	0
3	A	2	0	0	1	0
4	A	440	0	692	27	0
5	A	4	0	2	0	0
6	A	69	0	0	3	0
All	All	3451	0	3752	51	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 7.

All (51) 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:115:LEU:HD21	4:A:527:OLC:H2A	1.66	0.78
1:A:253:LYS:HB3	1:A:405:LEU:HD11	1.76	0.67
3:A:504:CL:CL	6:A:609:HOH:O	2.50	0.67
4:A:505:OLC:H14A	4:A:506:OLC:H11A	1.78	0.66
1:A:355:ILE:HG12	4:A:517:OLC:H18B	1.80	0.63
4:A:514:OLC:H15	4:A:515:OLC:H18	1.86	0.57
1:A:86:MET:O	1:A:90:ASN:ND2	2.30	0.57
1:A:47:ALA:HA	1:A:267:ALA:HB2	1.87	0.56
1:A:275:ASN:ND2	6:A:607:HOH:O	2.38	0.56
1:A:133:ALA:HA	1:A:374:LEU:HD22	1.88	0.55
1:A:237:HIS:HA	1:A:240:LEU:HD12	1.88	0.55
1:A:52:ILE:HG21	1:A:180:GLY:HA2	1.90	0.53
4:A:507:OLC:H14A	4:A:526:OLC:H13A	1.92	0.52
1:A:164:LEU:HD21	4:A:524:OLC:H15A	1.90	0.52
1:A:188:VAL:HG13	4:A:511:OLC:H8A	1.92	0.51
1:A:383:PHE:HD2	4:A:510:OLC:H18A	1.75	0.51
1:A:358:LEU:HD11	4:A:517:OLC:H18	1.91	0.51
1:A:52:ILE:HD11	1:A:184:LEU:HB2	1.93	0.51
1:A:108:ARG:NH1	1:A:341:GLY:O	2.42	0.50
1:A:420:VAL:HG11	4:A:521:OLC:H13	1.95	0.48
1:A:219:TYR:CG	4:A:514:OLC:H22	2.48	0.48
1:A:239:ALA:O	1:A:242:GLN:HG2	2.14	0.48
4:A:510:OLC:H18B	4:A:510:OLC:H15A	1.68	0.47
1:A:370:PRO:O	1:A:374:LEU:HG	2.15	0.47
4:A:510:OLC:H8A	4:A:510:OLC:H11	1.63	0.46
4:A:514:OLC:H12	4:A:514:OLC:H15A	1.65	0.46
1:A:103:LEU:HD11	1:A:391:PRO:HB2	1.98	0.46
4:A:512:OLC:H10	4:A:512:OLC:H13A	1.78	0.45
4:A:513:OLC:H8A	4:A:513:OLC:H11A	1.68	0.45
1:A:210:PRO:HD2	4:A:513:OLC:H21	1.97	0.45
1:A:308:LEU:HD13	1:A:315:LEU:HD12	1.99	0.45
1:A:249:THR:HG23	1:A:252:GLU:H	1.82	0.45
1:A:417:VAL:HG11	4:A:519:OLC:H13A	2.00	0.44
1:A:93:ALA:HB2	1:A:237:HIS:CE1	2.52	0.44
1:A:281:VAL:HG12	1:A:303:THR:HB	2.00	0.44
1:A:231:PRO:HG3	1:A:385:VAL:HG22	2.00	0.44
1:A:431:TRP:CE2	1:A:436:GLY:HA3	2.53	0.43
4:A:515:OLC:H14	4:A:515:OLC:H11	1.88	0.43
4:A:519:OLC:H10	4:A:519:OLC:H7A	1.70	0.42
1:A:113:ARG:NH2	6:A:614:HOH:O	2.52	0.42
4:A:506:OLC:H5A	4:A:506:OLC:H8	1.64	0.42
1:A:172:THR:HB	4:A:524:OLC:H14A	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:MET:HE1	1:A:347:ILE:HG23	2.00	0.41
4:A:519:OLC:H18A	4:A:519:OLC:H15A	1.82	0.41
1:A:236:LEU:O	1:A:239:ALA:N	2.51	0.41
1:A:76:TRP:CE2	1:A:210:PRO:HA	2.55	0.41
1:A:201:LEU:HD22	4:A:506:OLC:H9	2.02	0.41
4:A:522:OLC:H9	4:A:522:OLC:H6	1.79	0.41
1:A:121:ILE:HD12	4:A:515:OLC:H10	2.03	0.41
1:A:64:ILE:HG22	1:A:295:GLY:HA2	2.03	0.40
4:A:522:OLC:H2A	4:A:522:OLC:H21A	1.78	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	392/414 (95%)	385 (98%)	7 (2%)	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	298/321 (93%)	295 (99%)	3 (1%)	68	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	82	ASN
1	A	425	LEU

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	82	ASN
1	A	232	HIS
1	A	237	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\# Z > 2$
4	OLC	A	512	-	24,24,24	0.82	1 (4%)	25,25,25	1.02	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLC	A	506	-	21,21,24	0.87	2 (9%)	22,22,25	0.95	1 (4%)
4	OLC	A	514	-	24,24,24	0.82	2 (8%)	25,25,25	0.94	1 (4%)
4	OLC	A	522	-	24,24,24	0.80	2 (8%)	25,25,25	0.98	1 (4%)
4	OLC	A	527	-	11,11,24	1.16	2 (18%)	12,12,25	1.21	1 (8%)
4	OLC	A	505	-	21,21,24	0.87	2 (9%)	22,22,25	1.02	1 (4%)
4	OLC	A	519	-	16,16,24	0.33	0	15,15,25	0.77	0
4	OLC	A	507	-	24,24,24	0.82	2 (8%)	25,25,25	0.93	1 (4%)
4	OLC	A	517	-	24,24,24	0.81	2 (8%)	25,25,25	0.97	1 (4%)
5	PEG	A	528	-	3,3,6	0.30	0	2,2,5	0.12	0
4	OLC	A	523	-	7,7,24	0.33	0	6,6,25	0.65	0
4	OLC	A	510	-	24,24,24	0.82	2 (8%)	25,25,25	0.99	1 (4%)
4	OLC	A	515	-	24,24,24	0.80	2 (8%)	25,25,25	0.97	1 (4%)
4	OLC	A	526	-	10,10,24	0.41	0	9,9,25	0.92	0
4	OLC	A	520	-	24,24,24	0.81	2 (8%)	25,25,25	0.95	1 (4%)
4	OLC	A	508	-	17,17,24	0.32	0	16,16,25	0.81	0
4	OLC	A	513	-	24,24,24	0.81	2 (8%)	25,25,25	0.90	1 (4%)
4	OLC	A	511	-	16,16,24	0.33	0	15,15,25	0.77	0
4	OLC	A	521	-	22,22,24	0.85	2 (9%)	23,23,25	0.99	1 (4%)
4	OLC	A	509	-	17,17,24	0.97	2 (11%)	18,18,25	1.14	1 (5%)
4	OLC	A	524	-	8,8,24	0.30	0	7,7,25	0.78	0
4	OLC	A	525	-	7,7,24	0.31	0	6,6,25	0.71	0
4	OLC	A	516	-	15,15,24	1.00	2 (13%)	16,16,25	1.06	1 (6%)
4	OLC	A	518	-	13,13,24	0.35	0	12,12,25	0.75	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
4	OLC	A	512	-	-	11/24/24/24	-
4	OLC	A	506	-	-	10/21/21/24	-
4	OLC	A	514	-	-	14/24/24/24	-
4	OLC	A	522	-	-	10/24/24/24	-
4	OLC	A	527	-	-	6/11/11/24	-
4	OLC	A	505	-	-	12/21/21/24	-
4	OLC	A	519	-	-	4/14/14/24	-
4	OLC	A	507	-	-	13/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLC	A	517	-	-	12/24/24/24	-
5	PEG	A	528	-	-	0/0/1/4	-
4	OLC	A	523	-	-	3/5/5/24	-
4	OLC	A	510	-	-	14/24/24/24	-
4	OLC	A	515	-	-	8/24/24/24	-
4	OLC	A	526	-	-	4/8/8/24	-
4	OLC	A	520	-	-	13/24/24/24	-
4	OLC	A	508	-	-	8/15/15/24	-
4	OLC	A	513	-	-	14/24/24/24	-
4	OLC	A	511	-	-	7/14/14/24	-
4	OLC	A	521	-	-	16/22/22/24	-
4	OLC	A	509	-	-	10/17/17/24	-
4	OLC	A	524	-	-	4/6/6/24	-
4	OLC	A	525	-	-	3/5/5/24	-
4	OLC	A	516	-	-	11/15/15/24	-
4	OLC	A	518	-	-	7/11/11/24	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	512	OLC	O20-C1	2.56	1.40	1.33
4	A	507	OLC	O20-C1	2.48	1.40	1.33
4	A	509	OLC	O20-C1	2.47	1.40	1.33
4	A	505	OLC	O20-C1	2.47	1.40	1.33
4	A	515	OLC	O20-C1	2.44	1.40	1.33
4	A	527	OLC	O20-C1	2.44	1.40	1.33
4	A	510	OLC	O20-C1	2.44	1.40	1.33
4	A	521	OLC	O20-C1	2.43	1.40	1.33
4	A	516	OLC	O20-C1	2.43	1.40	1.33
4	A	514	OLC	O20-C1	2.43	1.40	1.33
4	A	522	OLC	O20-C1	2.42	1.40	1.33
4	A	506	OLC	O20-C1	2.41	1.40	1.33
4	A	517	OLC	O20-C1	2.40	1.40	1.33
4	A	520	OLC	O20-C1	2.40	1.40	1.33
4	A	513	OLC	O20-C1	2.39	1.40	1.33
4	A	521	OLC	O20-C21	-2.20	1.40	1.45
4	A	527	OLC	O20-C21	-2.19	1.40	1.45
4	A	516	OLC	O20-C21	-2.18	1.40	1.45
4	A	510	OLC	O20-C21	-2.15	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	506	OLC	O20-C21	-2.15	1.40	1.45
4	A	507	OLC	O20-C21	-2.15	1.40	1.45
4	A	517	OLC	O20-C21	-2.15	1.40	1.45
4	A	513	OLC	O20-C21	-2.14	1.40	1.45
4	A	520	OLC	O20-C21	-2.13	1.40	1.45
4	A	514	OLC	O20-C21	-2.13	1.40	1.45
4	A	505	OLC	O20-C21	-2.11	1.40	1.45
4	A	522	OLC	O20-C21	-2.09	1.40	1.45
4	A	509	OLC	O20-C21	-2.08	1.40	1.45
4	A	515	OLC	O20-C21	-2.07	1.40	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	527	OLC	O20-C1-C2	2.96	120.87	111.83
4	A	512	OLC	O20-C1-C2	2.95	120.83	111.83
4	A	509	OLC	O20-C1-C2	2.94	120.81	111.83
4	A	510	OLC	O20-C1-C2	2.83	120.47	111.83
4	A	505	OLC	O20-C1-C2	2.82	120.42	111.83
4	A	521	OLC	O20-C1-C2	2.80	120.37	111.83
4	A	516	OLC	O20-C1-C2	2.74	120.19	111.83
4	A	515	OLC	O20-C1-C2	2.73	120.15	111.83
4	A	514	OLC	O20-C1-C2	2.68	120.01	111.83
4	A	507	OLC	O20-C1-C2	2.66	119.95	111.83
4	A	517	OLC	O20-C1-C2	2.59	119.73	111.83
4	A	506	OLC	O20-C1-C2	2.59	119.73	111.83
4	A	522	OLC	O20-C1-C2	2.59	119.72	111.83
4	A	513	OLC	O20-C1-C2	2.57	119.68	111.83
4	A	520	OLC	O20-C1-C2	2.49	119.44	111.83

There are no chirality outliers.

All (214) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	507	OLC	C21-C22-C24-O25
4	A	509	OLC	C21-C22-C24-O25
4	A	509	OLC	O23-C22-C24-O25
4	A	509	OLC	O20-C21-C22-C24
4	A	509	OLC	O20-C21-C22-O23
4	A	510	OLC	C21-C22-C24-O25
4	A	510	OLC	O23-C22-C24-O25
4	A	515	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
4	A	515	OLC	O19-C1-O20-C21
4	A	516	OLC	C21-C22-C24-O25
4	A	516	OLC	O20-C21-C22-C24
4	A	516	OLC	O20-C21-C22-O23
4	A	517	OLC	O20-C21-C22-O23
4	A	520	OLC	O20-C21-C22-C24
4	A	520	OLC	O20-C21-C22-O23
4	A	522	OLC	C2-C1-O20-C21
4	A	522	OLC	O19-C1-O20-C21
4	A	516	OLC	O19-C1-O20-C21
4	A	520	OLC	O19-C1-O20-C21
4	A	520	OLC	C2-C1-O20-C21
4	A	516	OLC	C2-C1-O20-C21
4	A	506	OLC	C2-C1-O20-C21
4	A	513	OLC	C2-C1-O20-C21
4	A	513	OLC	O20-C21-C22-O23
4	A	506	OLC	O19-C1-O20-C21
4	A	513	OLC	O19-C1-O20-C21
4	A	514	OLC	C12-C13-C14-C15
4	A	507	OLC	C2-C1-O20-C21
4	A	517	OLC	C2-C1-O20-C21
4	A	521	OLC	C2-C1-O20-C21
4	A	527	OLC	C2-C1-O20-C21
4	A	506	OLC	O20-C21-C22-C24
4	A	517	OLC	O20-C21-C22-C24
4	A	522	OLC	O20-C21-C22-C24
4	A	522	OLC	O20-C21-C22-O23
4	A	527	OLC	C1-C2-C3-C4
4	A	517	OLC	O19-C1-O20-C21
4	A	521	OLC	O19-C1-O20-C21
4	A	527	OLC	O19-C1-O20-C21
4	A	507	OLC	C1-C2-C3-C4
4	A	523	OLC	C4-C5-C6-C7
4	A	509	OLC	C1-C2-C3-C4
4	A	510	OLC	C1-C2-C3-C4
4	A	515	OLC	C1-C2-C3-C4
4	A	517	OLC	C1-C2-C3-C4
4	A	510	OLC	C2-C1-O20-C21
4	A	507	OLC	O19-C1-O20-C21
4	A	506	OLC	O20-C21-C22-O23
4	A	520	OLC	C21-C22-C24-O25
4	A	521	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
4	A	509	OLC	C3-C4-C5-C6
4	A	513	OLC	C13-C14-C15-C16
4	A	517	OLC	C13-C14-C15-C16
4	A	524	OLC	C12-C13-C14-C15
4	A	510	OLC	O19-C1-O20-C21
4	A	507	OLC	O23-C22-C24-O25
4	A	516	OLC	O23-C22-C24-O25
4	A	521	OLC	O23-C22-C24-O25
4	A	511	OLC	C4-C5-C6-C7
4	A	514	OLC	C13-C14-C15-C16
4	A	515	OLC	C4-C5-C6-C7
4	A	526	OLC	C11-C12-C13-C14
4	A	507	OLC	C4-C5-C6-C7
4	A	510	OLC	C3-C4-C5-C6
4	A	519	OLC	C6-C7-C8-C9
4	A	506	OLC	C3-C4-C5-C6
4	A	519	OLC	C13-C14-C15-C16
4	A	515	OLC	C2-C3-C4-C5
4	A	517	OLC	C11-C12-C13-C14
4	A	516	OLC	C4-C5-C6-C7
4	A	521	OLC	C11-C12-C13-C14
4	A	512	OLC	C13-C14-C15-C16
4	A	508	OLC	C14-C15-C16-C17
4	A	512	OLC	C14-C15-C16-C17
4	A	523	OLC	C5-C6-C7-C8
4	A	512	OLC	C12-C13-C14-C15
4	A	521	OLC	C12-C13-C14-C15
4	A	505	OLC	C4-C5-C6-C7
4	A	505	OLC	C1-C2-C3-C4
4	A	524	OLC	C13-C14-C15-C16
4	A	513	OLC	C14-C15-C16-C17
4	A	521	OLC	C2-C3-C4-C5
4	A	510	OLC	C6-C7-C8-C9
4	A	512	OLC	C6-C7-C8-C9
4	A	526	OLC	C10-C11-C12-C13
4	A	512	OLC	C5-C6-C7-C8
4	A	505	OLC	C2-C3-C4-C5
4	A	507	OLC	C3-C4-C5-C6
4	A	513	OLC	C2-C3-C4-C5
4	A	514	OLC	C1-C2-C3-C4
4	A	520	OLC	C10-C11-C12-C13
4	A	513	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
4	A	518	OLC	C14-C15-C16-C17
4	A	516	OLC	C2-C3-C4-C5
4	A	522	OLC	C12-C13-C14-C15
4	A	525	OLC	C10-C11-C12-C13
4	A	513	OLC	C11-C12-C13-C14
4	A	505	OLC	C11-C12-C13-C14
4	A	506	OLC	C4-C5-C6-C7
4	A	520	OLC	O23-C22-C24-O25
4	A	507	OLC	C12-C13-C14-C15
4	A	505	OLC	C10-C11-C12-C13
4	A	509	OLC	C6-C7-C8-C9
4	A	518	OLC	C10-C11-C12-C13
4	A	512	OLC	C2-C3-C4-C5
4	A	515	OLC	C14-C15-C16-C17
4	A	510	OLC	C13-C14-C15-C16
4	A	514	OLC	C14-C15-C16-C17
4	A	517	OLC	C15-C16-C17-C18
4	A	525	OLC	C13-C14-C15-C16
4	A	514	OLC	C10-C11-C12-C13
4	A	521	OLC	C6-C7-C8-C9
4	A	508	OLC	C3-C4-C5-C6
4	A	521	OLC	C5-C6-C7-C8
4	A	509	OLC	C2-C1-O20-C21
4	A	507	OLC	C5-C6-C7-C8
4	A	520	OLC	C13-C14-C15-C16
4	A	524	OLC	C11-C12-C13-C14
4	A	506	OLC	C10-C11-C12-C13
4	A	521	OLC	C10-C11-C12-C13
4	A	522	OLC	C11-C12-C13-C14
4	A	507	OLC	C13-C14-C15-C16
4	A	513	OLC	C3-C4-C5-C6
4	A	519	OLC	C9-C10-C11-C12
4	A	517	OLC	C2-C3-C4-C5
4	A	525	OLC	C11-C12-C13-C14
4	A	508	OLC	C4-C5-C6-C7
4	A	510	OLC	C2-C3-C4-C5
4	A	514	OLC	C15-C16-C17-C18
4	A	521	OLC	C13-C14-C15-C16
4	A	512	OLC	C7-C8-C9-C10
4	A	518	OLC	C15-C16-C17-C18
4	A	509	OLC	O19-C1-O20-C21
4	A	507	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	A	505	OLC	C5-C6-C7-C8
4	A	510	OLC	C14-C15-C16-C17
4	A	511	OLC	C3-C4-C5-C6
4	A	520	OLC	C15-C16-C17-C18
4	A	507	OLC	C6-C7-C8-C9
4	A	511	OLC	C5-C6-C7-C8
4	A	516	OLC	C5-C6-C7-C8
4	A	514	OLC	C2-C3-C4-C5
4	A	523	OLC	C3-C4-C5-C6
4	A	519	OLC	C7-C8-C9-C10
4	A	505	OLC	O20-C21-C22-C24
4	A	521	OLC	O20-C21-C22-C24
4	A	506	OLC	O20-C1-C2-C3
4	A	505	OLC	O20-C21-C22-O23
4	A	521	OLC	O20-C21-C22-O23
4	A	512	OLC	C11-C12-C13-C14
4	A	520	OLC	C12-C13-C14-C15
4	A	521	OLC	C4-C5-C6-C7
4	A	508	OLC	C6-C7-C8-C9
4	A	510	OLC	C10-C11-C12-C13
4	A	508	OLC	C13-C14-C15-C16
4	A	516	OLC	C3-C4-C5-C6
4	A	527	OLC	C2-C3-C4-C5
4	A	512	OLC	C3-C4-C5-C6
4	A	514	OLC	C6-C7-C8-C9
4	A	521	OLC	C1-C2-C3-C4
4	A	505	OLC	C3-C4-C5-C6
4	A	522	OLC	C7-C8-C9-C10
4	A	506	OLC	C5-C6-C7-C8
4	A	515	OLC	C10-C11-C12-C13
4	A	517	OLC	C10-C11-C12-C13
4	A	514	OLC	O19-C1-O20-C21
4	A	520	OLC	C1-C2-C3-C4
4	A	514	OLC	C2-C1-O20-C21
4	A	507	OLC	C9-C10-C11-C12
4	A	514	OLC	C9-C10-C11-C12
4	A	521	OLC	C9-C10-C11-C12
4	A	526	OLC	C15-C16-C17-C18
4	A	509	OLC	C4-C5-C6-C7
4	A	511	OLC	C7-C8-C9-C10
4	A	508	OLC	C9-C10-C11-C12
4	A	513	OLC	C12-C13-C14-C15

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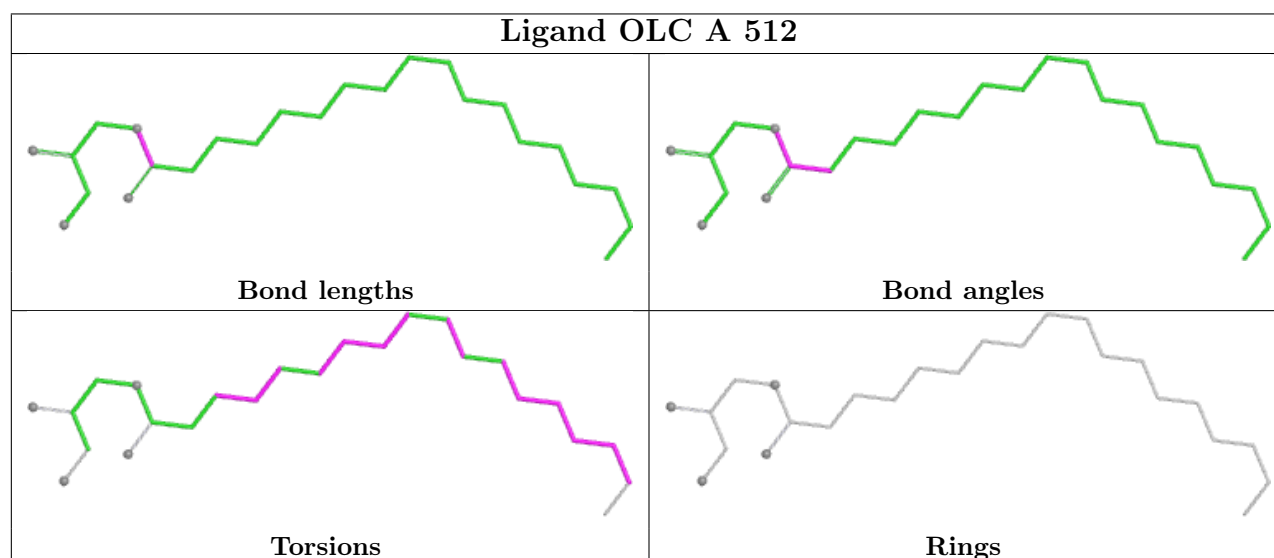
Mol	Chain	Res	Type	Atoms
4	A	511	OLC	C9-C10-C11-C12
4	A	518	OLC	C13-C14-C15-C16
4	A	511	OLC	C12-C13-C14-C15
4	A	513	OLC	O20-C21-C22-C24
4	A	522	OLC	C15-C16-C17-C18
4	A	524	OLC	C14-C15-C16-C17
4	A	508	OLC	C5-C6-C7-C8
4	A	511	OLC	C11-C12-C13-C14
4	A	512	OLC	C9-C10-C11-C12
4	A	505	OLC	C7-C8-C9-C10
4	A	514	OLC	C7-C8-C9-C10
4	A	527	OLC	O20-C21-C22-C24
4	A	526	OLC	C9-C10-C11-C12
4	A	514	OLC	O20-C1-C2-C3
4	A	520	OLC	C9-C10-C11-C12
4	A	513	OLC	C15-C16-C17-C18
4	A	505	OLC	O19-C1-O20-C21
4	A	508	OLC	C7-C8-C9-C10
4	A	518	OLC	C9-C10-C11-C12
4	A	510	OLC	C15-C16-C17-C18
4	A	522	OLC	C9-C10-C11-C12
4	A	512	OLC	C15-C16-C17-C18
4	A	505	OLC	C2-C1-O20-C21
4	A	527	OLC	O20-C21-C22-O23
4	A	506	OLC	O19-C1-C2-C3
4	A	510	OLC	O20-C1-C2-C3
4	A	517	OLC	O20-C1-C2-C3
4	A	514	OLC	C3-C4-C5-C6
4	A	520	OLC	C14-C15-C16-C17
4	A	513	OLC	O20-C1-C2-C3
4	A	518	OLC	C11-C12-C13-C14
4	A	515	OLC	O20-C1-C2-C3
4	A	517	OLC	O19-C1-C2-C3
4	A	513	OLC	O19-C1-C2-C3
4	A	516	OLC	O20-C1-C2-C3
4	A	522	OLC	C13-C14-C15-C16
4	A	510	OLC	O19-C1-C2-C3
4	A	518	OLC	C7-C8-C9-C10

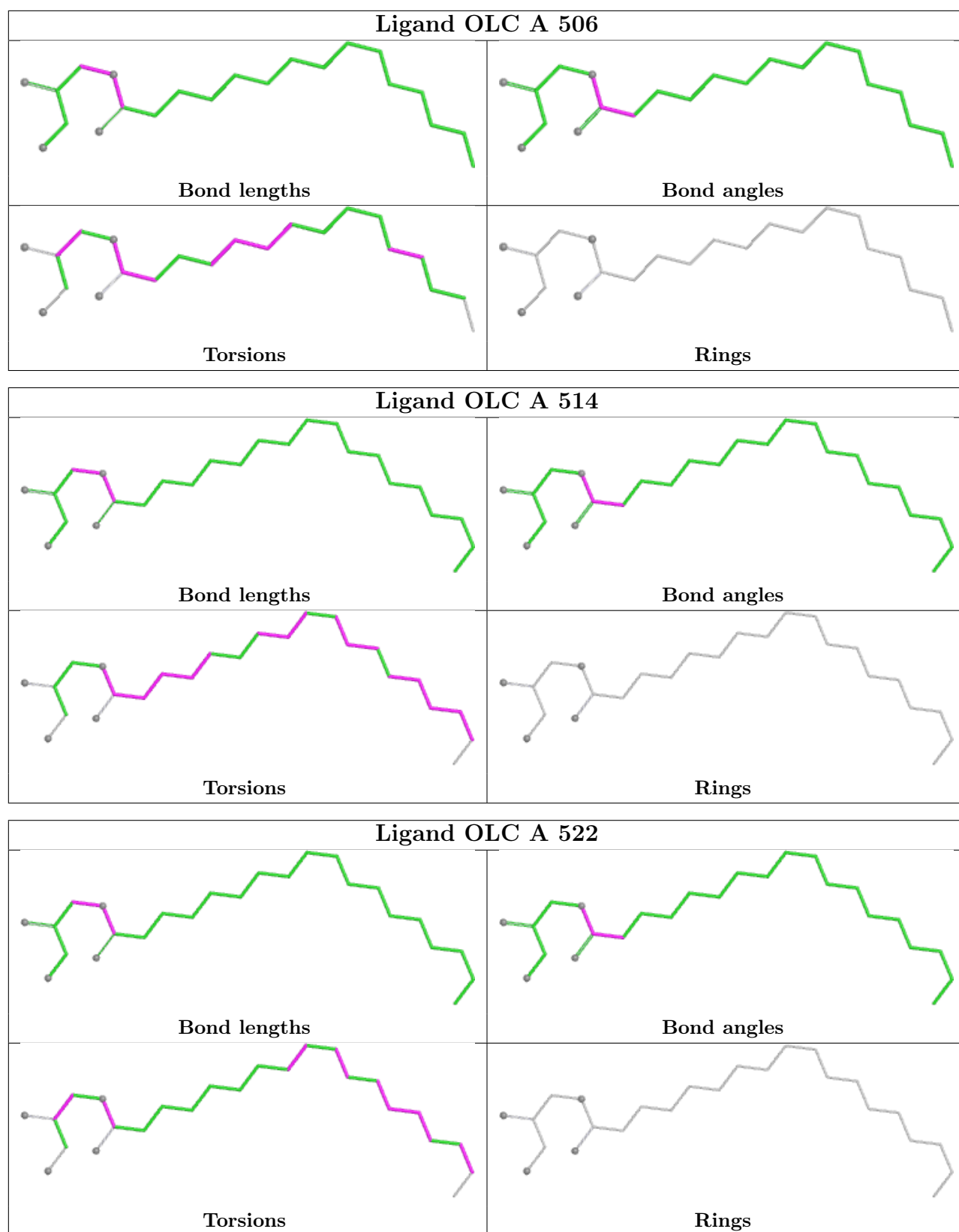
There are no ring outliers.

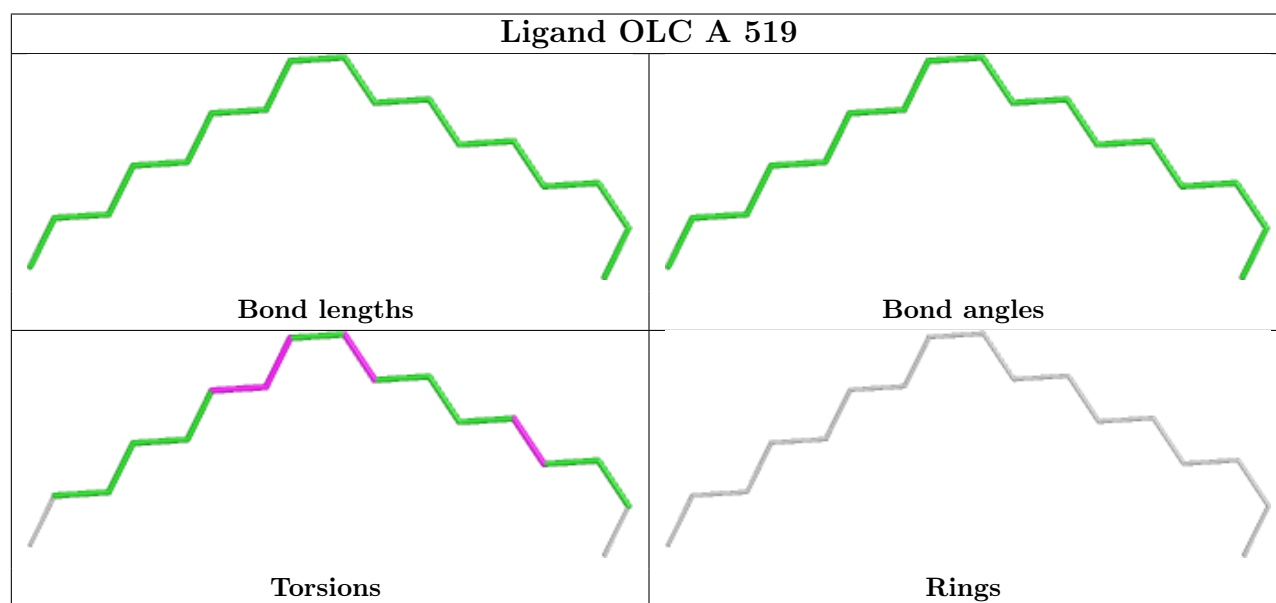
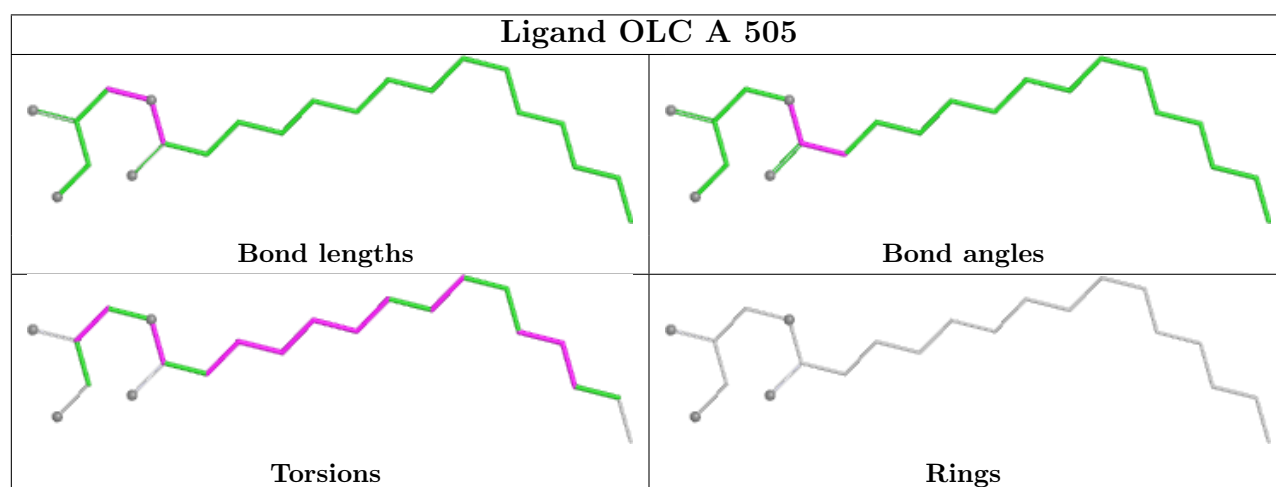
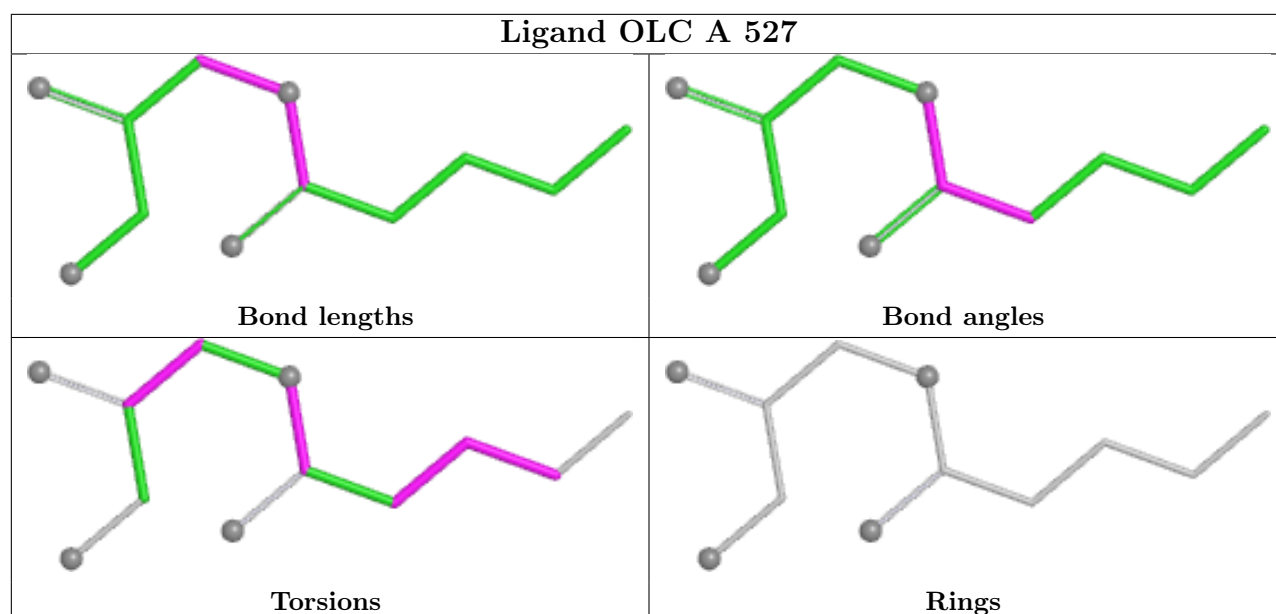
16 monomers are involved in 27 short contacts:

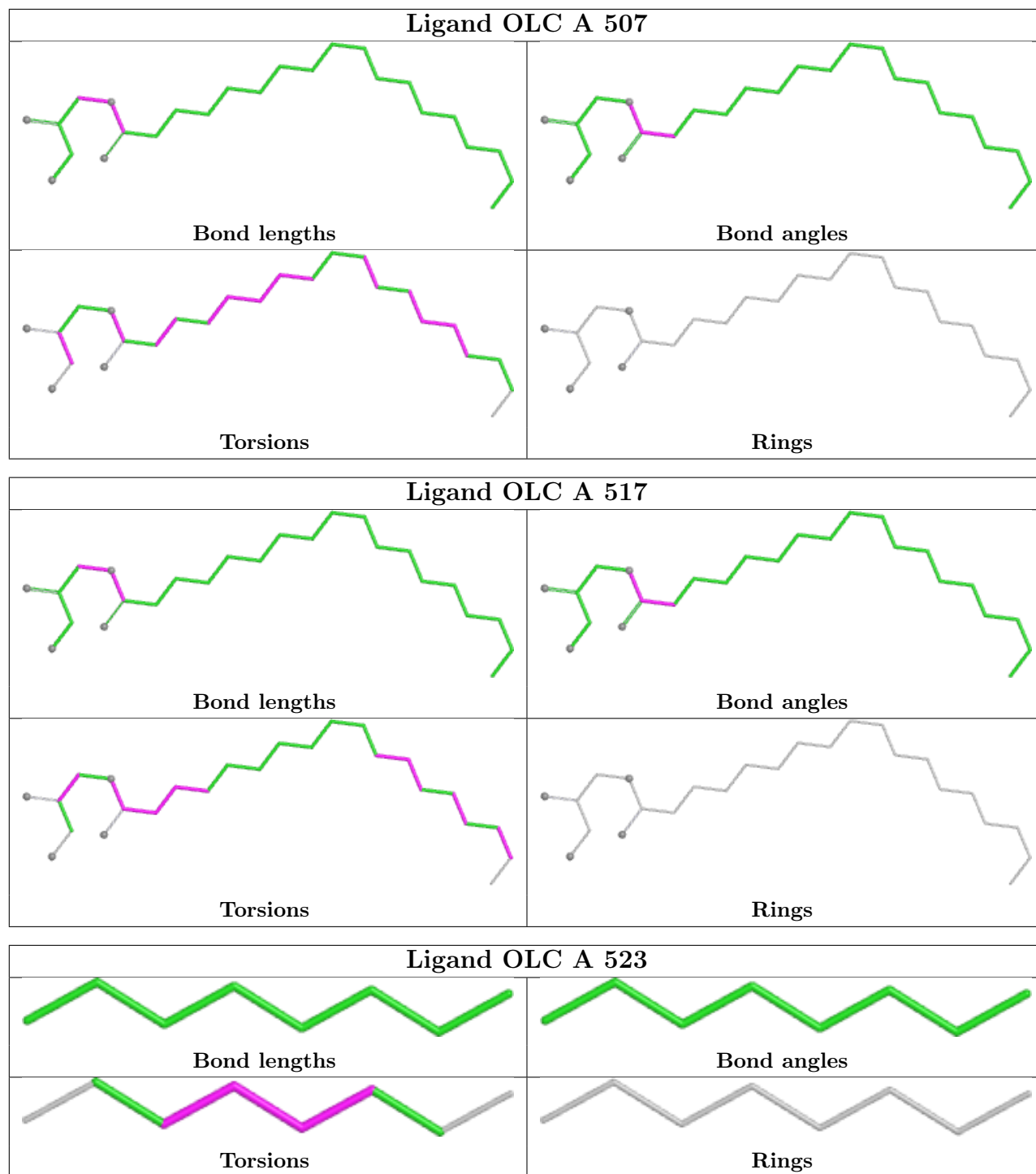
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	512	OLC	1	0
4	A	506	OLC	3	0
4	A	514	OLC	3	0
4	A	522	OLC	2	0
4	A	527	OLC	1	0
4	A	505	OLC	1	0
4	A	519	OLC	3	0
4	A	507	OLC	1	0
4	A	517	OLC	2	0
4	A	510	OLC	3	0
4	A	515	OLC	3	0
4	A	526	OLC	1	0
4	A	513	OLC	2	0
4	A	511	OLC	1	0
4	A	521	OLC	1	0
4	A	524	OLC	2	0

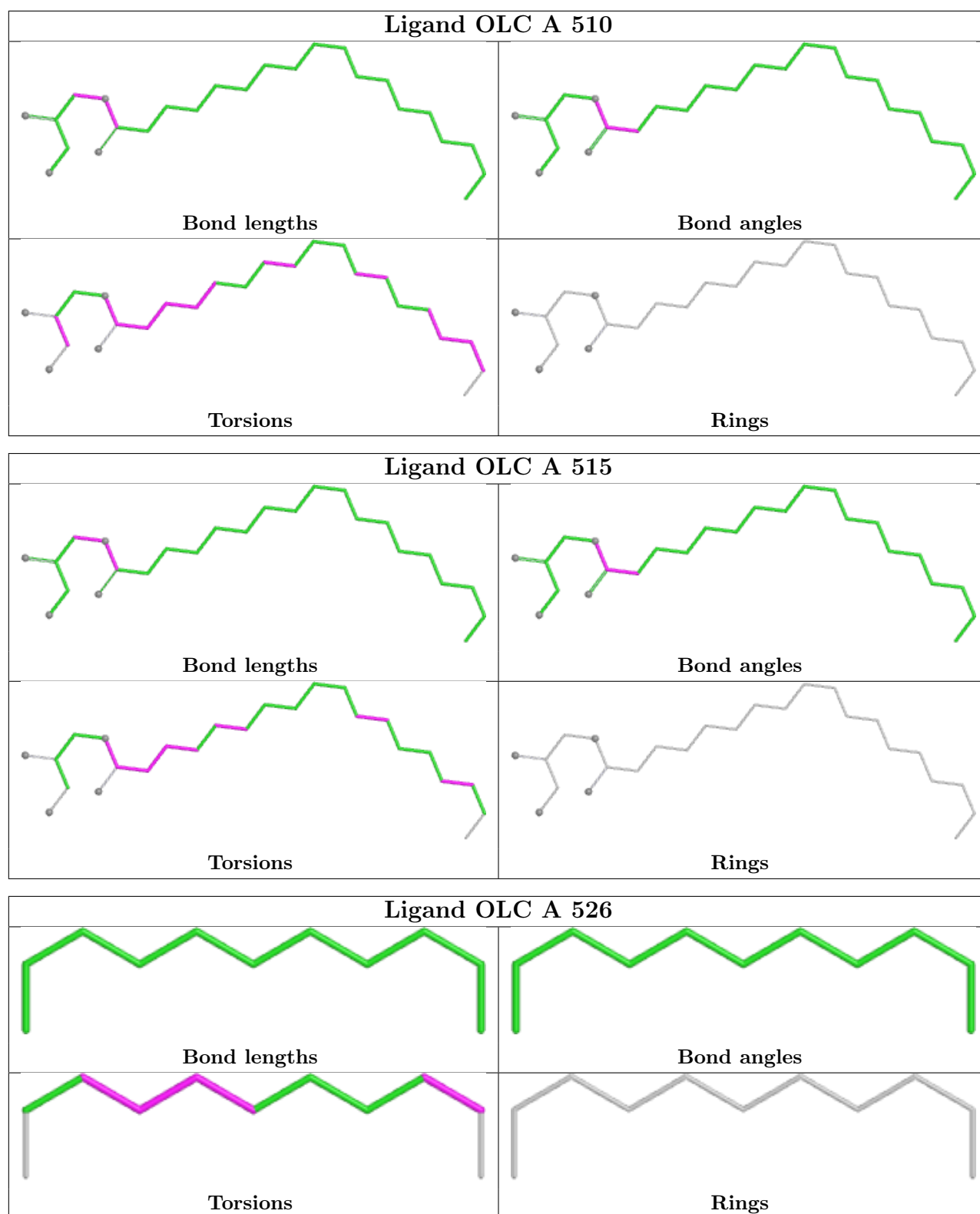
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

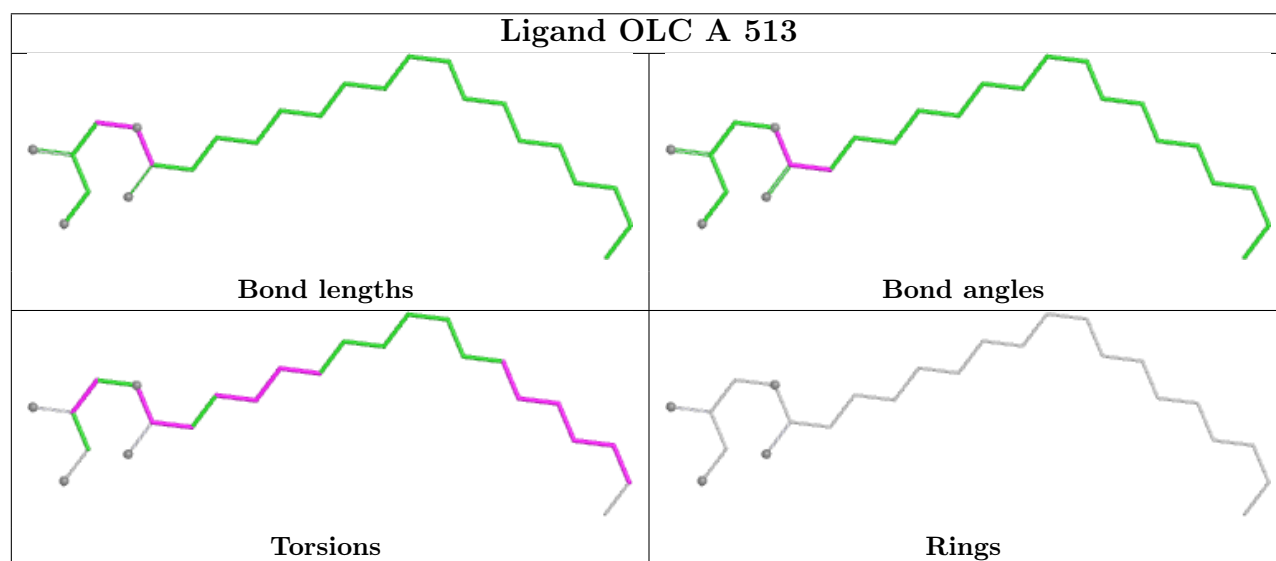
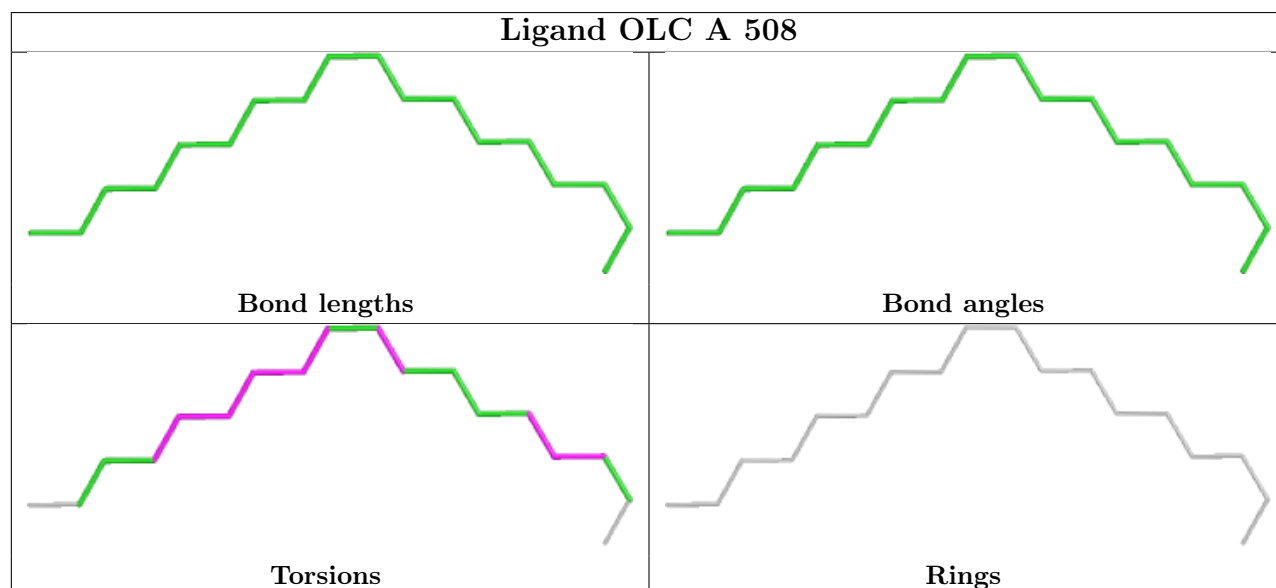
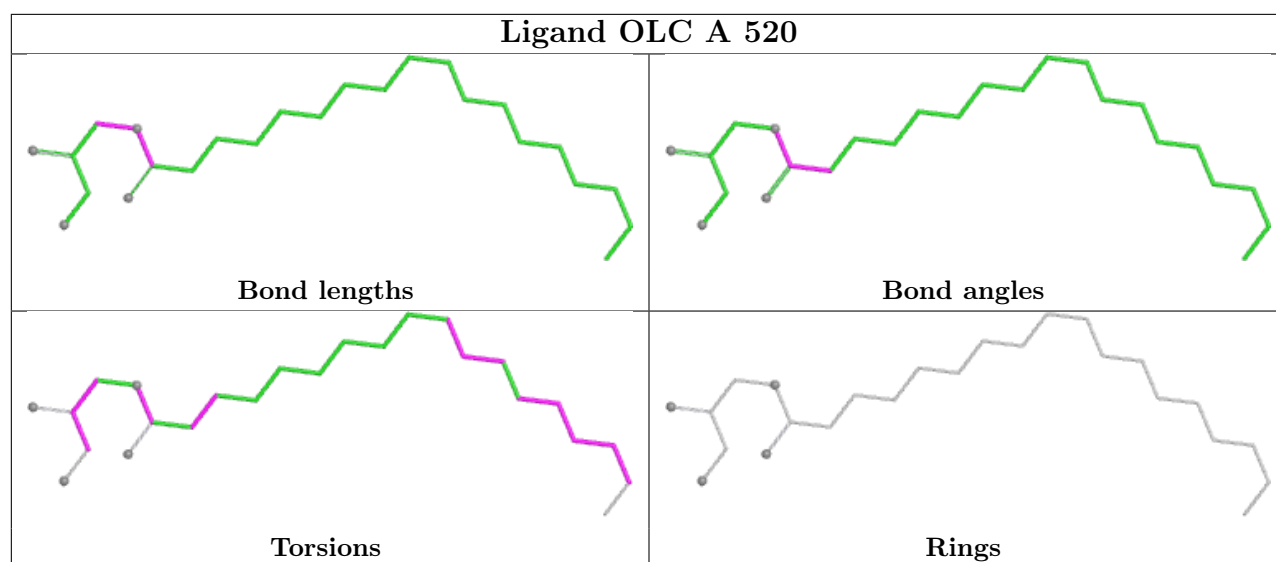


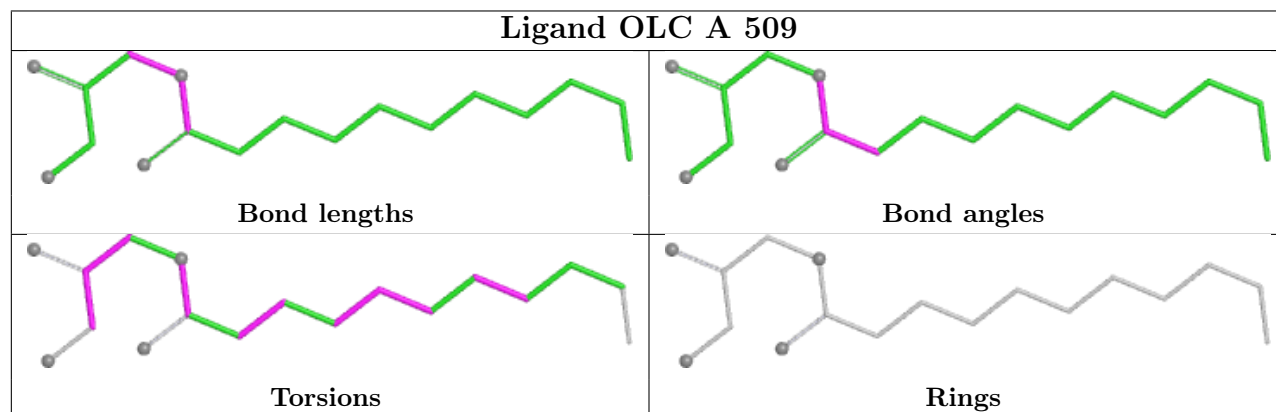
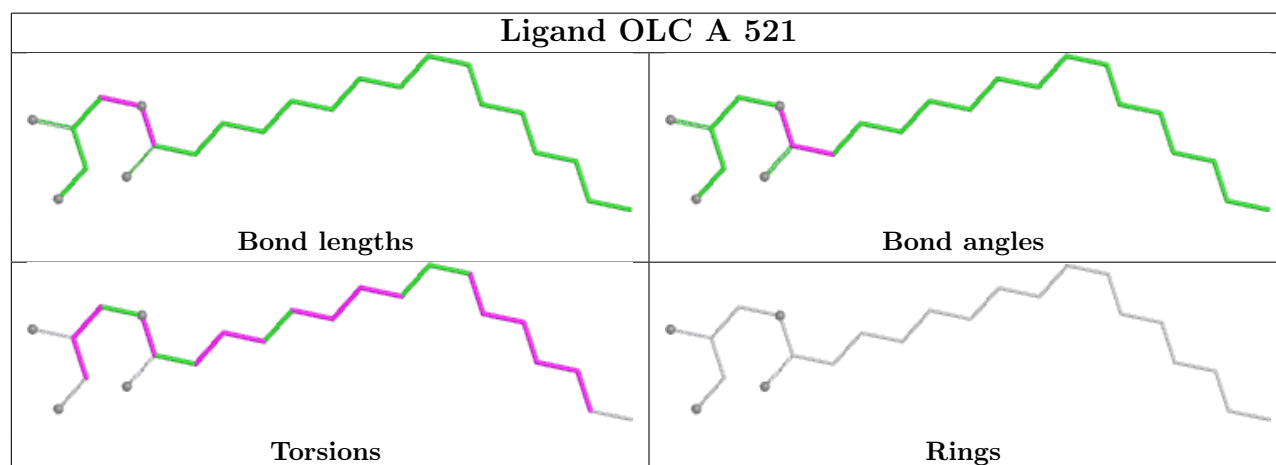
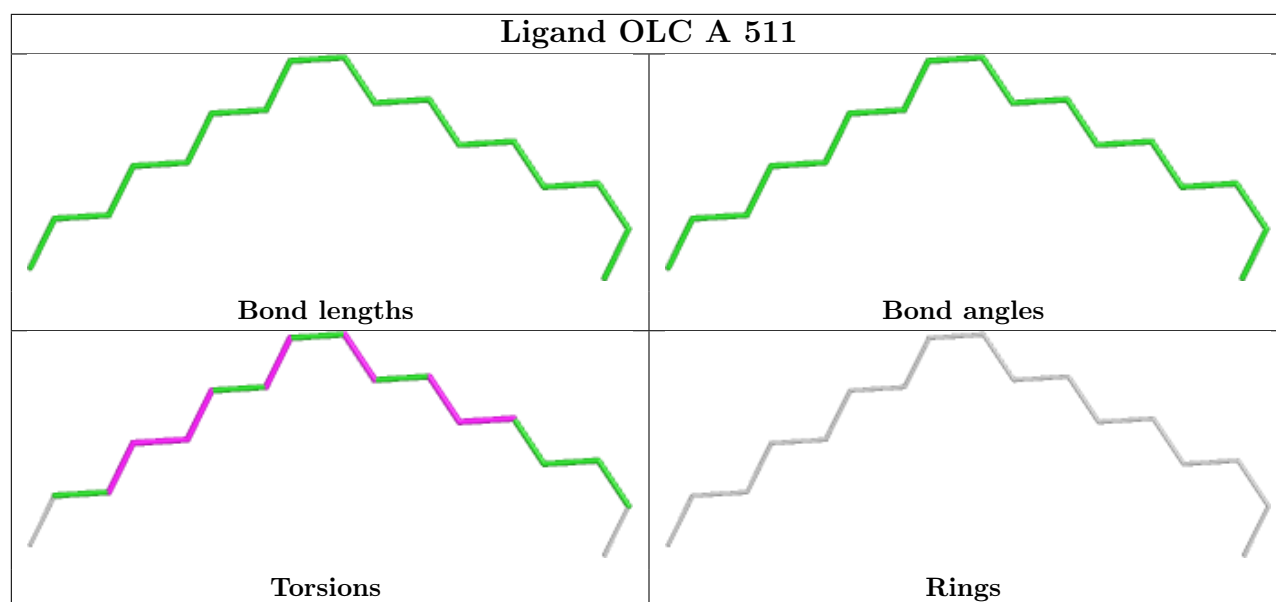


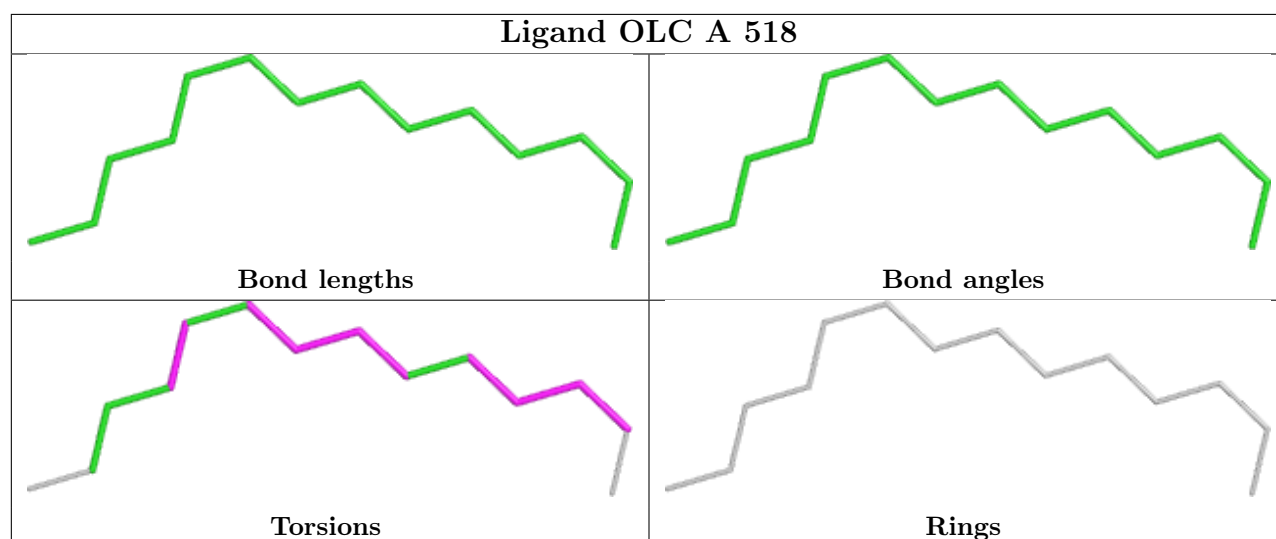
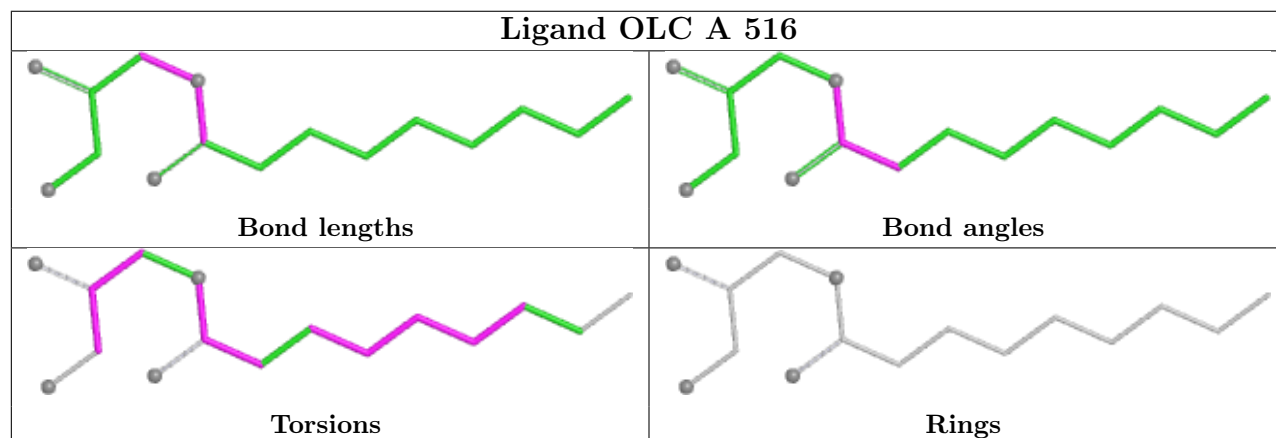
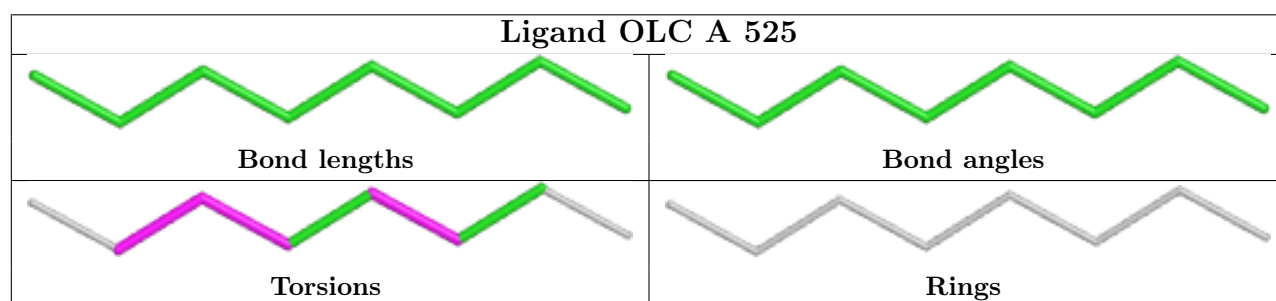
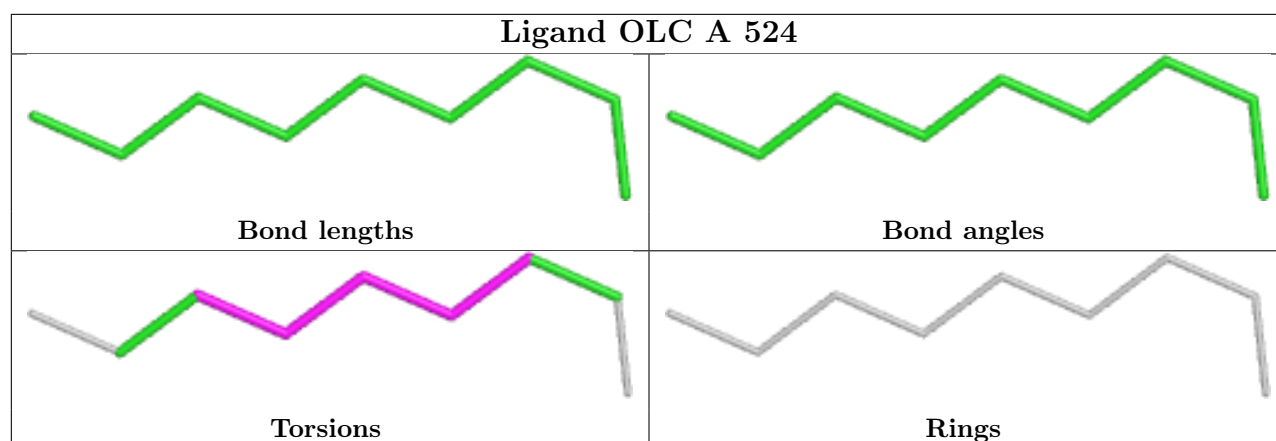












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	392/414 (94%)	0.41	21 (5%) 31 28	30, 56, 127, 195	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	ILE	3.4
1	A	245	ILE	3.1
1	A	48	VAL	3.0
1	A	436	GLY	2.7
1	A	243	GLY	2.5
1	A	244	ARG	2.5
1	A	53	ALA	2.4
1	A	213	GLN	2.4
1	A	117[A]	TRP	2.4
1	A	232	HIS	2.4
1	A	47	ALA	2.2
1	A	247	THR	2.2
1	A	46	PRO	2.2
1	A	241	THR	2.2
1	A	291	VAL	2.1
1	A	239	ALA	2.1
1	A	45	GLY	2.1
1	A	179	VAL	2.0
1	A	50	ALA	2.0
1	A	51	SER	2.0
1	A	54	TYR	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 ⓘ

There are no oligosaccharides in this entry.

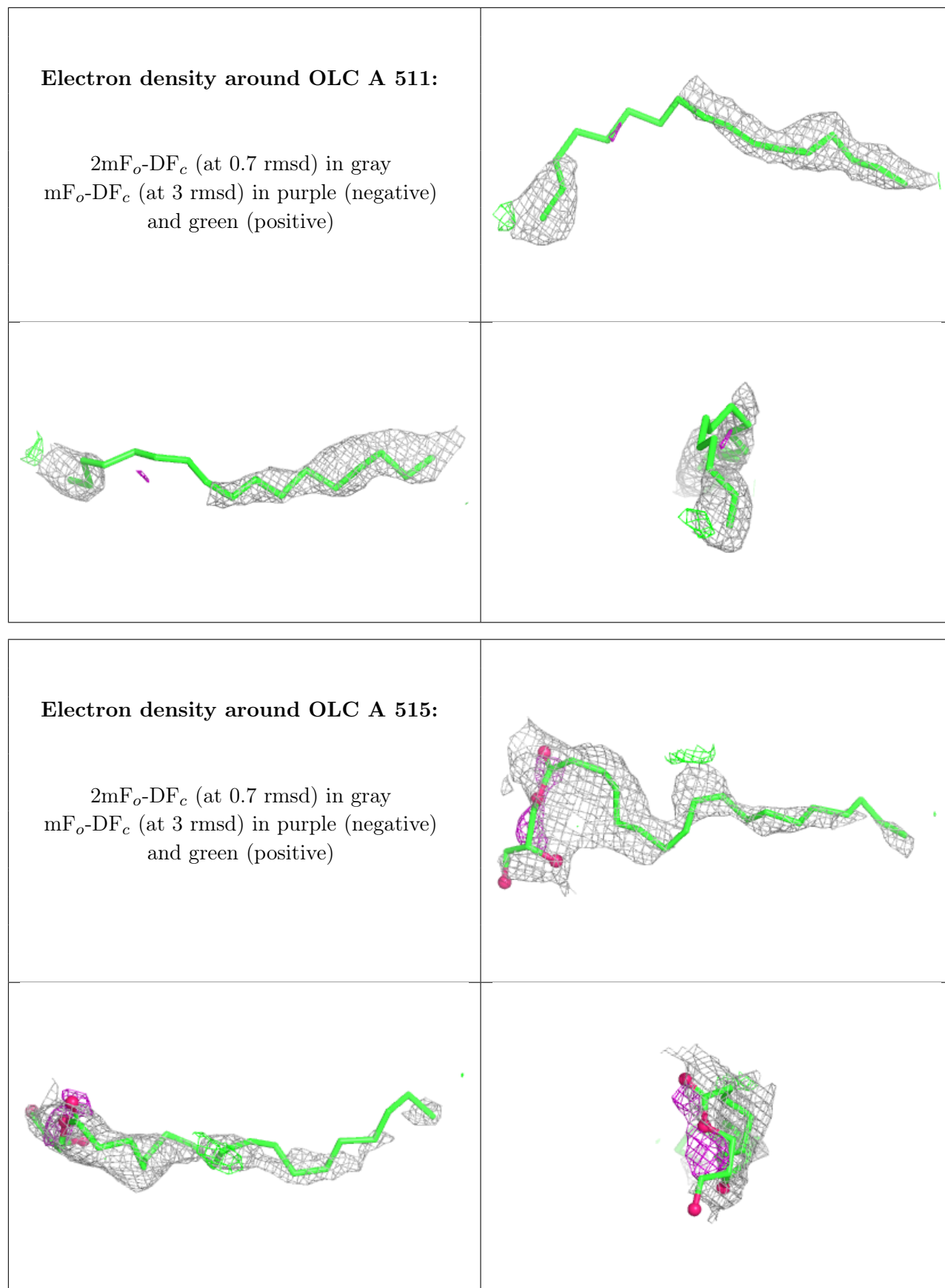
6.4 Ligands ⓘ

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
4	OLC	A	511	17/25	0.66	0.20	63,75,86,89	0
4	OLC	A	515	25/25	0.66	0.19	67,74,78,84	0
4	OLC	A	513	25/25	0.67	0.13	65,94,100,101	0
4	OLC	A	519	17/25	0.67	0.14	72,80,81,84	0
4	OLC	A	518	14/25	0.70	0.14	71,82,85,85	0
4	OLC	A	512	25/25	0.70	0.12	77,81,104,109	0
4	OLC	A	522	25/25	0.70	0.16	62,73,83,92	0
4	OLC	A	523	8/25	0.70	0.21	81,92,95,96	0
4	OLC	A	517	25/25	0.71	0.16	72,78,89,99	0
5	PEG	A	528	4/7	0.71	0.18	67,69,69,70	0
4	OLC	A	526	11/25	0.74	0.19	65,69,73,73	0
4	OLC	A	514	25/25	0.75	0.15	57,72,76,84	0
4	OLC	A	525	8/25	0.75	0.17	61,63,66,67	0
4	OLC	A	520	25/25	0.76	0.15	57,69,83,86	0
4	OLC	A	508	18/25	0.76	0.17	55,64,69,71	0
4	OLC	A	510	25/25	0.76	0.14	49,78,102,106	0
4	OLC	A	507	25/25	0.78	0.16	59,71,97,99	0
4	OLC	A	524	9/25	0.79	0.18	71,77,85,86	0
4	OLC	A	506	22/25	0.79	0.17	62,68,73,76	0
4	OLC	A	516	16/25	0.80	0.13	78,84,91,98	0
4	OLC	A	521	23/25	0.81	0.13	68,76,84,86	0
4	OLC	A	509	18/25	0.82	0.15	88,95,102,103	0
4	OLC	A	527	12/25	0.83	0.15	62,65,66,68	0
4	OLC	A	505	22/25	0.84	0.13	52,65,77,78	0
2	MN	A	502	1/1	0.94	0.07	71,71,71,71	1
3	CL	A	503	1/1	0.95	0.07	62,62,62,62	0
3	CL	A	504	1/1	0.96	0.14	64,64,64,64	0
2	MN	A	501	1/1	0.99	0.03	78,78,78,78	1

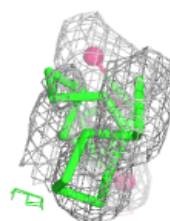
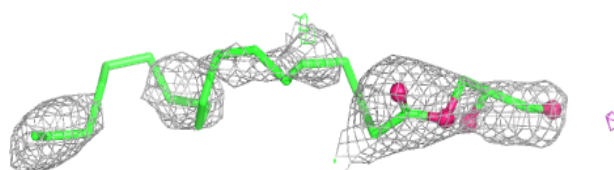
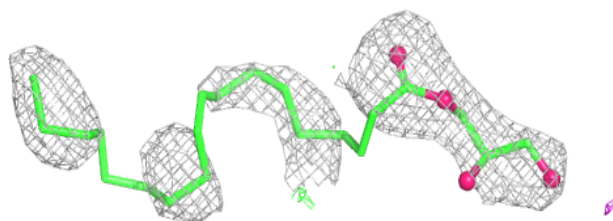
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

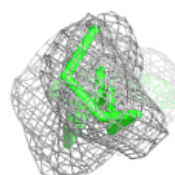
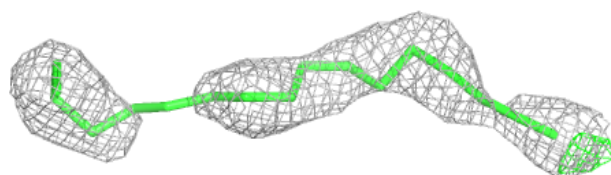
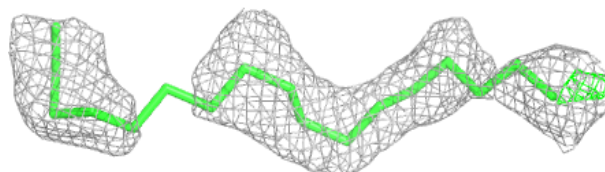


Electron density around OLC A 513:

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

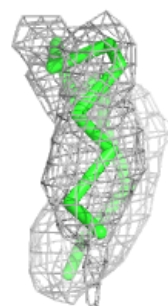
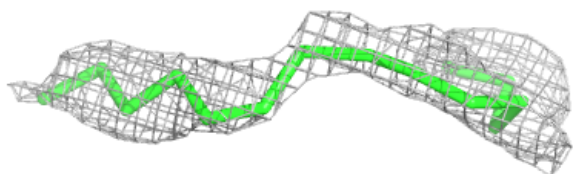
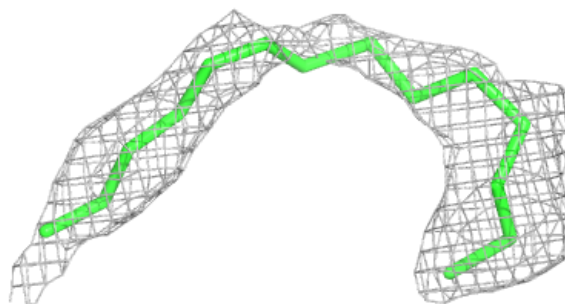
**Electron density around OLC A 519:**

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

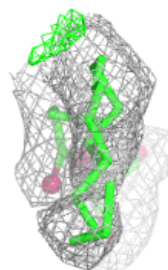
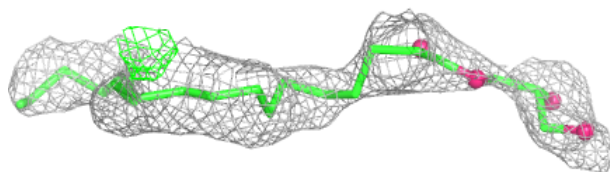
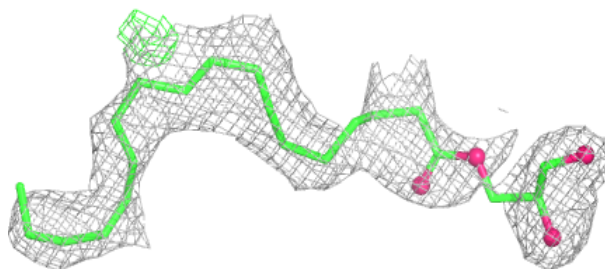


Electron density around OLC A 518:

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

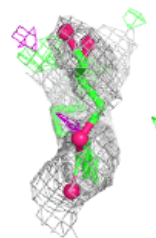
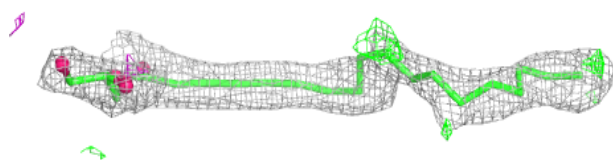
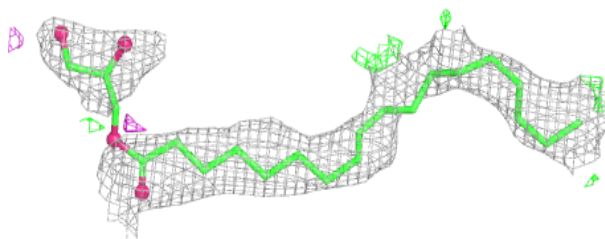
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and green (positive)

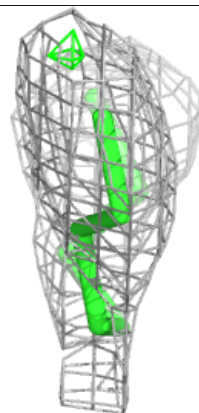
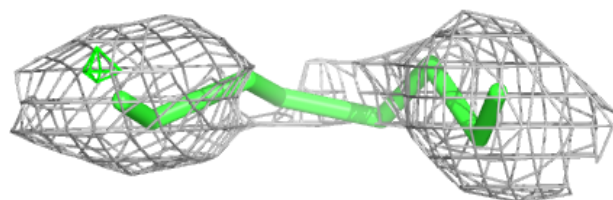
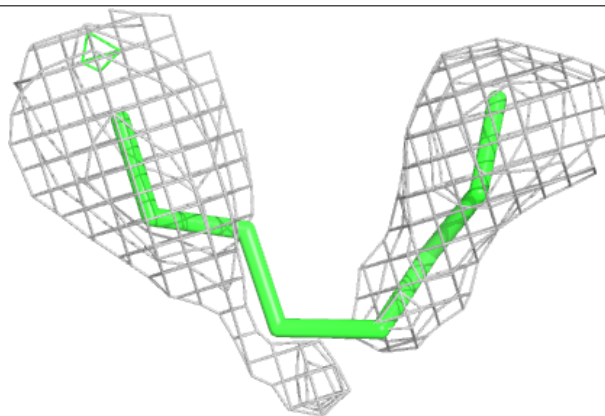


Electron density around OLC A 522:

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

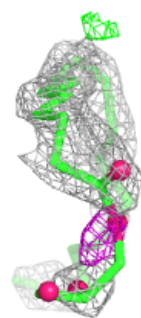
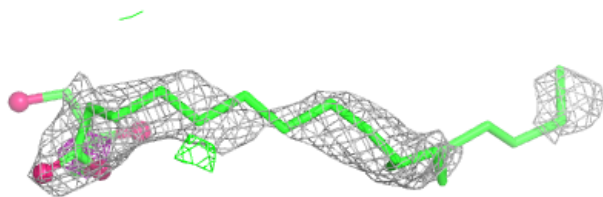
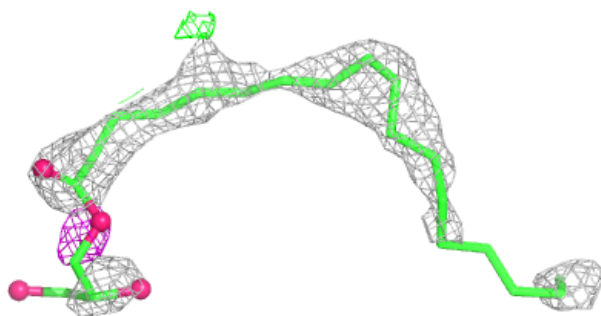
**Electron density around OLC A 523:**

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

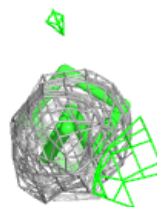
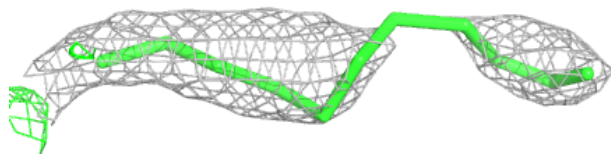
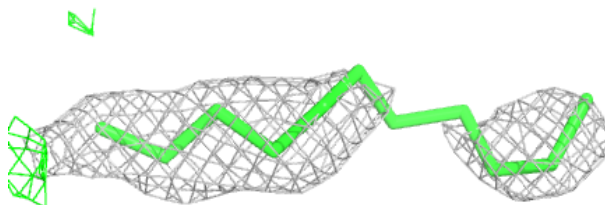


Electron density around OLC A 517:

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

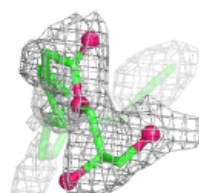
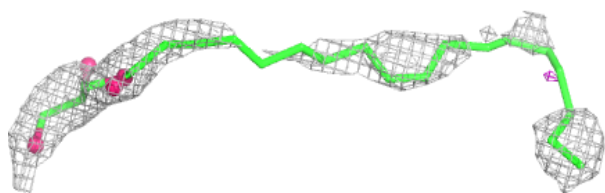
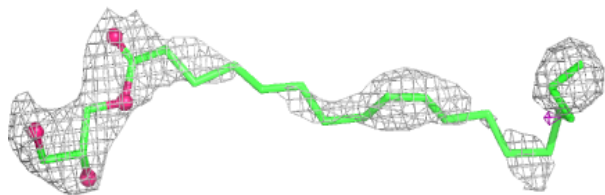
**Electron density around OLC A 526:**

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

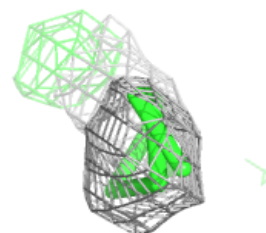
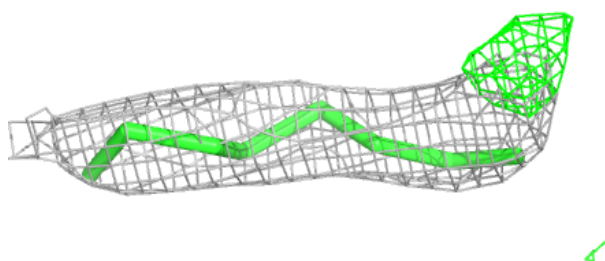
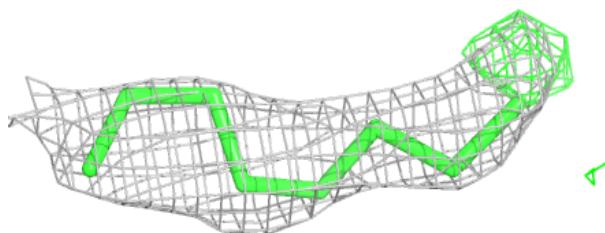


Electron density around OLC A 514:

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

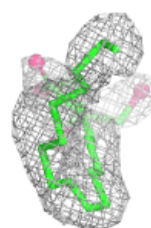
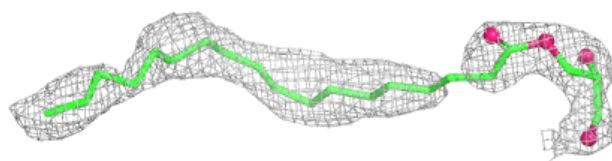
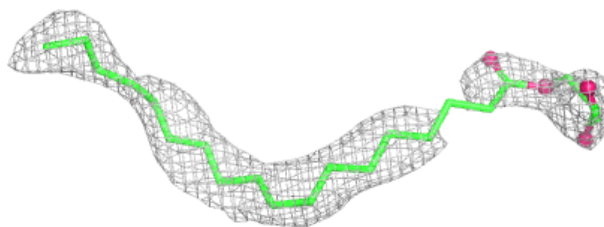
**Electron density around OLC A 525:**

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

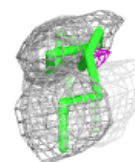
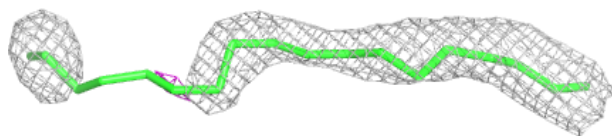
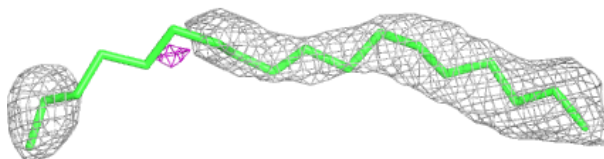


Electron density around OLC A 520:

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and green (positive)

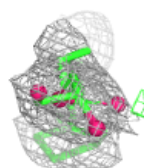
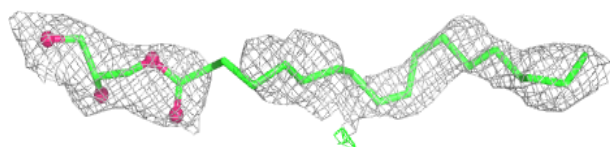
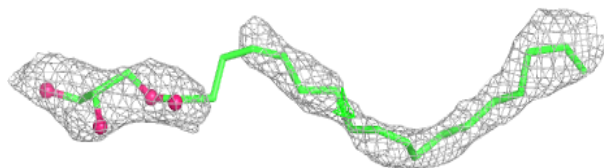
**Electron density around OLC A 508:**

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and green (positive)

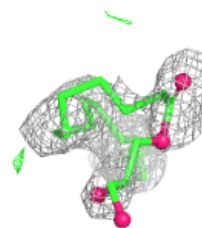
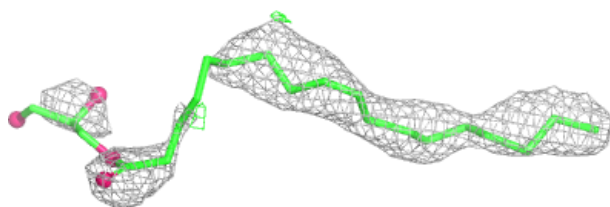
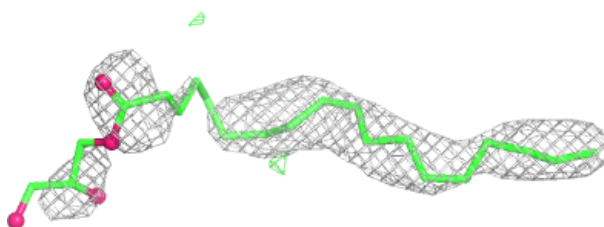


Electron density around OLC A 510:

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

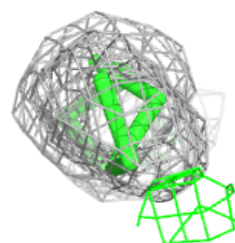
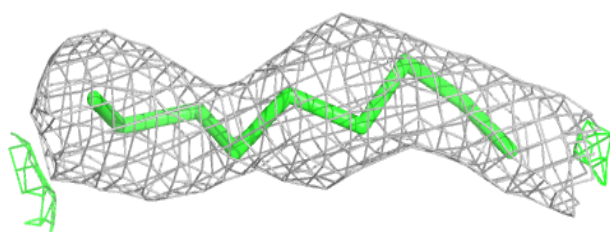
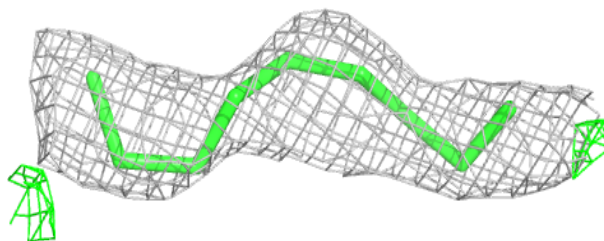
**Electron density around OLC A 507:**

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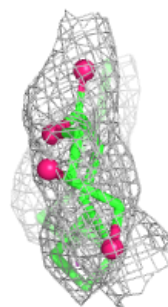
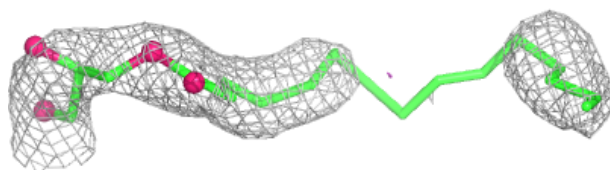
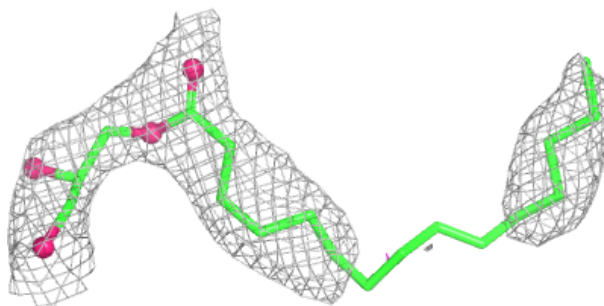


Electron density around OLC A 524:

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

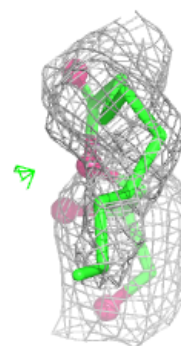
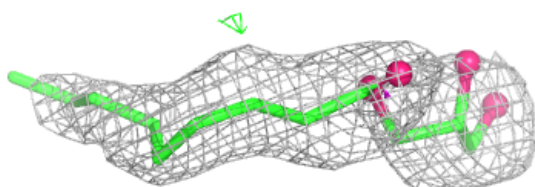
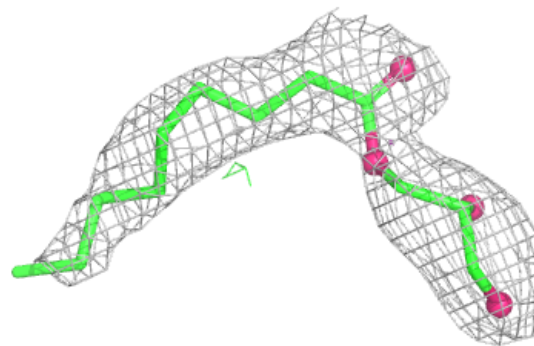
**Electron density around OLC A 506:**

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and green (positive)

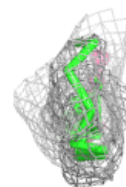
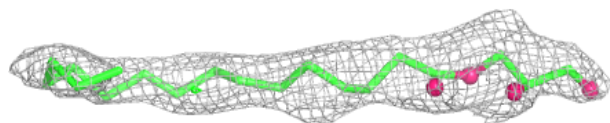
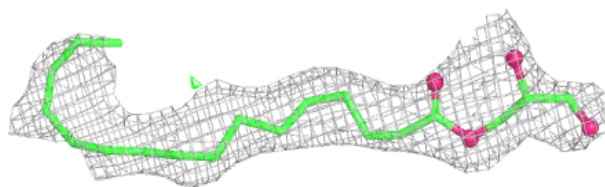


Electron density around OLC A 516:

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and green (positive)

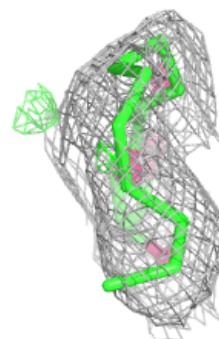
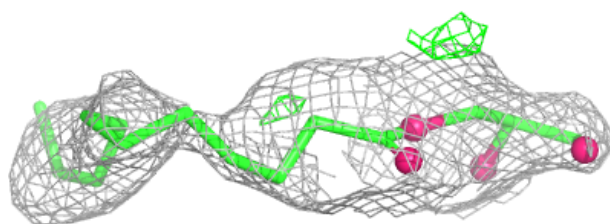
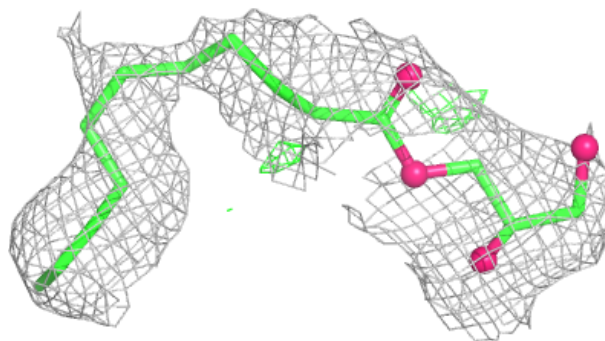
**Electron density around OLC A 521:**

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

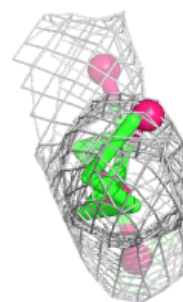
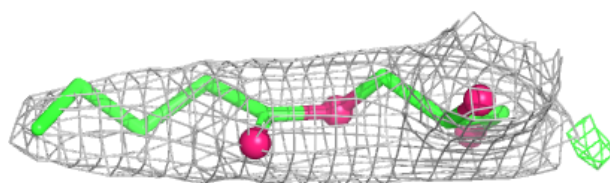
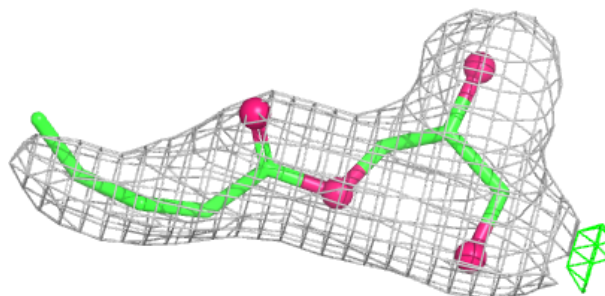


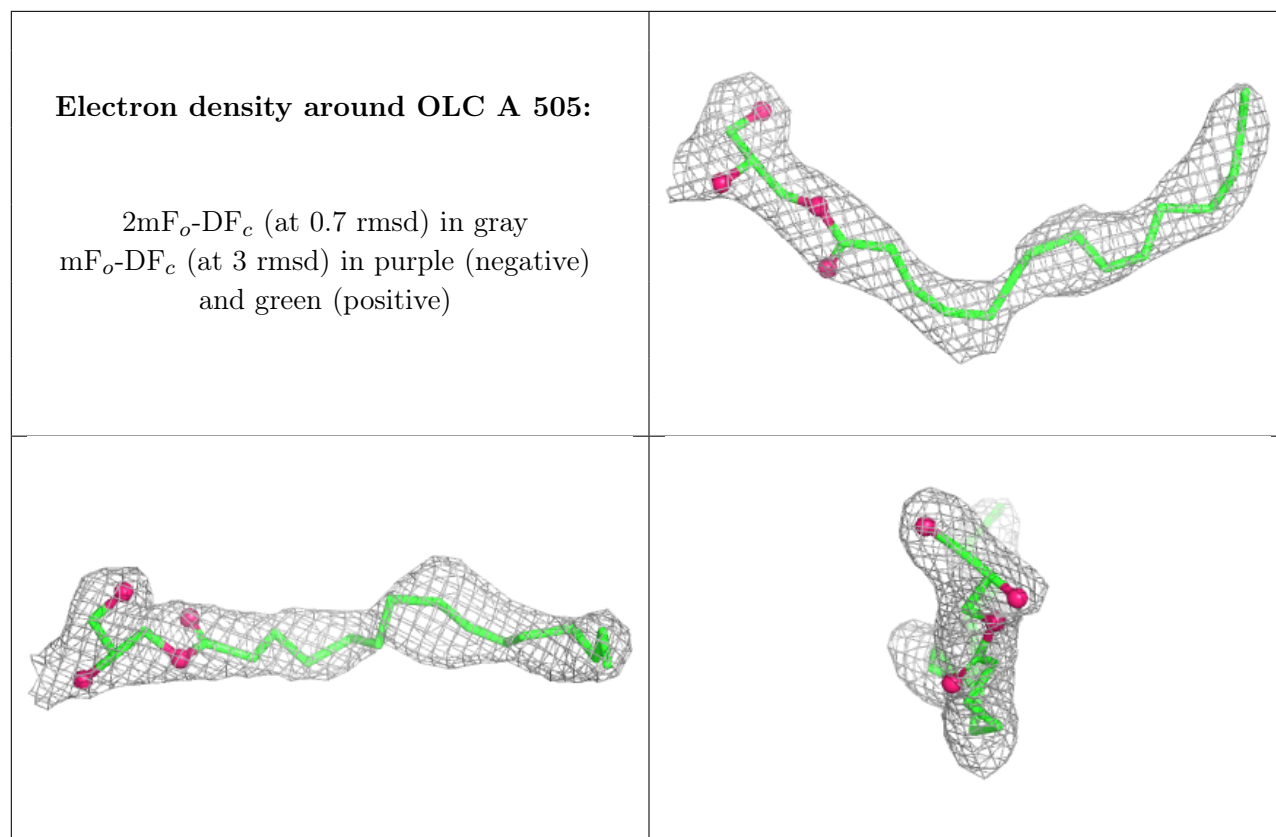
Electron density around OLC A 509:

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

**Electron density around OLC A 527:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.