



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:02 PM UTC

PDB ID : 8E6H / pdb_00008e6h
Title : X-ray structure of the Deinococcus radiodurans Nramp/MntH divalent transition metal transporter A47W mutant in an occluded, manganese-bound state
Authors : Ray, S.; Gaudet, R.
Deposited on : 2022-08-22
Resolution : 2.39 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

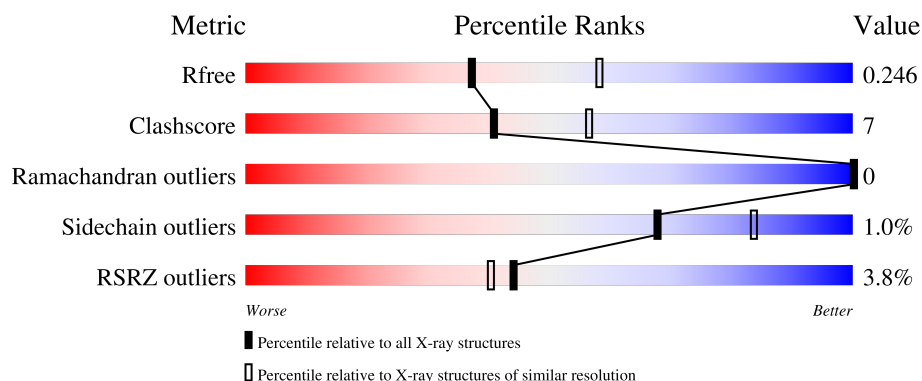
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	445	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3483 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	0	0
			2939	1932	491	499	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q9RTP8
A	-7	HIS	-	expression tag	UNP Q9RTP8
A	-6	HIS	-	expression tag	UNP Q9RTP8
A	-5	HIS	-	expression tag	UNP Q9RTP8
A	-4	HIS	-	expression tag	UNP Q9RTP8
A	-3	HIS	-	expression tag	UNP Q9RTP8
A	-2	HIS	-	expression tag	UNP Q9RTP8
A	-1	HIS	-	expression tag	UNP Q9RTP8
A	0	HIS	-	expression tag	UNP Q9RTP8
A	47	TRP	ALA	engineered mutation	UNP Q9RTP8

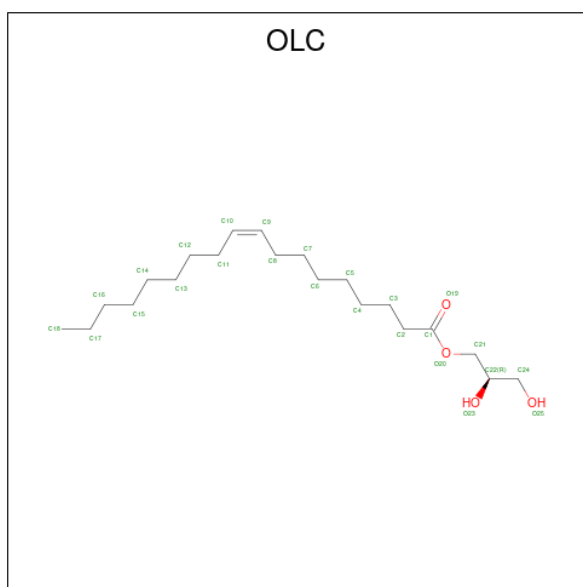
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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	1	Total	Cl	0	0
			1	1		

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



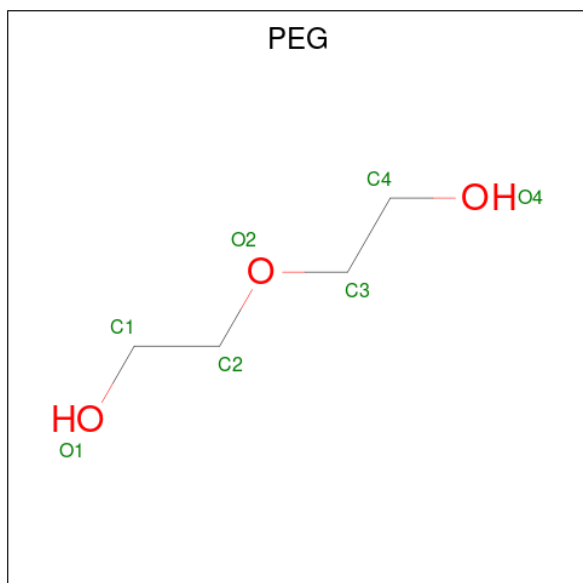
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 25	C 21	O 4	0	0
4	A	1	Total 25	C 21	O 4	0	0
4	A	1	Total 16	C 16		0	0
4	A	1	Total 24	C 20	O 4	0	0
4	A	1	Total 15	C 11	O 4	0	0
4	A	1	Total 25	C 21	O 4	0	0
4	A	1	Total 25	C 21	O 4	0	0
4	A	1	Total 25	C 21	O 4	0	0
4	A	1	Total 25	C 21	O 4	0	0
4	A	1	Total 25	C 21	O 4	0	0
4	A	1	Total 24	C 20	O 4	0	0
4	A	1	Total 18	C 18		0	0
4	A	1	Total 24	C 20	O 4	0	0
4	A	1	Total 23	C 19	O 4	0	0
4	A	1	Total 15	C 11	O 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 18 18	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C 15 15	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 9 9	0	0
4	A	1	Total C 14 14	0	0
4	A	1	Total C 6 6	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 5 3 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			3	2	1		

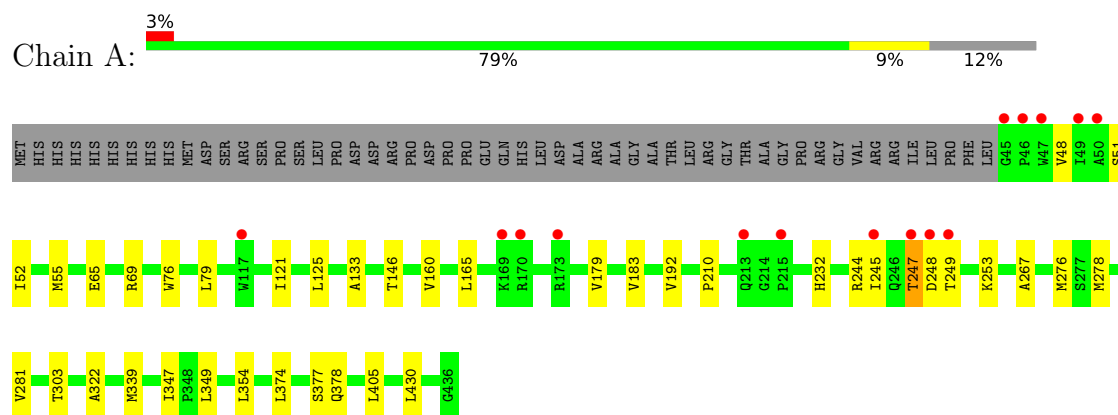
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	75	Total	O	0	0
			75	75		

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	58.98Å 70.93Å 98.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.35 – 2.39 45.35 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.35-2.39) 98.6 (45.35-2.39)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.246 0.206 , 0.246	Depositor DCC
R_{free} test set	1675 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.4	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	3483	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.09	0/3003	0.23	0/4105

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2939	0	3073	29	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	451	0	716	31	0
5	A	15	0	17	0	0
6	A	75	0	0	2	0
All	All	3483	0	3806	47	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 (47) 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:192:VAL:HA	4:A:505:OLC:H2A	1.70	0.74
1:A:65:GLU:OE2	1:A:69:ARG:NH1	2.29	0.66
4:A:513:OLC:H12	4:A:522:OLC:H5A	1.81	0.62
1:A:267:ALA:HB2	4:A:523:OLC:H5	1.83	0.61
1:A:79:LEU:HD23	4:A:518:OLC:H18A	1.88	0.56
1:A:165:LEU:HD21	1:A:349:LEU:HB3	1.89	0.55
1:A:52:ILE:HD11	1:A:183:VAL:HG21	1.88	0.55
4:A:523:OLC:H10	4:A:526:OLC:H13A	1.88	0.54
1:A:354:LEU:HD21	4:A:510:OLC:H10	1.91	0.52
1:A:245:ILE:HD13	1:A:248:ASP:HA	1.93	0.51
1:A:48:VAL:HG11	4:A:526:OLC:H6A	1.93	0.50
1:A:253:LYS:HB3	1:A:405:LEU:HD11	1.94	0.50
1:A:244:ARG:NH2	6:A:610:HOH:O	2.45	0.50
4:A:507:OLC:H5A	4:A:511:OLC:H7	1.93	0.49
1:A:76:TRP:CE2	1:A:210:PRO:HA	2.48	0.48
1:A:48:VAL:HG12	4:A:526:OLC:H11	1.96	0.48
1:A:281:VAL:HG12	1:A:303:THR:HB	1.96	0.47
1:A:374:LEU:O	1:A:378:GLN:HG2	2.15	0.47
1:A:146:THR:HG22	4:A:512:OLC:H7	1.97	0.47
1:A:339:MET:HE1	1:A:347:ILE:HG23	1.96	0.47
1:A:55:MET:HE1	1:A:278:MET:HE1	1.98	0.46
4:A:511:OLC:H6	4:A:511:OLC:H9	1.49	0.46
1:A:76:TRP:CD2	1:A:210:PRO:HA	2.50	0.46
4:A:521:OLC:H14A	4:A:521:OLC:H11A	1.59	0.46
4:A:509:OLC:H2A	4:A:509:OLC:H5	1.70	0.46
1:A:179:VAL:HG22	1:A:322:ALA:HB1	1.98	0.46
4:A:512:OLC:H8A	4:A:512:OLC:H11A	1.67	0.46
1:A:232:HIS:ND1	6:A:603:HOH:O	2.36	0.45
4:A:507:OLC:H12A	4:A:507:OLC:H9	1.60	0.45
4:A:518:OLC:H16A	4:A:518:OLC:H13	1.70	0.45
1:A:276:MET:HE1	4:A:507:OLC:H12	1.98	0.45
1:A:133:ALA:HB2	1:A:377:SER:OG	2.17	0.45
4:A:511:OLC:H5	4:A:511:OLC:H2A	1.79	0.45
4:A:516:OLC:H3A	4:A:516:OLC:H6	1.27	0.44
4:A:504:OLC:H11	4:A:504:OLC:H8	1.66	0.44
1:A:125:LEU:HD11	4:A:519:OLC:H15	1.98	0.44
1:A:160:VAL:HG21	4:A:514:OLC:H17	2.00	0.44
1:A:76:TRP:HB2	4:A:518:OLC:H17	2.01	0.43
4:A:515:OLC:H6A	4:A:515:OLC:H9	1.66	0.43
1:A:146:THR:O	4:A:512:OLC:H2	2.19	0.42
4:A:505:OLC:H11A	4:A:505:OLC:H8A	1.82	0.41
4:A:514:OLC:H11A	4:A:514:OLC:H8A	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:526:OLC:H13A	4:A:526:OLC:H16	1.80	0.41
4:A:522:OLC:H8	4:A:522:OLC:H5	1.86	0.41
1:A:121:ILE:HD12	4:A:509:OLC:H4A	2.02	0.41
4:A:519:OLC:H11A	4:A:519:OLC:H8	1.65	0.41
1:A:247:THR:O	1:A:249:THR:HG23	2.22	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	390/445 (88%)	389 (100%)	1 (0%)	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	301/349 (86%)	298 (99%)	3 (1%)	68	84

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

Mol	Chain	Res	Type
1	A	51	SER

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Mol	Chain	Res	Type
1	A	247	THR
1	A	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	82	ASN
1	A	232	HIS
1	A	340	GLN
1	A	426	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 3 are monoatomic - leaving 27 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	517	-	14,14,24	1.02	2 (14%)	15,15,25	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLC	A	511	-	24,24,24	0.80	2 (8%)	25,25,25	0.92	1 (4%)
4	OLC	A	521	-	24,24,24	0.81	2 (8%)	25,25,25	0.94	1 (4%)
5	PEG	A	528	-	4,4,6	0.42	0	3,3,5	0.30	0
4	OLC	A	510	-	24,24,24	0.82	2 (8%)	25,25,25	0.92	1 (4%)
4	OLC	A	507	-	23,23,24	0.83	2 (8%)	24,24,25	0.96	1 (4%)
4	OLC	A	516	-	22,22,24	0.85	2 (9%)	23,23,25	0.92	1 (4%)
4	OLC	A	519	-	24,24,24	0.81	2 (8%)	25,25,25	0.95	1 (4%)
4	OLC	A	523	-	7,7,24	0.44	0	6,6,25	0.88	0
5	PEG	A	530	-	2,2,6	0.49	0	1,1,5	0.41	0
4	OLC	A	508	-	14,14,24	1.02	2 (14%)	15,15,25	1.05	1 (6%)
4	OLC	A	506	-	15,15,24	0.34	0	14,14,25	0.74	0
4	OLC	A	513	-	23,23,24	0.83	2 (8%)	24,24,25	0.98	1 (4%)
4	OLC	A	512	-	24,24,24	0.81	2 (8%)	25,25,25	0.96	1 (4%)
5	PEG	A	529	-	6,6,6	0.51	0	5,5,5	0.23	0
4	OLC	A	515	-	23,23,24	0.83	2 (8%)	24,24,25	1.00	1 (4%)
4	OLC	A	509	-	24,24,24	0.81	2 (8%)	25,25,25	0.96	1 (4%)
4	OLC	A	505	-	24,24,24	0.82	2 (8%)	25,25,25	0.96	1 (4%)
4	OLC	A	522	-	14,14,24	0.34	0	13,13,25	0.73	0
4	OLC	A	514	-	17,17,24	0.33	0	16,16,25	0.75	0
4	OLC	A	504	-	24,24,24	0.82	2 (8%)	25,25,25	0.97	1 (4%)
4	OLC	A	527	-	5,5,24	0.33	0	4,4,25	0.58	0
4	OLC	A	518	-	17,17,24	0.33	0	16,16,25	0.80	0
4	OLC	A	520	-	10,10,24	0.40	0	9,9,25	0.89	0
4	OLC	A	524	-	10,10,24	0.42	0	9,9,25	0.85	0
4	OLC	A	526	-	13,13,24	0.35	0	12,12,25	0.72	0
4	OLC	A	525	-	8,8,24	0.32	0	7,7,25	0.69	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	517	-	-	9/14/14/24	-
4	OLC	A	511	-	-	17/24/24/24	-
4	OLC	A	521	-	-	10/24/24/24	-
5	PEG	A	528	-	-	1/2/2/4	-
4	OLC	A	510	-	-	14/24/24/24	-
4	OLC	A	507	-	-	14/23/23/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLC	A	516	-	-	11/22/22/24	-
4	OLC	A	519	-	-	11/24/24/24	-
4	OLC	A	523	-	-	2/5/5/24	-
4	OLC	A	508	-	-	3/14/14/24	-
4	OLC	A	506	-	-	8/13/13/24	-
4	OLC	A	513	-	-	8/23/23/24	-
4	OLC	A	512	-	-	7/24/24/24	-
5	PEG	A	529	-	-	1/4/4/4	-
4	OLC	A	515	-	-	12/23/23/24	-
4	OLC	A	509	-	-	11/24/24/24	-
4	OLC	A	505	-	-	11/24/24/24	-
4	OLC	A	522	-	-	5/12/12/24	-
4	OLC	A	514	-	-	8/15/15/24	-
4	OLC	A	504	-	-	13/24/24/24	-
4	OLC	A	527	-	-	2/3/3/24	-
4	OLC	A	518	-	-	9/15/15/24	-
4	OLC	A	520	-	-	2/8/8/24	-
4	OLC	A	524	-	-	5/8/8/24	-
4	OLC	A	526	-	-	6/11/11/24	-
4	OLC	A	525	-	-	5/6/6/24	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	515	OLC	O20-C1	2.50	1.40	1.33
4	A	512	OLC	O20-C1	2.45	1.40	1.33
4	A	516	OLC	O20-C1	2.44	1.40	1.33
4	A	521	OLC	O20-C1	2.42	1.40	1.33
4	A	505	OLC	O20-C1	2.41	1.40	1.33
4	A	517	OLC	O20-C1	2.41	1.40	1.33
4	A	509	OLC	O20-C1	2.41	1.40	1.33
4	A	507	OLC	O20-C1	2.40	1.40	1.33
4	A	519	OLC	O20-C1	2.39	1.40	1.33
4	A	511	OLC	O20-C1	2.38	1.40	1.33
4	A	504	OLC	O20-C1	2.38	1.40	1.33
4	A	508	OLC	O20-C1	2.38	1.40	1.33
4	A	510	OLC	O20-C1	2.37	1.40	1.33
4	A	513	OLC	O20-C1	2.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	OLC	O20-C21	-2.22	1.40	1.45
4	A	508	OLC	O20-C21	-2.20	1.40	1.45
4	A	507	OLC	O20-C21	-2.19	1.40	1.45
4	A	513	OLC	O20-C21	-2.19	1.40	1.45
4	A	519	OLC	O20-C21	-2.17	1.40	1.45
4	A	517	OLC	O20-C21	-2.16	1.40	1.45
4	A	504	OLC	O20-C21	-2.16	1.40	1.45
4	A	505	OLC	O20-C21	-2.16	1.40	1.45
4	A	509	OLC	O20-C21	-2.15	1.40	1.45
4	A	512	OLC	O20-C21	-2.11	1.40	1.45
4	A	521	OLC	O20-C21	-2.11	1.40	1.45
4	A	511	OLC	O20-C21	-2.11	1.40	1.45
4	A	516	OLC	O20-C21	-2.08	1.40	1.45
4	A	515	OLC	O20-C21	-2.06	1.40	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	OLC	O20-C1-C2	2.80	120.37	111.83
4	A	517	OLC	O20-C1-C2	2.77	120.29	111.83
4	A	515	OLC	O20-C1-C2	2.77	120.29	111.83
4	A	516	OLC	O20-C1-C2	2.76	120.24	111.83
4	A	505	OLC	O20-C1-C2	2.74	120.19	111.83
4	A	509	OLC	O20-C1-C2	2.73	120.16	111.83
4	A	513	OLC	O20-C1-C2	2.71	120.10	111.83
4	A	507	OLC	O20-C1-C2	2.63	119.87	111.83
4	A	508	OLC	O20-C1-C2	2.62	119.83	111.83
4	A	521	OLC	O20-C1-C2	2.58	119.72	111.83
4	A	512	OLC	O20-C1-C2	2.57	119.67	111.83
4	A	519	OLC	O20-C1-C2	2.55	119.60	111.83
4	A	510	OLC	O20-C1-C2	2.53	119.54	111.83
4	A	511	OLC	O20-C1-C2	2.43	119.24	111.83

There are no chirality outliers.

All (205) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	OLC	C21-C22-C24-O25
4	A	509	OLC	C21-C22-C24-O25
4	A	511	OLC	C6-C7-C8-C9
4	A	511	OLC	C21-C22-C24-O25
4	A	515	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
4	A	515	OLC	O20-C21-C22-C24
4	A	515	OLC	O20-C21-C22-O23
4	A	515	OLC	C2-C1-O20-C21
4	A	515	OLC	O19-C1-O20-C21
4	A	519	OLC	C21-C22-C24-O25
4	A	519	OLC	O20-C21-C22-C24
4	A	519	OLC	O20-C21-C22-O23
4	A	511	OLC	O19-C1-O20-C21
4	A	509	OLC	C2-C1-O20-C21
4	A	509	OLC	O19-C1-O20-C21
4	A	516	OLC	O19-C1-O20-C21
4	A	511	OLC	C2-C1-O20-C21
4	A	516	OLC	C2-C1-O20-C21
4	A	519	OLC	C2-C1-O20-C21
4	A	519	OLC	O19-C1-O20-C21
4	A	516	OLC	C3-C4-C5-C6
4	A	507	OLC	C2-C1-O20-C21
4	A	508	OLC	C2-C1-O20-C21
4	A	508	OLC	O19-C1-O20-C21
4	A	510	OLC	C2-C1-O20-C21
4	A	504	OLC	C4-C5-C6-C7
4	A	504	OLC	O20-C21-C22-C24
4	A	510	OLC	O19-C1-O20-C21
4	A	509	OLC	O23-C22-C24-O25
4	A	515	OLC	C1-C2-C3-C4
4	A	517	OLC	C1-C2-C3-C4
4	A	514	OLC	C5-C6-C7-C8
4	A	521	OLC	C11-C12-C13-C14
4	A	507	OLC	O19-C1-O20-C21
4	A	504	OLC	O20-C21-C22-O23
4	A	517	OLC	O20-C21-C22-O23
5	A	528	PEG	O2-C3-C4-O4
4	A	517	OLC	O20-C21-C22-C24
4	A	504	OLC	C2-C1-O20-C21
4	A	506	OLC	C2-C3-C4-C5
4	A	511	OLC	C4-C5-C6-C7
4	A	522	OLC	C12-C13-C14-C15
4	A	510	OLC	C14-C15-C16-C17
4	A	514	OLC	C4-C5-C6-C7
4	A	504	OLC	O23-C22-C24-O25
4	A	511	OLC	O23-C22-C24-O25
4	A	515	OLC	O23-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
4	A	519	OLC	O23-C22-C24-O25
4	A	507	OLC	C11-C12-C13-C14
4	A	517	OLC	C2-C3-C4-C5
4	A	518	OLC	C5-C6-C7-C8
4	A	507	OLC	C3-C4-C5-C6
4	A	505	OLC	C2-C3-C4-C5
4	A	513	OLC	C1-C2-C3-C4
4	A	510	OLC	C13-C14-C15-C16
4	A	511	OLC	C2-C3-C4-C5
4	A	524	OLC	C11-C12-C13-C14
4	A	510	OLC	C3-C4-C5-C6
4	A	516	OLC	C2-C3-C4-C5
4	A	525	OLC	C13-C14-C15-C16
4	A	521	OLC	C14-C15-C16-C17
4	A	525	OLC	C14-C15-C16-C17
4	A	504	OLC	C11-C12-C13-C14
4	A	504	OLC	O19-C1-O20-C21
4	A	507	OLC	C10-C11-C12-C13
4	A	517	OLC	C2-C1-O20-C21
4	A	522	OLC	C11-C12-C13-C14
4	A	524	OLC	C12-C13-C14-C15
4	A	517	OLC	C4-C5-C6-C7
4	A	510	OLC	C4-C5-C6-C7
4	A	520	OLC	C13-C14-C15-C16
4	A	519	OLC	C14-C15-C16-C17
4	A	511	OLC	C13-C14-C15-C16
4	A	505	OLC	C6-C7-C8-C9
4	A	521	OLC	C10-C11-C12-C13
4	A	505	OLC	C11-C12-C13-C14
4	A	505	OLC	C3-C4-C5-C6
4	A	506	OLC	C12-C13-C14-C15
4	A	521	OLC	C13-C14-C15-C16
4	A	517	OLC	O19-C1-O20-C21
4	A	509	OLC	C2-C3-C4-C5
4	A	514	OLC	C11-C12-C13-C14
4	A	518	OLC	C11-C12-C13-C14
4	A	514	OLC	C10-C11-C12-C13
4	A	509	OLC	C3-C4-C5-C6
4	A	506	OLC	C11-C12-C13-C14
4	A	507	OLC	C7-C8-C9-C10
4	A	526	OLC	C12-C13-C14-C15
4	A	509	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	515	OLC	C5-C6-C7-C8
4	A	511	OLC	C14-C15-C16-C17
4	A	514	OLC	C3-C4-C5-C6
4	A	505	OLC	C14-C15-C16-C17
4	A	507	OLC	C2-C3-C4-C5
4	A	504	OLC	C10-C11-C12-C13
4	A	507	OLC	C6-C7-C8-C9
4	A	509	OLC	C10-C11-C12-C13
4	A	516	OLC	C10-C11-C12-C13
4	A	524	OLC	C10-C11-C12-C13
4	A	526	OLC	C6-C7-C8-C9
4	A	516	OLC	O20-C21-C22-O23
4	A	505	OLC	C1-C2-C3-C4
4	A	505	OLC	C12-C13-C14-C15
4	A	513	OLC	C2-C3-C4-C5
4	A	507	OLC	C13-C14-C15-C16
4	A	507	OLC	C12-C13-C14-C15
4	A	512	OLC	C3-C4-C5-C6
4	A	518	OLC	C9-C10-C11-C12
4	A	506	OLC	C6-C7-C8-C9
4	A	510	OLC	C10-C11-C12-C13
4	A	518	OLC	C10-C11-C12-C13
4	A	521	OLC	C2-C1-O20-C21
4	A	521	OLC	C3-C4-C5-C6
4	A	516	OLC	C21-C22-C24-O25
4	A	509	OLC	C5-C6-C7-C8
4	A	505	OLC	C2-C1-O20-C21
4	A	514	OLC	C13-C14-C15-C16
4	A	516	OLC	C4-C5-C6-C7
4	A	517	OLC	C3-C4-C5-C6
4	A	514	OLC	C6-C7-C8-C9
4	A	509	OLC	C4-C5-C6-C7
4	A	524	OLC	C15-C16-C17-C18
4	A	506	OLC	C4-C5-C6-C7
4	A	510	OLC	C5-C6-C7-C8
4	A	525	OLC	C12-C13-C14-C15
4	A	507	OLC	C14-C15-C16-C17
4	A	504	OLC	C15-C16-C17-C18
4	A	518	OLC	C12-C13-C14-C15
4	A	521	OLC	O19-C1-O20-C21
4	A	519	OLC	C15-C16-C17-C18
4	A	505	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
4	A	516	OLC	C5-C6-C7-C8
4	A	511	OLC	C3-C4-C5-C6
4	A	518	OLC	C4-C5-C6-C7
4	A	508	OLC	C4-C5-C6-C7
4	A	525	OLC	C15-C16-C17-C18
4	A	512	OLC	C4-C5-C6-C7
4	A	509	OLC	C9-C10-C11-C12
4	A	512	OLC	C6-C7-C8-C9
4	A	522	OLC	C13-C14-C15-C16
4	A	511	OLC	C11-C12-C13-C14
4	A	506	OLC	C5-C6-C7-C8
4	A	512	OLC	C5-C6-C7-C8
4	A	519	OLC	C10-C11-C12-C13
4	A	513	OLC	C3-C4-C5-C6
4	A	519	OLC	C3-C4-C5-C6
4	A	517	OLC	C5-C6-C7-C8
4	A	512	OLC	C2-C3-C4-C5
4	A	511	OLC	C10-C11-C12-C13
5	A	529	PEG	C1-C2-O2-C3
4	A	521	OLC	C15-C16-C17-C18
4	A	514	OLC	C2-C3-C4-C5
4	A	505	OLC	C15-C16-C17-C18
4	A	516	OLC	C11-C12-C13-C14
4	A	523	OLC	C6-C7-C8-C9
4	A	515	OLC	C11-C12-C13-C14
4	A	523	OLC	C4-C5-C6-C7
4	A	515	OLC	C12-C13-C14-C15
4	A	526	OLC	C5-C6-C7-C8
4	A	511	OLC	C5-C6-C7-C8
4	A	527	OLC	C14-C15-C16-C17
4	A	521	OLC	O20-C1-C2-C3
4	A	519	OLC	C11-C12-C13-C14
4	A	510	OLC	C12-C13-C14-C15
4	A	522	OLC	C15-C16-C17-C18
4	A	526	OLC	C11-C12-C13-C14
4	A	513	OLC	C5-C6-C7-C8
4	A	507	OLC	O23-C22-C24-O25
4	A	518	OLC	C1-C2-C3-C4
4	A	513	OLC	C7-C8-C9-C10
4	A	505	OLC	C13-C14-C15-C16
4	A	506	OLC	C3-C4-C5-C6
4	A	504	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	A	516	OLC	O23-C22-C24-O25
4	A	526	OLC	C15-C16-C17-C18
4	A	504	OLC	O20-C1-C2-C3
4	A	513	OLC	C9-C10-C11-C12
4	A	524	OLC	C9-C10-C11-C12
4	A	506	OLC	C9-C10-C11-C12
4	A	507	OLC	C9-C10-C11-C12
4	A	510	OLC	C1-C2-C3-C4
4	A	520	OLC	C9-C10-C11-C12
4	A	521	OLC	C9-C10-C11-C12
4	A	522	OLC	C9-C10-C11-C12
4	A	507	OLC	C4-C5-C6-C7
4	A	510	OLC	C15-C16-C17-C18
4	A	510	OLC	O20-C1-C2-C3
4	A	510	OLC	C9-C10-C11-C12
4	A	504	OLC	C13-C14-C15-C16
4	A	518	OLC	C7-C8-C9-C10
4	A	525	OLC	C10-C11-C12-C13
4	A	515	OLC	C3-C4-C5-C6
4	A	513	OLC	O19-C1-O20-C21
4	A	526	OLC	C13-C14-C15-C16
4	A	515	OLC	C13-C14-C15-C16
4	A	513	OLC	C2-C1-O20-C21
4	A	518	OLC	C13-C14-C15-C16
4	A	512	OLC	O20-C1-C2-C3
4	A	510	OLC	O19-C1-C2-C3
4	A	511	OLC	O20-C1-C2-C3
4	A	527	OLC	C13-C14-C15-C16
4	A	511	OLC	C15-C16-C17-C18
4	A	511	OLC	C9-C10-C11-C12
4	A	511	OLC	O19-C1-C2-C3
4	A	512	OLC	C1-C2-C3-C4

There are no ring outliers.

17 monomers are involved in 31 short contacts:

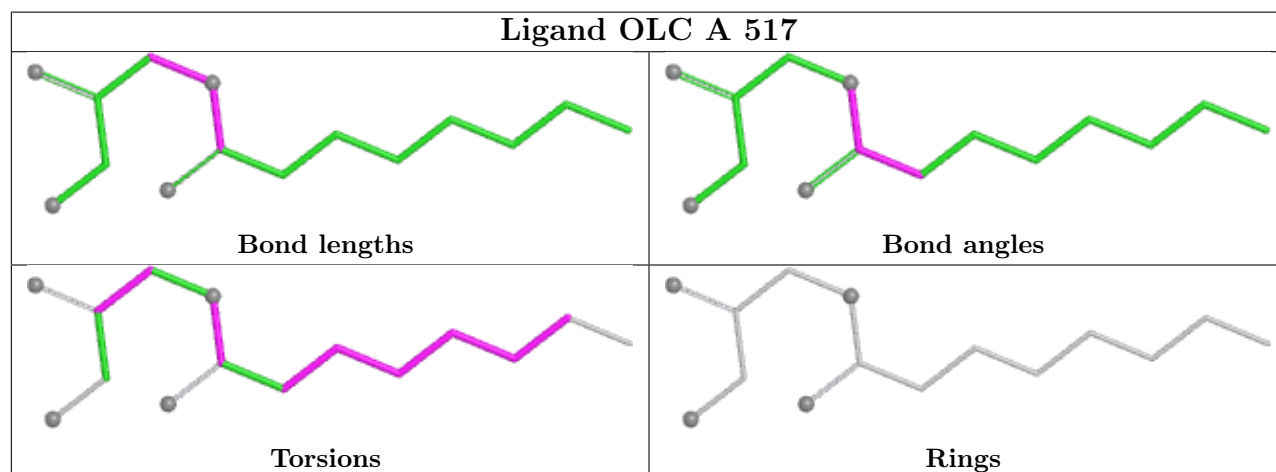
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	511	OLC	3	0
4	A	521	OLC	1	0
4	A	510	OLC	1	0
4	A	507	OLC	3	0
4	A	516	OLC	1	0

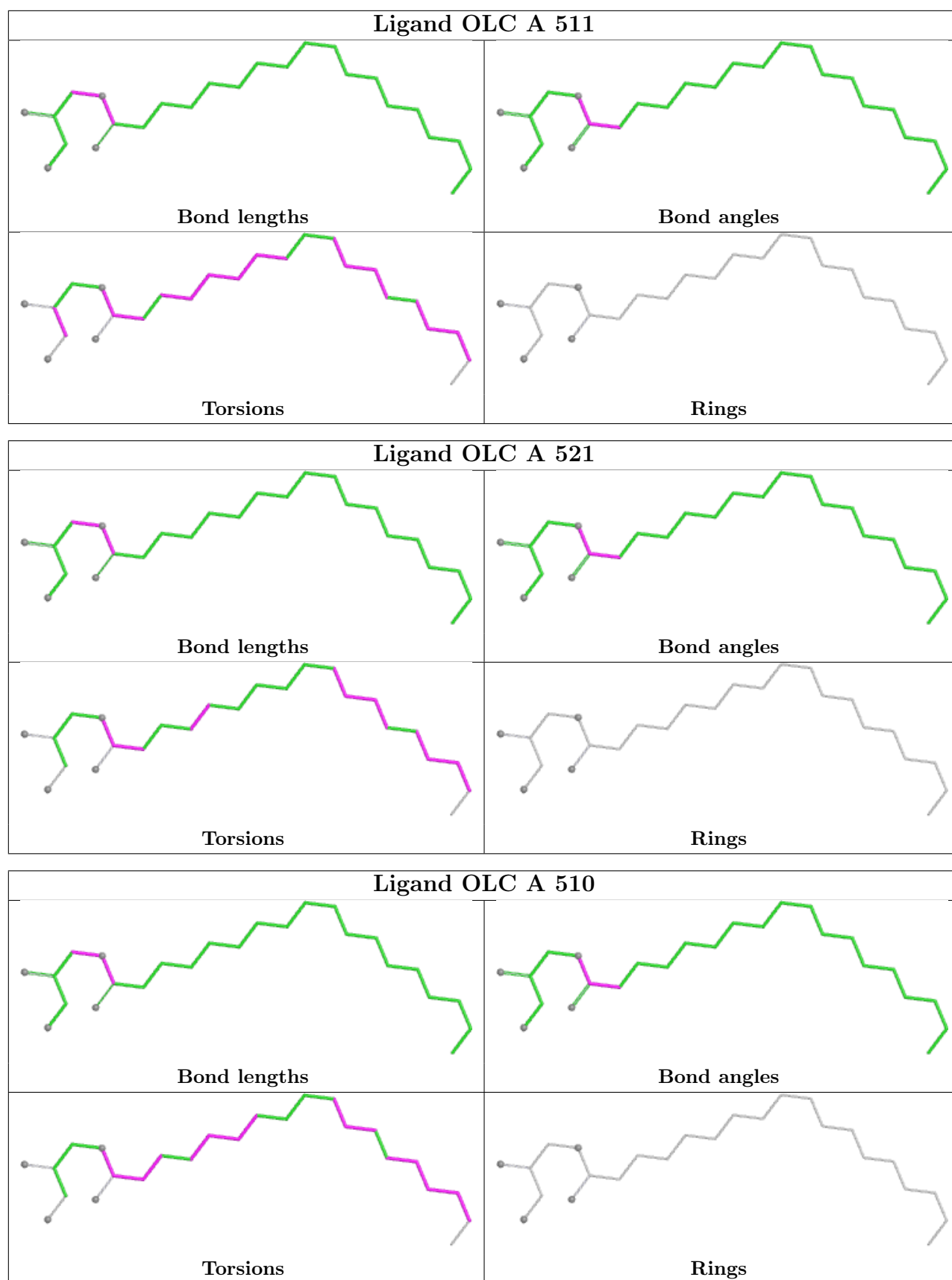
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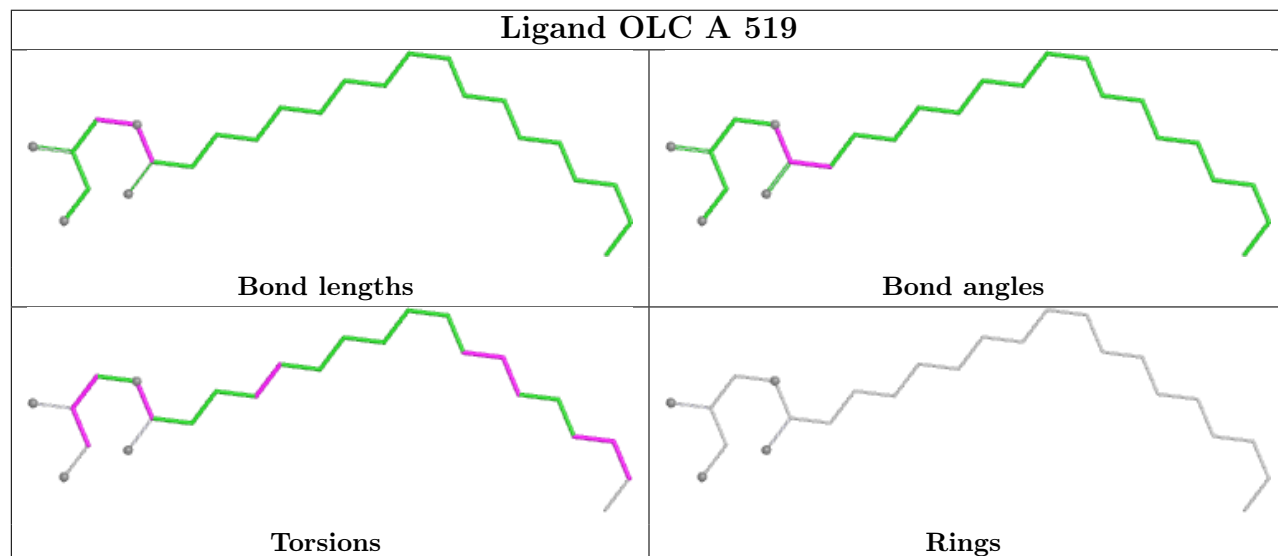
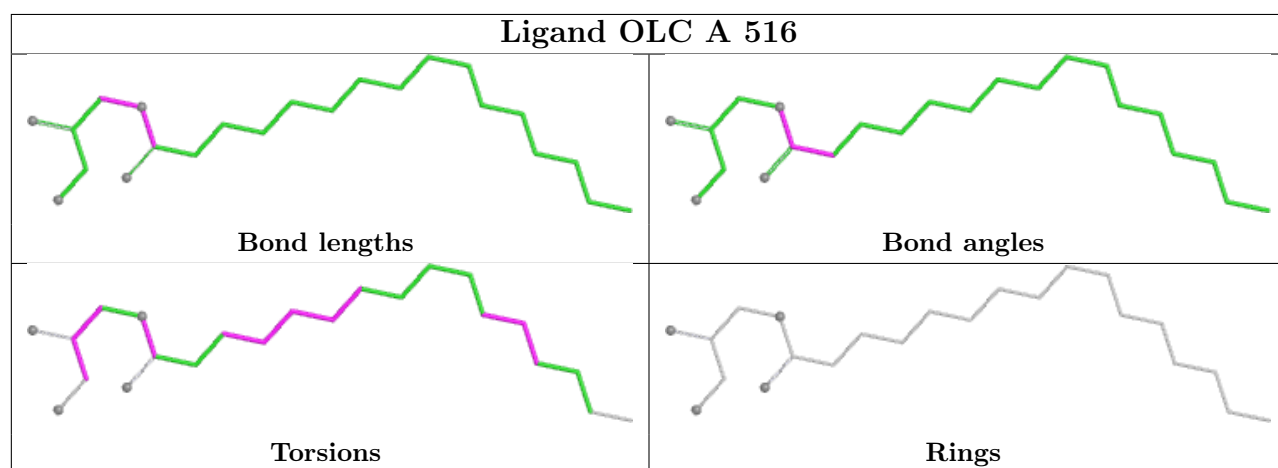
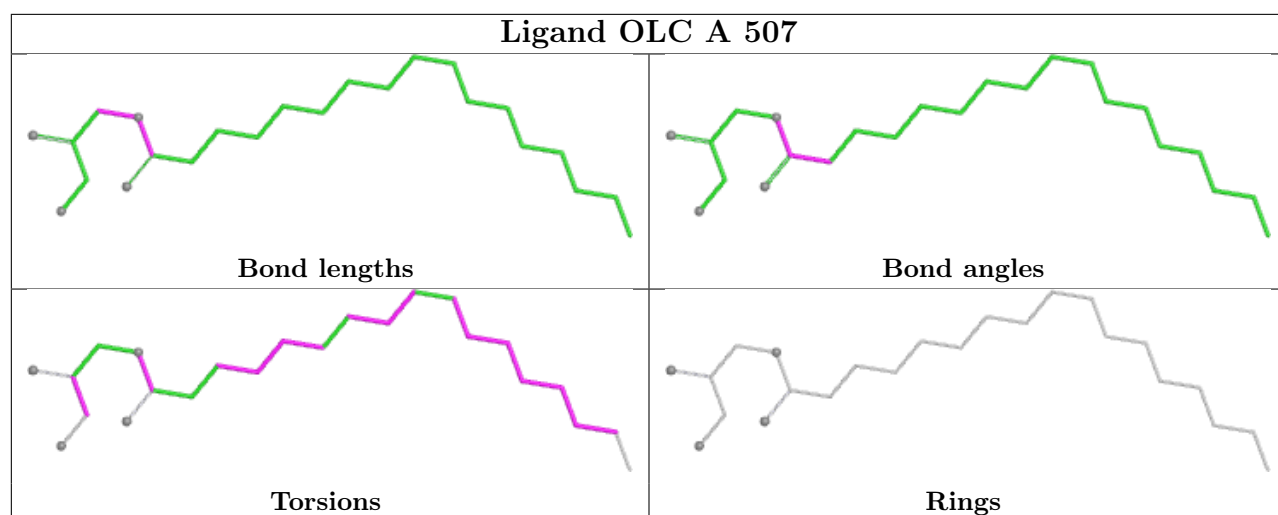
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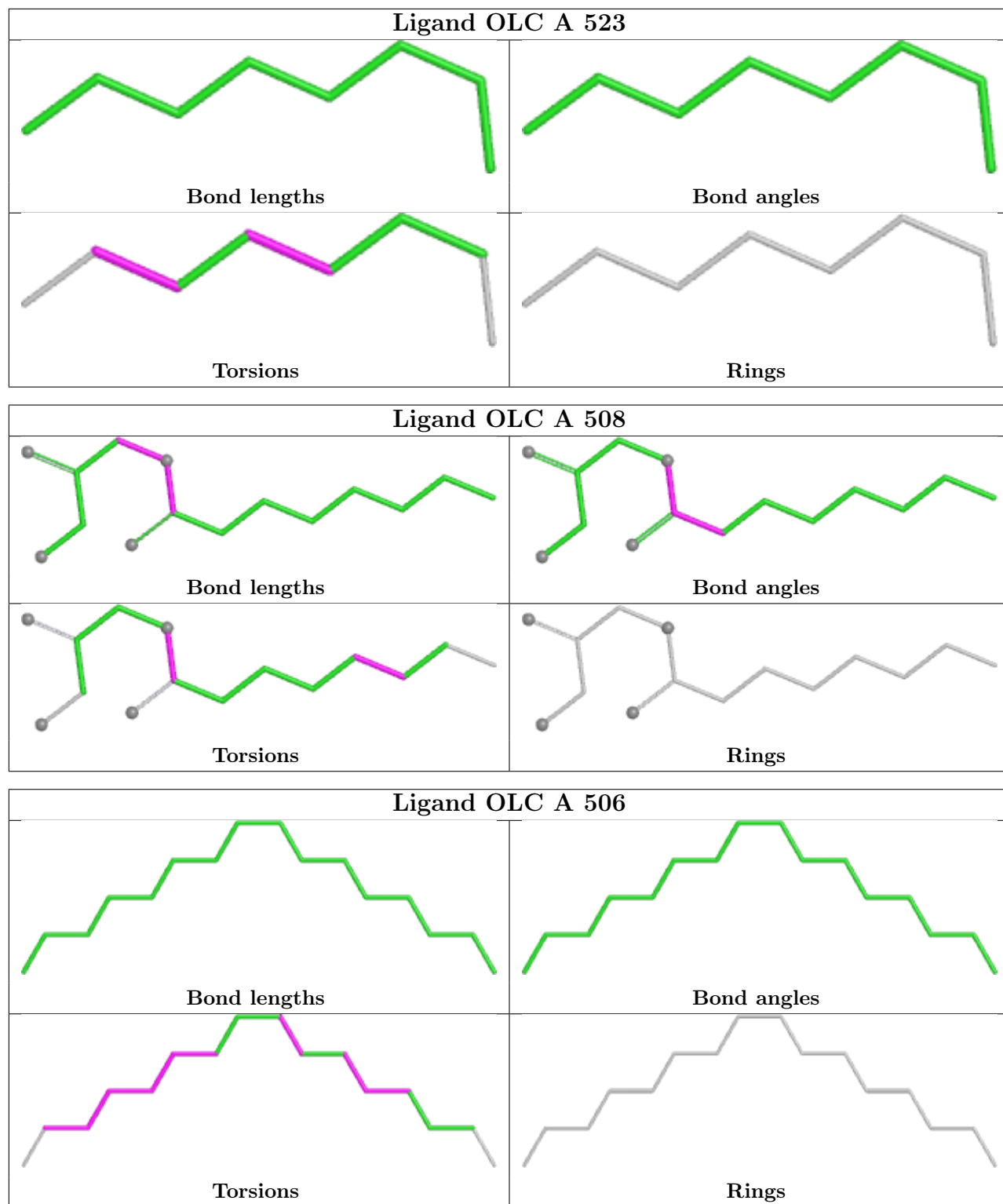
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	519	OLC	2	0
4	A	523	OLC	2	0
4	A	513	OLC	1	0
4	A	512	OLC	3	0
4	A	515	OLC	1	0
4	A	509	OLC	2	0
4	A	505	OLC	2	0
4	A	522	OLC	2	0
4	A	514	OLC	2	0
4	A	504	OLC	1	0
4	A	518	OLC	3	0
4	A	526	OLC	4	0

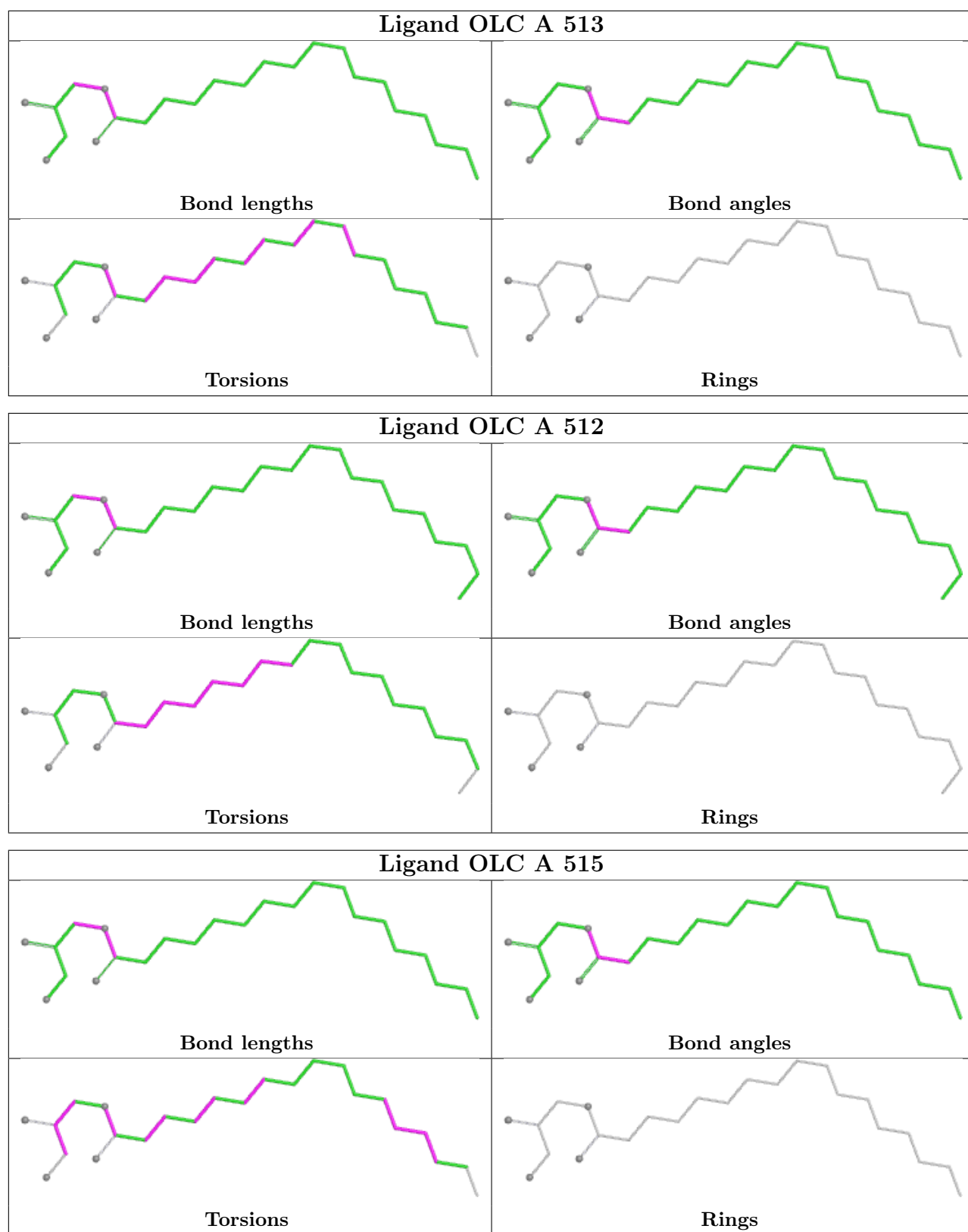
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

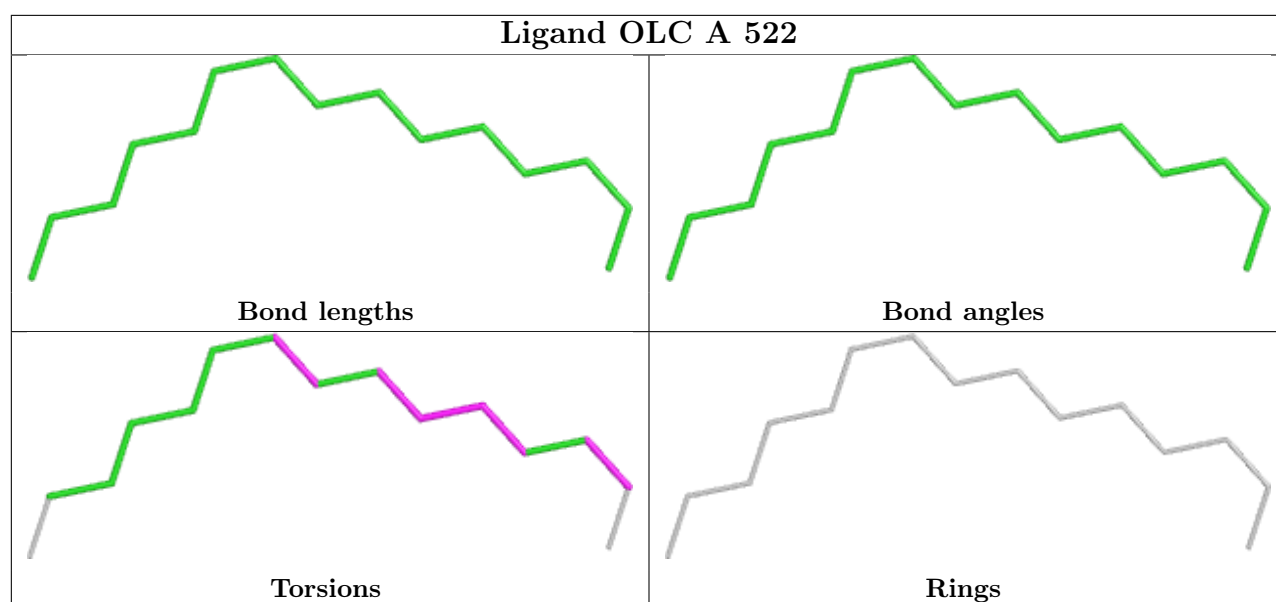
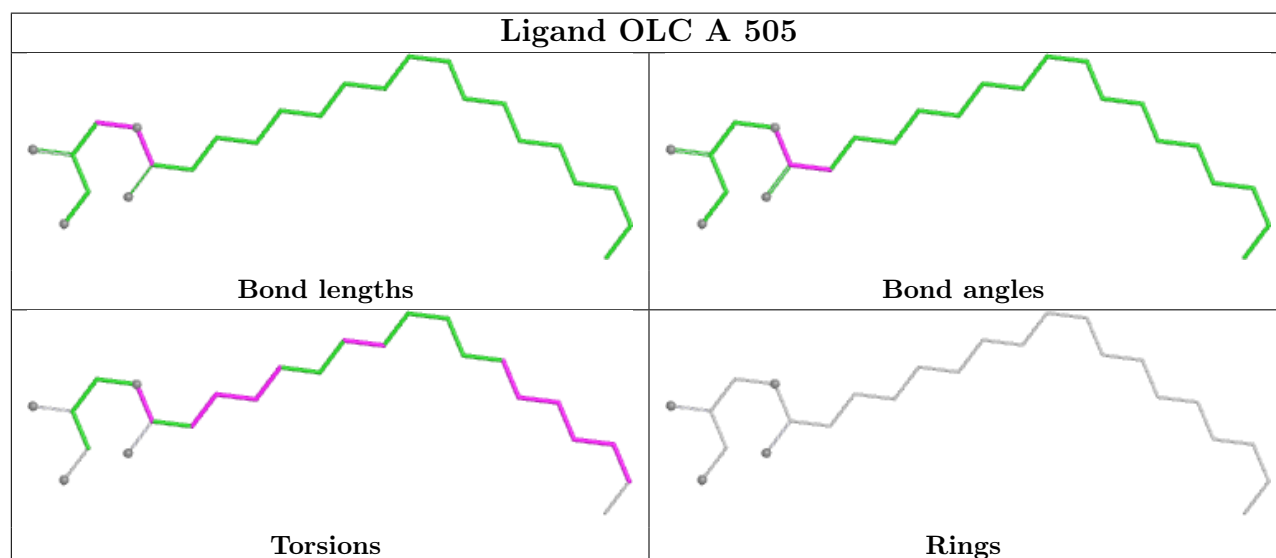
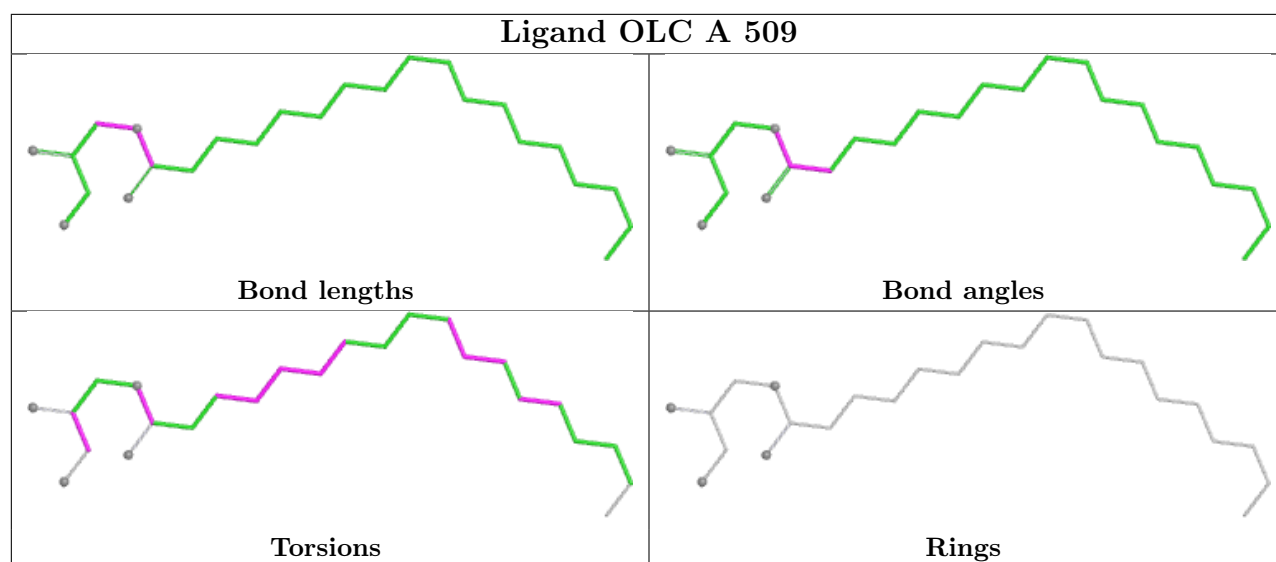


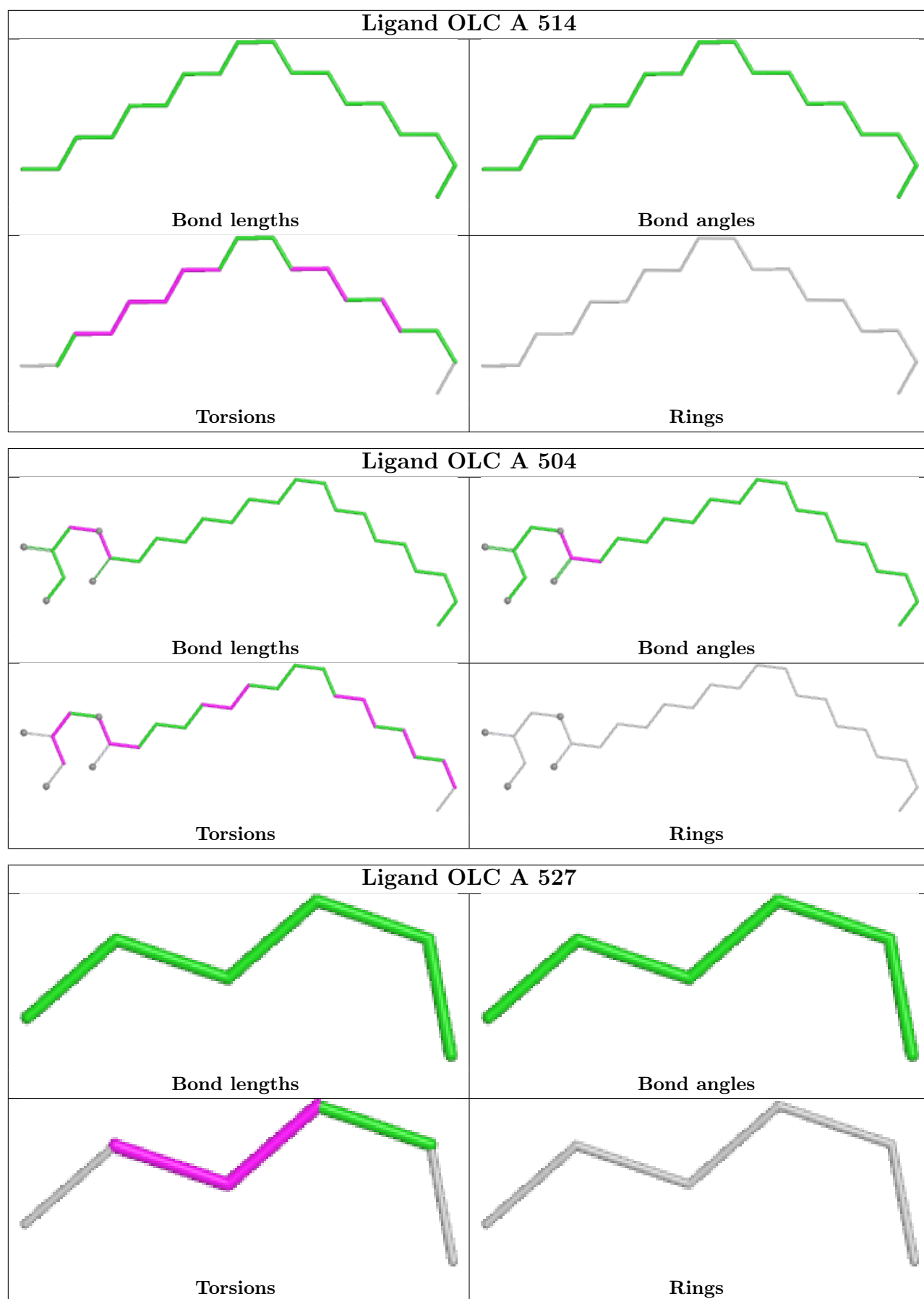


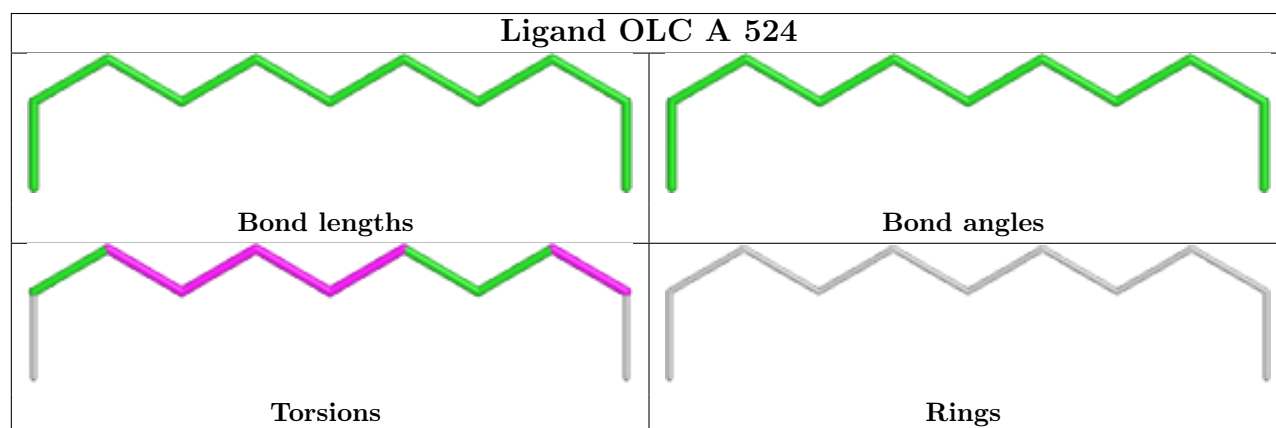
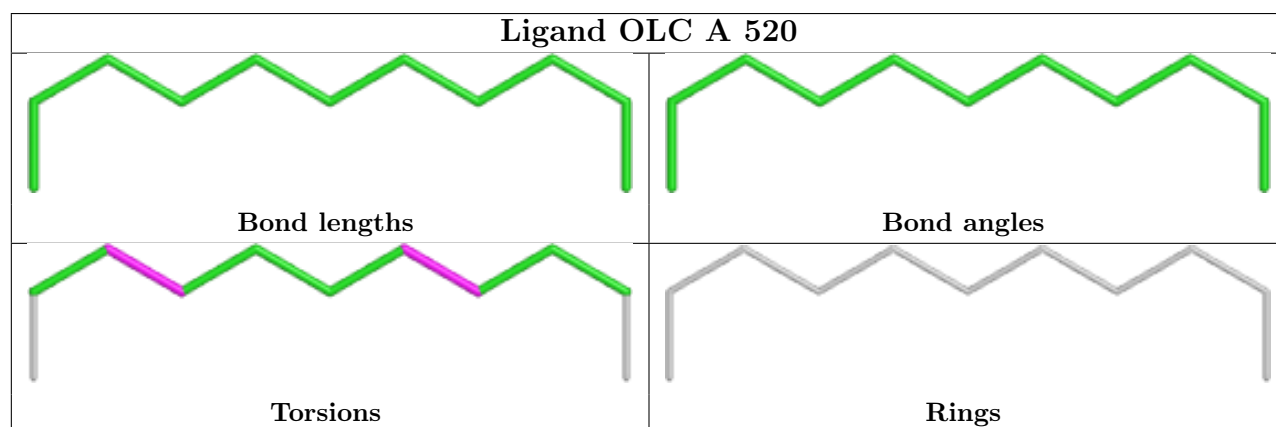
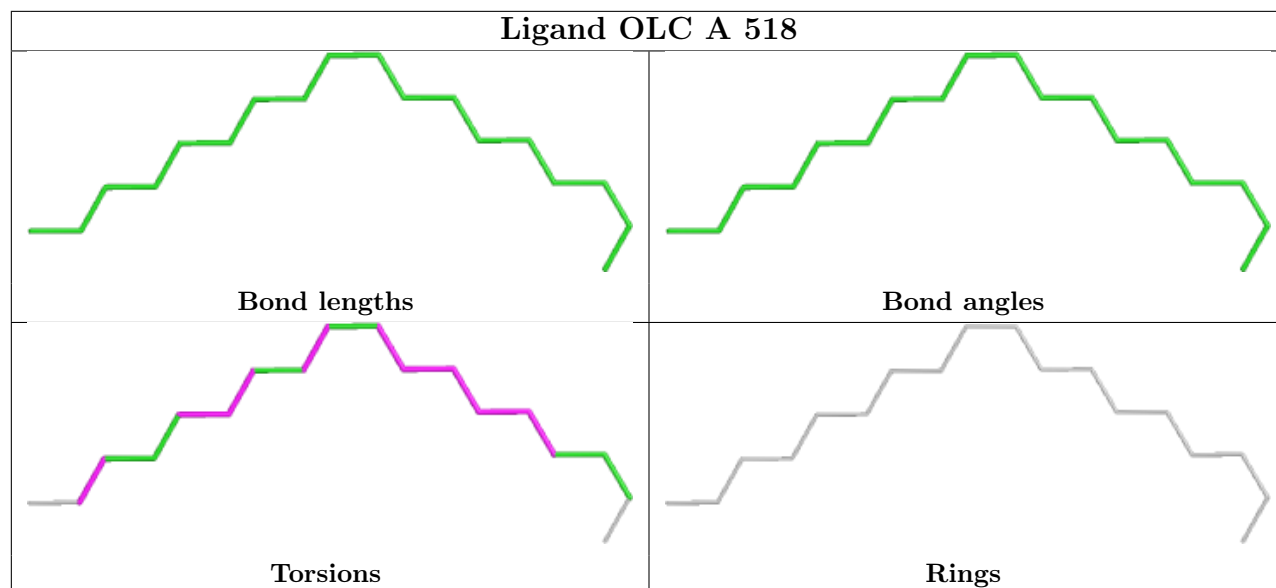


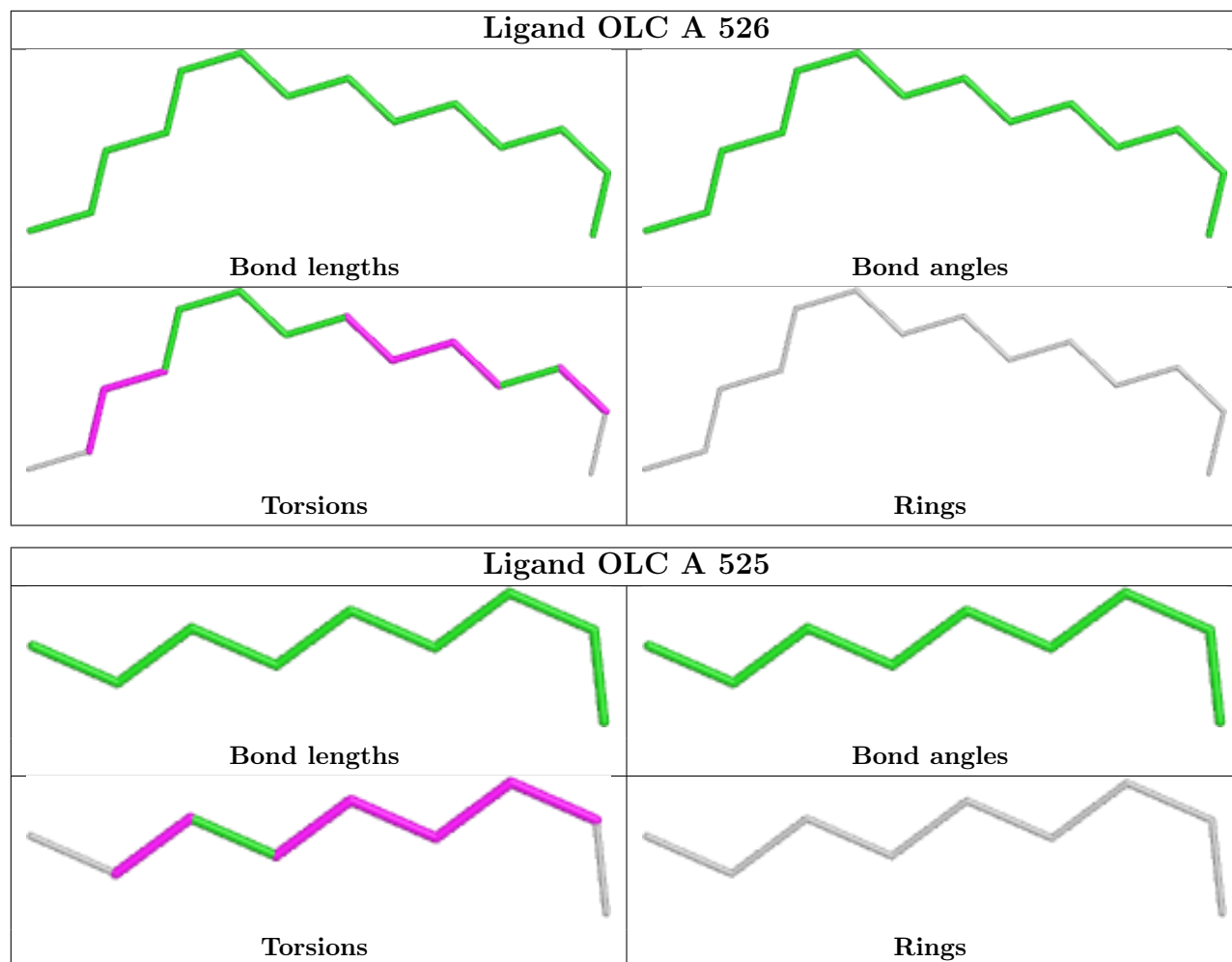












5.7 Other polymers [i](#)

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	392/445 (88%)	0.29	15 (3%) 44 40	28, 41, 83, 135	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	TRP	5.0
1	A	245	ILE	3.4
1	A	50	ALA	2.9
1	A	215	PRO	2.8
1	A	247	THR	2.4
1	A	46	PRO	2.4
1	A	213	GLN	2.4
1	A	249	THR	2.3
1	A	170	ARG	2.3
1	A	45	GLY	2.3
1	A	248	ASP	2.2
1	A	49	ILE	2.2
1	A	117	TRP	2.1
1	A	173	ARG	2.1
1	A	169	LYS	2.1

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 ⓘ

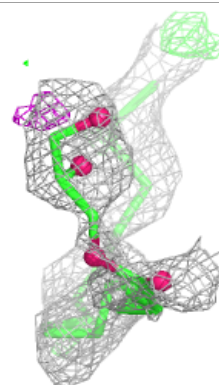
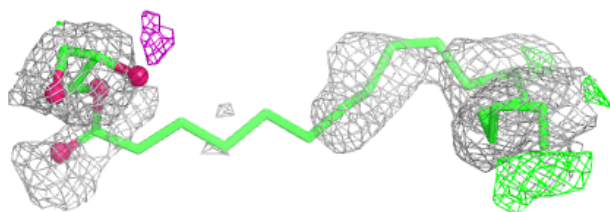
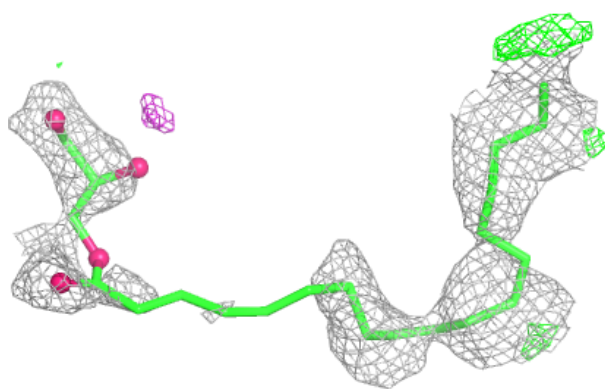
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLC	A	521	25/25	0.58	0.16	68,83,101,104	0
4	OLC	A	520	11/25	0.66	0.22	66,77,85,92	0
5	PEG	A	530	3/7	0.66	0.17	51,51,64,66	0
4	OLC	A	519	25/25	0.69	0.16	45,80,98,100	0
4	OLC	A	514	18/25	0.69	0.18	47,72,79,81	0
4	OLC	A	515	24/25	0.71	0.17	44,75,92,94	0
4	OLC	A	517	15/25	0.71	0.15	67,80,88,98	0
4	OLC	A	513	24/25	0.71	0.17	57,69,77,83	0
4	OLC	A	512	25/25	0.72	0.17	51,75,98,103	0
4	OLC	A	522	15/25	0.73	0.18	49,63,71,80	0
4	OLC	A	526	14/25	0.73	0.19	64,81,88,89	0
4	OLC	A	527	6/25	0.73	0.18	45,47,55,63	0
5	PEG	A	529	7/7	0.73	0.18	46,51,68,74	0
4	OLC	A	518	18/25	0.73	0.19	52,68,82,82	0
4	OLC	A	510	25/25	0.74	0.16	52,65,82,85	0
4	OLC	A	507	24/25	0.74	0.15	57,69,76,80	0
4	OLC	A	508	15/25	0.74	0.17	50,75,94,95	0
4	OLC	A	511	25/25	0.75	0.17	47,65,82,86	0
4	OLC	A	524	11/25	0.75	0.23	49,80,101,101	0
4	OLC	A	516	23/25	0.76	0.14	49,76,94,99	0
4	OLC	A	504	25/25	0.76	0.16	46,58,72,75	0
4	OLC	A	509	25/25	0.76	0.15	40,69,78,83	0
4	OLC	A	523	8/25	0.77	0.16	63,71,80,81	0
4	OLC	A	525	9/25	0.77	0.17	50,58,71,81	0
4	OLC	A	506	16/25	0.82	0.14	36,55,63,64	0
4	OLC	A	505	25/25	0.83	0.14	40,56,69,73	0
5	PEG	A	528	5/7	0.86	0.14	46,47,56,69	0
2	MN	A	501	1/1	0.98	0.05	39,39,39,39	1
3	CL	A	503	1/1	0.99	0.12	43,43,43,43	0
2	MN	A	502	1/1	0.99	0.04	42,42,42,42	0

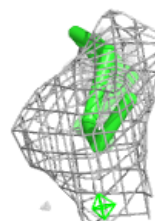
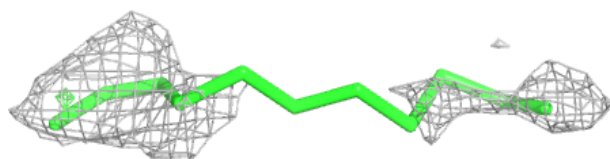
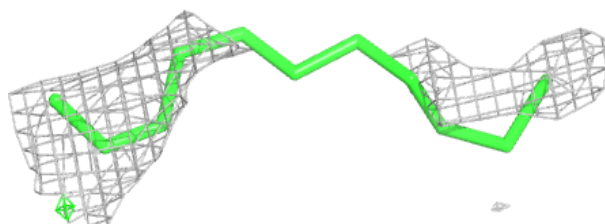
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 521:

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

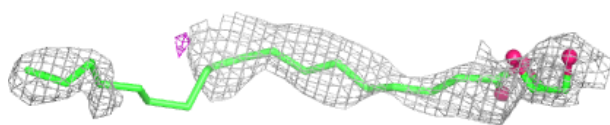
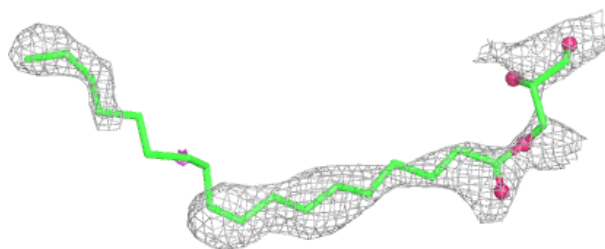
**Electron density around OLC A 520:**

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

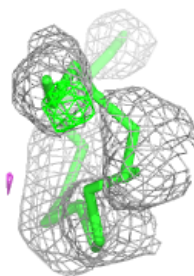
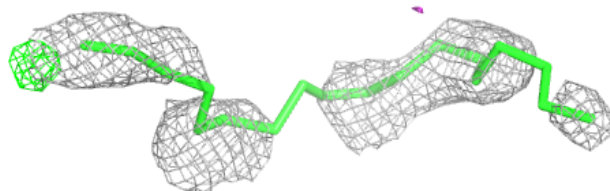
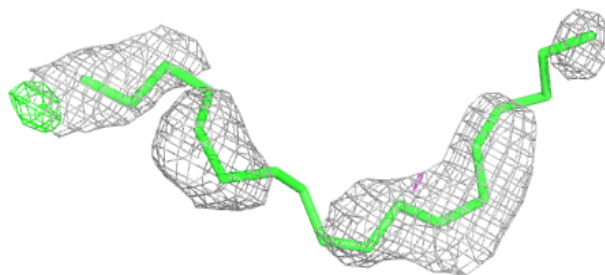


Electron density around OLC A 519:

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

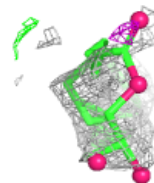
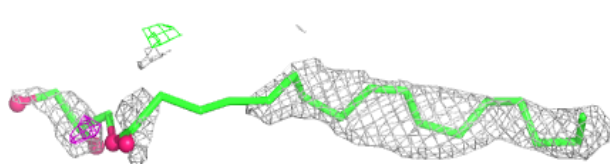
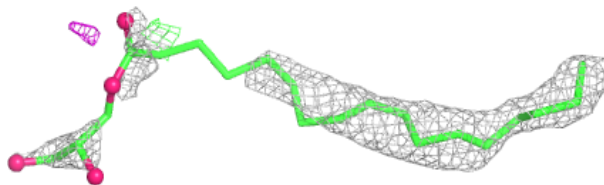
**Electron density around OLC A 514:**

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

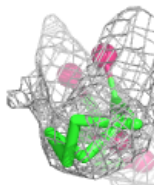
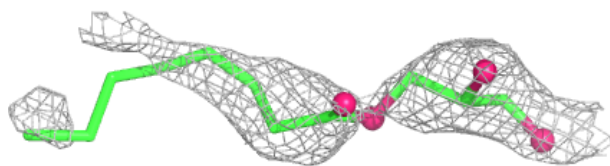
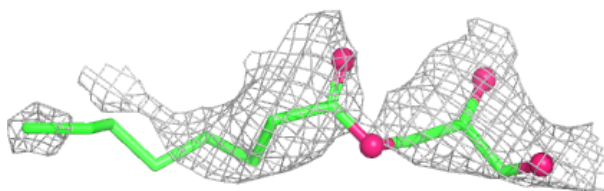


Electron density around OLC A 515:

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

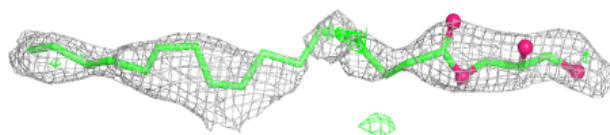
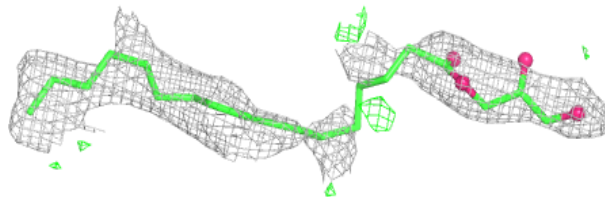
**Electron density around OLC A 517:**

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

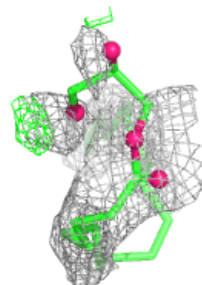
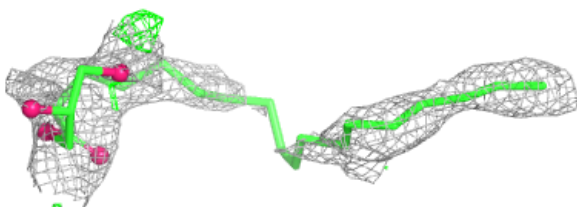
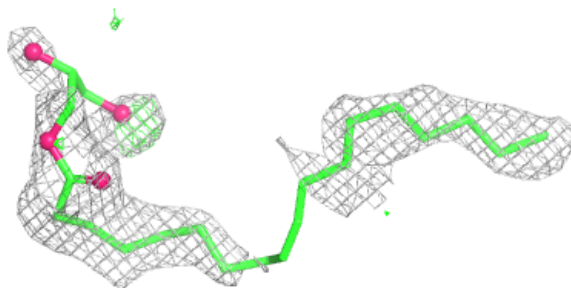


Electron density around OLC A 513:

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

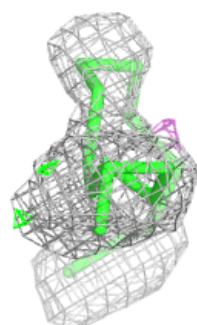
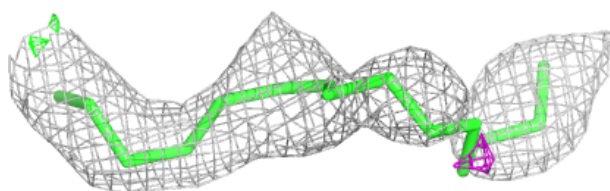
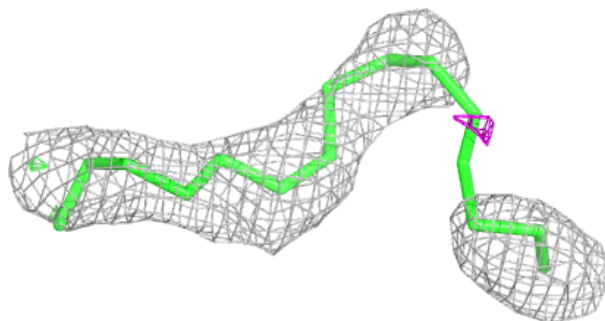
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

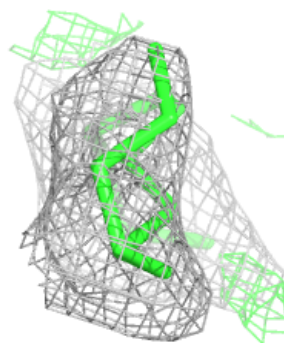
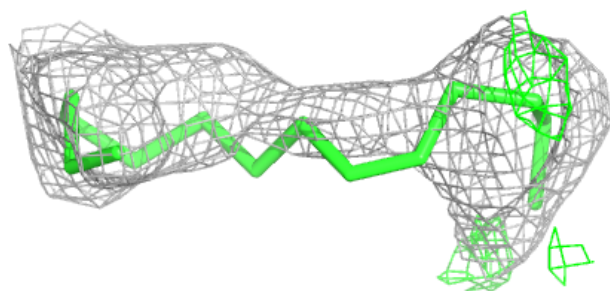
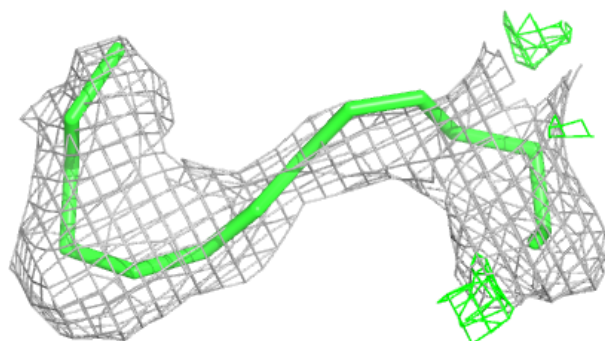


Electron density around OLC A 522:

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

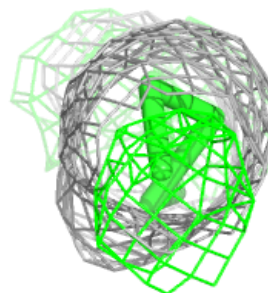
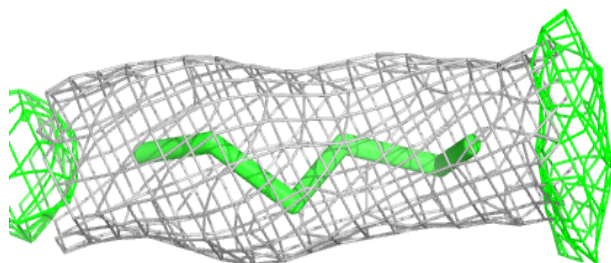
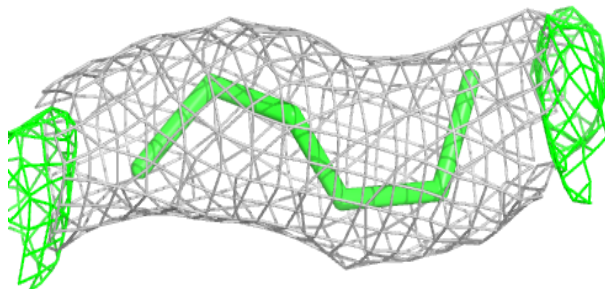
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

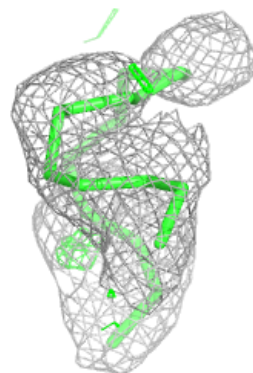
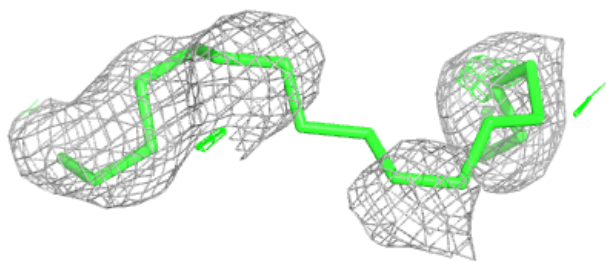
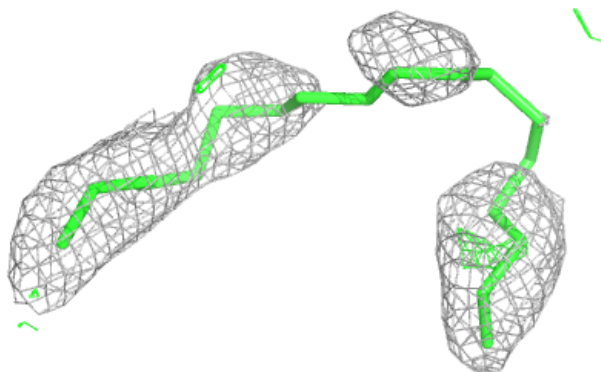


Electron density around OLC A 527:

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

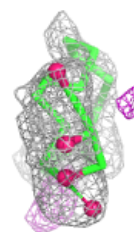
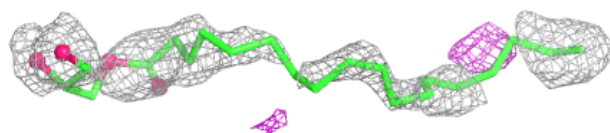
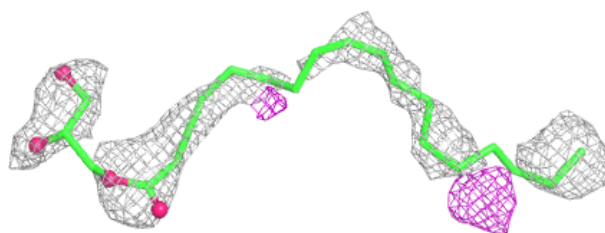
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

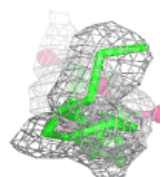
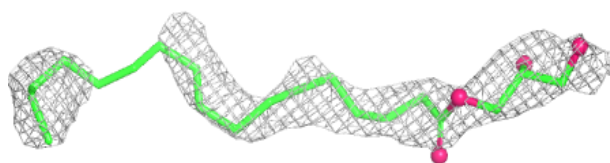
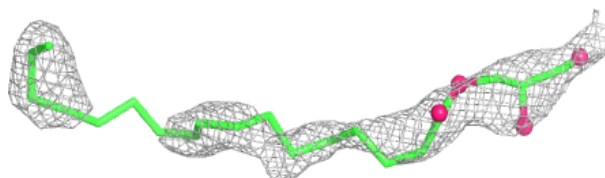


Electron density around OLC A 510:

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

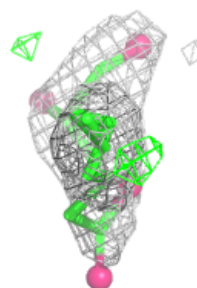
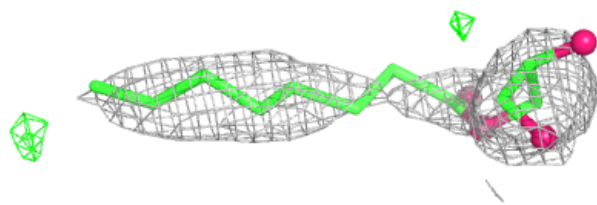
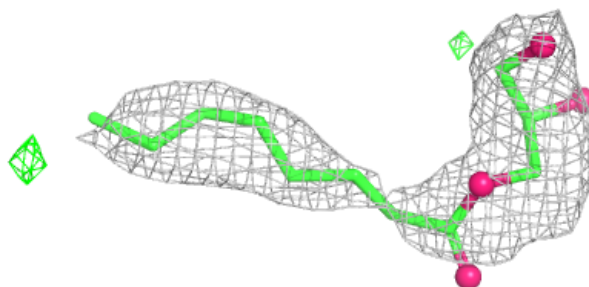
**Electron density around OLC A 507:**

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and green (positive)

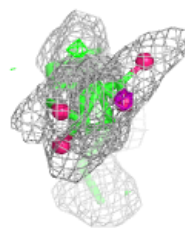
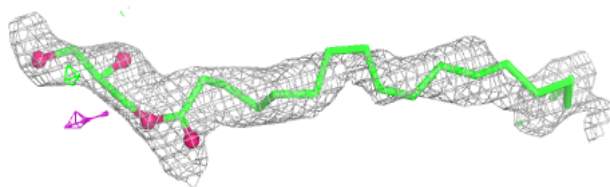
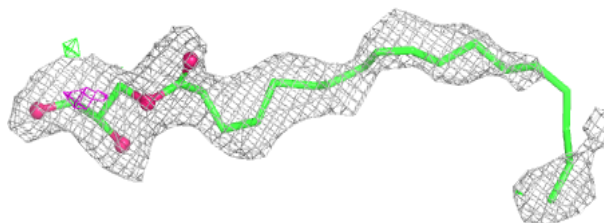


Electron density around OLC A 508:

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

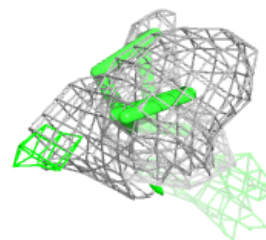
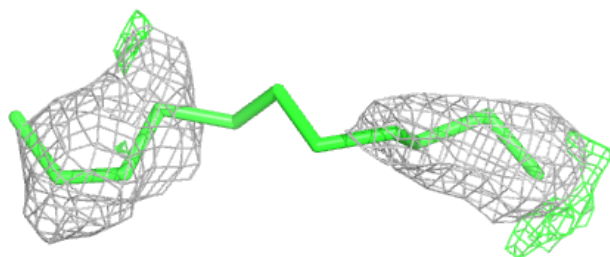
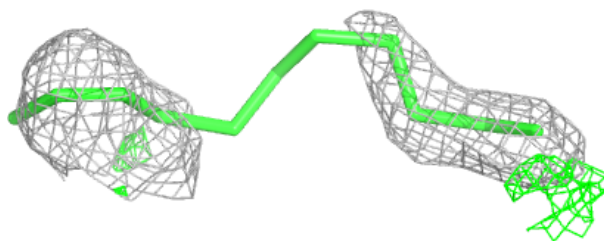
**Electron density around OLC A 511:**

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

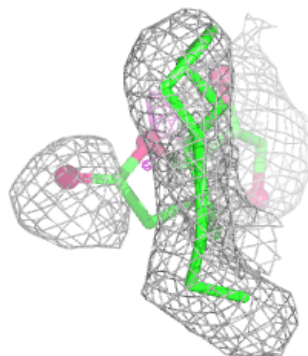
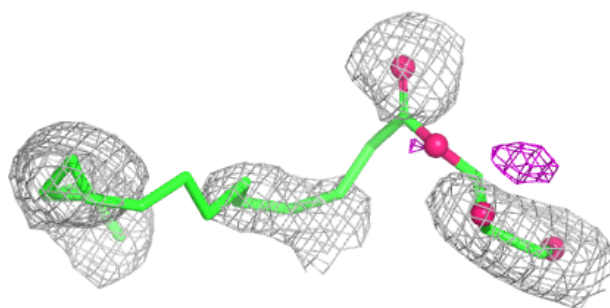
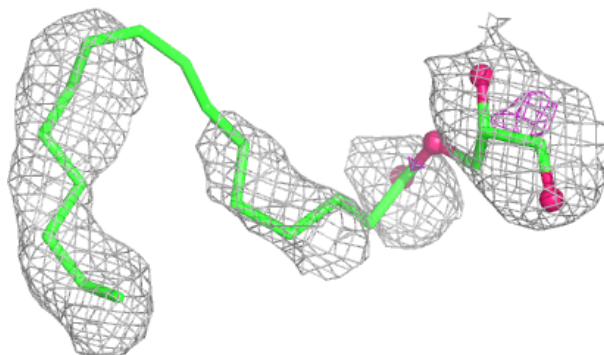


Electron density around OLC A 524:

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

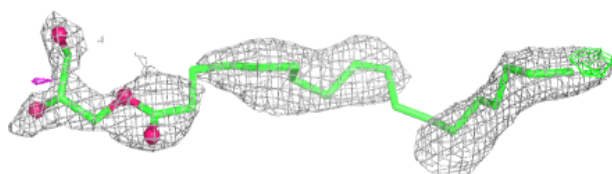
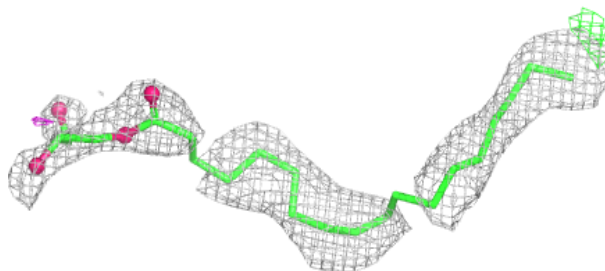
**Electron density around OLC A 516:**

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

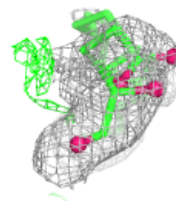
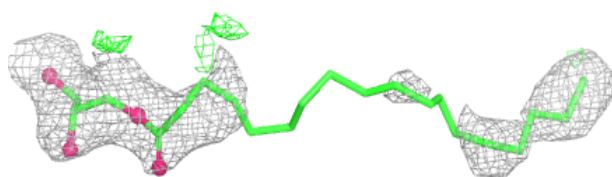
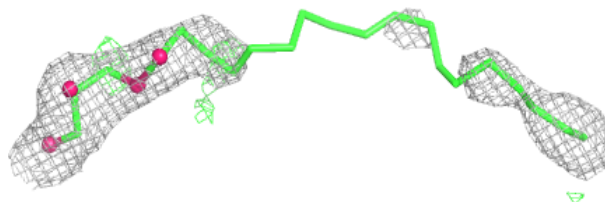


Electron density around OLC A 504:

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

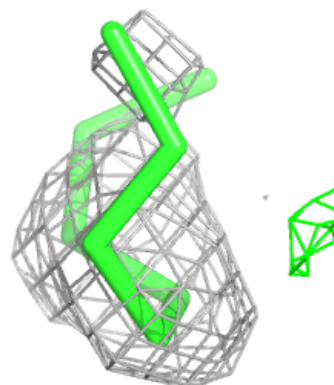
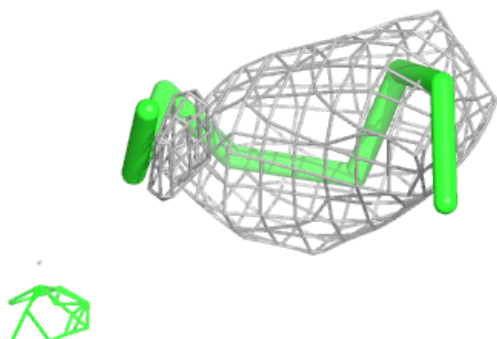
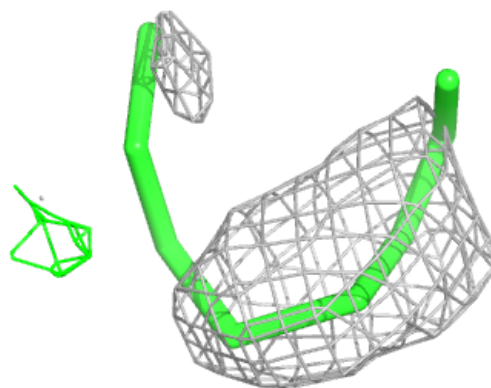
**Electron density around OLC A 509:**

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and green (positive)

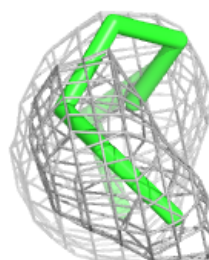
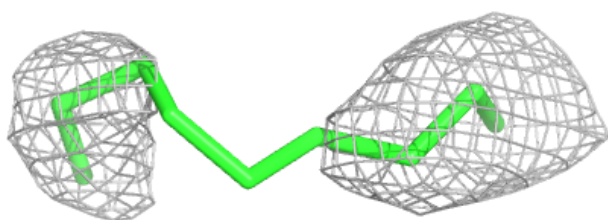
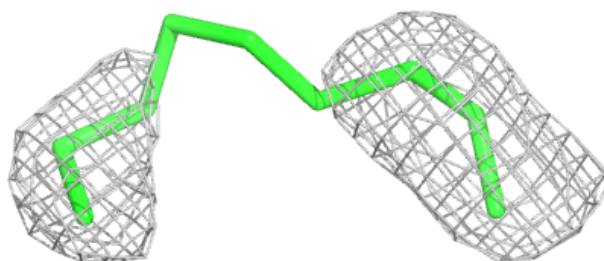


Electron density around OLC A 523:

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

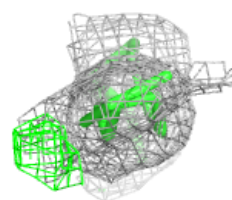
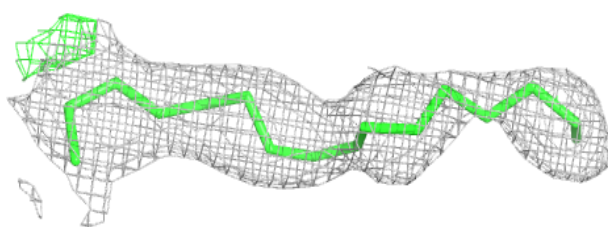
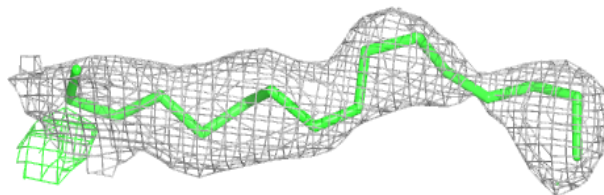
**Electron density around OLC A 525:**

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

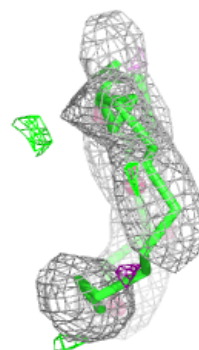
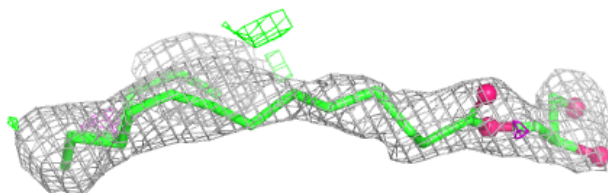
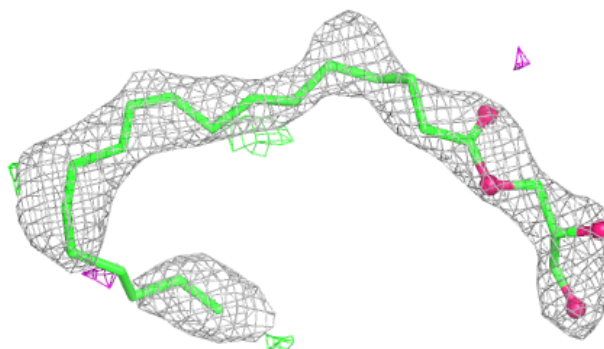


Electron density around OLC A 506:

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

**Electron density around OLC 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.