



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 12:50 AM EDT

PDB ID : 8E60
Title : X-ray structure of the Deinococcus radiodurans Nramp/MntH divalent transition metal transporter WT in an occluded, manganese-bound state
Authors : Ray, S.; Gaudet, R.
Deposited on : 2022-08-22
Resolution : 2.38 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

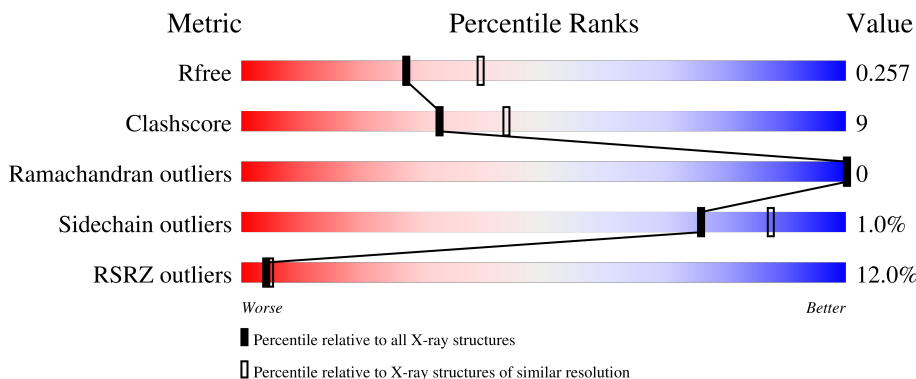
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLC	A	509	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLC	A	519	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3385 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
			Total	C	N	O	S			
1	A	393	2933	1927	489	500	17	0	1	0

There are 9 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

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is CHLORIDE ION (three-letter code: 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 (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



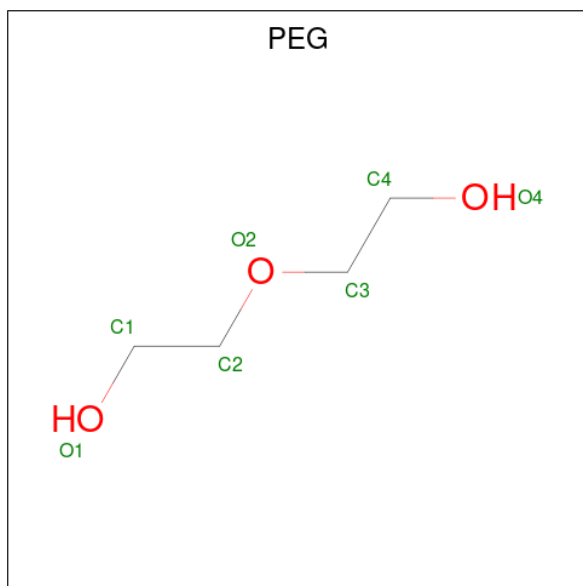
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C 14 14	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 18 14 4	0	0
4	A	1	Total C O 16 12 4	0	0
4	A	1	Total C 13 13	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C 17 17	0	0
4	A	1	Total C O 13 9 4	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 15 15	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C O 24 20 4	0	0
4	A	1	Total C O 16 12 4	0	0
4	A	1	Total C O 18 14 4	0	0
4	A	1	Total C 16 16	0	0
4	A	1	Total C O 19 15 4	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C O 15 11 4	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

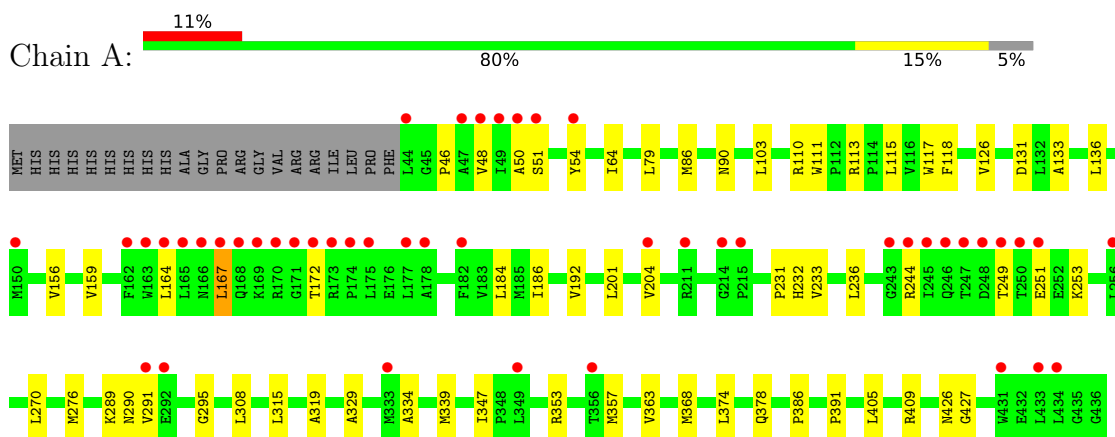
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	47	Total	O	0	0
			47	47		

3 Residue-property plots [i](#)

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

- Molecule 1: Divalent metal cation transporter MntH



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.08Å 71.10Å 98.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.28 – 2.38 41.28 – 2.38	Depositor EDS
% Data completeness (in resolution range)	95.1 (41.28-2.38) 95.1 (41.28-2.38)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.259 0.207 , 0.257	Depositor DCC
R_{free} test set	1642 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3385	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.38% 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: MN, OLC, GOL, CL, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/2996	0.44	0/4097

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	2933	0	3058	45	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	377	0	590	35	0
5	A	19	0	25	3	0
6	A	6	0	8	0	0
7	A	47	0	0	0	0
All	All	3385	0	3681	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (61) 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:386:PRO:HG2	4:A:511:OLC:H16	1.67	0.76
1:A:270:LEU:HB2	4:A:514:OLC:H6A	1.69	0.75
1:A:201:LEU:HD11	4:A:522:OLC:H3	1.75	0.68
4:A:506:OLC:H6	4:A:520:OLC:H7	1.74	0.68
1:A:133:ALA:HA	1:A:374:LEU:HD22	1.82	0.61
1:A:115:LEU:HD21	4:A:505:OLC:H9	1.82	0.60
1:A:110:ARG:HB3	5:A:527:PEG:H11	1.82	0.60
1:A:167:LEU:HD23	1:A:172:THR:HG22	1.84	0.59
1:A:113:ARG:HG3	5:A:529:PEG:H32	1.86	0.57
1:A:184:LEU:HD21	4:A:523:OLC:H16	1.87	0.57
4:A:515:OLC:H12A	4:A:515:OLC:H18A	1.87	0.56
1:A:156:VAL:HG22	4:A:517:OLC:H17A	1.85	0.56
1:A:48:VAL:HG22	4:A:523:OLC:H7	1.88	0.56
1:A:363:VAL:HG13	1:A:368:MET:HB2	1.88	0.55
1:A:86:MET:O	1:A:90:ASN:ND2	2.32	0.54
1:A:236:LEU:HD22	1:A:334:ALA:HB2	1.90	0.54
4:A:504:OLC:H8A	4:A:518:OLC:H10	1.90	0.54
1:A:79:LEU:HD23	4:A:515:OLC:H17	1.90	0.52
1:A:339:MET:HE3	1:A:347:ILE:H	1.74	0.52
1:A:409:ARG:HD3	4:A:507:OLC:H24A	1.91	0.52
1:A:276:MET:HE1	4:A:506:OLC:H13A	1.92	0.51
1:A:192:VAL:HG22	4:A:510:OLC:H6	1.93	0.51
1:A:50:ALA:HB1	1:A:54:TYR:HE1	1.76	0.50
1:A:164:LEU:HD23	1:A:329:ALA:HB2	1.94	0.50
1:A:51:SER:HB3	4:A:523:OLC:H16A	1.95	0.49
1:A:103:LEU:HD11	1:A:391:PRO:HB2	1.94	0.48
1:A:353:ARG:HG3	1:A:357:MET:HE3	1.94	0.48
4:A:524:OLC:H6	4:A:524:OLC:H9	1.67	0.47
1:A:270:LEU:HD23	4:A:523:OLC:H13A	1.97	0.47
1:A:118:PHE:HD1	4:A:512:OLC:H5A	1.79	0.46
4:A:516:OLC:H14	4:A:516:OLC:H17A	1.82	0.46
4:A:524:OLC:H2	4:A:524:OLC:H21	1.53	0.46
1:A:339:MET:HB3	1:A:339:MET:HE2	1.80	0.45
1:A:159:VAL:HG21	4:A:517:OLC:H18B	1.96	0.45
1:A:232:HIS:CE1	1:A:233:VAL:HG23	2.51	0.45
1:A:374:LEU:O	1:A:378:GLN:HG2	2.17	0.45
1:A:111:TRP:CZ2	4:A:505:OLC:H7A	2.51	0.45
1:A:204:VAL:HG11	4:A:520:OLC:H11	1.98	0.45
4:A:516:OLC:H10	4:A:516:OLC:H13	1.51	0.44
1:A:111:TRP:HE1	5:A:527:PEG:H42	1.82	0.44
4:A:511:OLC:H14	4:A:511:OLC:H11A	1.73	0.44
1:A:426:ASN:HB2	4:A:511:OLC:H15	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:517:OLC:H15	4:A:517:OLC:H18A	1.75	0.43
4:A:516:OLC:H2A	4:A:516:OLC:H21	1.79	0.43
1:A:136:LEU:HD23	1:A:136:LEU:HA	1.83	0.43
4:A:522:OLC:H7	4:A:522:OLC:H4	1.74	0.43
4:A:507:OLC:H6A	4:A:507:OLC:H3	1.67	0.42
1:A:64:ILE:HG22	1:A:295:GLY:HA2	2.01	0.42
1:A:253:LYS:HB3	1:A:405:LEU:HD11	2.00	0.42
4:A:505:OLC:H11A	4:A:505:OLC:H8A	1.86	0.41
1:A:186:ILE:HG13	1:A:319:ALA:HB2	2.02	0.41
1:A:427:GLY:HA3	4:A:511:OLC:H7	2.01	0.41
4:A:523:OLC:H5	4:A:523:OLC:H8A	1.77	0.41
1:A:131:ASP:OD2	1:A:353:ARG:NH2	2.53	0.41
4:A:510:OLC:H8	4:A:510:OLC:H11	1.77	0.41
4:A:511:OLC:H7	4:A:511:OLC:H10	1.76	0.41
1:A:308:LEU:HD13	1:A:315:LEU:HD12	2.02	0.40
1:A:289:LYS:HB2	1:A:291:VAL:HG23	2.04	0.40
1:A:46:PRO:HD3	1:A:244:ARG:NH1	2.35	0.40
1:A:249:THR:HG22	1:A:251:GLU:H	1.86	0.40
1:A:126:VAL:HG11	1:A:231:PRO:HB2	2.04	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%)	386 (98%)	6 (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	299/322 (93%)	296 (99%)	3 (1%)	76 87

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

Mol	Chain	Res	Type
1	A	117	TRP
1	A	167	LEU
1	A	290	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	232	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 monosaccharides 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
5	PEG	A	529	-	4,4,6	0.42	0	3,3,5	0.30	0
4	OLC	A	509	-	12,12,24	0.34	0	11,11,25	0.72	0
5	PEG	A	528	-	6,6,6	0.49	0	5,5,5	0.27	0
4	OLC	A	518	-	14,14,24	0.33	0	13,13,25	0.73	0
4	OLC	A	510	-	24,24,24	0.81	2 (8%)	25,25,25	0.95	1 (4%)
4	OLC	A	524	-	18,18,24	0.94	2 (11%)	18,19,25	1.05	1 (5%)
4	OLC	A	525	-	6,6,24	0.31	0	5,5,25	0.66	0
4	OLC	A	514	-	15,15,24	0.33	0	14,14,25	0.72	0
4	OLC	A	508	-	15,15,24	0.99	2 (13%)	16,16,25	1.11	1 (6%)
4	OLC	A	521	-	15,15,24	0.99	2 (13%)	16,16,25	1.08	1 (6%)
4	OLC	A	506	-	24,24,24	0.81	2 (8%)	25,25,25	1.00	1 (4%)
4	OLC	A	523	-	15,15,24	0.34	0	14,14,25	0.69	0
5	PEG	A	527	-	6,6,6	0.48	0	5,5,5	0.25	0
4	OLC	A	513	-	6,6,24	0.31	0	5,5,25	0.68	0
4	OLC	A	511	-	16,16,24	0.32	0	15,15,25	0.81	0
4	OLC	A	516	-	24,24,24	0.81	2 (8%)	25,25,25	0.94	1 (4%)
4	OLC	A	520	-	23,23,24	0.82	2 (8%)	24,24,25	0.92	1 (4%)
4	OLC	A	512	-	12,12,24	1.09	2 (16%)	13,13,25	1.03	1 (7%)
6	GOL	A	530	-	5,5,5	0.56	0	5,5,5	0.23	0
4	OLC	A	519	-	15,15,24	0.33	0	14,14,25	0.77	0
4	OLC	A	504	-	24,24,24	0.81	2 (8%)	25,25,25	0.95	1 (4%)
4	OLC	A	526	-	14,14,24	1.03	2 (14%)	15,15,25	1.04	1 (6%)
4	OLC	A	515	-	8,8,24	0.31	0	7,7,25	0.73	0
4	OLC	A	505	-	13,13,24	0.32	0	12,12,25	0.69	0
4	OLC	A	522	-	17,17,24	0.95	2 (11%)	18,18,25	1.05	1 (5%)
4	OLC	A	507	-	17,17,24	0.95	2 (11%)	18,18,25	1.10	1 (5%)
4	OLC	A	517	-	7,7,24	0.30	0	6,6,25	0.72	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
5	PEG	A	529	-	-	1/2/2/4	-
4	OLC	A	509	-	-	4/10/10/24	-
5	PEG	A	528	-	-	1/4/4/4	-
4	OLC	A	518	-	-	3/12/12/24	-
4	OLC	A	510	-	-	6/24/24/24	-
4	OLC	A	524	-	-	6/18/18/24	-
4	OLC	A	525	-	-	1/4/4/24	-
4	OLC	A	514	-	-	4/13/13/24	-
4	OLC	A	508	-	-	8/15/15/24	-
4	OLC	A	521	-	-	8/15/15/24	-
4	OLC	A	506	-	-	11/24/24/24	-
4	OLC	A	523	-	-	5/13/13/24	-
5	PEG	A	527	-	-	1/4/4/4	-
4	OLC	A	513	-	-	1/4/4/24	-
4	OLC	A	511	-	-	6/14/14/24	-
4	OLC	A	516	-	-	8/24/24/24	-
4	OLC	A	520	-	-	14/23/23/24	-
4	OLC	A	512	-	-	7/12/12/24	-
6	GOL	A	530	-	-	3/4/4/4	-
4	OLC	A	519	-	-	7/13/13/24	-
4	OLC	A	504	-	-	13/24/24/24	-
4	OLC	A	526	-	-	8/14/14/24	-
4	OLC	A	515	-	-	5/6/6/24	-
4	OLC	A	505	-	-	6/11/11/24	-
4	OLC	A	522	-	-	8/17/17/24	-
4	OLC	A	507	-	-	8/17/17/24	-
4	OLC	A	517	-	-	1/5/5/24	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	524	OLC	O20-C1	2.49	1.40	1.33
4	A	510	OLC	O20-C1	2.46	1.40	1.33
4	A	526	OLC	O20-C1	2.45	1.40	1.33
4	A	508	OLC	O20-C1	2.44	1.40	1.33
4	A	520	OLC	O20-C1	2.44	1.40	1.33
4	A	506	OLC	O20-C1	2.43	1.40	1.33
4	A	521	OLC	O20-C1	2.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	OLC	O20-C1	2.40	1.40	1.33
4	A	522	OLC	O20-C1	2.40	1.40	1.33
4	A	512	OLC	O20-C1	2.39	1.40	1.33
4	A	516	OLC	O20-C1	2.38	1.40	1.33
4	A	507	OLC	O20-C1	2.38	1.40	1.33
4	A	522	OLC	O20-C21	-2.18	1.40	1.45
4	A	512	OLC	O20-C21	-2.17	1.40	1.45
4	A	507	OLC	O20-C21	-2.15	1.40	1.45
4	A	516	OLC	O20-C21	-2.13	1.40	1.45
4	A	510	OLC	O20-C21	-2.10	1.40	1.45
4	A	526	OLC	O20-C21	-2.10	1.40	1.45
4	A	524	OLC	O20-C21	-2.09	1.40	1.45
4	A	521	OLC	O20-C21	-2.09	1.40	1.45
4	A	506	OLC	O20-C21	-2.08	1.40	1.45
4	A	520	OLC	O20-C21	-2.06	1.40	1.45
4	A	504	OLC	O20-C21	-2.05	1.40	1.45
4	A	508	OLC	O20-C21	-2.05	1.40	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	508	OLC	O20-C1-C2	2.87	120.93	111.91
4	A	524	OLC	O20-C1-C2	2.83	120.78	111.91
4	A	506	OLC	O20-C1-C2	2.74	120.49	111.91
4	A	521	OLC	O20-C1-C2	2.71	120.42	111.91
4	A	507	OLC	O20-C1-C2	2.71	120.41	111.91
4	A	526	OLC	O20-C1-C2	2.67	120.28	111.91
4	A	516	OLC	O20-C1-C2	2.67	120.27	111.91
4	A	504	OLC	O20-C1-C2	2.56	119.94	111.91
4	A	520	OLC	O20-C1-C2	2.56	119.93	111.91
4	A	510	OLC	O20-C1-C2	2.54	119.87	111.91
4	A	512	OLC	O20-C1-C2	2.47	119.66	111.91
4	A	522	OLC	O20-C1-C2	2.42	119.49	111.91

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	OLC	C2-C1-O20-C21
4	A	504	OLC	O19-C1-O20-C21
4	A	512	OLC	O20-C21-C22-C24
4	A	512	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
4	A	524	OLC	C2-C1-O20-C21
4	A	524	OLC	O19-C1-O20-C21
4	A	526	OLC	O20-C21-C22-C24
4	A	516	OLC	O19-C1-O20-C21
4	A	526	OLC	O19-C1-O20-C21
4	A	516	OLC	C2-C1-O20-C21
4	A	526	OLC	C2-C1-O20-C21
4	A	520	OLC	O19-C1-O20-C21
4	A	512	OLC	C2-C1-O20-C21
4	A	508	OLC	O19-C1-O20-C21
4	A	508	OLC	C2-C1-O20-C21
4	A	520	OLC	C2-C1-O20-C21
4	A	507	OLC	C2-C1-O20-C21
4	A	512	OLC	O19-C1-O20-C21
4	A	507	OLC	O19-C1-O20-C21
4	A	520	OLC	C1-C2-C3-C4
4	A	508	OLC	O20-C21-C22-C24
4	A	508	OLC	O20-C21-C22-O23
4	A	512	OLC	C1-C2-C3-C4
4	A	521	OLC	C1-C2-C3-C4
4	A	526	OLC	C1-C2-C3-C4
4	A	510	OLC	C1-C2-C3-C4
4	A	523	OLC	C13-C14-C15-C16
4	A	516	OLC	C10-C11-C12-C13
4	A	526	OLC	O20-C21-C22-O23
4	A	522	OLC	C4-C5-C6-C7
4	A	521	OLC	C5-C6-C7-C8
4	A	508	OLC	C2-C3-C4-C5
4	A	518	OLC	C13-C14-C15-C16
4	A	510	OLC	C4-C5-C6-C7
4	A	515	OLC	C14-C15-C16-C17
4	A	505	OLC	C5-C6-C7-C8
4	A	521	OLC	C2-C3-C4-C5
4	A	504	OLC	C14-C15-C16-C17
4	A	504	OLC	C11-C12-C13-C14
4	A	506	OLC	C12-C13-C14-C15
4	A	506	OLC	C4-C5-C6-C7
4	A	508	OLC	C3-C4-C5-C6
4	A	504	OLC	C21-C22-C24-O25
4	A	512	OLC	C21-C22-C24-O25
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	522	OLC	C21-C22-C24-O25
6	A	530	GOL	O1-C1-C2-C3
4	A	504	OLC	C3-C4-C5-C6
4	A	520	OLC	C5-C6-C7-C8
4	A	520	OLC	C2-C3-C4-C5
4	A	519	OLC	C10-C11-C12-C13
4	A	520	OLC	C10-C11-C12-C13
4	A	511	OLC	C3-C4-C5-C6
4	A	514	OLC	C13-C14-C15-C16
4	A	521	OLC	C3-C4-C5-C6
4	A	522	OLC	C2-C3-C4-C5
4	A	521	OLC	C4-C5-C6-C7
4	A	510	OLC	C3-C4-C5-C6
4	A	519	OLC	C13-C14-C15-C16
4	A	507	OLC	C5-C6-C7-C8
4	A	518	OLC	C14-C15-C16-C17
4	A	519	OLC	C5-C6-C7-C8
4	A	504	OLC	O23-C22-C24-O25
4	A	522	OLC	O23-C22-C24-O25
4	A	506	OLC	C10-C11-C12-C13
4	A	506	OLC	C6-C7-C8-C9
4	A	520	OLC	C6-C7-C8-C9
4	A	523	OLC	C6-C7-C8-C9
4	A	516	OLC	C11-C12-C13-C14
4	A	520	OLC	C3-C4-C5-C6
4	A	504	OLC	C1-C2-C3-C4
4	A	505	OLC	C6-C7-C8-C9
4	A	507	OLC	C4-C5-C6-C7
4	A	511	OLC	C6-C7-C8-C9
4	A	516	OLC	C6-C7-C8-C9
4	A	519	OLC	C4-C5-C6-C7
4	A	523	OLC	C11-C12-C13-C14
4	A	506	OLC	C3-C4-C5-C6
4	A	526	OLC	C3-C4-C5-C6
4	A	508	OLC	C6-C7-C8-C9
4	A	508	OLC	C1-C2-C3-C4
4	A	521	OLC	O23-C22-C24-O25
4	A	522	OLC	O20-C21-C22-O23
4	A	507	OLC	C2-C3-C4-C5
4	A	511	OLC	C7-C8-C9-C10
4	A	511	OLC	C15-C16-C17-C18
4	A	520	OLC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	A	522	OLC	C5-C6-C7-C8
4	A	519	OLC	C11-C12-C13-C14
4	A	504	OLC	O20-C21-C22-O23
4	A	507	OLC	C1-C2-C3-C4
4	A	509	OLC	C6-C7-C8-C9
4	A	516	OLC	C15-C16-C17-C18
4	A	506	OLC	C2-C1-O20-C21
4	A	513	OLC	C14-C15-C16-C17
4	A	504	OLC	O20-C21-C22-C24
4	A	504	OLC	C10-C11-C12-C13
4	A	514	OLC	C3-C4-C5-C6
4	A	505	OLC	C11-C12-C13-C14
4	A	515	OLC	C11-C12-C13-C14
4	A	521	OLC	C6-C7-C8-C9
4	A	526	OLC	C2-C3-C4-C5
4	A	506	OLC	O19-C1-O20-C21
4	A	511	OLC	C13-C14-C15-C16
4	A	505	OLC	C13-C14-C15-C16
4	A	519	OLC	C12-C13-C14-C15
4	A	514	OLC	C4-C5-C6-C7
4	A	515	OLC	C12-C13-C14-C15
4	A	506	OLC	C11-C12-C13-C14
4	A	506	OLC	C2-C3-C4-C5
4	A	507	OLC	C3-C4-C5-C6
4	A	522	OLC	C1-C2-C3-C4
4	A	515	OLC	C10-C11-C12-C13
4	A	516	OLC	C1-C2-C3-C4
4	A	506	OLC	C7-C8-C9-C10
4	A	516	OLC	C9-C10-C11-C12
4	A	504	OLC	C2-C3-C4-C5
4	A	526	OLC	C5-C6-C7-C8
6	A	530	GOL	C1-C2-C3-O3
4	A	512	OLC	O23-C22-C24-O25
4	A	523	OLC	C4-C5-C6-C7
4	A	519	OLC	C9-C10-C11-C12
4	A	510	OLC	C13-C14-C15-C16
4	A	518	OLC	C7-C8-C9-C10
4	A	511	OLC	C5-C6-C7-C8
4	A	509	OLC	C7-C8-C9-C10
5	A	529	PEG	C4-C3-O2-C2
5	A	527	PEG	O1-C1-C2-O2
4	A	504	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	524	OLC	C7-C8-C9-C10
4	A	514	OLC	C11-C12-C13-C14
5	A	528	PEG	C1-C2-O2-C3
4	A	510	OLC	C6-C7-C8-C9
4	A	520	OLC	C9-C10-C11-C12
4	A	506	OLC	C15-C16-C17-C18
4	A	507	OLC	C7-C8-C9-C10
4	A	509	OLC	C14-C15-C16-C17
4	A	523	OLC	C5-C6-C7-C8
4	A	520	OLC	O20-C1-C2-C3
4	A	520	OLC	O23-C22-C24-O25
6	A	530	GOL	O1-C1-C2-O2
4	A	515	OLC	C13-C14-C15-C16
4	A	525	OLC	C12-C13-C14-C15
4	A	509	OLC	C15-C16-C17-C18
4	A	517	OLC	C14-C15-C16-C17
4	A	520	OLC	O19-C1-C2-C3
4	A	505	OLC	C10-C11-C12-C13
4	A	510	OLC	C10-C11-C12-C13
4	A	524	OLC	C9-C10-C11-C12
4	A	522	OLC	C7-C8-C9-C10
4	A	524	OLC	O20-C1-C2-C3
4	A	505	OLC	C4-C5-C6-C7
4	A	524	OLC	O19-C1-C2-C3

There are no ring outliers.

18 monomers are involved in 38 short contacts:

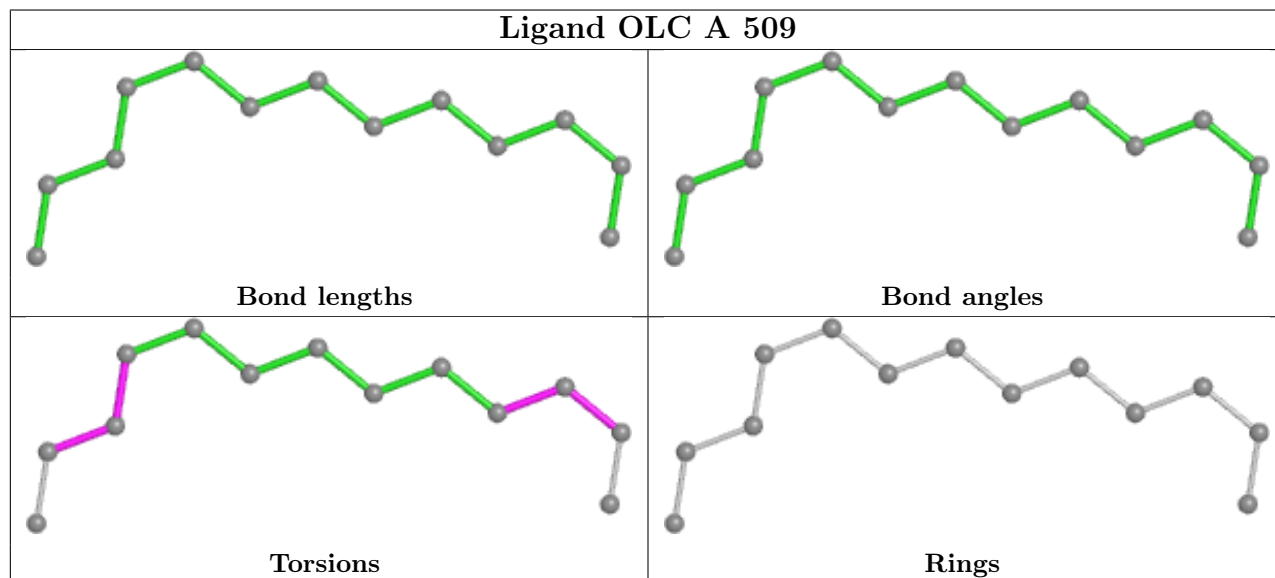
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	529	PEG	1	0
4	A	518	OLC	1	0
4	A	510	OLC	2	0
4	A	524	OLC	2	0
4	A	514	OLC	1	0
4	A	506	OLC	2	0
4	A	523	OLC	5	0
5	A	527	PEG	2	0
4	A	511	OLC	5	0
4	A	516	OLC	3	0
4	A	520	OLC	2	0
4	A	512	OLC	1	0
4	A	504	OLC	1	0

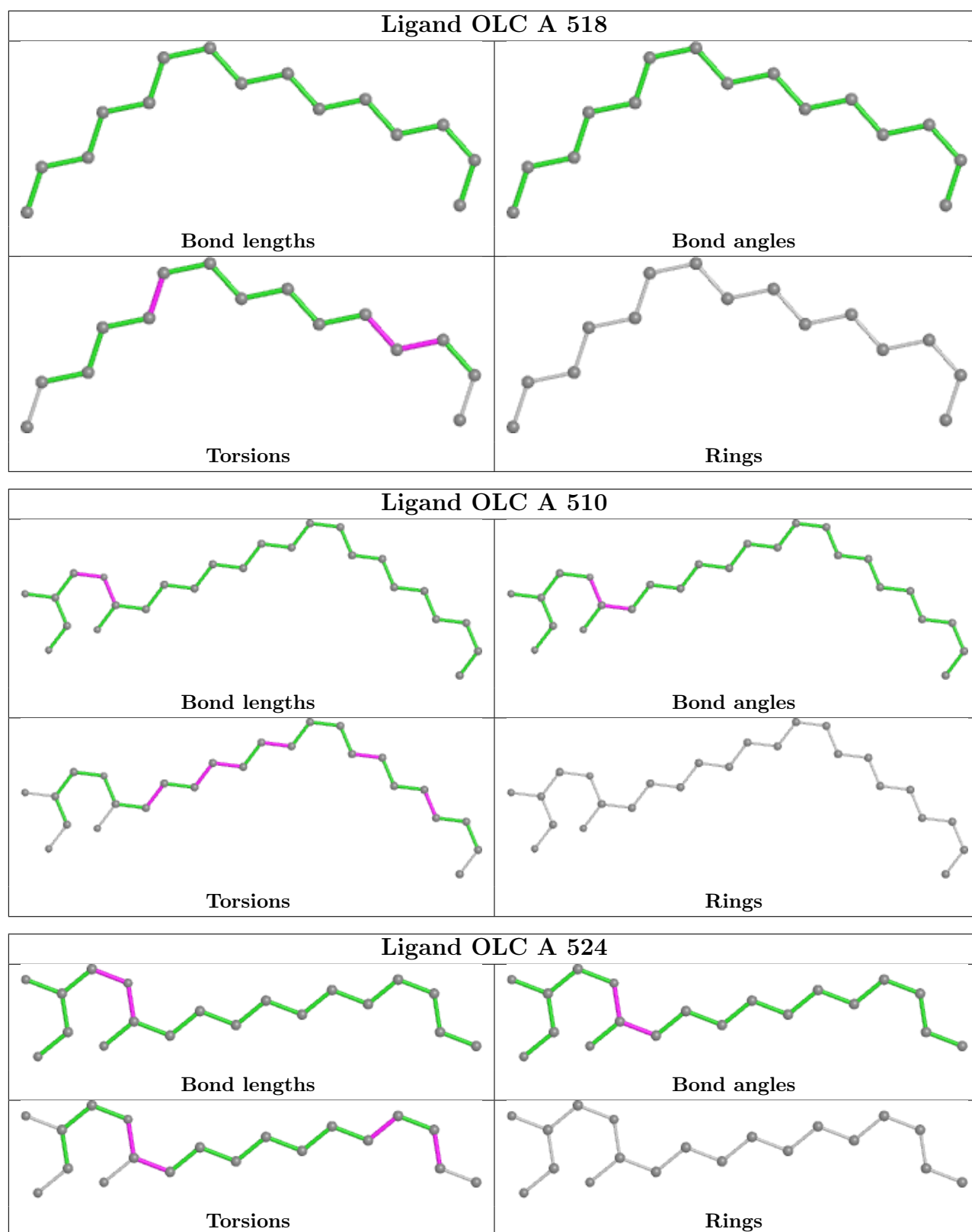
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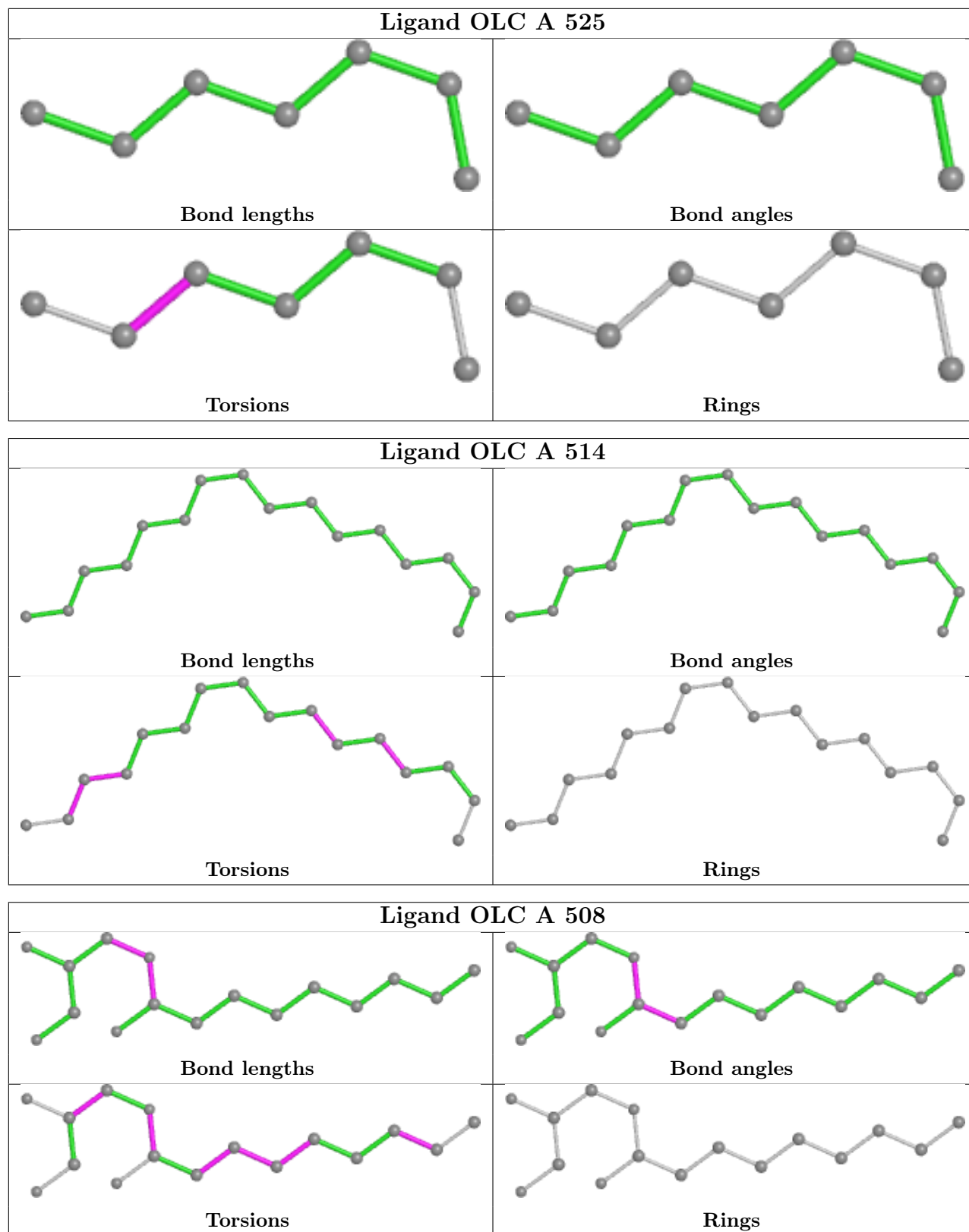
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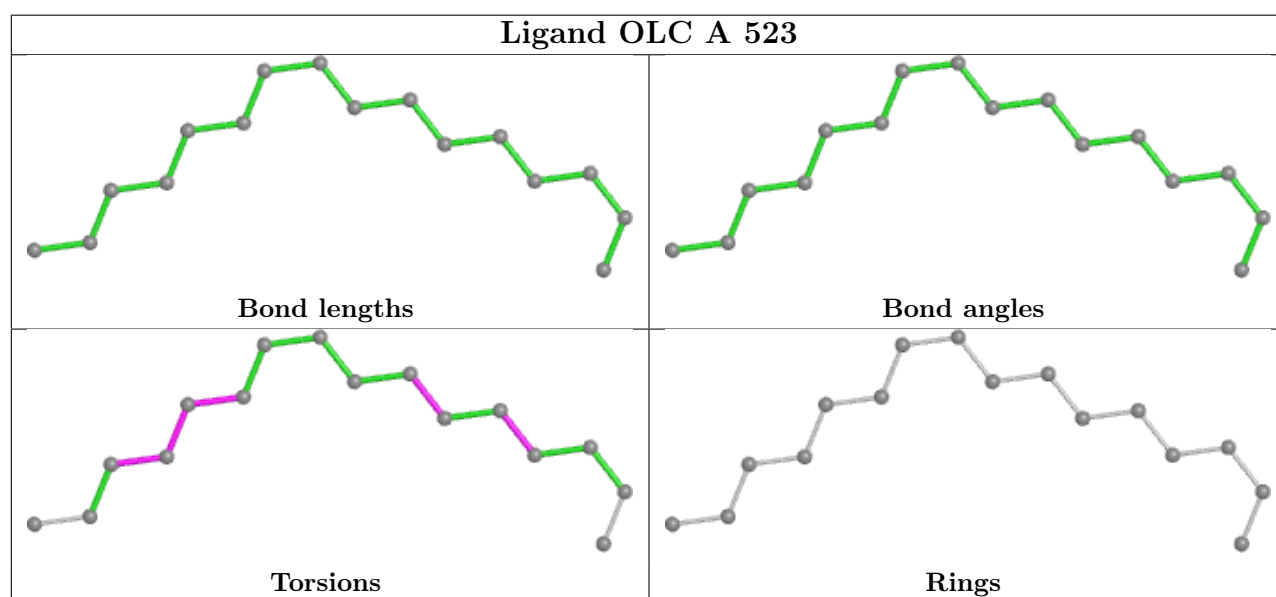
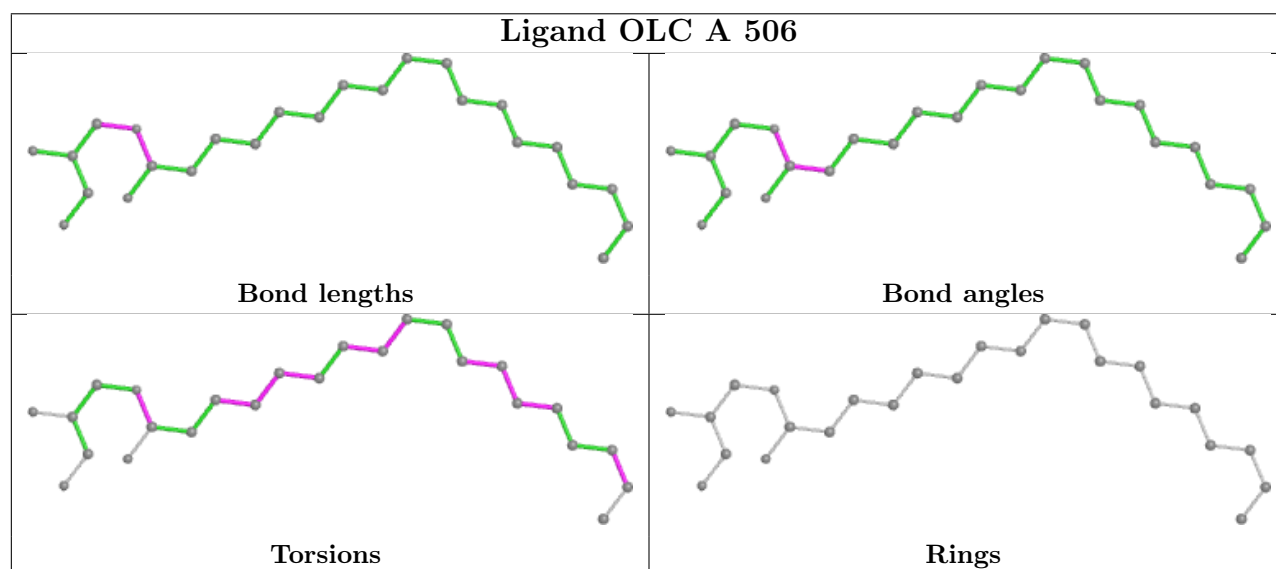
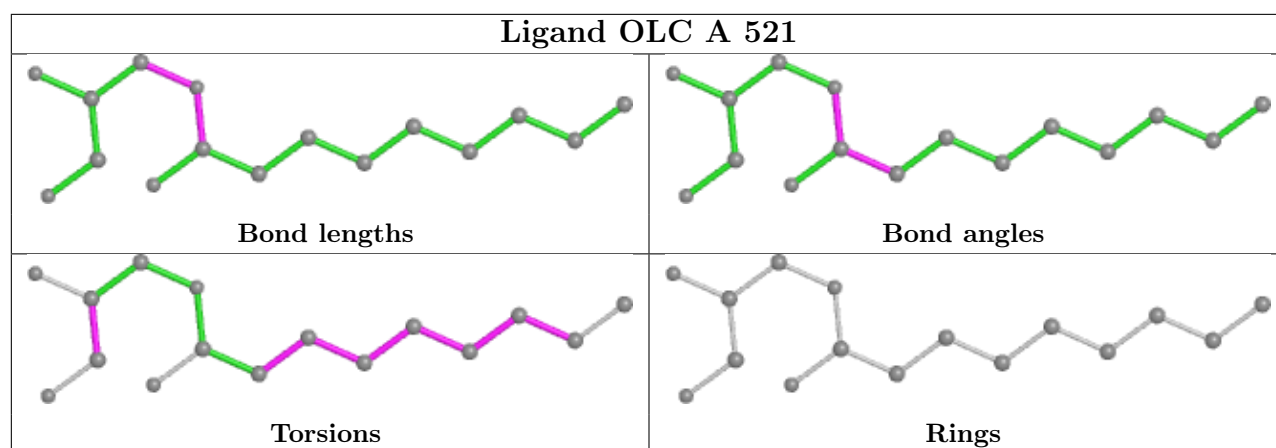
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	515	OLC	2	0
4	A	505	OLC	3	0
4	A	522	OLC	2	0
4	A	507	OLC	2	0
4	A	517	OLC	3	0

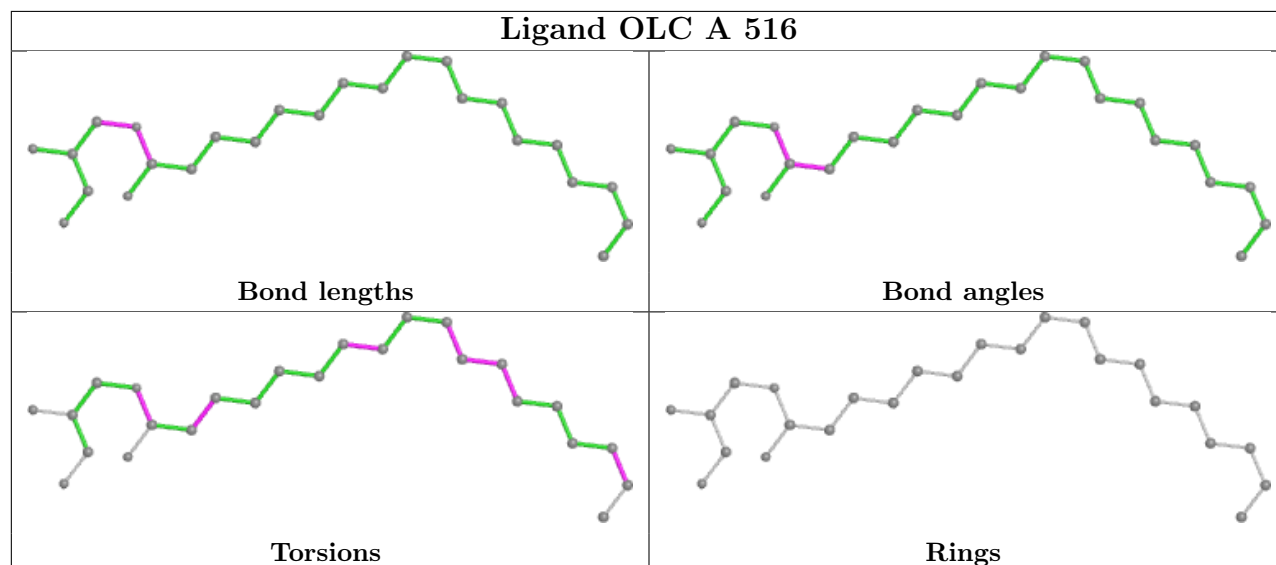
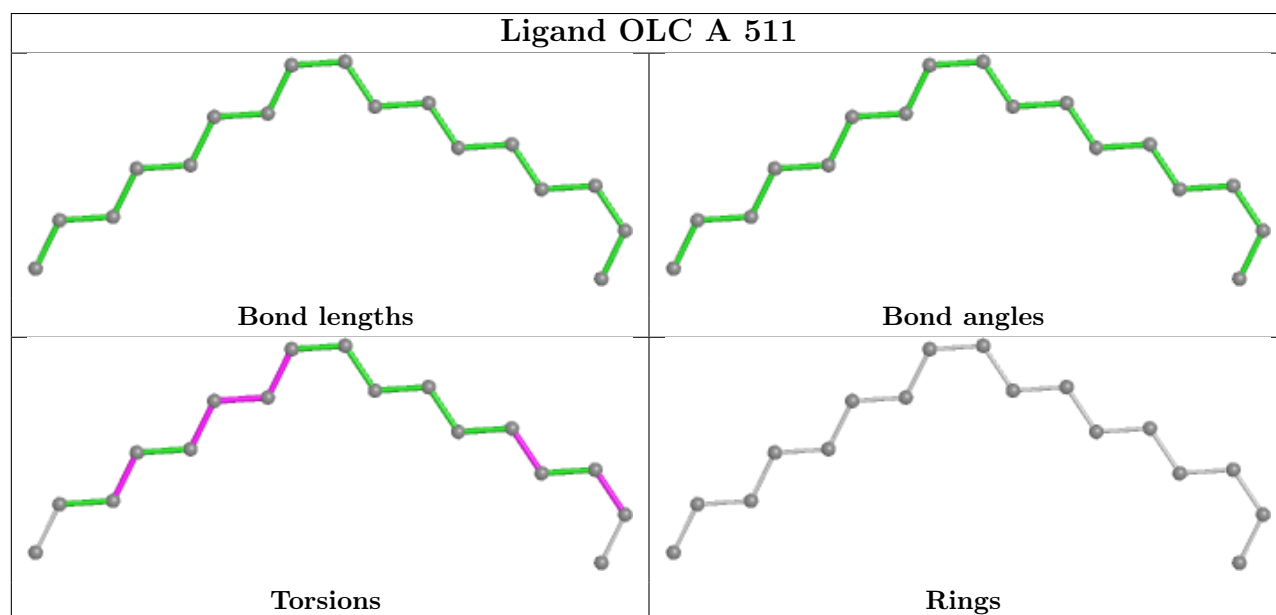
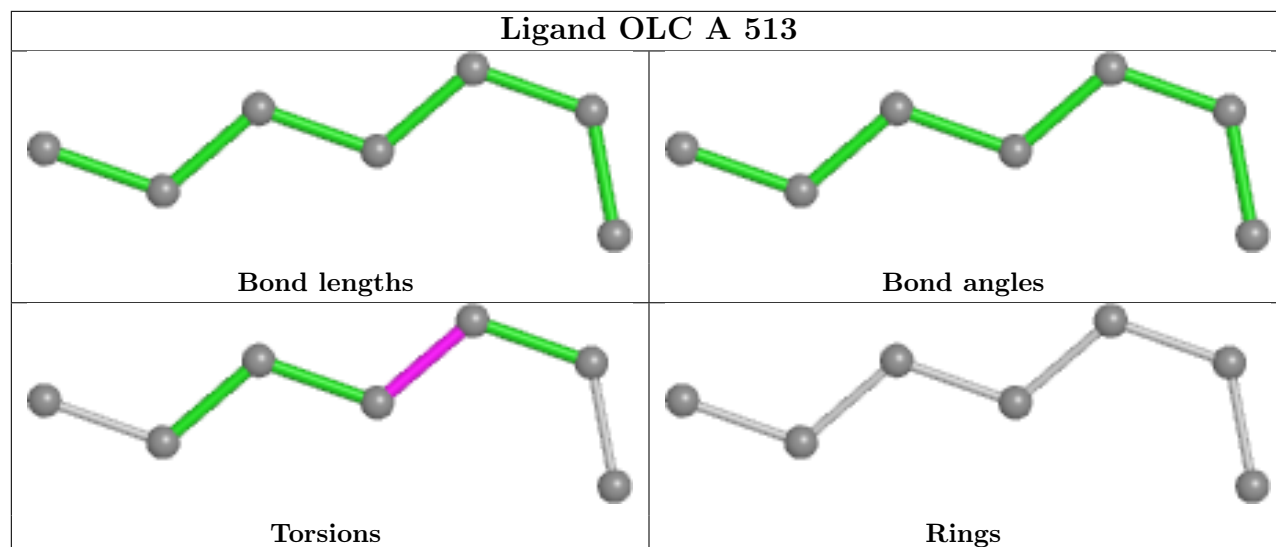
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

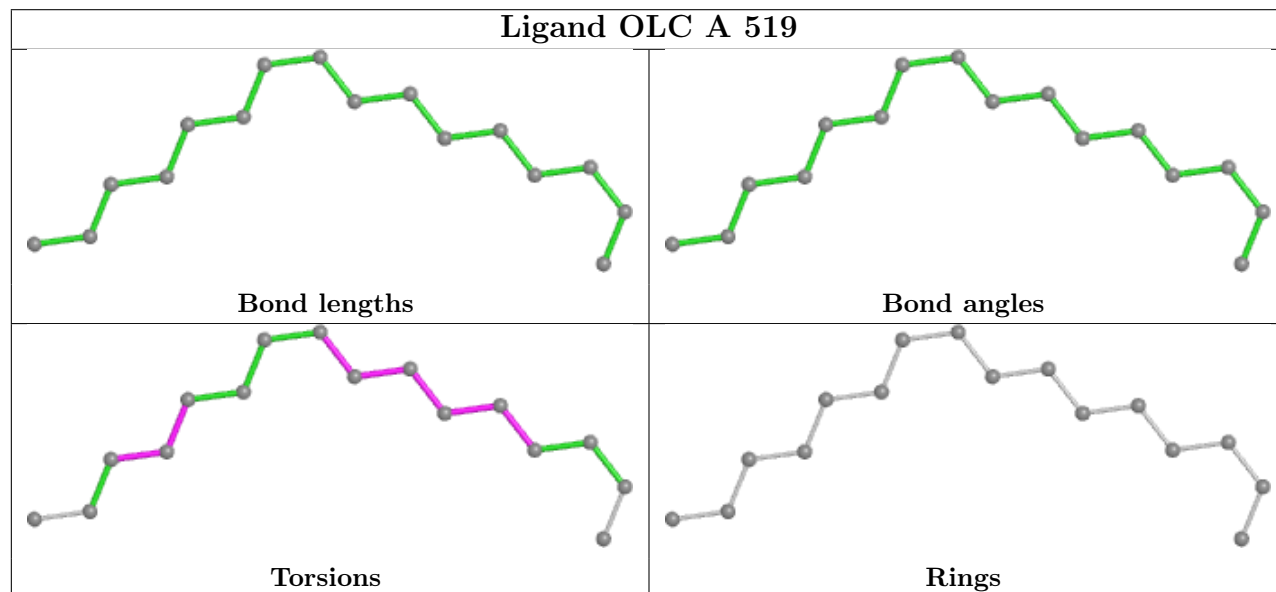
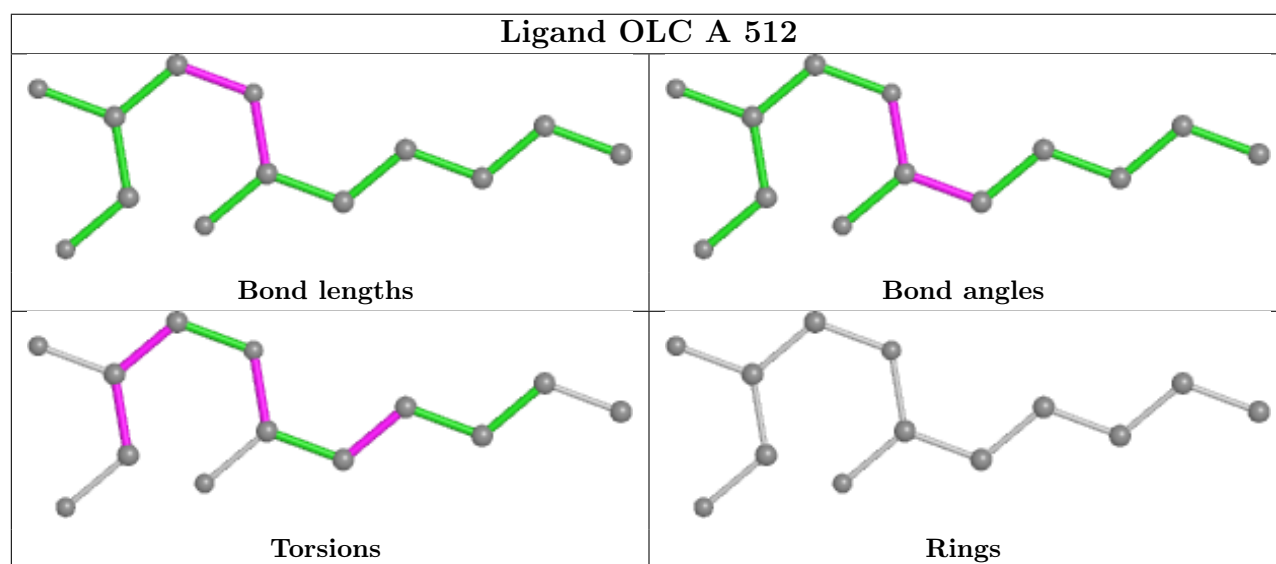
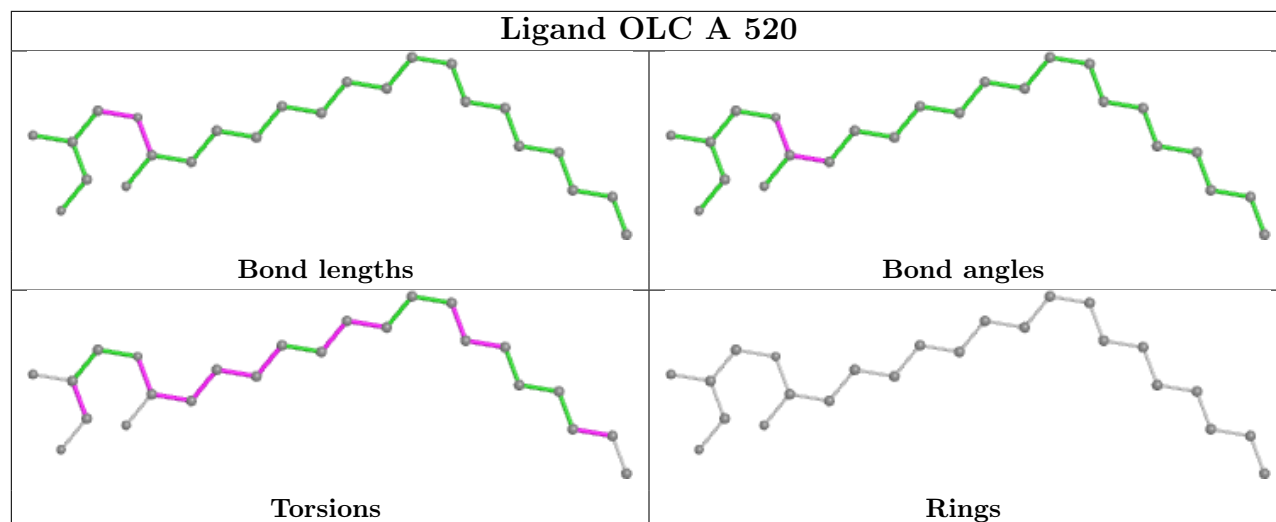


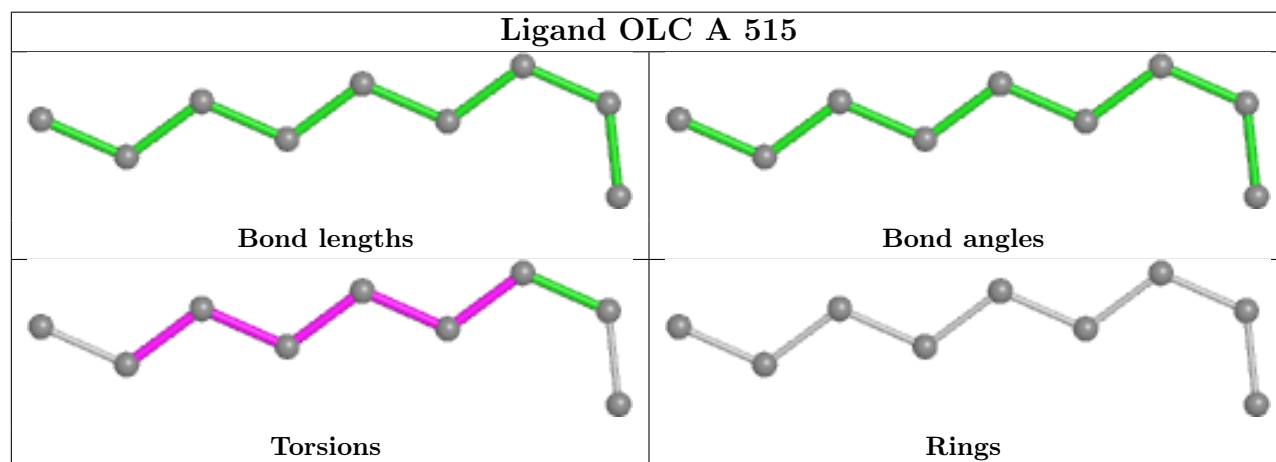
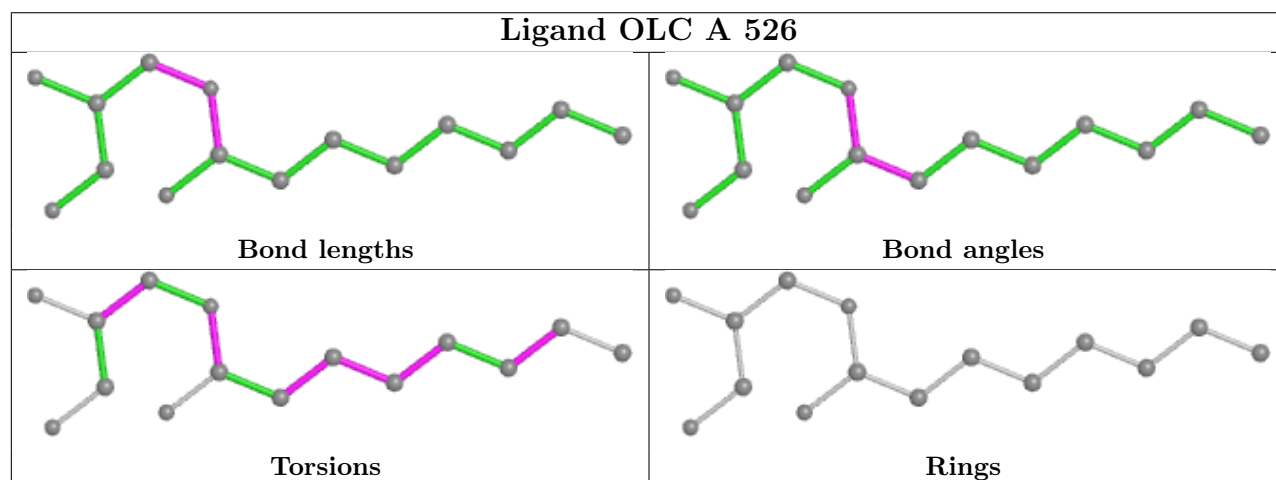
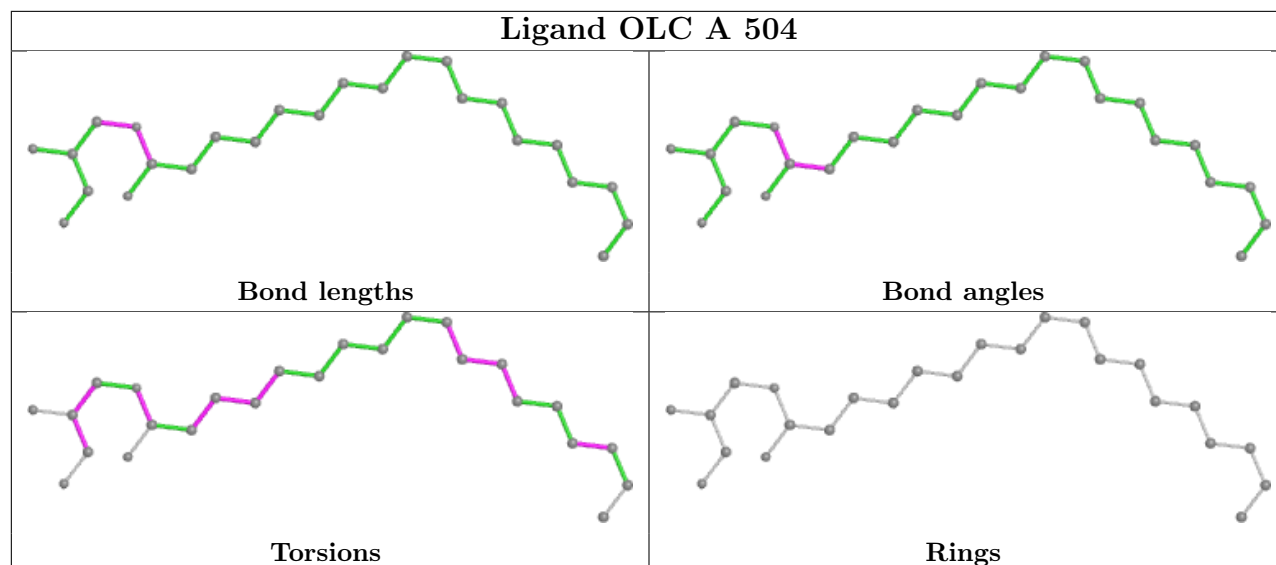


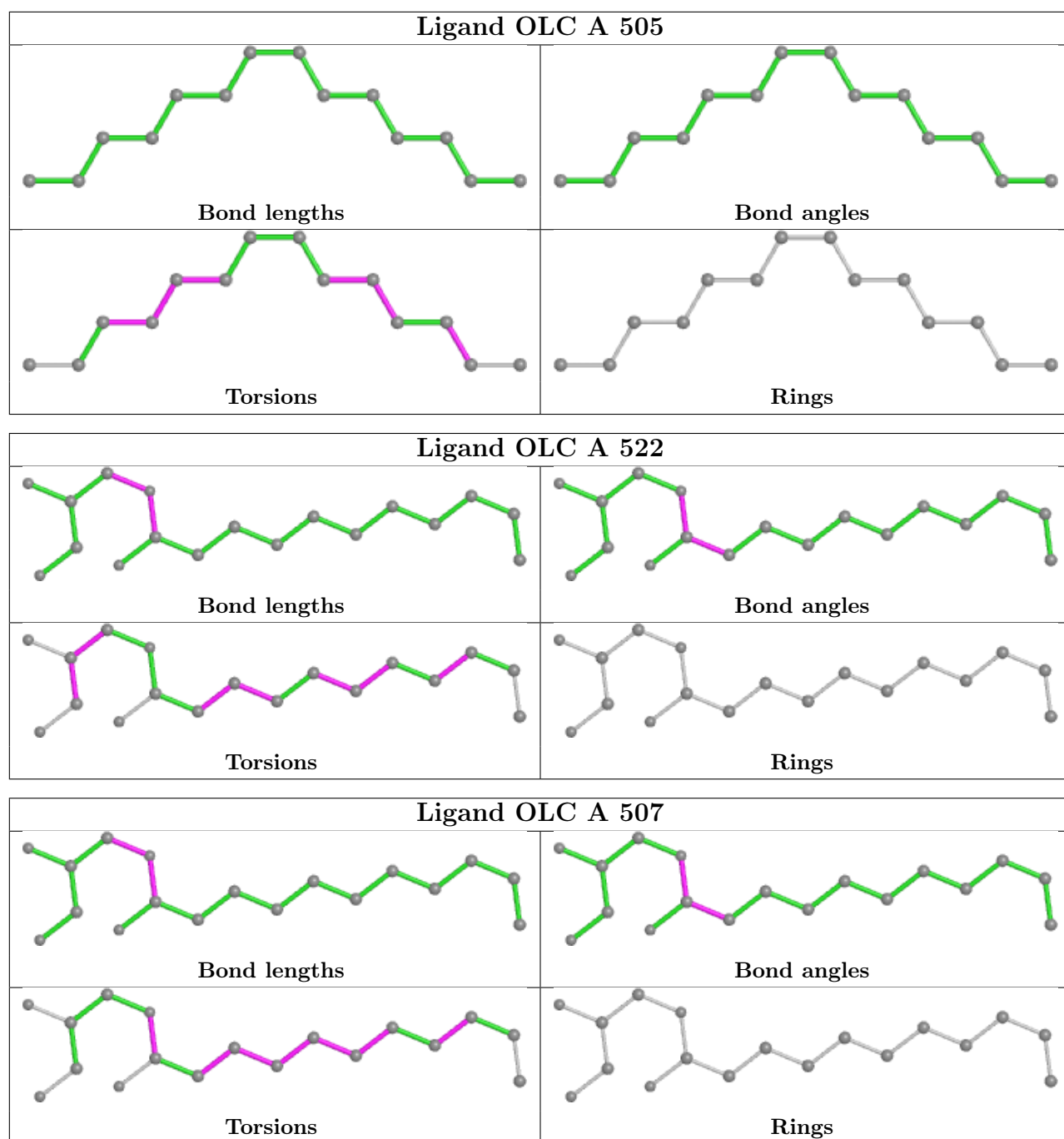


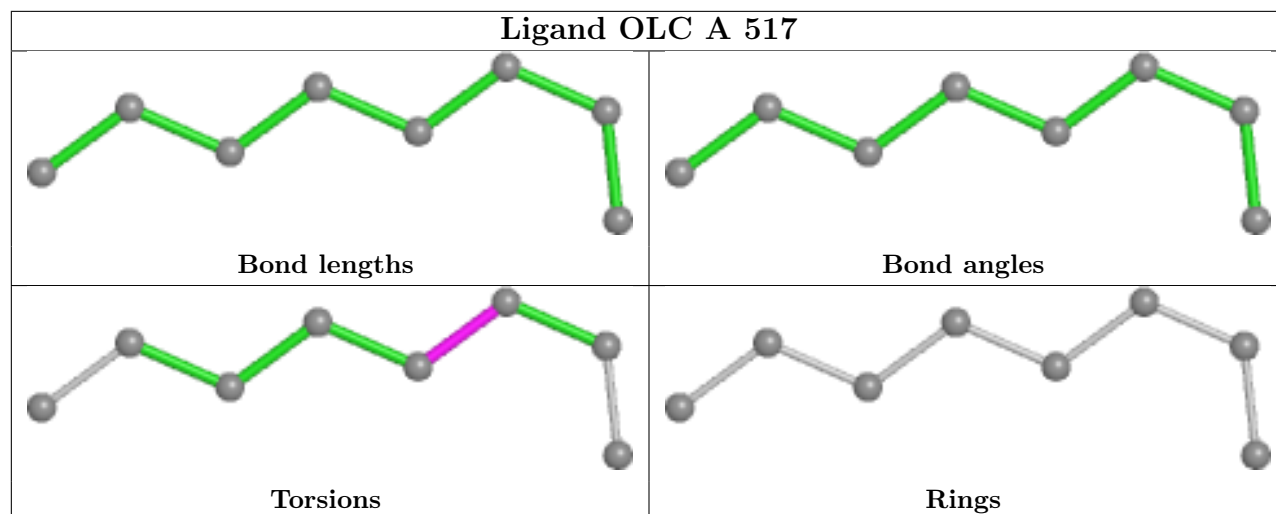












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/414 (94%)	0.71	47 (11%) 4 5	35, 53, 120, 177	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	PRO	11.3
1	A	246	GLN	8.4
1	A	168	GLN	8.3
1	A	292	GLU	7.3
1	A	162	PHE	7.2
1	A	171	GLY	7.0
1	A	170	ARG	6.4
1	A	172	THR	6.3
1	A	434	LEU	5.7
1	A	244	ARG	5.4
1	A	175	LEU	5.3
1	A	166	ASN	5.1
1	A	177	LEU	5.0
1	A	433	LEU	4.4
1	A	245	ILE	4.2
1	A	247	THR	4.2
1	A	333	MET	4.1
1	A	167	LEU	4.0
1	A	163	TRP	3.9
1	A	349	LEU	3.9
1	A	173	ARG	3.9
1	A	54	TYR	3.7
1	A	250	THR	3.6
1	A	165	LEU	3.5
1	A	169	LYS	3.5
1	A	243	GLY	3.2
1	A	178	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	215	PRO	3.0
1	A	431	TRP	2.9
1	A	51	SER	2.7
1	A	48	VAL	2.7
1	A	356	THR	2.6
1	A	249	THR	2.5
1	A	291	VAL	2.5
1	A	47	ALA	2.3
1	A	49	ILE	2.3
1	A	204	VAL	2.2
1	A	214	GLY	2.2
1	A	150	MET	2.2
1	A	211	ARG	2.1
1	A	182	PHE	2.1
1	A	164	LEU	2.1
1	A	44	LEU	2.1
1	A	251	GLU	2.1
1	A	256	LEU	2.1
1	A	50	ALA	2.1
1	A	248	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLC	A	509	13/25	0.40	0.45	61,88,99,102	0
4	OLC	A	526	15/25	0.40	0.35	78,102,117,120	0
4	OLC	A	523	16/25	0.50	0.37	73,85,96,101	0

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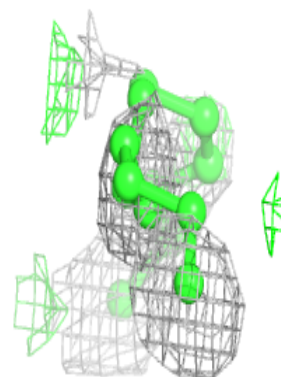
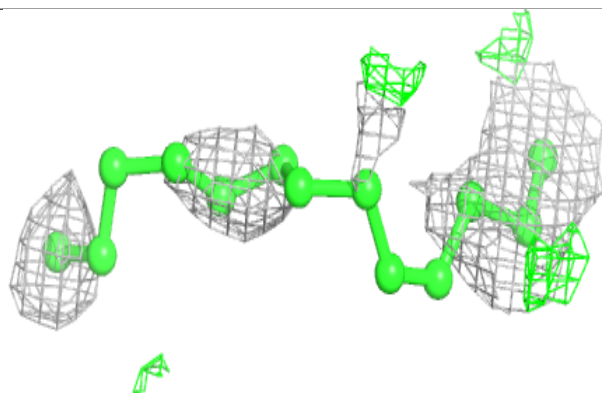
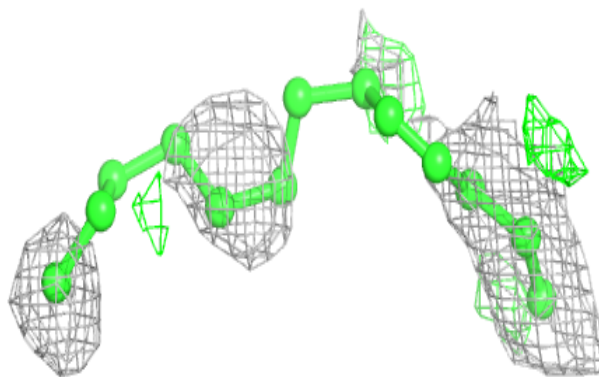
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	OLC	A	507	18/25	0.62	0.31	67,78,108,109	0
4	OLC	A	504	25/25	0.65	0.27	50,66,73,78	0
4	OLC	A	524	19/25	0.66	0.26	71,90,108,112	0
4	OLC	A	516	25/25	0.66	0.34	69,83,93,99	0
4	OLC	A	517	8/25	0.69	0.33	70,78,95,98	0
4	OLC	A	520	24/25	0.70	0.39	58,72,81,83	0
4	OLC	A	519	16/25	0.70	0.44	60,75,85,87	0
5	PEG	A	528	7/7	0.70	0.26	69,76,93,97	0
4	OLC	A	506	25/25	0.71	0.34	52,79,91,109	0
4	OLC	A	505	14/25	0.73	0.35	58,68,77,83	0
4	OLC	A	513	7/25	0.73	0.32	55,65,87,93	0
4	OLC	A	518	15/25	0.73	0.37	78,89,102,103	0
4	OLC	A	508	16/25	0.75	0.25	66,76,88,91	0
4	OLC	A	521	16/25	0.75	0.27	57,79,101,103	0
4	OLC	A	511	17/25	0.77	0.29	53,73,84,88	0
4	OLC	A	514	16/25	0.77	0.23	52,79,83,83	0
4	OLC	A	522	18/25	0.78	0.25	56,74,97,99	0
4	OLC	A	515	9/25	0.79	0.34	57,66,91,91	0
4	OLC	A	512	13/25	0.79	0.20	53,71,79,80	0
5	PEG	A	527	7/7	0.81	0.26	47,57,64,67	0
4	OLC	A	510	25/25	0.83	0.27	41,65,96,103	0
5	PEG	A	529	5/7	0.83	0.25	57,64,74,78	0
4	OLC	A	525	7/25	0.88	0.21	60,64,71,72	0
2	MN	A	501	1/1	0.89	0.07	63,63,63,63	1
2	MN	A	502	1/1	0.90	0.05	75,75,75,75	0
6	GOL	A	530	6/6	0.90	0.27	58,71,75,88	0
3	CL	A	503	1/1	0.91	0.24	54,54,54,54	0

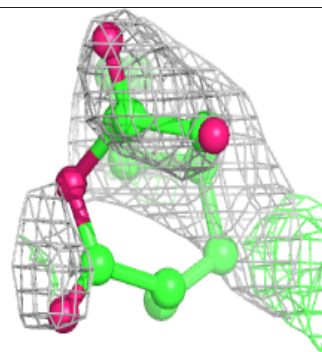
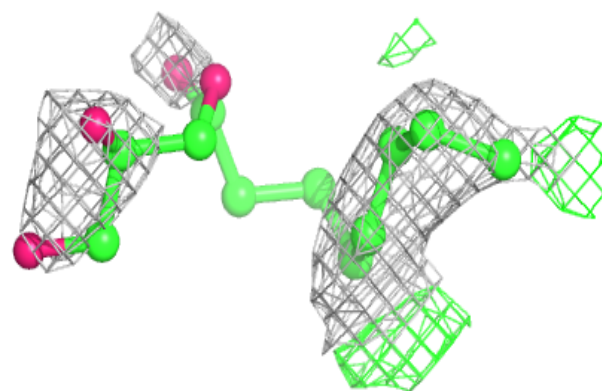
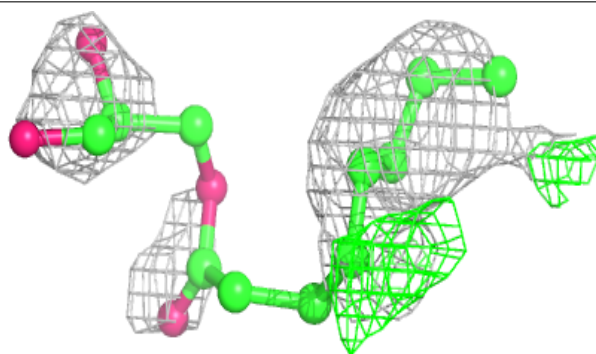
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 509:

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

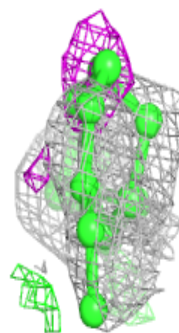
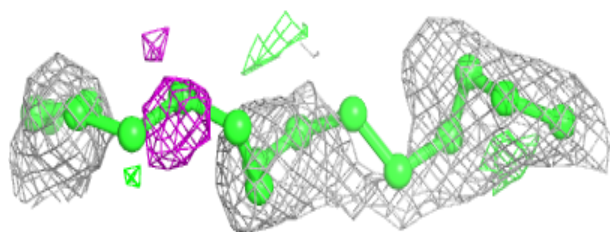
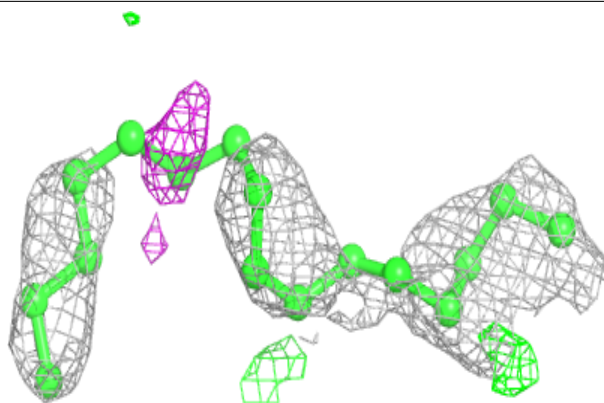
**Electron density around OLC A 526:**

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

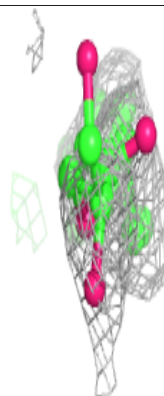
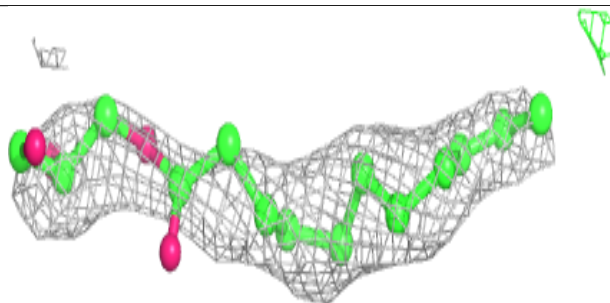
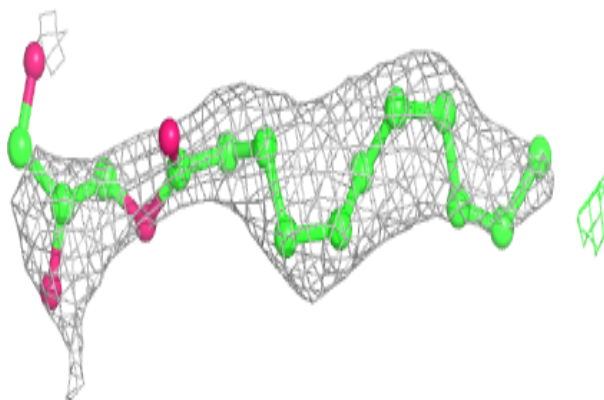


Electron density around OLC A 523:

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

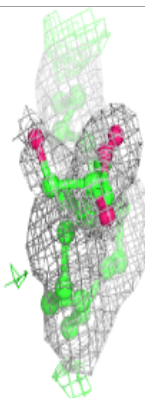
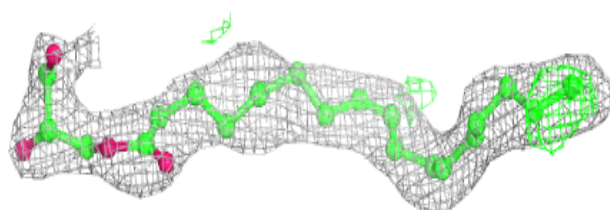
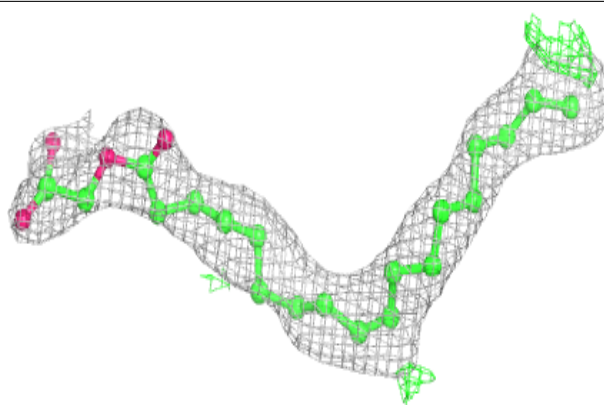
**Electron density around OLC A 507:**

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

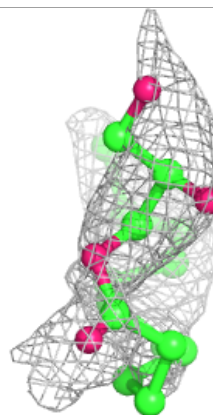
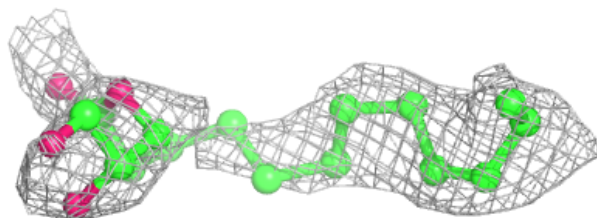
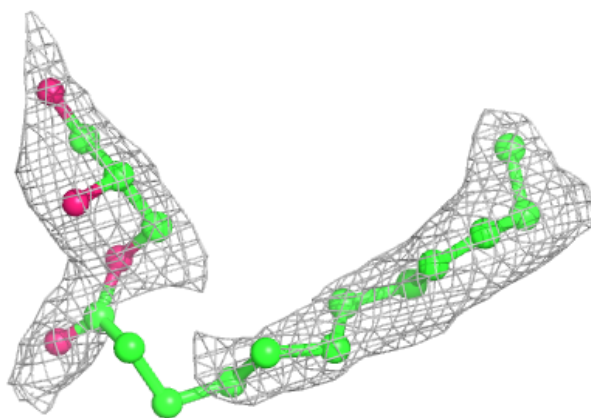


Electron density around OLC A 504:

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

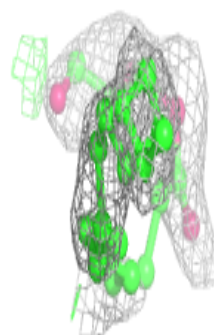
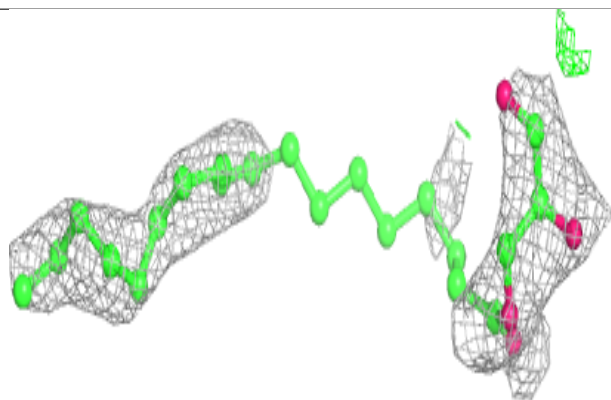
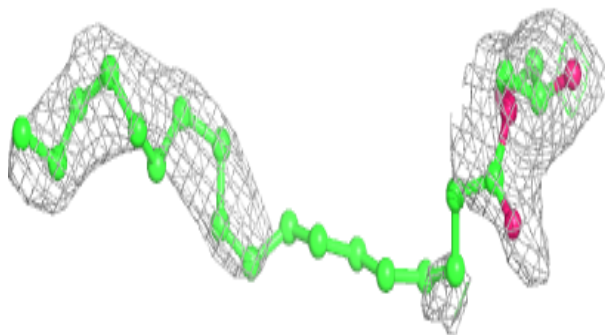
**Electron density around OLC A 524:**

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

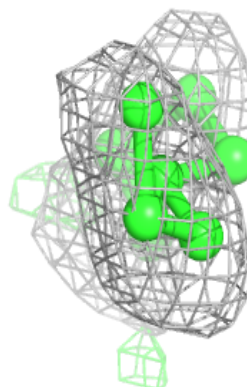
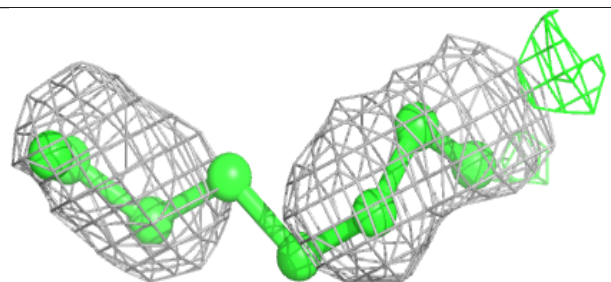
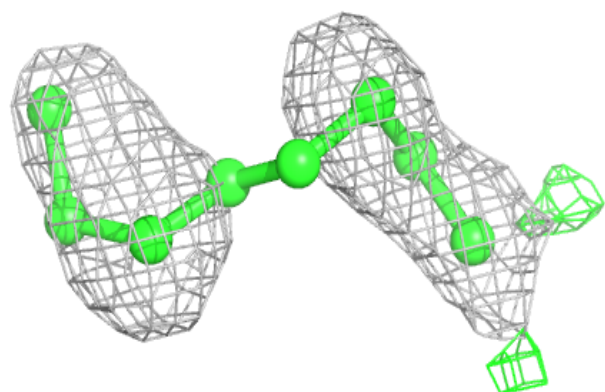


Electron density around OLC A 516:

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

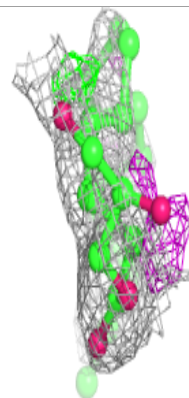
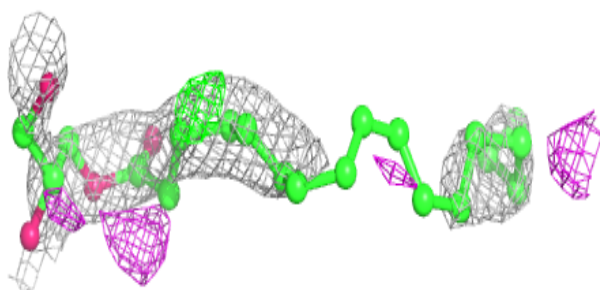
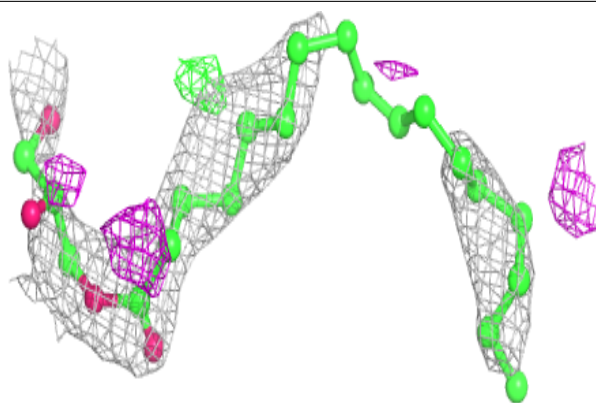
**Electron density around OLC A 517:**

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

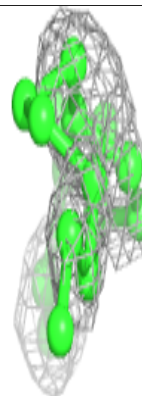
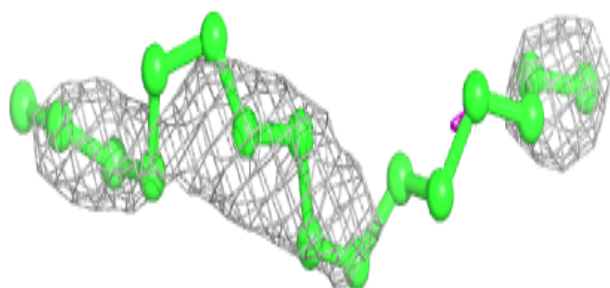
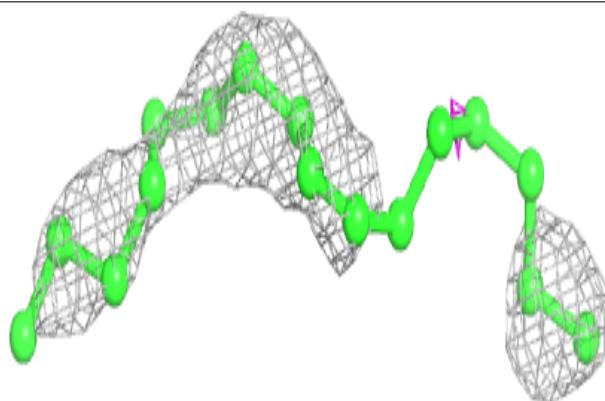


Electron density around OLC A 520:

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

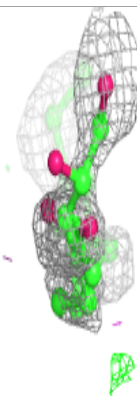
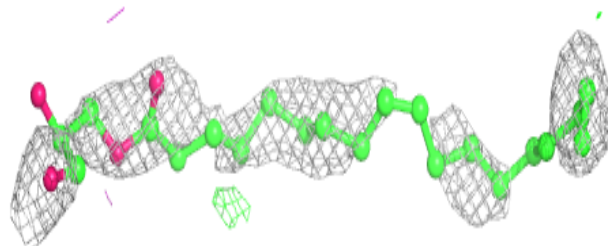
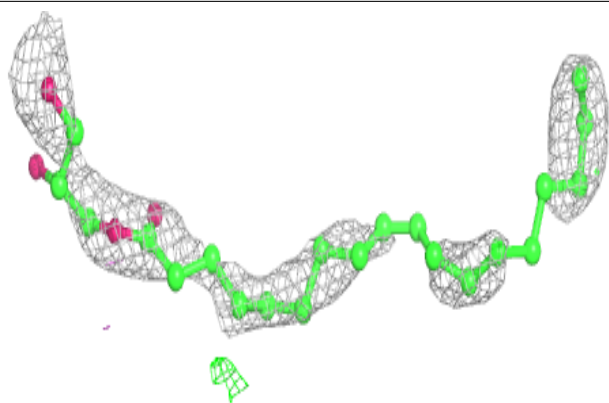
**Electron density around OLC A 519:**

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

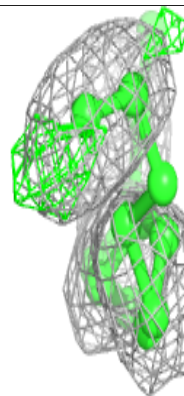
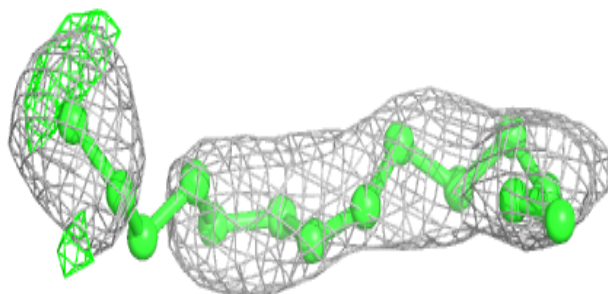
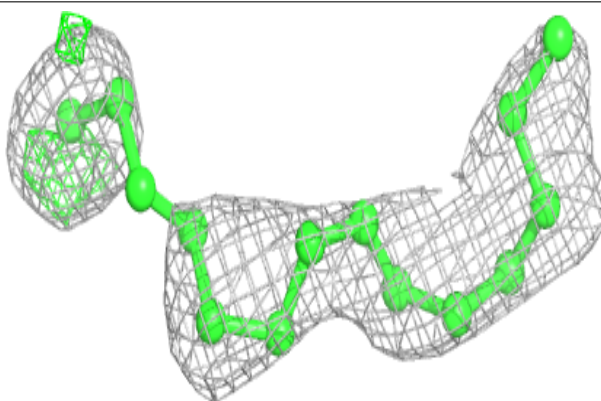


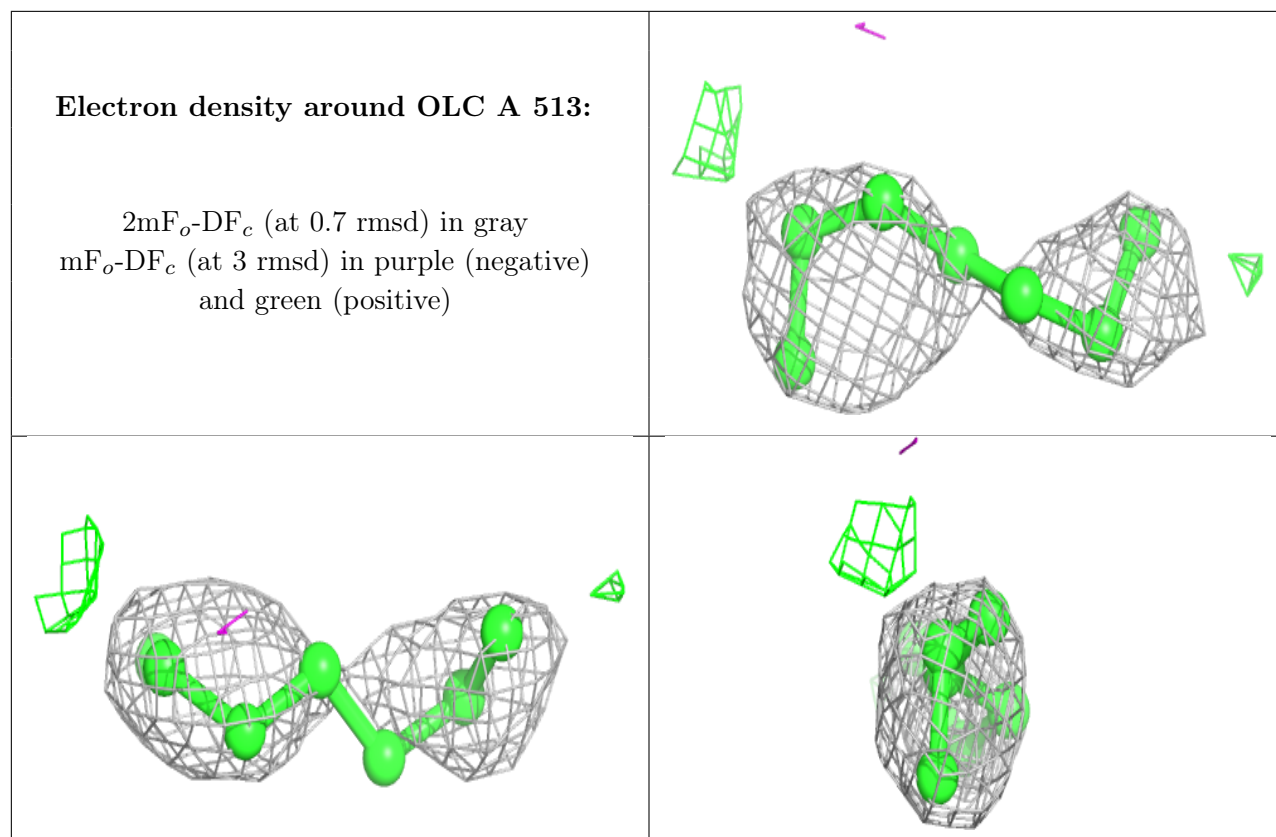
Electron density around OLC A 506:

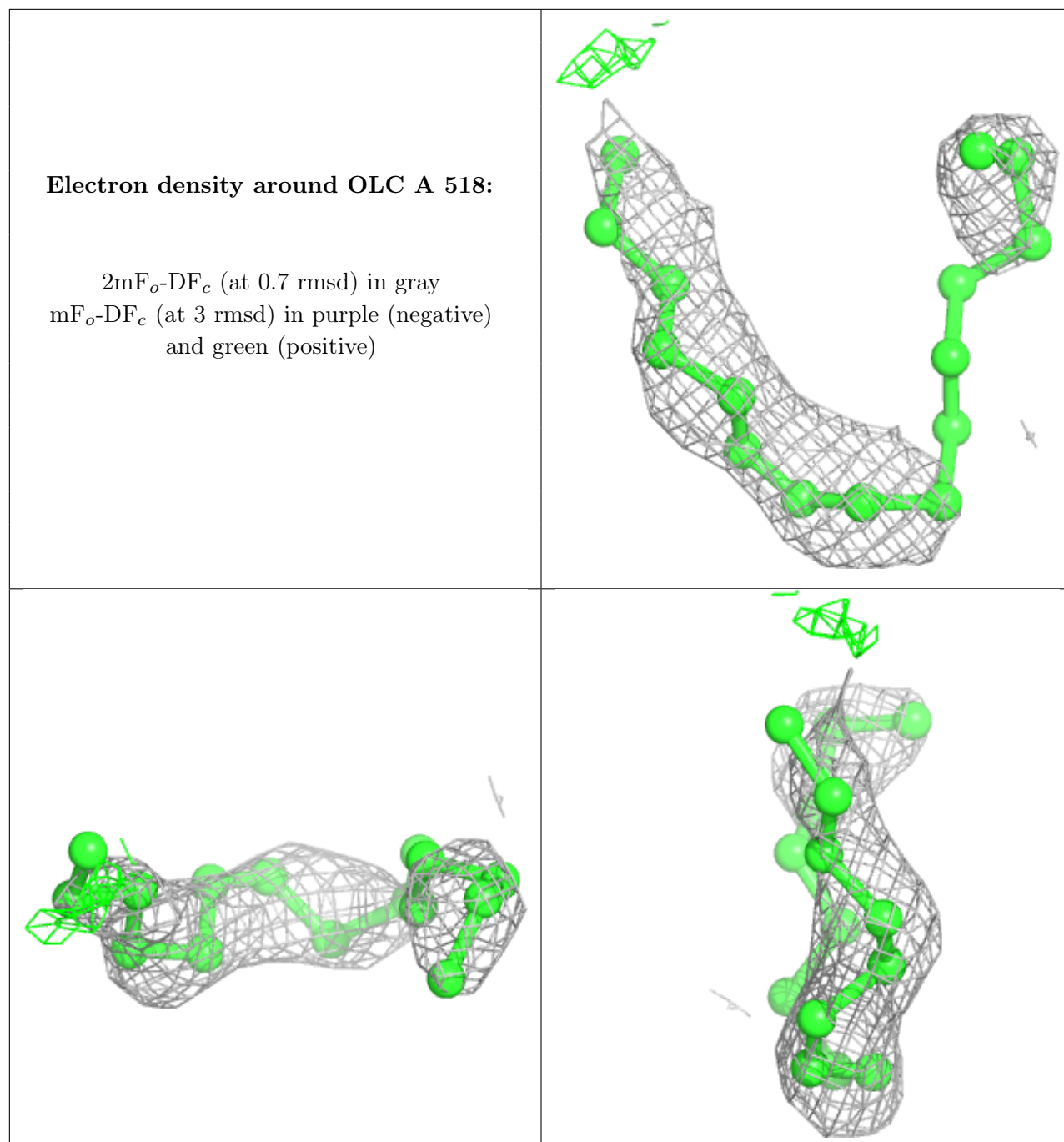
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**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)

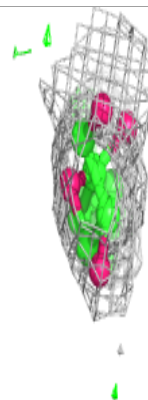
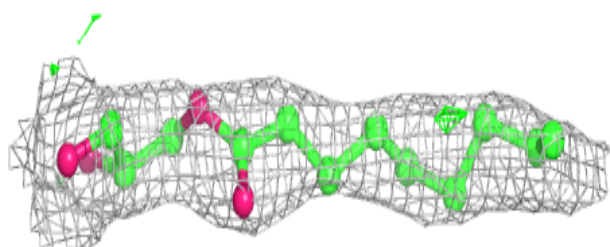
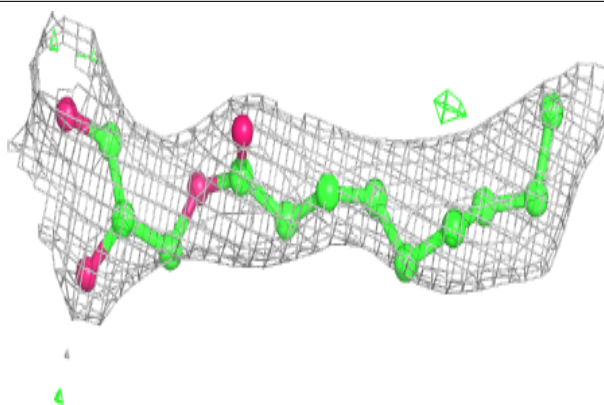




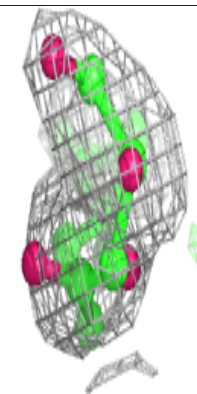
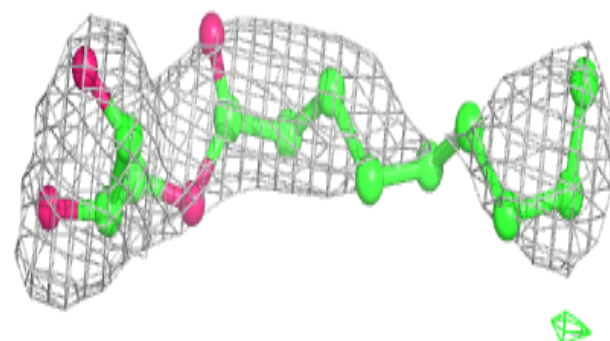
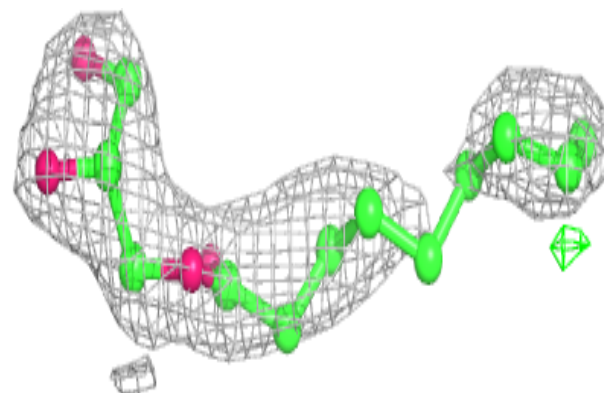


Electron density around OLC A 508:

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

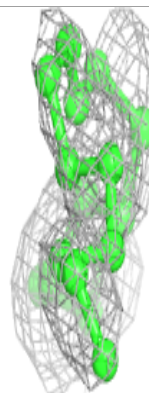
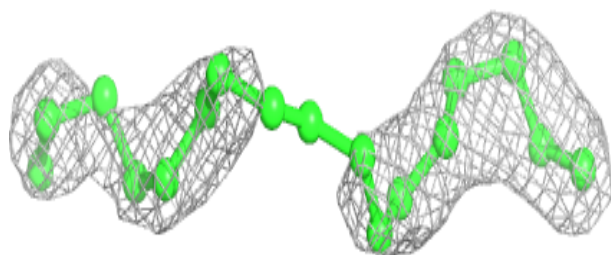
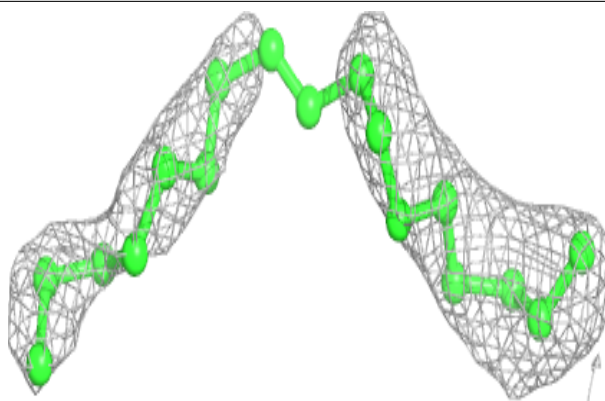
**Electron density around OLC A 521:**

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

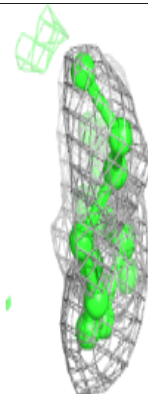
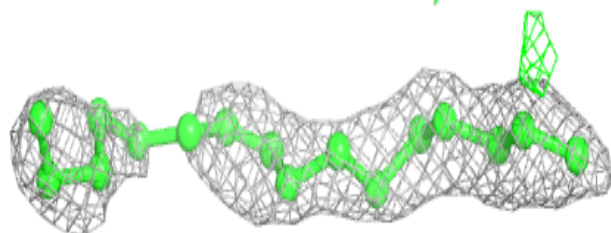
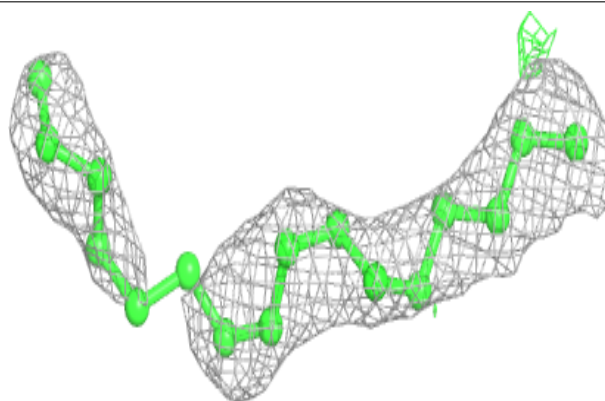


Electron density around OLC A 511:

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

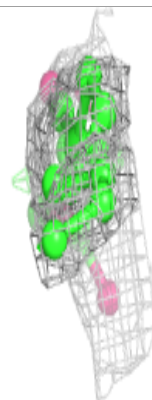
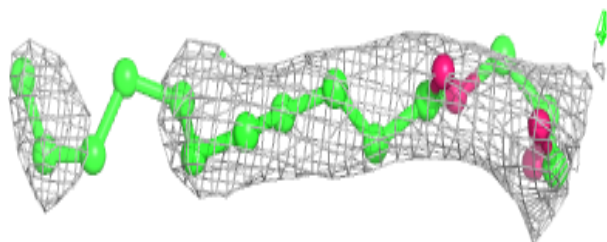
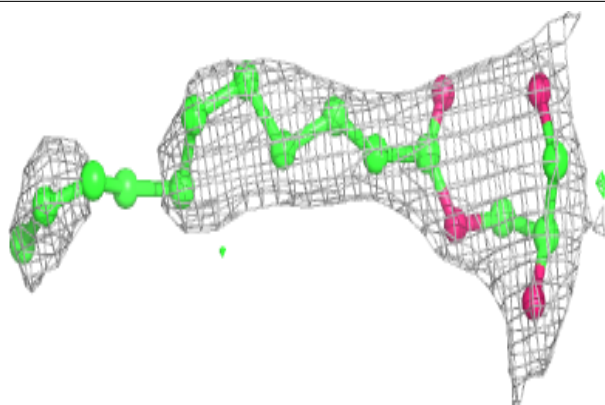
**Electron density around OLC A 514:**

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

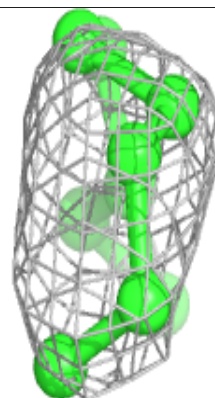
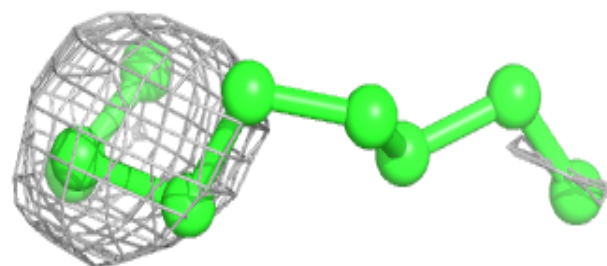
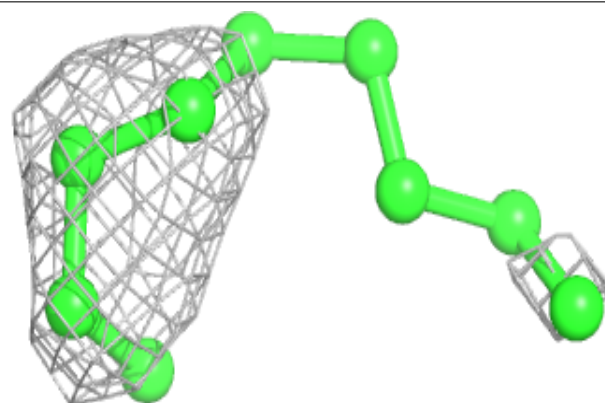


Electron density around OLC A 522:

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

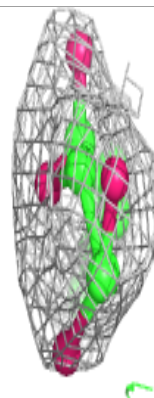
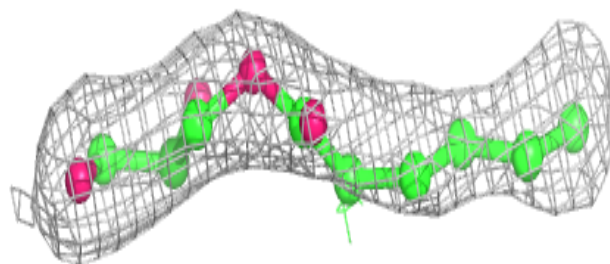
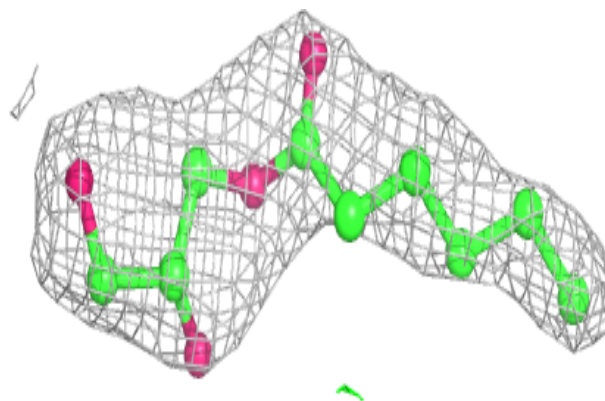
**Electron density around OLC A 515:**

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

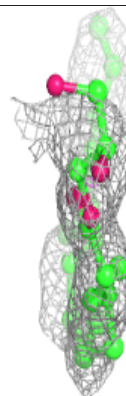
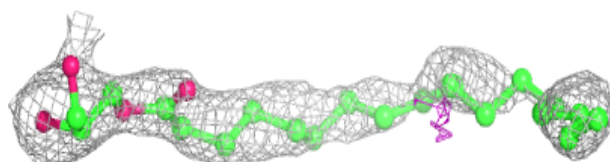
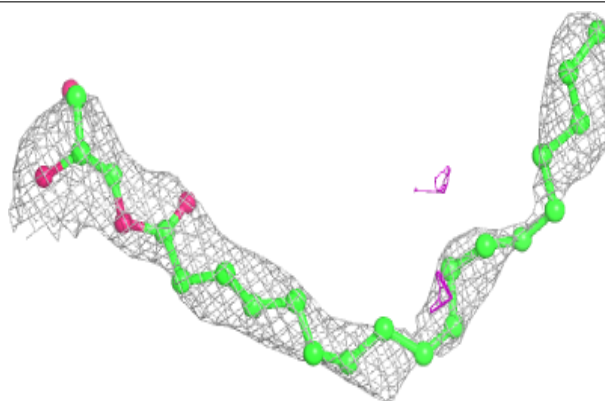


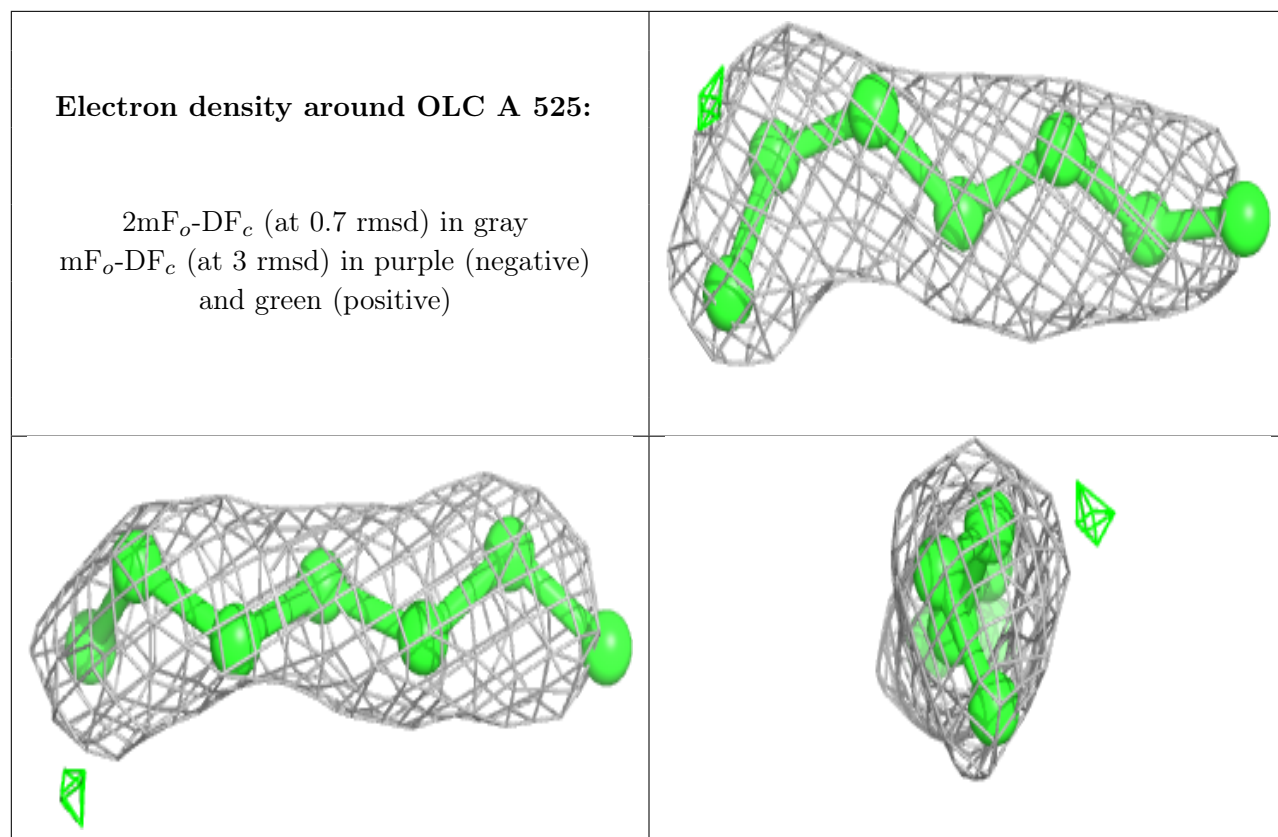
Electron density around OLC A 512:

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

**Electron density around OLC A 510:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.