Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 02:04 AM EDT

PDB ID	:	8E5V
Title	:	X-ray structure of the Deinococcus radiodurans Nramp/MntH divalent transition metal transporter WTsoak in an occluded state
Authors	:	Ray, S.; Gaudet, R.
Deposited on	:	2022-08-22
Resolution	:	2.36 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:

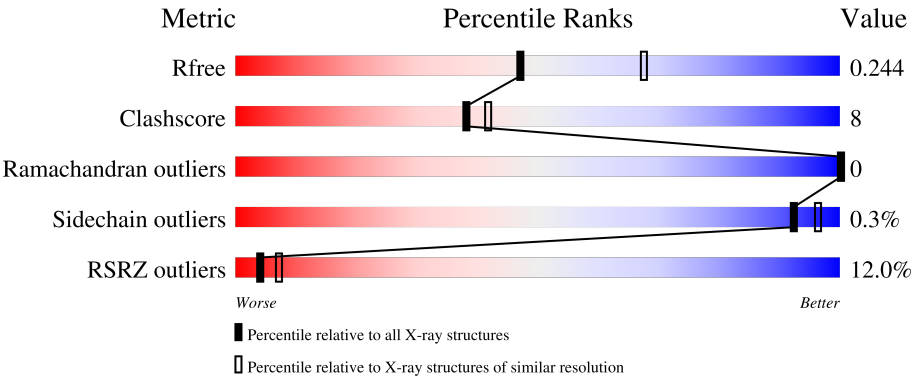
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 <=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	11% 83% 11% 5%

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	515	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OLC	A	517	-	-	-	X
4	OLC	A	520	-	-	-	X
4	OLC	A	524	-	-	-	X
5	PEG	A	530	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3449 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	3	0
			2945	1939	487	502	17			

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

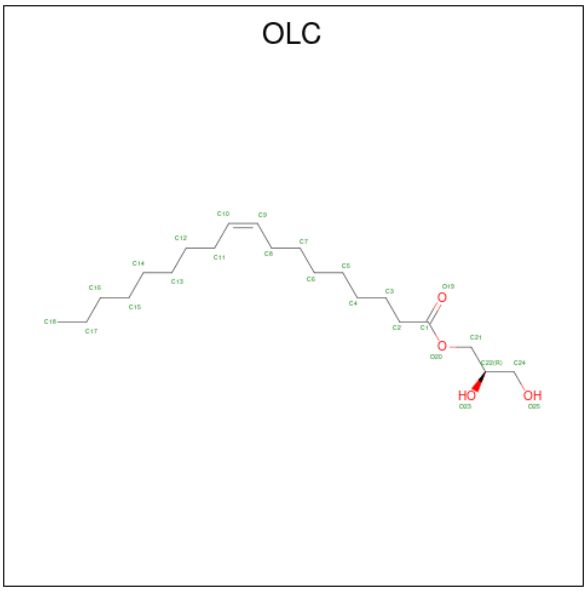
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- 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: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 19 15 4	0	0
4	A	1	Total C O 18 14 4	0	0
4	A	1	Total C O 13 9 4	0	0
4	A	1	Total C O 18 14 4	0	0
4	A	1	Total C O 23 19 4	0	0
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 O 14 10 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 7 7	0	0
4	A	1	Total C 8 8	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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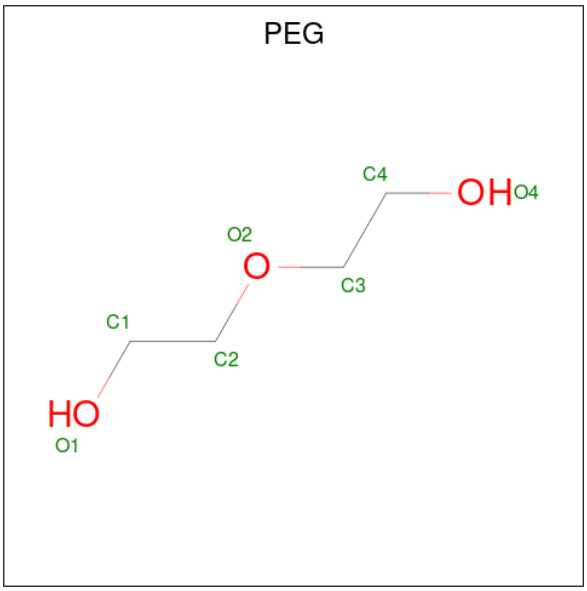
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 16 16	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C 9 9	0	0
4	A	1	Total C O 23 19 4	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C 18 18	0	0
4	A	1	Total C O 25 21 4	0	0
4	A	1	Total C O 22 18 4	0	0
4	A	1	Total C 9 9	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 6 is water.

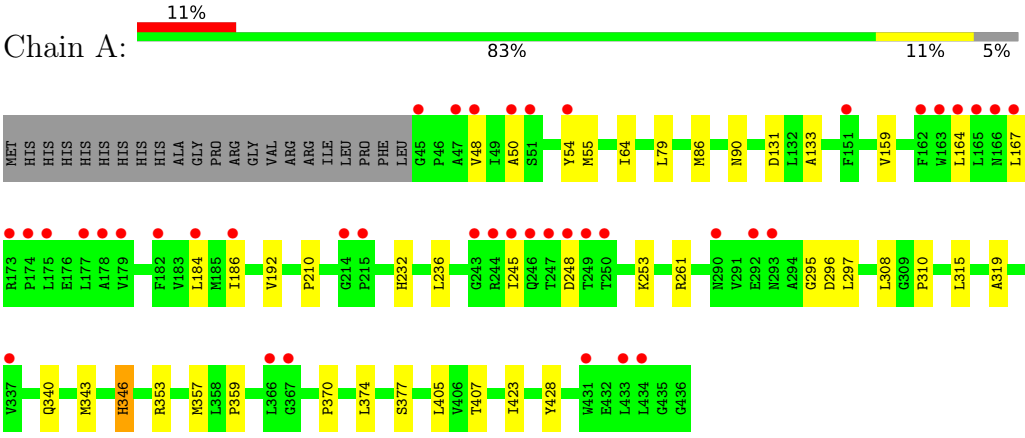
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.95Å 71.04Å 98.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.23 – 2.36 41.23 – 2.36	Depositor EDS
% Data completeness (in resolution range)	98.7 (41.23-2.36) 98.7 (41.23-2.36)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.217 , 0.246 0.216 , 0.244	Depositor DCC
R_{free} test set	1743 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3449	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/3009	0.43	0/4116

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2945	0	3072	38	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	427	0	664	31	0
5	A	14	0	20	1	0
6	A	61	0	0	1	0
All	All	3449	0	3756	54	0

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

All (54) 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:232:HIS:ND1	6:A:603:HOH:O	2.30	0.64
1:A:359:PRO:HB3	4:A:515:OLC:H14A	1.80	0.64
1:A:253:LYS:HB3	1:A:405:LEU:HD11	1.81	0.61
1:A:423:ILE:HG23	4:A:508:OLC:H14	1.83	0.59
1:A:333:MET:HB3	4:A:525:OLC:H14A	1.85	0.58
1:A:343:MET:HA	5:A:530:PEG:H32	1.85	0.58
1:A:159:VAL:HG11	4:A:516:OLC:H8	1.88	0.55
1:A:407:THR:HA	4:A:527:OLC:H21A	1.89	0.55
1:A:164:LEU:HD22	4:A:529:OLC:H15A	1.88	0.54
1:A:86:MET:O	1:A:90:ASN:ND2	2.28	0.54
1:A:428:TYR:HB2	4:A:520:OLC:H14	1.90	0.54
1:A:184:LEU:HD11	4:A:524:OLC:H14A	1.89	0.54
1:A:333:MET:HB2	4:A:525:OLC:H16	1.89	0.53
4:A:515:OLC:H14	4:A:515:OLC:H8	1.93	0.51
1:A:133:ALA:HA	1:A:374[B]:LEU:HD22	1.94	0.50
1:A:210:PRO:HD3	4:A:517:OLC:H9	1.93	0.50
1:A:133:ALA:HA	1:A:374[A]:LEU:HD22	1.94	0.50
1:A:353:ARG:HG3	1:A:357:MET:HE3	1.93	0.50
1:A:167:LEU:HB3	1:A:172:THR:HG23	1.94	0.49
1:A:48:VAL:HG13	4:A:524:OLC:H13A	1.93	0.49
1:A:340:GLN:HG2	1:A:346:HIS:HB3	1.94	0.49
1:A:131:ASP:OD2	1:A:353:ARG:NH2	2.46	0.49
1:A:261:ARG:HH22	4:A:510:OLC:H24A	1.79	0.48
4:A:516:OLC:H4A	4:A:516:OLC:H7A	1.59	0.48
1:A:308:LEU:HD13	1:A:315:LEU:HD12	1.98	0.46
4:A:525:OLC:H15A	4:A:525:OLC:H12	1.54	0.46
4:A:529:OLC:H13A	4:A:529:OLC:H16A	1.81	0.46
1:A:64:ILE:HG22	1:A:295:GLY:HA2	1.97	0.46
4:A:525:OLC:H17	4:A:525:OLC:H14	1.54	0.46
1:A:245:ILE:HD12	1:A:253:LYS:HG3	1.99	0.45
4:A:528:OLC:H4	4:A:528:OLC:H7	1.71	0.45
4:A:508:OLC:H7	4:A:522:OLC:H17	1.99	0.45
4:A:519:OLC:H2	4:A:519:OLC:H21	1.72	0.45
1:A:79:LEU:HG	4:A:517:OLC:H14A	1.99	0.45
1:A:310:PRO:HB3	4:A:519:OLC:H3	1.98	0.44
4:A:517:OLC:H13	4:A:517:OLC:H16	1.68	0.44
1:A:50:ALA:HB1	1:A:54:TYR:HE2	1.83	0.43
1:A:245:ILE:HD13	1:A:248:ASP:HA	2.00	0.43
1:A:192:VAL:HA	4:A:507:OLC:H2	2.00	0.43
4:A:515:OLC:H18A	4:A:515:OLC:H15	1.73	0.43
1:A:133:ALA:HB2	1:A:377:SER:OG	2.19	0.42
4:A:508:OLC:H18A	4:A:508:OLC:H15	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:O	1:A:323:SER:OG	2.28	0.42
4:A:517:OLC:H5	4:A:517:OLC:H8	1.74	0.42
4:A:505:OLC:H5	4:A:505:OLC:H2A	1.89	0.42
4:A:523:OLC:H2	4:A:523:OLC:H21A	1.71	0.42
1:A:296:ASP:OD1	1:A:297:LEU:N	2.53	0.42
4:A:512:OLC:H11	4:A:512:OLC:H8A	1.73	0.42
1:A:236:LEU:HD22	1:A:334:ALA:HB2	2.03	0.41
1:A:167:LEU:HB3	1:A:172:THR:CG2	2.51	0.41
4:A:512:OLC:H15	4:A:512:OLC:H18A	1.86	0.41
1:A:186:ILE:HG13	1:A:319:ALA:HB2	2.02	0.40
1:A:370:PRO:O	1:A:374[B]:LEU:HG	2.21	0.40
1:A:370:PRO:O	1:A:374[A]:LEU:HG	2.21	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	393/414 (95%)	387 (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	301/322 (94%)	300 (100%)	1 (0%)	92 96

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

Mol	Chain	Res	Type
1	A	346	HIS

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	59	ASN
1	A	82	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 2 are monoatomic - leaving 29 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	513	-	6,6,24	0.31	0	5,5,25	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OLC	A	506	-	17,17,24	0.95	2 (11%)	18,18,25	1.03	1 (5%)
4	OLC	A	524	-	7,7,24	0.31	0	6,6,25	0.71	0
4	OLC	A	518	-	10,10,24	0.40	0	9,9,25	0.88	0
4	OLC	A	526	-	17,17,24	0.33	0	16,16,25	0.77	0
5	PEG	A	530	-	6,6,6	0.11	0	5,5,5	0.08	0
4	OLC	A	507	-	22,22,24	0.83	2 (9%)	23,23,25	0.98	1 (4%)
4	OLC	A	528	-	21,21,24	0.85	2 (9%)	22,22,25	0.93	1 (4%)
4	OLC	A	505	-	12,12,24	1.10	2 (16%)	13,13,25	1.01	1 (7%)
4	OLC	A	522	-	8,8,24	0.30	0	7,7,25	0.75	0
4	OLC	A	517	-	15,15,24	0.33	0	14,14,25	0.70	0
4	OLC	A	519	-	24,24,24	0.81	2 (8%)	25,25,25	0.98	1 (4%)
4	OLC	A	520	-	6,6,24	0.31	0	5,5,25	0.65	0
4	OLC	A	515	-	24,24,24	0.81	2 (8%)	25,25,25	0.98	1 (4%)
4	OLC	A	511	-	10,10,24	0.41	0	9,9,25	0.86	0
4	OLC	A	508	-	17,17,24	0.32	0	16,16,25	0.81	0
5	PEG	A	531	-	6,6,6	0.12	0	5,5,5	0.03	0
4	OLC	A	523	-	22,22,24	0.83	2 (9%)	23,23,25	1.03	1 (4%)
4	OLC	A	521	-	10,10,24	0.35	0	9,9,25	0.67	0
4	OLC	A	503	-	18,18,24	0.92	2 (11%)	18,19,25	1.13	1 (5%)
4	OLC	A	516	-	7,7,24	0.31	0	6,6,25	0.69	0
4	OLC	A	514	-	7,7,24	0.30	0	6,6,25	0.72	0
4	OLC	A	512	-	24,24,24	0.81	2 (8%)	25,25,25	1.00	1 (4%)
4	OLC	A	529	-	8,8,24	0.30	0	7,7,25	0.75	0
4	OLC	A	510	-	13,13,24	1.06	2 (15%)	14,14,25	1.06	1 (7%)
4	OLC	A	527	-	24,24,24	0.80	2 (8%)	25,25,25	0.94	1 (4%)
4	OLC	A	504	-	17,17,24	0.95	2 (11%)	18,18,25	1.05	1 (5%)
4	OLC	A	509	-	24,24,24	0.81	2 (8%)	25,25,25	0.97	1 (4%)
4	OLC	A	525	-	10,10,24	0.41	0	9,9,25	0.85	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	513	-	-	0/4/4/24	-
4	OLC	A	506	-	-	12/17/17/24	-
4	OLC	A	524	-	-	3/5/5/24	-
4	OLC	A	518	-	-	5/8/8/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLC	A	526	-	-	9/15/15/24	-
5	PEG	A	530	-	-	1/4/4/4	-
4	OLC	A	507	-	-	11/22/22/24	-
4	OLC	A	528	-	-	11/21/21/24	-
4	OLC	A	505	-	-	3/12/12/24	-
4	OLC	A	522	-	-	4/6/6/24	-
4	OLC	A	517	-	-	8/13/13/24	-
4	OLC	A	519	-	-	14/24/24/24	-
4	OLC	A	520	-	-	2/4/4/24	-
4	OLC	A	515	-	-	12/24/24/24	-
4	OLC	A	511	-	-	4/8/8/24	-
4	OLC	A	508	-	-	6/15/15/24	-
5	PEG	A	531	-	-	3/4/4/4	-
4	OLC	A	523	-	-	10/22/22/24	-
4	OLC	A	521	-	-	2/8/8/24	-
4	OLC	A	503	-	-	13/18/18/24	-
4	OLC	A	516	-	-	4/5/5/24	-
4	OLC	A	514	-	-	1/5/5/24	-
4	OLC	A	512	-	-	15/24/24/24	-
4	OLC	A	529	-	-	2/6/6/24	-
4	OLC	A	510	-	-	9/13/13/24	-
4	OLC	A	527	-	-	14/24/24/24	-
4	OLC	A	504	-	-	8/17/17/24	-
4	OLC	A	509	-	-	14/24/24/24	-
4	OLC	A	525	-	-	4/8/8/24	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	OLC	O20-C1	2.49	1.40	1.33
4	A	504	OLC	O20-C1	2.46	1.40	1.33
4	A	519	OLC	O20-C1	2.46	1.40	1.33
4	A	523	OLC	O20-C1	2.46	1.40	1.33
4	A	505	OLC	O20-C1	2.43	1.40	1.33
4	A	512	OLC	O20-C1	2.41	1.40	1.33
4	A	515	OLC	O20-C1	2.41	1.40	1.33
4	A	503	OLC	O20-C1	2.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	527	OLC	O20-C1	2.39	1.40	1.33
4	A	528	OLC	O20-C1	2.38	1.40	1.33
4	A	507	OLC	O20-C1	2.38	1.40	1.33
4	A	506	OLC	O20-C1	2.38	1.40	1.33
4	A	509	OLC	O20-C1	2.38	1.40	1.33
4	A	509	OLC	O20-C21	-2.15	1.40	1.45
4	A	505	OLC	O20-C21	-2.14	1.40	1.45
4	A	512	OLC	O20-C21	-2.14	1.40	1.45
4	A	519	OLC	O20-C21	-2.11	1.40	1.45
4	A	528	OLC	O20-C21	-2.11	1.40	1.45
4	A	507	OLC	O20-C21	-2.10	1.40	1.45
4	A	506	OLC	O20-C21	-2.10	1.40	1.45
4	A	515	OLC	O20-C21	-2.10	1.40	1.45
4	A	510	OLC	O20-C21	-2.08	1.40	1.45
4	A	523	OLC	O20-C21	-2.07	1.40	1.45
4	A	527	OLC	O20-C21	-2.07	1.40	1.45
4	A	503	OLC	O20-C21	-2.04	1.40	1.45
4	A	504	OLC	O20-C21	-2.03	1.40	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	OLC	O20-C1-C2	3.02	121.38	111.91
4	A	512	OLC	O20-C1-C2	2.81	120.73	111.91
4	A	515	OLC	O20-C1-C2	2.76	120.56	111.91
4	A	519	OLC	O20-C1-C2	2.74	120.51	111.91
4	A	510	OLC	O20-C1-C2	2.71	120.42	111.91
4	A	523	OLC	O20-C1-C2	2.70	120.37	111.91
4	A	507	OLC	O20-C1-C2	2.68	120.31	111.91
4	A	504	OLC	O20-C1-C2	2.59	120.03	111.91
4	A	509	OLC	O20-C1-C2	2.56	119.94	111.91
4	A	506	OLC	O20-C1-C2	2.50	119.75	111.91
4	A	505	OLC	O20-C1-C2	2.48	119.68	111.91
4	A	527	OLC	O20-C1-C2	2.47	119.67	111.91
4	A	528	OLC	O20-C1-C2	2.42	119.49	111.91

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	OLC	C9-C10-C11-C12
4	A	503	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
4	A	504	OLC	C2-C1-O20-C21
4	A	504	OLC	O19-C1-O20-C21
4	A	507	OLC	O20-C21-C22-C24
4	A	507	OLC	O20-C21-C22-O23
4	A	509	OLC	C21-C22-C24-O25
4	A	510	OLC	O20-C21-C22-C24
4	A	510	OLC	C2-C1-O20-C21
4	A	510	OLC	O19-C1-O20-C21
4	A	519	OLC	O20-C21-C22-C24
4	A	519	OLC	O20-C21-C22-O23
4	A	519	OLC	C2-C1-O20-C21
4	A	519	OLC	O19-C1-O20-C21
4	A	523	OLC	C2-C1-O20-C21
4	A	523	OLC	O19-C1-O20-C21
4	A	527	OLC	C21-C22-C24-O25
4	A	528	OLC	C21-C22-C24-O25
4	A	512	OLC	O19-C1-O20-C21
4	A	528	OLC	O19-C1-O20-C21
4	A	512	OLC	C2-C1-O20-C21
4	A	528	OLC	C2-C1-O20-C21
4	A	506	OLC	O20-C21-C22-O23
4	A	510	OLC	O20-C21-C22-O23
4	A	515	OLC	C2-C1-O20-C21
4	A	503	OLC	O20-C21-C22-C24
4	A	527	OLC	O20-C21-C22-C24
4	A	527	OLC	O20-C21-C22-O23
4	A	515	OLC	O19-C1-O20-C21
4	A	509	OLC	C1-C2-C3-C4
4	A	509	OLC	O23-C22-C24-O25
4	A	523	OLC	O23-C22-C24-O25
4	A	503	OLC	C1-C2-C3-C4
4	A	507	OLC	C1-C2-C3-C4
5	A	531	PEG	O2-C3-C4-O4
4	A	503	OLC	C3-C4-C5-C6
4	A	525	OLC	C14-C15-C16-C17
4	A	527	OLC	C1-C2-C3-C4
4	A	525	OLC	C12-C13-C14-C15
4	A	503	OLC	O20-C21-C22-O23
4	A	512	OLC	O20-C21-C22-O23
4	A	506	OLC	C2-C1-O20-C21
4	A	509	OLC	C2-C1-O20-C21
4	A	507	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
4	A	503	OLC	C5-C6-C7-C8
4	A	512	OLC	C13-C14-C15-C16
4	A	518	OLC	C11-C12-C13-C14
4	A	506	OLC	O20-C21-C22-C24
4	A	512	OLC	O20-C21-C22-C24
4	A	509	OLC	C5-C6-C7-C8
4	A	510	OLC	C2-C3-C4-C5
4	A	522	OLC	C11-C12-C13-C14
4	A	503	OLC	C4-C5-C6-C7
4	A	515	OLC	C5-C6-C7-C8
4	A	509	OLC	C3-C4-C5-C6
4	A	506	OLC	C2-C3-C4-C5
4	A	510	OLC	C3-C4-C5-C6
4	A	519	OLC	C5-C6-C7-C8
4	A	527	OLC	C3-C4-C5-C6
4	A	508	OLC	C2-C3-C4-C5
4	A	512	OLC	C12-C13-C14-C15
4	A	523	OLC	C2-C3-C4-C5
4	A	506	OLC	O19-C1-O20-C21
4	A	508	OLC	C11-C12-C13-C14
4	A	524	OLC	C13-C14-C15-C16
4	A	506	OLC	C21-C22-C24-O25
4	A	523	OLC	C21-C22-C24-O25
4	A	517	OLC	C12-C13-C14-C15
4	A	519	OLC	C10-C11-C12-C13
4	A	526	OLC	C14-C15-C16-C17
4	A	525	OLC	C11-C12-C13-C14
4	A	515	OLC	C13-C14-C15-C16
4	A	509	OLC	O19-C1-O20-C21
4	A	515	OLC	C4-C5-C6-C7
4	A	526	OLC	C3-C4-C5-C6
4	A	503	OLC	O23-C22-C24-O25
4	A	527	OLC	O23-C22-C24-O25
4	A	528	OLC	O23-C22-C24-O25
4	A	511	OLC	C12-C13-C14-C15
4	A	509	OLC	C10-C11-C12-C13
4	A	509	OLC	C6-C7-C8-C9
4	A	515	OLC	C6-C7-C8-C9
5	A	531	PEG	C4-C3-O2-C2
4	A	504	OLC	C5-C6-C7-C8
4	A	507	OLC	O19-C1-O20-C21
4	A	519	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	A	527	OLC	C5-C6-C7-C8
4	A	518	OLC	C12-C13-C14-C15
4	A	507	OLC	C4-C5-C6-C7
4	A	518	OLC	C10-C11-C12-C13
4	A	523	OLC	C10-C11-C12-C13
4	A	512	OLC	C14-C15-C16-C17
4	A	523	OLC	C4-C5-C6-C7
4	A	508	OLC	C3-C4-C5-C6
4	A	511	OLC	C10-C11-C12-C13
4	A	512	OLC	C6-C7-C8-C9
4	A	525	OLC	C10-C11-C12-C13
4	A	526	OLC	C10-C11-C12-C13
4	A	527	OLC	C10-C11-C12-C13
4	A	527	OLC	C11-C12-C13-C14
4	A	516	OLC	C3-C4-C5-C6
4	A	521	OLC	C11-C12-C13-C14
4	A	506	OLC	C5-C6-C7-C8
4	A	507	OLC	C5-C6-C7-C8
4	A	512	OLC	C5-C6-C7-C8
4	A	514	OLC	C6-C7-C8-C9
4	A	529	OLC	C10-C11-C12-C13
4	A	511	OLC	C13-C14-C15-C16
4	A	503	OLC	C2-C3-C4-C5
4	A	516	OLC	C2-C3-C4-C5
4	A	517	OLC	C7-C8-C9-C10
4	A	526	OLC	C6-C7-C8-C9
4	A	527	OLC	C6-C7-C8-C9
4	A	528	OLC	C6-C7-C8-C9
4	A	509	OLC	C4-C5-C6-C7
4	A	524	OLC	C15-C16-C17-C18
4	A	515	OLC	O20-C21-C22-O23
4	A	506	OLC	C1-C2-C3-C4
4	A	508	OLC	C12-C13-C14-C15
4	A	515	OLC	O20-C21-C22-C24
4	A	519	OLC	C15-C16-C17-C18
4	A	504	OLC	C2-C3-C4-C5
4	A	507	OLC	C3-C4-C5-C6
4	A	504	OLC	C21-C22-C24-O25
4	A	522	OLC	C14-C15-C16-C17
4	A	526	OLC	C2-C3-C4-C5
4	A	506	OLC	O23-C22-C24-O25
4	A	528	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	517	OLC	C13-C14-C15-C16
4	A	519	OLC	C3-C4-C5-C6
4	A	527	OLC	C15-C16-C17-C18
4	A	522	OLC	C10-C11-C12-C13
4	A	507	OLC	C13-C14-C15-C16
4	A	526	OLC	C1-C2-C3-C4
4	A	512	OLC	C2-C3-C4-C5
4	A	526	OLC	C11-C12-C13-C14
4	A	510	OLC	O23-C22-C24-O25
4	A	508	OLC	C10-C11-C12-C13
4	A	516	OLC	C6-C7-C8-C9
4	A	522	OLC	C13-C14-C15-C16
4	A	520	OLC	C12-C13-C14-C15
4	A	512	OLC	C11-C12-C13-C14
4	A	503	OLC	C6-C7-C8-C9
4	A	508	OLC	C4-C5-C6-C7
4	A	515	OLC	C14-C15-C16-C17
4	A	518	OLC	C15-C16-C17-C18
4	A	528	OLC	C2-C3-C4-C5
5	A	531	PEG	C1-C2-O2-C3
4	A	528	OLC	O20-C21-C22-O23
4	A	518	OLC	C14-C15-C16-C17
4	A	515	OLC	C1-C2-C3-C4
4	A	526	OLC	C5-C6-C7-C8
4	A	503	OLC	C2-C1-O20-C21
4	A	516	OLC	C4-C5-C6-C7
4	A	506	OLC	C3-C4-C5-C6
4	A	523	OLC	C7-C8-C9-C10
4	A	503	OLC	O19-C1-O20-C21
4	A	512	OLC	C21-C22-C24-O25
4	A	517	OLC	C9-C10-C11-C12
4	A	512	OLC	C3-C4-C5-C6
4	A	523	OLC	C5-C6-C7-C8
4	A	524	OLC	C11-C12-C13-C14
4	A	517	OLC	C14-C15-C16-C17
4	A	520	OLC	C14-C15-C16-C17
4	A	519	OLC	C14-C15-C16-C17
4	A	517	OLC	C6-C7-C8-C9
4	A	521	OLC	C10-C11-C12-C13
4	A	528	OLC	C9-C10-C11-C12
4	A	528	OLC	C7-C8-C9-C10
4	A	511	OLC	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	A	523	OLC	C3-C4-C5-C6
4	A	519	OLC	C9-C10-C11-C12
4	A	527	OLC	C13-C14-C15-C16
4	A	526	OLC	C15-C16-C17-C18
4	A	505	OLC	C21-C22-C24-O25
4	A	510	OLC	C21-C22-C24-O25
4	A	515	OLC	C7-C8-C9-C10
4	A	528	OLC	C5-C6-C7-C8
4	A	517	OLC	C4-C5-C6-C7
4	A	505	OLC	O23-C22-C24-O25
4	A	517	OLC	C3-C4-C5-C6
4	A	519	OLC	C7-C8-C9-C10
4	A	527	OLC	C9-C10-C11-C12
4	A	509	OLC	O20-C1-C2-C3
4	A	509	OLC	C7-C8-C9-C10
4	A	512	OLC	O20-C1-C2-C3
4	A	519	OLC	O20-C1-C2-C3
4	A	507	OLC	C12-C13-C14-C15
4	A	506	OLC	C7-C8-C9-C10
4	A	510	OLC	C1-C2-C3-C4
4	A	504	OLC	C4-C5-C6-C7
4	A	505	OLC	C2-C3-C4-C5
4	A	529	OLC	C11-C12-C13-C14
4	A	509	OLC	C2-C3-C4-C5
4	A	509	OLC	O19-C1-C2-C3
4	A	512	OLC	O19-C1-C2-C3
5	A	530	PEG	C1-C2-O2-C3
4	A	515	OLC	O23-C22-C24-O25
4	A	507	OLC	C9-C10-C11-C12
4	A	504	OLC	O20-C1-C2-C3
4	A	506	OLC	C4-C5-C6-C7
4	A	519	OLC	O19-C1-C2-C3
4	A	527	OLC	C7-C8-C9-C10
4	A	504	OLC	O19-C1-C2-C3

There are no ring outliers.

18 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	524	OLC	2	0
5	A	530	PEG	1	0
4	A	507	OLC	1	0

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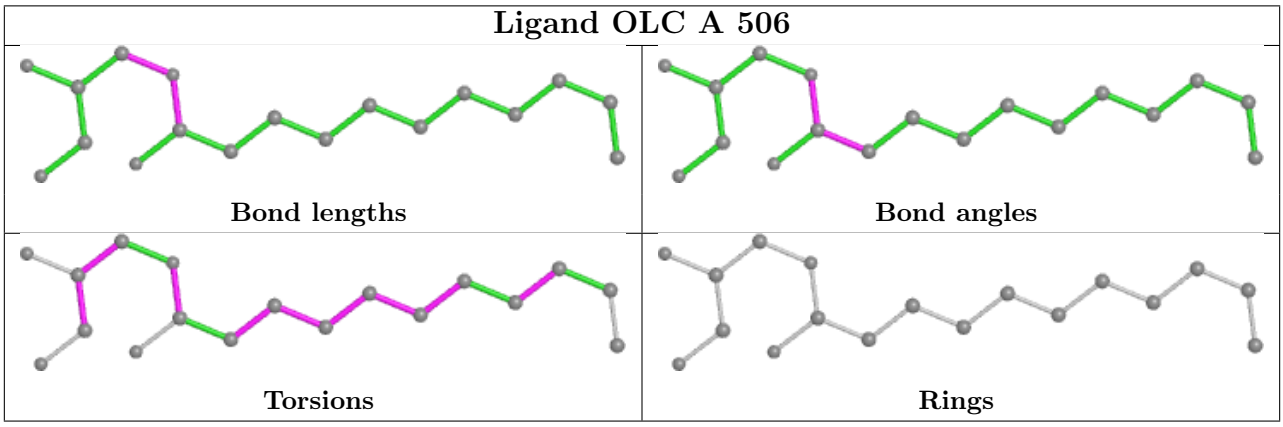
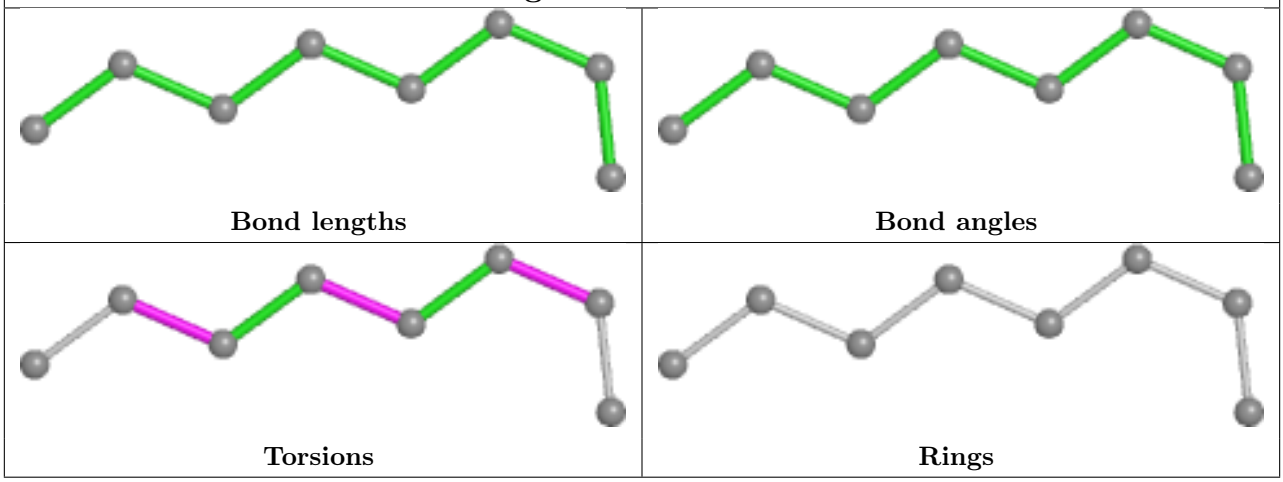
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	528	OLC	1	0
4	A	505	OLC	1	0
4	A	522	OLC	1	0
4	A	517	OLC	4	0
4	A	519	OLC	2	0
4	A	520	OLC	1	0
4	A	515	OLC	3	0
4	A	508	OLC	3	0
4	A	523	OLC	1	0
4	A	516	OLC	2	0
4	A	512	OLC	2	0
4	A	529	OLC	2	0
4	A	510	OLC	1	0
4	A	527	OLC	1	0
4	A	525	OLC	4	0

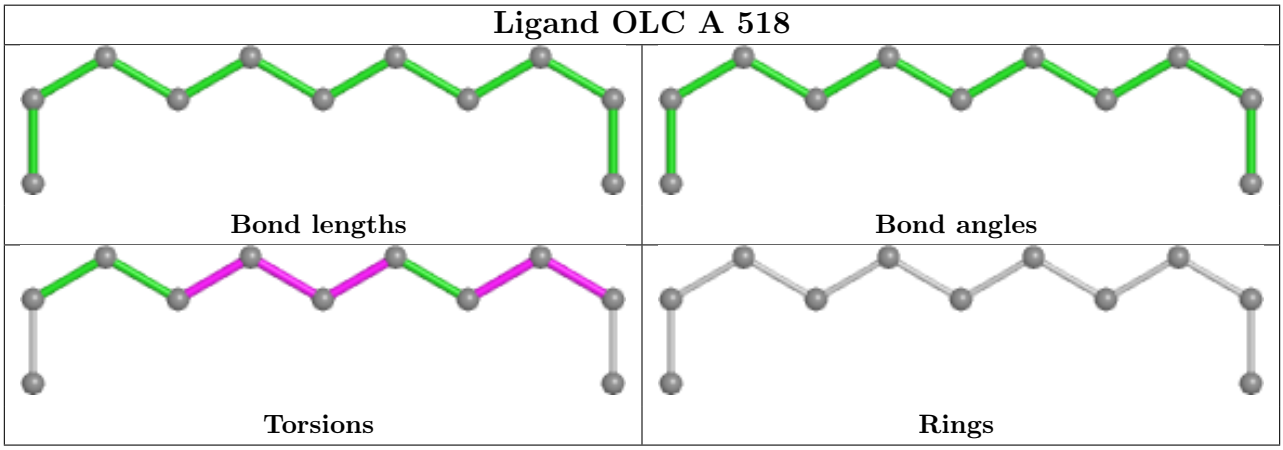
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



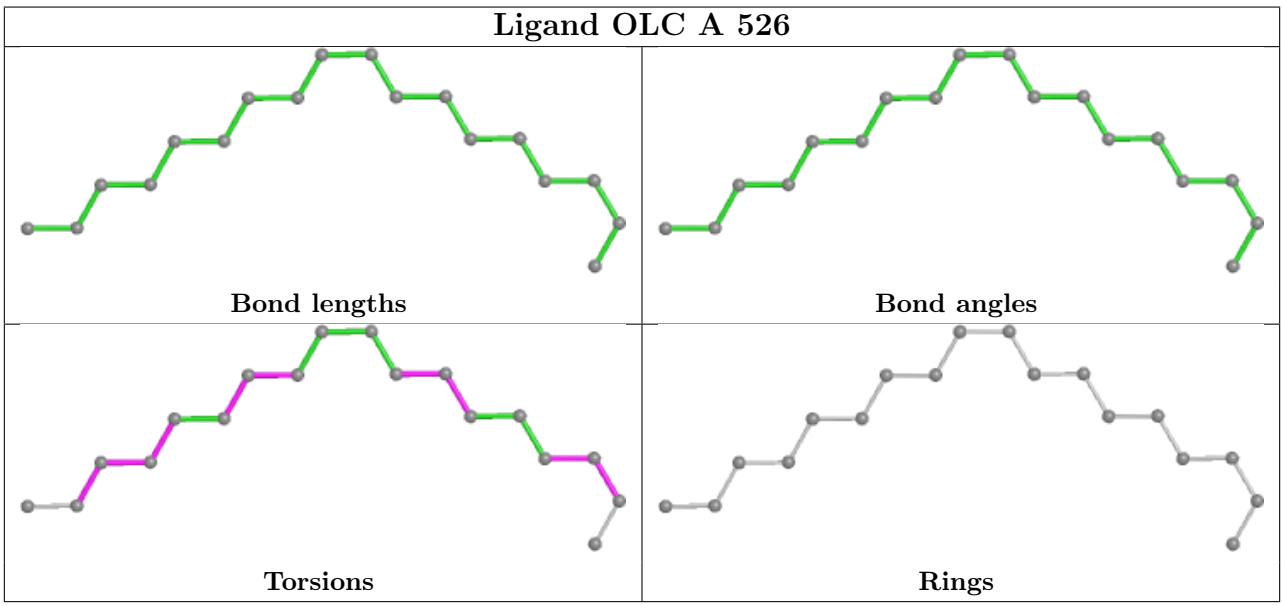
Ligand OLC A 524



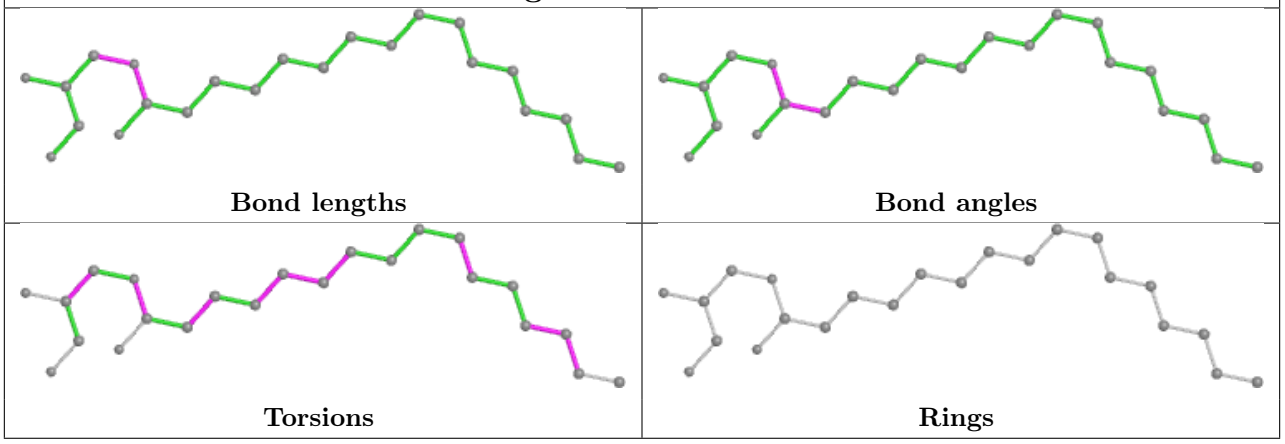
Ligand OLC A 518



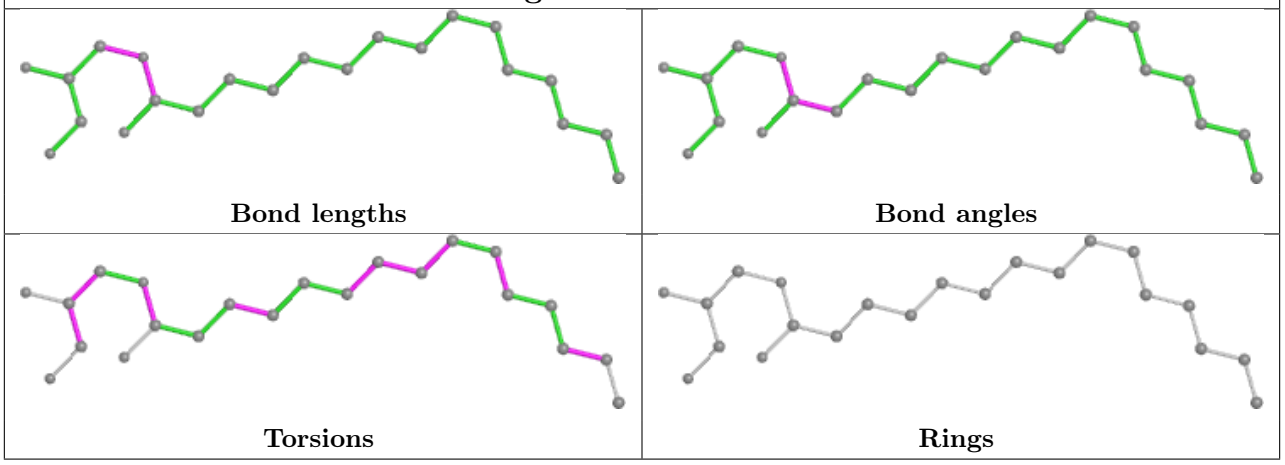
Ligand OLC A 526



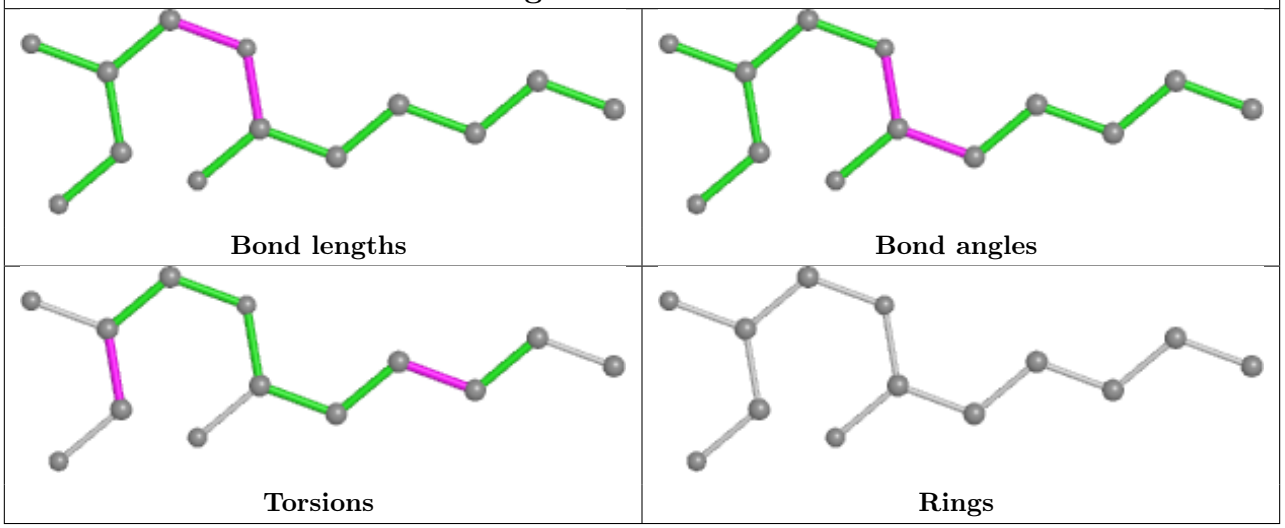
Ligand OLC A 507



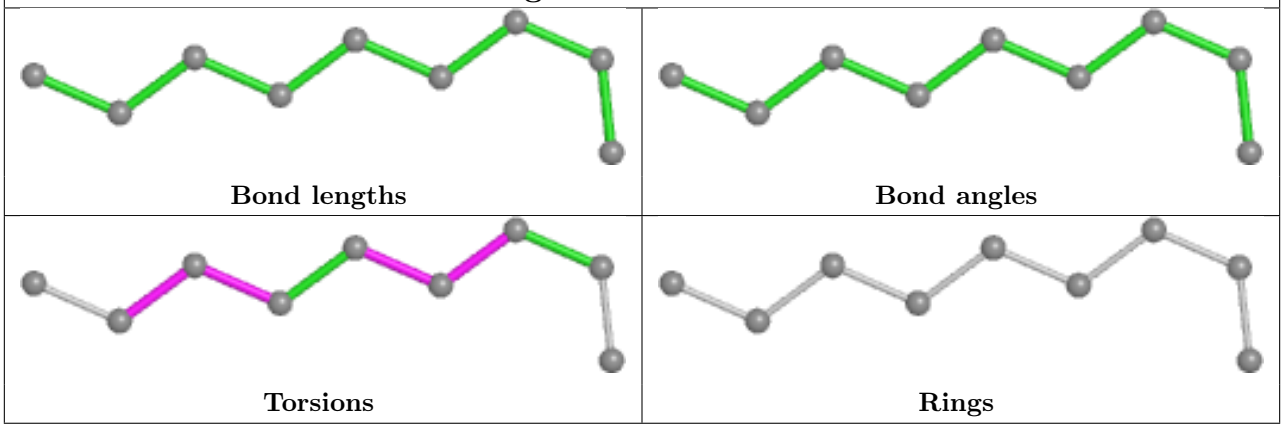
Ligand OLC A 528



Ligand OLC A 505



Ligand OLC A 522



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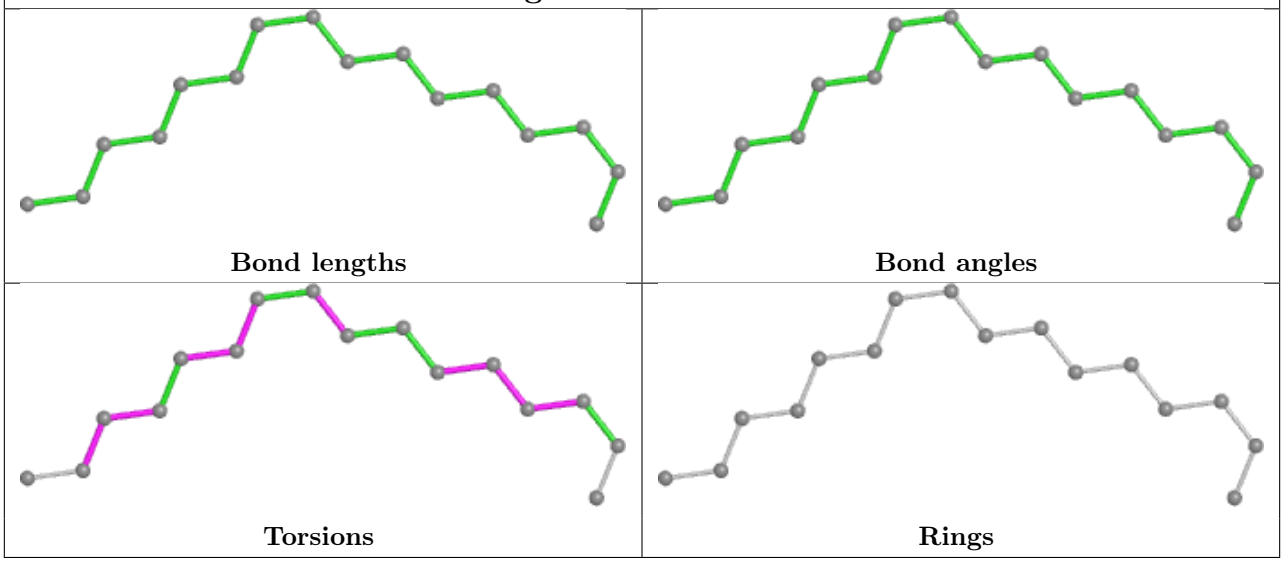

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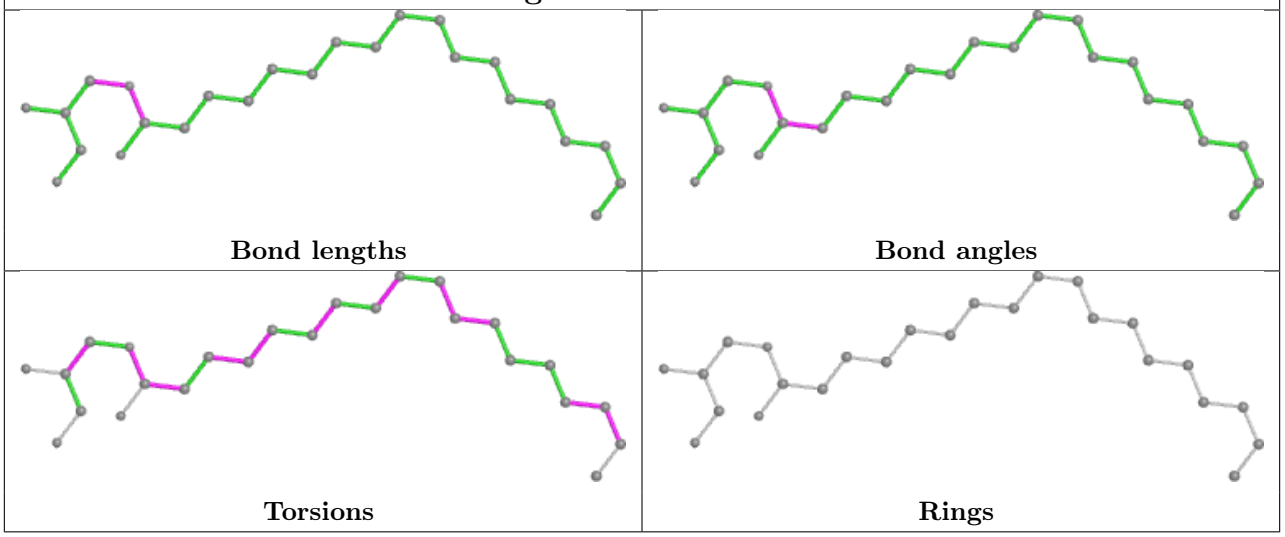

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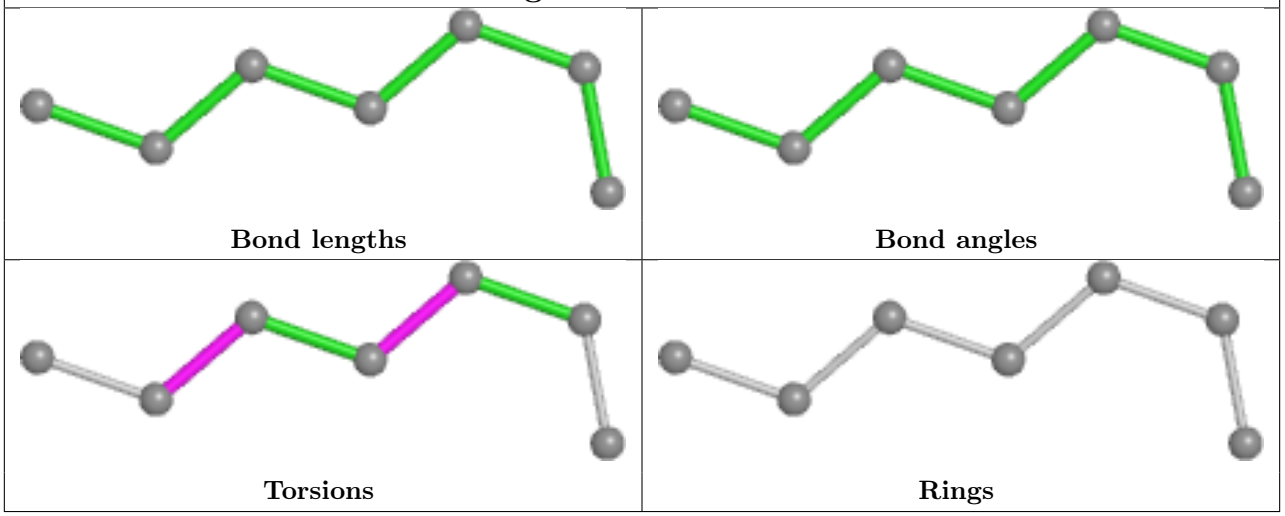

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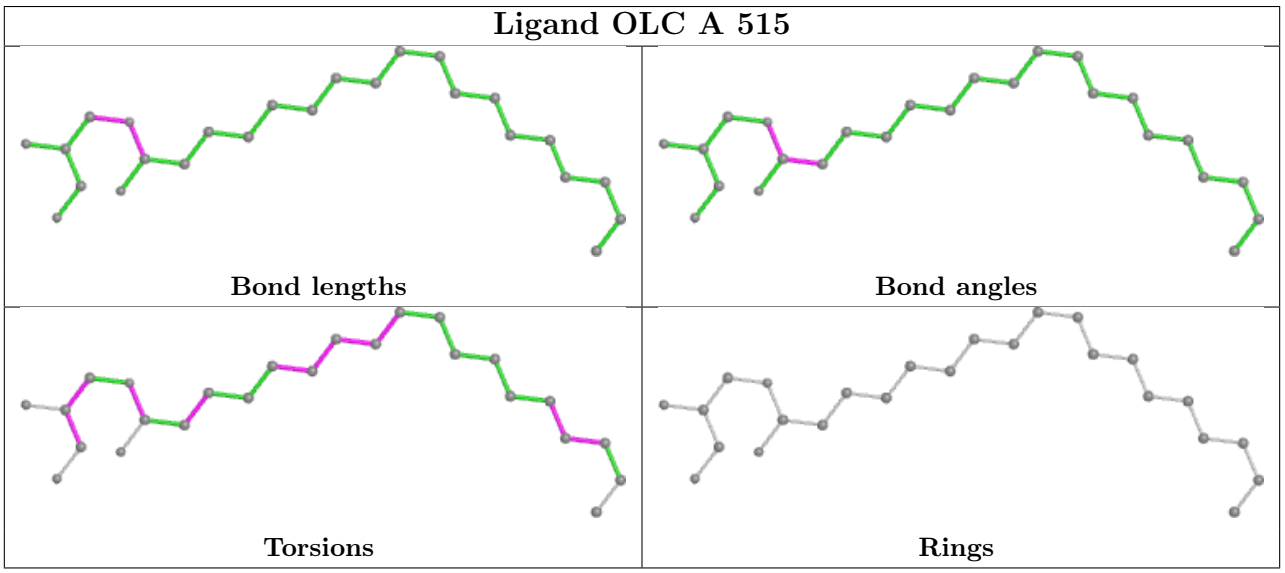

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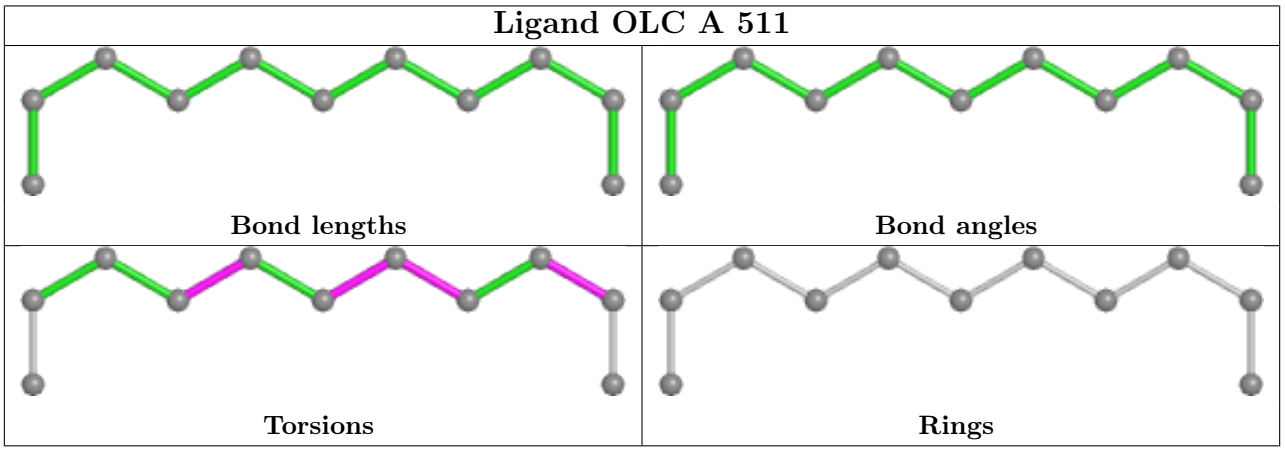

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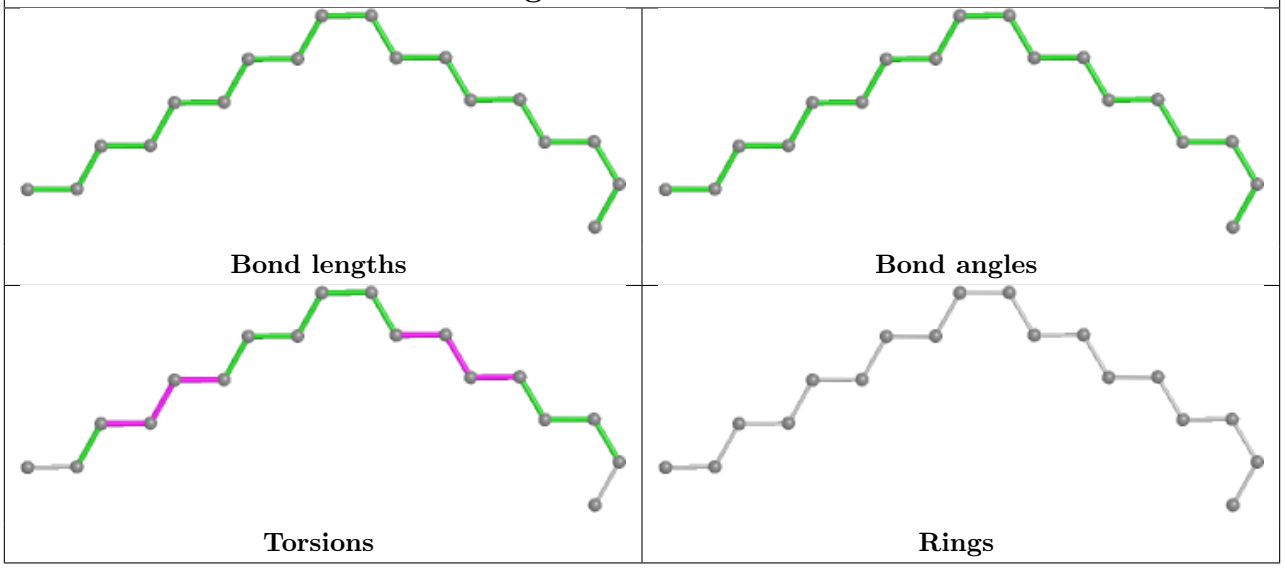

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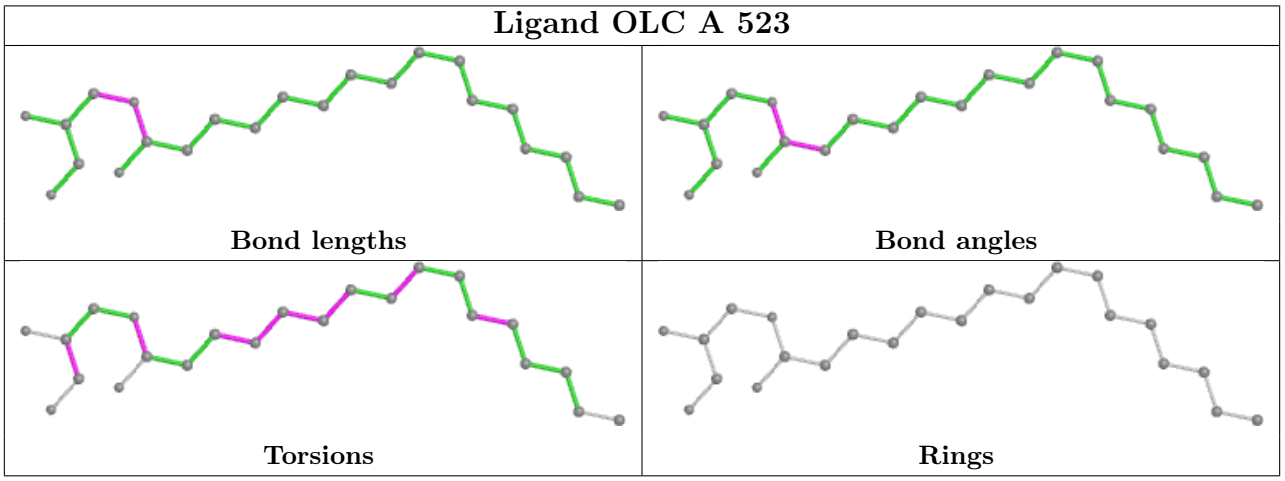

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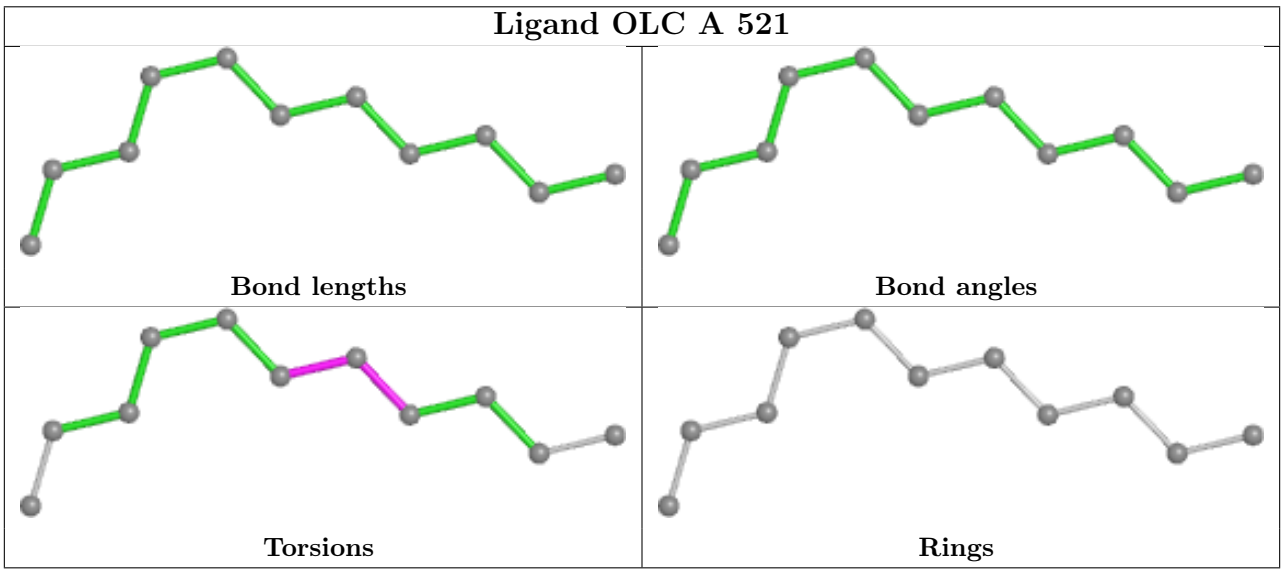
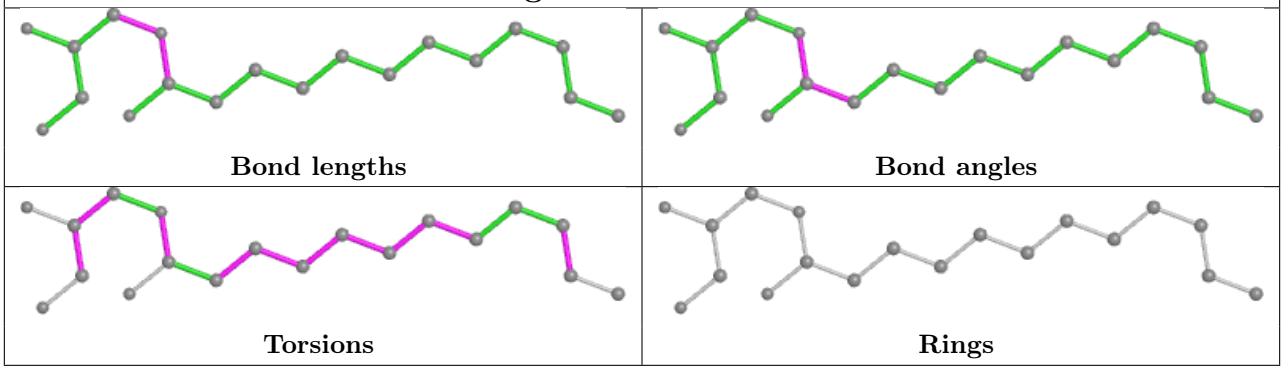
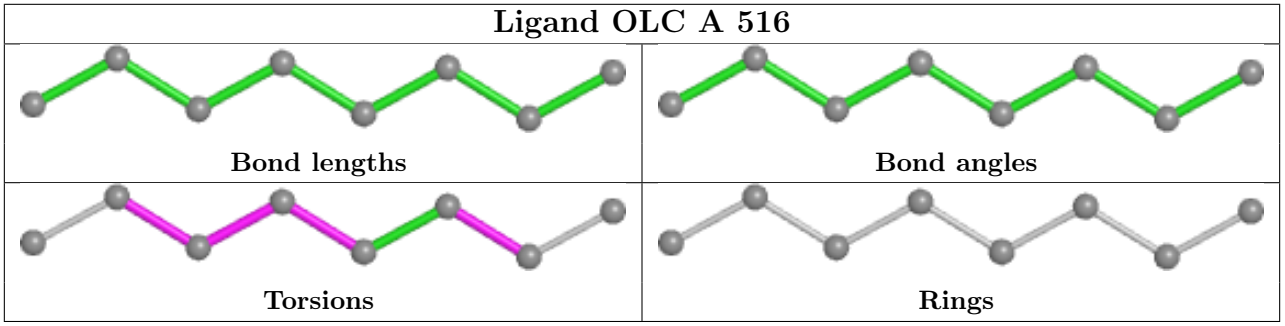


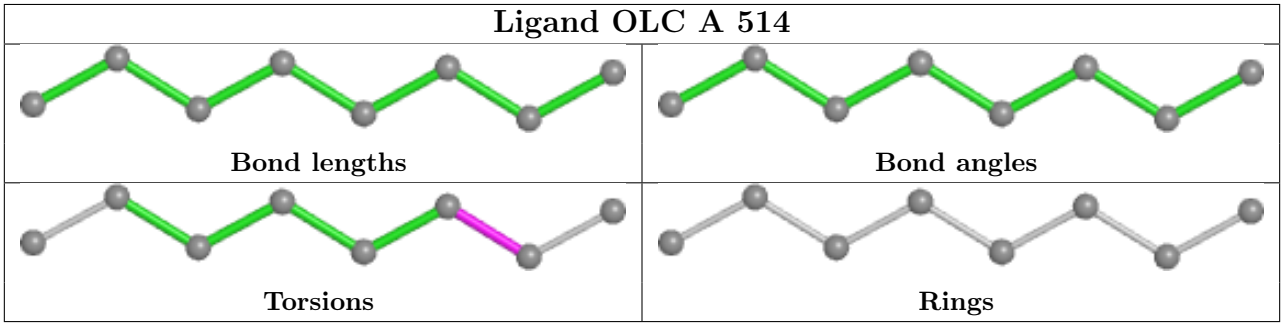
Ligand OLC A 503



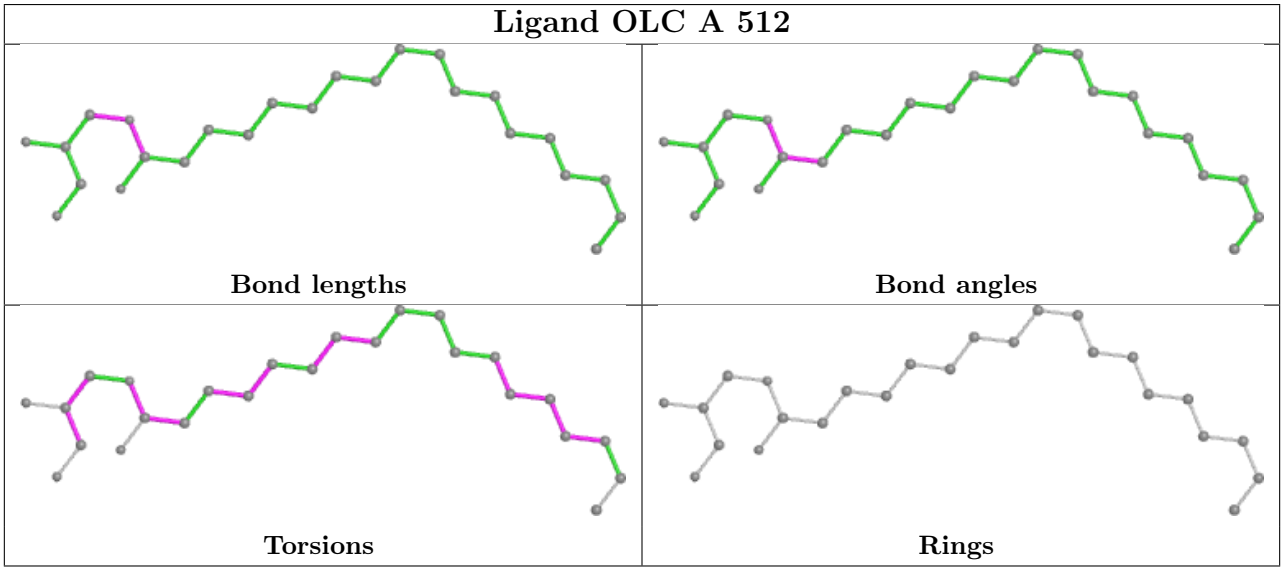
Ligand OLC A 516



Ligand OLC A 514



Ligand OLC A 512



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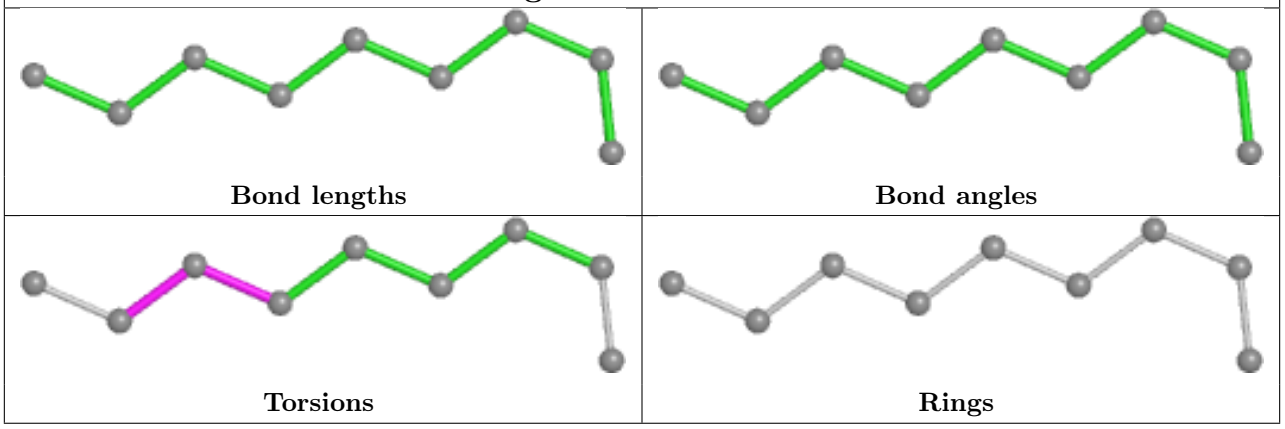

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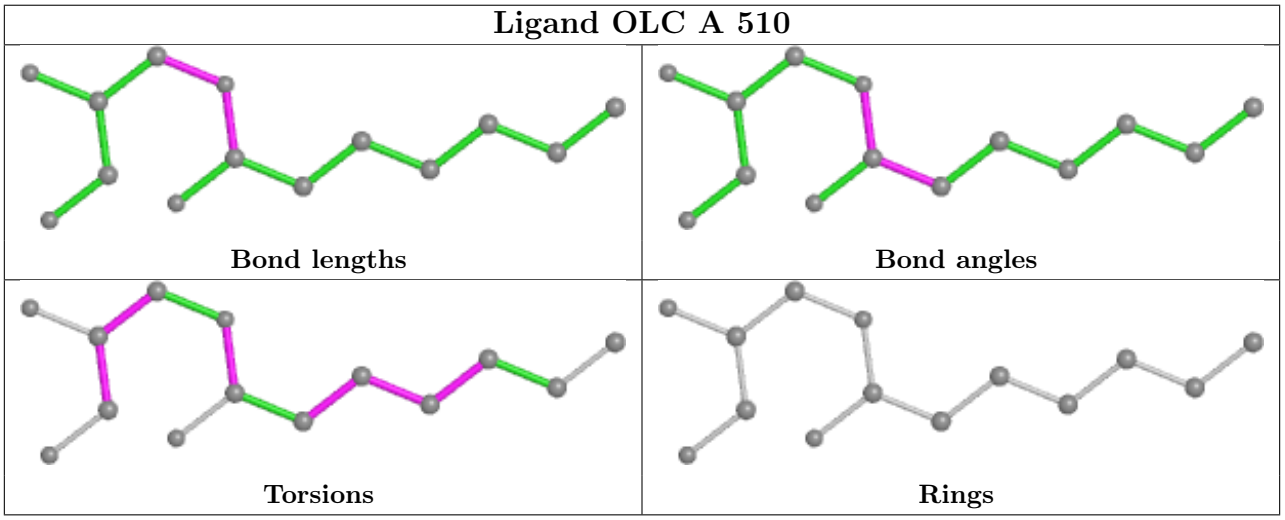
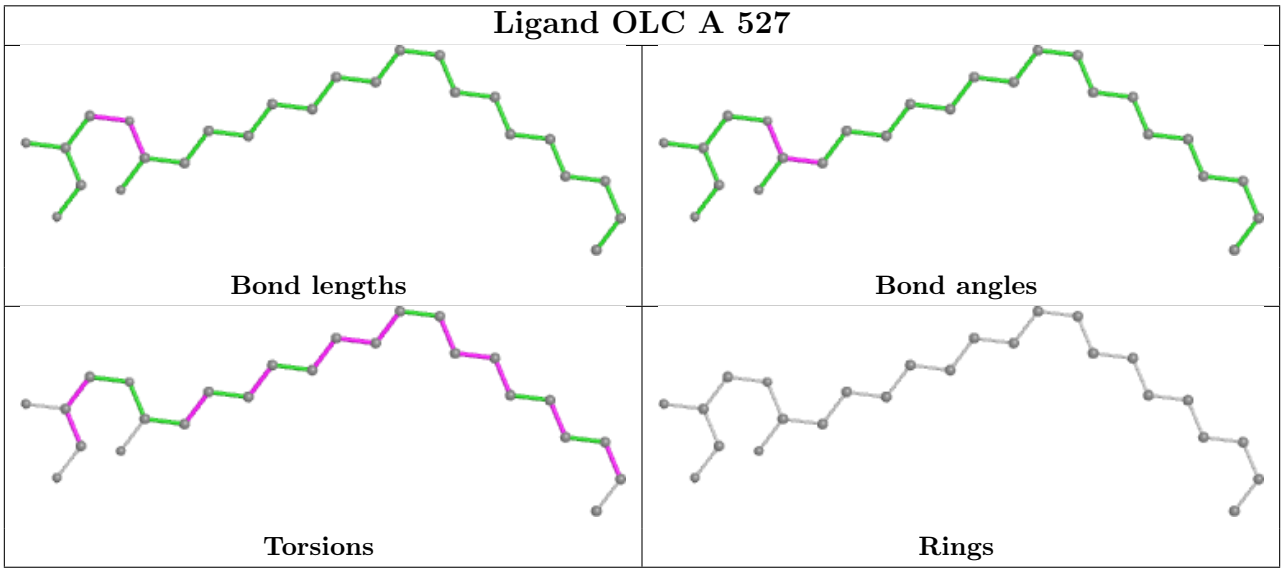
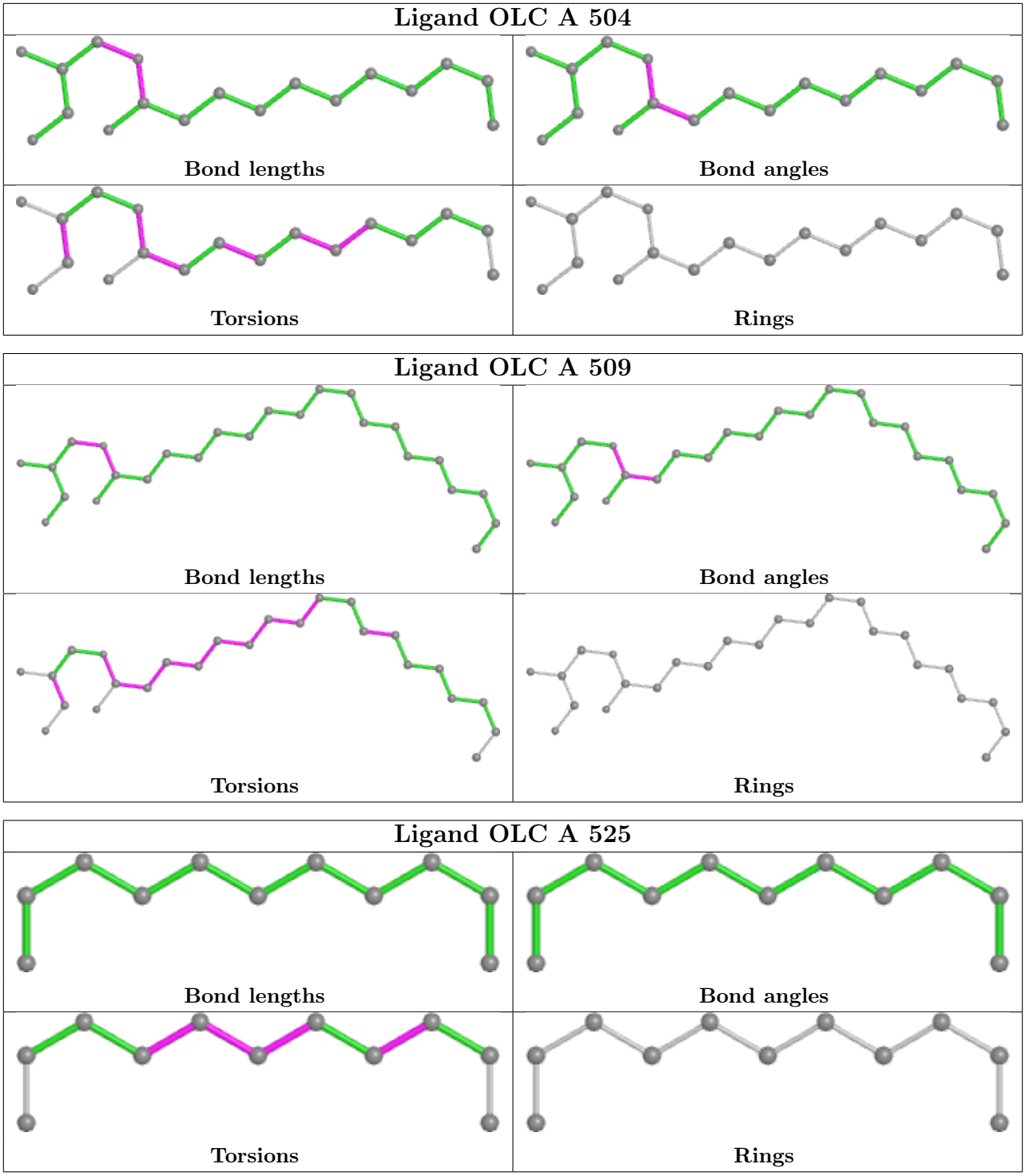


Ligand OLC A 527





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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	392/414 (94%)	0.86	47 (11%) 4 7	36, 54, 120, 169	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	GLN	11.2
1	A	174	PRO	10.6
1	A	171	GLY	10.3
1	A	167	LEU	9.5
1	A	246	GLN	9.1
1	A	292	GLU	8.8
1	A	170	ARG	8.7
1	A	172	THR	7.9
1	A	173	ARG	7.2
1	A	243	GLY	6.4
1	A	434	LEU	6.3
1	A	162	PHE	6.0
1	A	244	ARG	5.7
1	A	247	THR	5.7
1	A	175	LEU	5.7
1	A	163	TRP	5.6
1	A	169	LYS	5.0
1	A	50	ALA	5.0
1	A	51	SER	4.4
1	A	245	ILE	3.8
1	A	433	LEU	3.8
1	A	165	LEU	3.7
1	A	166	ASN	3.6
1	A	48	VAL	3.4
1	A	249	THR	3.4
1	A	178	ALA	3.4
1	A	164	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	333	MET	3.3
1	A	366	LEU	3.2
1	A	431	TRP	3.1
1	A	293	ASN	3.0
1	A	290	ASN	3.0
1	A	177	LEU	3.0
1	A	214	GLY	2.9
1	A	54	TYR	2.8
1	A	179	VAL	2.7
1	A	45	GLY	2.7
1	A	367	GLY	2.5
1	A	215	PRO	2.5
1	A	248	ASP	2.4
1	A	182	PHE	2.3
1	A	47	ALA	2.3
1	A	250	THR	2.3
1	A	186	ILE	2.2
1	A	184	LEU	2.1
1	A	151	PHE	2.1
1	A	337	VAL	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, 95^{th} 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	524	8/25	0.29	0.68	94,110,123,128	0
4	OLC	A	520	7/25	0.48	0.50	73,78,83,83	0
5	PEG	A	531	7/7	0.51	0.35	75,84,98,100	0

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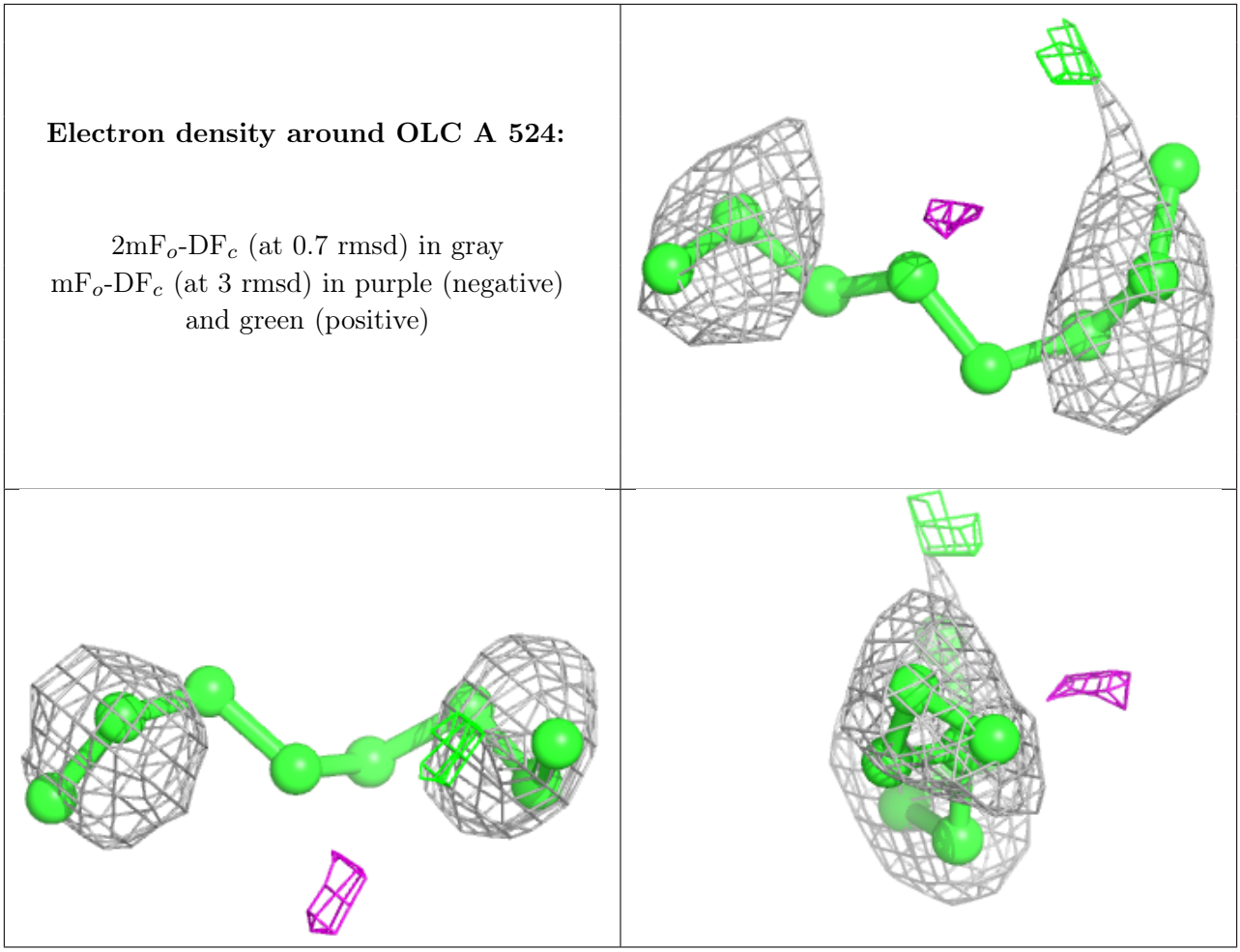
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLC	A	517	16/25	0.52	0.49	63,82,89,96	0
4	OLC	A	529	9/25	0.64	0.23	85,91,96,97	0
4	OLC	A	526	18/25	0.65	0.36	54,62,74,76	0
4	OLC	A	527	25/25	0.65	0.30	52,63,88,91	0
4	OLC	A	516	8/25	0.67	0.31	82,85,89,91	0
4	OLC	A	515	25/25	0.67	0.46	64,89,109,115	0
4	OLC	A	525	11/25	0.68	0.30	74,79,88,95	0
4	OLC	A	508	18/25	0.69	0.35	53,79,87,87	0
4	OLC	A	521	11/25	0.69	0.26	62,72,81,84	0
5	PEG	A	530	7/7	0.70	0.42	55,69,74,81	0
4	OLC	A	510	14/25	0.70	0.29	74,82,96,104	0
4	OLC	A	528	22/25	0.71	0.32	64,70,80,89	0
4	OLC	A	512	25/25	0.71	0.34	67,74,102,118	0
4	OLC	A	522	9/25	0.73	0.36	73,78,83,85	0
4	OLC	A	523	23/25	0.73	0.31	71,83,92,102	0
4	OLC	A	509	25/25	0.74	0.27	56,72,82,86	0
4	OLC	A	518	11/25	0.74	0.36	63,68,80,81	0
4	OLC	A	504	18/25	0.76	0.25	63,78,102,105	0
4	OLC	A	507	23/25	0.76	0.33	49,68,88,95	0
4	OLC	A	519	25/25	0.77	0.26	64,78,100,111	0
4	OLC	A	505	13/25	0.79	0.23	70,80,86,96	0
4	OLC	A	511	11/25	0.82	0.22	63,69,73,82	0
4	OLC	A	513	7/25	0.83	0.25	63,67,71,73	0
4	OLC	A	503	19/25	0.83	0.22	60,66,71,73	0
4	OLC	A	514	8/25	0.84	0.24	72,74,76,79	0
4	OLC	A	506	18/25	0.88	0.17	67,74,89,92	0
3	CL	A	502	1/1	0.90	0.18	60,60,60,60	0
2	NA	A	501	1/1	0.96	0.07	51,51,51,51	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.

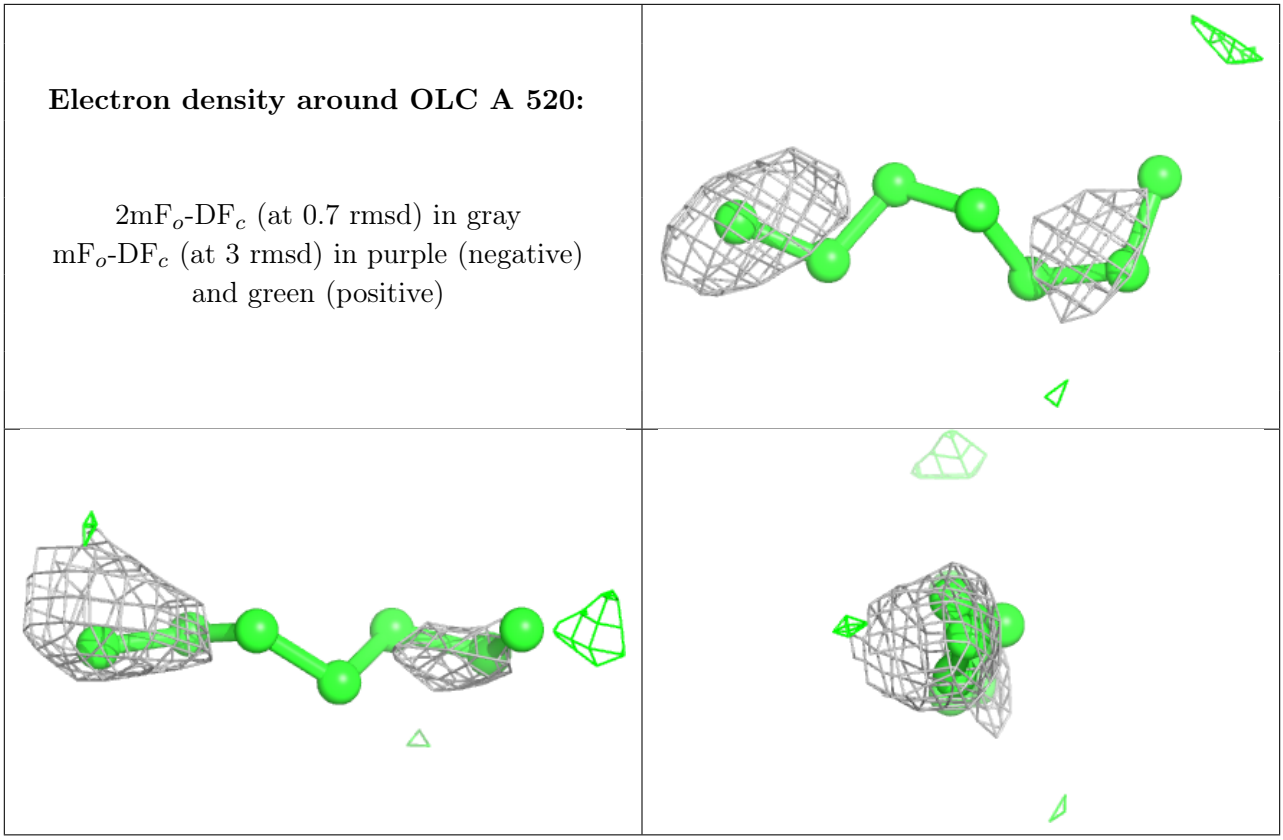
Electron density around OLC A 524:

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



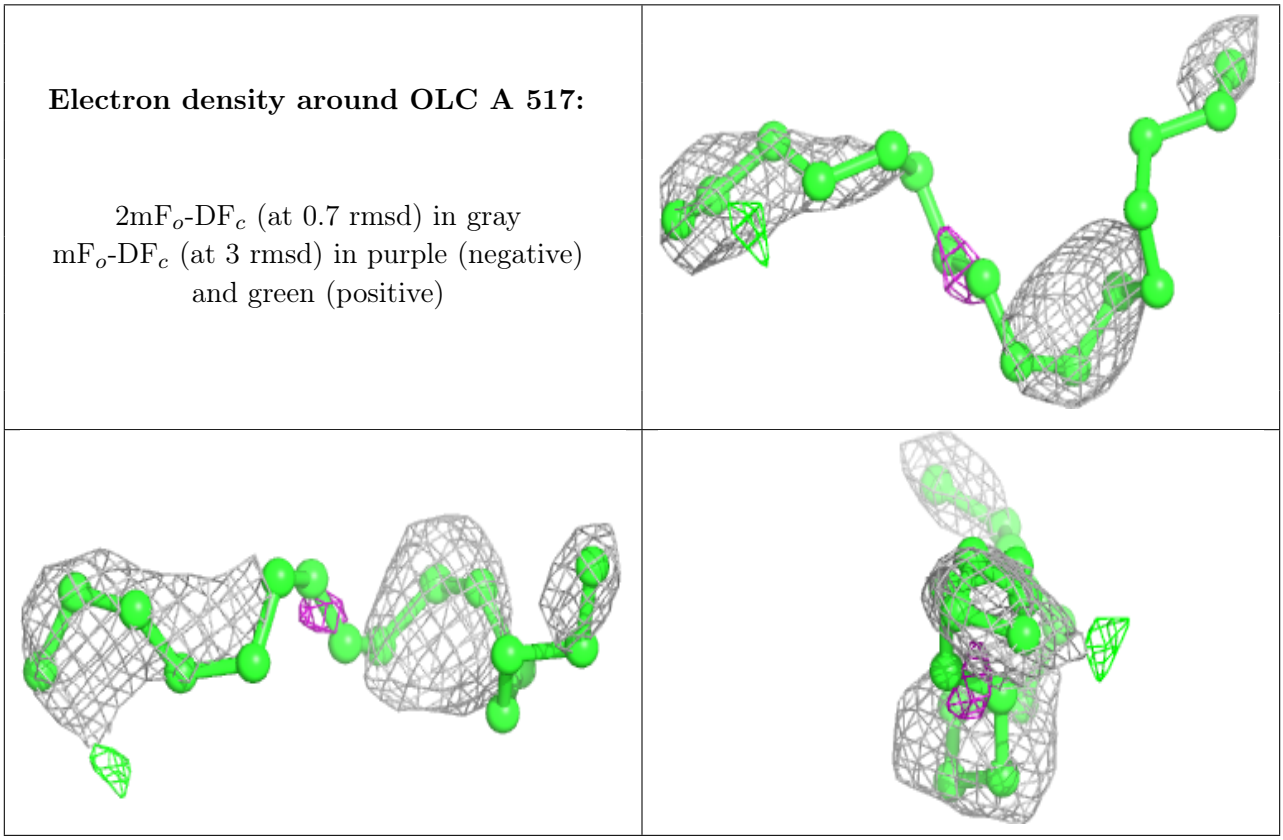
Electron density around OLC A 520:

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



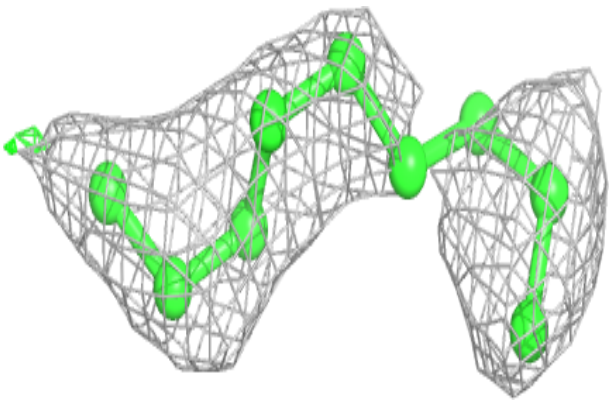
Electron density around OLC A 517:

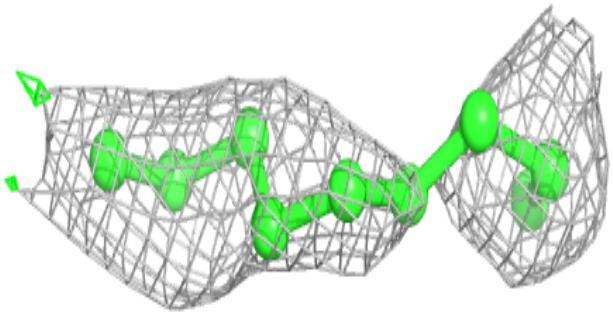
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

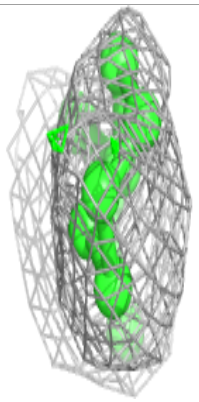


Electron density around OLC A 529:

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

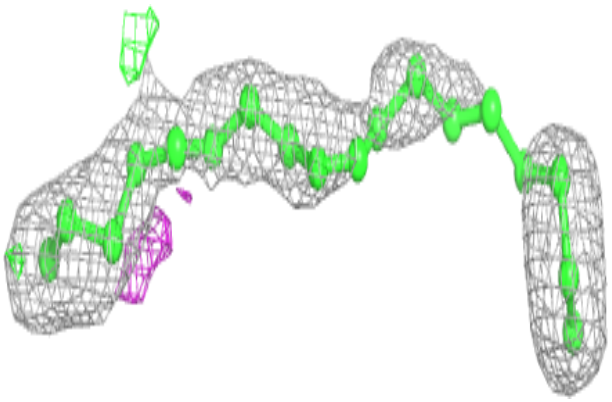


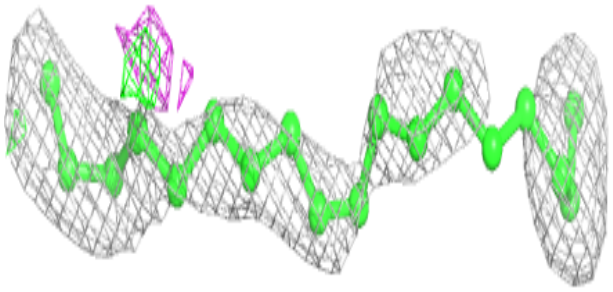


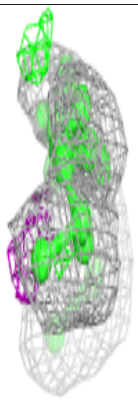


Electron density around OLC A 526:

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

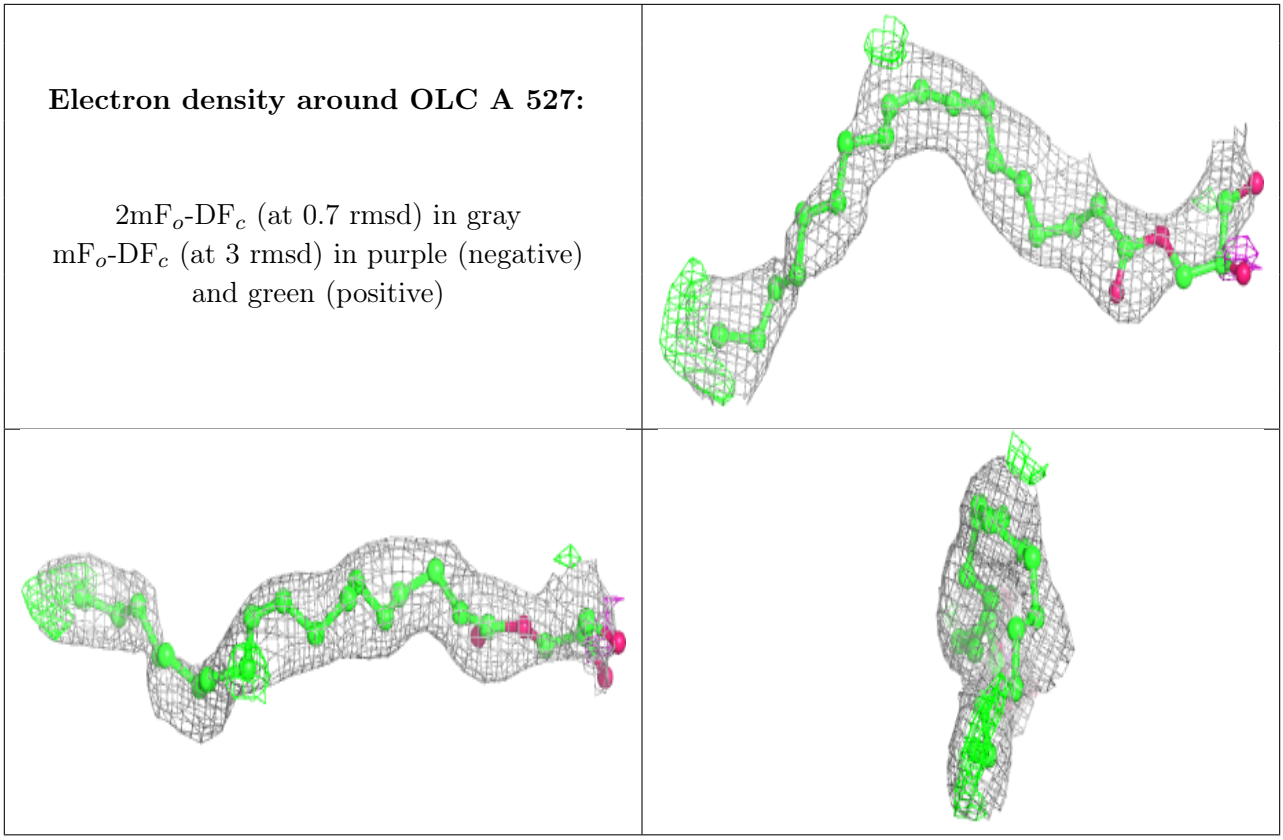






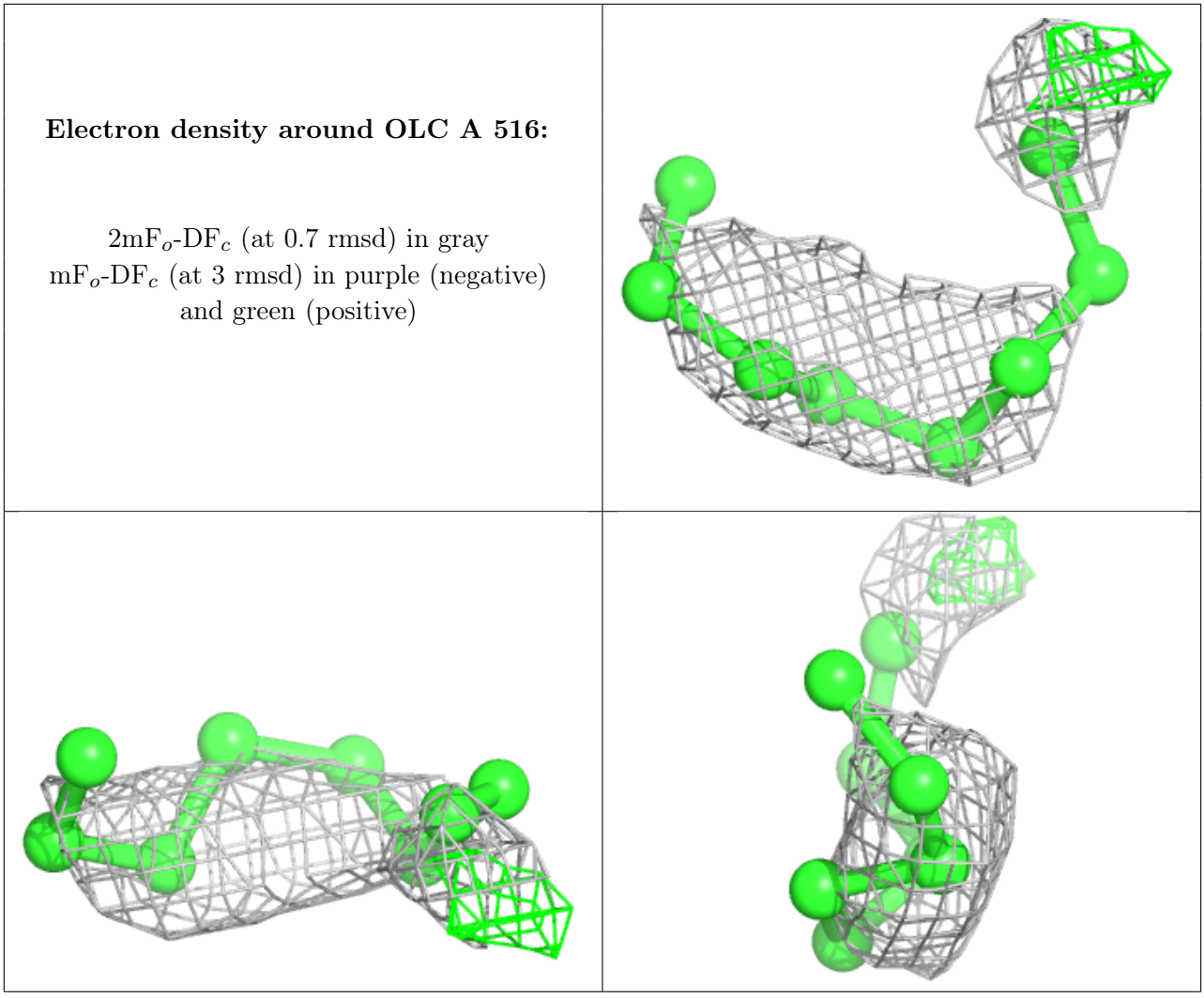
Electron density around OLC A 527:

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



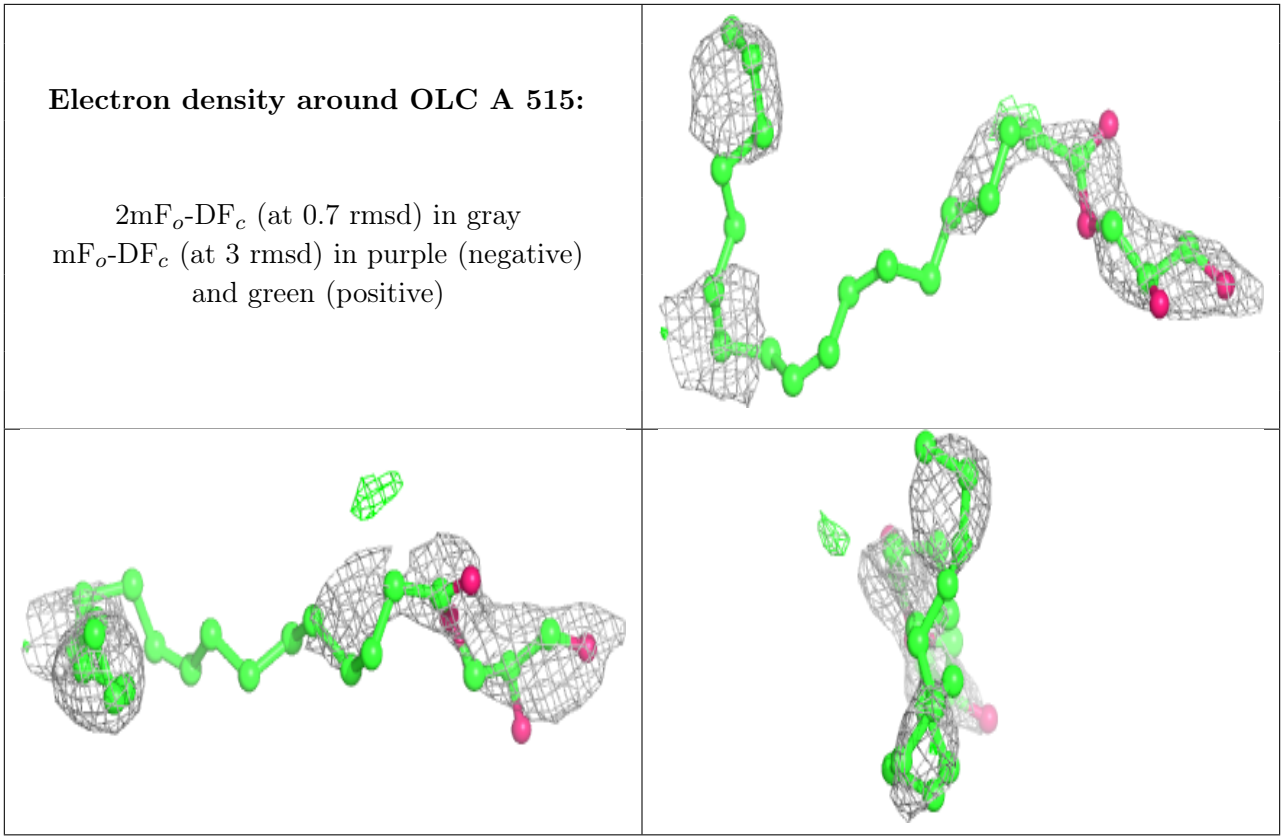
Electron density around OLC A 516:

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



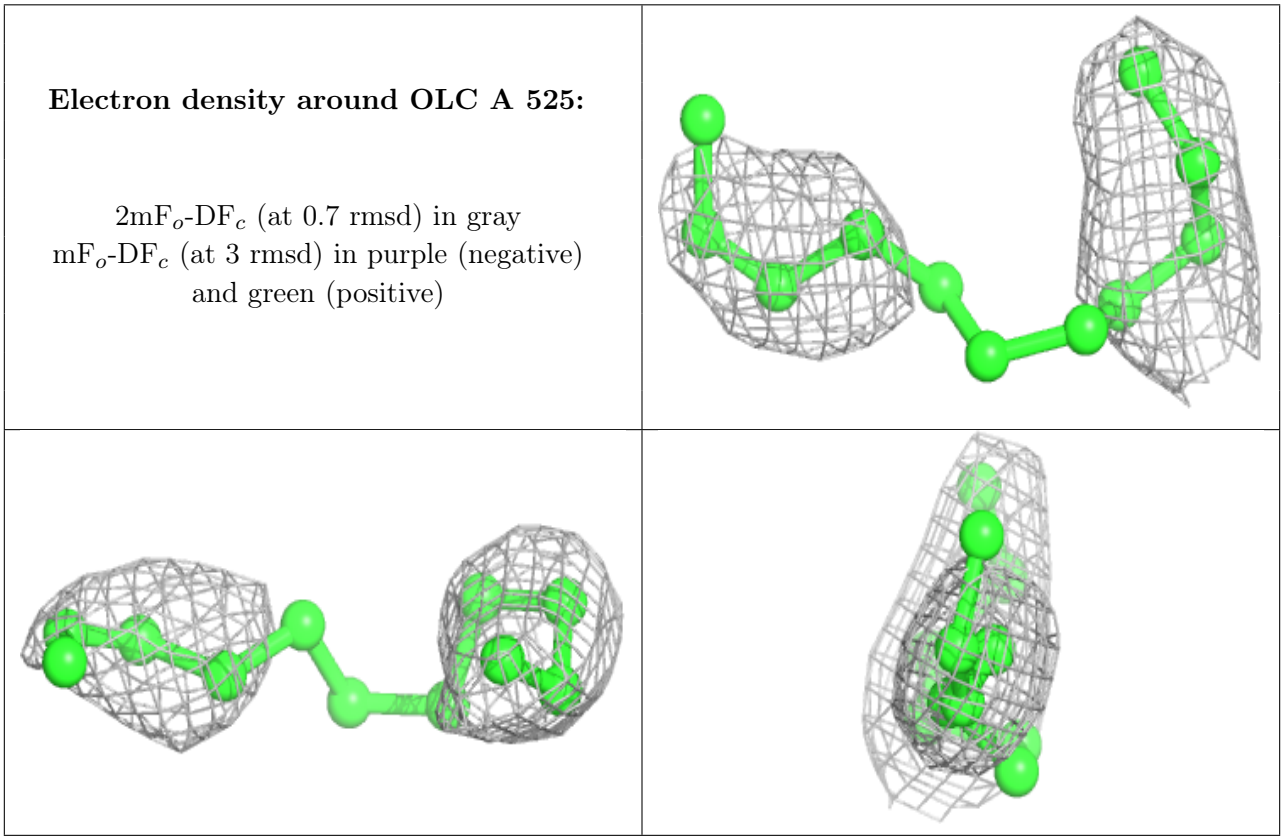
Electron density around OLC A 515:

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



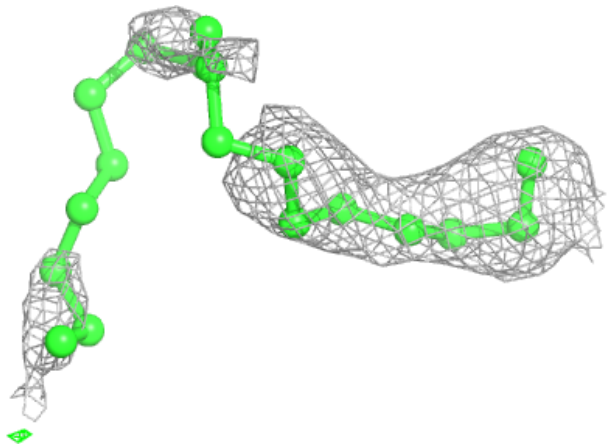
Electron density around OLC A 525:

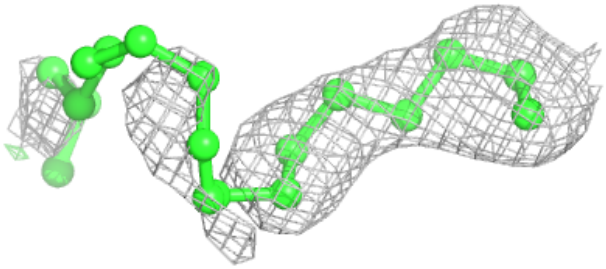
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

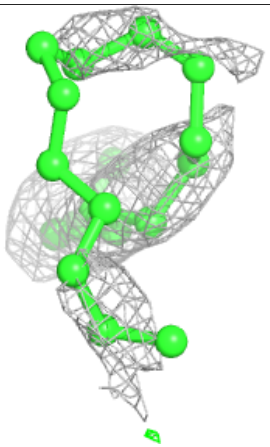


Electron density around OLC A 508:

$2mF_o$-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:

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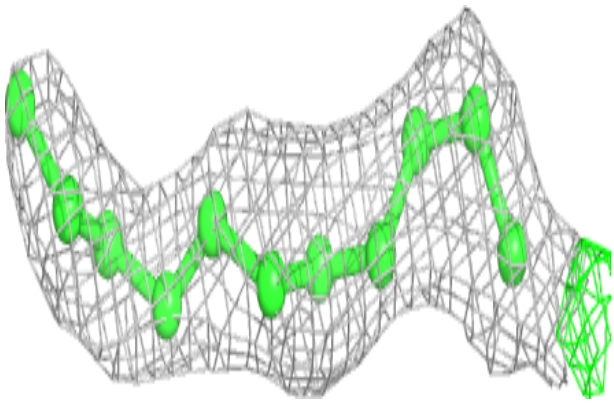
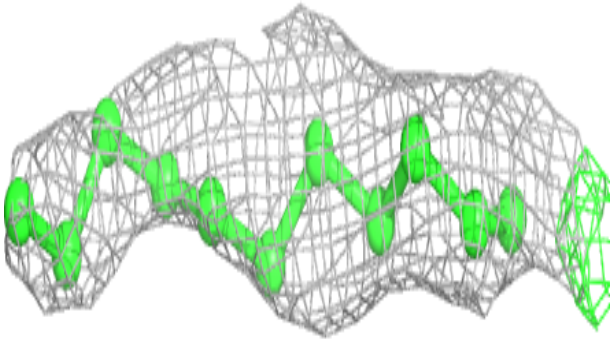
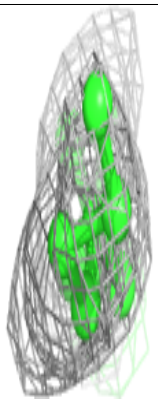
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

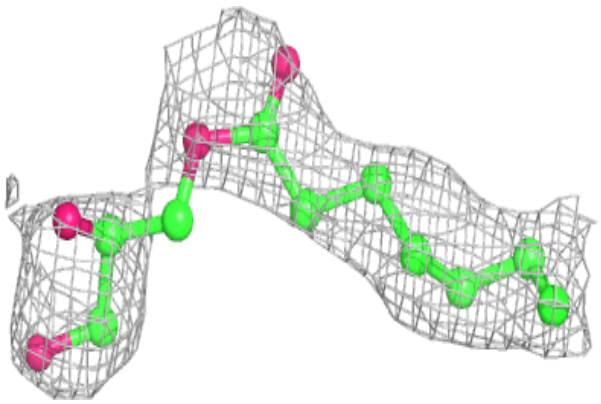


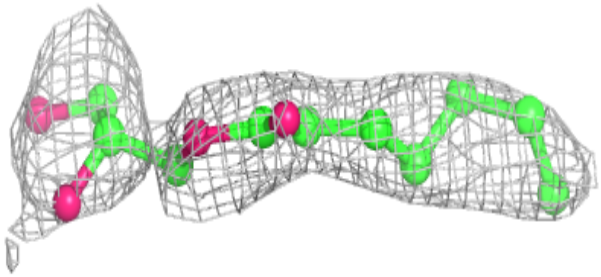


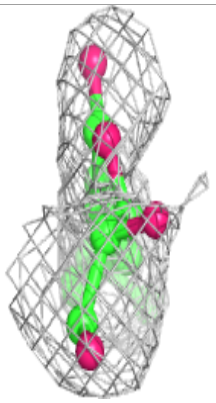


Electron density around OLC A 510:

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

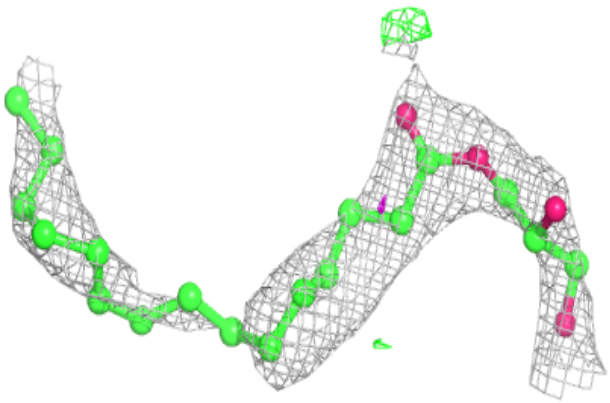


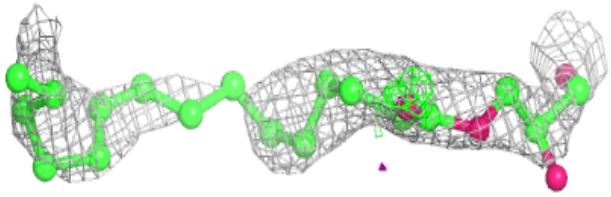


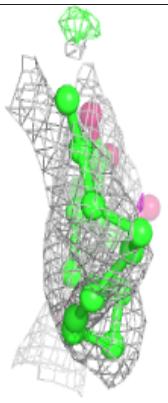


Electron density around OLC A 528:

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

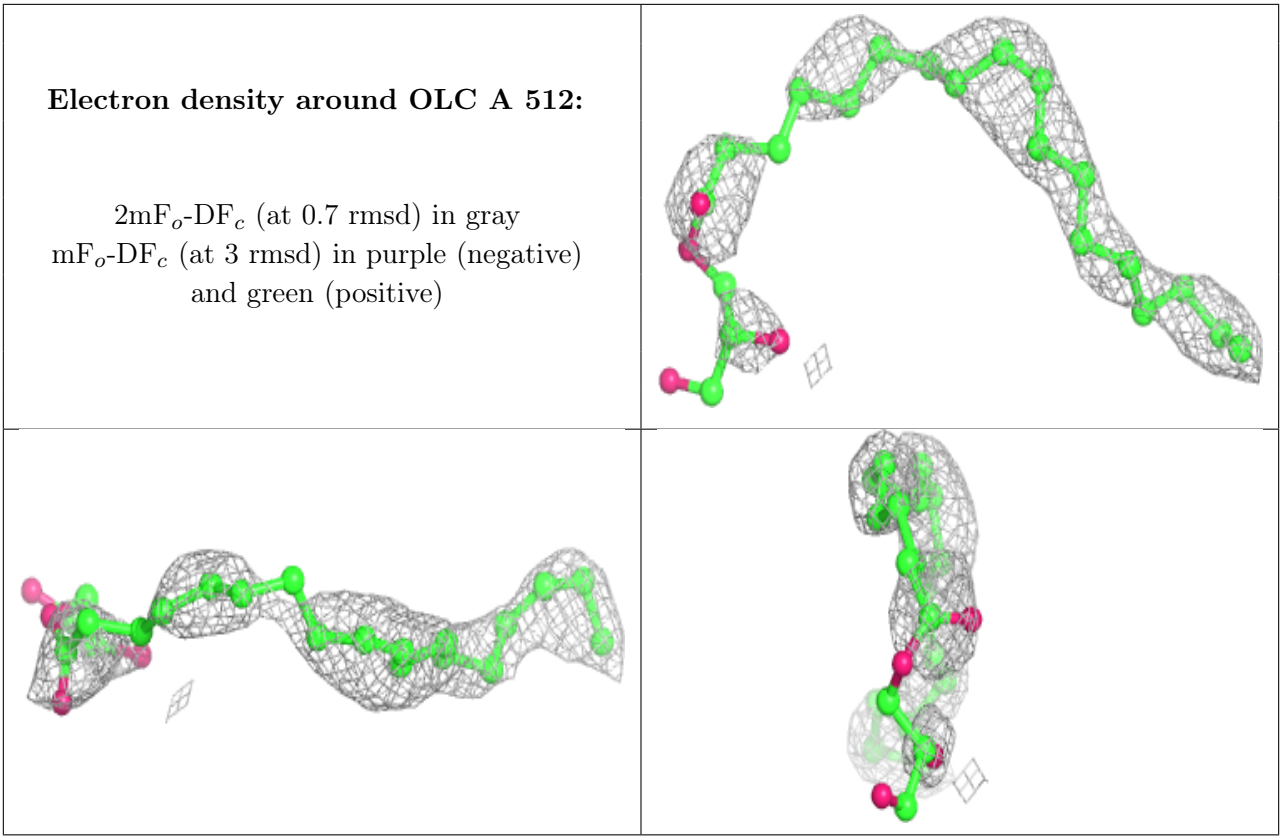






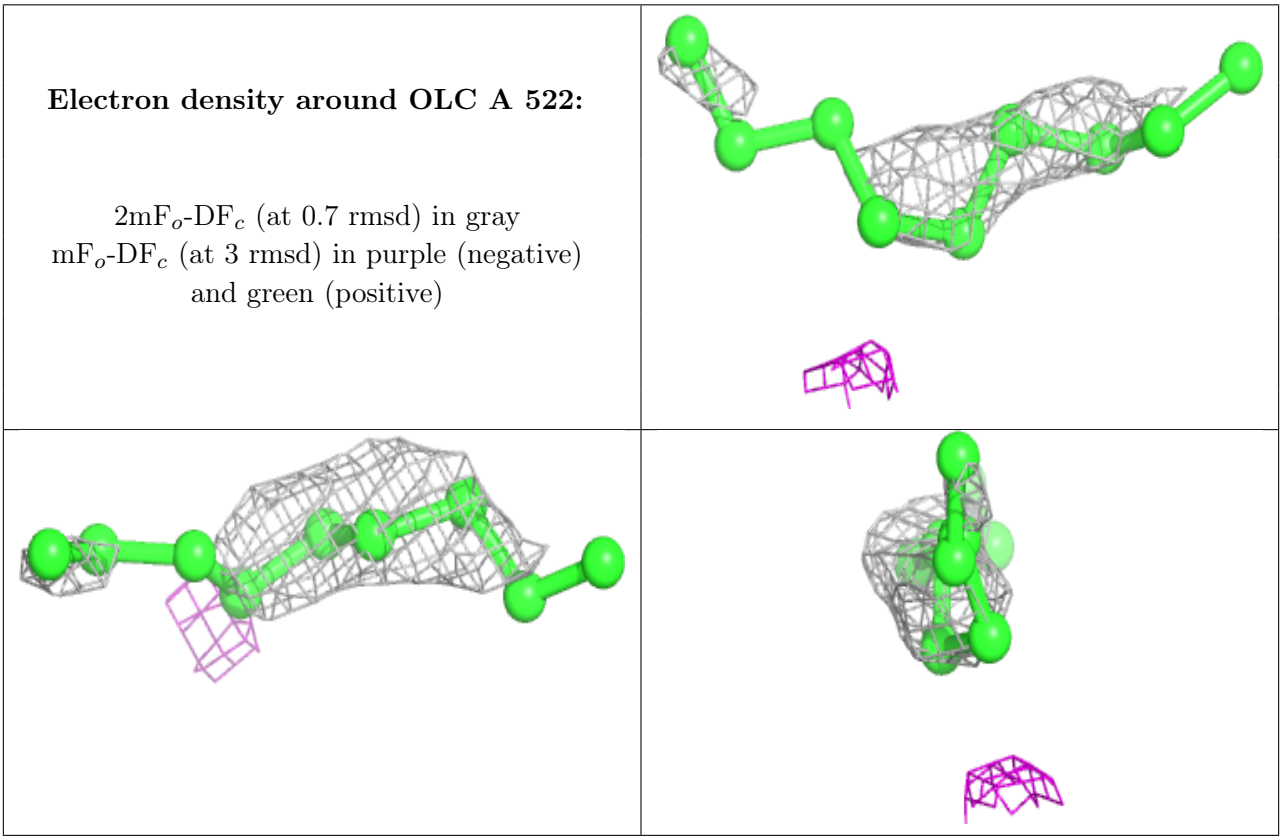
Electron density around OLC A 512:

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



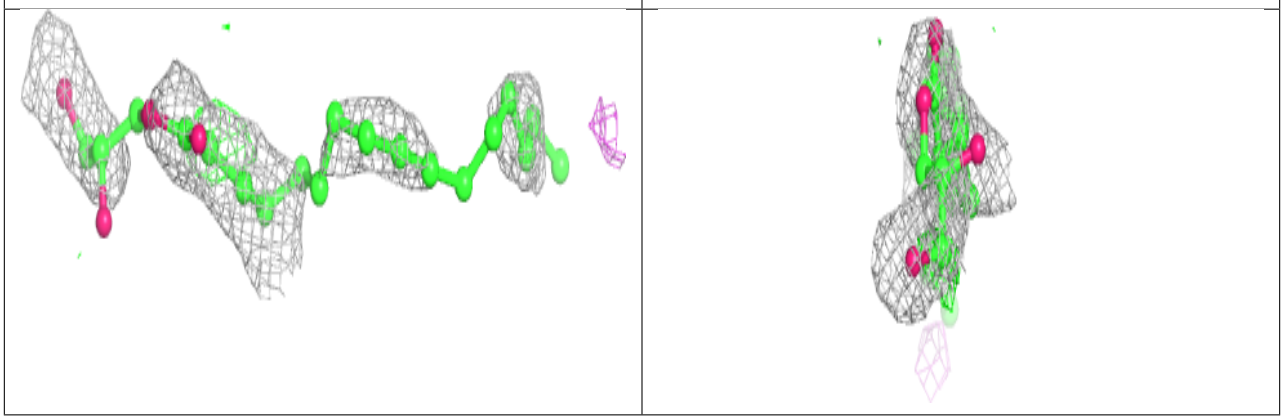
Electron density around OLC A 522:

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



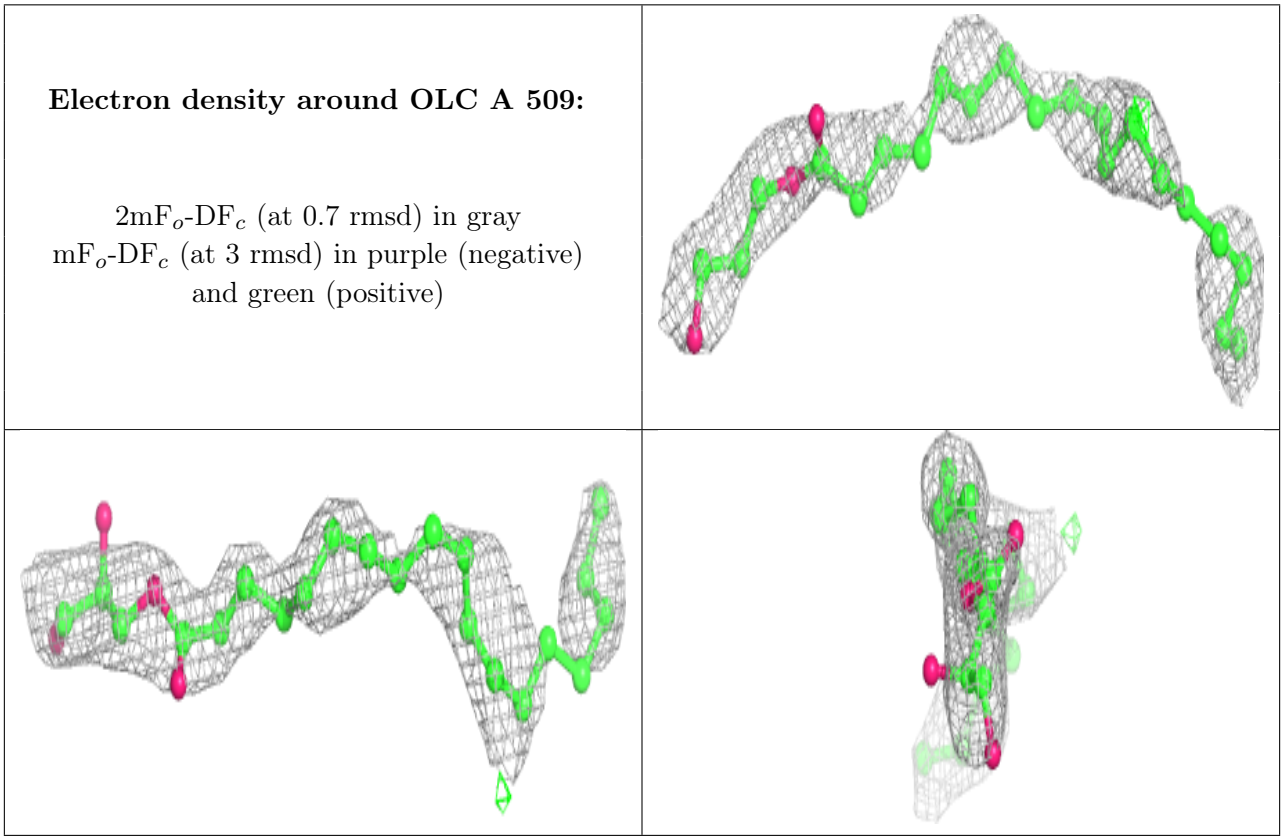
Electron density around OLC A 523:

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



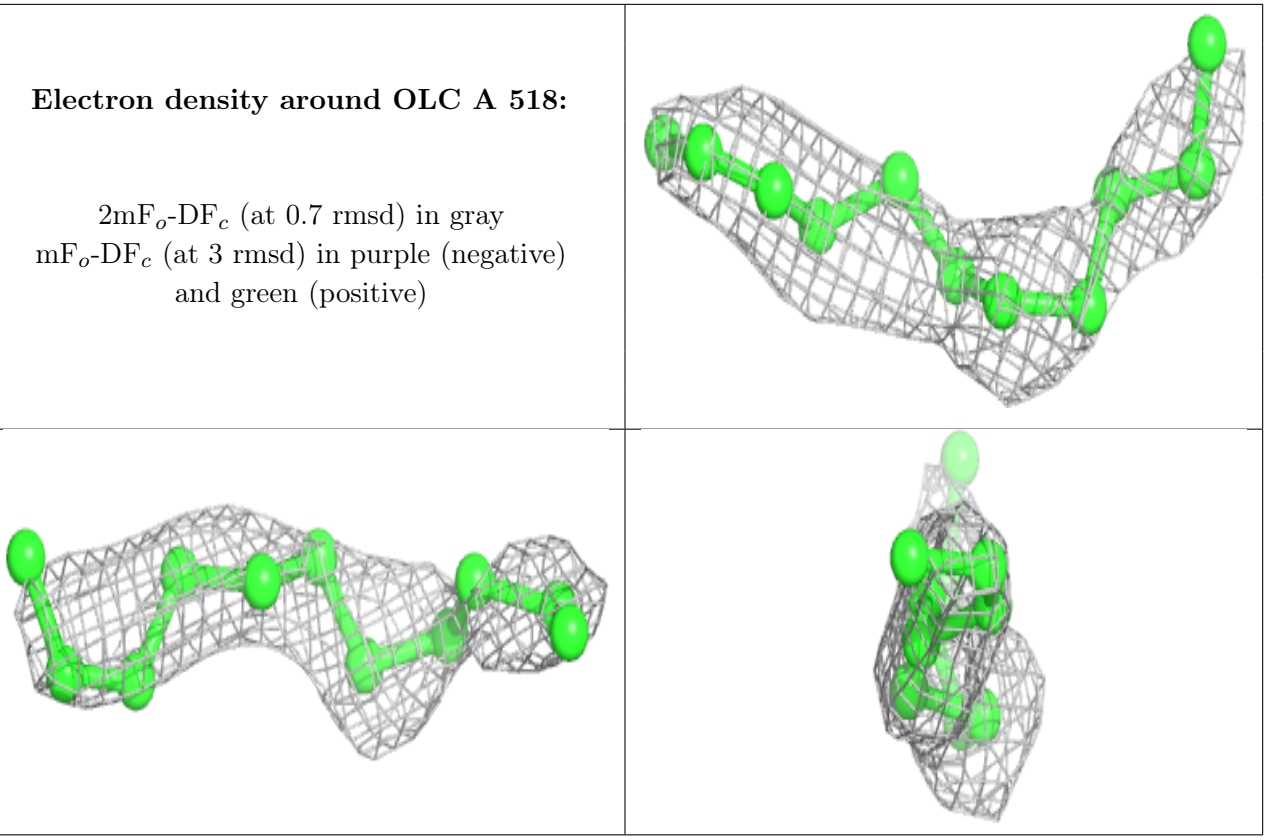
Electron density around OLC A 509:

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



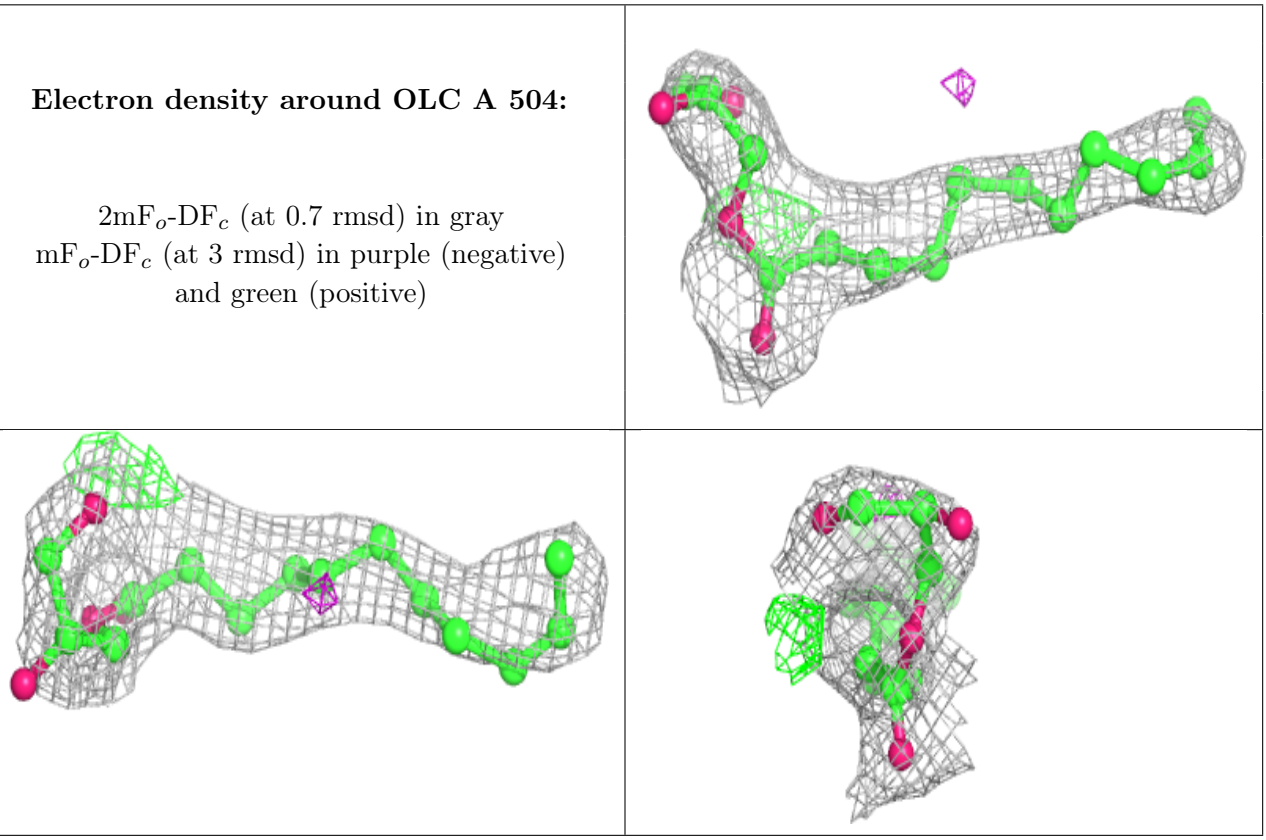
Electron density around OLC A 518:

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



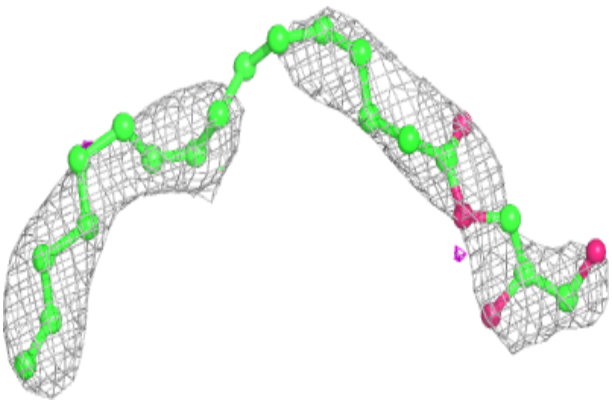
Electron density around OLC A 504:

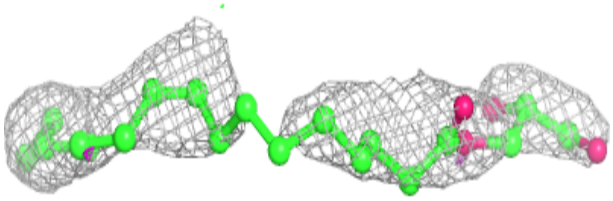
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

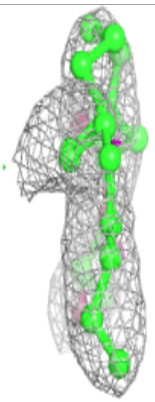


Electron density around OLC A 507:

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

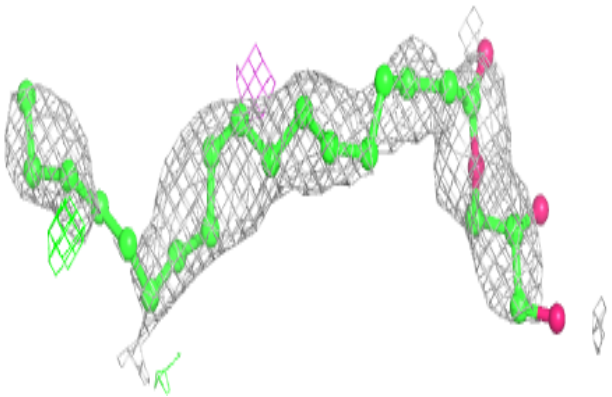


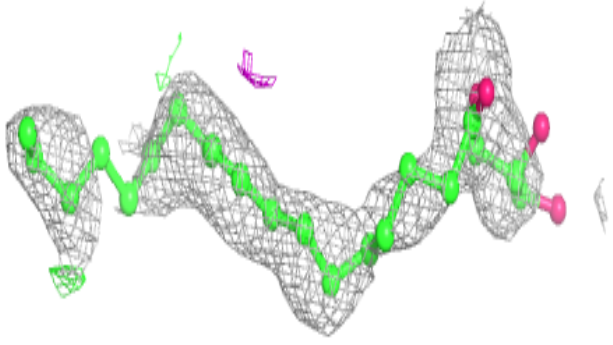


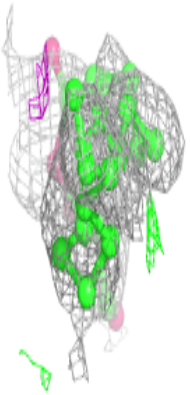


Electron density around OLC A 519:

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

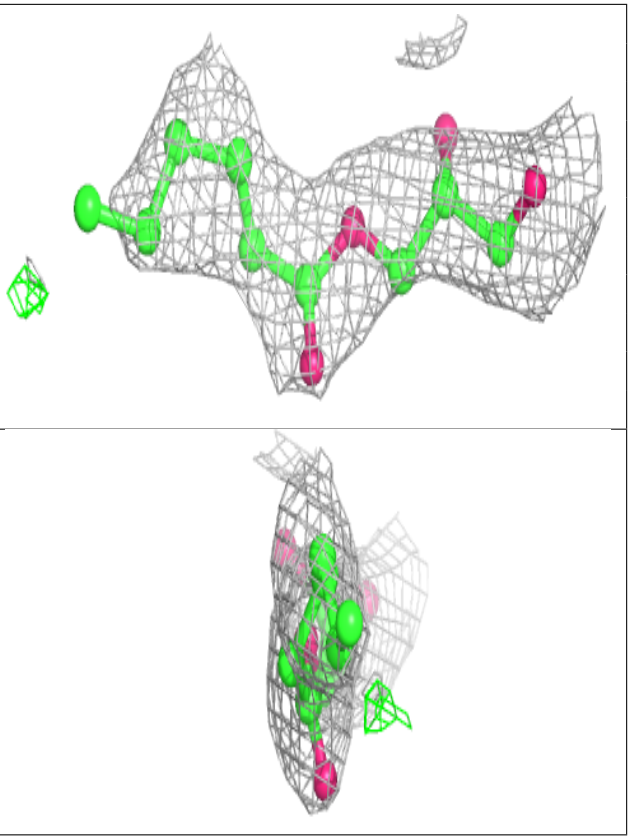






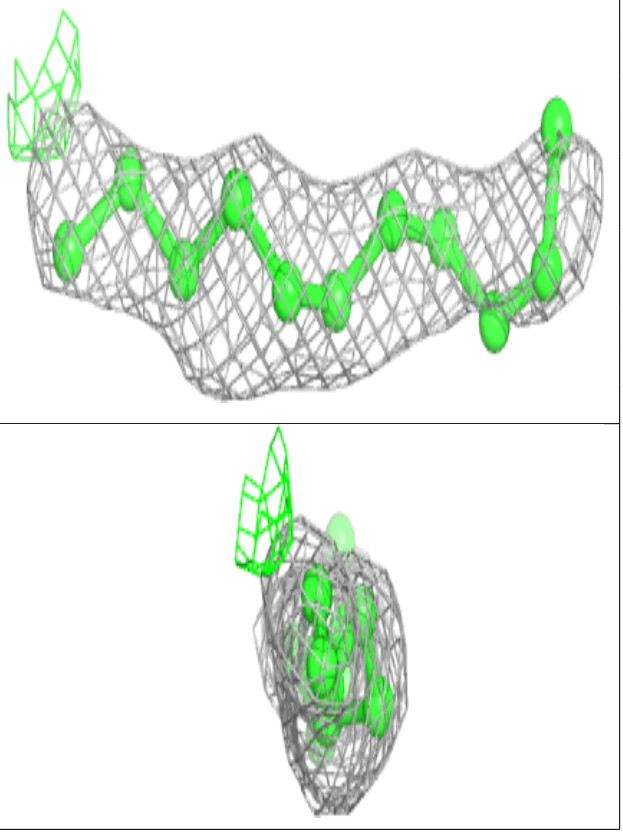
Electron density around OLC A 505:

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



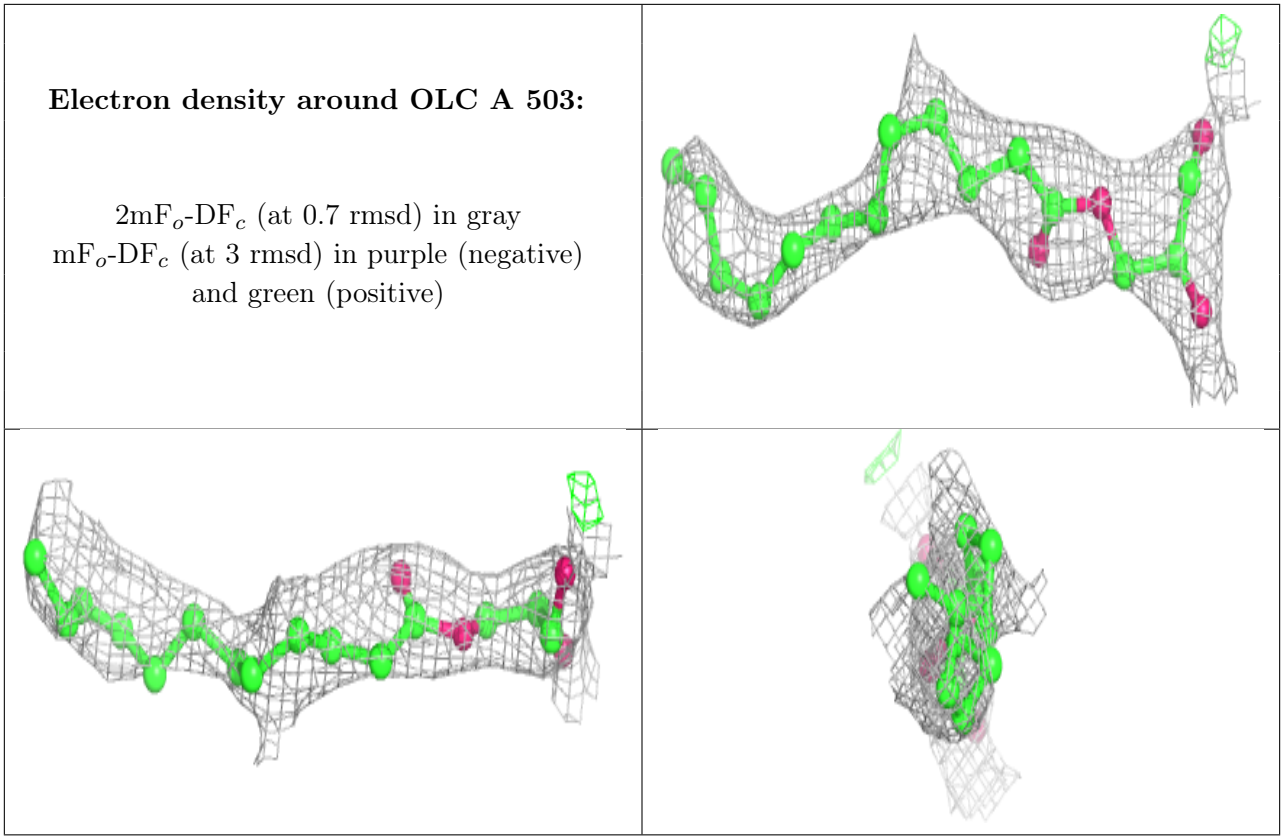
Electron density around OLC A 511:

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



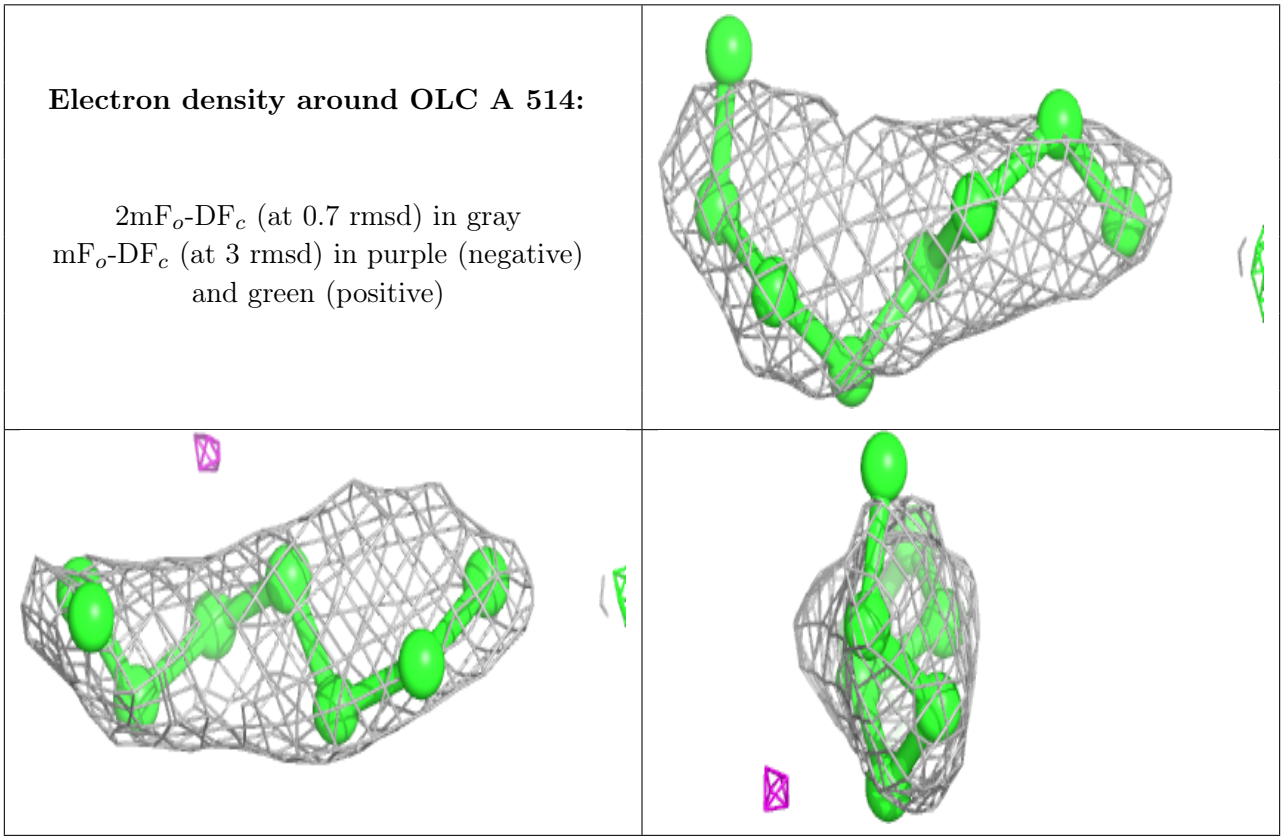
Electron density around OLC A 503:

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



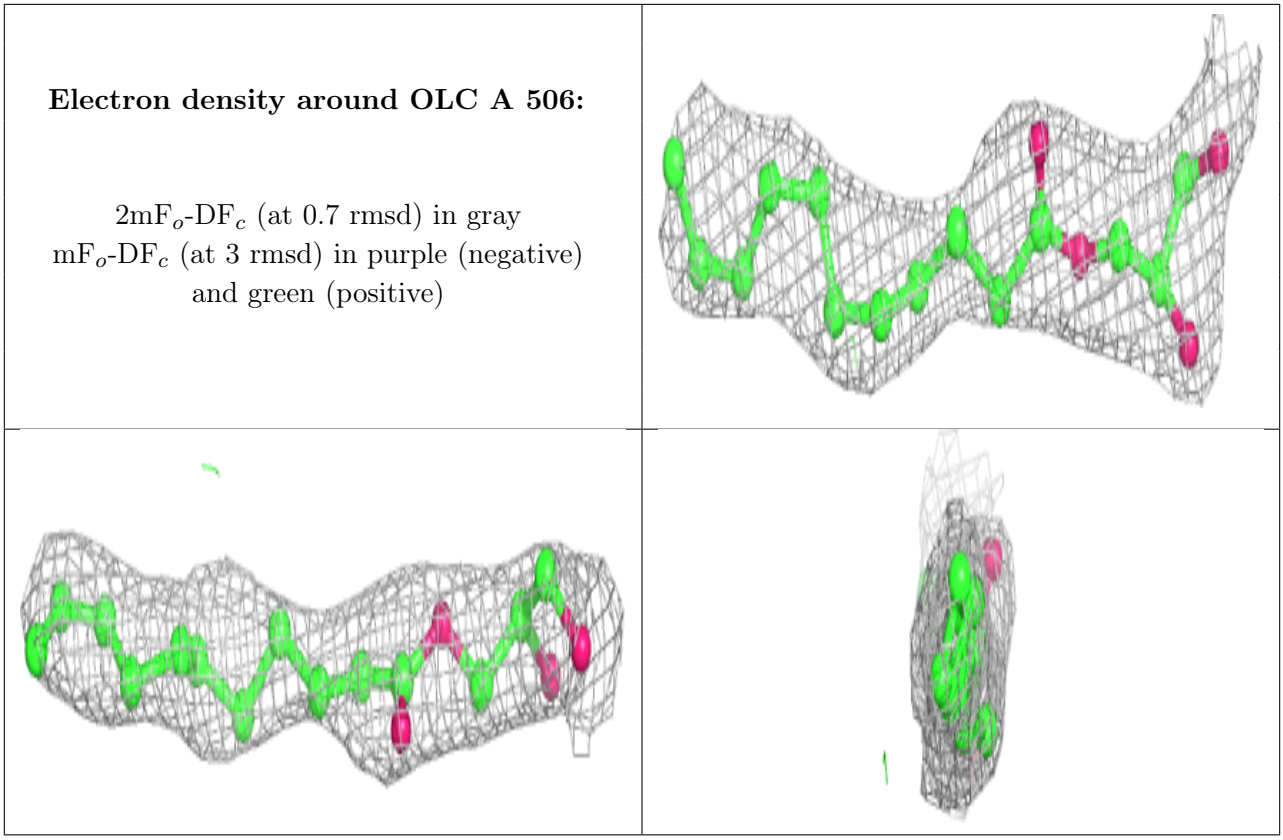
Electron density around OLC A 514:

$2mF_o$-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 506:

$2mF_o$-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.