



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:10 am BST

PDB ID : 6OB7  
Title : Human equilibrative nucleoside transporter-1, dilazep bound  
Authors : Wright, N.J.; Lee, S.-Y.  
Deposited on : 2019-03-19  
Resolution : 2.30 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](mailto: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.

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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 : 2.11  
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) : 2.11

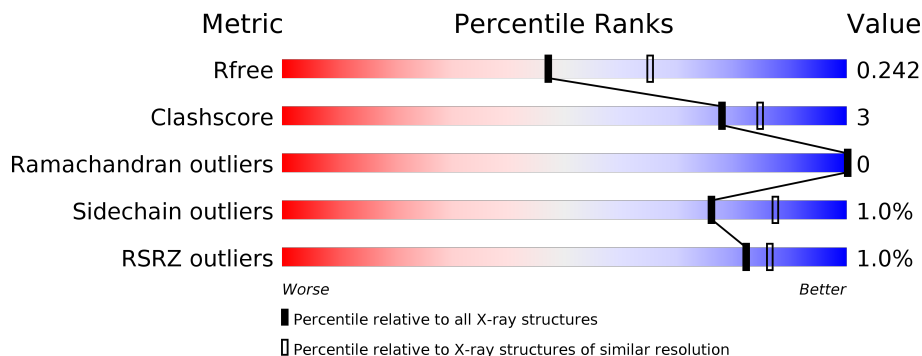
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	442	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6618 atoms, of which 3332 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 Equilibrative nucleoside transporter 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	381	5953	1991	3005	449	485	23	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

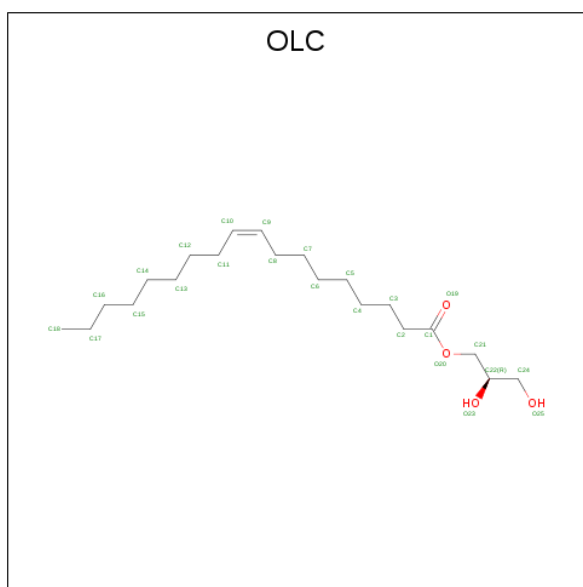
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q99808
A	1	ALA	-	expression tag	UNP Q99808
A	168	PHE	LEU	engineered mutation	UNP Q99808
A	175	ALA	PRO	engineered mutation	UNP Q99808
A	?	-	PRO	deletion	UNP Q99808
A	?	-	GLY	deletion	UNP Q99808
A	?	-	GLU	deletion	UNP Q99808
A	?	-	GLN	deletion	UNP Q99808
A	?	-	GLU	deletion	UNP Q99808
A	?	-	THR	deletion	UNP Q99808
A	?	-	LYS	deletion	UNP Q99808
A	?	-	LEU	deletion	UNP Q99808
A	?	-	ASP	deletion	UNP Q99808
A	?	-	LEU	deletion	UNP Q99808
A	?	-	ILE	deletion	UNP Q99808
A	?	-	SER	deletion	UNP Q99808
A	?	-	LYS	deletion	UNP Q99808
A	?	-	GLY	deletion	UNP Q99808
A	?	-	GLU	deletion	UNP Q99808
A	?	-	GLU	deletion	UNP Q99808
A	?	-	PRO	deletion	UNP Q99808
A	?	-	ARG	deletion	UNP Q99808
A	?	-	ALA	deletion	UNP Q99808
A	?	-	GLY	deletion	UNP Q99808
A	?	-	LYS	deletion	UNP Q99808
A	?	-	GLU	deletion	UNP Q99808
A	?	-	GLU	deletion	UNP Q99808

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q99808
A	?	-	GLY	deletion	UNP Q99808
A	?	-	VAL	deletion	UNP Q99808
A	?	-	SER	deletion	UNP Q99808
A	?	-	VAL	deletion	UNP Q99808
A	?	-	SER	deletion	UNP Q99808
A	?	-	ASN	deletion	UNP Q99808
A	?	-	SER	deletion	UNP Q99808
A	?	-	GLN	deletion	UNP Q99808
A	288	LYS	ASN	engineered mutation	UNP Q99808
A	457	GLY	-	expression tag	UNP Q99808
A	458	THR	-	expression tag	UNP Q99808
A	459	GLU	-	expression tag	UNP Q99808
A	460	LEU	-	expression tag	UNP Q99808
A	461	LEU	-	expression tag	UNP Q99808
A	462	GLN	-	expression tag	UNP Q99808
A	463	VAL	-	expression tag	UNP Q99808
A	464	ASP	-	expression tag	UNP Q99808
A	465	THR	-	expression tag	UNP Q99808
A	466	ASN	-	expression tag	UNP Q99808
A	467	SER	-	expression tag	UNP Q99808
A	468	LEU	-	expression tag	UNP Q99808
A	469	GLU	-	expression tag	UNP Q99808
A	470	VAL	-	expression tag	UNP Q99808
A	471	LEU	-	expression tag	UNP Q99808
A	472	PHE	-	expression tag	UNP Q99808
A	473	GLN	-	expression tag	UNP Q99808

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



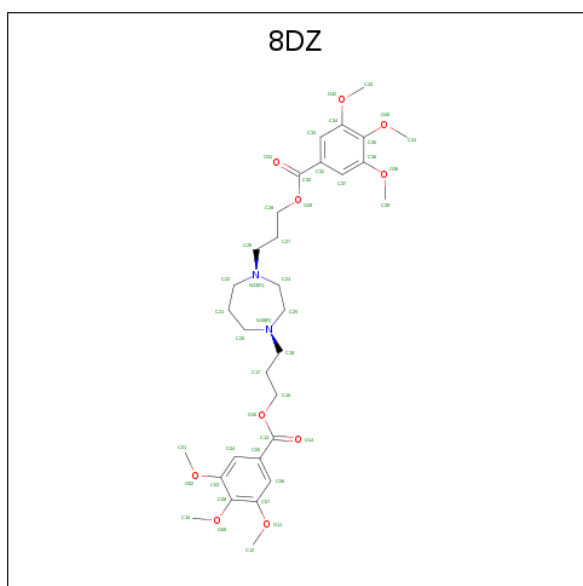
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			31	10	17	4		
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	A	1	Total	C	H	O	0	0
			34	11	19	4		
2	A	1	Total	C	H	O	0	0
			25	8	13	4		
2	A	1	Total	C	H	O	0	0
			34	11	19	4		
2	A	1	Total	C	H	O	0	0
			28	9	15	4		
2	A	1	Total	C	H	O	0	0
			22	7	11	4		
2	A	1	Total	C	H	O	0	0
			19	6	9	4		
2	A	1	Total	C	H		0	0
			15	7	8			
2	A	1	Total	C	H	O	0	0
			34	11	19	4		
2	A	1	Total	C	H	O	0	0
			28	9	15	4		
2	A	1	Total	C	H	O	0	0
			15	4	7	4		
2	A	1	Total	C	H	O	0	0
			16	5	7	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			13	5	6	2		
2	A	1	Total	C	H	O	0	0
			22	7	11	4		
2	A	1	Total	C	H		0	0
			27	11	16			
2	A	1	Total	C	H	O	0	0
			22	7	11	4		

- Molecule 3 is (1,4-diazepane-1,4-diyl)di(propane-3,1-diyl) bis(3,4,5-trimethoxybenzoate) (three-letter code: 8DZ) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>2</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			87	31	44	2	10		

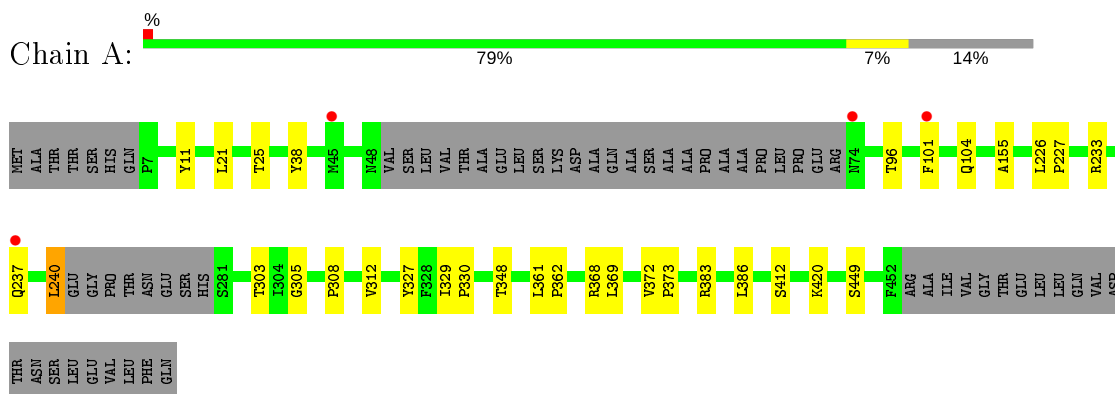
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Equilibrative nucleoside transporter 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.04Å 72.04Å 173.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	62.39 – 2.30 62.39 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.8 (62.39-2.30) 91.8 (62.39-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.203 , 0.243 0.205 , 0.242	Depositor DCC
$R_{free}$ test set	1098 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OLC, 8DZ

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	0.31	0/3029	0.43	0/4120

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	2948	3005	3005	19	0
2	A	232	283	283	1	0
3	A	43	44	0	0	0
4	A	63	0	0	1	0
All	All	3286	3332	3288	19	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 3.

All (19) 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:420:LYS:NZ	4:A:701:HOH:O	2.21	0.73
1:A:21:LEU:O	1:A:25:THR:HG23	1.99	0.60
1:A:96:THR:HG23	1:A:155:ALA:HB1	1.86	0.55
1:A:303:THR:OG1	1:A:368:ARG:NH2	2.36	0.55
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.90	0.53
1:A:348:THR:HG21	1:A:412:SER:HB3	1.91	0.51
1:A:11:TYR:O	2:A:602:OLC:H3A	2.14	0.48
1:A:240:LEU:N	1:A:240:LEU:HD23	2.30	0.47
1:A:101:PHE:O	1:A:104:GLN:NE2	2.44	0.46
1:A:327:TYR:HA	1:A:330:PRO:HG2	1.98	0.45
1:A:361:LEU:HB3	1:A:362:PRO:HD3	1.99	0.43
1:A:308:PRO:O	1:A:312:VAL:HG22	2.19	0.43
1:A:308:PRO:O	1:A:312:VAL:HG13	2.18	0.43
1:A:383:ARG:CD	1:A:386:LEU:O	2.67	0.43
1:A:312:VAL:HA	1:A:329:ILE:HD12	2.01	0.43
1:A:233:ARG:O	1:A:237:GLN:HB2	2.19	0.42
1:A:383:ARG:HD3	1:A:386:LEU:O	2.19	0.41
1:A:226:LEU:N	1:A:227:PRO:CD	2.84	0.41
1:A:305:GLY:HA2	1:A:449:SER:HB3	2.03	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	375/442 (85%)	370 (99%)	5 (1%)	0	100 100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	309/371 (83%)	306 (99%)	3 (1%)	76 87

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

Mol	Chain	Res	Type
1	A	38	TYR
1	A	240	LEU
1	A	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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
2	OLC	A	611	-	14,14,24	1.03	2 (14%)	15,15,25	0.98	1 (6%)
2	OLC	A	607	-	12,12,24	1.10	1 (8%)	13,13,25	1.12	1 (7%)
2	OLC	A	604	-	14,14,24	1.02	1 (7%)	15,15,25	0.86	1 (6%)
2	OLC	A	614	-	8,8,24	1.08	1 (12%)	9,9,25	0.88	0
2	OLC	A	601	-	13,13,24	1.05	1 (7%)	14,14,25	1.09	1 (7%)
2	OLC	A	608	-	10,10,24	1.20	2 (20%)	11,11,25	1.20	1 (9%)
2	OLC	A	610	-	6,6,24	0.48	0	4,5,25	0.46	0
2	OLC	A	605	-	11,11,24	1.16	1 (9%)	12,12,25	0.94	1 (8%)
2	OLC	A	613	-	7,7,24	0.96	0	6,7,25	0.38	0
2	OLC	A	602	-	24,24,24	0.83	2 (8%)	25,25,25	0.83	1 (4%)
2	OLC	A	609	-	9,9,24	1.23	1 (11%)	10,10,25	1.28	1 (10%)
2	OLC	A	617	-	10,10,24	0.38	0	9,9,25	0.64	0
2	OLC	A	606	-	14,14,24	1.01	2 (14%)	15,15,25	0.99	1 (6%)
2	OLC	A	612	-	12,12,24	1.08	1 (8%)	13,13,25	1.03	1 (7%)
2	OLC	A	615	-	3,6,24	0.32	0	2,6,25	0.37	0
3	8DZ	A	619	-	45,45,45	2.71	13 (28%)	55,59,59	1.67	12 (21%)
2	OLC	A	618	-	10,10,24	1.19	1 (10%)	11,11,25	0.96	1 (9%)
2	OLC	A	616	-	10,10,24	1.18	2 (20%)	11,11,25	1.12	1 (9%)
2	OLC	A	603	-	24,24,24	0.81	2 (8%)	25,25,25	0.92	1 (4%)

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
2	OLC	A	611	-	-	10/14/14/24	-
2	OLC	A	607	-	-	7/12/12/24	-
2	OLC	A	604	-	-	3/14/14/24	-
2	OLC	A	614	-	-	4/7/7/24	-
2	OLC	A	601	-	-	5/13/13/24	-
2	OLC	A	608	-	-	4/10/10/24	-
2	OLC	A	610	-	-	2/4/4/24	-
2	OLC	A	605	-	-	2/11/11/24	-
2	OLC	A	613	-	-	4/6/6/24	-
2	OLC	A	602	-	-	15/24/24/24	-
2	OLC	A	609	-	-	5/9/9/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	617	-	-	3/8/8/24	-
2	OLC	A	606	-	-	3/14/14/24	-
2	OLC	A	612	-	-	4/12/12/24	-
2	OLC	A	615	-	-	2/2/4/24	-
3	8DZ	A	619	-	-	9/34/45/45	0/3/3/3
2	OLC	A	618	-	-	2/10/10/24	-
2	OLC	A	616	-	-	6/10/10/24	-
2	OLC	A	603	-	-	17/24/24/24	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	619	8DZ	C26-N23	-9.81	1.24	1.47
3	A	619	8DZ	C18-N19	-9.23	1.26	1.47
3	A	619	8DZ	C20-N19	-4.10	1.34	1.46
3	A	619	8DZ	C25-N19	-4.02	1.35	1.46
3	A	619	8DZ	C24-N23	-3.93	1.35	1.46
3	A	619	8DZ	C22-N23	-3.57	1.36	1.46
3	A	619	8DZ	O31-C30	-3.53	1.13	1.22
3	A	619	8DZ	C32-C30	3.27	1.57	1.50
3	A	619	8DZ	O14-C13	-2.89	1.14	1.22
3	A	619	8DZ	O11-C07	2.73	1.41	1.37
3	A	619	8DZ	O15-C16	-2.66	1.37	1.45
2	A	605	OLC	O20-C1	2.60	1.40	1.33
2	A	604	OLC	O20-C1	2.55	1.40	1.33
2	A	618	OLC	O20-C1	2.51	1.40	1.33
2	A	608	OLC	O20-C1	2.50	1.40	1.33
2	A	607	OLC	O20-C1	2.48	1.40	1.33
2	A	601	OLC	O20-C1	2.48	1.40	1.33
2	A	609	OLC	O20-C1	2.48	1.40	1.33
2	A	602	OLC	O20-C1	2.47	1.40	1.33
2	A	612	OLC	O20-C1	2.44	1.40	1.33
2	A	606	OLC	O20-C1	2.43	1.40	1.33
2	A	616	OLC	O20-C1	2.42	1.40	1.33
2	A	611	OLC	O20-C1	2.40	1.40	1.33
2	A	603	OLC	O20-C1	2.34	1.40	1.33
3	A	619	8DZ	O02-C03	2.29	1.40	1.37
2	A	603	OLC	O20-C21	-2.18	1.40	1.45
2	A	611	OLC	O20-C21	-2.14	1.40	1.45
2	A	614	OLC	O20-C21	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	606	OLC	O20-C21	-2.05	1.40	1.45
2	A	602	OLC	O20-C21	-2.05	1.40	1.45
2	A	608	OLC	O20-C21	-2.05	1.40	1.45
2	A	616	OLC	O20-C21	-2.02	1.40	1.45
3	A	619	8DZ	O29-C30	2.01	1.38	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	619	8DZ	C28-O29-C30	4.62	126.16	116.43
3	A	619	8DZ	O15-C13-C05	4.47	119.93	112.14
3	A	619	8DZ	O38-C36-C35	3.87	121.96	115.16
2	A	609	OLC	O20-C1-C2	3.39	120.28	111.38
3	A	619	8DZ	O02-C03-C08	3.12	120.64	115.16
2	A	608	OLC	O20-C1-C2	2.92	121.08	111.91
2	A	607	OLC	O20-C1-C2	2.89	120.98	111.91
2	A	601	OLC	O20-C1-C2	2.76	120.56	111.91
2	A	616	OLC	O20-C1-C2	2.72	120.46	111.91
3	A	619	8DZ	O02-C03-C04	-2.59	119.67	124.12
2	A	612	OLC	O20-C1-C2	2.57	119.99	111.91
3	A	619	8DZ	O09-C08-C03	2.56	123.81	120.12
3	A	619	8DZ	O38-C36-C37	-2.50	119.81	124.12
3	A	619	8DZ	O29-C30-C32	2.50	116.49	112.14
2	A	611	OLC	O20-C1-C2	2.47	119.65	111.91
2	A	606	OLC	O20-C1-C2	2.46	119.61	111.91
3	A	619	8DZ	O15-C13-O14	-2.46	118.69	123.67
2	A	603	OLC	O20-C1-C2	2.43	119.53	111.91
2	A	605	OLC	O20-C1-C2	2.42	119.49	111.91
2	A	602	OLC	O20-C1-C2	2.40	119.44	111.91
2	A	618	OLC	O20-C1-C2	2.33	119.23	111.91
3	A	619	8DZ	C36-C35-C34	2.24	121.86	119.57
2	A	604	OLC	O20-C1-C2	2.16	118.68	111.91
3	A	619	8DZ	C10-O09-C08	-2.09	109.04	114.78
3	A	619	8DZ	C12-O11-C07	-2.01	114.50	117.53

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	608	OLC	O20-C21-C22-C24
2	A	608	OLC	O20-C21-C22-O23
2	A	610	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	A	613	OLC	C21-C22-C24-O25
2	A	613	OLC	O23-C22-C24-O25
2	A	609	OLC	O20-C21-C22-O23
2	A	618	OLC	C21-C22-C24-O25
2	A	615	OLC	C1-C2-C3-C4
3	A	619	8DZ	C17-C18-N19-C20
3	A	619	8DZ	C17-C18-N19-C25
2	A	611	OLC	C21-C22-C24-O25
2	A	611	OLC	O23-C22-C24-O25
2	A	611	OLC	O20-C21-C22-C24
2	A	616	OLC	C21-C22-C24-O25
2	A	616	OLC	O20-C21-C22-C24
2	A	616	OLC	O20-C21-C22-O23
2	A	608	OLC	O19-C1-O20-C21
2	A	608	OLC	C2-C1-O20-C21
2	A	603	OLC	C2-C1-O20-C21
2	A	614	OLC	C2-C1-O20-C21
2	A	607	OLC	C2-C1-O20-C21
2	A	607	OLC	O19-C1-O20-C21
2	A	603	OLC	O19-C1-O20-C21
2	A	611	OLC	O20-C21-C22-O23
2	A	616	OLC	C2-C1-O20-C21
2	A	603	OLC	O20-C21-C22-O23
2	A	614	OLC	O19-C1-O20-C21
2	A	618	OLC	O23-C22-C24-O25
2	A	612	OLC	C1-C2-C3-C4
2	A	616	OLC	O19-C1-O20-C21
2	A	614	OLC	O20-C21-C22-O23
2	A	605	OLC	O20-C21-C22-O23
2	A	602	OLC	O20-C21-C22-O23
2	A	606	OLC	C2-C1-O20-C21
3	A	619	8DZ	C16-C17-C18-N19
2	A	614	OLC	O20-C21-C22-C24
2	A	605	OLC	O20-C21-C22-C24
2	A	602	OLC	O20-C21-C22-C24
2	A	609	OLC	O20-C21-C22-C24
2	A	603	OLC	O20-C21-C22-C24
2	A	602	OLC	C5-C6-C7-C8
2	A	603	OLC	C1-C2-C3-C4
2	A	602	OLC	C21-C22-C24-O25
2	A	609	OLC	C21-C22-C24-O25
2	A	603	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
2	A	604	OLC	C1-C2-C3-C4
2	A	607	OLC	C1-C2-C3-C4
2	A	611	OLC	C2-C1-O20-C21
2	A	603	OLC	C5-C6-C7-C8
2	A	611	OLC	C3-C4-C5-C6
2	A	606	OLC	O19-C1-O20-C21
2	A	603	OLC	C14-C15-C16-C17
2	A	601	OLC	C2-C1-O20-C21
2	A	602	OLC	O23-C22-C24-O25
2	A	602	OLC	C11-C12-C13-C14
2	A	601	OLC	O19-C1-O20-C21
2	A	611	OLC	O19-C1-O20-C21
2	A	603	OLC	C10-C11-C12-C13
2	A	603	OLC	C6-C7-C8-C9
2	A	617	OLC	C5-C6-C7-C8
2	A	602	OLC	C10-C11-C12-C13
2	A	602	OLC	C6-C7-C8-C9
3	A	619	8DZ	C08-C03-O02-C01
2	A	615	OLC	C2-C3-C4-C5
2	A	603	OLC	C15-C16-C17-C18
2	A	603	OLC	O23-C22-C24-O25
2	A	606	OLC	C5-C6-C7-C8
2	A	607	OLC	C3-C4-C5-C6
2	A	604	OLC	C4-C5-C6-C7
2	A	602	OLC	C14-C15-C16-C17
2	A	601	OLC	C4-C5-C6-C7
2	A	607	OLC	O20-C21-C22-C24
2	A	612	OLC	O20-C21-C22-C24
2	A	613	OLC	O20-C21-C22-O23
2	A	603	OLC	C3-C4-C5-C6
2	A	616	OLC	O23-C22-C24-O25
3	A	619	8DZ	C04-C03-O02-C01
2	A	603	OLC	C12-C13-C14-C15
3	A	619	8DZ	O31-C30-O29-C28
2	A	610	OLC	C9-C10-C11-C12
2	A	611	OLC	C1-C2-C3-C4
2	A	612	OLC	O20-C21-C22-O23
2	A	604	OLC	C5-C6-C7-C8
2	A	602	OLC	C3-C4-C5-C6
2	A	603	OLC	C4-C5-C6-C7
2	A	613	OLC	O19-C1-O20-C21
3	A	619	8DZ	C26-C27-C28-O29

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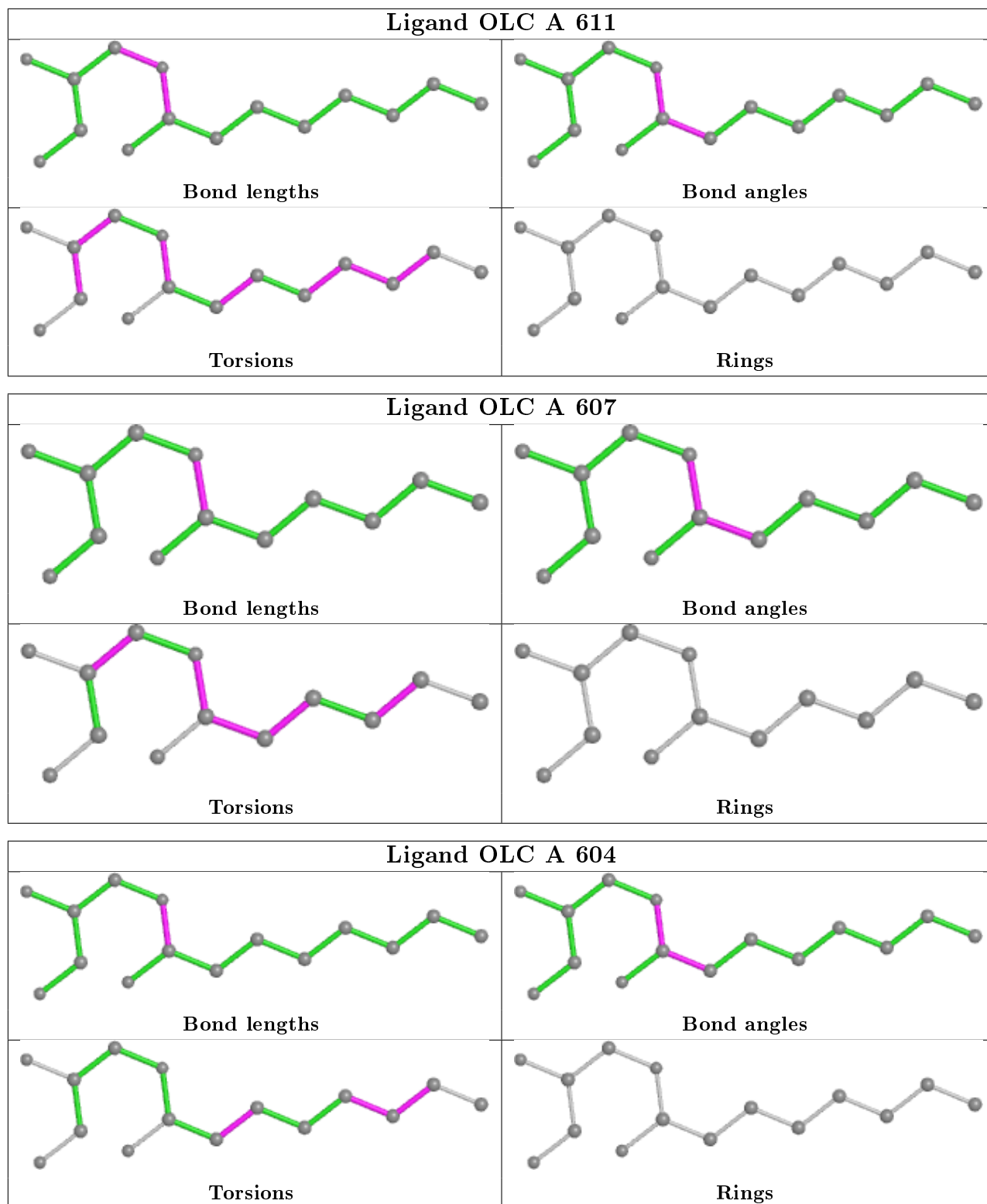
Mol	Chain	Res	Type	Atoms
2	A	603	OLC	C9-C10-C11-C12
2	A	602	OLC	C2-C1-O20-C21
2	A	611	OLC	C4-C5-C6-C7
2	A	602	OLC	O19-C1-O20-C21
2	A	617	OLC	C6-C7-C8-C9
3	A	619	8DZ	N23-C26-C27-C28
2	A	602	OLC	C4-C5-C6-C7
2	A	601	OLC	O20-C21-C22-C24
2	A	611	OLC	C5-C6-C7-C8
2	A	607	OLC	O20-C21-C22-O23
2	A	617	OLC	C7-C8-C9-C10
2	A	603	OLC	C7-C8-C9-C10
3	A	619	8DZ	C32-C30-O29-C28
2	A	601	OLC	O20-C21-C22-O23
2	A	602	OLC	C22-C21-O20-C1
2	A	607	OLC	O20-C1-C2-C3
2	A	612	OLC	O23-C22-C24-O25
2	A	609	OLC	O19-C1-O20-C21
2	A	602	OLC	C15-C16-C17-C18
2	A	609	OLC	C2-C1-O20-C21

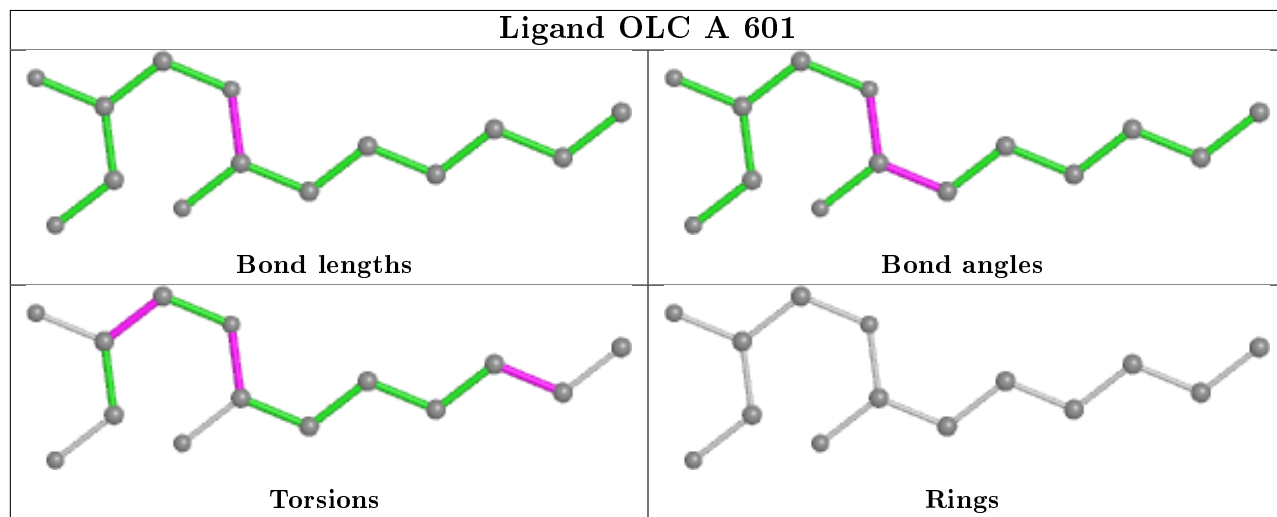
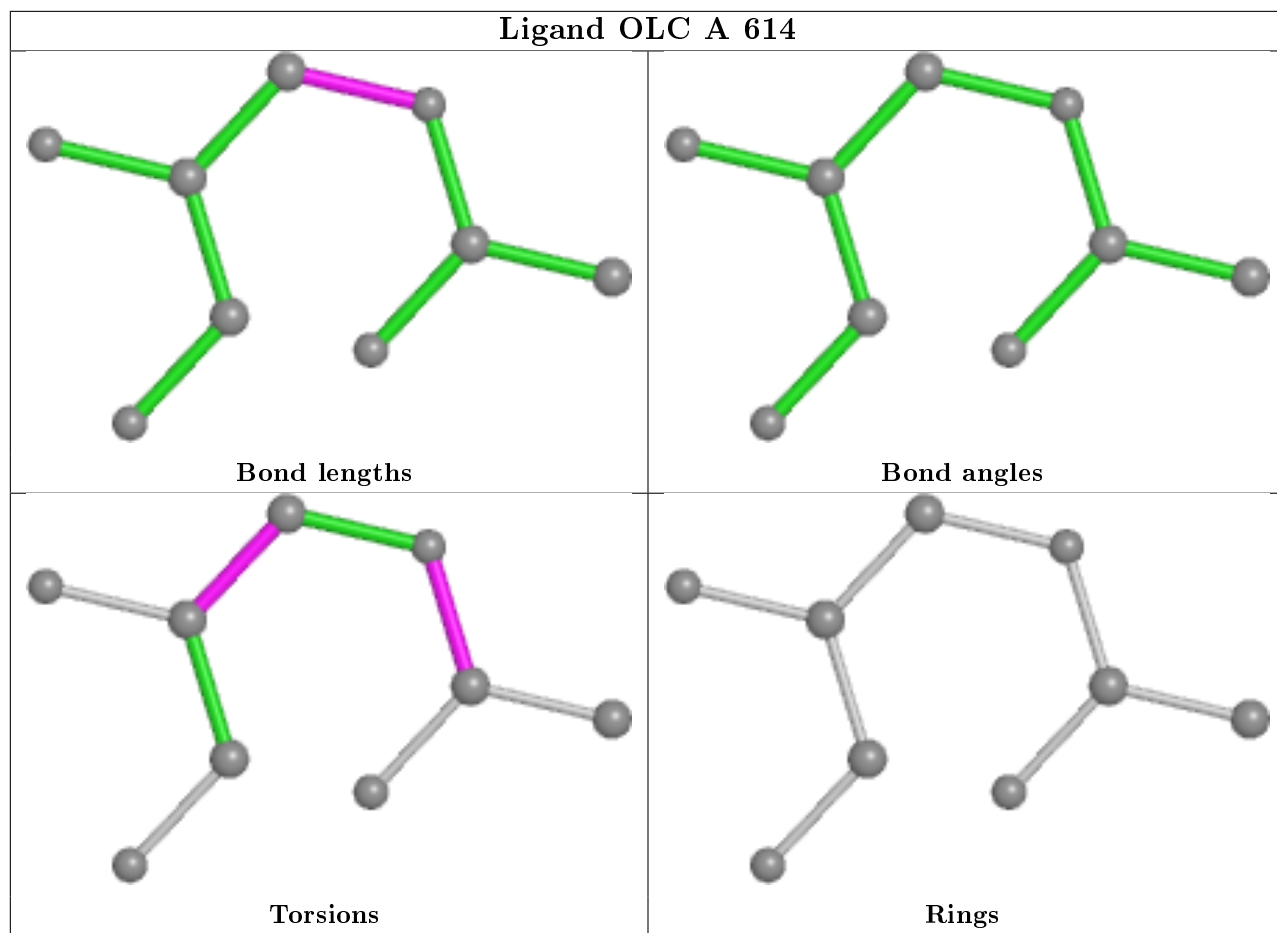
There are no ring outliers.

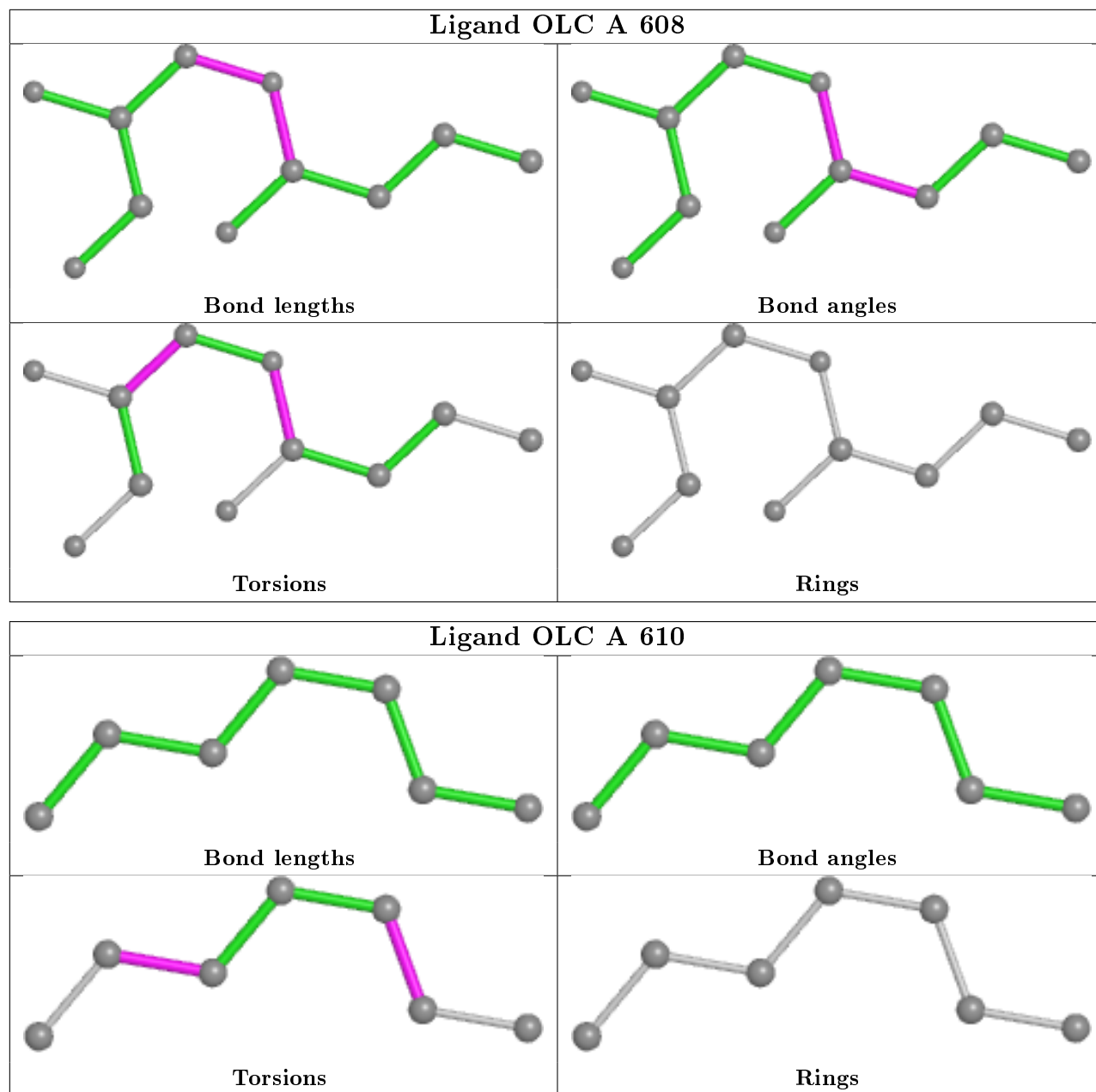
1 monomer is involved in 1 short contact:

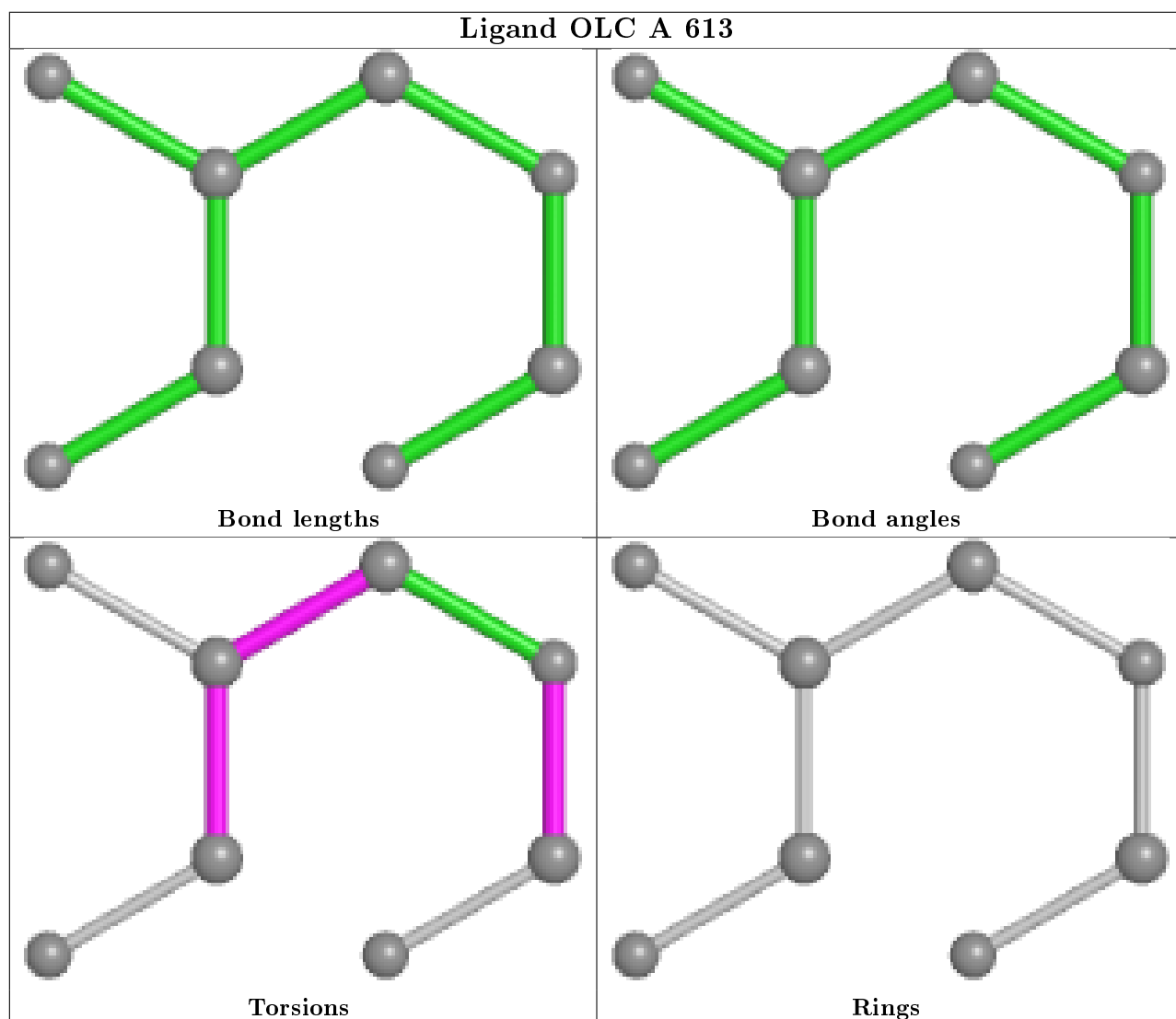
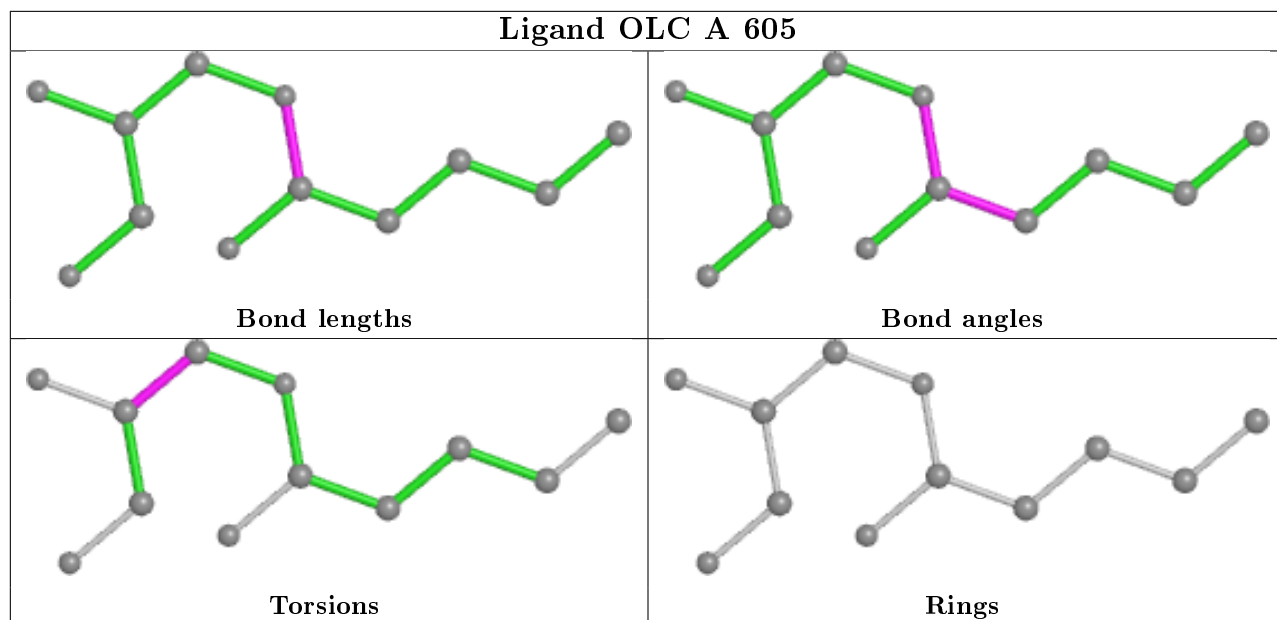
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	OLC	1	0

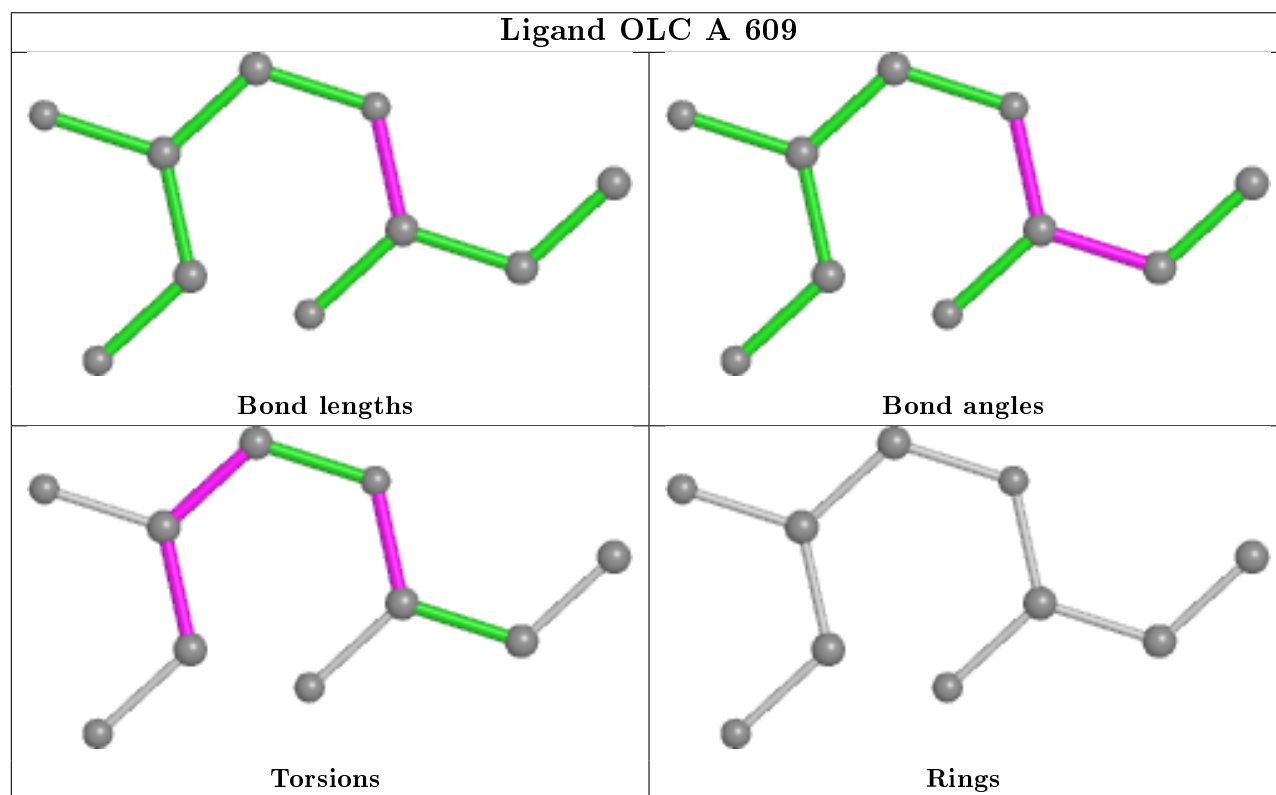
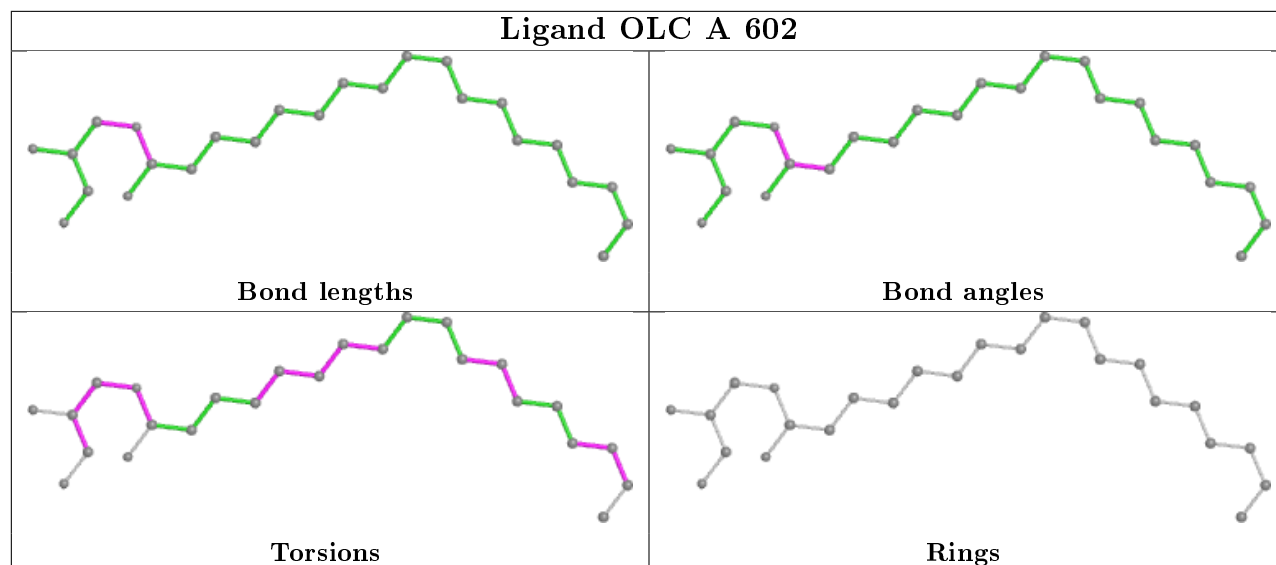
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

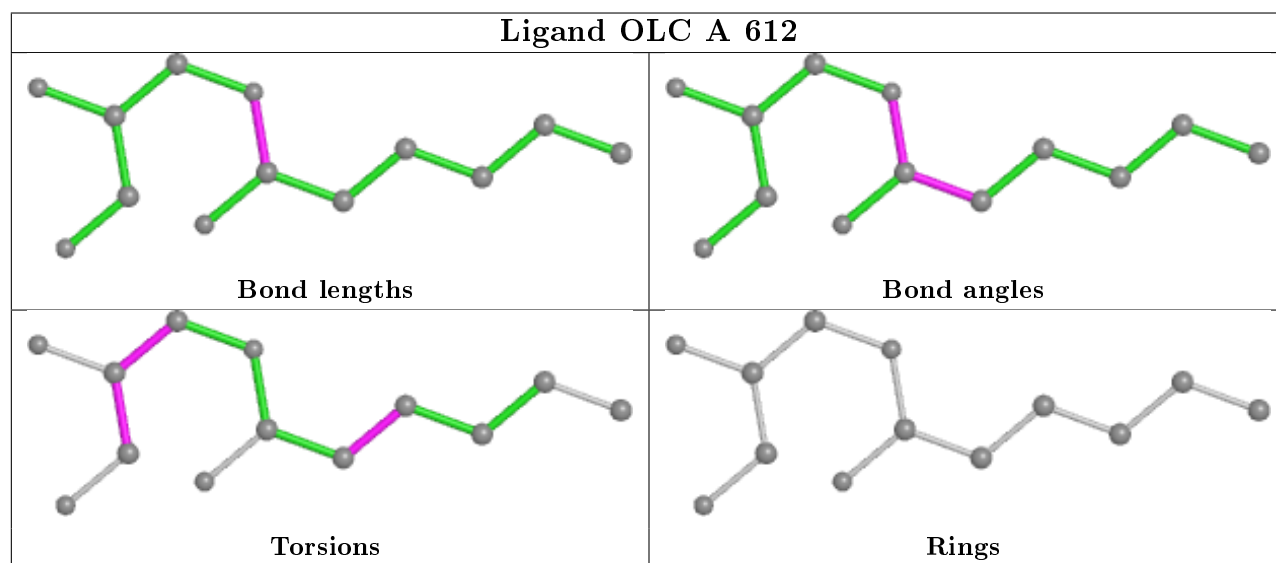
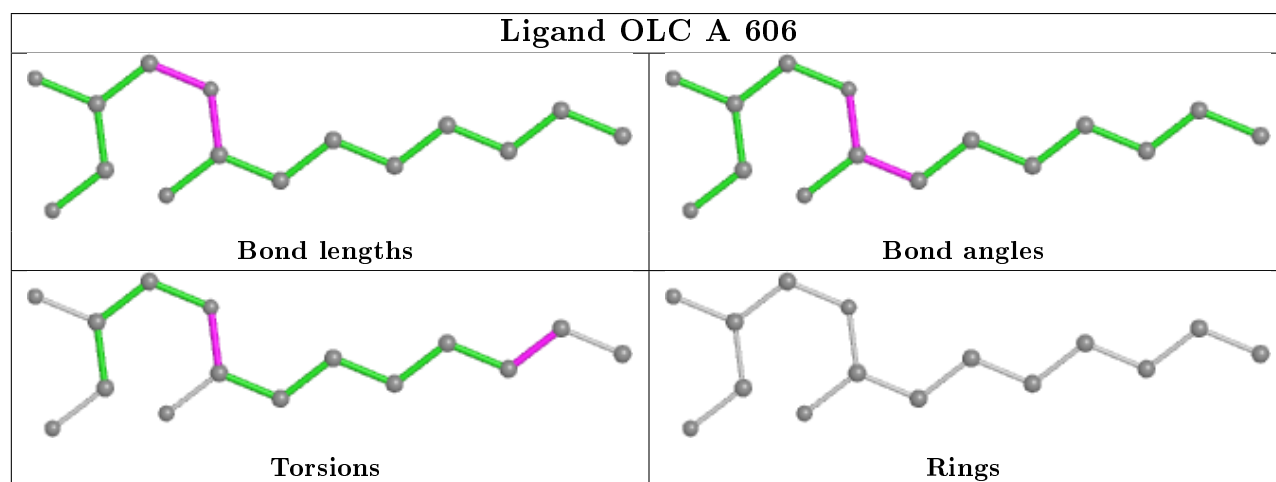
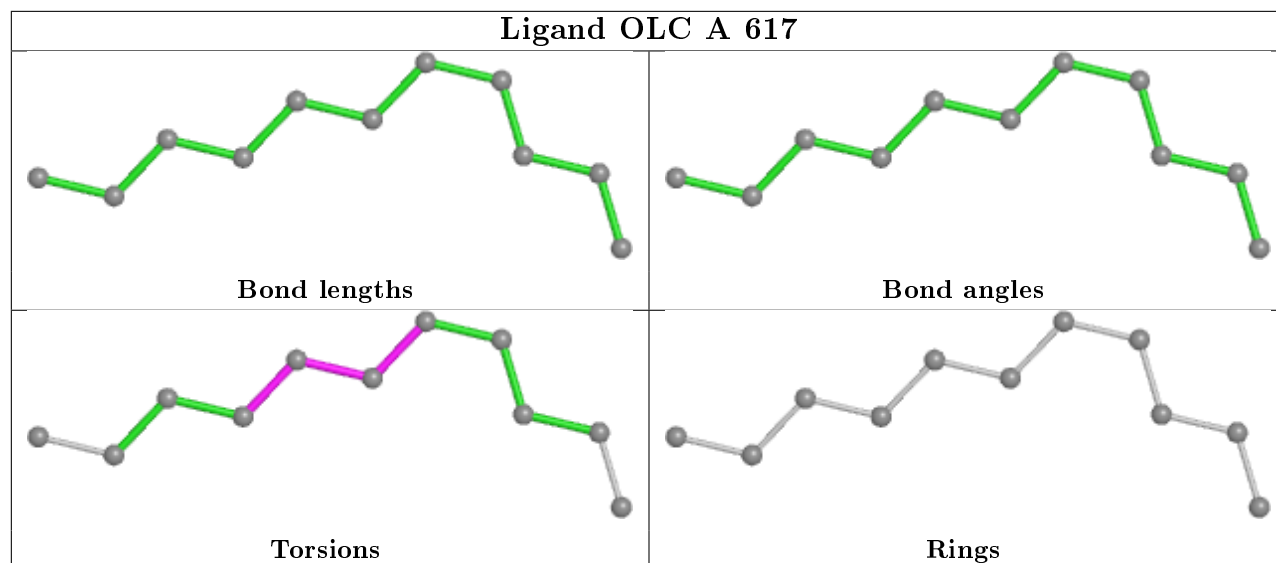


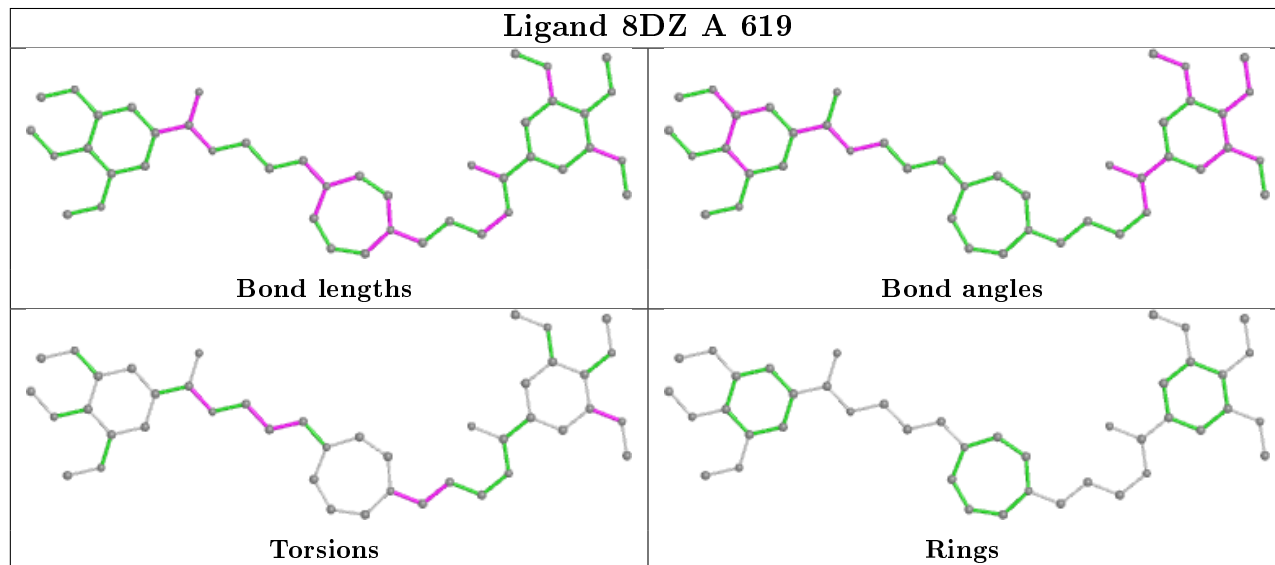
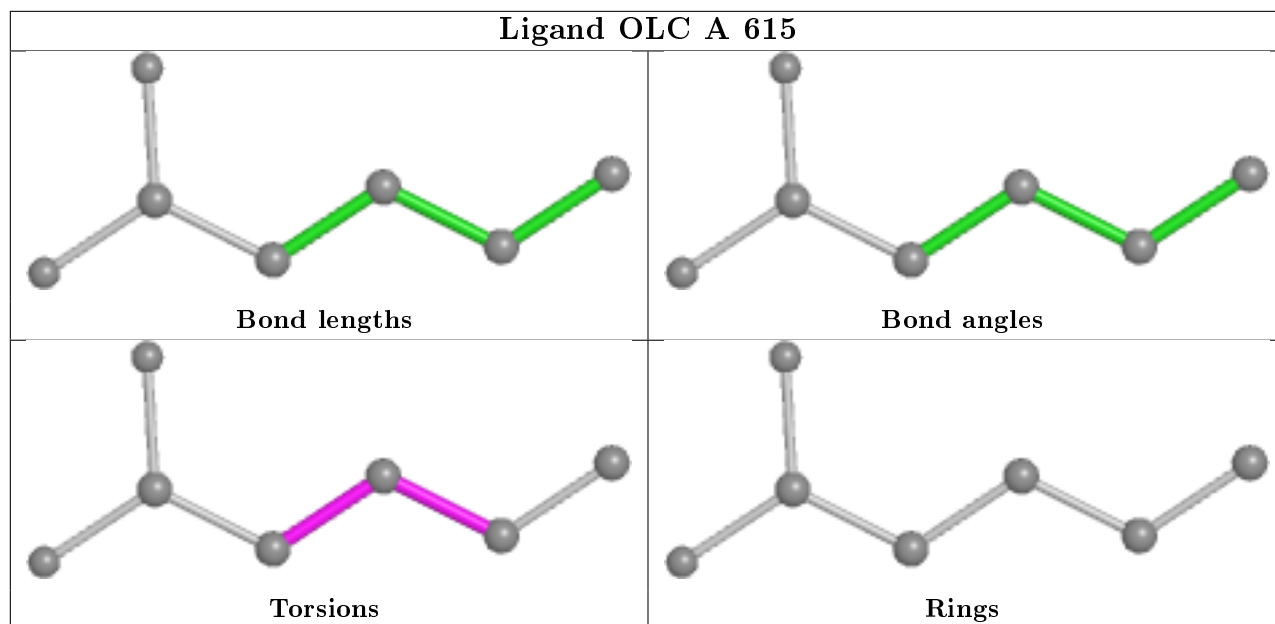




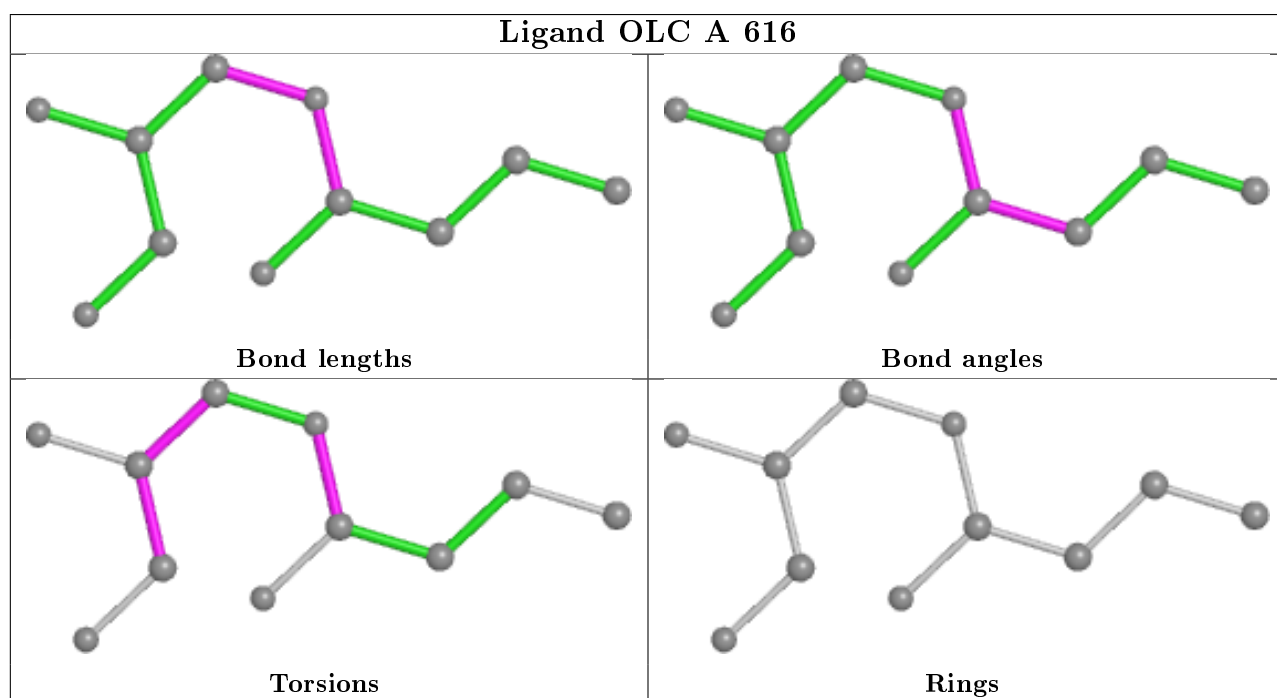
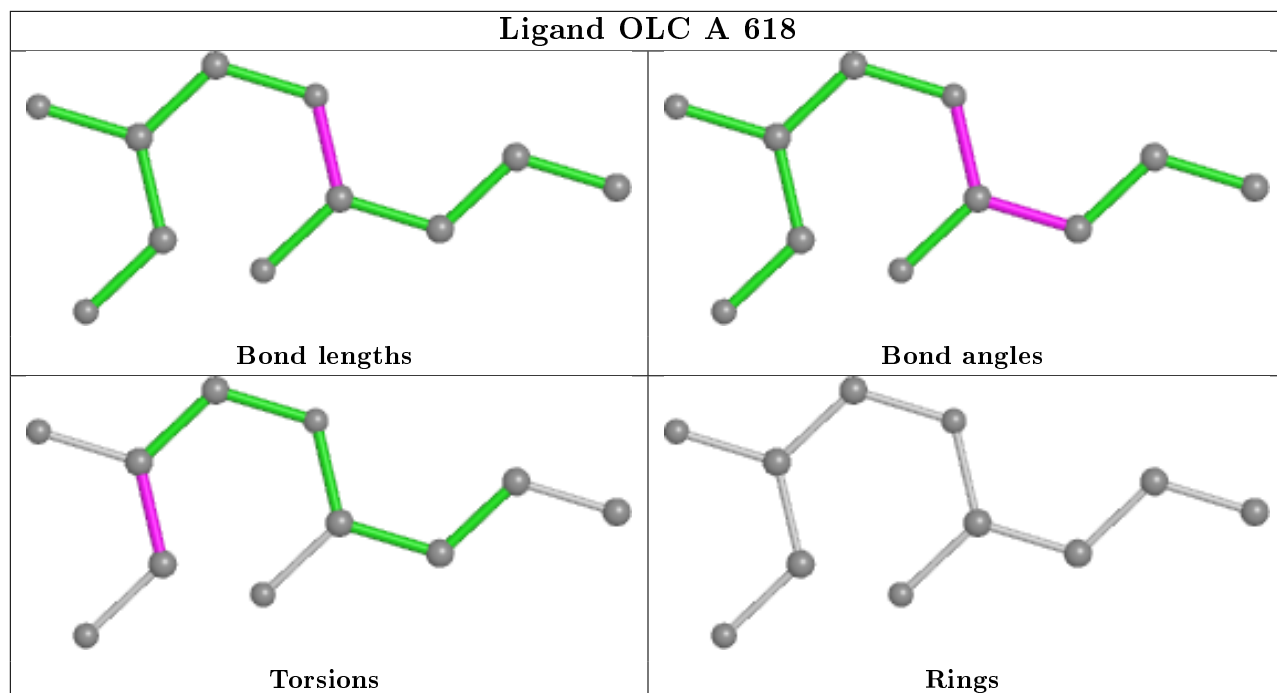


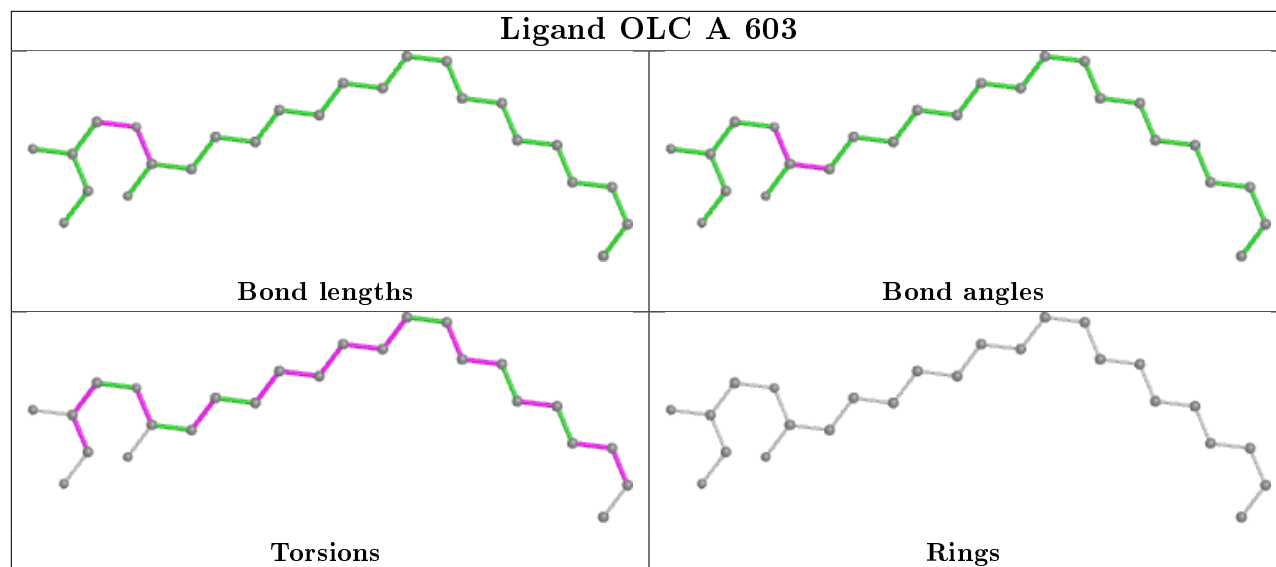












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	381/442 (86%)	-0.22	4 (1%) 82 86	13, 22, 39, 52	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	ASN	4.1
1	A	45	MET	2.6
1	A	237	GLN	2.0
1	A	101	PHE	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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.

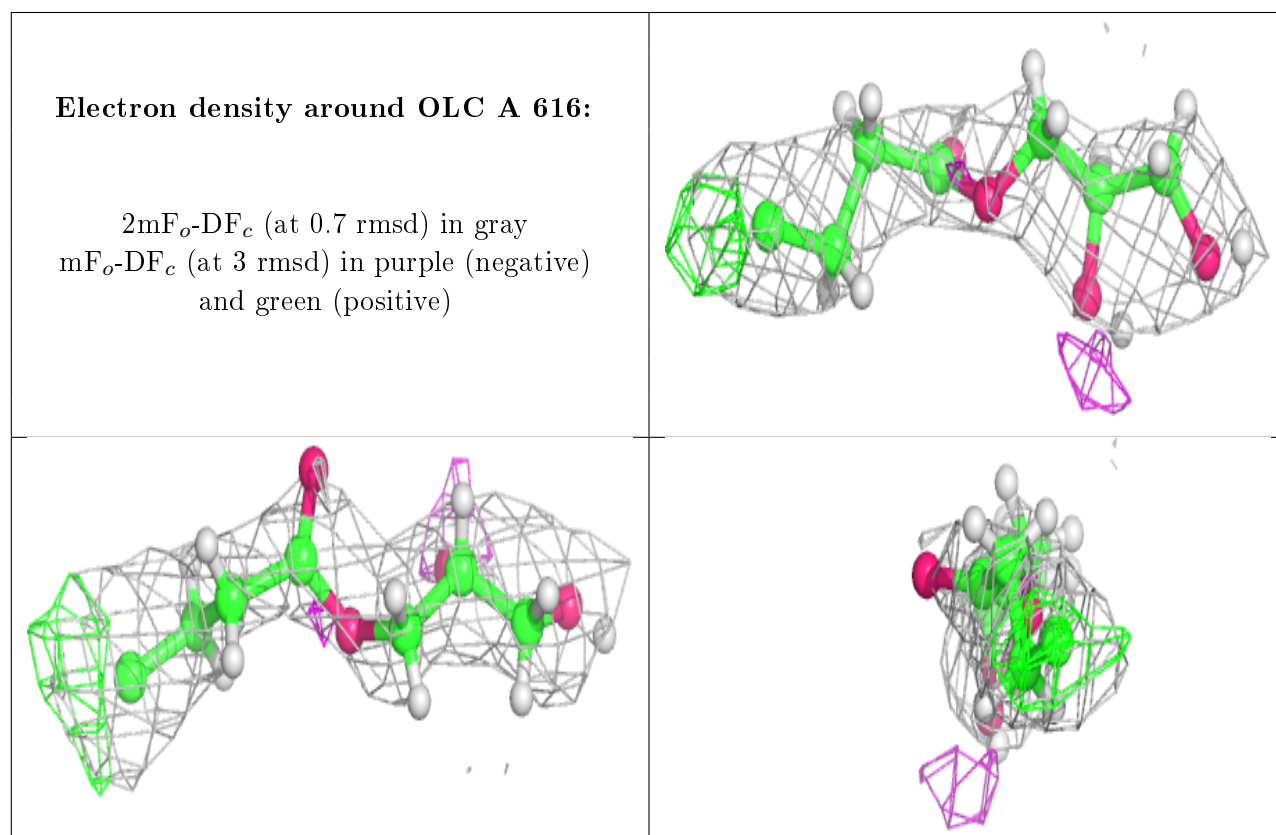
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OLC	A	616	11/25	0.67	0.31	26,42,49,56	0
2	OLC	A	602	25/25	0.73	0.28	23,41,50,55	0
2	OLC	A	605	12/25	0.73	0.18	28,45,53,59	0

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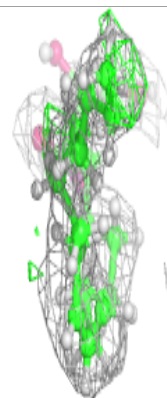
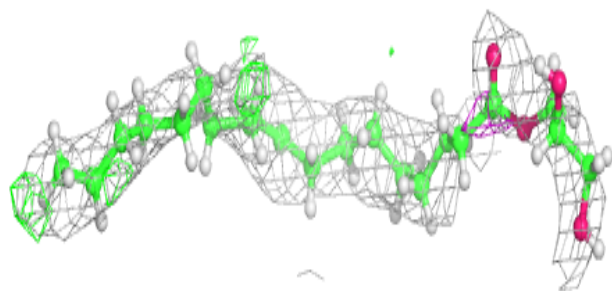
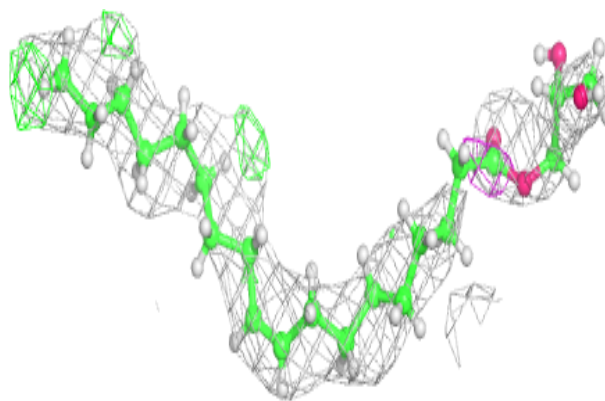
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OLC	A	601	14/25	0.75	0.19	23,30,52,54	0
2	OLC	A	603	25/25	0.76	0.19	32,40,49,51	0
2	OLC	A	606	15/25	0.77	0.14	22,36,55,57	0
2	OLC	A	611	15/25	0.78	0.28	26,36,52,57	0
2	OLC	A	617	11/25	0.78	0.18	27,36,41,41	0
2	OLC	A	618	11/25	0.78	0.24	39,46,51,53	0
2	OLC	A	610	7/25	0.79	0.18	24,34,41,41	0
2	OLC	A	612	13/25	0.79	0.28	31,40,56,58	0
2	OLC	A	614	9/25	0.82	0.29	41,48,66,66	0
2	OLC	A	607	13/25	0.85	0.22	33,41,48,48	0
2	OLC	A	613	8/25	0.85	0.19	40,45,52,52	0
2	OLC	A	604	15/25	0.86	0.20	29,33,44,48	0
2	OLC	A	615	7/25	0.88	0.16	29,34,36,38	0
2	OLC	A	609	10/25	0.88	0.19	34,44,50,50	0
2	OLC	A	608	11/25	0.91	0.17	32,42,46,54	0
3	8DZ	A	619	43/43	0.93	0.11	20,20,20,20	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.

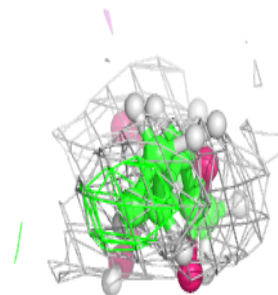
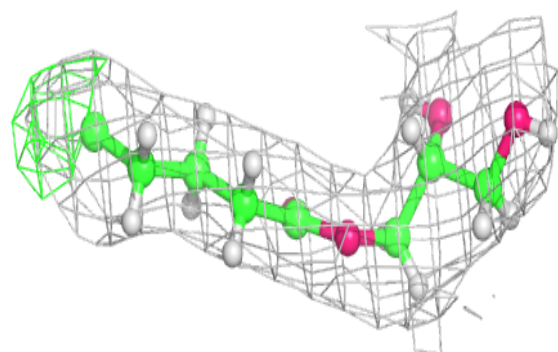
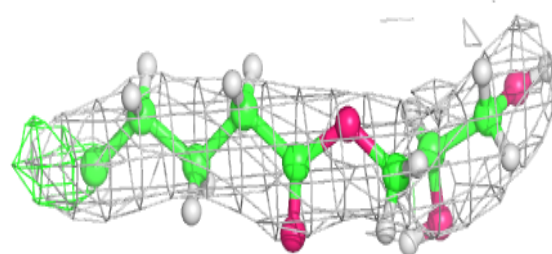


**Electron density around OLC A 602:**

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

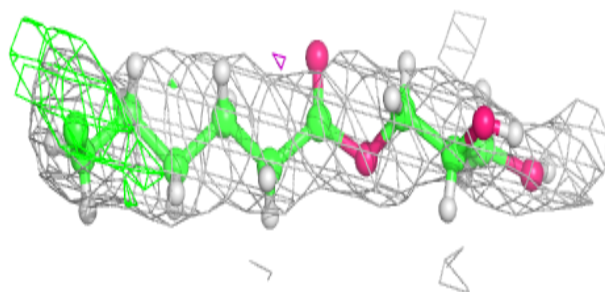
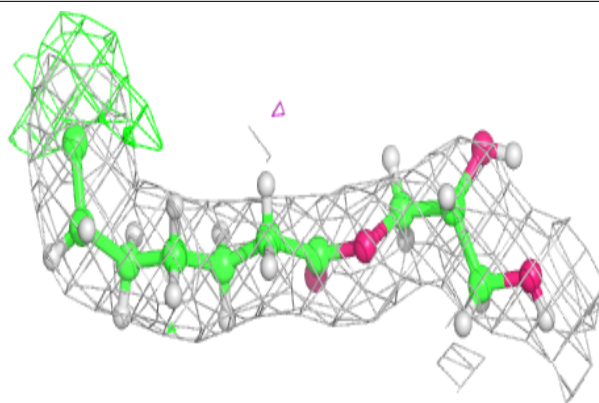
**Electron density around OLC A 605:**

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

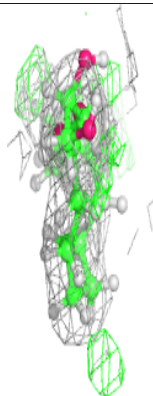
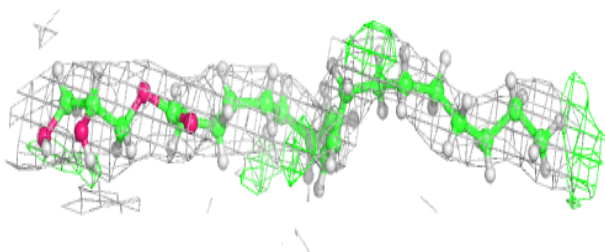
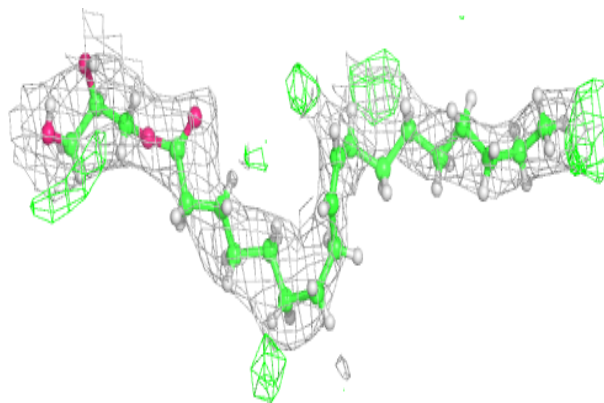


**Electron density around OLC A 601:**

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

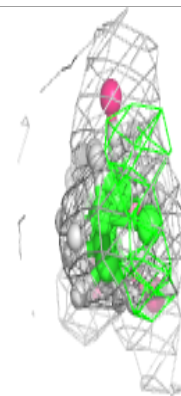
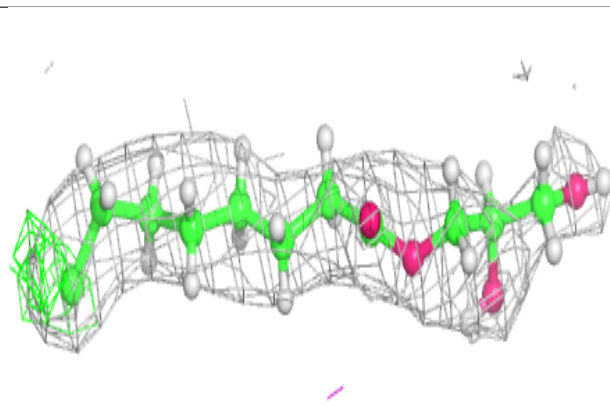
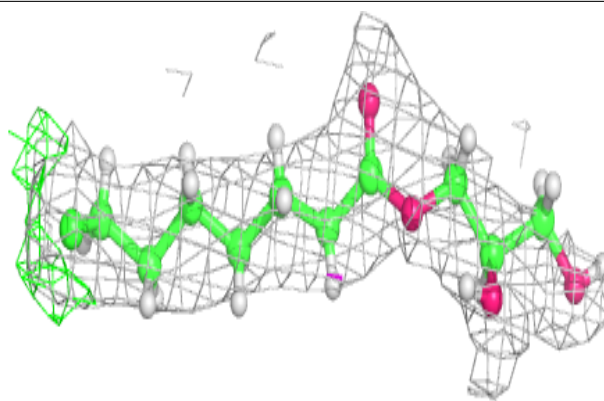
**Electron density around OLC A 603:**

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

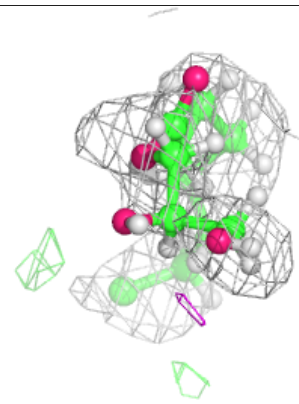
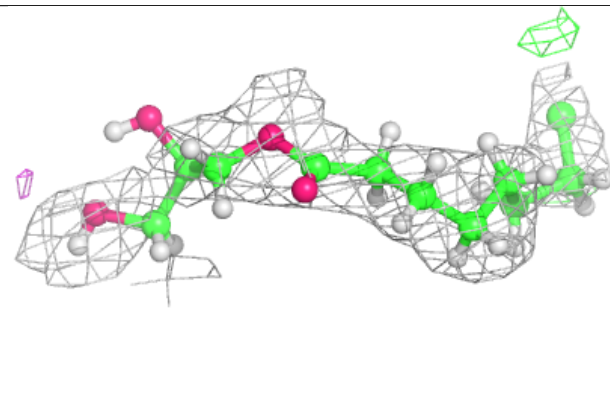
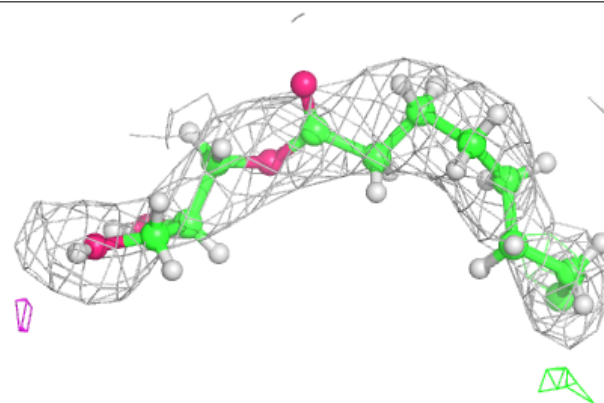


**Electron density around OLC A 606:**

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

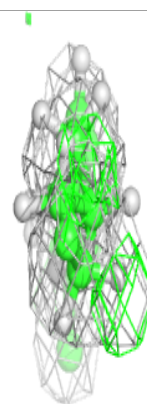
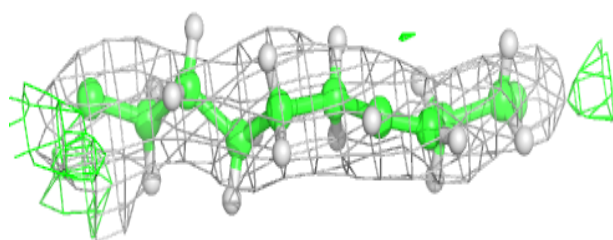
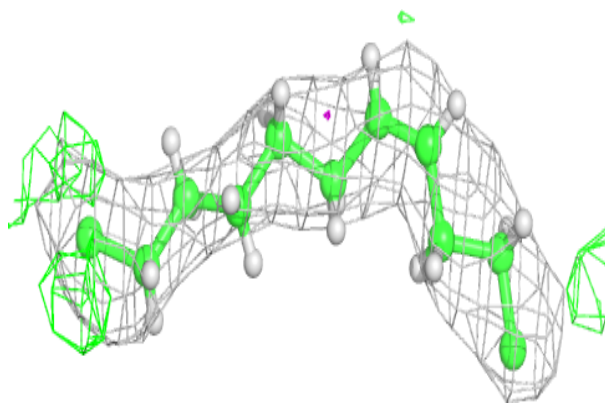
**Electron density around OLC A 611:**

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

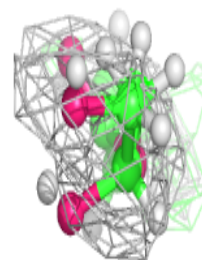
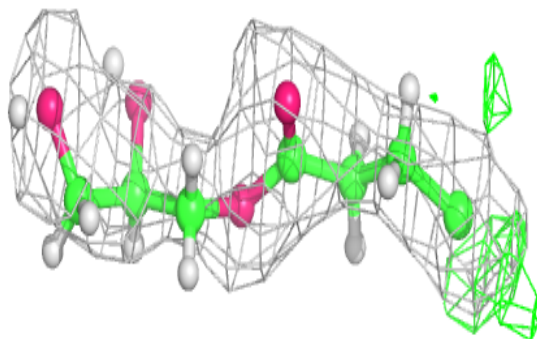
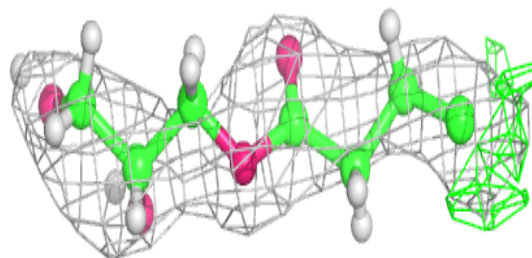


**Electron density around OLC A 617:**

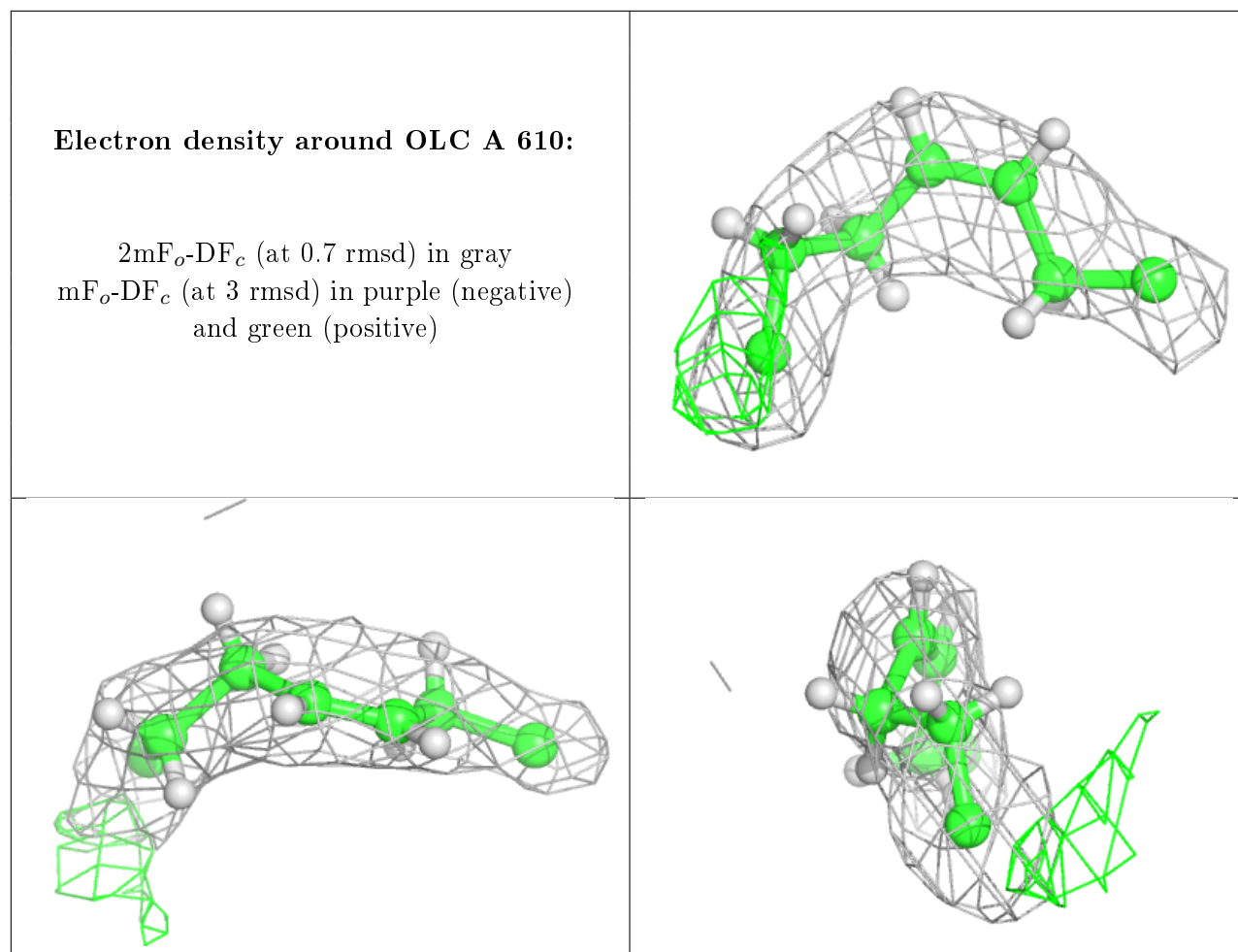
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around OLC A 618:**

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

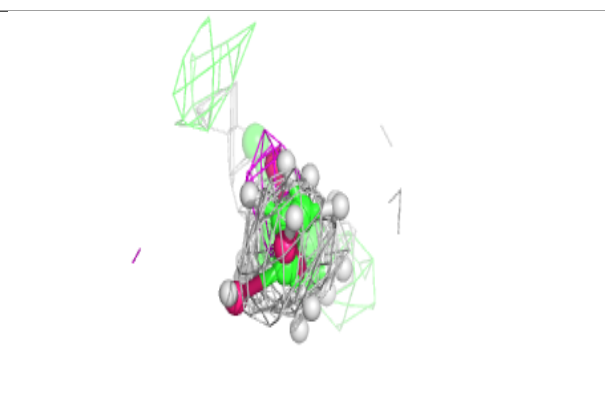
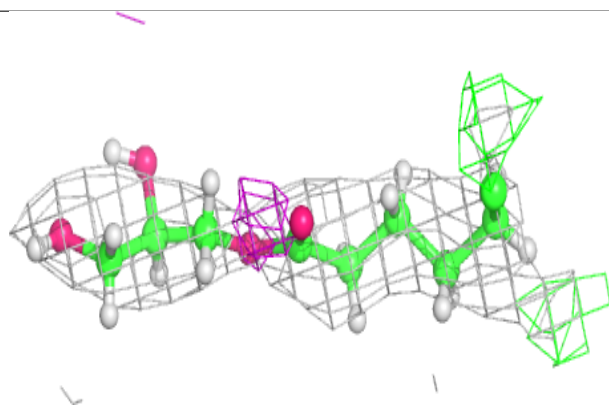
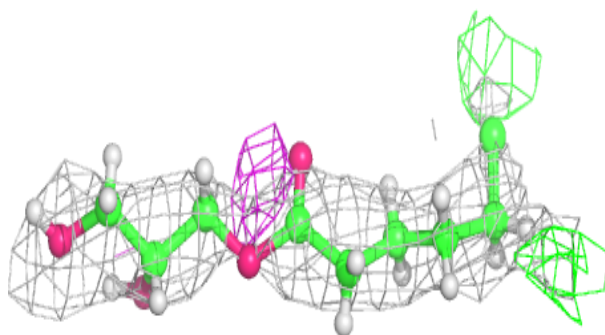




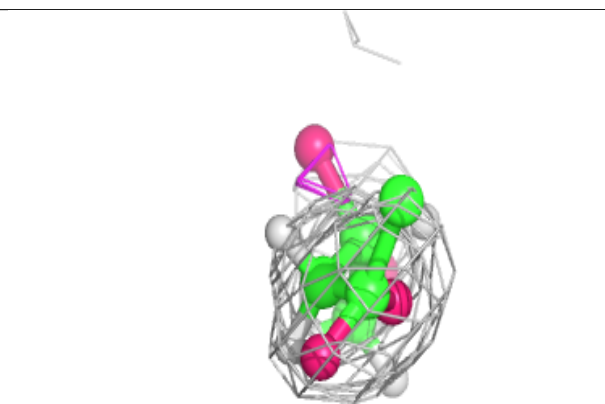
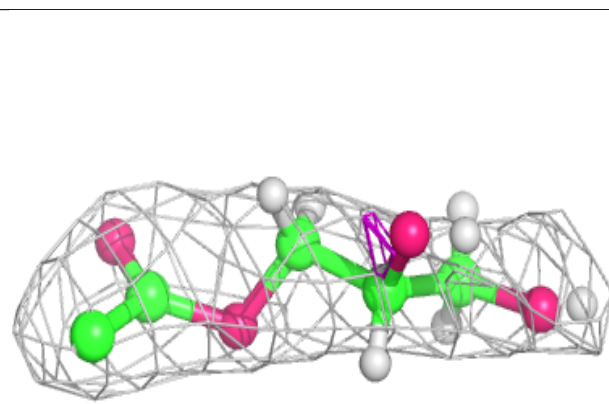
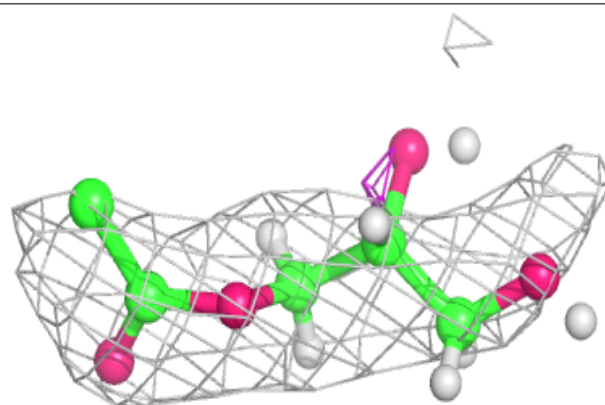


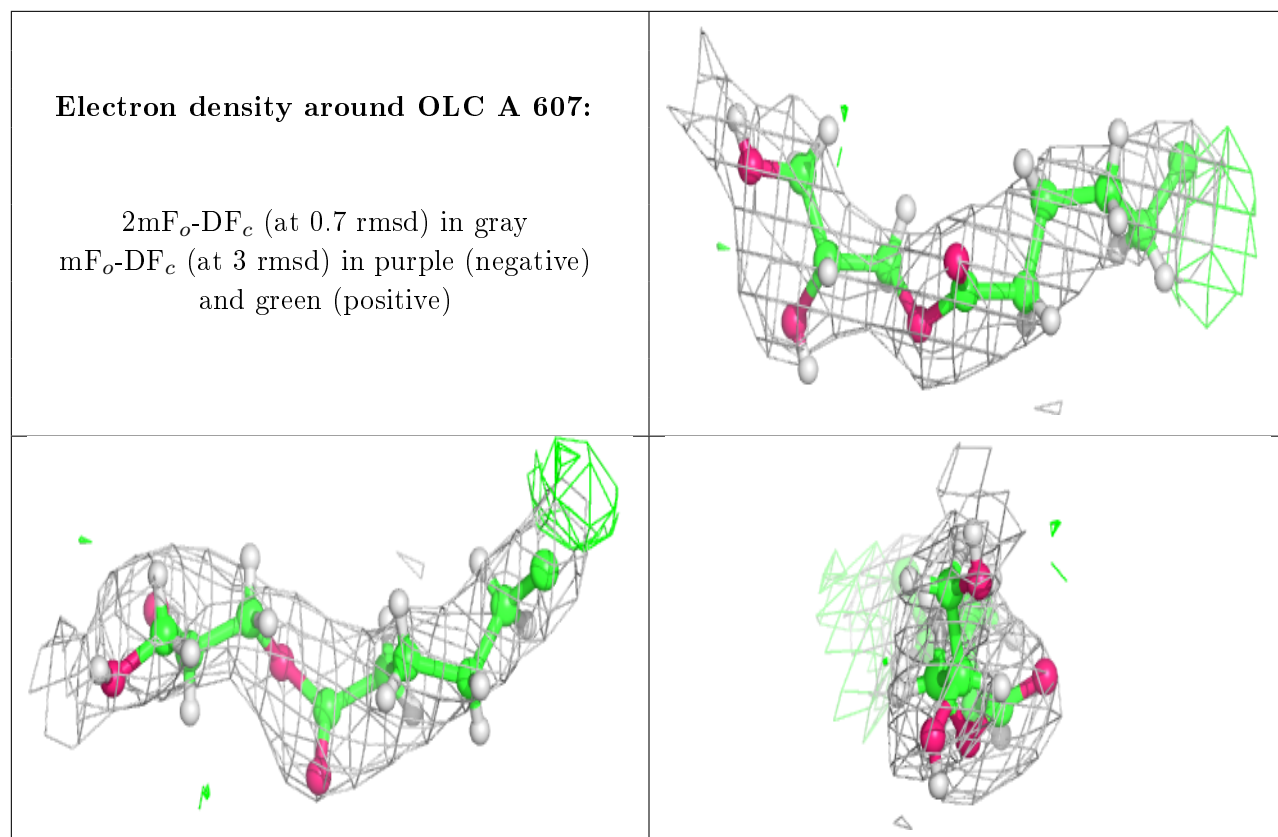
**Electron density around OLC A 612:**

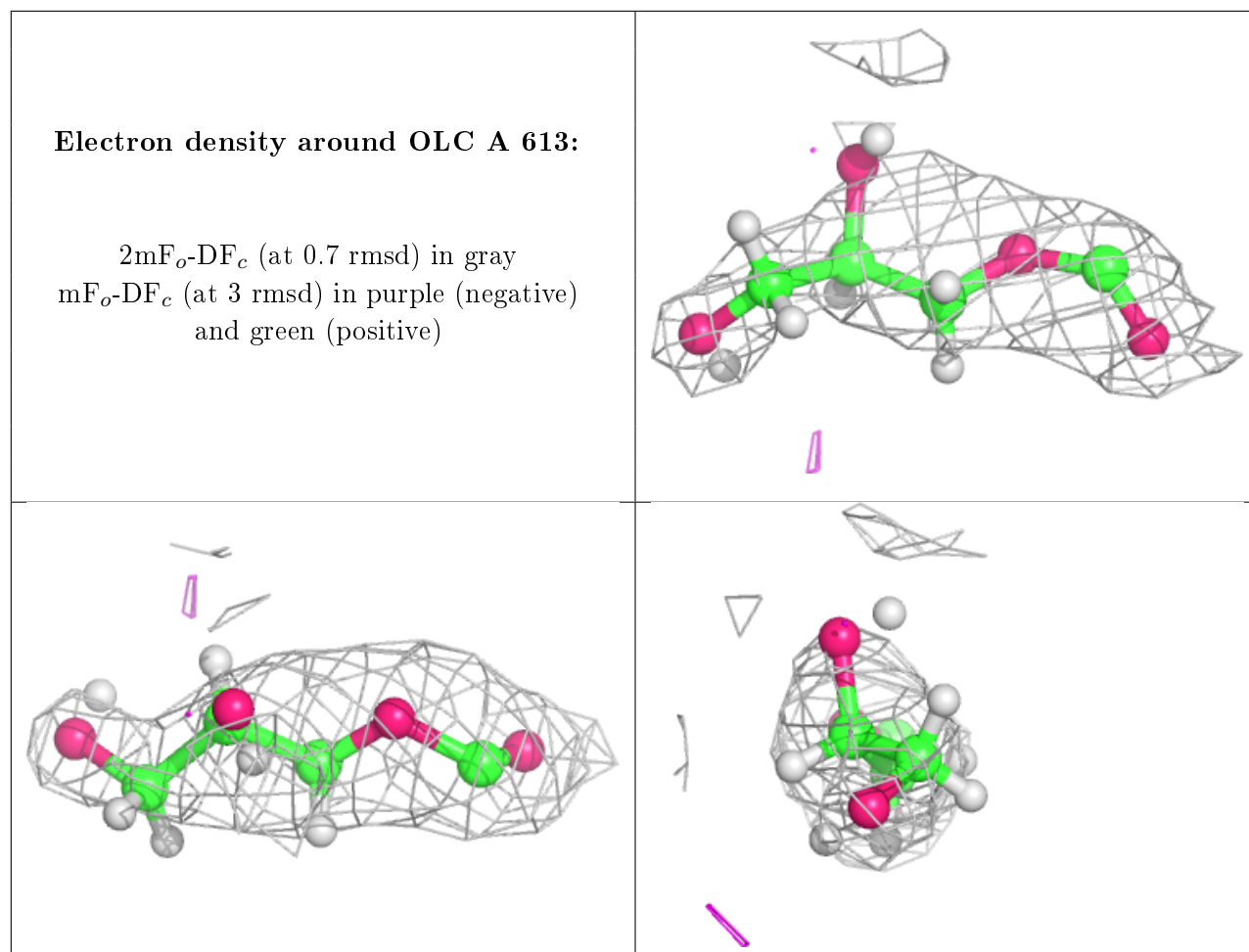
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around OLC A 614:**

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

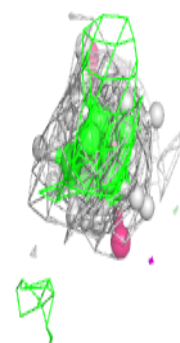
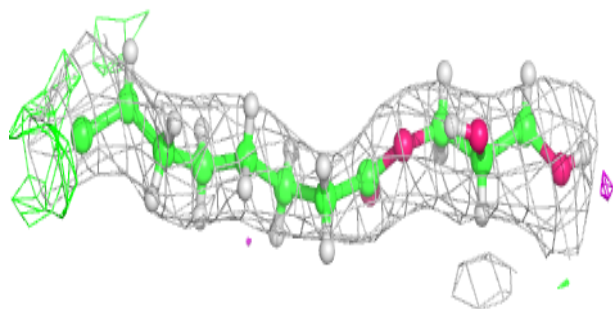
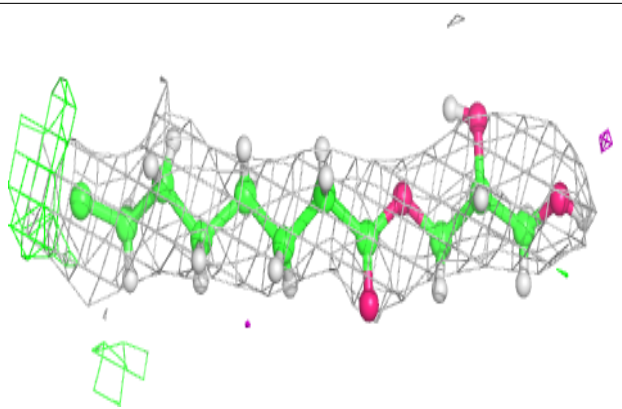




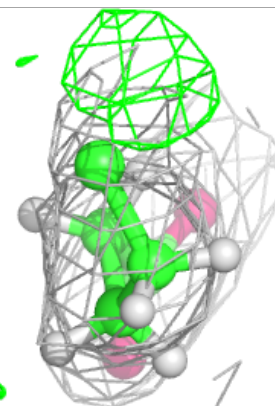
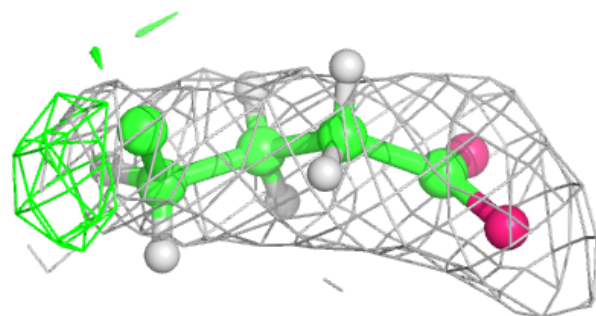
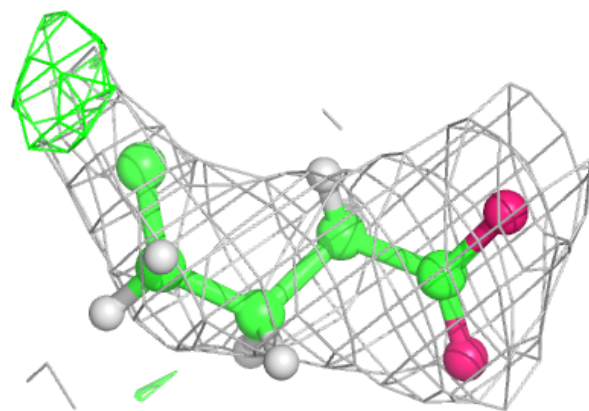


**Electron density around OLC A 604:**

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

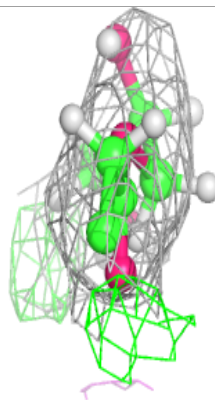
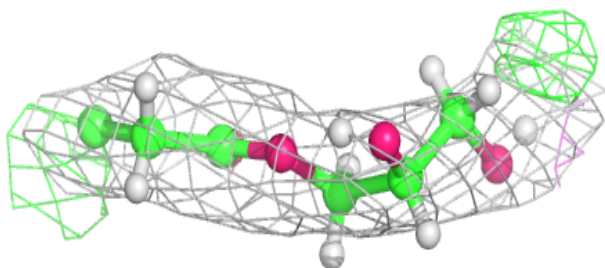
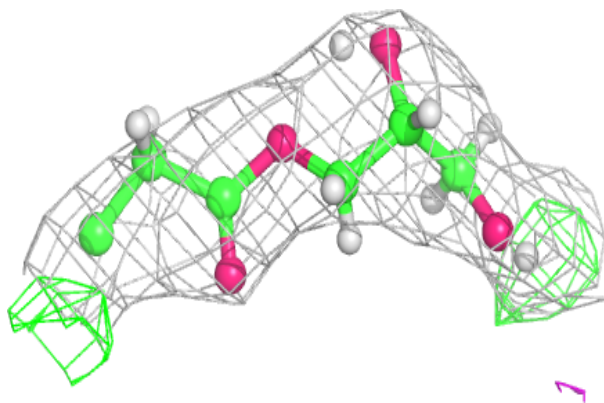
**Electron density around OLC A 615:**

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

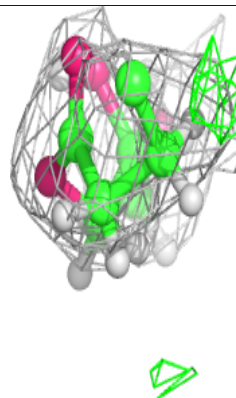
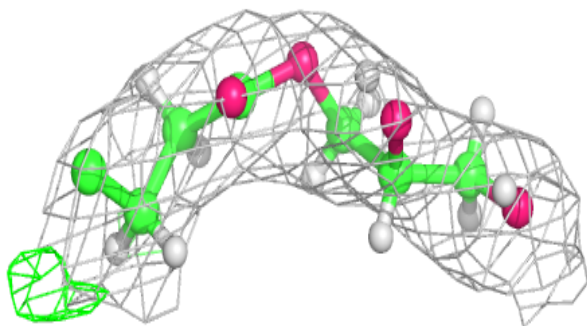
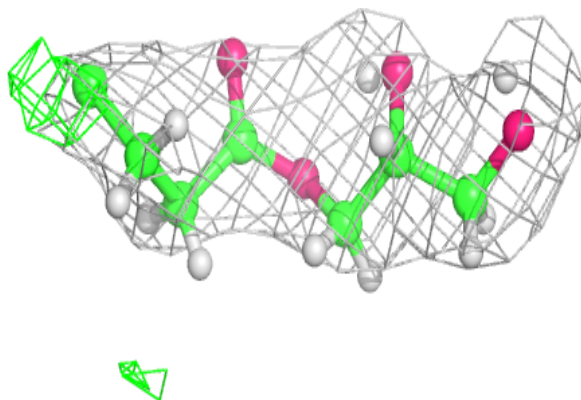


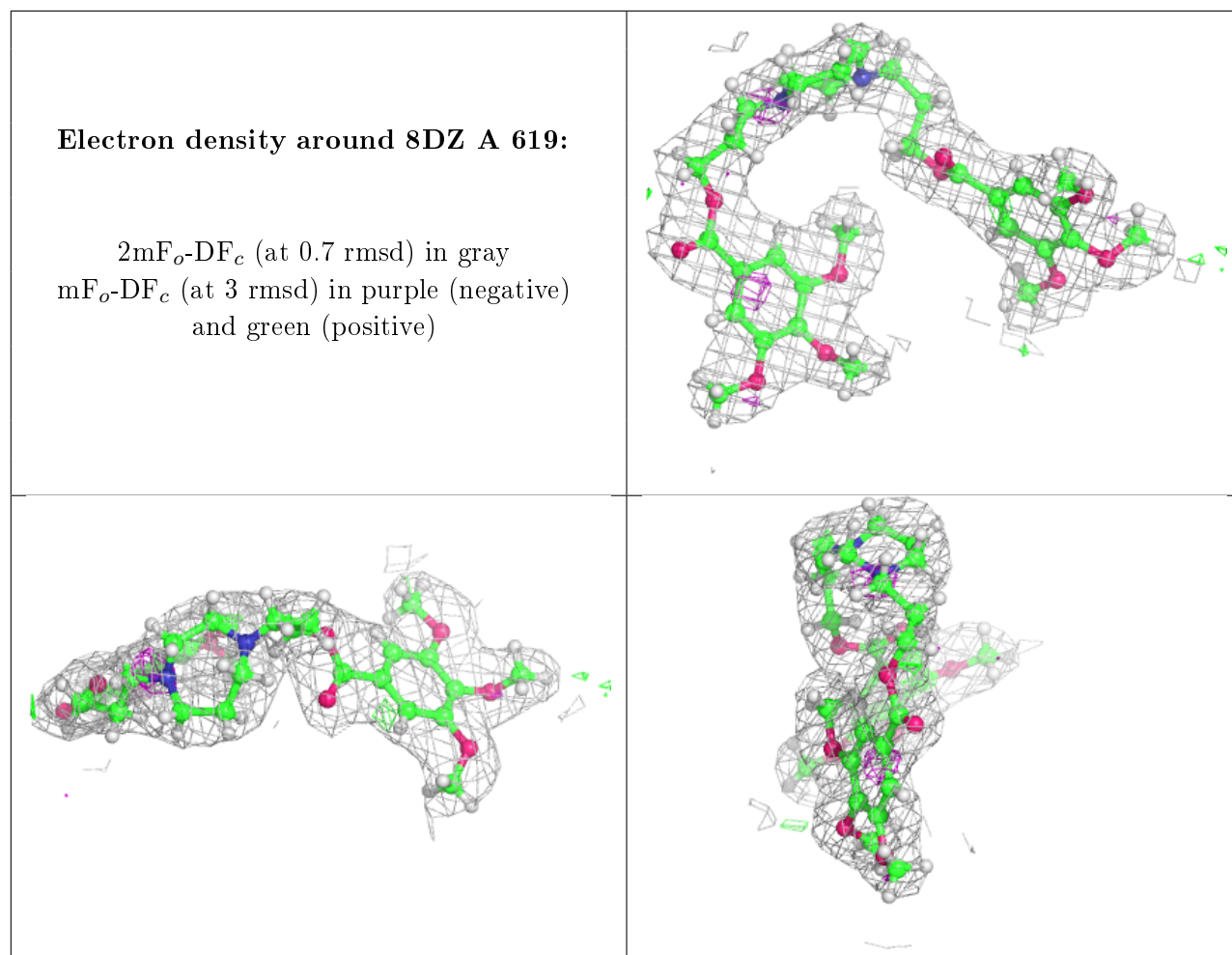
**Electron density around OLC A 609:**

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

**Electron density around OLC A 608:**

$2mF_o-DF_c$  (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.