



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 01:21 pm BST

PDB ID : 4N4Y  
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant G232V from *Thermus thermophilus*  
Authors : Li, Y.; Chen, Y.; Stout, C.D.  
Deposited on : 2013-10-08  
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

---

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

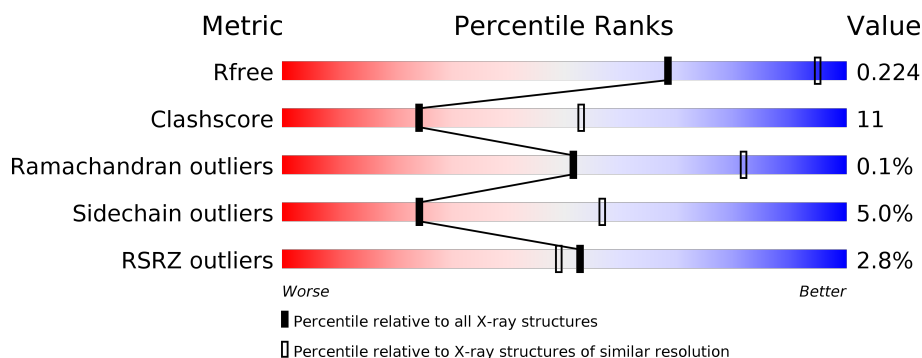
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	568	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>••</div> </div> </div>
2	B	168	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>••</div> </div> </div>
3	C	34	<div> <div></div> <div> <div></div> <div>71%</div> <div>18%</div> <div>•</div> <div>9%</div> </div> </div>

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
8	OLC	A	611	-	-	-	X
8	OLC	C	102	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6549 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	4	0
			4371	2970	696	689	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	232	VAL	GLY	ENGINEERED MUTATION	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	1	0
			1288	837	214	233	4			

- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			241	169	37	35			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

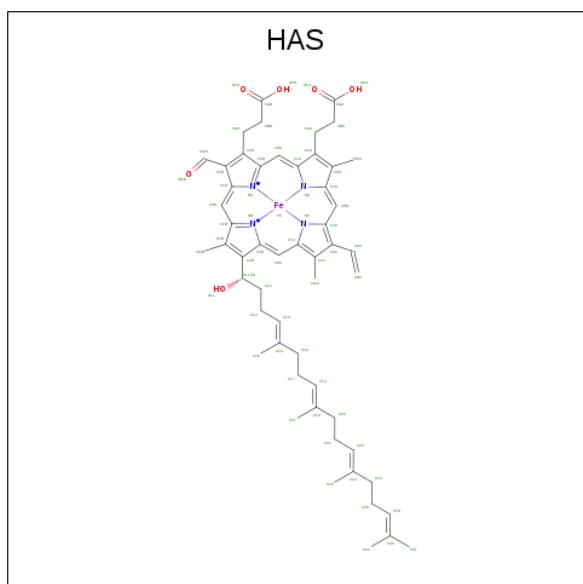
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



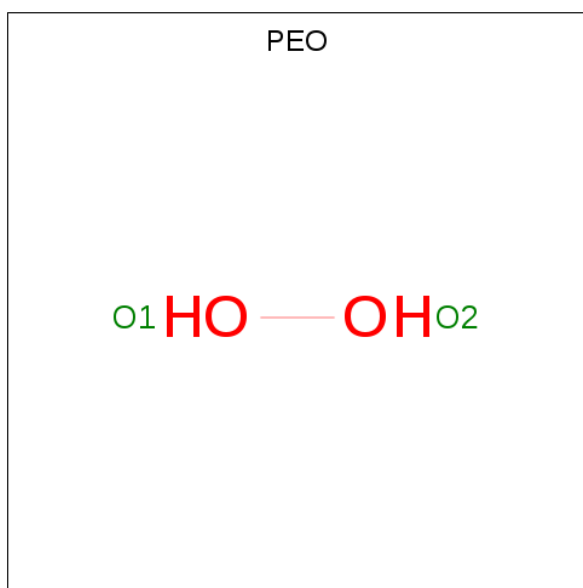
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula:  $C_{54}H_{64}FeN_4O_6$ ).



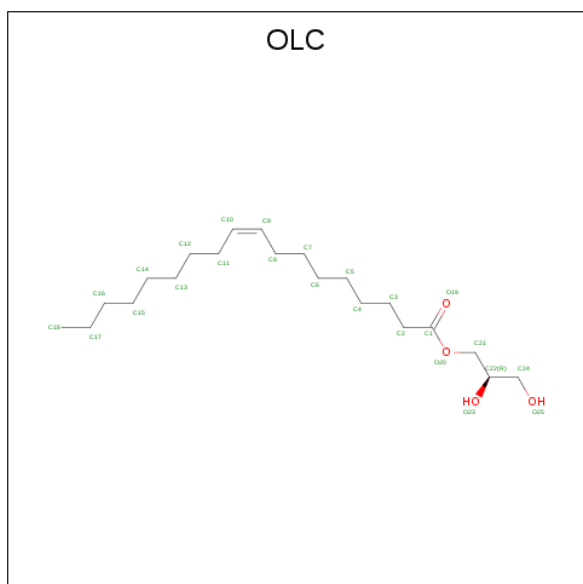
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula:  $\text{H}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			2	2		

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula:  $\text{C}_{21}\text{H}_{40}\text{O}_4$ ).



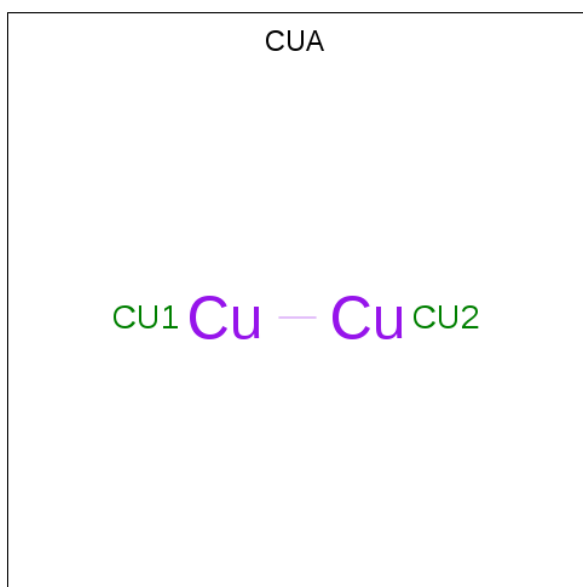
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			23	19	4		
8	A	1	Total	C	O	0	0
			21	19	2		
8	A	1	Total	C	O	0	0
			18	14	4		
8	A	1	Total	C	O	0	0
			17	13	4		
8	A	1	Total	C	O	0	0
			8	4	4		
8	A	1	Total	C	O	0	0
			15	11	4		
8	A	1	Total	C	O	0	0
			20	16	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			21	17	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	C	1	Total	C	O	0	0
			25	21	4		
8	C	1	Total	C	O	0	0
			25	21	4		

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cu 2 2	0	0

- Molecule 10 is water.

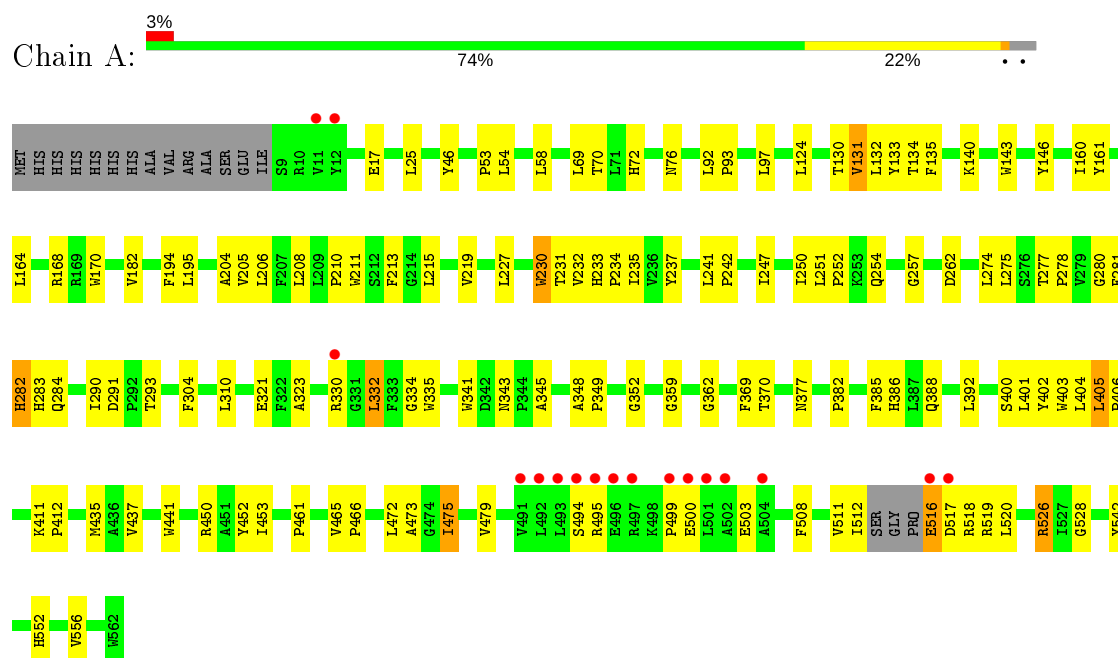
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	118	Total O 118 118	0	0
10	B	72	Total O 72 72	0	0
10	C	3	Total O 3 3	0	0



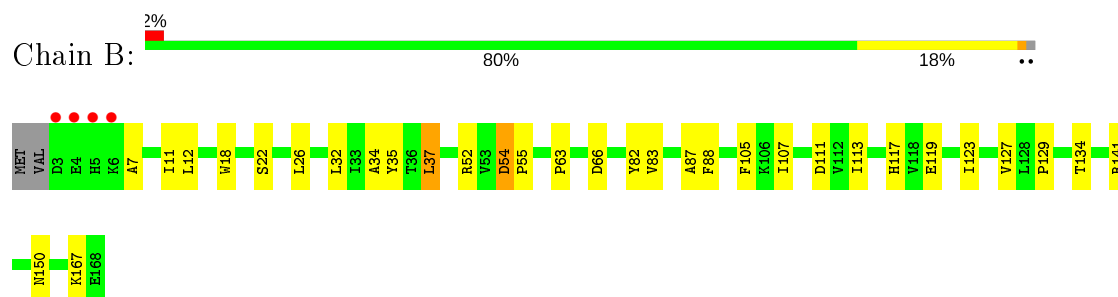
### 3 Residue-property plots [i](#)

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.

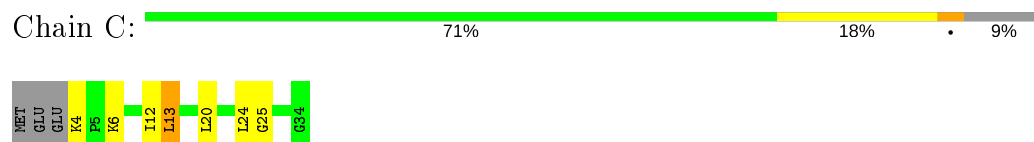
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • Molecule 2: Cytochrome c oxidase subunit 2



#### • Molecule 3: Cytochrome c oxidase polypeptide 2A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.15Å 98.40Å 114.10Å 90.00° 138.93° 90.00°	Depositor
Resolution (Å)	74.96 – 2.90 49.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (74.96-2.90) 98.5 (49.20-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.177 , 0.225 0.180 , 0.224	Depositor DCC
$R_{free}$ test set	1192 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6549	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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, PEO, CUA, HEM, HAS, CU

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	0.78	0/4537	0.77	2/6228 (0.0%)
2	B	0.80	0/1330	0.74	1/1817 (0.1%)
3	C	0.84	0/247	0.82	1/335 (0.3%)
All	All	0.79	0/6114	0.77	4/8380 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	VAL	N-CA-C	-6.50	93.46	111.00
2	B	54	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	332	LEU	CA-CB-CG	5.27	127.43	115.30
3	C	13	LEU	CA-CB-CG	5.27	127.43	115.30

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	4371	0	4473	110	0
2	B	1288	0	1260	21	1
3	C	241	0	267	3	0
4	A	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	43	0	30	6	0
6	A	65	0	62	1	0
7	A	2	0	0	0	0
8	A	218	0	313	23	0
8	B	75	0	120	8	0
8	C	50	0	80	5	0
9	B	2	0	0	0	0
10	A	118	0	0	6	1
10	B	72	0	0	2	1
10	C	3	0	0	0	0
All	All	6549	0	6605	142	2

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 11.

The worst 5 of 142 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:233:HIS:NE2	1:A:237:TYR:HE2	0.87	1.34
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.79	1.26
1:A:168:ARG:HH22	8:A:611:OLC:H6A	1.18	1.05
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:HG2	1.61	1.04
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.73	1.01

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:317:HOH:O	10:B:340:HOH:O[2_656]	2.06	0.14
2:B:66:ASP:OD2	10:A:716:HOH:O[2_656]	2.13	0.07

## 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	550/568 (97%)	519 (94%)	30 (6%)	1 (0%)	47	78
2	B	165/168 (98%)	163 (99%)	2 (1%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	744/770 (97%)	711 (96%)	32 (4%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	HIS

### 5.3.2 Protein sidechains ⓘ

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	448/463 (97%)	426 (95%)	22 (5%)	25	57
2	B	134/138 (97%)	129 (96%)	5 (4%)	34	68
3	C	24/27 (89%)	21 (88%)	3 (12%)	4	14
All	All	606/628 (96%)	576 (95%)	30 (5%)	24	57

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	TYR
1	A	495	ARG
3	C	13	LEU
1	A	494	SER
1	A	500	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	446	ASN
2	B	69	GLN
2	B	117	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\# Z  > 2$
9	CUA	B	201	2	0,1,1	0.00	-	-		
8	OLC	A	607	-	20,20,24	0.66	1 (5%)	20,20,25	0.48	0
8	OLC	A	608	-	17,17,24	0.59	0	18,18,25	0.48	0
7	PEO	A	604	4,6	1,1,1	0.50	0	-		
8	OLC	A	614	-	20,20,24	0.56	0	21,21,25	0.62	0
8	OLC	A	613	-	24,24,24	0.66	1 (4%)	25,25,25	1.03	3 (12%)
8	OLC	A	606	-	22,22,24	0.56	0	23,23,25	0.71	0
8	OLC	A	610	-	7,7,24	0.46	0	6,7,25	0.70	0
8	OLC	A	615	-	24,24,24	0.52	0	25,25,25	0.68	0
5	HEM	A	602	1	27,50,50	3.06	12 (44%)	17,82,82	1.80	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	OLC	A	605	-	24,24,24	0.49	0	25,25,25	0.64	0
8	OLC	A	611	-	14,14,24	0.61	0	15,15,25	0.50	0
8	OLC	A	609	-	16,16,24	0.78	0	17,17,25	0.80	1 (5%)
8	OLC	B	203	-	24,24,24	0.76	1 (4%)	25,25,25	1.01	2 (8%)
6	HAS	A	603	1,7	56,72,72	4.45	14 (25%)	50,109,109	3.04	16 (32%)
8	OLC	A	612	-	19,19,24	0.49	0	20,20,25	0.78	1 (5%)
8	OLC	C	101	-	24,24,24	0.49	0	25,25,25	0.77	0
8	OLC	B	202	-	24,24,24	0.63	1 (4%)	25,25,25	0.76	0
8	OLC	C	102	-	24,24,24	0.57	0	25,25,25	0.59	0
8	OLC	B	204	-	24,24,24	0.49	0	25,25,25	0.68	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
8	OLC	A	607	-	-	11/19/19/24	-
8	OLC	A	608	-	-	7/17/17/24	-
8	OLC	A	614	-	-	11/20/20/24	-
8	OLC	A	613	-	-	16/24/24/24	-
8	OLC	A	606	-	-	12/22/22/24	-
8	OLC	A	610	-	-	2/6/6/24	-
8	OLC	A	615	-	-	11/24/24/24	-
5	HEM	A	602	1	-	0/6/54/54	-
8	OLC	A	605	-	-	11/24/24/24	-
8	OLC	A	611	-	-	7/14/14/24	-
8	OLC	A	609	-	-	5/16/16/24	-
8	OLC	B	203	-	-	13/24/24/24	-
6	HAS	A	603	1,7	-	1/35/122/122	-
8	OLC	A	612	-	-	8/19/19/24	-
8	OLC	C	101	-	-	12/24/24/24	-
8	OLC	B	202	-	-	15/24/24/24	-
8	OLC	C	102	-	-	16/24/24/24	-
8	OLC	B	204	-	-	8/24/24/24	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHD-C4A	-18.50	1.32	1.51
6	A	603	HAS	CHC-C4B	-11.40	1.33	1.53
6	A	603	HAS	C4B-NB	-10.82	1.34	1.49
6	A	603	HAS	C1B-NB	-10.73	1.35	1.49
6	A	603	HAS	C1A-C2A	9.33	1.50	1.38

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CHB-C1B-NB	11.76	125.56	110.94
6	A	603	HAS	CHB-C1D-ND	8.00	120.88	110.94
6	A	603	HAS	CHC-C4B-NB	7.23	124.38	110.75
6	A	603	HAS	CHD-C4A-C3A	-5.83	119.78	129.53
6	A	603	HAS	CHA-C4D-ND	5.77	121.62	110.75

There are no chirality outliers.

5 of 166 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	614	OLC	C21-C22-C24-O25
8	A	614	OLC	O20-C21-C22-C24
8	A	614	OLC	O20-C21-C22-O23
8	A	606	OLC	C21-C22-C24-O25
8	A	606	OLC	O23-C22-C24-O25

There are no ring outliers.

15 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	607	OLC	2	0
8	A	614	OLC	1	0
8	A	613	OLC	6	0
8	A	606	OLC	5	0
8	A	610	OLC	2	0
8	A	615	OLC	2	0
5	A	602	HEM	6	0
8	A	605	OLC	2	0
8	A	611	OLC	6	0
8	B	203	OLC	4	0
6	A	603	HAS	1	0
8	A	612	OLC	1	0
8	C	101	OLC	4	0

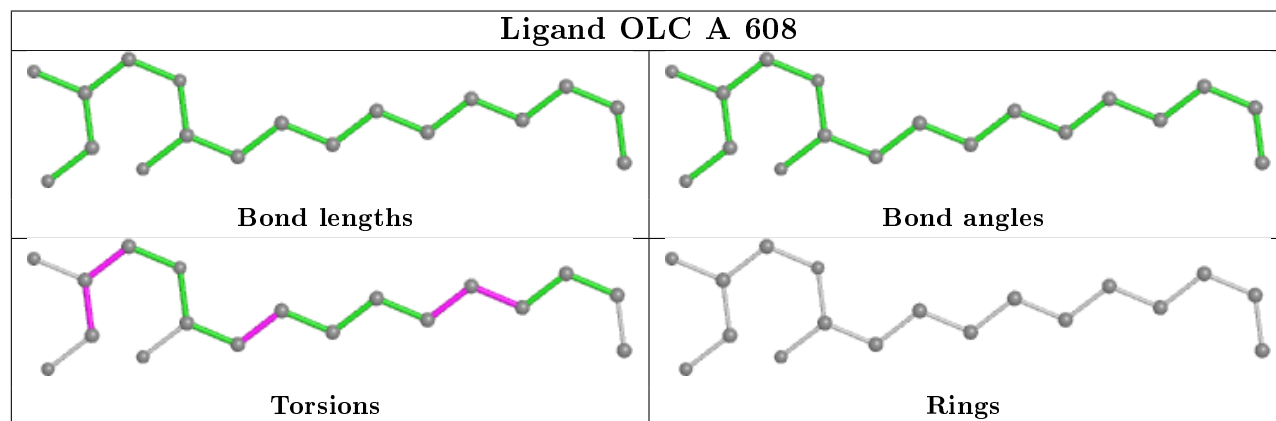
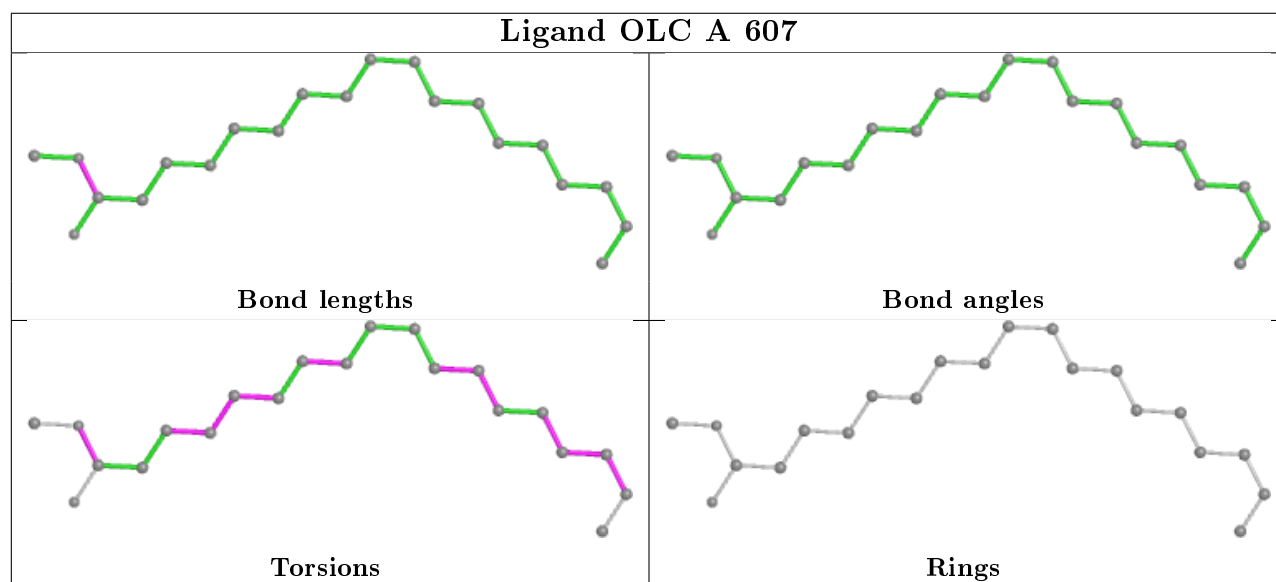
*Continued on next page...*

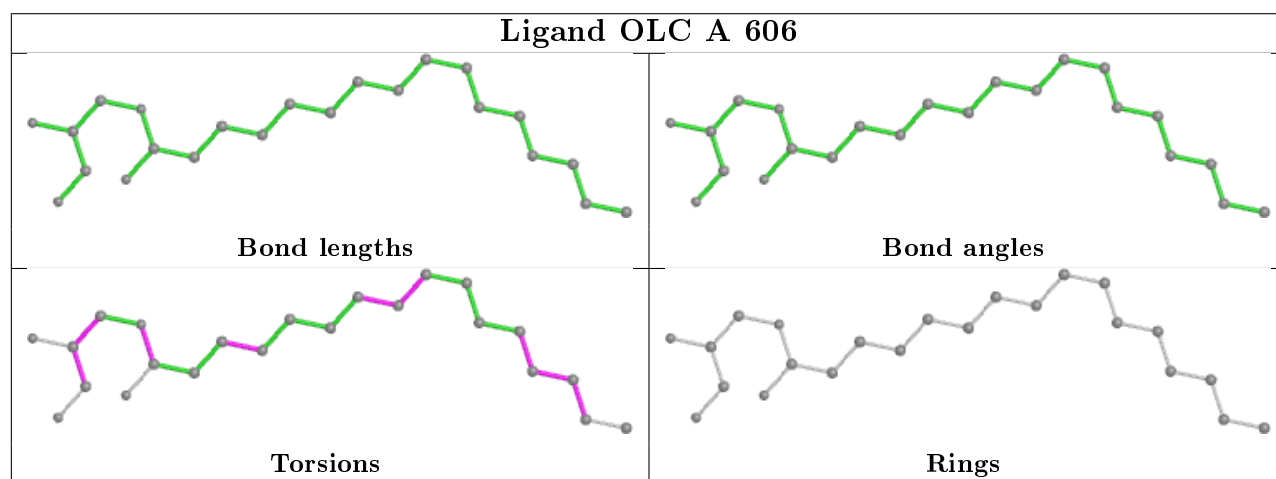
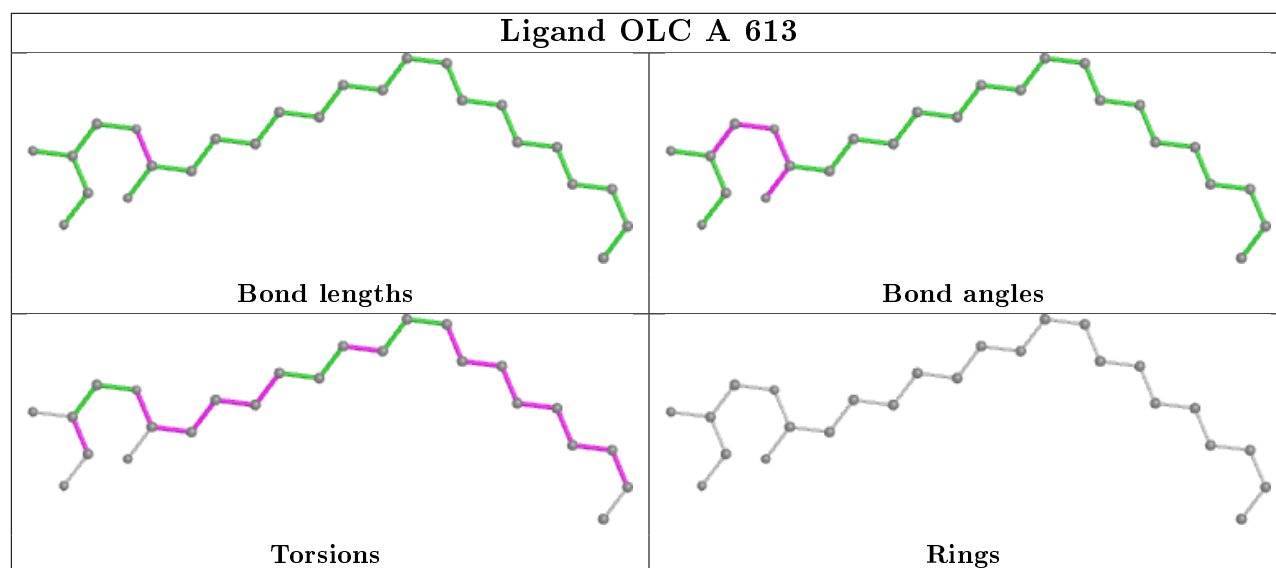
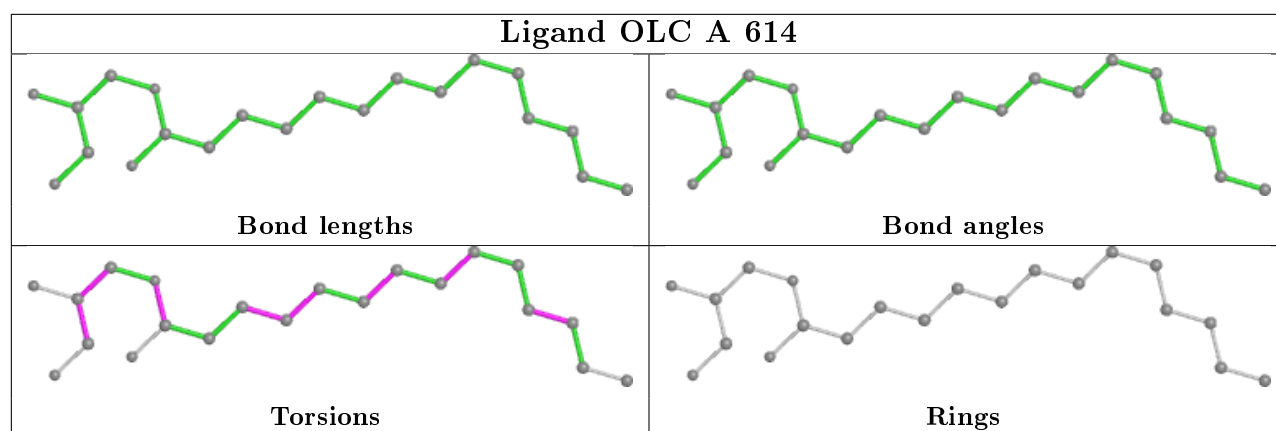


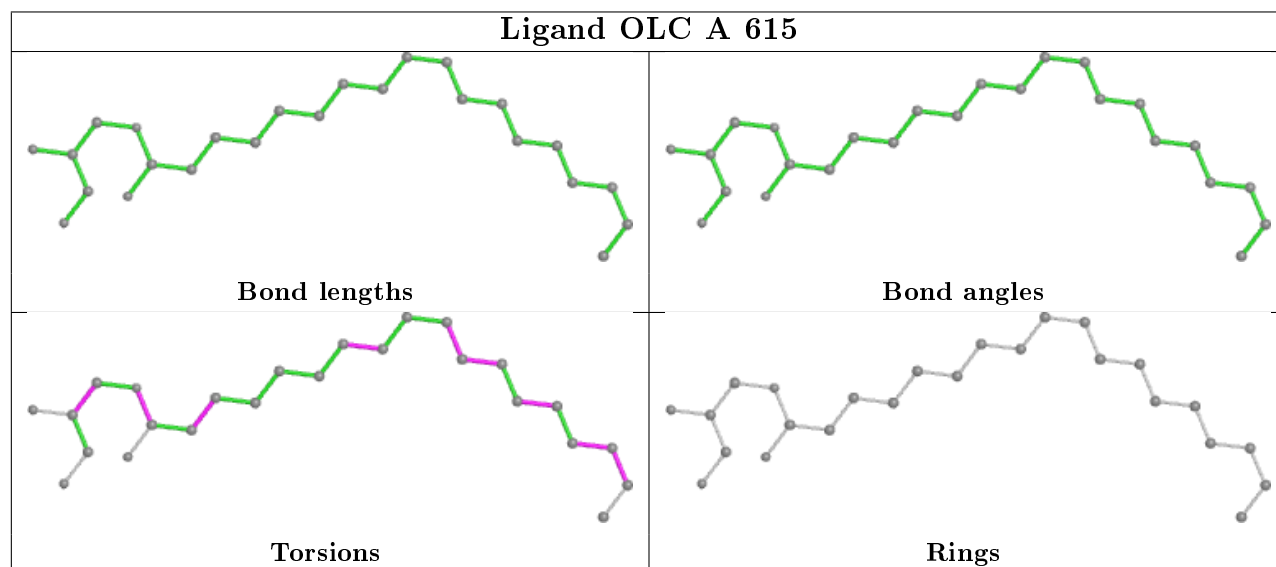
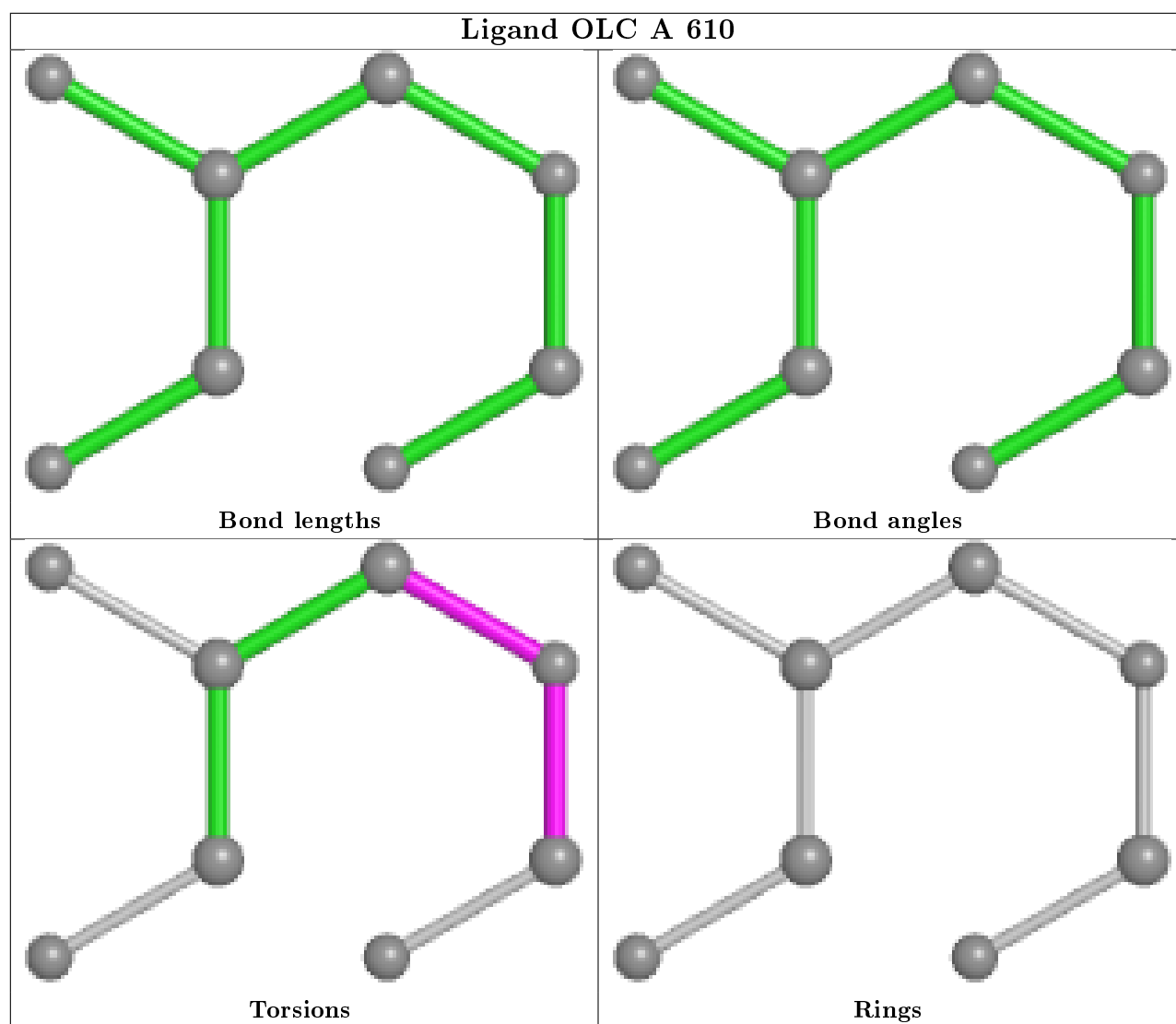
*Continued from previous page...*

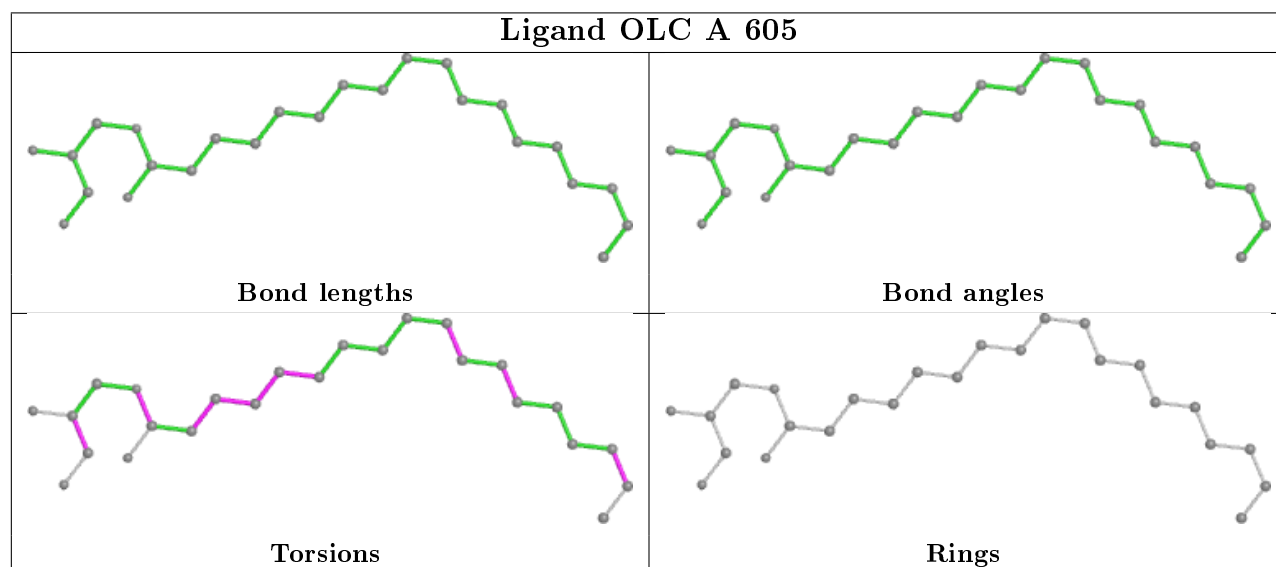
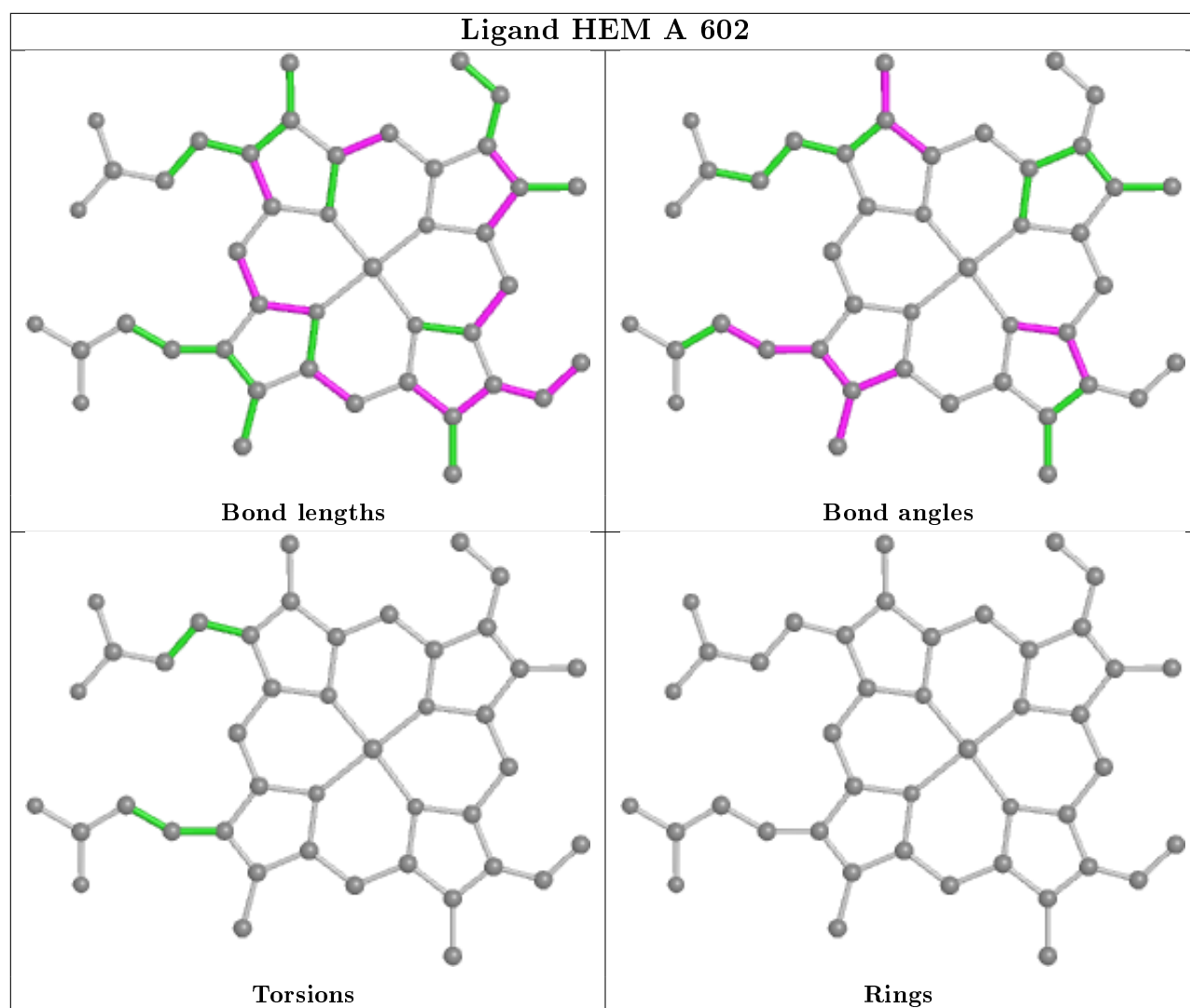
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	202	OLC	4	0
8	C	102	OLC	2	0

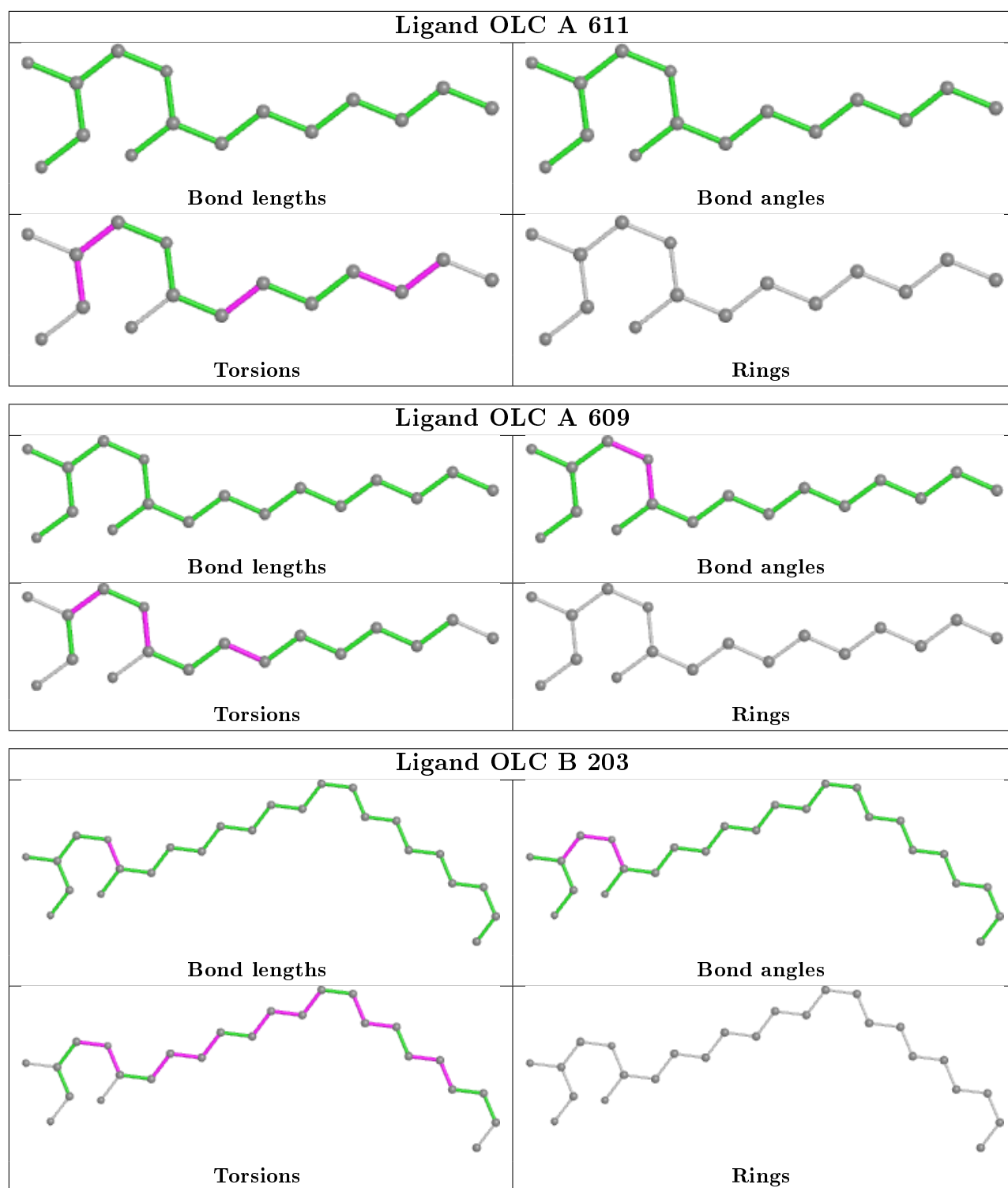
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

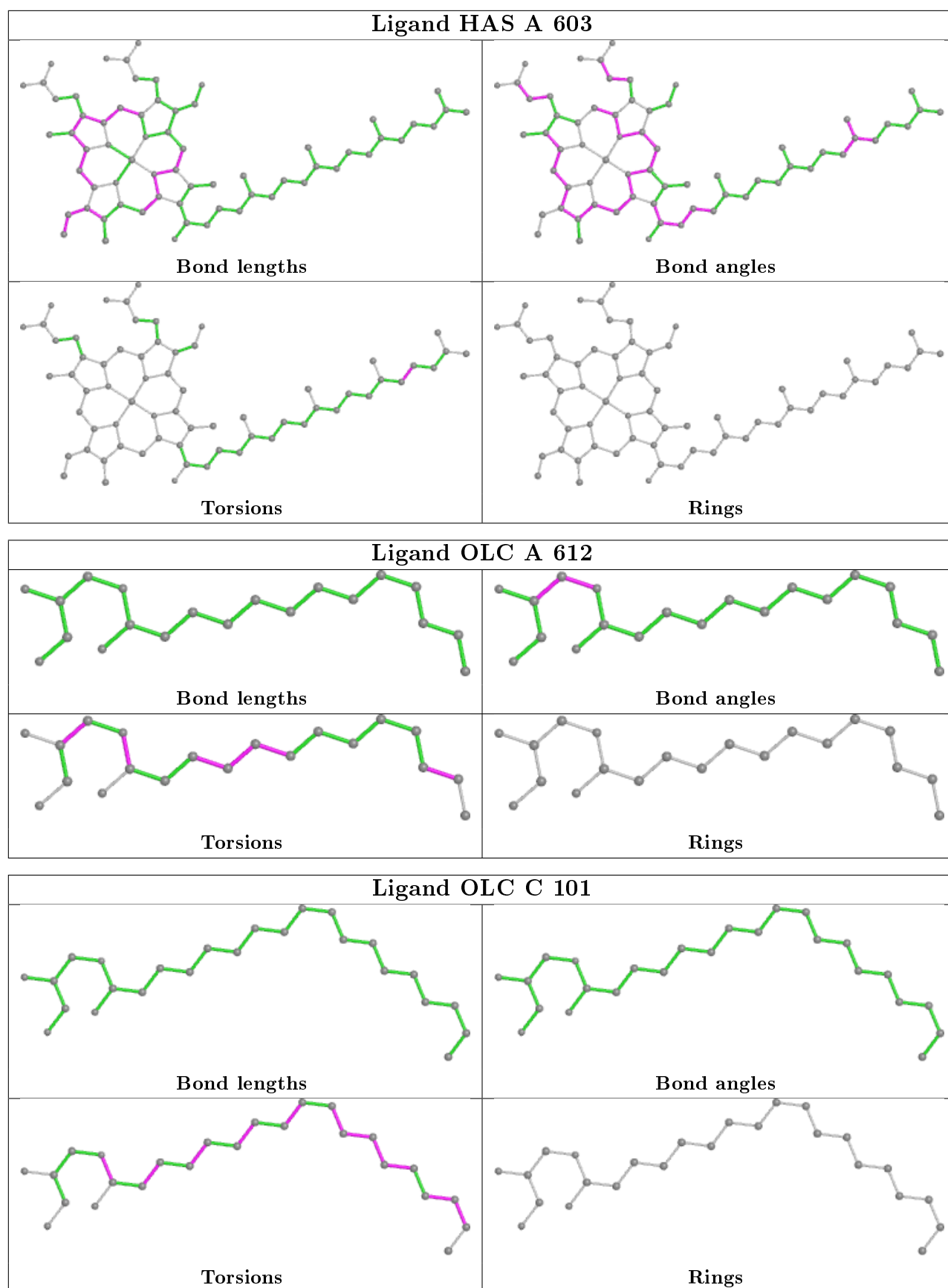


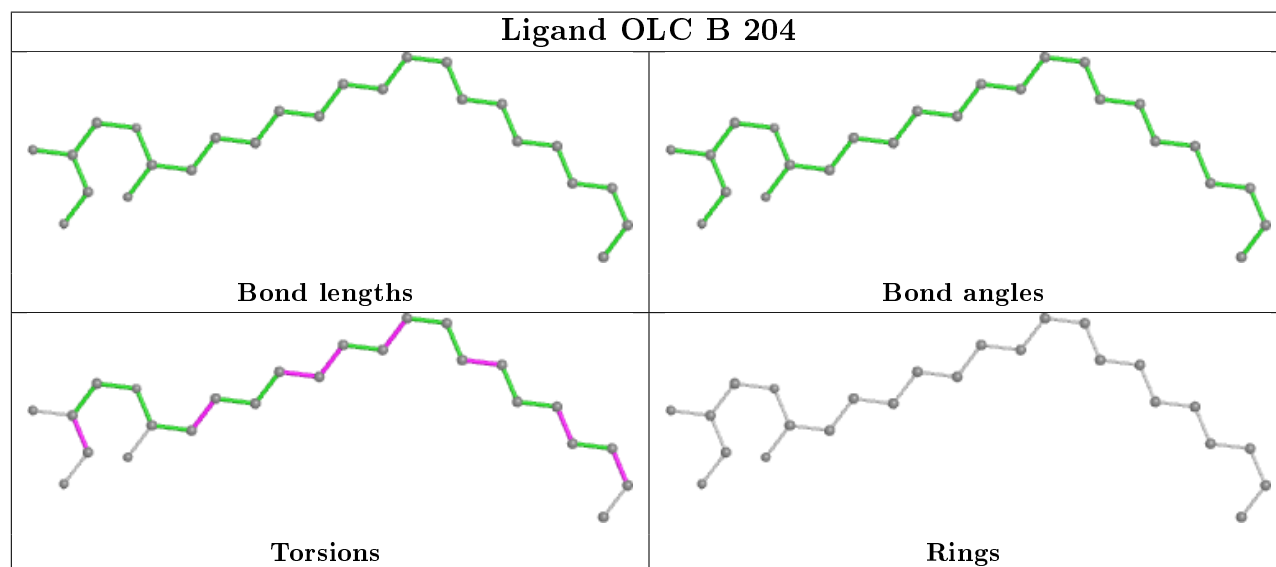
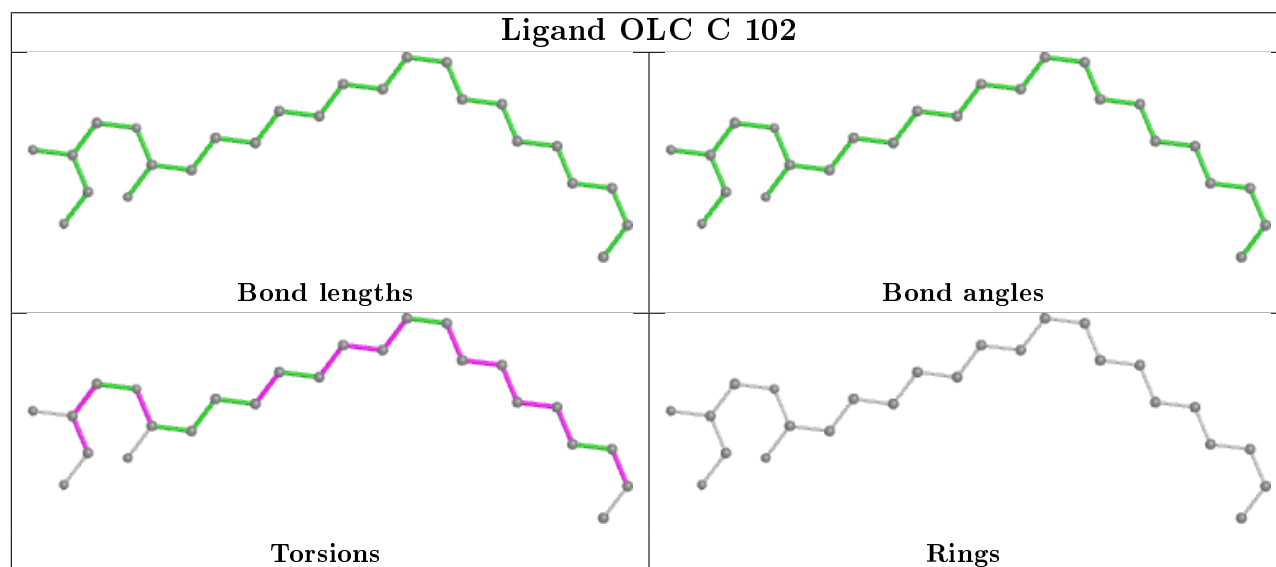
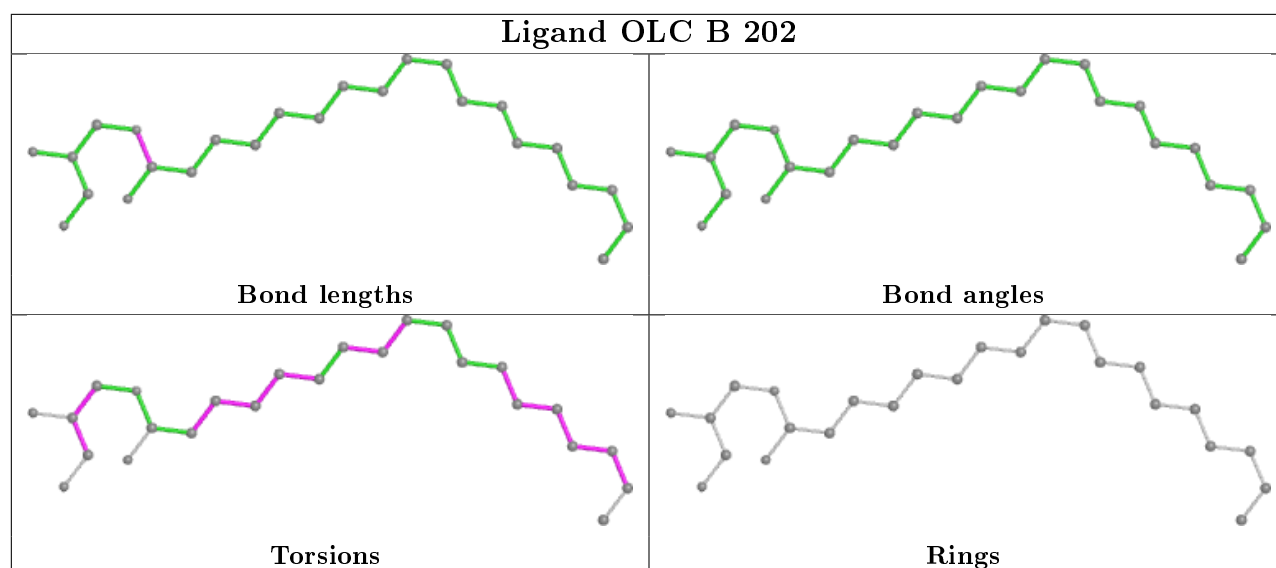












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	551/568 (97%)	-0.34	17 (3%) 49 44	14, 26, 50, 80	0
2	B	166/168 (98%)	-0.18	4 (2%) 59 56	16, 27, 41, 65	0
3	C	31/34 (91%)	-0.60	0 100 100	19, 25, 38, 44	0
All	All	748/770 (97%)	-0.31	21 (2%) 53 49	14, 26, 46, 80	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	GLU	5.0
1	A	495	ARG	4.5
1	A	494	SER	4.2
2	B	4	GLU	4.2
1	A	493	LEU	4.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

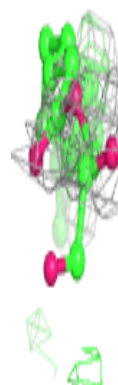
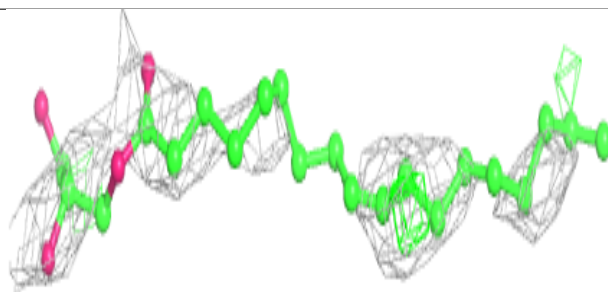
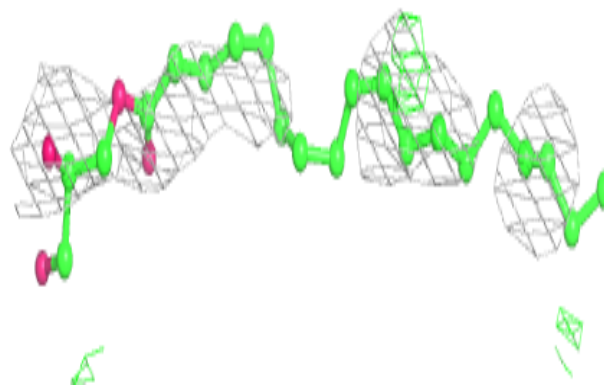
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	OLC	C	102	25/25	0.61	0.44	82,91,98,98	0
8	OLC	A	609	17/25	0.64	0.39	61,66,77,80	0
8	OLC	B	203	25/25	0.71	0.30	52,67,78,79	0
8	OLC	A	614	21/25	0.71	0.36	57,63,78,78	0
8	OLC	A	613	25/25	0.75	0.35	54,58,61,62	0
8	OLC	A	605	25/25	0.78	0.35	60,68,81,81	0
8	OLC	A	612	20/25	0.78	0.34	60,62,70,72	0
8	OLC	C	101	25/25	0.78	0.33	54,56,77,78	0
8	OLC	A	611	15/25	0.78	0.53	51,68,81,81	0
8	OLC	A	608	18/25	0.79	0.32	47,60,71,71	0
8	OLC	B	204	25/25	0.81	0.27	61,69,72,76	0
8	OLC	A	607	21/25	0.82	0.27	49,55,70,70	0
8	OLC	A	615	25/25	0.82	0.33	57,60,68,69	0
8	OLC	B	202	25/25	0.83	0.26	57,59,62,63	0
8	OLC	A	606	23/25	0.87	0.25	35,41,46,47	0
8	OLC	A	610	8/25	0.91	0.32	55,56,59,60	0
5	HEM	A	602	43/43	0.97	0.12	7,14,17,20	0
6	HAS	A	603	65/65	0.98	0.14	13,19,23,29	0
4	CU	A	601	1/1	1.00	0.07	20,20,20,20	0
9	CUA	B	201	2/2	1.00	0.05	19,19,19,19	0
7	PEO	A	604	2/2	1.00	0.12	18,18,18,19	0

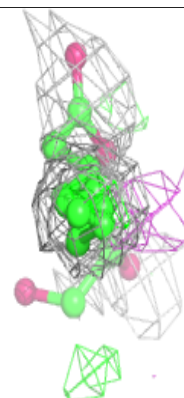
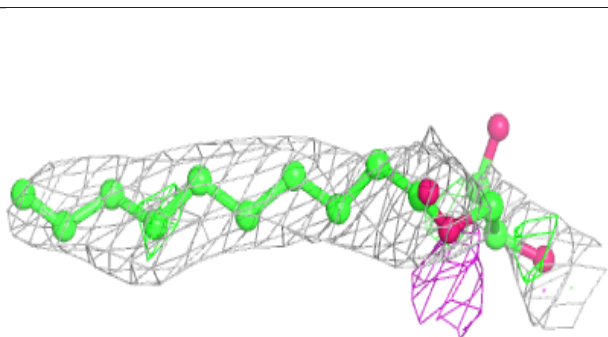
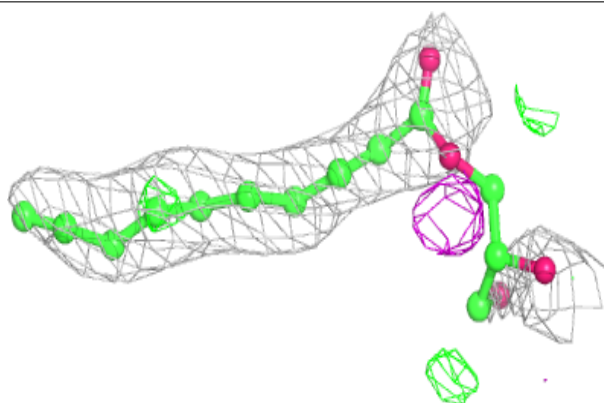
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC C 102:**

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

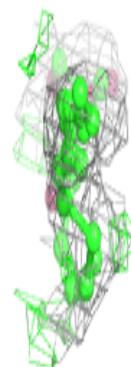
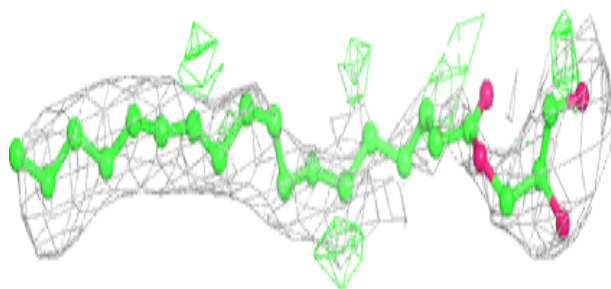
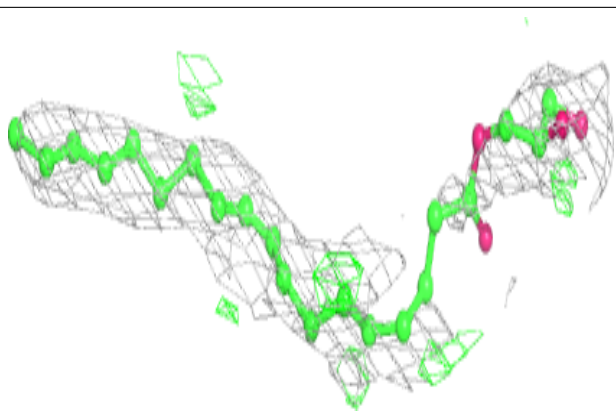
**Electron density around OLC A 609:**

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

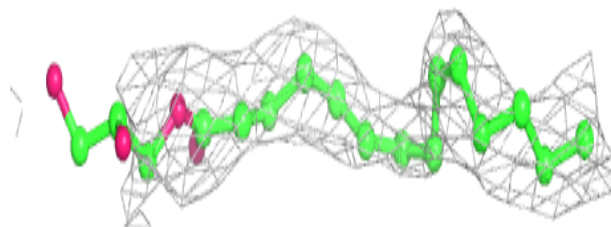
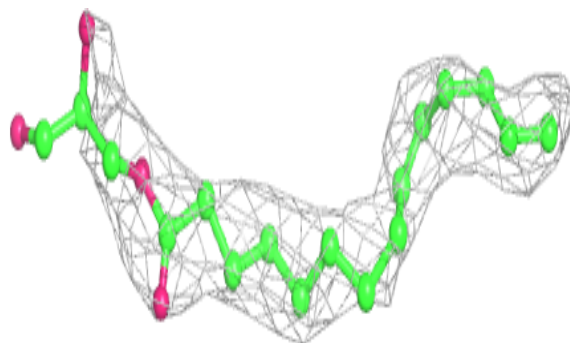


**Electron density around OLC B 203:**

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

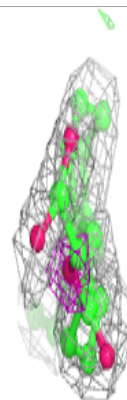
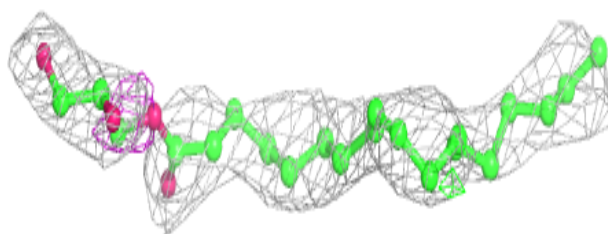
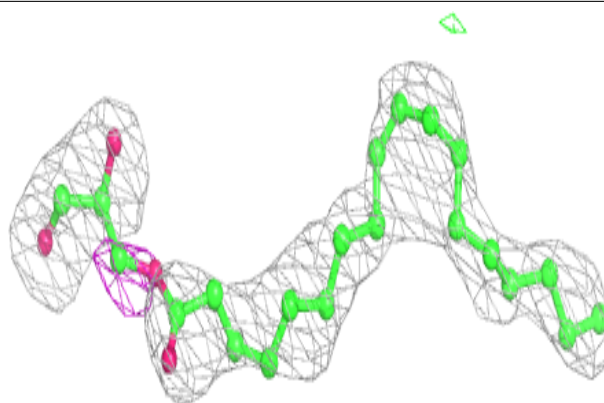
**Electron density around OLC A 614:**

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

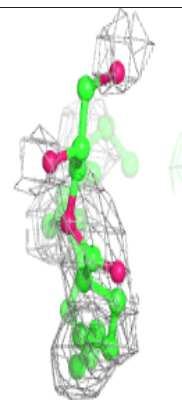
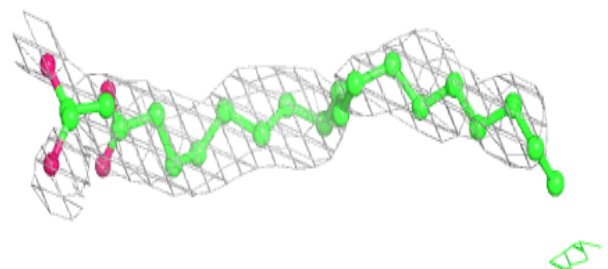
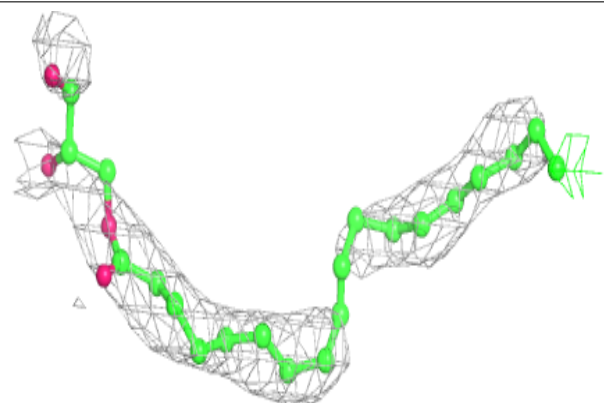


**Electron density around OLC A 613:**

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

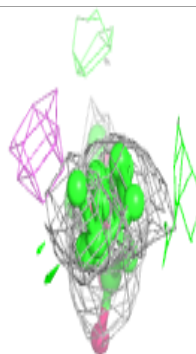
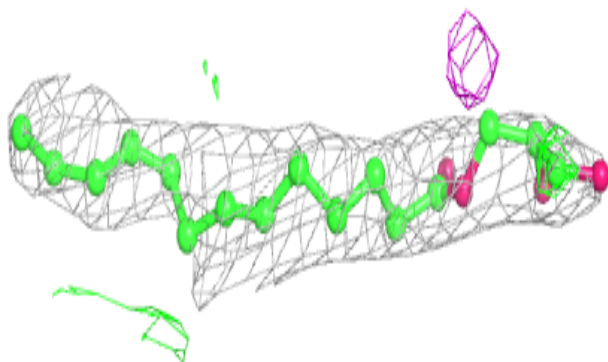
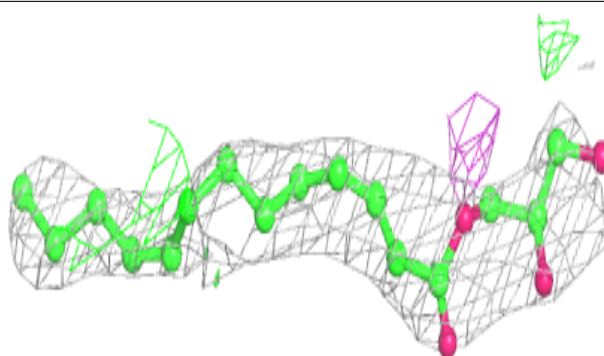
**Electron density around OLC A 605:**

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

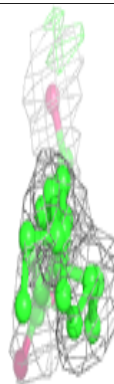
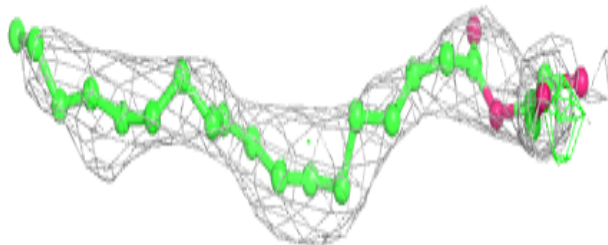
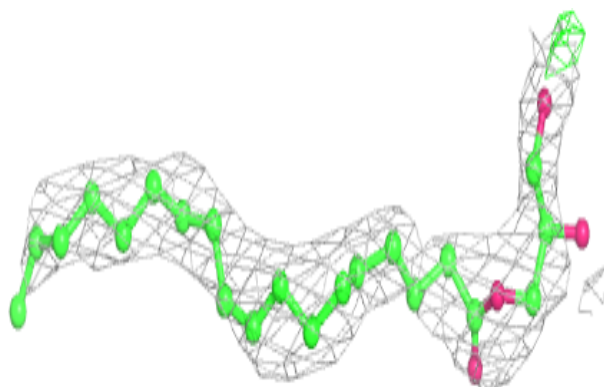


**Electron density around OLC A 612:**

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

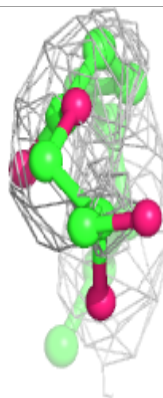
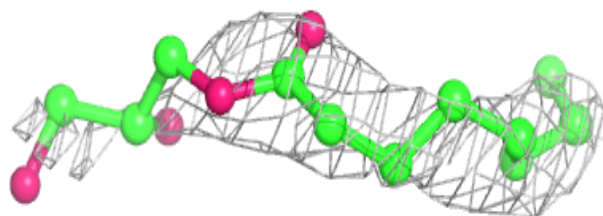
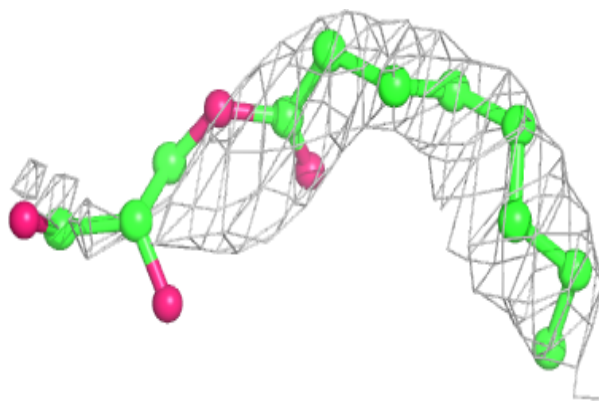
**Electron density around OLC C 101:**

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

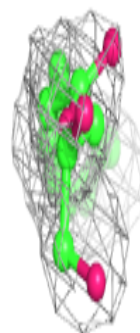
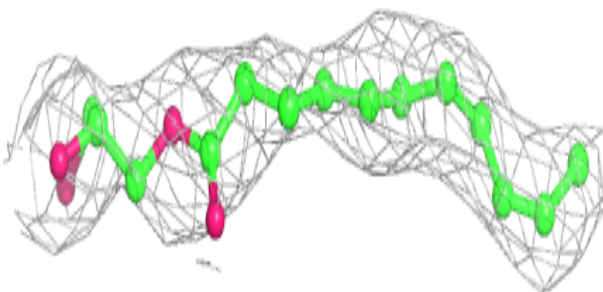
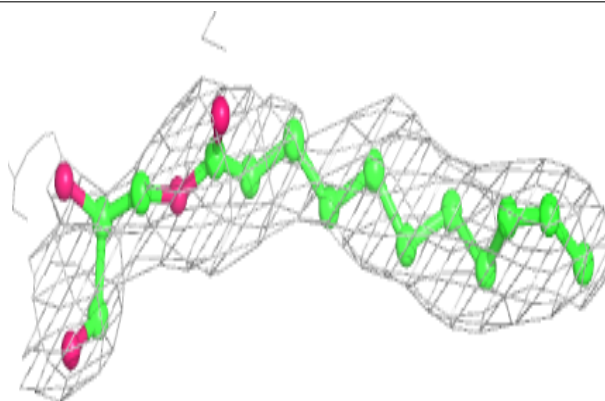


**Electron density around OLC A 611:**

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

**Electron density around OLC A 608:**

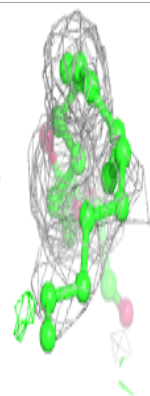
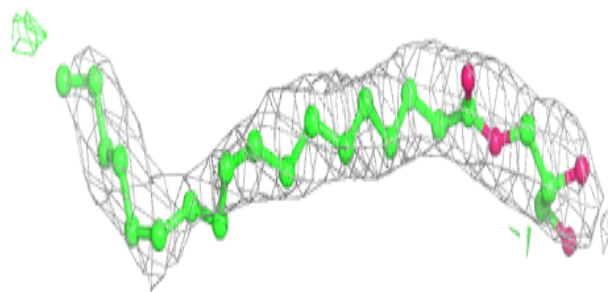
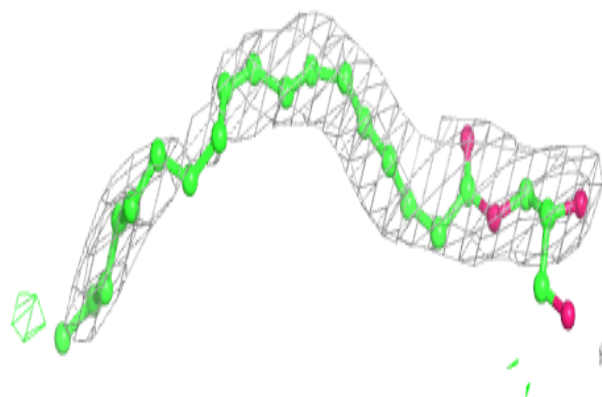
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



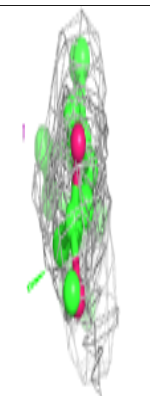
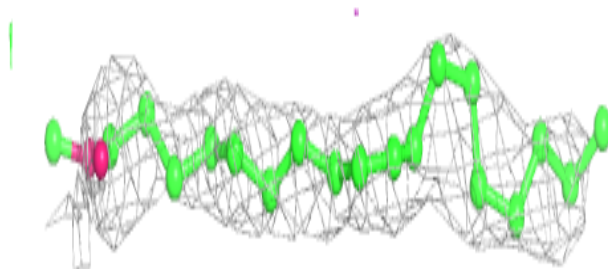
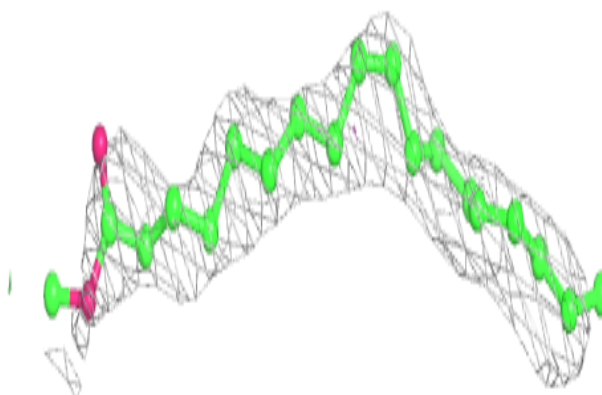


**Electron density around OLC B 204:**

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

**Electron density around OLC A 607:**

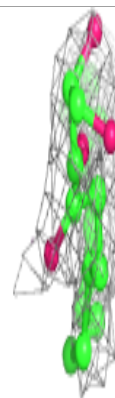
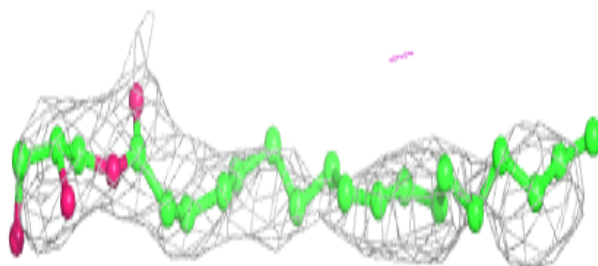
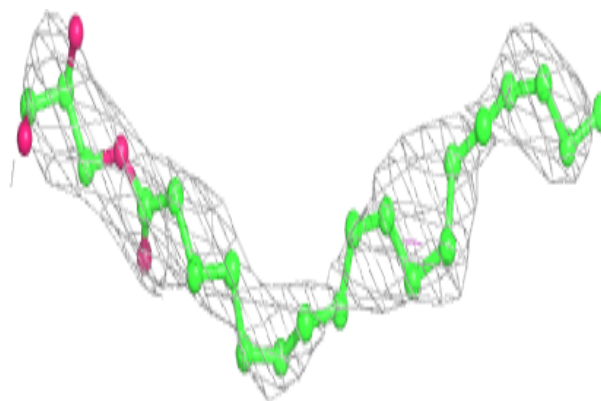
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



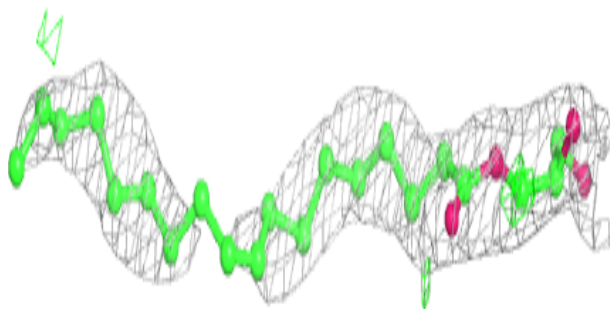
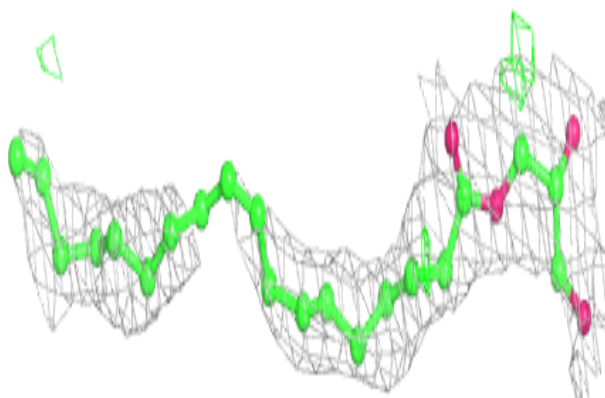


**Electron density around OLC A 615:**

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

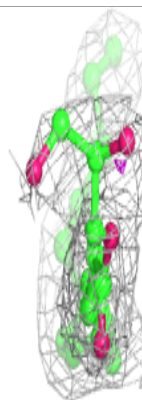
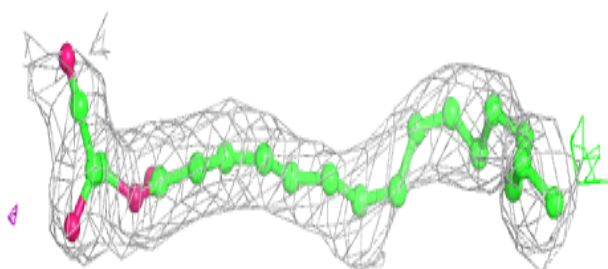
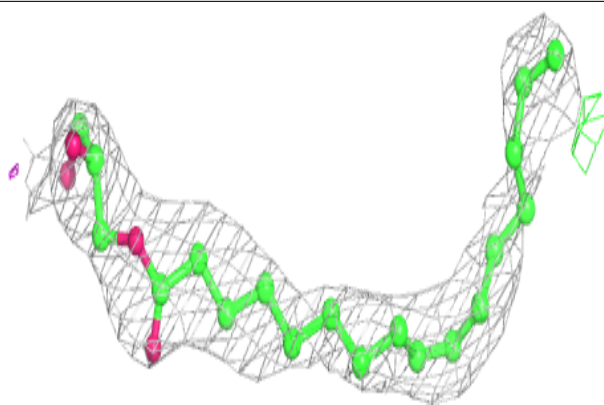
**Electron density around OLC B 202:**

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

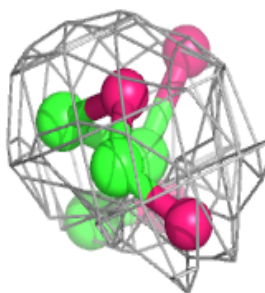
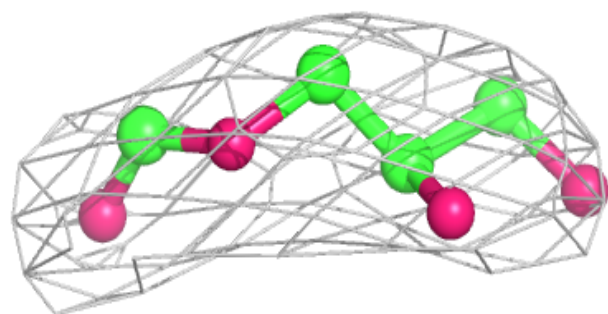
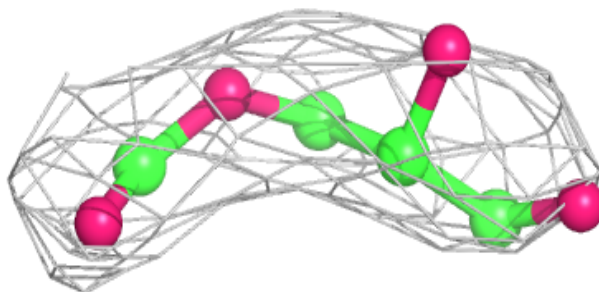


**Electron density around OLC A 606:**

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

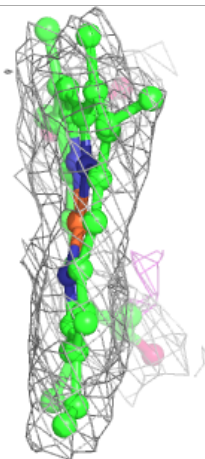
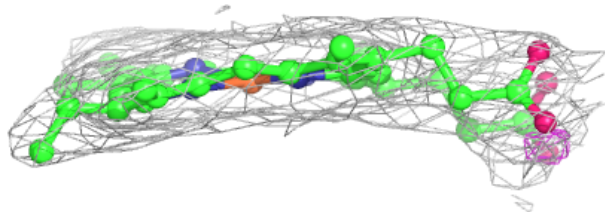
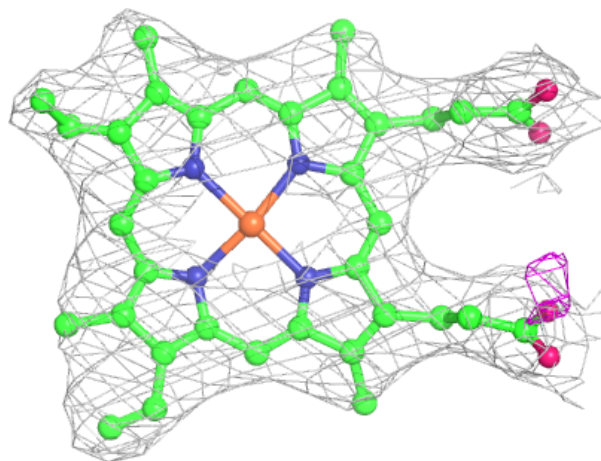
**Electron density around OLC A 610:**

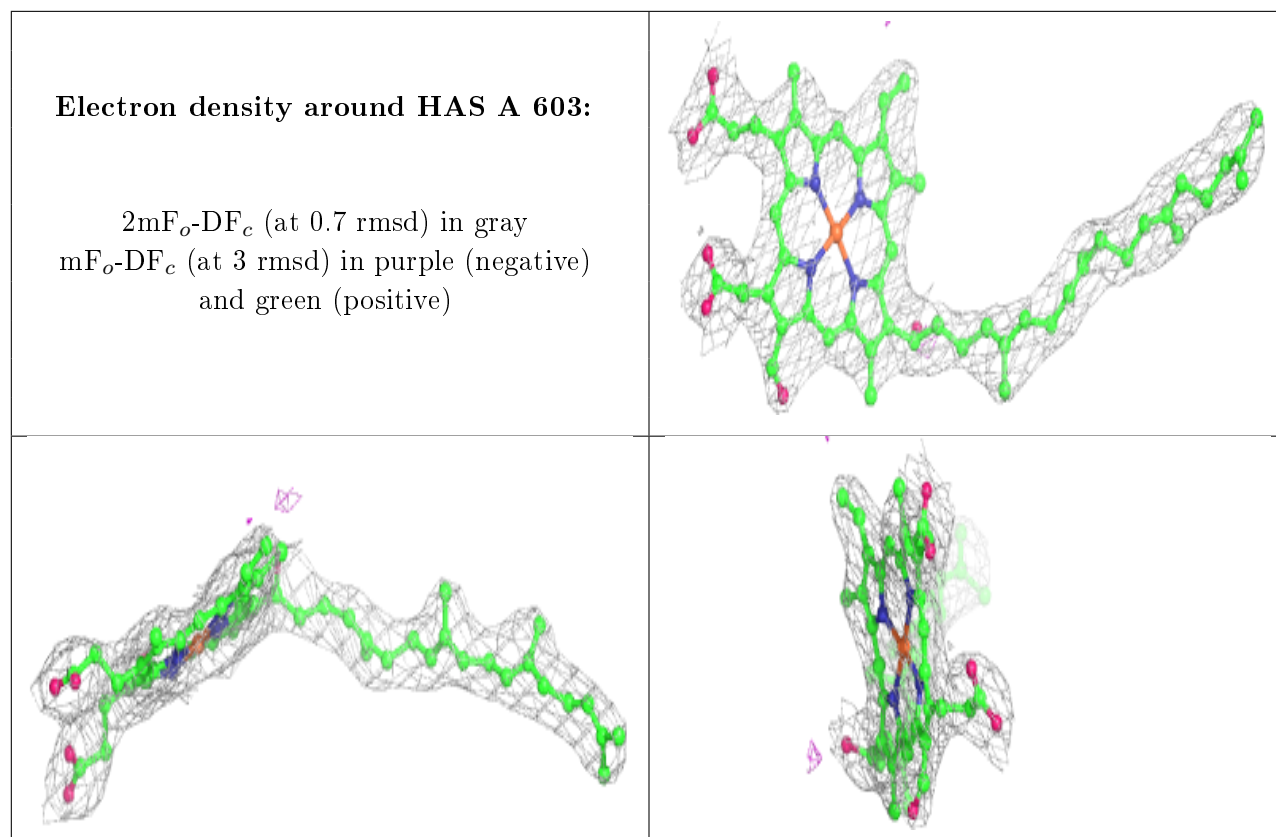
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.