



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:12 AM UTC

PDB ID : 9VDJ / pdb\_00009vdj  
Title : Serial synchrotron crystallography structure of a ba3-type cytochrome c oxidase using a goniometer-compatible chip-based platform  
Authors : Kabbinala, A.; Branden, G.; Neutze, R.; Ghosh, S.  
Deposited on : 2025-06-08  
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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

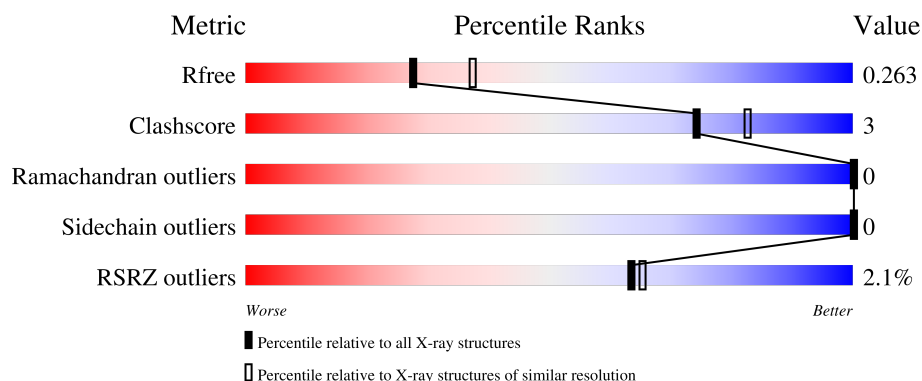
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

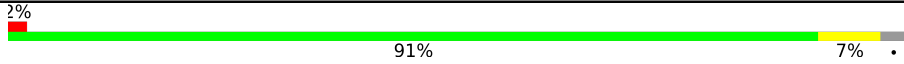
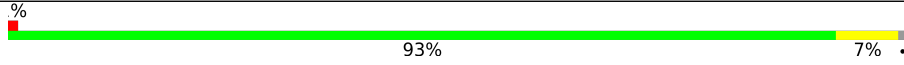

The reported resolution of this entry is 2.30 Å.

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))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of 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	569	
2	B	168	
3	C	34	

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
6	HAS	A	603	X	-	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6426 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	554	Total	C	N	O	S	0	0	0
			4367	2963	698	690	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q5SJ79
A	-5	HIS	-	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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1300	846	216	234	4			

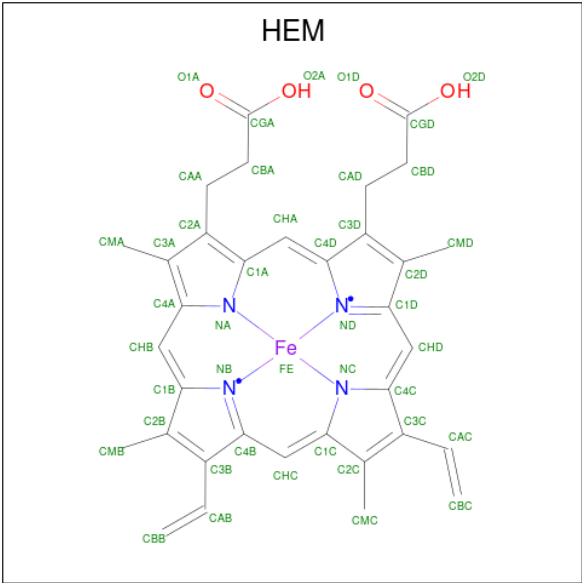
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			240	169	37	34			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

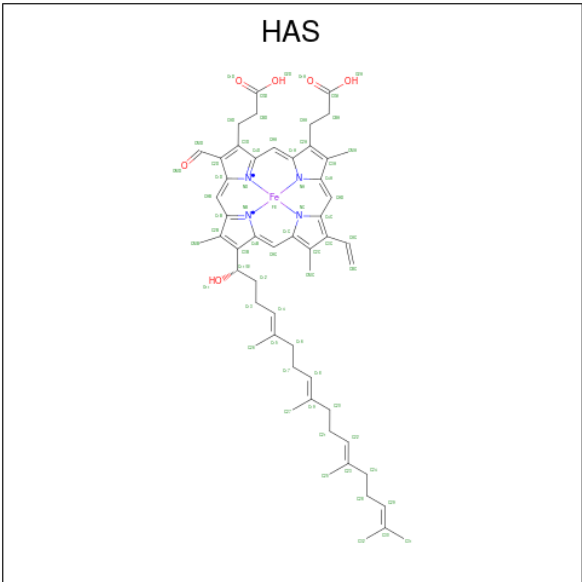
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Cu			0	0
			1	1				

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



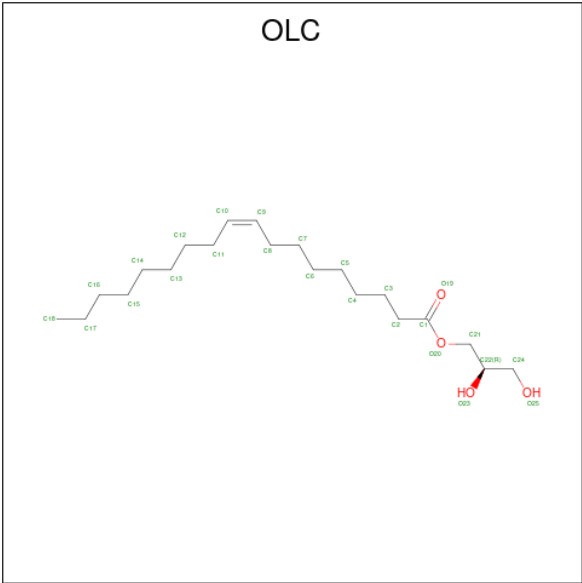
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 6 is HEME-AS (CCD ID: HAS) (formula:  $C_{54}H_{64}FeN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



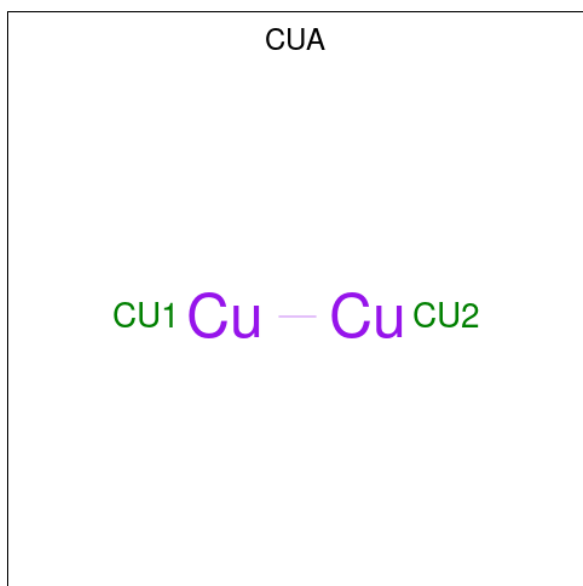
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			23	19	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			17	13	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			20	16	4		
7	A	1	Total	C	O	0	0
			21	17	4		
7	A	1	Total	C		0	0
			9	9			
7	A	1	Total	C		0	0
			9	9			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			24	20	4		
7	B	1	Total	C	O	0	0
			20	18	2		
7	B	1	Total	C	O	0	0
			25	21	4		
7	B	1	Total	C	O	0	0
			24	20	4		
7	C	1	Total	C	O	0	0
			15	11	4		

- Molecule 8 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



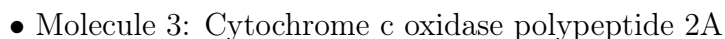
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cu	0	0
			2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	74	Total	O	0	0
			74	74		
9	B	59	Total	O	0	0
			59	59		
9	C	2	Total	O	0	0
			2	2		



- Molecule 1: Cytochrome c oxidase subunit 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.85Å 100.32Å 96.62Å 90.00° 126.76° 90.00°	Depositor
Resolution (Å)	32.15 – 2.30 32.15 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (32.15-2.30) 100.0 (32.15-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 1.47Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.209 , 0.264 0.207 , 0.263	Depositor DCC
$R_{free}$ test set	7692 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 92.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: CU, OLC, HEM, CUA, HAS

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	0.40	0/4524	0.58	0/6213
2	B	0.39	0/1337	0.58	0/1828
3	C	0.33	0/246	0.52	0/335
All	All	0.40	0/6107	0.57	0/8376

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	4367	0	4468	31	0
2	B	1300	0	1278	8	0
3	C	240	0	267	1	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
6	A	65	0	62	0	0
7	A	189	0	264	1	0
7	B	69	0	103	2	0
7	C	15	0	19	0	0
8	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	74	0	0	3	0
9	B	59	0	0	1	0
9	C	2	0	0	0	0
All	All	6426	0	6491	39	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 (39) 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	1.67	0.91
1:A:100:ARG:HD2	9:A:704:HOH:O	1.81	0.79
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.53	0.74
1:A:177:LYS:HE3	1:A:178:VAL:H	1.56	0.69
1:A:15:TYR:HA	9:A:704:HOH:O	2.00	0.61
5:A:602:HEM:HBC2	5:A:602:HEM:HMC1	1.84	0.59
2:B:17:GLY:HA3	7:B:204:OLC:H3A	1.85	0.58
1:A:516:GLU:HG2	1:A:520:LEU:HD11	1.88	0.56
1:A:302:THR:O	1:A:305:VAL:HG12	2.06	0.56
1:A:332:LEU:HD23	1:A:333:PHE:HE2	1.70	0.55
1:A:411:LYS:HZ1	1:A:494:SER:C	2.16	0.53
2:B:138:THR:O	2:B:140:LYS:NZ	2.38	0.52
2:B:144:GLU:HG2	2:B:165:VAL:HG22	1.92	0.51
1:A:314:PHE:HE2	3:C:9:LEU:HD23	1.77	0.49
1:A:421:GLY:O	1:A:425:VAL:HG13	2.13	0.48
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.48	0.47
1:A:128:GLU:HB3	1:A:142:HIS:HB2	1.97	0.47
2:B:105:PHE:O	2:B:134:THR:HA	2.13	0.47
2:B:32:LEU:HD21	7:B:203:OLC:H7A	1.96	0.47
1:A:233:HIS:CE1	1:A:237:TYR:HE2	2.30	0.47
2:B:106:LYS:HB3	2:B:106:LYS:HE3	1.54	0.47
1:A:233:HIS:CE1	1:A:237:TYR:CE2	3.02	0.47
1:A:398:MET:O	1:A:401:LEU:HB2	2.15	0.46
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.97	0.45
1:A:233:HIS:CD2	1:A:237:TYR:HE2	2.34	0.45
2:B:51:GLU:OE2	9:B:301:HOH:O	2.21	0.45
1:A:253:LYS:HD2	1:A:509:ALA:HA	2.00	0.44
1:A:362:GLY:HA3	9:A:753:HOH:O	2.19	0.43
1:A:100:ARG:N	1:A:100:ARG:HD3	2.33	0.42
1:A:254:GLN:HE22	1:A:403:TRP:CD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:VAL:HG12	1:A:512:ILE:O	2.20	0.42
1:A:562:TRP:HA	2:B:155:LEU:HG	2.02	0.42
1:A:385:PHE:O	1:A:389:VAL:HG12	2.20	0.42
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.85	0.41
1:A:69:LEU:HD11	5:A:602:HEM:HBD2	2.01	0.41
1:A:216:VAL:HG12	7:A:610:OLC:H24A	2.03	0.41
1:A:177:LYS:HD2	1:A:177:LYS:HA	1.77	0.41
1:A:217:GLU:OE2	1:A:217:GLU:HA	2.20	0.40
1:A:282:HIS:CD2	1:A:283:HIS:CD2	3.10	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	552/569 (97%)	536 (97%)	16 (3%)	0	100	100
2	B	165/168 (98%)	161 (98%)	4 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	746/771 (97%)	726 (97%)	20 (3%)	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	447/463 (96%)	447 (100%)	0	100	100
2	B	136/138 (99%)	136 (100%)	0	100	100
3	C	24/27 (89%)	24 (100%)	0	100	100
All	All	607/628 (97%)	607 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	159	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\# Z  > 2$
7	OLC	A	614	-	23,23,24	0.21	0	24,24,25	0.28	0
7	OLC	B	201	-	19,19,24	0.25	0	19,19,25	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	OLC	A	606	-	16,16,24	0.27	0	17,17,25	0.30	0
8	CUA	B	202	2	0,1,1	-	-	-		
7	OLC	A	612	-	8,8,24	0.13	0	7,7,25	0.13	0
5	HEM	A	602	1	50,50,50	1.61	9 (18%)	67,82,82	1.93	14 (20%)
6	HAS	A	603	1	72,72,72	2.40	28 (38%)	87,109,109	2.46	36 (41%)
7	OLC	B	204	-	23,23,24	0.24	0	24,24,25	0.31	0
7	OLC	A	605	-	17,17,24	0.26	0	18,18,25	0.31	0
7	OLC	A	608	-	17,17,24	0.24	0	18,18,25	0.31	0
7	OLC	A	613	-	8,8,24	0.14	0	7,7,25	0.25	0
7	OLC	C	101	-	14,14,24	0.26	0	15,15,25	0.36	0
7	OLC	A	610	-	19,19,24	0.25	0	20,20,25	0.39	0
7	OLC	A	607	-	14,14,24	0.21	0	15,15,25	0.31	0
7	OLC	A	611	-	20,20,24	0.25	0	21,21,25	0.38	0
7	OLC	B	203	-	24,24,24	0.20	0	25,25,25	0.33	0
7	OLC	A	609	-	14,14,24	0.23	0	15,15,25	0.30	0
7	OLC	A	604	-	22,22,24	0.23	0	23,23,25	0.33	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
7	OLC	A	614	-	-	2/23/23/24	-
7	OLC	B	201	-	-	3/18/18/24	-
7	OLC	A	606	-	-	2/16/16/24	-
7	OLC	A	612	-	-	0/6/6/24	-
5	HEM	A	602	1	-	3/14/54/54	-
6	HAS	A	603	1	1/1/8/18	7/42/82/82	-
7	OLC	B	204	-	-	6/23/23/24	-
7	OLC	A	605	-	-	3/17/17/24	-
7	OLC	A	608	-	-	2/17/17/24	-
7	OLC	A	613	-	-	1/6/6/24	-
7	OLC	C	101	-	-	5/14/14/24	-
7	OLC	A	610	-	-	2/19/19/24	-
7	OLC	A	607	-	-	2/14/14/24	-
7	OLC	A	611	-	-	4/20/20/24	-
7	OLC	B	203	-	-	2/24/24/24	-
7	OLC	A	609	-	-	4/14/14/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	A	604	-	-	2/22/22/24	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	FE-NB	5.65	2.12	1.94
6	A	603	HAS	FE-ND	5.36	2.11	1.94
6	A	603	HAS	C3B-C2B	5.31	1.46	1.34
5	A	602	HEM	FE-NB	5.24	2.11	1.94
6	A	603	HAS	CHD-C4A	5.14	1.48	1.38
6	A	603	HAS	C2A-C3A	4.90	1.47	1.36
6	A	603	HAS	FE-NC	4.75	2.10	1.95
6	A	603	HAS	FE-NA	4.68	2.10	1.95
6	A	603	HAS	CHB-C1D	4.36	1.47	1.38
6	A	603	HAS	CHA-C1A	4.26	1.46	1.38
6	A	603	HAS	CHC-C4B	4.17	1.46	1.38
6	A	603	HAS	CHC-C1C	3.87	1.48	1.39
5	A	602	HEM	FE-NC	3.78	2.07	1.95
6	A	603	HAS	CHB-C1B	3.74	1.47	1.39
6	A	603	HAS	CHA-C4D	3.55	1.47	1.39
6	A	603	HAS	C2D-C3D	3.44	1.45	1.37
6	A	603	HAS	CHD-C4C	3.31	1.46	1.39
5	A	602	HEM	C1B-NB	-3.18	1.34	1.40
6	A	603	HAS	C1D-ND	-3.13	1.34	1.40
5	A	602	HEM	C4D-ND	-3.06	1.34	1.40
6	A	603	HAS	C4D-C3D	2.92	1.50	1.45
6	A	603	HAS	C4B-NB	-2.89	1.35	1.40
6	A	603	HAS	C11-C3B	-2.74	1.48	1.51
6	A	603	HAS	C1C-C2C	2.62	1.49	1.43
6	A	603	HAS	C4A-NA	-2.49	1.34	1.39
6	A	603	HAS	C4C-NC	-2.47	1.35	1.39
5	A	602	HEM	C3C-C4C	-2.45	1.41	1.46
6	A	603	HAS	C4B-C3B	2.43	1.49	1.44
5	A	602	HEM	FE-ND	-2.36	1.87	1.94
5	A	602	HEM	FE-NA	2.31	2.02	1.95
6	A	603	HAS	C1A-NA	-2.27	1.35	1.39
6	A	603	HAS	C1B-NB	-2.25	1.34	1.38
5	A	602	HEM	C1C-NC	-2.12	1.35	1.39
6	A	603	HAS	C3C-C2C	2.11	1.48	1.41
5	A	602	HEM	C1C-C2C	-2.10	1.41	1.45
6	A	603	HAS	C1C-NC	-2.08	1.35	1.39
6	A	603	HAS	C3C-C4C	2.07	1.48	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2D-C3D-C4D	-8.16	100.53	106.43
5	A	602	HEM	CHC-C4B-NB	7.31	132.29	124.42
5	A	602	HEM	CHD-C1D-ND	6.05	130.94	124.42
6	A	603	HAS	C2A-C1A-NA	5.70	115.83	110.32
6	A	603	HAS	C2B-C1B-NB	5.67	116.46	109.90
6	A	603	HAS	C3D-C4D-ND	5.51	115.67	110.35
6	A	603	HAS	C3B-C4B-NB	5.45	116.10	109.84
6	A	603	HAS	C3C-C2C-C1C	-5.12	101.13	107.17
6	A	603	HAS	C3C-C4C-NC	4.97	113.98	109.80
6	A	603	HAS	CAD-C3D-C4D	4.14	131.91	124.70
5	A	602	HEM	CHD-C1D-C2D	-3.82	118.99	125.03
6	A	603	HAS	C1B-C2B-C3B	-3.73	102.48	106.80
5	A	602	HEM	C1B-NB-C4B	3.71	109.60	105.21
6	A	603	HAS	C2C-C1C-NC	3.49	115.74	110.14
6	A	603	HAS	C1A-C2A-C3A	-3.49	102.51	107.11
6	A	603	HAS	CAA-CBA-CGA	-3.44	104.55	113.67
5	A	602	HEM	C1A-CHA-C4D	-3.42	118.20	126.25
6	A	603	HAS	OMD-CMD-C2D	-3.31	118.16	125.62
5	A	602	HEM	C3B-C4B-NB	-3.26	107.12	109.47
6	A	603	HAS	CHA-C4D-ND	-3.24	120.94	124.42
6	A	603	HAS	C4B-C3B-C2B	-3.09	102.24	107.44
5	A	602	HEM	C4A-CHB-C1B	-3.04	119.09	126.25
5	A	602	HEM	C4C-NC-C1C	3.02	110.74	105.82
6	A	603	HAS	C27-C19-C20	3.00	120.43	115.23
6	A	603	HAS	C3A-C4A-NA	3.00	115.18	109.64
6	A	603	HAS	CHB-C1B-C2B	-2.88	120.47	125.03
6	A	603	HAS	C4A-C3A-C2A	-2.82	102.79	106.97
6	A	603	HAS	C25-C23-C24	2.76	120.02	115.23
6	A	603	HAS	C17-C18-C19	-2.75	121.33	127.62
6	A	603	HAS	O11-C11-C3B	-2.74	106.24	111.26
5	A	602	HEM	O2D-CGD-O1D	-2.69	116.41	123.33
6	A	603	HAS	C32-C30-C31	2.68	120.76	114.59
6	A	603	HAS	CMA-C3A-C4A	2.59	129.29	124.73
5	A	602	HEM	CHA-C4D-ND	2.54	127.51	124.37
5	A	602	HEM	CHB-C4A-NA	2.53	128.44	123.86
5	A	602	HEM	O2A-CGA-CBA	2.50	121.89	114.00
5	A	602	HEM	CHA-C1A-NA	2.48	128.37	123.86
6	A	603	HAS	CAD-CBD-CGD	-2.45	107.17	113.67
6	A	603	HAS	CMC-C2C-C3C	2.42	132.24	126.55
6	A	603	HAS	CHC-C1C-C2C	-2.36	120.57	127.43
6	A	603	HAS	C4C-C3C-C2C	-2.32	104.42	107.30
6	A	603	HAS	CMB-C2B-C1B	2.31	128.65	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C12-C13-C14	-2.27	106.19	112.16
6	A	603	HAS	CHC-C4B-NB	-2.27	121.56	124.37
5	A	602	HEM	CHC-C4B-C3B	-2.25	120.59	125.07
6	A	603	HAS	O1A-CGA-CBA	-2.21	116.09	123.09
6	A	603	HAS	C21-C22-C23	-2.16	122.67	127.62
6	A	603	HAS	C4B-NB-C1B	-2.13	102.68	105.21
6	A	603	HAS	CHD-C4A-NA	-2.03	122.24	124.45
6	A	603	HAS	CHA-C1A-NA	-2.01	122.27	124.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	HEM	C2B-C3B-CAB-CBB
6	A	603	HAS	C1D-C2D-CMD-OMD
6	A	603	HAS	C3D-C2D-CMD-OMD
7	A	609	OLC	C21-C22-C24-O25
6	A	603	HAS	C23-C24-C28-C29
7	A	605	OLC	C2-C1-O20-C21
7	A	611	OLC	C1-C2-C3-C4
7	C	101	OLC	C2-C3-C4-C5
7	A	609	OLC	O23-C22-C24-O25
7	A	605	OLC	O19-C1-O20-C21
7	B	201	OLC	C11-C12-C13-C14
7	B	201	OLC	C1-C2-C3-C4
7	A	611	OLC	O20-C21-C22-O23
5	A	602	HEM	C4B-C3B-CAB-CBB
7	A	609	OLC	C2-C3-C4-C5
7	A	609	OLC	C1-C2-C3-C4
7	B	203	OLC	C14-C15-C16-C17
7	C	101	OLC	C2-C1-O20-C21
7	B	204	OLC	C13-C14-C15-C16
7	A	606	OLC	C6-C7-C8-C9
7	C	101	OLC	O19-C1-O20-C21
7	B	204	OLC	C3-C4-C5-C6
7	A	607	OLC	C22-C21-O20-C1
7	A	606	OLC	C3-C4-C5-C6
7	A	610	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	A	610	OLC	C7-C8-C9-C10
7	A	607	OLC	C1-C2-C3-C4
7	B	203	OLC	C9-C10-C11-C12
7	C	101	OLC	C1-C2-C3-C4
7	C	101	OLC	C3-C4-C5-C6
7	B	204	OLC	C10-C11-C12-C13
7	A	608	OLC	C4-C5-C6-C7
7	B	204	OLC	C11-C12-C13-C14
6	A	603	HAS	CAA-CBA-CGA-O1A
6	A	603	HAS	CAA-CBA-CGA-O2A
7	A	611	OLC	C7-C8-C9-C10
6	A	603	HAS	CAD-CBD-CGD-O1D
6	A	603	HAS	CAD-CBD-CGD-O2D
7	A	614	OLC	C7-C8-C9-C10
7	A	608	OLC	C7-C8-C9-C10
7	B	204	OLC	C7-C8-C9-C10
7	A	605	OLC	C4-C5-C6-C7
7	A	604	OLC	C7-C8-C9-C10
7	A	614	OLC	C9-C10-C11-C12
7	A	611	OLC	C9-C10-C11-C12
7	A	613	OLC	C10-C11-C12-C13
7	A	604	OLC	C2-C3-C4-C5
7	B	201	OLC	C7-C8-C9-C10
7	B	204	OLC	C9-C10-C11-C12
5	A	602	HEM	CAA-CBA-CGA-O2A

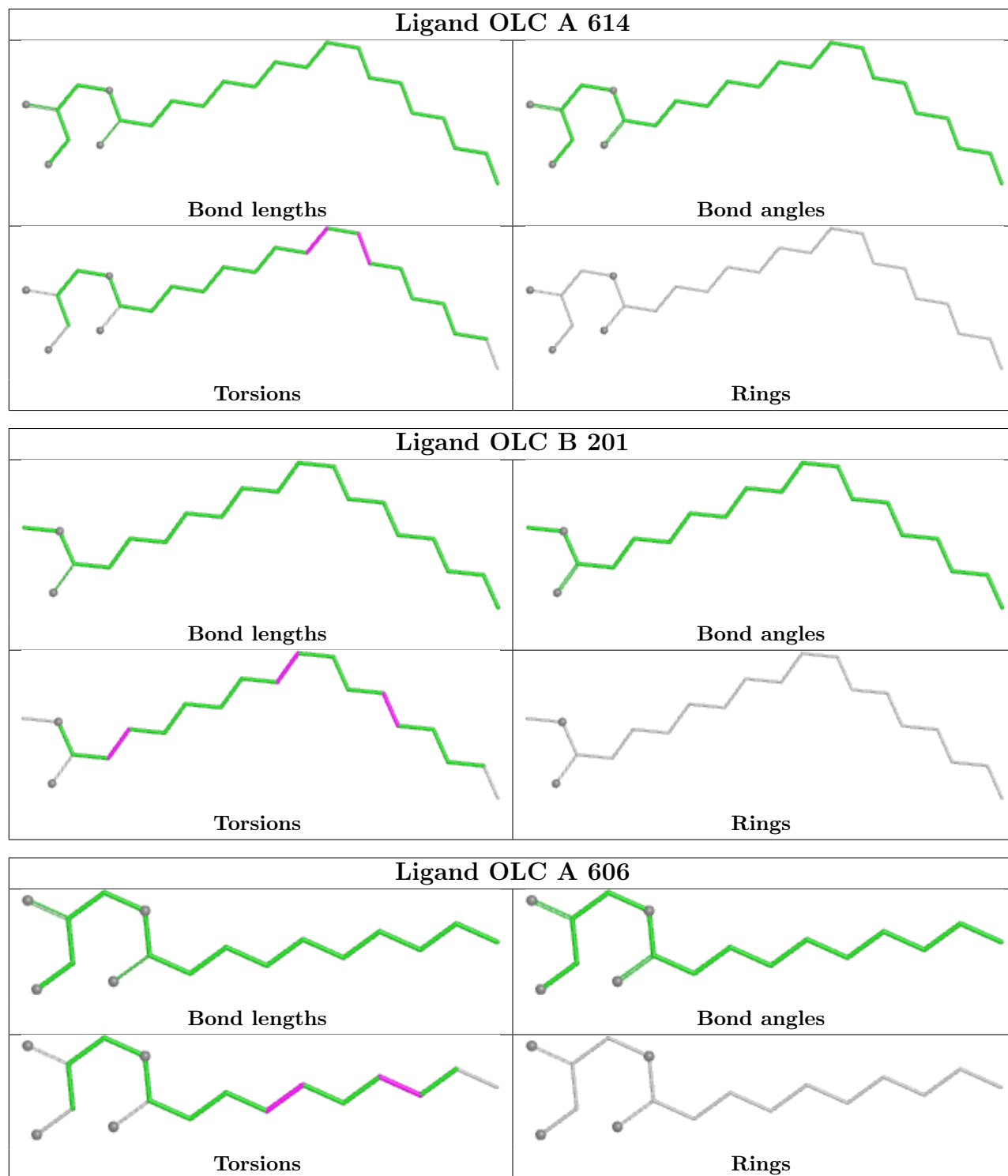
There are no ring outliers.

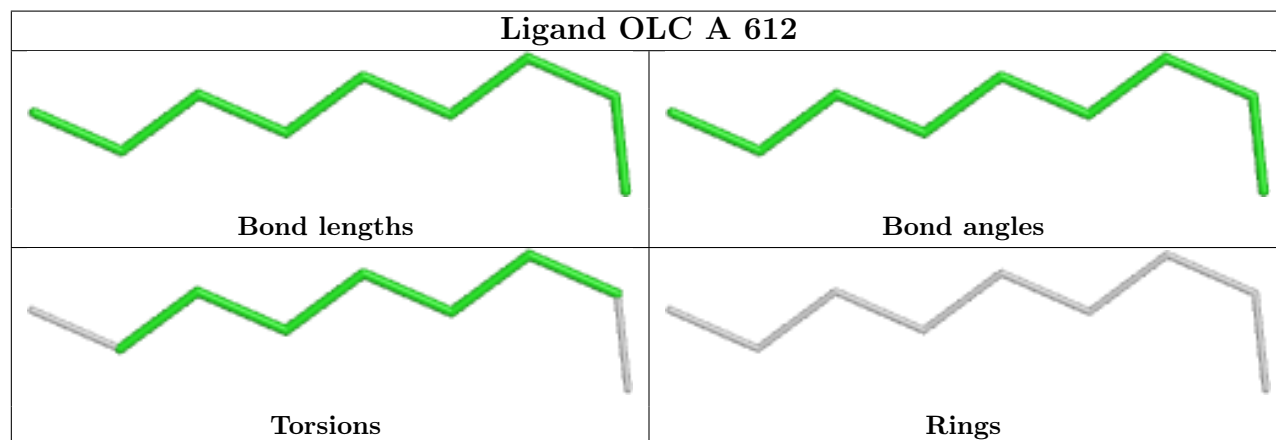
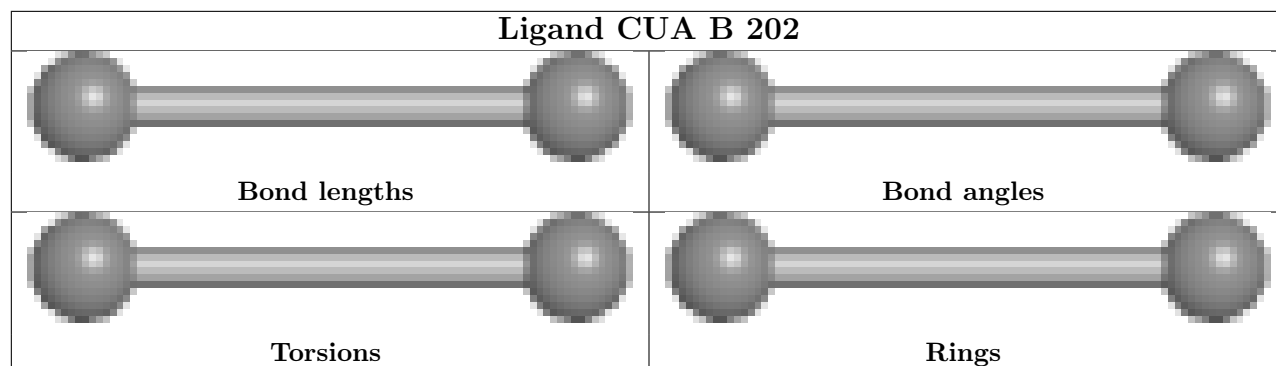
4 monomers are involved in 5 short contacts:

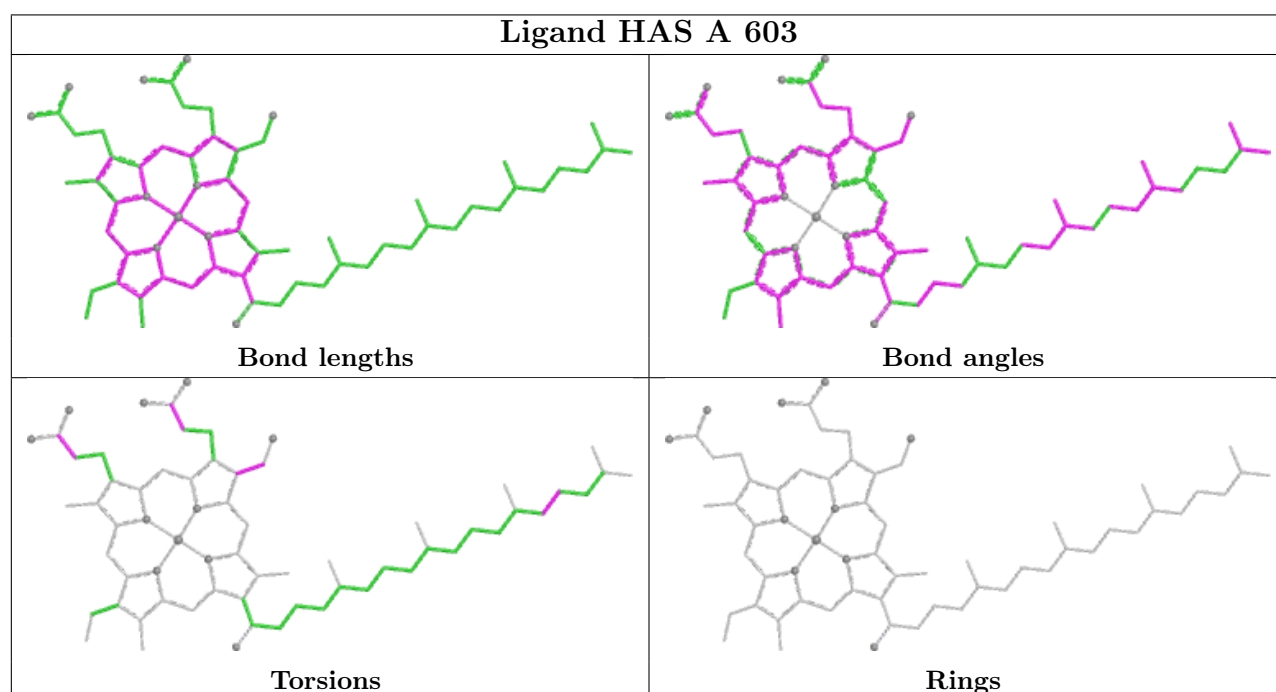
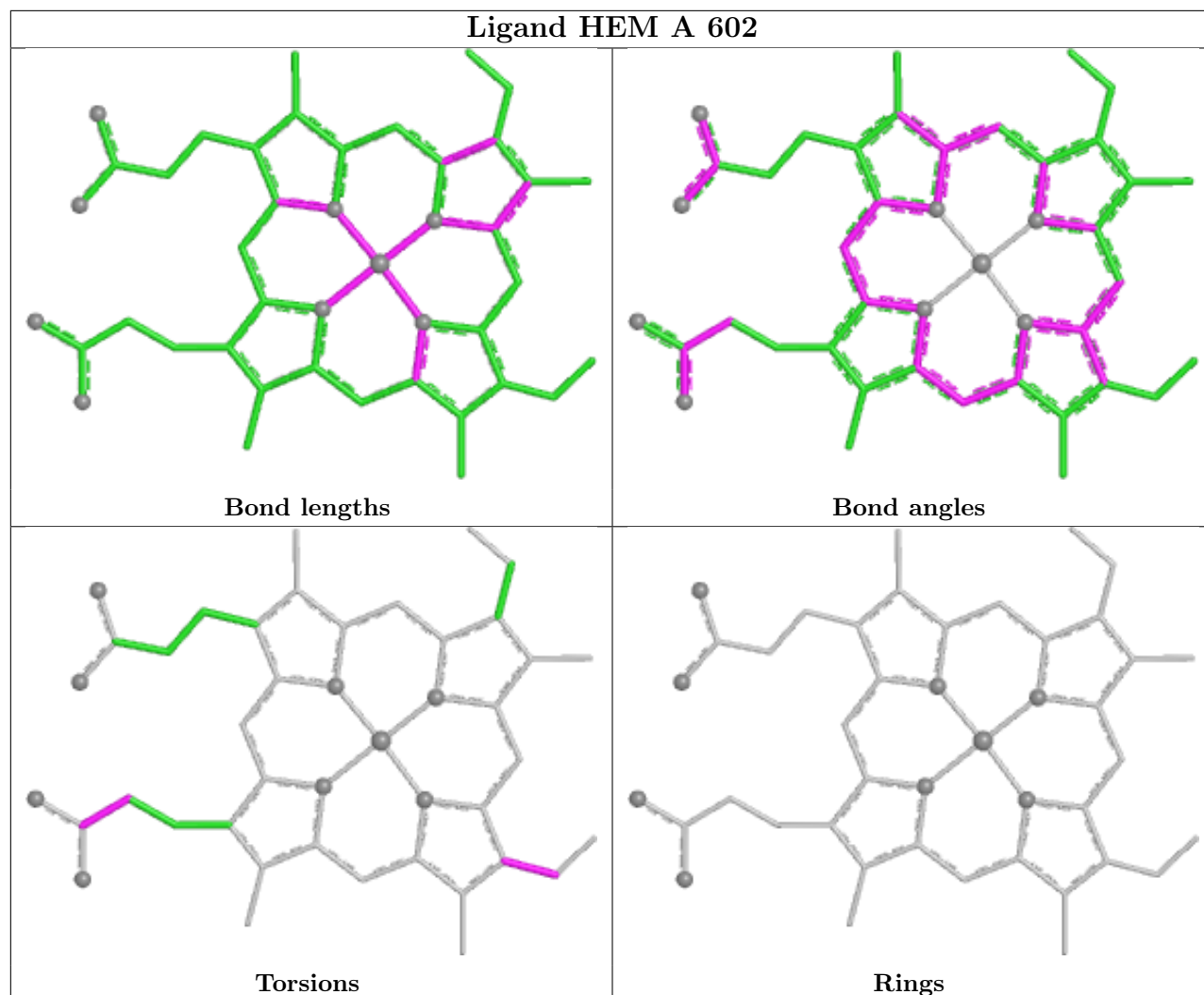
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	HEM	2	0
7	B	204	OLC	1	0
7	A	610	OLC	1	0
7	B	203	OLC	1	0

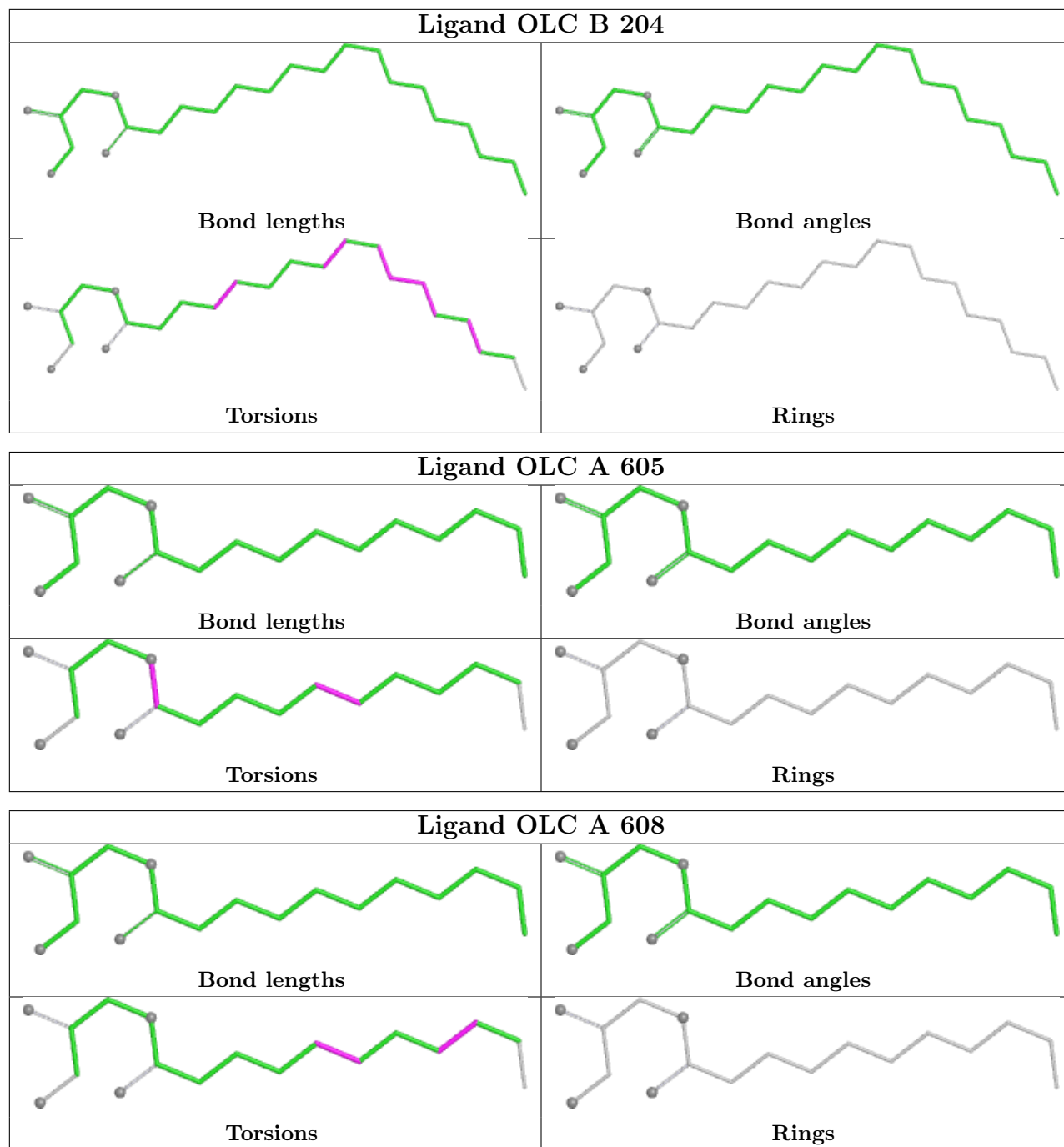
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

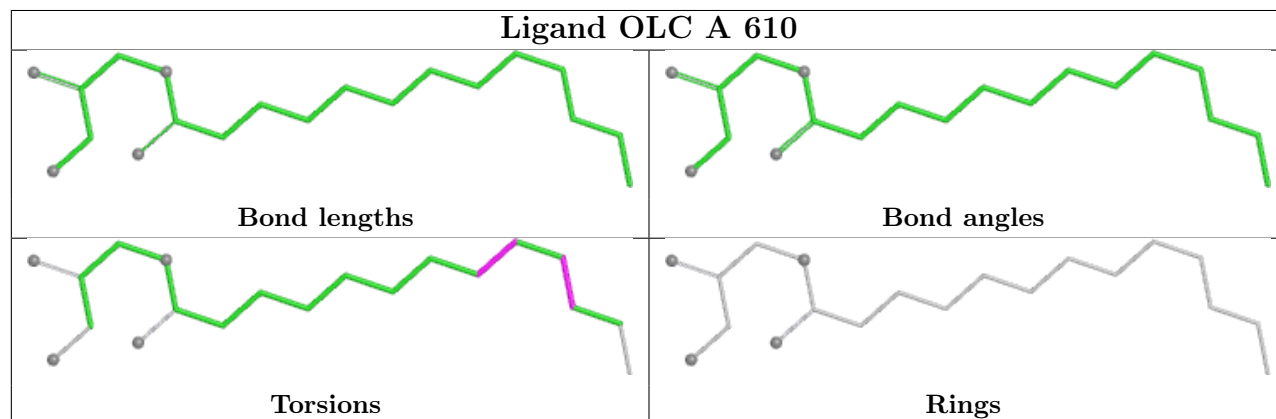
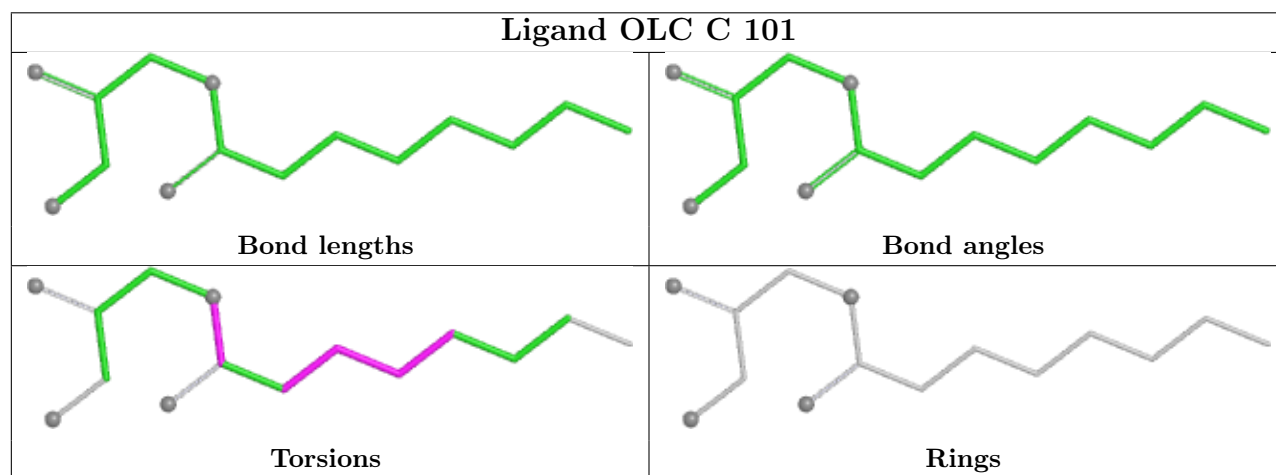
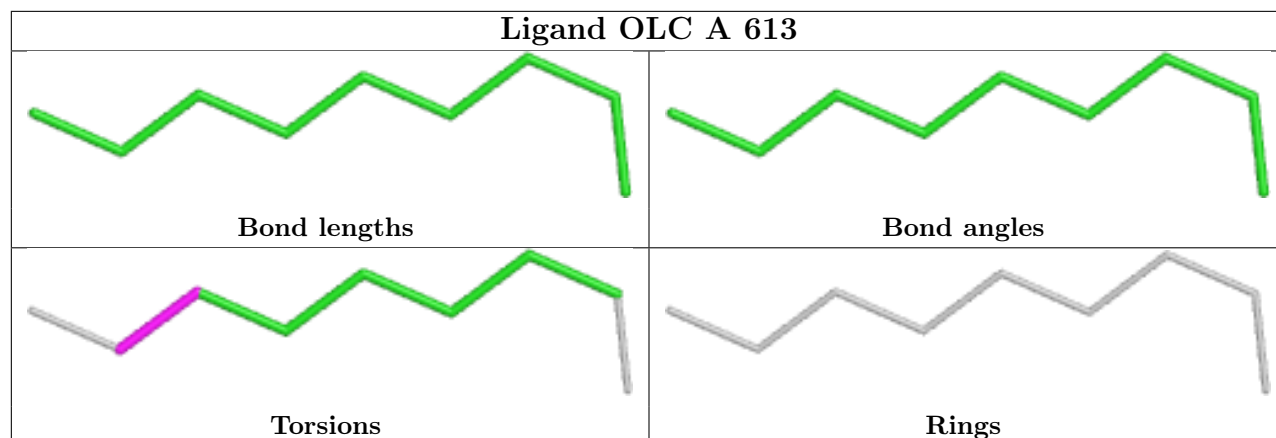
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

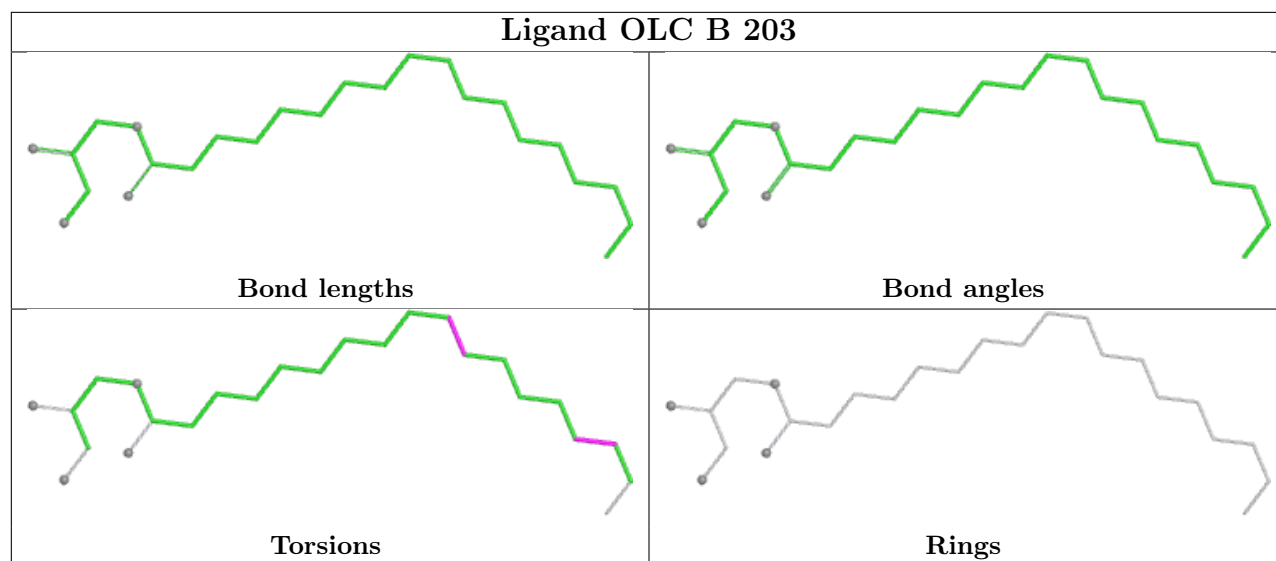
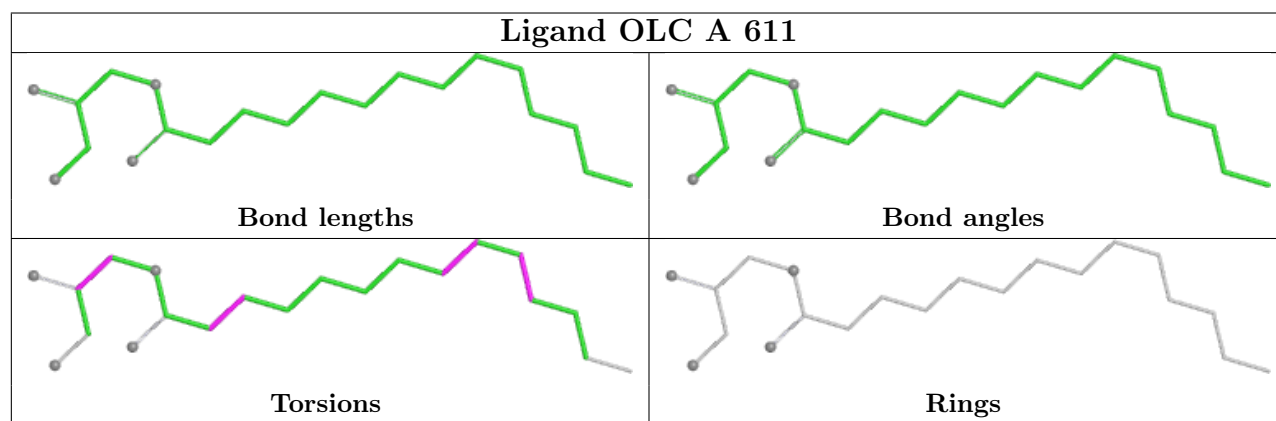
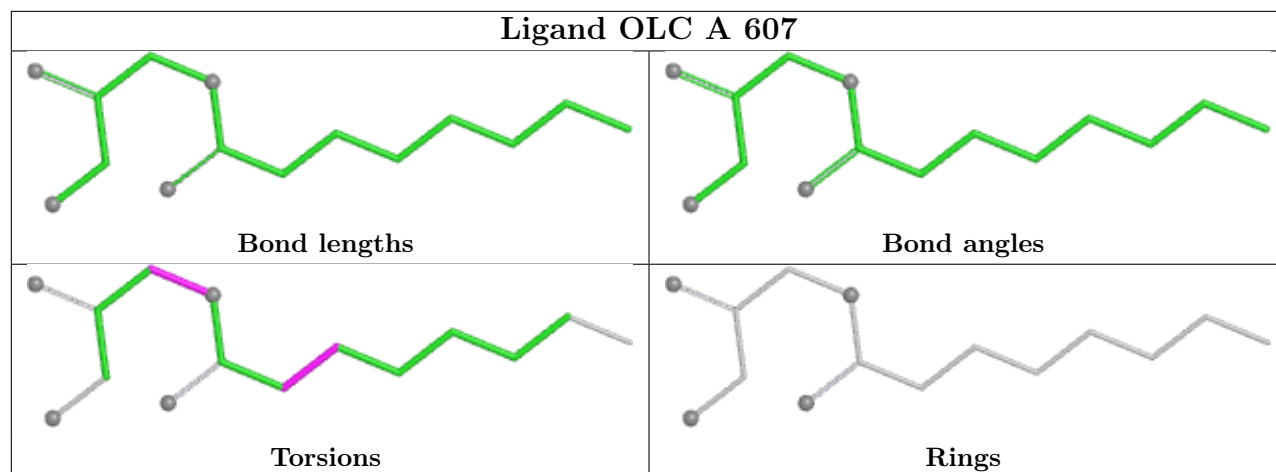




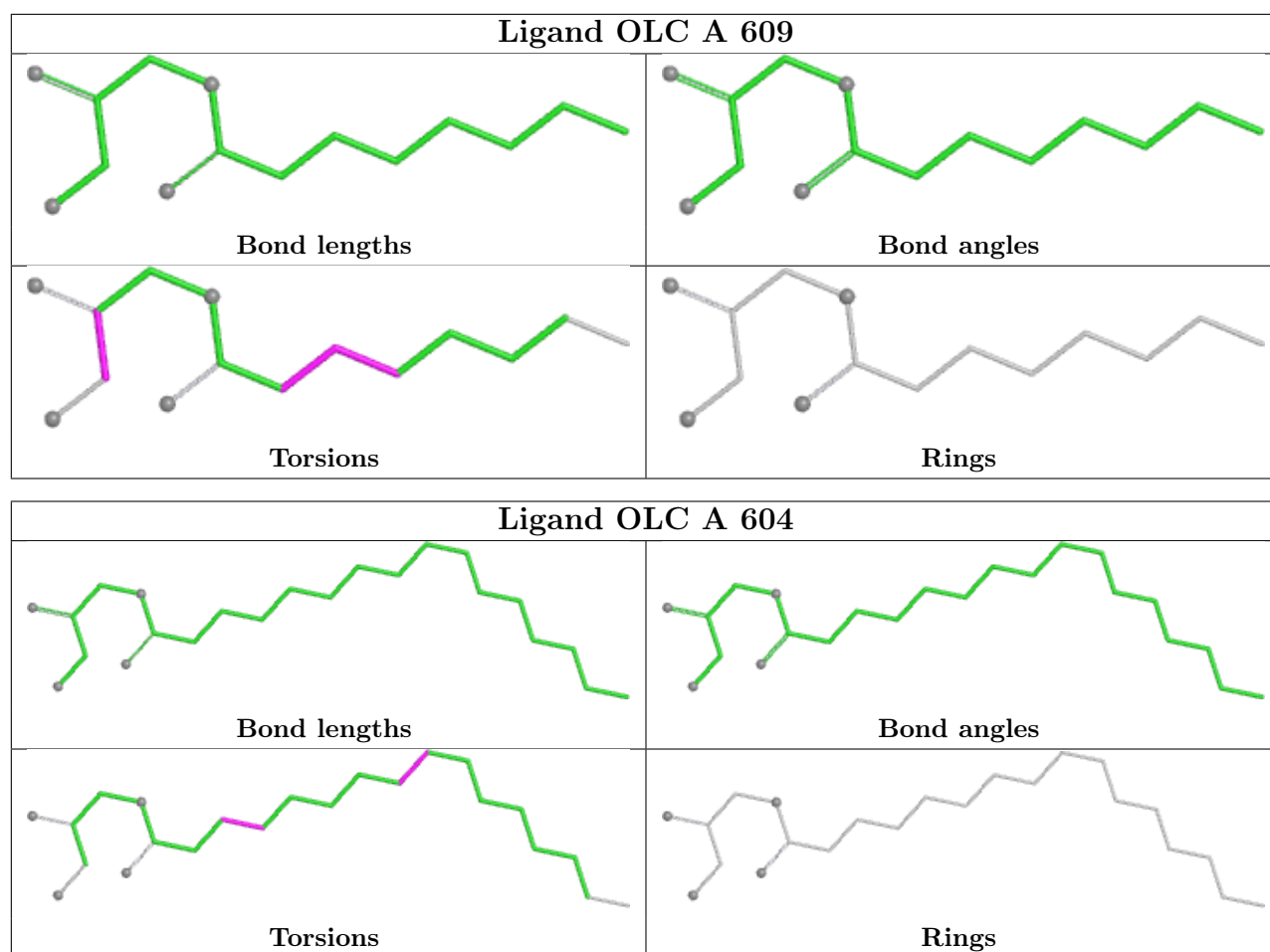












## 5.7 Other polymers [i](#)

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	554/569 (97%)	0.26	14 (2%) 58 60	25, 41, 72, 112	0
2	B	167/168 (99%)	0.12	2 (1%) 76 77	26, 41, 67, 120	0
3	C	31/34 (91%)	0.28	0 100 100	35, 42, 56, 69	0
All	All	752/771 (97%)	0.23	16 (2%) 63 65	25, 41, 71, 120	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	4.3
1	A	504	ALA	3.6
1	A	523	ALA	3.6
1	A	515	PRO	3.3
1	A	491	VAL	3.0
2	B	3	ASP	2.7
1	A	501	LEU	2.5
1	A	514	GLY	2.5
1	A	548	GLN	2.5
1	A	333	PHE	2.4
1	A	513	SER	2.4
1	A	517	ASP	2.3
1	A	342	ASP	2.2
1	A	505	PRO	2.2
1	A	518	ARG	2.2
1	A	499	PRO	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

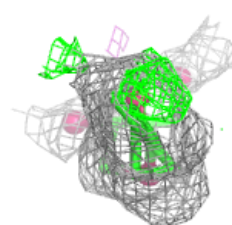
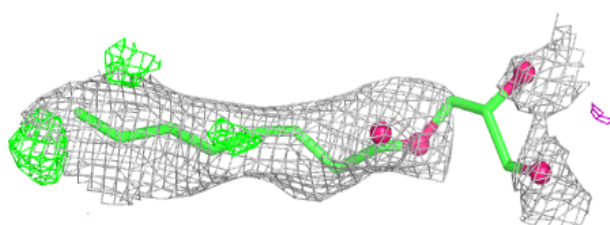
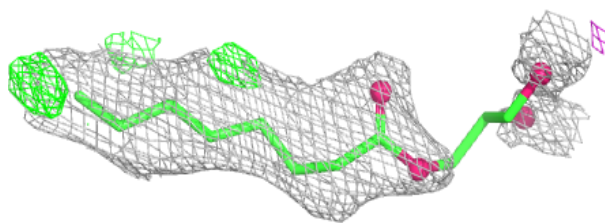
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	OLC	C	101	15/25	0.68	0.28	86,106,116,117	0
7	OLC	A	607	15/25	0.72	0.22	77,84,106,113	0
7	OLC	A	610	20/25	0.76	0.21	82,99,115,123	0
7	OLC	A	606	17/25	0.76	0.20	68,86,105,108	0
7	OLC	B	204	24/25	0.80	0.19	75,85,117,120	0
7	OLC	A	613	9/25	0.80	0.22	70,77,81,82	0
7	OLC	B	201	20/25	0.81	0.23	76,93,105,110	0
7	OLC	A	611	21/25	0.81	0.17	72,80,94,97	0
7	OLC	A	608	18/25	0.81	0.17	69,87,101,101	0
7	OLC	B	203	25/25	0.82	0.16	65,81,109,116	0
7	OLC	A	609	15/25	0.82	0.20	77,88,93,93	0
7	OLC	A	612	9/25	0.82	0.27	94,97,109,111	0
7	OLC	A	604	23/25	0.83	0.18	57,77,86,92	0
7	OLC	A	614	24/25	0.83	0.16	54,74,96,101	0
7	OLC	A	605	18/25	0.84	0.15	72,78,97,100	0
6	HAS	A	603	65/65	0.97	0.08	20,33,45,57	0
4	CU	A	601	1/1	0.97	0.04	34,34,34,34	0
5	HEM	A	602	43/43	0.98	0.06	20,30,38,39	0
8	CUA	B	202	2/2	0.99	0.03	32,32,32,38	0

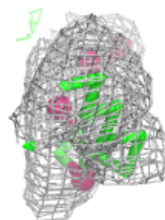
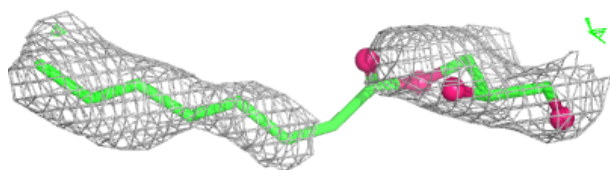
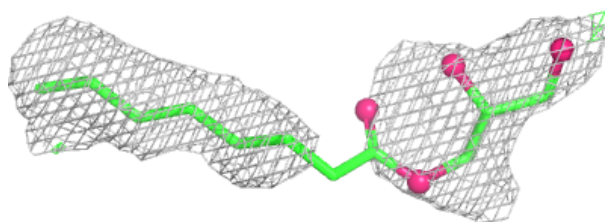
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLC C 101:**

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

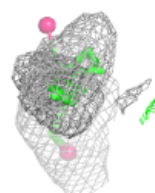
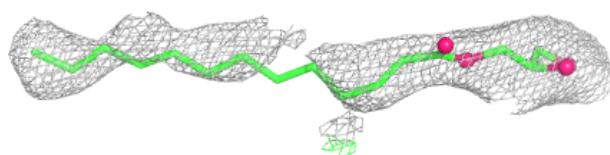
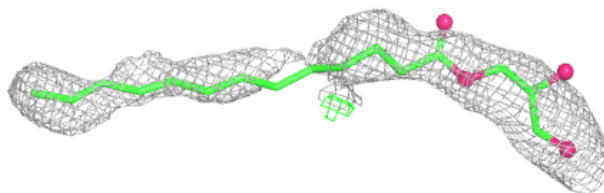
**Electron density around OLC A 607:**

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

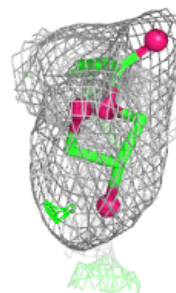
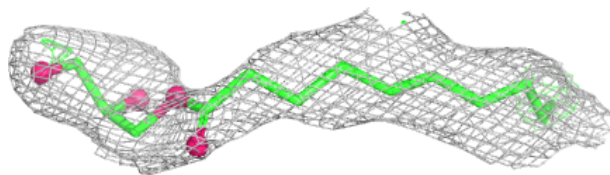
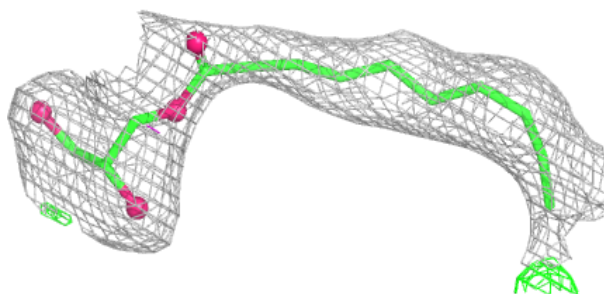


**Electron density around OLC A 610:**

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

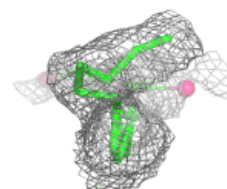
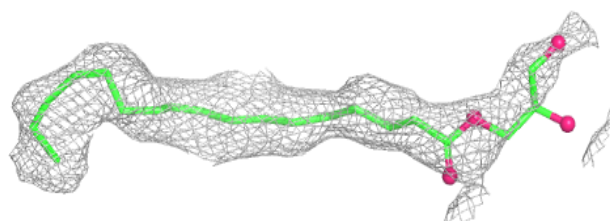
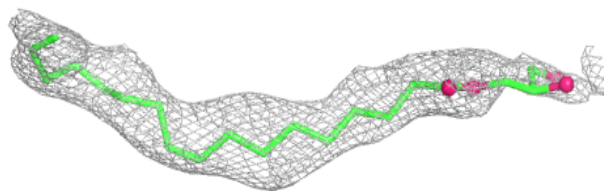
**Electron density around OLC A 606:**

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

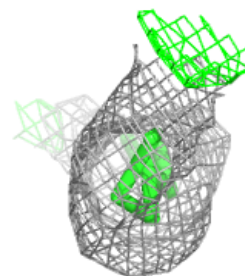
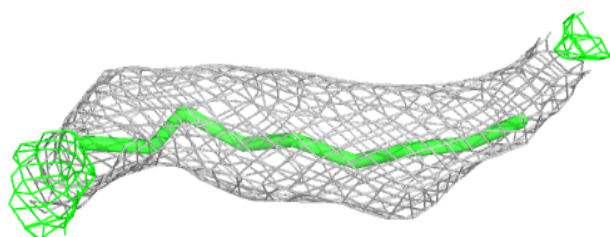
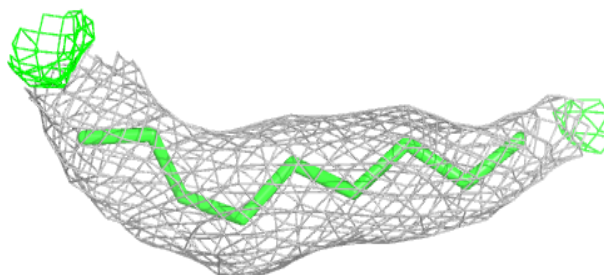


**Electron density around OLC B 204:**

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

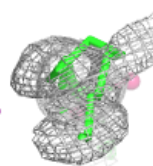
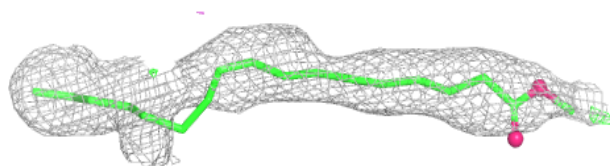
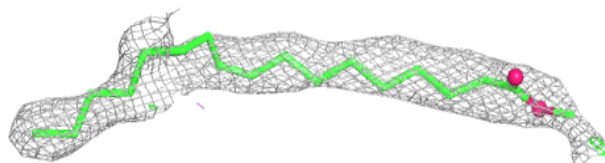
**Electron density around OLC A 613:**

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

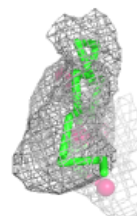
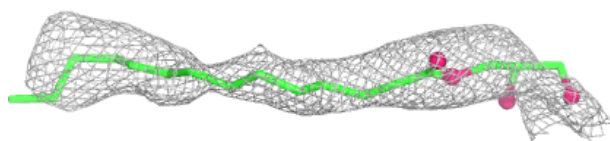
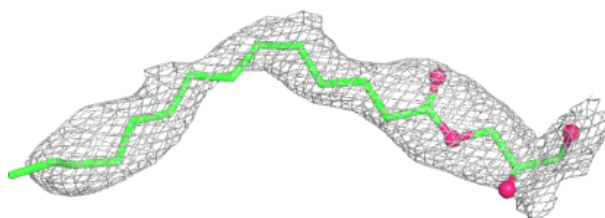


**Electron density around OLC B 201:**

$2mF_o-DF_c$  (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:**

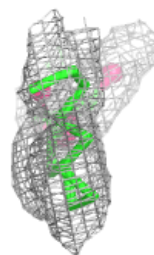
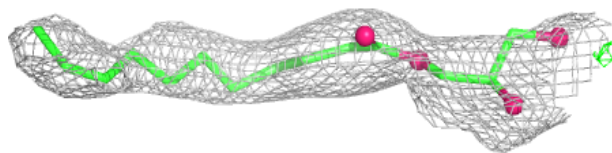
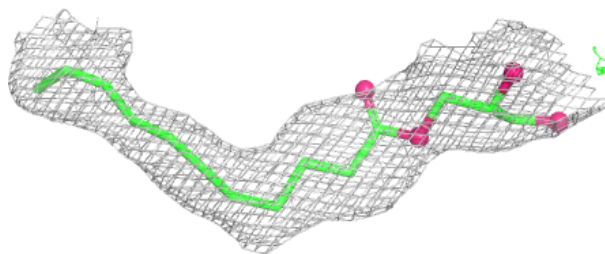
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



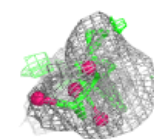
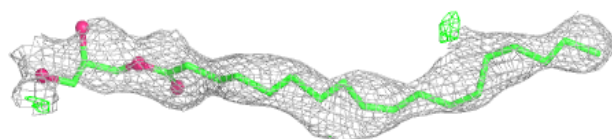
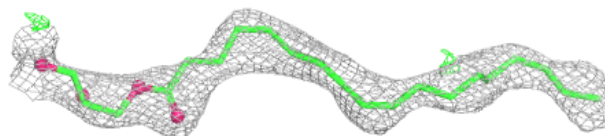


**Electron density around OLC A 608:**

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

**Electron density around OLC B 203:**

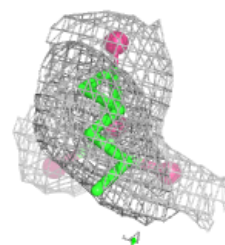
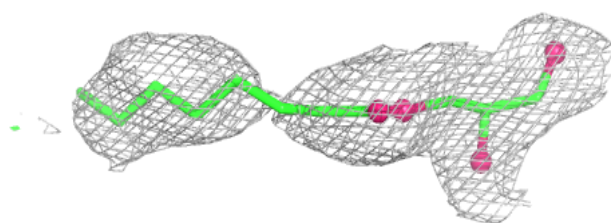
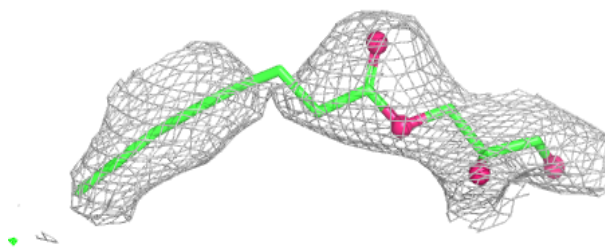
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



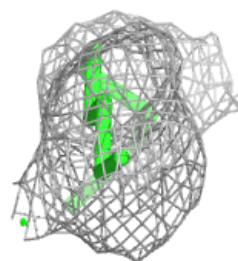
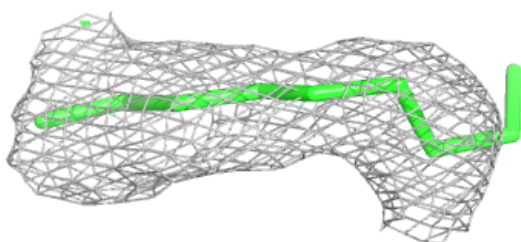
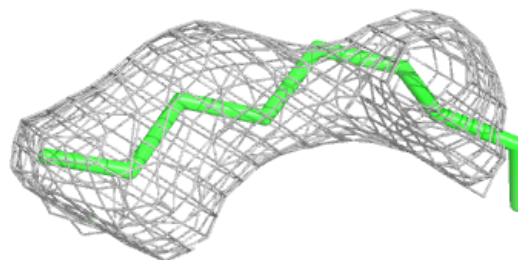


**Electron density around OLC A 609:**

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

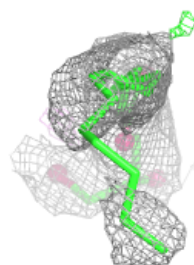
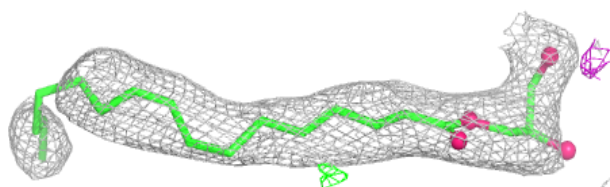
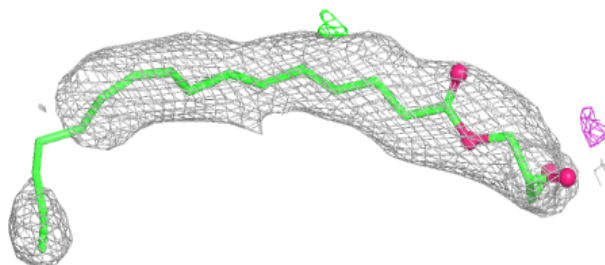
**Electron density around OLC A 612:**

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

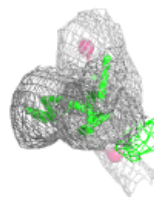
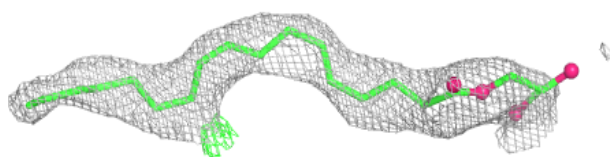
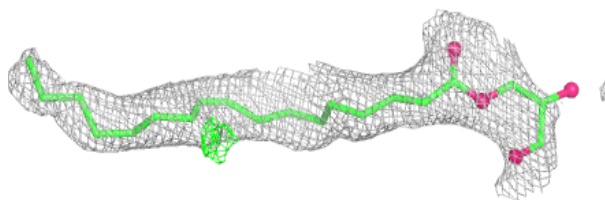


**Electron density around OLC A 604:**

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

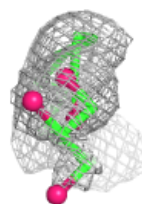
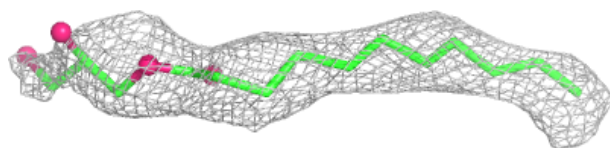
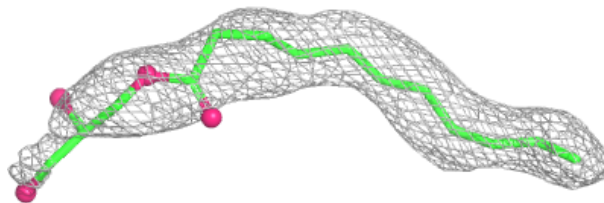
**Electron density around OLC A 614:**

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

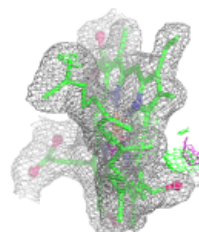
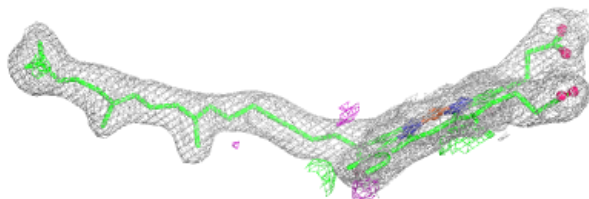
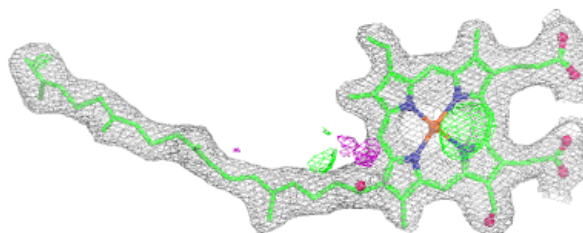


**Electron density around OLC A 605:**

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

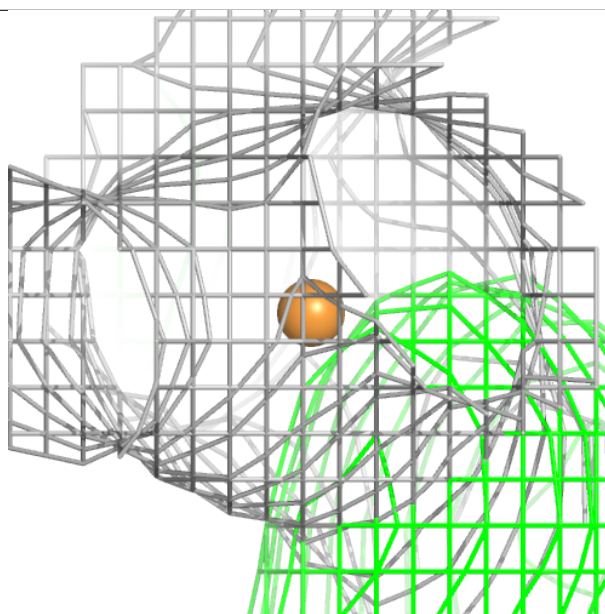
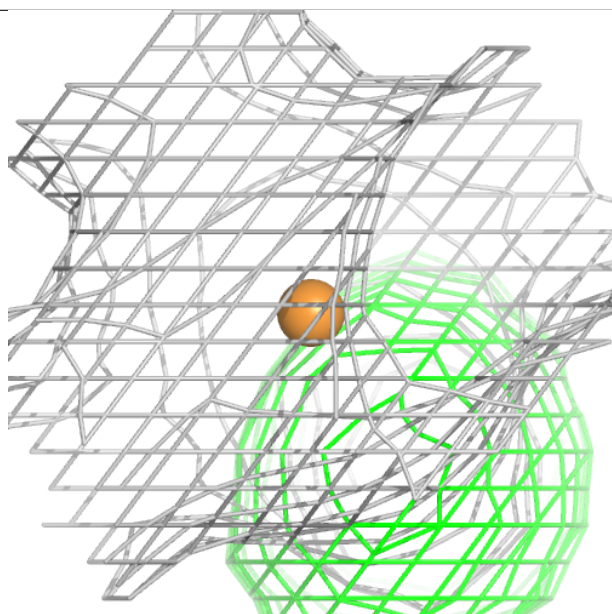
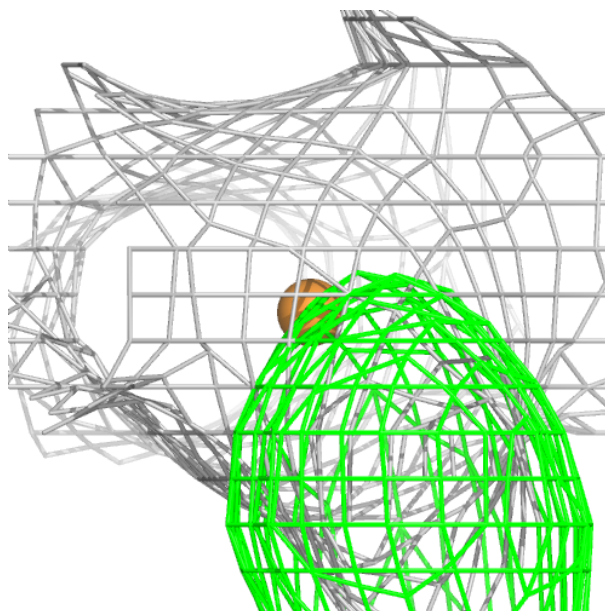
**Electron density around HAS A 603:**

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



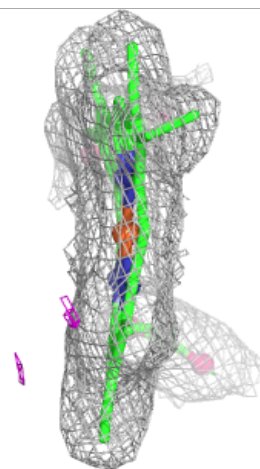
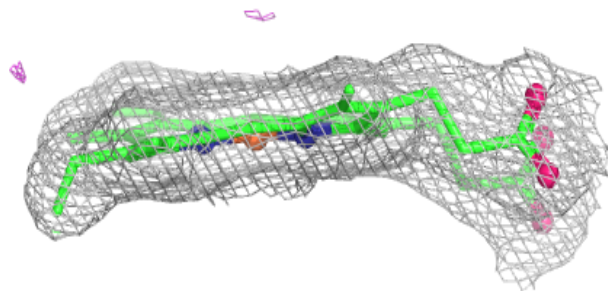
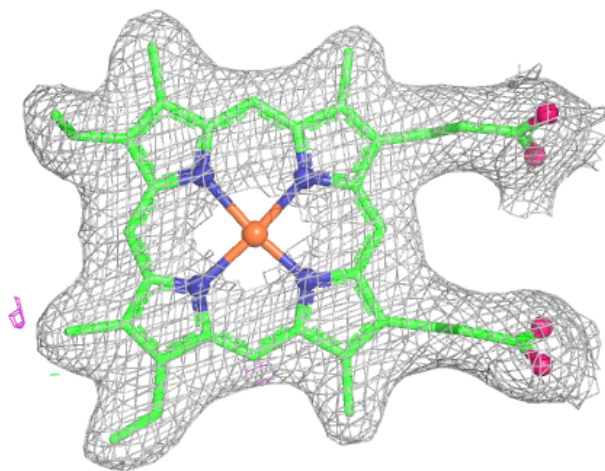
**Electron density around CU A 601:**

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

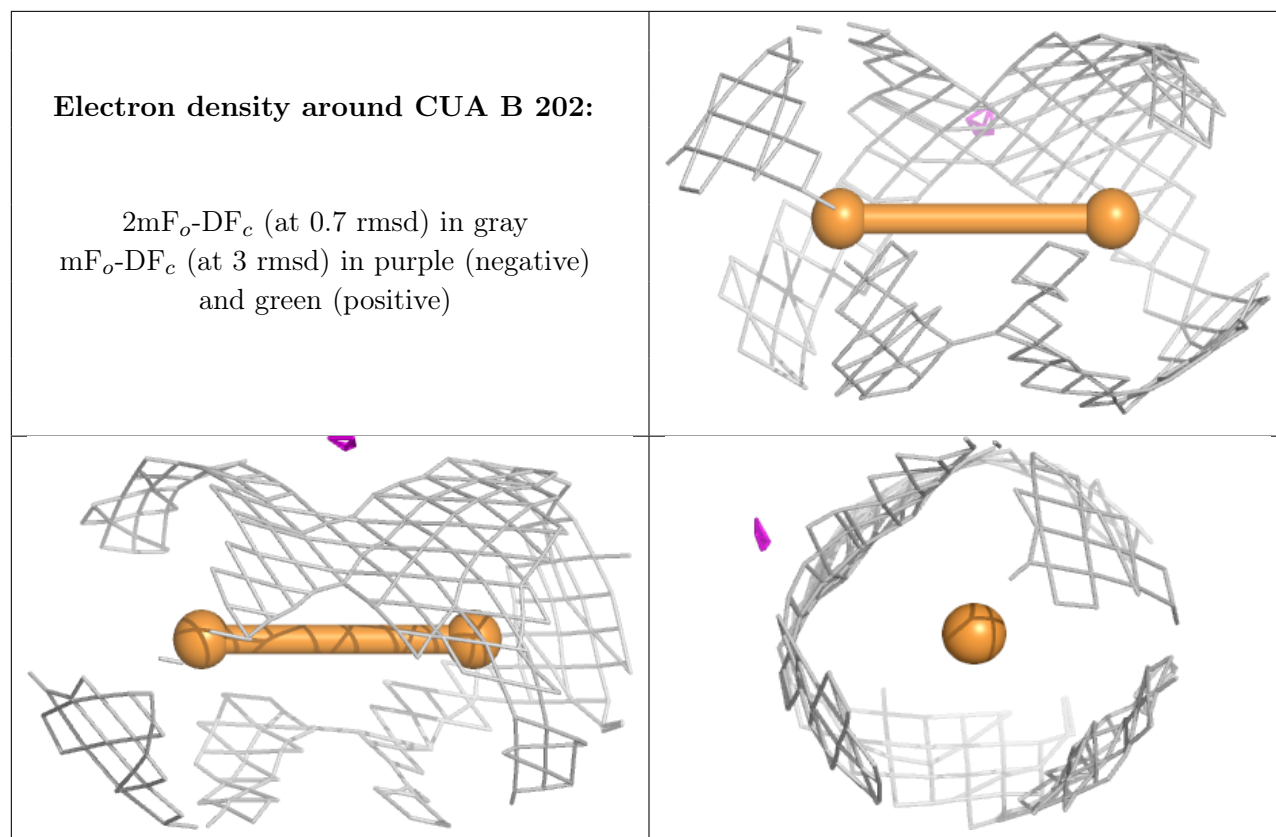


**Electron density around HEM A 602:**

$2mF_o-DF_c$  (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.