



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 04:14 PM JST

PDB ID : 8K65  
Title : Serial femtosecond crystallography structure of CO bound ba3- type cytochrome c oxidase without pump laser irradiation  
Authors : Safari, C.; Ghosh, S.; Andersson, R.; Johannesson, J.; Donoso, A.V.; Bath, P.; Zoric, D.; Sandelin, E.; Nango, E.; Tanaka, R.; Iwata, S.; Neutze, R.; Branden, G.  
Deposited on : 2023-07-25  
Resolution : 2.00 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](#) ①) were used in the production of this report:

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

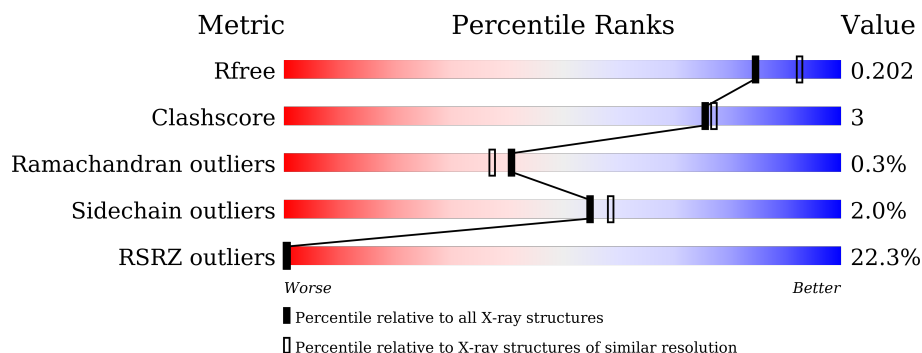
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	 25% 91% 6%
2	B	168	 14% 91% 8%
3	C	34	 6% 85% 6% 9%

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 [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6487 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
			Total	C	N	O	S			
1	A	554	4368	2963	698	691	16	0	0	0

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
			Total	C	N	O	S			
2	B	167	1301	846	216	235	4	0	0	0

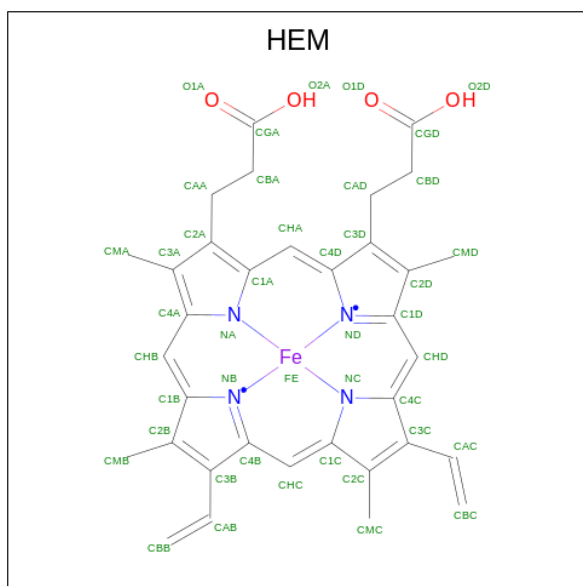
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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

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

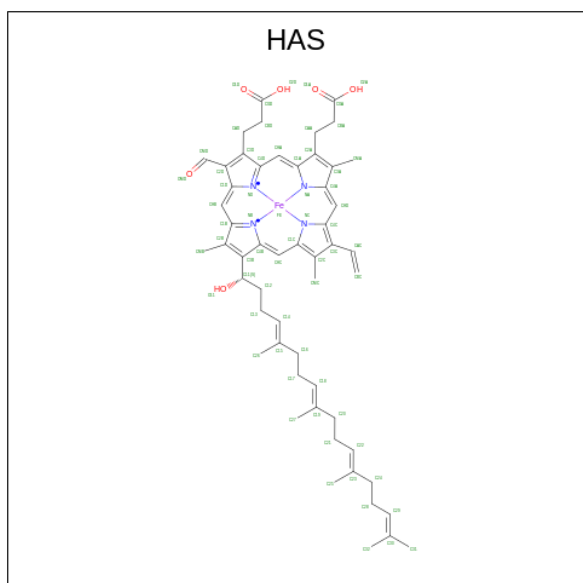
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

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



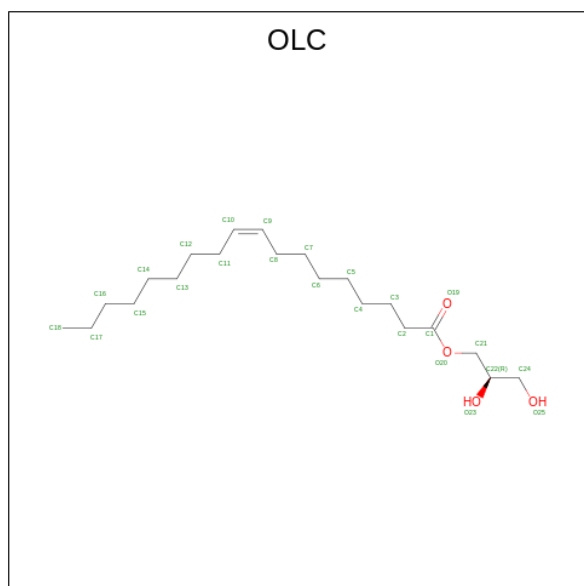
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Fe N O 43 34 1 4 4	0	0

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



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

- Molecule 7 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>) (labeled as "Ligand of Interest" by depositor).



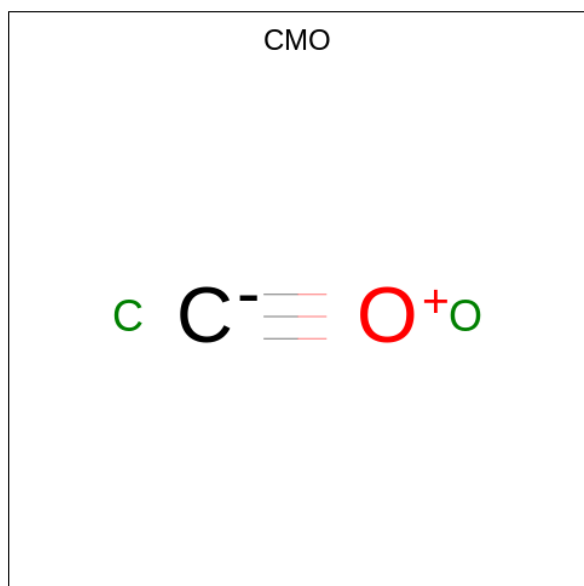
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			23	19	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			17	13	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			18	14	4		
7	A	1	Total	C	O	0	0
			15	11	4		
7	A	1	Total	C	O	0	0
			20	16	4		
7	A	1	Total	C	O	0	0
			21	17	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	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
			24	20	4		
7	C	1	Total	C	O	0	0
			15	11	4		

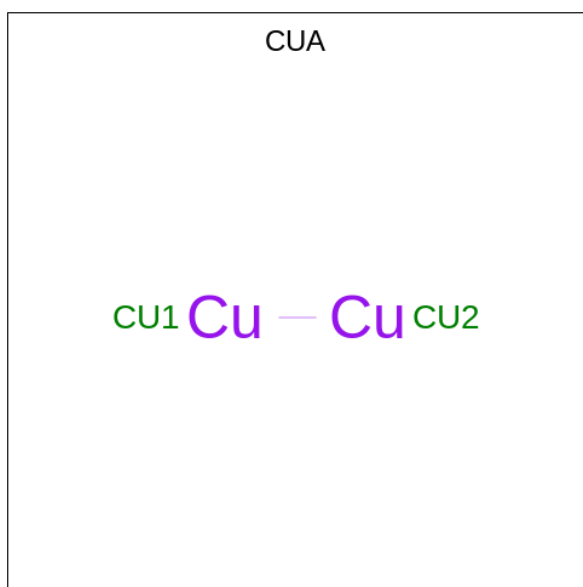
- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





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

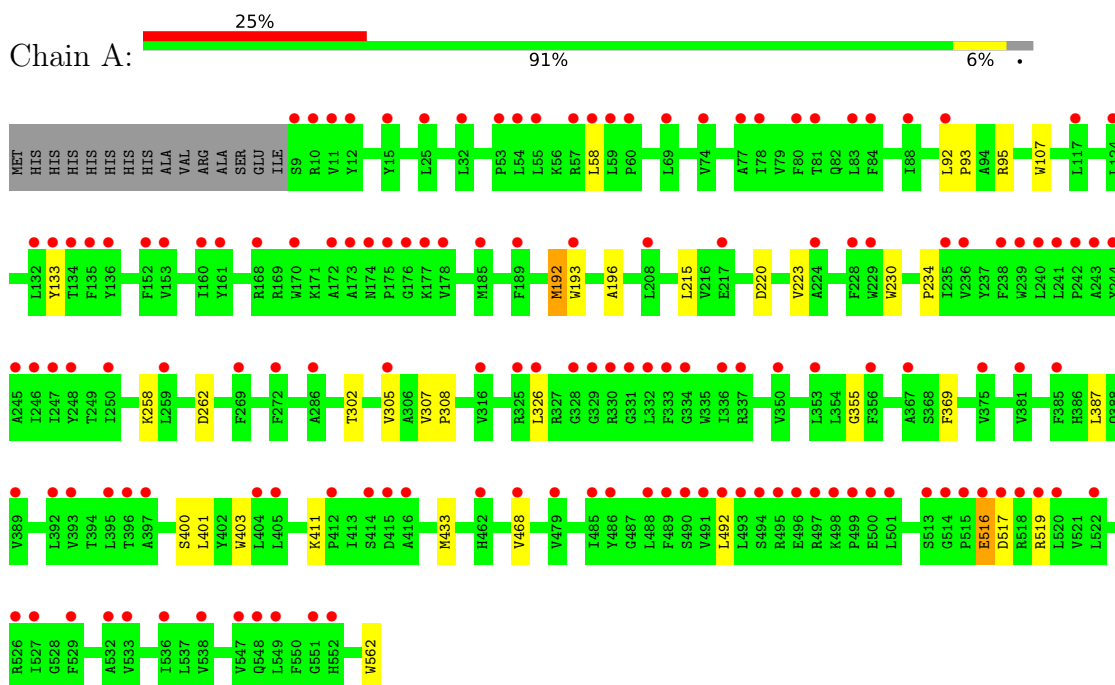
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	99	Total O 100 100	0	1
10	B	88	Total O 88 88	0	0
10	C	3	Total O 3 3	0	0

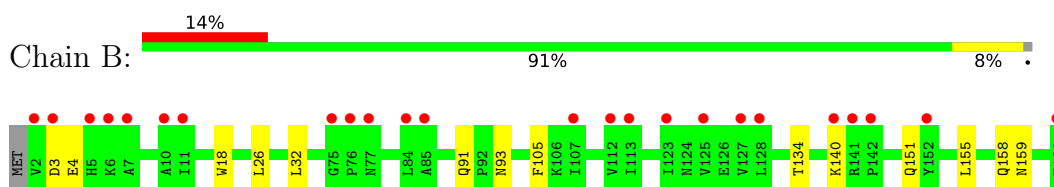
### 3 Residue-property plots [i](#)

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

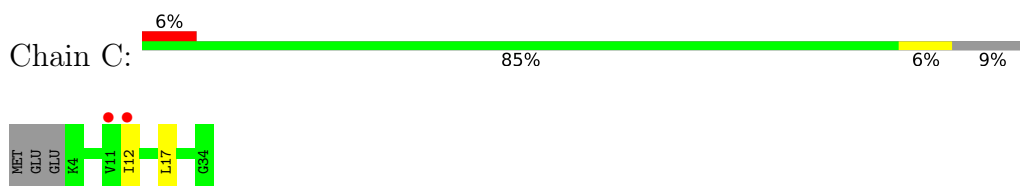
- Molecule 1: Cytochrome c oxidase subunit 1



- 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, $\alpha$ , $\beta$ , $\gamma$	145.85Å 100.32Å 96.62Å 90.00° 126.76° 90.00°	Depositor
Resolution (Å)	37.20 – 2.00 38.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.20-2.00) 100.0 (38.70-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.00Å)	Xtrriage
Refinement program	REFMAC v8.0	Depositor
R, $R_{free}$	0.170 , 0.196 0.177 , 0.202	Depositor DCC
$R_{free}$ test set	3773 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 84.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6487	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: CMO, OLC, HAS, CUA, CU, HEM

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	0.75	1/4525 (0.0%)	0.82	1/6213 (0.0%)
2	B	0.80	1/1338 (0.1%)	0.82	0/1828
3	C	0.72	0/247	0.76	0/335
All	All	0.76	2/6110 (0.0%)	0.82	1/8376 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	GLU	CD-OE2	5.74	1.31	1.25
2	B	151	GLN	C-O	5.17	1.33	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	NE-CZ-NH1	-5.93	117.34	120.30

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	4368	0	4467	29	0
2	B	1301	0	1278	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	241	0	267	1	0
4	A	1	0	0	0	0
5	A	43	0	30	1	0
6	A	65	0	62	1	0
7	A	165	0	229	2	0
7	B	69	0	103	2	0
7	C	39	0	54	0	0
8	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	100	0	0	1	0
10	B	88	0	0	4	0
10	C	3	0	0	0	0
All	All	6487	0	6490	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:192:MET:CE	1:A:196:ALA:HB2	1.82	1.10
1:A:192:MET:HE3	1:A:196:ALA:HB2	1.49	0.90
1:A:192:MET:CE	1:A:196:ALA:CB	2.55	0.85
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.64	0.80
1:A:192:MET:HE2	1:A:192:MET:O	1.84	0.78
1:A:258:LYS:NZ	2:B:4:GLU:OE1	2.27	0.64
1:A:220:ASP:HB3	1:A:223:VAL:CG1	2.29	0.62
1:A:192:MET:HE1	1:A:196:ALA:CB	2.30	0.62
1:A:192:MET:HE2	1:A:192:MET:C	2.22	0.60
6:A:603:HAS:HMC1	6:A:603:HAS:HBC1	1.85	0.57
2:B:93:ASN:CG	10:B:311:HOH:O	2.43	0.56
5:A:602:HEM:HBC2	5:A:602:HEM:HMC1	1.88	0.55
2:B:32:LEU:HD21	7:B:203:OLC:H7A	1.87	0.55
1:A:411:LYS:NZ	1:A:492:LEU:O	2.40	0.53
1:A:192:MET:HE2	1:A:193:TRP:HA	1.93	0.51
1:A:519:ARG:N	1:A:519:ARG:HD3	2.26	0.50
2:B:91:GLN:NE2	10:B:301:HOH:O	2.19	0.50
1:A:107:TRP:CE3	7:A:606:OLC:H21	2.47	0.50
2:B:159:ASN:HB2	10:B:343:HOH:O	2.11	0.49
1:A:220:ASP:CB	1:A:223:VAL:HG12	2.40	0.49
1:A:519:ARG:HD3	1:A:519:ARG:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD22	1:A:433:MET:HE1	1.97	0.47
1:A:307:VAL:N	1:A:308:PRO:HD2	2.30	0.46
1:A:355:GLY:HA3	1:A:433:MET:HE1	1.98	0.46
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.52	0.45
1:A:192:MET:HE1	1:A:234:PRO:HB2	1.99	0.44
1:A:516:GLU:OE2	1:A:517:ASP:OD1	2.36	0.44
1:A:516:GLU:HG2	1:A:517:ASP:N	2.34	0.43
1:A:400:SER:HA	1:A:403:TRP:NE1	2.34	0.42
1:A:468:VAL:HG21	7:A:608:OLC:H2	2.01	0.42
1:A:516:GLU:HG2	1:A:517:ASP:OD1	2.20	0.42
1:A:562:TRP:HA	2:B:155:LEU:HG	2.02	0.41
1:A:302:THR:O	1:A:305:VAL:HG12	2.20	0.41
2:B:105:PHE:O	2:B:134:THR:HA	2.20	0.41
2:B:32:LEU:CD2	7:B:203:OLC:H7A	2.51	0.41
1:A:92:LEU:HB2	1:A:93:PRO:HD3	2.03	0.40
1:A:400:SER:CA	10:A:719:HOH:O	2.69	0.40
2:B:91:GLN:HG3	10:B:386:HOH:O	2.21	0.40
1:A:192:MET:HE2	1:A:196:ALA:CB	2.49	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%)	537 (97%)	14 (2%)	1 (0%)	47	44
2	B	165/168 (98%)	162 (98%)	2 (1%)	1 (1%)	25	19
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	746/771 (97%)	728 (98%)	16 (2%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	ASP
1	A	369	PHE

### 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%)	439 (98%)	8 (2%)	59 63
2	B	136/138 (99%)	133 (98%)	3 (2%)	52 55
3	C	24/27 (89%)	23 (96%)	1 (4%)	30 27
All	All	607/628 (97%)	595 (98%)	12 (2%)	55 58

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	133	TYR
1	A	192	MET
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	326	LEU
1	A	401	LEU
2	B	26	LEU
2	B	140	LYS
2	B	158	GLN
3	C	17	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	446	ASN
2	B	60	GLN
2	B	99	GLN

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Mol	Chain	Res	Type
2	B	158	GLN
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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	609	-	14,14,24	0.27	0	15,15,25	0.26	0
7	OLC	A	610	-	19,19,24	0.27	0	20,20,25	0.32	0
7	OLC	A	612	-	8,8,24	0.15	0	7,7,25	0.12	0
9	CUA	B	202	2	0,1,1	-	-	-		
7	OLC	A	605	-	17,17,24	0.29	0	18,18,25	0.28	0
7	OLC	A	606	-	16,16,24	0.33	0	17,17,25	0.35	0
7	OLC	B	204	-	23,23,24	0.27	0	24,24,25	0.24	0
7	OLC	C	101	-	23,23,24	0.28	0	24,24,25	0.32	0
8	CMO	A	614	4	0,1,1	-	-	-		
7	OLC	C	102	-	14,14,24	0.26	0	15,15,25	0.33	0
7	OLC	A	607	-	14,14,24	0.26	0	15,15,25	0.31	0
7	OLC	A	613	-	8,8,24	0.20	0	7,7,25	0.19	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	OLC	B	201	-	19,19,24	0.24	0	19,19,25	0.21	0
7	OLC	B	203	-	24,24,24	0.27	0	25,25,25	0.23	0
5	HEM	A	602	1	41,50,50	1.56	9 (21%)	45,82,82	1.84	12 (26%)
6	HAS	A	603	1	69,72,72	2.18	20 (28%)	73,109,109	2.24	23 (31%)
7	OLC	A	608	-	17,17,24	0.34	0	18,18,25	0.42	0
7	OLC	A	604	-	22,22,24	0.25	0	23,23,25	0.40	0
7	OLC	A	611	-	20,20,24	0.26	0	21,21,25	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	602	1	-	1/12/54/54	-
7	OLC	A	606	-	-	8/16/16/24	-
6	HAS	A	603	1	1/1/8/18	5/40/82/82	-
7	OLC	A	608	-	-	8/17/17/24	-
7	OLC	A	609	-	-	5/14/14/24	-
7	OLC	A	610	-	-	6/19/19/24	-
7	OLC	A	612	-	-	3/6/6/24	-
7	OLC	A	605	-	-	6/17/17/24	-
7	OLC	A	613	-	-	2/6/6/24	-
7	OLC	B	204	-	-	10/23/23/24	-
7	OLC	B	201	-	-	11/18/18/24	-
7	OLC	B	203	-	-	10/24/24/24	-
7	OLC	A	604	-	-	4/22/22/24	-
7	OLC	C	101	-	-	9/23/23/24	-
7	OLC	A	611	-	-	6/20/20/24	-
7	OLC	C	102	-	-	6/14/14/24	-
7	OLC	A	607	-	-	9/14/14/24	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHD-C4A	7.02	1.45	1.35
6	A	603	HAS	CHC-C4B	4.41	1.46	1.35
6	A	603	HAS	C3B-C2B	4.40	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C4B-NB	-4.35	1.32	1.40
6	A	603	HAS	C3C-C2C	4.10	1.46	1.40
5	A	602	HEM	C1B-NB	-4.07	1.33	1.40
6	A	603	HAS	C1D-ND	-4.02	1.33	1.40
6	A	603	HAS	FE-NA	4.00	2.11	1.95
6	A	603	HAS	C1B-NB	-3.90	1.30	1.38
6	A	603	HAS	C2A-C3A	3.78	1.44	1.36
6	A	603	HAS	C4A-NA	-3.60	1.32	1.39
6	A	603	HAS	CHB-C1D	3.48	1.45	1.38
6	A	603	HAS	CHB-C1B	3.04	1.46	1.39
5	A	602	HEM	C4B-NB	-2.96	1.32	1.38
6	A	603	HAS	CHA-C4D	2.93	1.45	1.39
6	A	603	HAS	C1C-CHC	2.89	1.49	1.41
5	A	602	HEM	C3C-C2C	-2.84	1.36	1.40
6	A	603	HAS	CHA-C1A	2.81	1.43	1.38
5	A	602	HEM	FE-NB	2.73	2.10	1.96
6	A	603	HAS	C4A-C3A	2.70	1.50	1.45
5	A	602	HEM	CMD-C2D	2.68	1.56	1.50
5	A	602	HEM	CHB-C1B	2.64	1.41	1.35
6	A	603	HAS	FE-NB	2.63	2.11	1.97
5	A	602	HEM	C4D-ND	-2.53	1.35	1.40
6	A	603	HAS	C4D-ND	-2.21	1.34	1.38
6	A	603	HAS	C1A-NA	-2.20	1.35	1.39
5	A	602	HEM	C1A-NA	2.19	1.40	1.36
5	A	602	HEM	C4A-NA	2.08	1.40	1.36
6	A	603	HAS	C2D-C3D	2.02	1.41	1.36

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2D-C3D-C4D	-6.15	102.11	106.49
5	A	602	HEM	CHC-C4B-NB	5.77	130.70	124.43
6	A	603	HAS	CMC-C2C-C3C	5.09	134.20	124.68
6	A	603	HAS	C2A-C1A-NA	5.05	115.24	110.32
6	A	603	HAS	CAD-C3D-C4D	4.80	133.04	124.66
6	A	603	HAS	C13-C12-C11	-4.60	107.43	114.35
6	A	603	HAS	C3B-C4B-NB	4.42	115.07	109.84
5	A	602	HEM	C1B-NB-C4B	4.36	109.57	105.07
6	A	603	HAS	C3D-C4D-ND	4.06	114.29	110.36
6	A	603	HAS	CAA-CBA-CGA	-4.06	104.86	113.60
5	A	602	HEM	CHD-C1D-ND	3.96	128.73	124.43
6	A	603	HAS	C3C-C4C-NC	3.90	114.26	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2B-C1B-NB	3.87	114.52	109.88
6	A	603	HAS	OMD-CMD-C2D	-3.38	118.05	125.69
6	A	603	HAS	C4B-C3B-C2B	-3.08	102.14	107.41
6	A	603	HAS	C1B-C2B-C3B	-3.08	103.12	106.80
6	A	603	HAS	C4A-C3A-C2A	-2.99	102.58	106.94
6	A	603	HAS	C1A-C2A-C3A	-2.85	103.41	107.13
6	A	603	HAS	CMA-C3A-C4A	2.84	129.71	124.71
6	A	603	HAS	C3A-C4A-NA	2.58	114.44	109.69
5	A	602	HEM	CHC-C4B-C3B	-2.53	120.69	124.57
6	A	603	HAS	CMB-C2B-C1B	2.48	128.82	125.04
5	A	602	HEM	O2A-CGA-CBA	2.48	122.00	114.03
6	A	603	HAS	CMC-C2C-C1C	-2.42	124.74	128.46
5	A	602	HEM	CAB-C3B-C2B	2.42	136.56	128.60
5	A	602	HEM	CHA-C4D-ND	2.42	127.37	124.38
6	A	603	HAS	CHA-C4D-ND	-2.36	121.85	124.42
5	A	602	HEM	O1A-CGA-CBA	-2.36	115.51	123.08
5	A	602	HEM	O2D-CGD-O1D	-2.35	117.45	123.30
6	A	603	HAS	C32-C30-C31	2.32	119.72	114.60
5	A	602	HEM	CHA-C4D-C3D	-2.28	121.04	125.33
6	A	603	HAS	O1D-CGD-CBD	-2.24	115.88	123.08
5	A	602	HEM	CHD-C1D-C2D	-2.23	121.49	124.98
5	A	602	HEM	O2D-CGD-CBD	2.14	120.90	114.03
6	A	603	HAS	CAA-C2A-C1A	2.02	128.70	124.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	605	OLC	O20-C21-C22-O23
7	A	607	OLC	C21-C22-C24-O25
7	A	607	OLC	O20-C21-C22-C24
7	A	607	OLC	O20-C21-C22-O23
7	A	610	OLC	C10-C11-C12-C13
7	C	101	OLC	O19-C1-O20-C21
7	C	101	OLC	C2-C1-O20-C21
7	A	613	OLC	C11-C12-C13-C14
7	A	608	OLC	C2-C1-O20-C21
7	C	102	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
7	C	102	OLC	O19-C1-O20-C21
7	A	608	OLC	O19-C1-O20-C21
7	A	607	OLC	C2-C1-O20-C21
7	B	204	OLC	C2-C1-O20-C21
7	A	607	OLC	O19-C1-O20-C21
7	B	204	OLC	O19-C1-O20-C21
7	A	610	OLC	O20-C21-C22-O23
7	B	204	OLC	O20-C21-C22-O23
7	A	606	OLC	C1-C2-C3-C4
7	A	610	OLC	O20-C21-C22-C24
7	B	204	OLC	O20-C21-C22-C24
7	B	204	OLC	C11-C12-C13-C14
7	A	612	OLC	C12-C13-C14-C15
7	A	605	OLC	C21-C22-C24-O25
7	A	611	OLC	C21-C22-C24-O25
7	C	102	OLC	C21-C22-C24-O25
7	A	606	OLC	O20-C21-C22-O23
7	B	203	OLC	C4-C5-C6-C7
7	C	101	OLC	C3-C4-C5-C6
7	A	606	OLC	C3-C4-C5-C6
7	C	101	OLC	C1-C2-C3-C4
7	B	203	OLC	C13-C14-C15-C16
7	A	610	OLC	C5-C6-C7-C8
7	A	610	OLC	C2-C3-C4-C5
7	C	102	OLC	O23-C22-C24-O25
7	C	102	OLC	C4-C5-C6-C7
7	A	604	OLC	C11-C12-C13-C14
7	B	203	OLC	C11-C12-C13-C14
7	B	204	OLC	C12-C13-C14-C15
7	B	201	OLC	C1-C2-C3-C4
7	A	613	OLC	C14-C15-C16-C17
7	B	204	OLC	C2-C3-C4-C5
7	A	606	OLC	C6-C7-C8-C9
7	A	608	OLC	C3-C4-C5-C6
7	B	201	OLC	C11-C12-C13-C14
7	B	201	OLC	C13-C14-C15-C16
7	A	607	OLC	O23-C22-C24-O25
7	B	201	OLC	C6-C7-C8-C9
7	C	101	OLC	C6-C7-C8-C9
7	A	611	OLC	C3-C4-C5-C6
7	A	611	OLC	C5-C6-C7-C8
7	A	604	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	B	203	OLC	C2-C1-O20-C21
7	A	612	OLC	C14-C15-C16-C17
7	B	201	OLC	C2-C1-O20-C21
7	B	201	OLC	C2-C3-C4-C5
7	A	605	OLC	O20-C21-C22-C24
7	B	203	OLC	C3-C4-C5-C6
7	A	609	OLC	C4-C5-C6-C7
7	A	607	OLC	C5-C6-C7-C8
7	A	604	OLC	C10-C11-C12-C13
7	B	204	OLC	C10-C11-C12-C13
7	A	606	OLC	C5-C6-C7-C8
7	C	101	OLC	C5-C6-C7-C8
7	B	203	OLC	C5-C6-C7-C8
7	B	203	OLC	O19-C1-O20-C21
7	C	101	OLC	C10-C11-C12-C13
7	A	606	OLC	O20-C21-C22-C24
7	A	608	OLC	C4-C5-C6-C7
7	B	203	OLC	C9-C10-C11-C12
7	A	605	OLC	C1-C2-C3-C4
7	B	201	OLC	O19-C1-O20-C21
7	B	201	OLC	C10-C11-C12-C13
7	A	607	OLC	C2-C3-C4-C5
7	A	608	OLC	C7-C8-C9-C10
7	A	611	OLC	O23-C22-C24-O25
7	A	608	OLC	O20-C21-C22-O23
7	B	201	OLC	C14-C15-C16-C17
7	B	204	OLC	C7-C8-C9-C10
7	B	203	OLC	C12-C13-C14-C15
6	A	603	HAS	CAD-CBD-CGD-O1D
7	A	609	OLC	C2-C3-C4-C5
7	A	611	OLC	C11-C12-C13-C14
7	B	201	OLC	C11-C10-C9-C8
6	A	603	HAS	CAA-CBA-CGA-O2A
6	A	603	HAS	CAA-CBA-CGA-O1A
7	A	605	OLC	C3-C4-C5-C6
7	A	611	OLC	C9-C10-C11-C12
6	A	603	HAS	C23-C24-C28-C29
7	A	608	OLC	O20-C21-C22-C24
7	B	203	OLC	O20-C21-C22-C24
7	A	606	OLC	O20-C1-C2-C3
6	A	603	HAS	CAD-CBD-CGD-O2D
7	B	201	OLC	C9-C10-C11-C12

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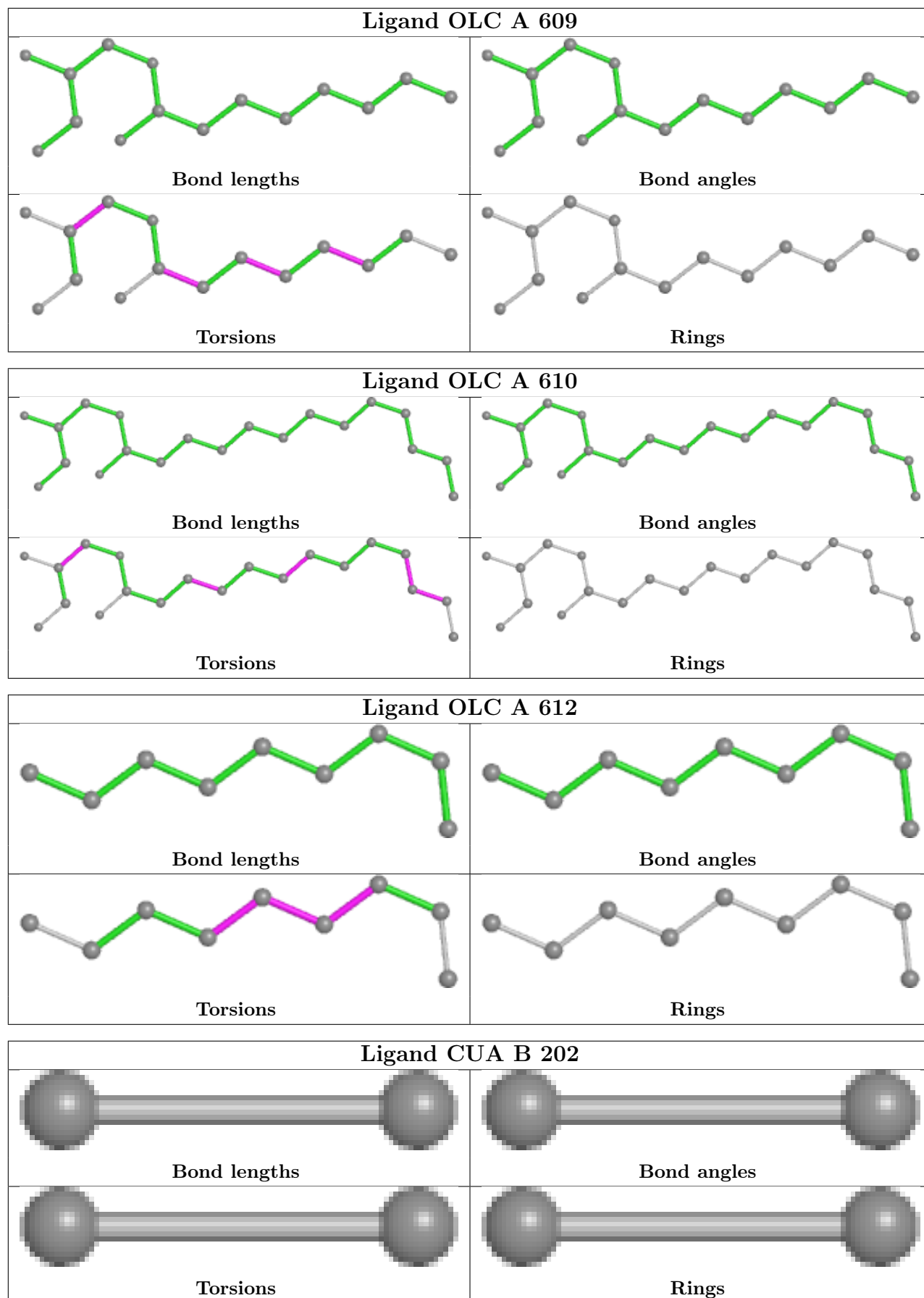
Mol	Chain	Res	Type	Atoms
7	C	102	OLC	C5-C6-C7-C8
7	C	101	OLC	C7-C8-C9-C10
7	A	605	OLC	O23-C22-C24-O25
7	A	608	OLC	O20-C1-C2-C3
7	A	610	OLC	C9-C10-C11-C12
7	A	604	OLC	C7-C8-C9-C10
7	C	101	OLC	C9-C10-C11-C12
7	A	606	OLC	O19-C1-C2-C3
7	A	612	OLC	C13-C14-C15-C16
7	B	204	OLC	C3-C4-C5-C6
7	A	609	OLC	O20-C1-C2-C3
7	A	607	OLC	O20-C1-C2-C3
7	A	609	OLC	O20-C21-C22-O23
7	A	609	OLC	O19-C1-C2-C3
5	A	602	HEM	CAD-CBD-CGD-O2D

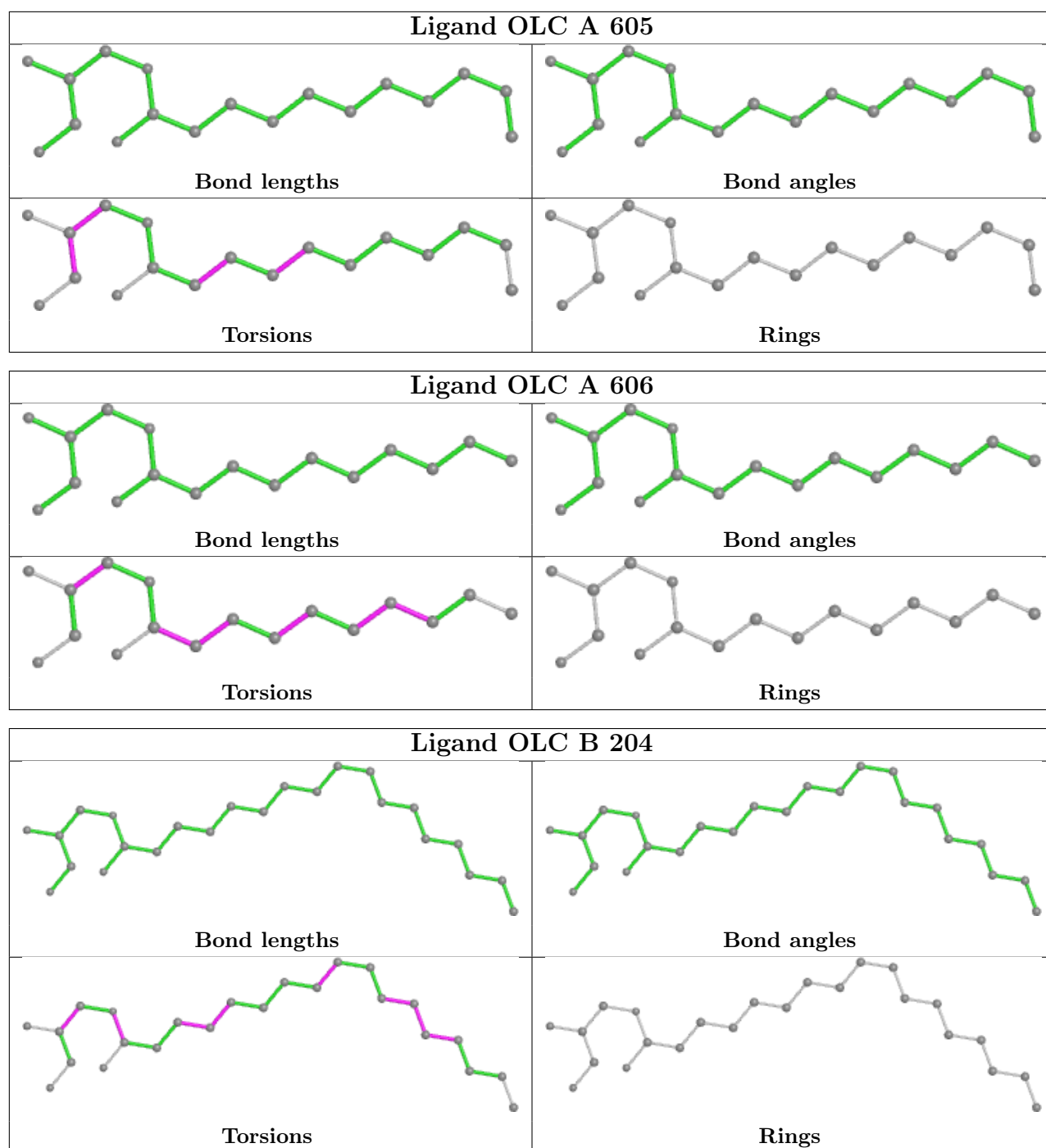
There are no ring outliers.

5 monomers are involved in 6 short contacts:

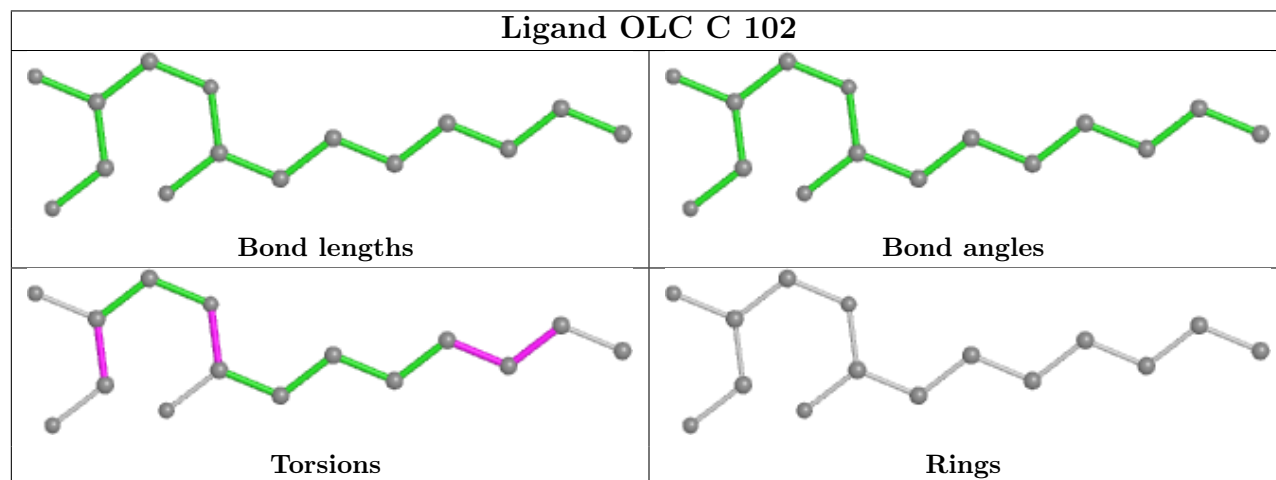
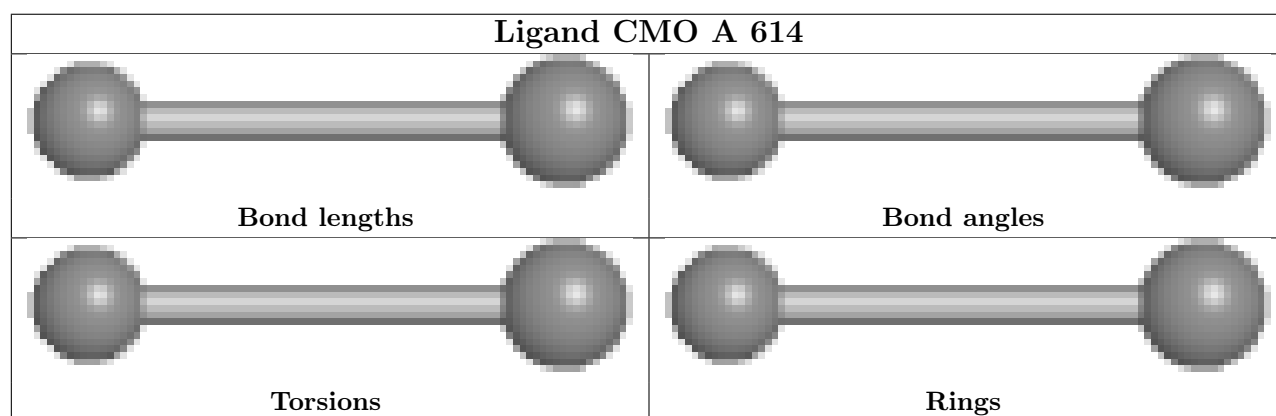
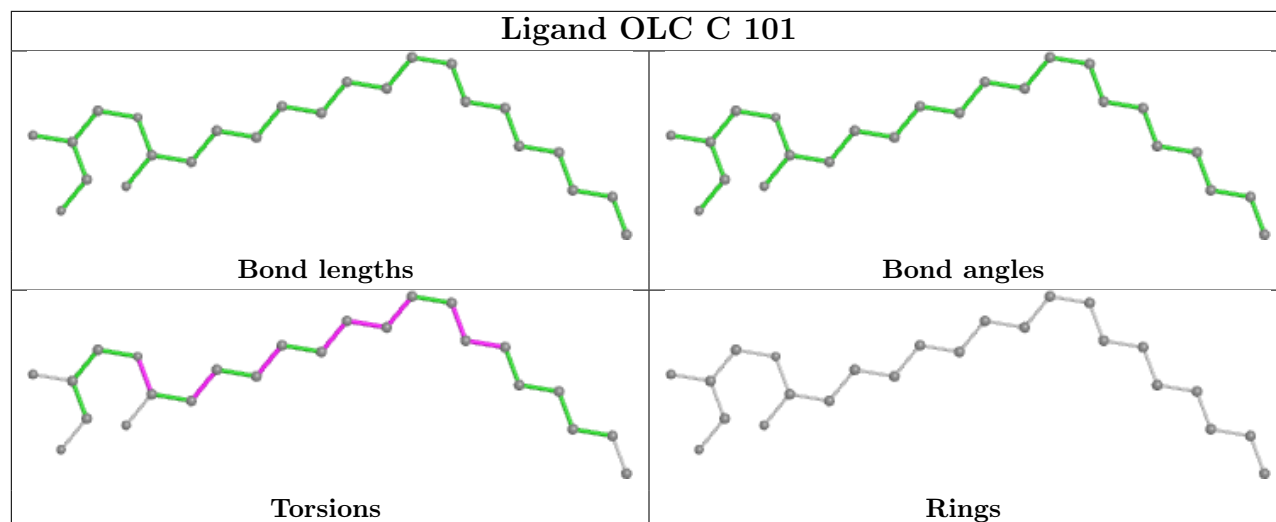
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	606	OLC	1	0
7	B	203	OLC	2	0
5	A	602	HEM	1	0
6	A	603	HAS	1	0
7	A	608	OLC	1	0

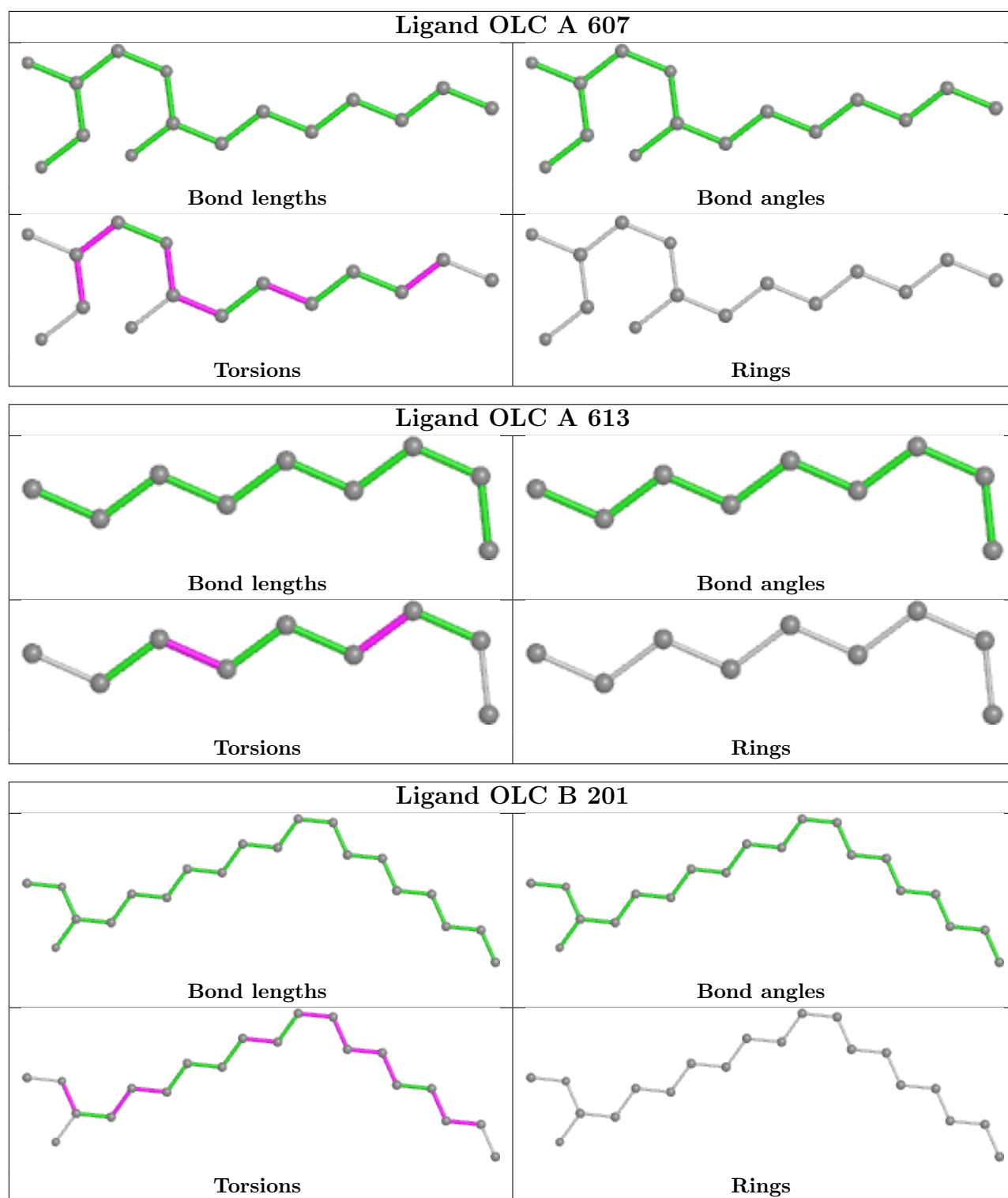
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

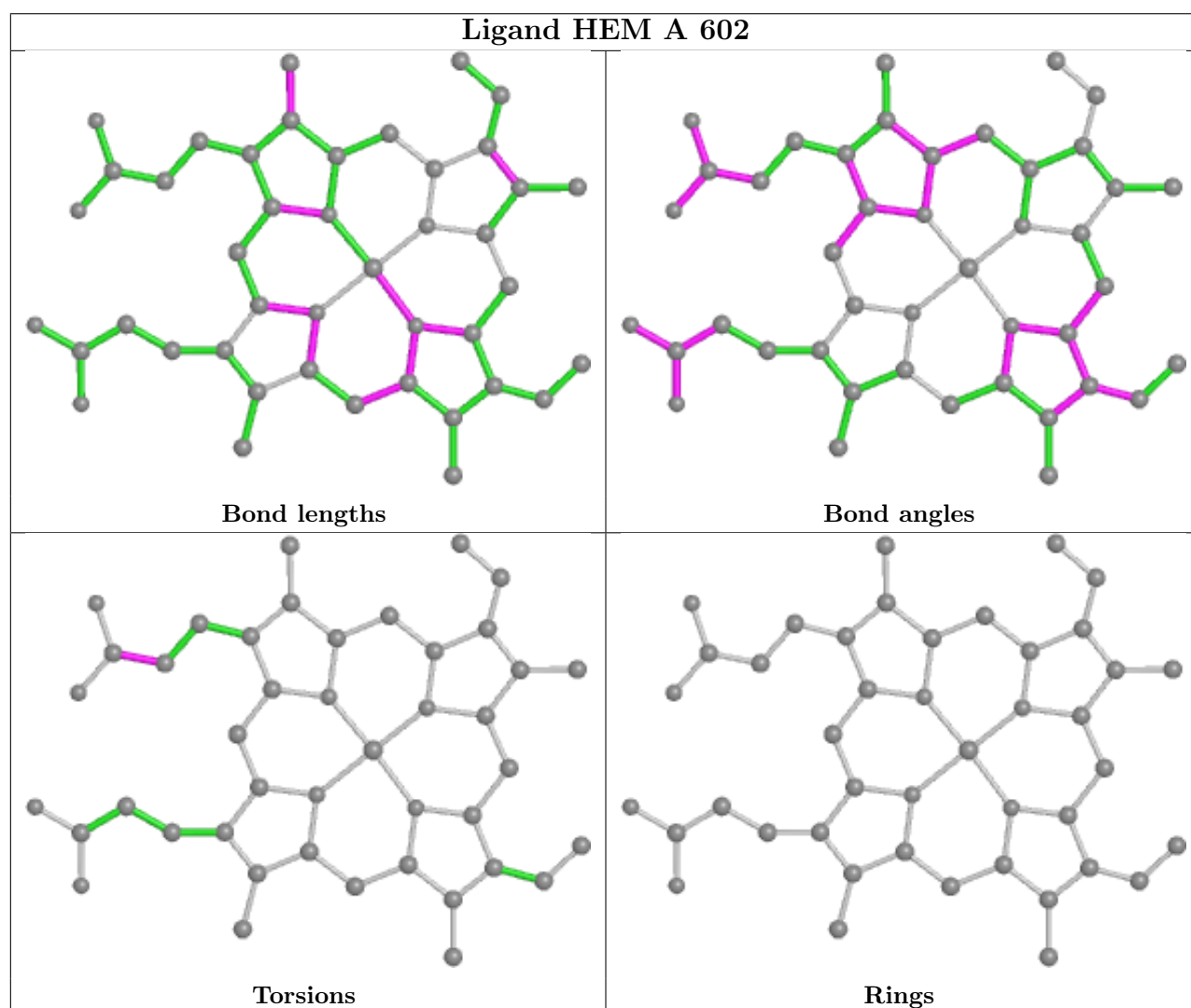
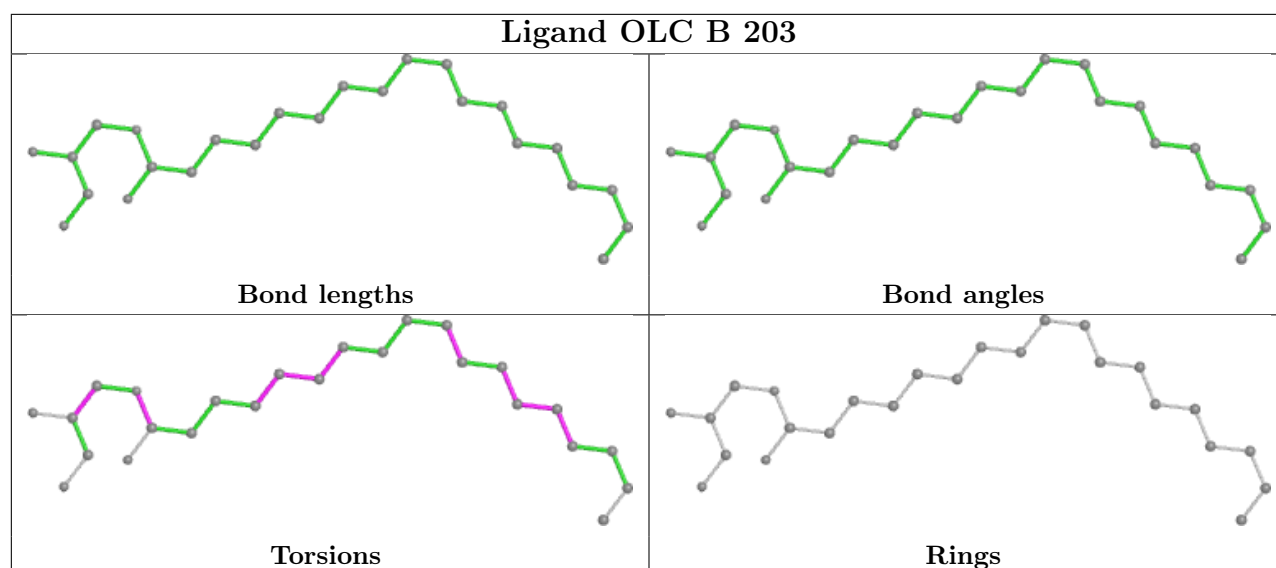


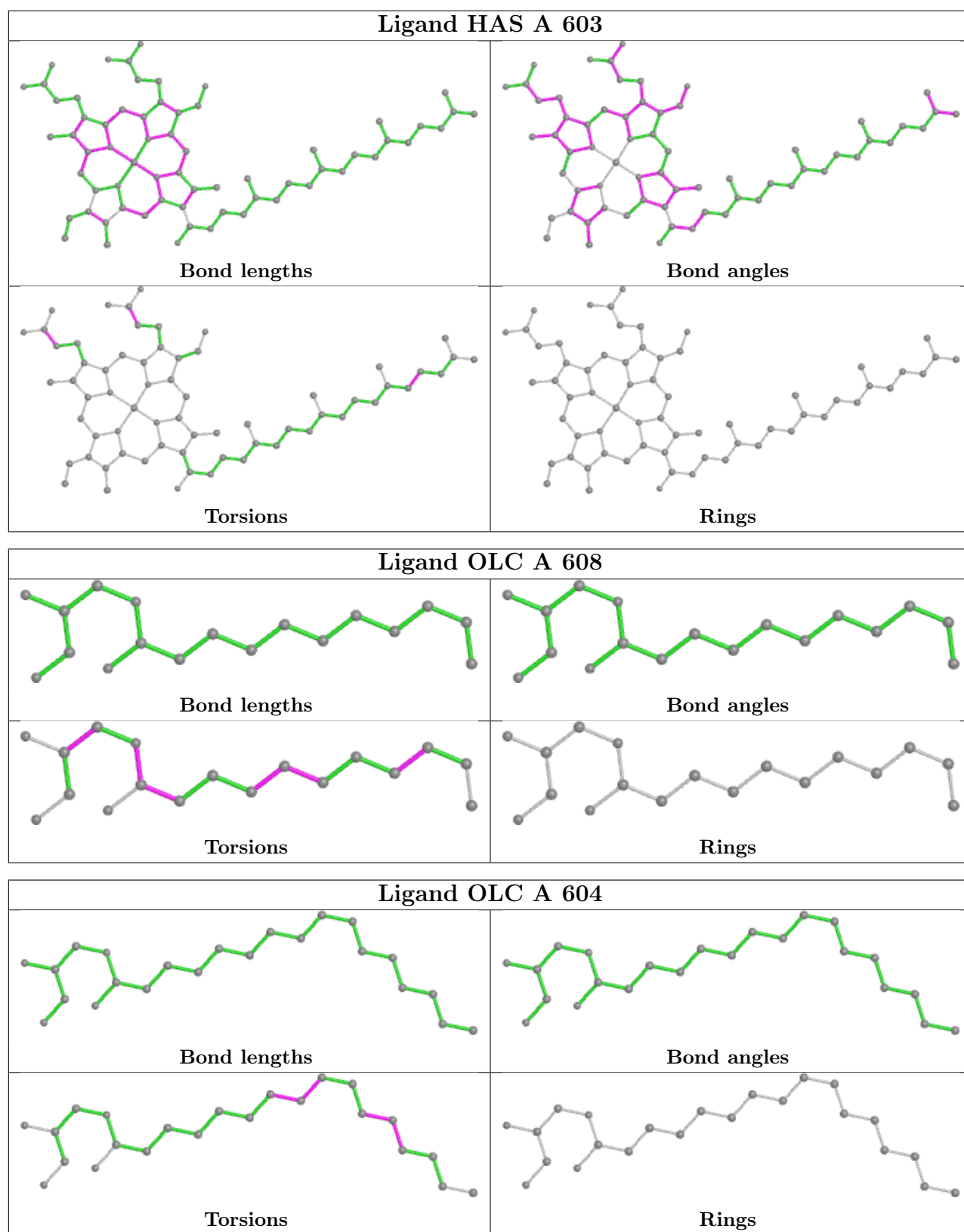


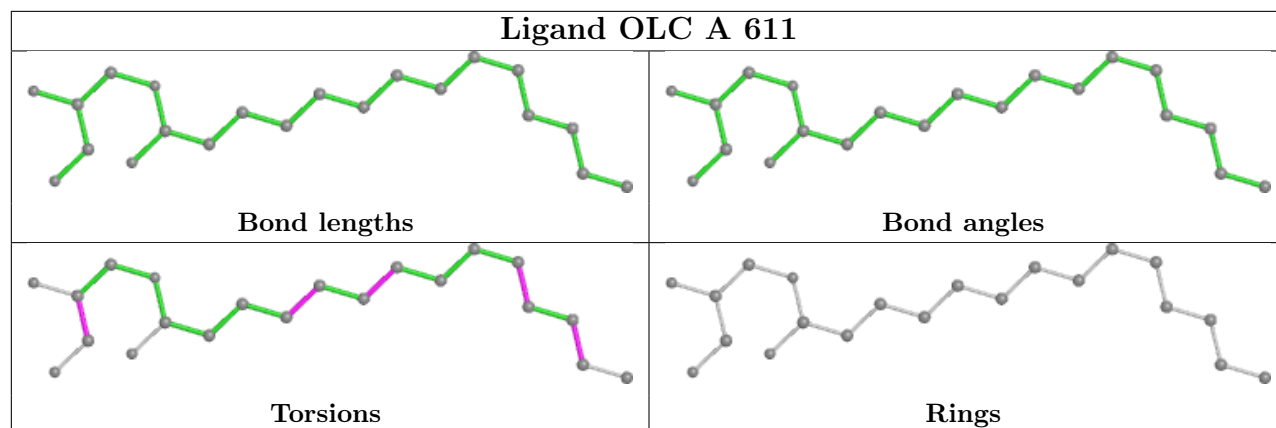












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	1.47	142 (25%) 0 0	21, 32, 59, 91	0
2	B	167/168 (99%)	1.14	24 (14%) 2 2	22, 32, 57, 104	0
3	C	31/34 (91%)	1.07	2 (6%) 18 18	27, 34, 42, 66	0
All	All	752/771 (97%)	1.38	168 (22%) 0 0	21, 32, 59, 104	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	16.2
1	A	519	ARG	6.6
1	A	515	PRO	6.5
1	A	495	ARG	6.5
1	A	333	PHE	6.4
1	A	9	SER	5.5
1	A	494	SER	5.5
1	A	331	GLY	5.3
1	A	175	PRO	5.3
2	B	5	HIS	5.1
1	A	60	PRO	5.0
2	B	3	ASP	4.9
1	A	493	LEU	4.9
1	A	57	ARG	4.8
1	A	389	VAL	4.7
2	B	76	PRO	4.6
1	A	496	GLU	4.6
1	A	235	ILE	4.5
1	A	11	VAL	4.4
1	A	172	ALA	4.4
1	A	58	LEU	4.1
1	A	240	LEU	4.1
1	A	241	LEU	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	247	ILE	4.1
1	A	236	VAL	4.0
1	A	551	GLY	3.9
1	A	334	GLY	3.9
1	A	492	LEU	3.9
1	A	491	VAL	3.9
1	A	514	GLY	3.9
1	A	173	ALA	3.8
1	A	332	LEU	3.8
1	A	246	ILE	3.8
1	A	393	VAL	3.8
2	B	168	GLU	3.7
1	A	239	TRP	3.6
1	A	10	ARG	3.6
1	A	497	ARG	3.6
1	A	381	VAL	3.6
1	A	499	PRO	3.5
1	A	337	ARG	3.5
2	B	140	LYS	3.5
1	A	518	ARG	3.5
1	A	490	SER	3.5
1	A	53	PRO	3.5
1	A	174	ASN	3.4
1	A	238	PHE	3.4
1	A	176	GLY	3.4
1	A	78	ILE	3.3
1	A	326	LEU	3.3
1	A	392	LEU	3.3
1	A	397	ALA	3.3
1	A	88	ILE	3.3
1	A	412	PRO	3.2
1	A	486	TYR	3.2
1	A	330	ARG	3.2
1	A	536	ILE	3.2
2	B	75	GLY	3.1
1	A	55	LEU	3.1
2	B	7	ALA	3.0
1	A	32	LEU	3.0
1	A	353	LEU	3.0
1	A	489	PHE	3.0
1	A	54	LEU	3.0
1	A	84	PHE	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	522	LEU	3.0
1	A	517	ASP	3.0
1	A	132	LEU	3.0
1	A	385	PHE	3.0
2	B	6	LYS	3.0
1	A	329	GLY	2.9
1	A	405	LEU	2.9
1	A	133	TYR	2.9
1	A	83	LEU	2.9
1	A	547	VAL	2.8
1	A	513	SER	2.8
1	A	242	PRO	2.8
1	A	488	LEU	2.8
1	A	501	LEU	2.8
3	C	12	ILE	2.8
1	A	498	LYS	2.8
1	A	77	ALA	2.8
1	A	69	LEU	2.8
1	A	217	GLU	2.7
1	A	414	SER	2.7
1	A	396	THR	2.7
1	A	500	GLU	2.7
1	A	189	PHE	2.7
1	A	92	LEU	2.7
1	A	244	TYR	2.7
1	A	479	VAL	2.6
1	A	269	PHE	2.6
1	A	529	PHE	2.6
3	C	11	VAL	2.6
1	A	160	ILE	2.6
1	A	134	THR	2.6
1	A	245	ALA	2.6
1	A	59	LEU	2.6
2	B	113	ILE	2.5
1	A	15	TYR	2.5
1	A	520	LEU	2.5
1	A	415	ASP	2.5
1	A	516	GLU	2.5
1	A	25	LEU	2.5
1	A	178	VAL	2.5
1	A	136	TYR	2.5
1	A	356	PHE	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	117	LEU	2.4
1	A	395	LEU	2.4
1	A	527	ILE	2.4
2	B	85	ALA	2.4
1	A	80	PHE	2.4
1	A	416	ALA	2.4
1	A	12	TYR	2.4
1	A	336	ILE	2.4
1	A	168	ARG	2.4
2	B	142	PRO	2.4
2	B	141	ARG	2.4
1	A	153	VAL	2.3
1	A	325	ARG	2.3
1	A	552	HIS	2.3
1	A	81	THR	2.3
1	A	124	LEU	2.3
1	A	229	TRP	2.3
1	A	532	ALA	2.3
1	A	404	LEU	2.3
2	B	152	TYR	2.3
1	A	228	PHE	2.3
1	A	305	VAL	2.3
1	A	316	VAL	2.2
1	A	375	VAL	2.2
2	B	123	ILE	2.2
1	A	161	TYR	2.2
2	B	112	VAL	2.2
1	A	74	VAL	2.2
1	A	328	GLY	2.2
1	A	367	ALA	2.2
1	A	485	ILE	2.2
1	A	538	VAL	2.2
2	B	11	ILE	2.2
1	A	135	PHE	2.2
1	A	170	TRP	2.1
2	B	127	VAL	2.1
1	A	526	ARG	2.1
1	A	462	HIS	2.1
2	B	107	ILE	2.1
1	A	208	LEU	2.1
2	B	84	LEU	2.1
1	A	185	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	193	TRP	2.1
2	B	77	ASN	2.1
1	A	549	LEU	2.1
2	B	128	LEU	2.1
1	A	350	VAL	2.1
1	A	243	ALA	2.1
2	B	10	ALA	2.1
1	A	248	TYR	2.1
1	A	177	LYS	2.1
1	A	250	ILE	2.1
1	A	468	VAL	2.1
1	A	533	VAL	2.1
1	A	272	PHE	2.1
1	A	259	LEU	2.0
2	B	125	VAL	2.0
1	A	152	PHE	2.0
1	A	286	ALA	2.0
1	A	548	GLN	2.0
1	A	224	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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.

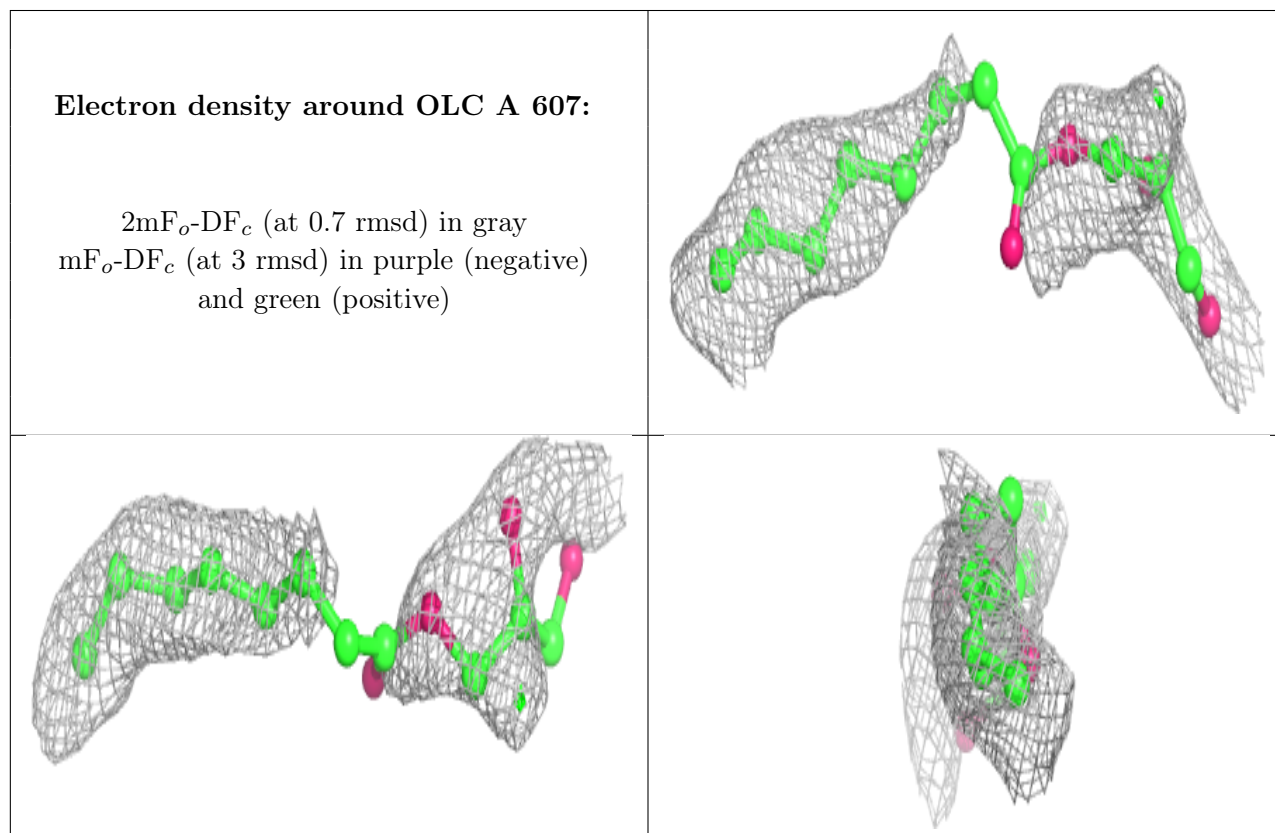
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	OLC	A	607	15/25	0.16	0.37	67,84,97,99	0
7	OLC	C	102	15/25	0.41	0.27	67,74,89,92	0
7	OLC	C	101	24/25	0.44	0.27	54,66,98,101	0
7	OLC	A	609	15/25	0.51	0.22	80,94,101,102	0

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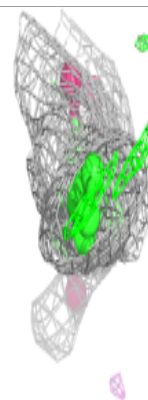
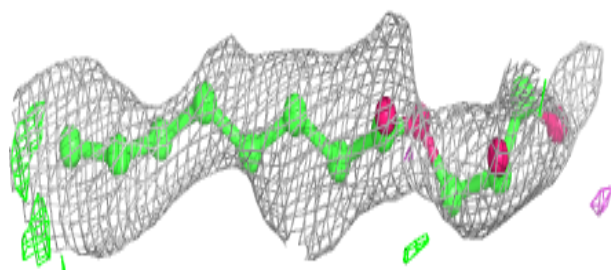
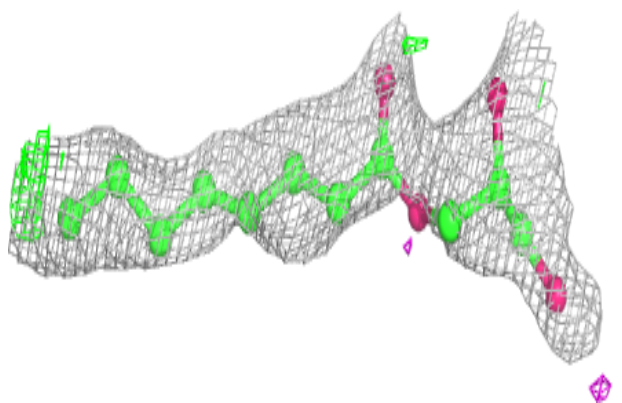
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	OLC	A	608	18/25	0.55	0.23	62,79,91,92	0
7	OLC	A	606	17/25	0.59	0.26	70,73,88,91	0
7	OLC	B	203	25/25	0.60	0.20	64,68,86,101	0
7	OLC	A	611	21/25	0.64	0.26	56,77,94,105	0
7	OLC	A	605	18/25	0.65	0.21	61,77,95,102	0
7	OLC	A	610	20/25	0.68	0.21	70,80,96,100	0
7	OLC	B	204	24/25	0.68	0.20	68,80,93,103	0
7	OLC	B	201	20/25	0.69	0.14	69,77,86,97	0
7	OLC	A	613	9/25	0.71	0.19	56,59,75,76	0
7	OLC	A	604	23/25	0.79	0.15	42,60,91,94	0
5	HEM	A	602	43/43	0.80	0.23	20,23,27,36	0
6	HAS	A	603	65/65	0.80	0.26	20,26,44,59	0
8	CMO	A	614	2/2	0.83	0.22	20,20,20,26	0
7	OLC	A	612	9/25	0.85	0.11	64,69,74,77	0
9	CUA	B	202	2/2	0.98	0.10	25,25,25,26	0
4	CU	A	601	1/1	0.99	0.13	29,29,29,29	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.

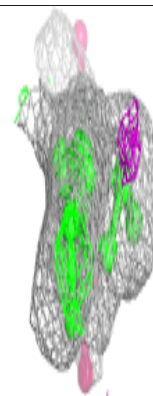
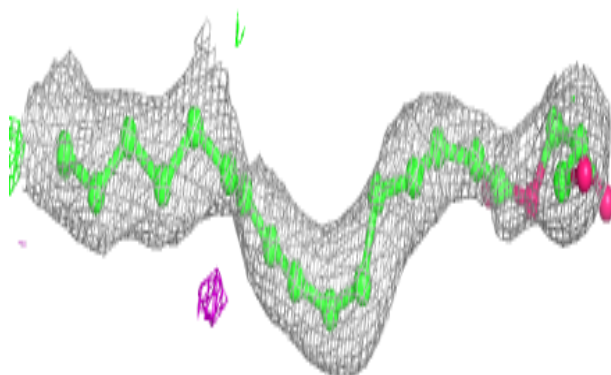
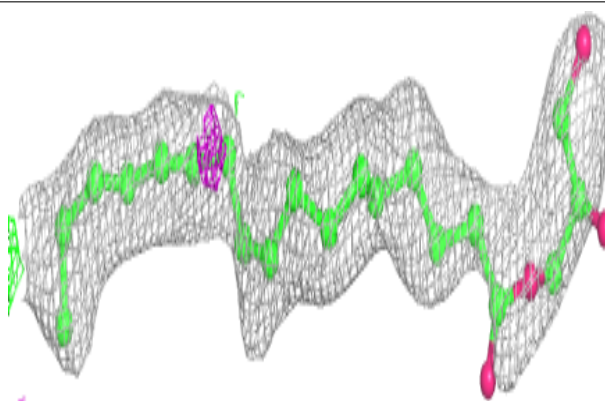


**Electron density around OLC C 102:**

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

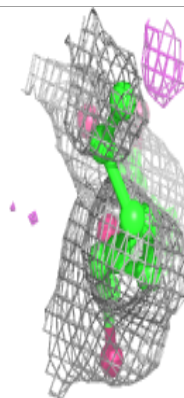
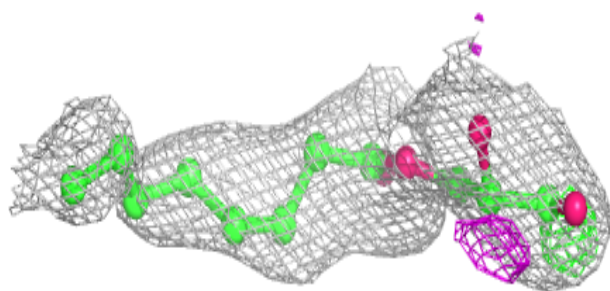
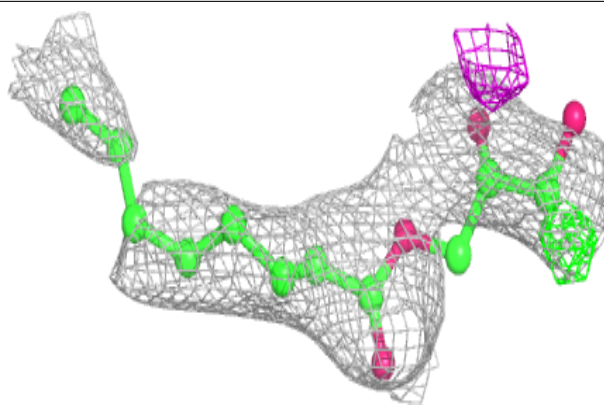
**Electron density around OLC C 101:**

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

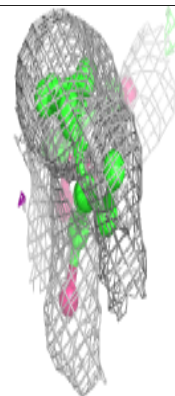
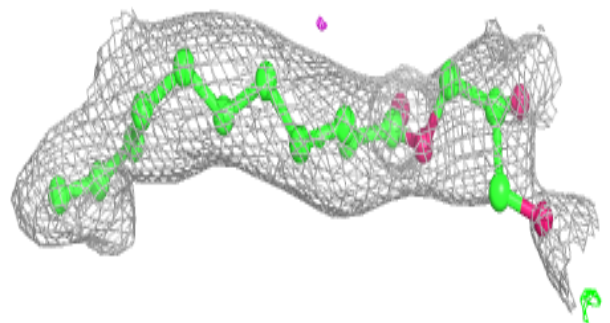
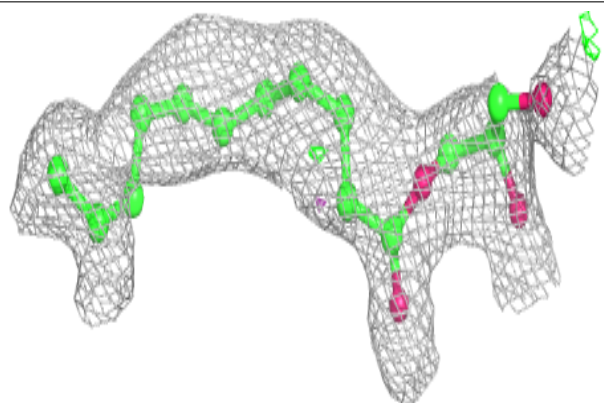


**Electron density around OLC A 609:**

$2mF_o-DF_c$  (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:**

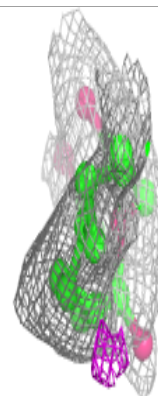
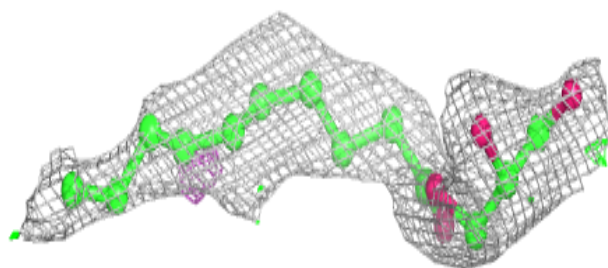
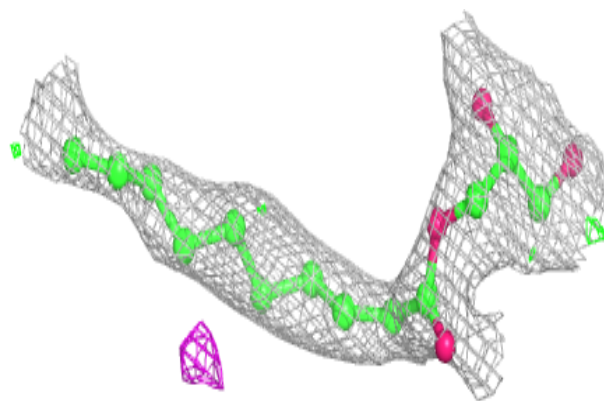
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



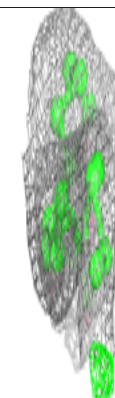
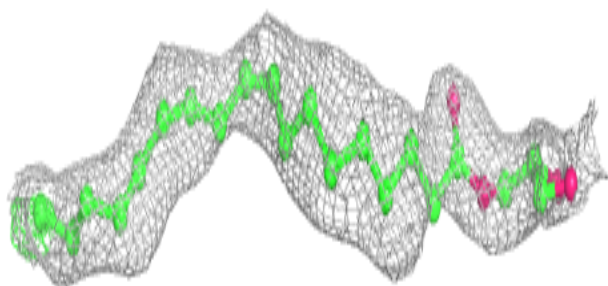
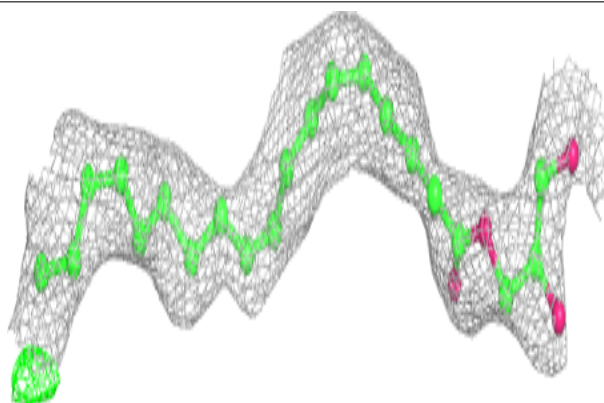


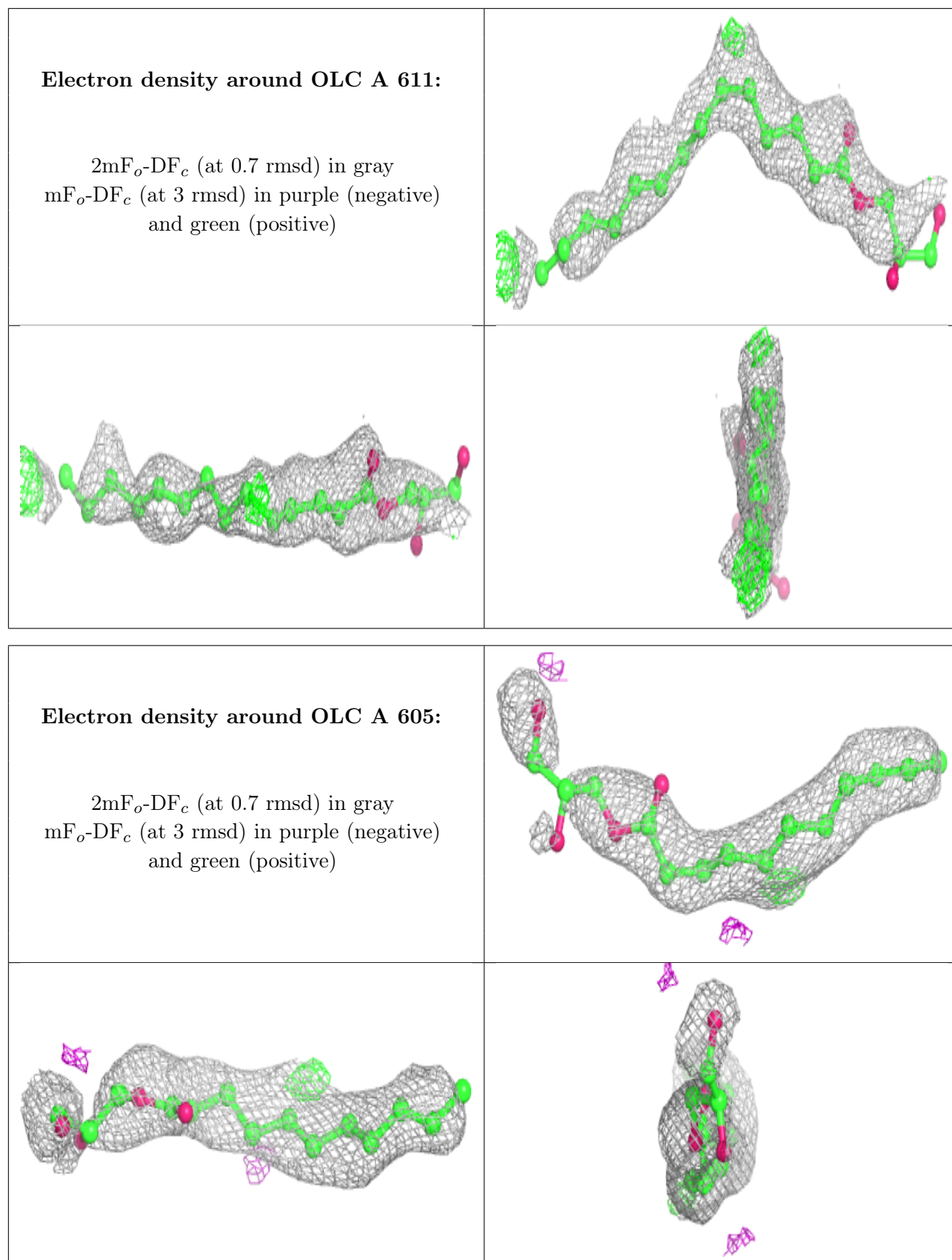
**Electron density around OLC A 606:**

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

**Electron density around OLC B 203:**

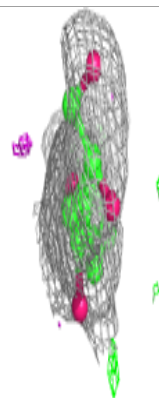
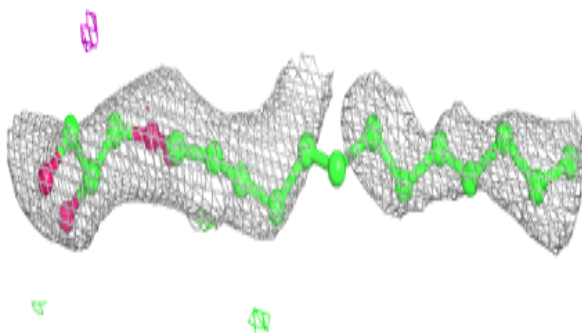
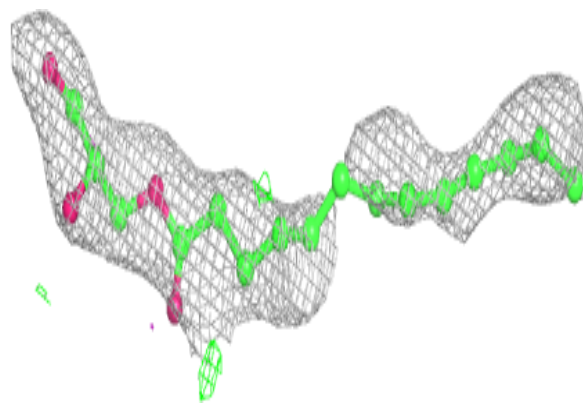
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



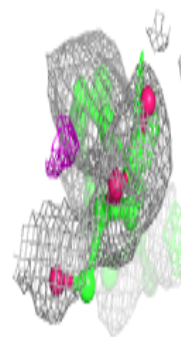
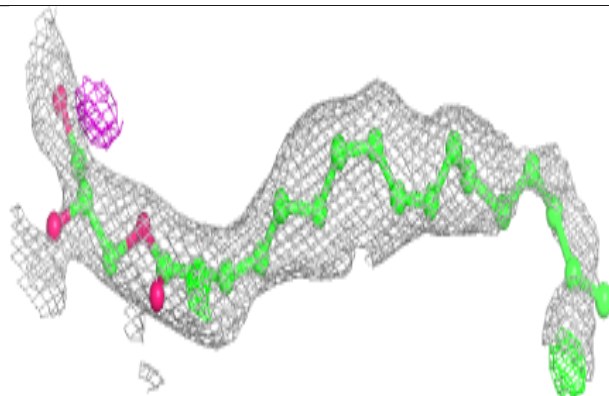
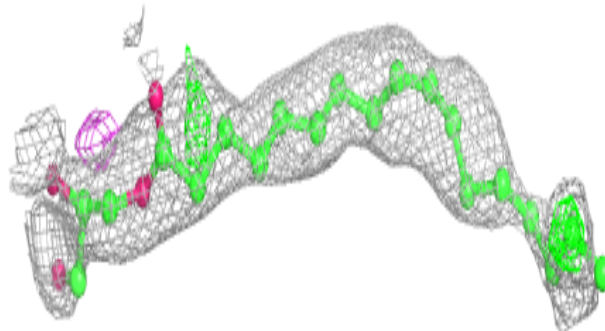


**Electron density around OLC A 610:**

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

**Electron density around OLC B 204:**

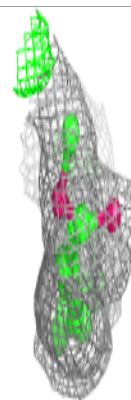
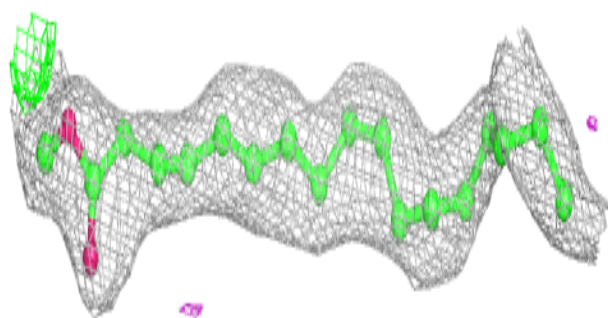
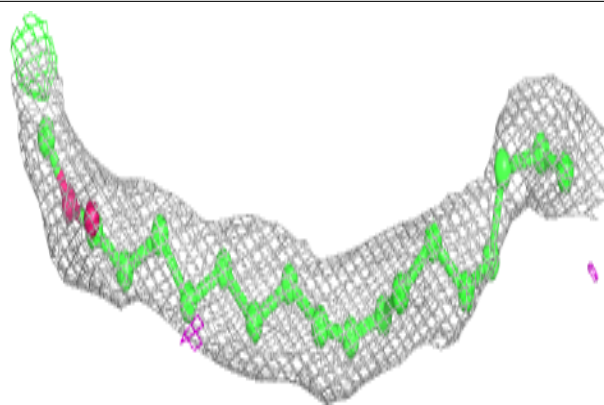
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



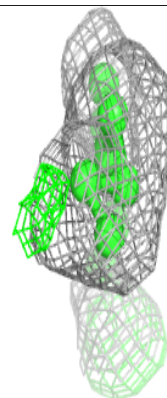
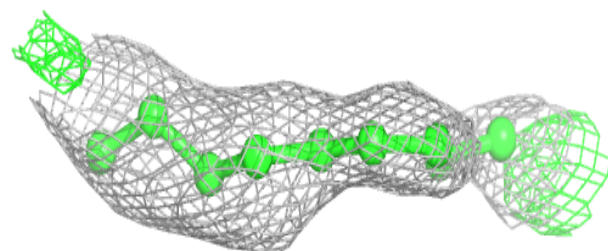
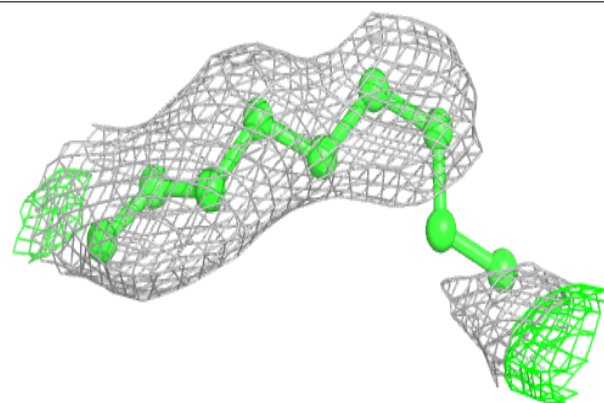


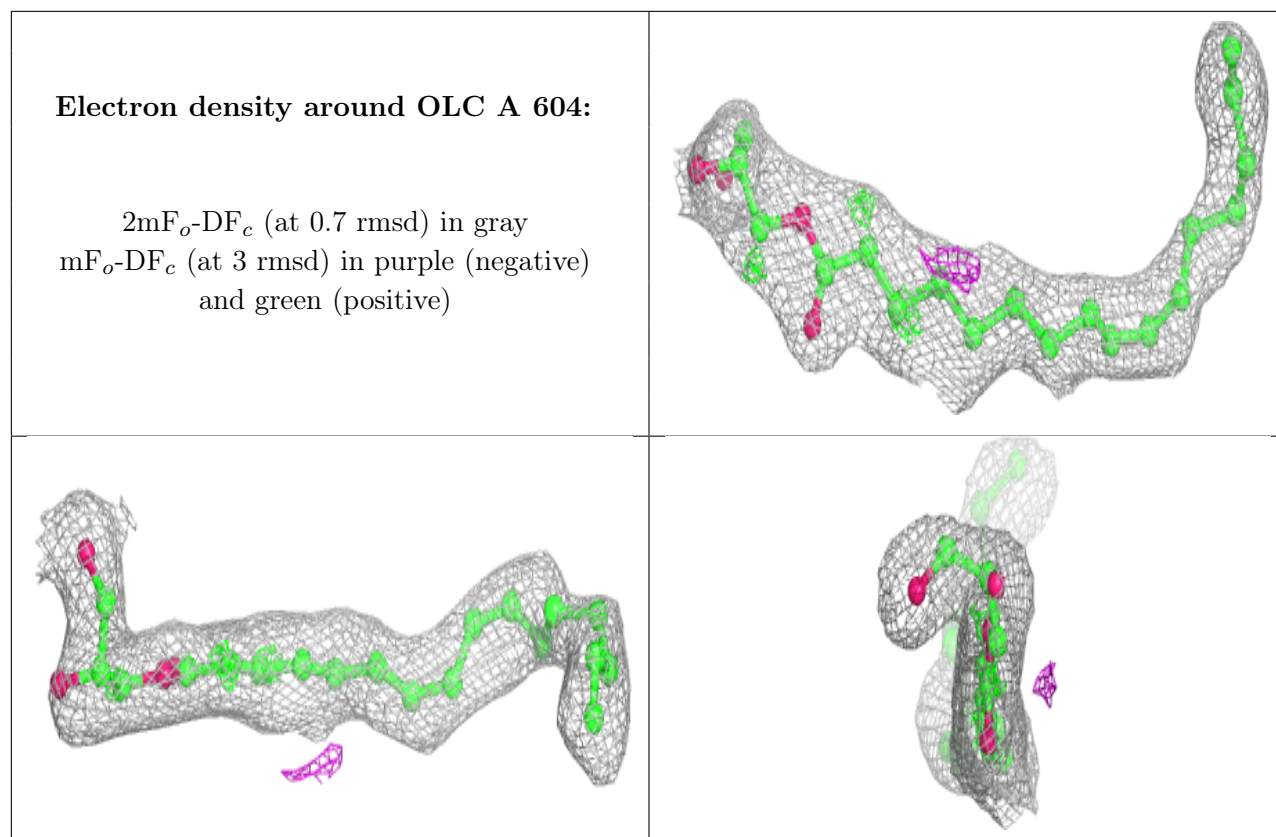
**Electron density around OLC B 201:**

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

**Electron density around OLC A 613:**

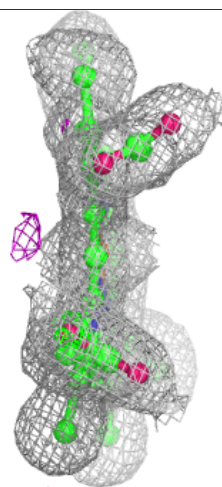
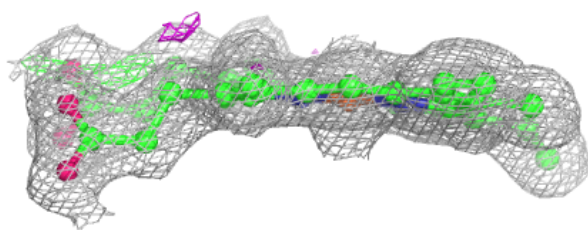
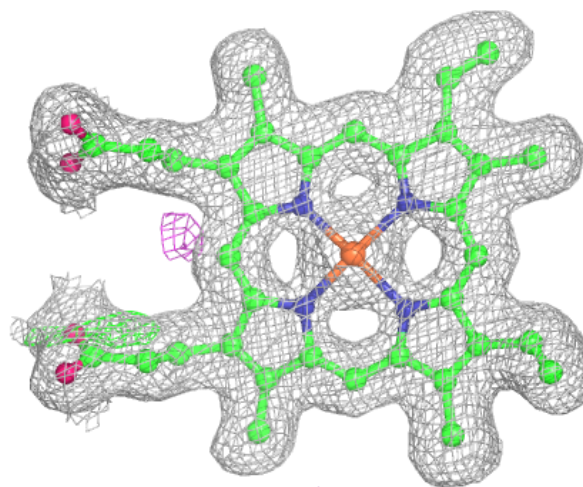
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

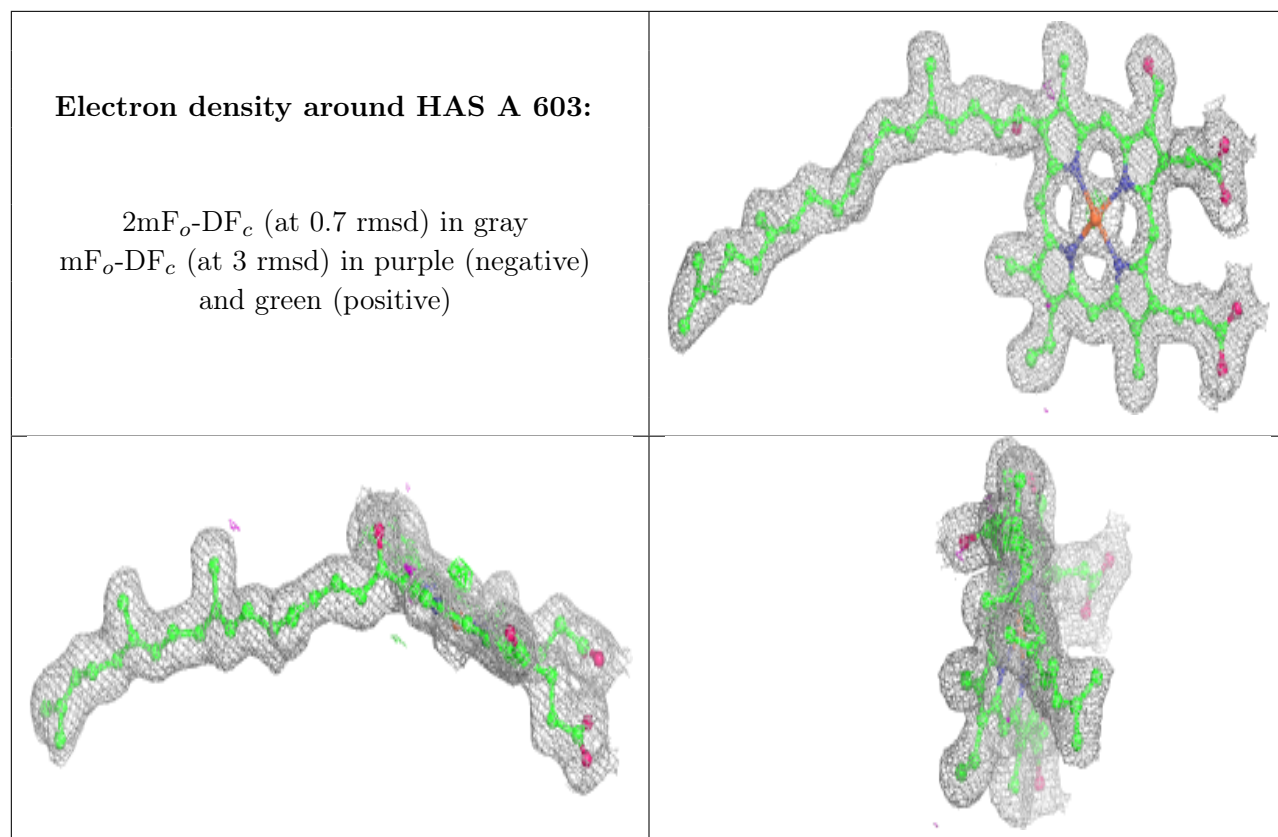




**Electron density around HEM A 602:**

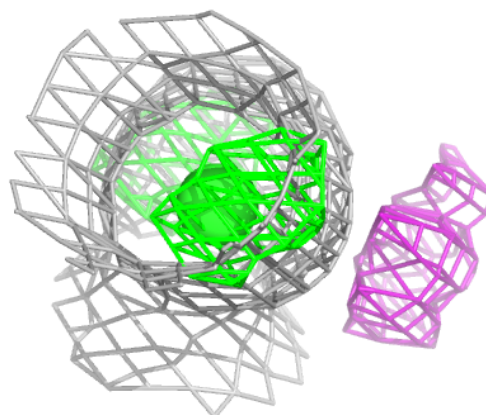
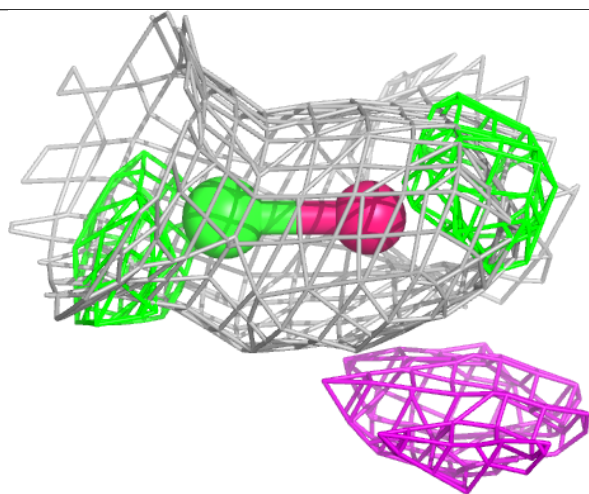
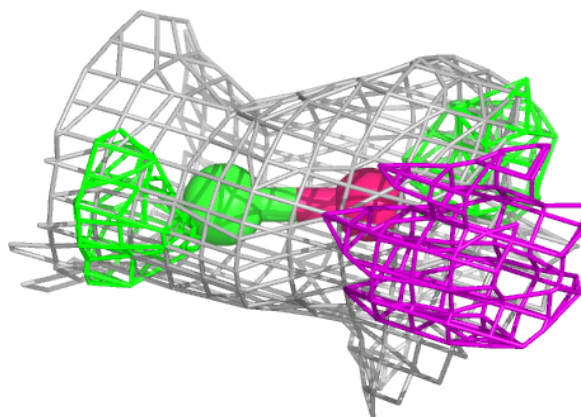
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



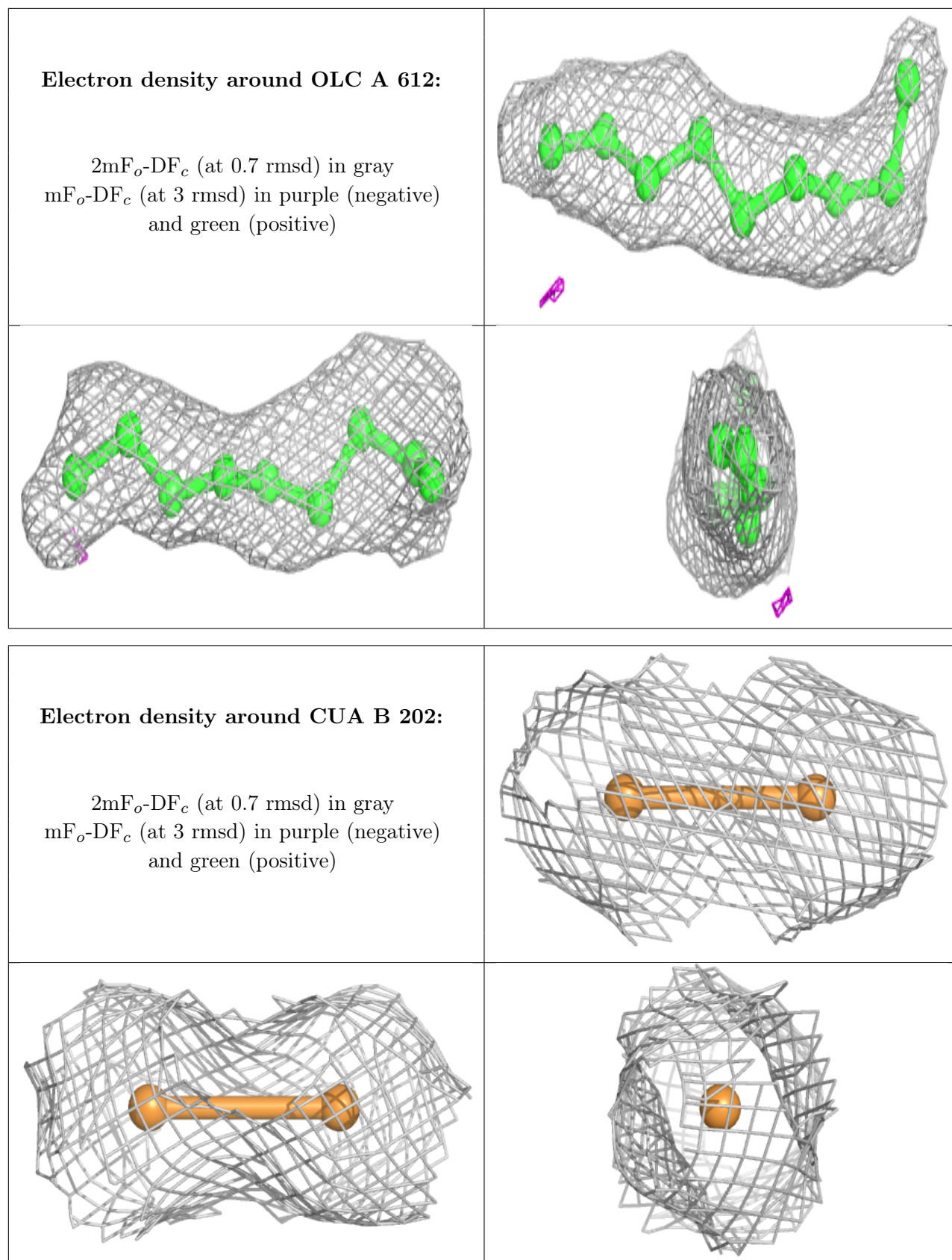


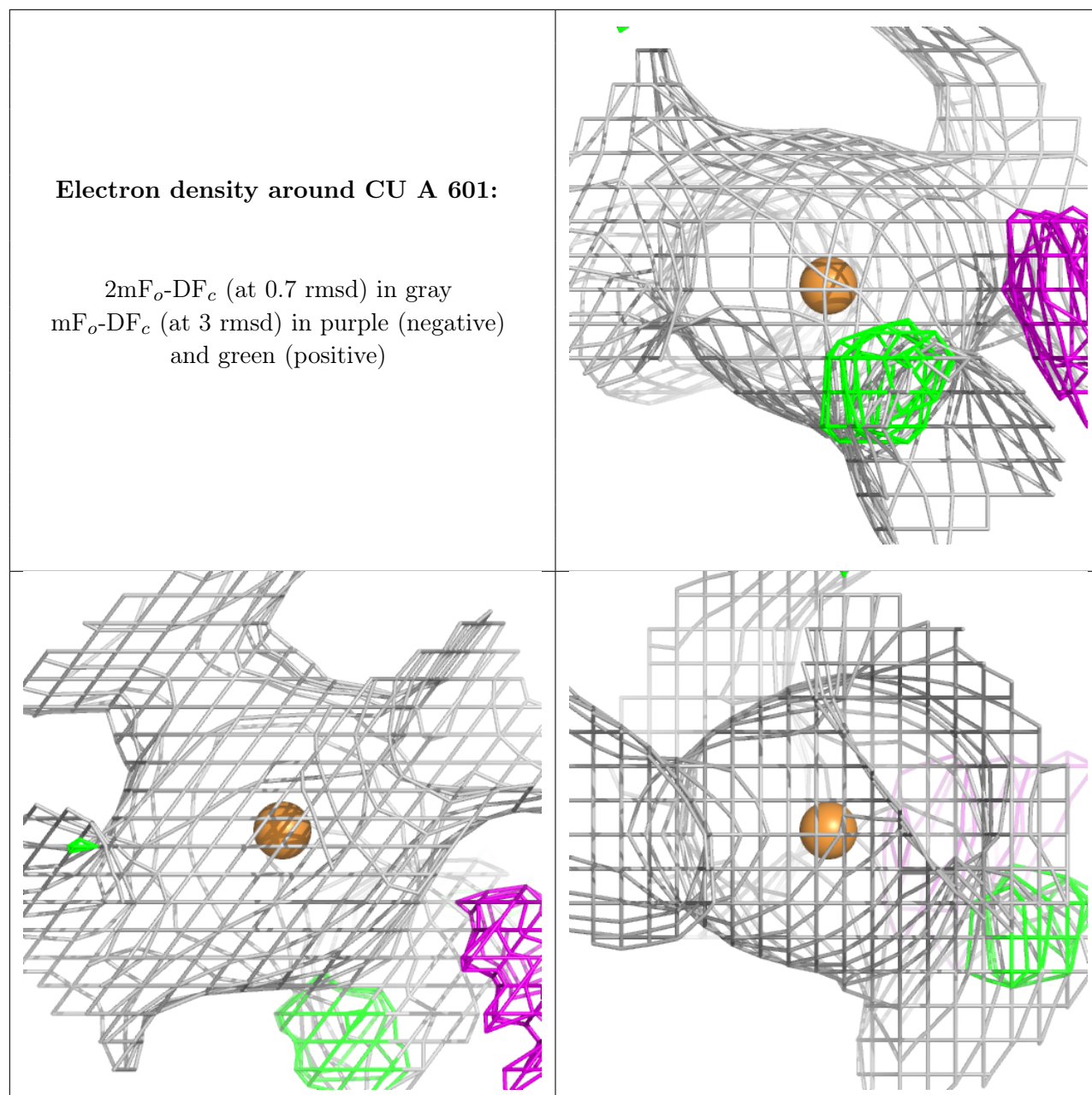
**Electron density around CMO A 614:**

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









## 6.5 Other polymers ⓘ

There are no such residues in this entry.