



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 01:31 pm GMT

PDB ID : 5NDC  
Title : Structure of ba3-type cytochrome c oxidase from *Thermus thermophilus* by serial femtosecond crystallography  
Authors : Andersson, R.; Safari, C.; Dods, R.; Nango, E.; Tanaka, R.; Nakane, T.; Tono, K.; Joti, Y.; Bath, P.; Dunevall, E.; Bosman, E.; Nureki, O.; Iwata, S.; Neutze, R.; Branden, G.  
Deposited on : 2017-03-08  
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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, 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

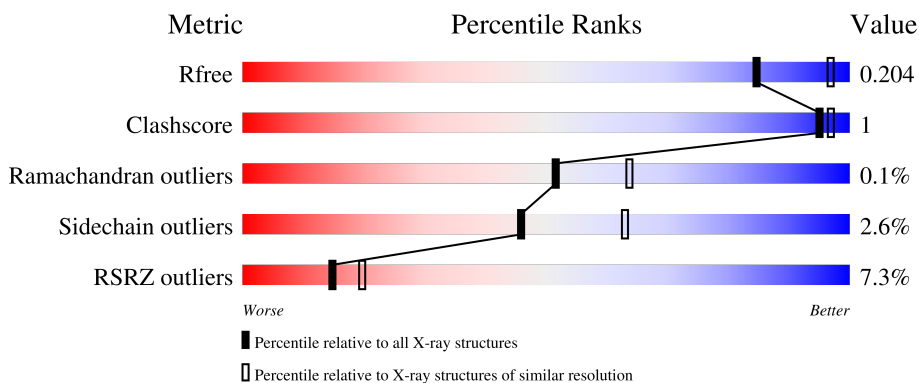
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	 9% 92% 5% . .
2	B	168	 4% 95% . .
3	C	34	 91% 9%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6386 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

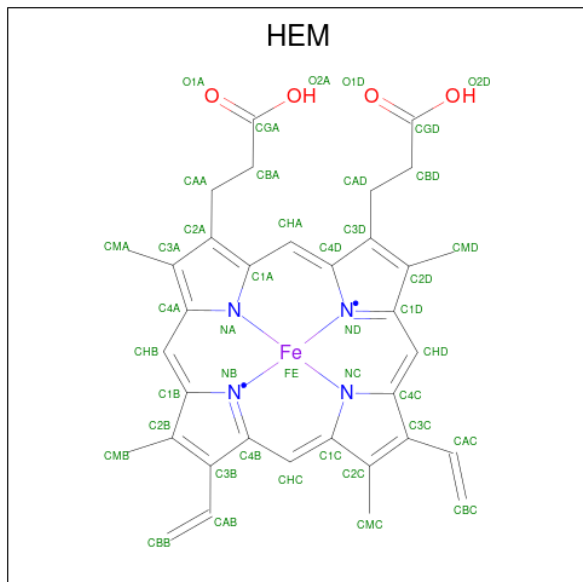
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide IIA.

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).

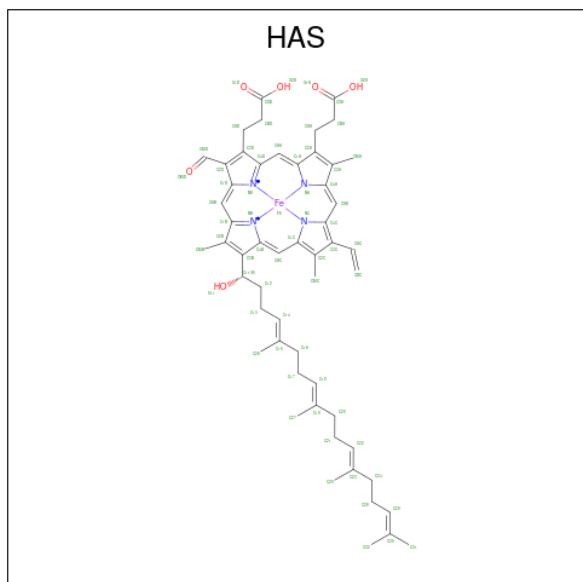
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



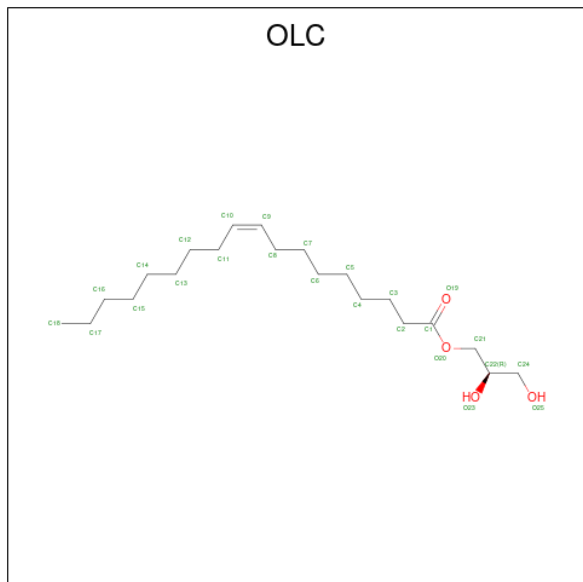
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
5	A	1	43	34	1	4	4	0	0

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



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>).



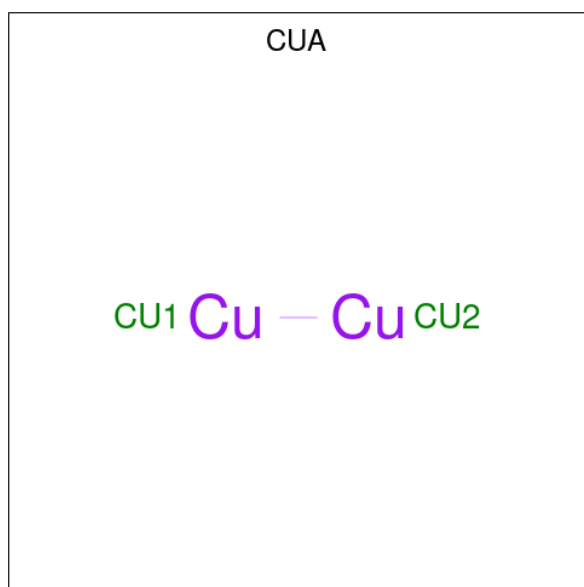
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C O	0	0
			23	19 4		
7	A	1	Total	C O	0	0
			18	14 4		
7	A	1	Total	C O	0	0
			17	13 4		
7	A	1	Total	C O	0	0
			15	11 4		
7	A	1	Total	C O	0	0
			18	14 4		
7	A	1	Total	C O	0	0
			15	11 4		
7	A	1	Total	C O	0	0
			20	16 4		
7	A	1	Total	C O	0	0
			21	17 4		
7	A	1	Total	C O	0	0
			20	18 2		
7	A	1	Total	C	0	0
			9	9		
7	A	1	Total	C	0	0
			9	9		
7	B	1	Total	C O	0	0
			25	21 4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			24	20	4		
7	C	1	Total	C	O	0	0
			15	11	4		
7	C	1	Total	C	O	0	0
			24	20	4		

- Molecule 8 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

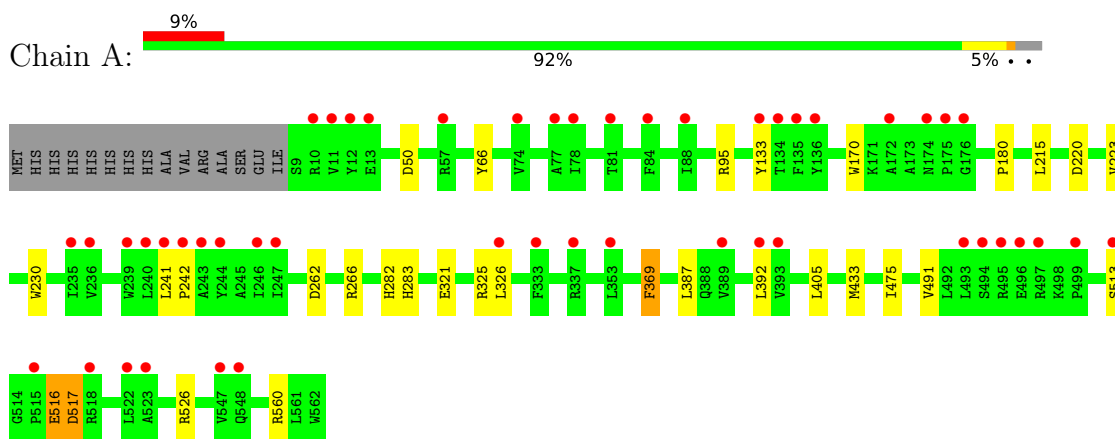
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	58	Total	O	0	0
			58	58		
9	B	34	Total	O	0	0
			34	34		

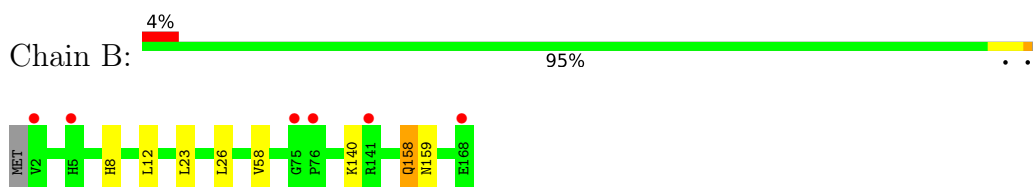
### 3 Residue-property plots [i](#)

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.

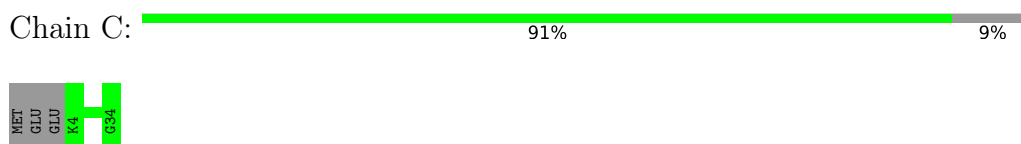
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase polypeptide IIA





## 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)	36.40 – 2.30 36.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.40-2.30) 99.9 (36.31-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.162 , 0.197 0.173 , 0.204	Depositor DCC
$R_{free}$ test set	2511 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 72.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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, CUA, HEM, OLC, 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	0.59	1/4525 (0.0%)	0.72	8/6213 (0.1%)
2	B	0.57	0/1338	0.70	0/1828
3	C	0.56	0/247	0.60	0/335
All	All	0.59	1/6110 (0.0%)	0.71	8/8376 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	GLU	CD-OE2	5.15	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	ASP	CB-CG-OD1	10.99	128.19	118.30
1	A	95	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	517	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	50	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	95	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	266	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	266	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	560	ARG	NE-CZ-NH1	-5.14	117.73	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	12	0
2	B	1301	0	1278	2	0
3	C	241	0	267	0	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
6	A	65	0	62	1	0
7	A	185	0	257	0	0
7	B	25	0	40	0	0
7	C	63	0	89	0	0
8	B	2	0	0	0	0
9	A	58	0	0	1	1
9	B	34	0	0	0	0
All	All	6386	0	6490	15	1

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 1.

All (15) 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:516:GLU:OE2	2:B:8:HIS:NE2	2.01	0.94
1:A:516:GLU:OE2	1:A:517:ASP:OD1	1.88	0.91
5:A:602:HEM:HBC2	5:A:602:HEM:HMC2	1.72	0.71
6:A:603:HAS:HBC1	6:A:603:HAS:HMC1	1.75	0.67
1:A:387:LEU:HD22	1:A:433:MET:HE1	1.82	0.62
1:A:321:GLU:OE1	1:A:325:ARG:NH1	2.40	0.52
5:A:602:HEM:HBC2	5:A:602:HEM:CMC	2.40	0.50
1:A:282:HIS:CD2	1:A:283:HIS:CD2	3.00	0.49
1:A:516:GLU:CD	1:A:517:ASP:OD1	2.51	0.47
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.96	0.47
1:A:66:TYR:OH	2:B:158:GLN:NE2	2.50	0.43
1:A:526:ARG:NH2	9:A:703:HOH:O	2.51	0.43
1:A:405:LEU:HD23	1:A:491:VAL:HG11	2.02	0.41
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.56	0.40
1:A:241:LEU:N	1:A:242:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:706:HOH:O	9:A:706:HOH:O[2_656]	2.06	0.14

### 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%)	534 (97%)	17 (3%)	1 (0%)	47	58
2	B	165/168 (98%)	162 (98%)	3 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	746/771 (97%)	725 (97%)	20 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	438 (98%)	9 (2%)	55	72
2	B	136/138 (99%)	129 (95%)	7 (5%)	24	33
3	C	24/27 (89%)	24 (100%)	0	100	100
All	All	607/628 (97%)	591 (97%)	16 (3%)	46	63

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	TYR
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	326	LEU
1	A	369	PHE
1	A	392	LEU
1	A	475	ILE
1	A	513	SER
2	B	12	LEU
2	B	23	LEU
2	B	26	LEU
2	B	58	VAL
2	B	140	LYS
2	B	158	GLN
2	B	159	ASN

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

Mol	Chain	Res	Type
1	A	254	GLN
1	A	462	HIS
2	B	60	GLN
2	B	158	GLN

### 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 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	C	103	-	23,23,24	0.98	1 (4%)	24,24,25	0.97	1 (4%)
8	CUA	B	201	2	0,1,1	-	-	-		
7	OLC	A	613	-	8,8,24	0.26	0	7,7,25	0.46	0
7	OLC	B	202	-	24,24,24	1.07	1 (4%)	25,25,25	0.88	1 (4%)
7	OLC	A	611	-	20,20,24	1.06	1 (5%)	21,21,25	0.82	1 (4%)
7	OLC	A	612	-	19,19,24	1.20	1 (5%)	19,19,25	1.01	2 (10%)
7	OLC	A	605	-	17,17,24	1.13	1 (5%)	18,18,25	1.12	2 (11%)
7	OLC	A	607	-	14,14,24	1.35	1 (7%)	15,15,25	1.15	2 (13%)
7	OLC	C	102	-	14,14,24	1.35	1 (7%)	15,15,25	1.16	2 (13%)
6	HAS	A	603	1	69,72,72	2.23	20 (28%)	73,109,109	2.57	25 (34%)
7	OLC	A	610	-	19,19,24	1.19	1 (5%)	20,20,25	1.11	2 (10%)
7	OLC	A	614	-	8,8,24	0.32	0	7,7,25	0.34	0
7	OLC	A	608	-	17,17,24	1.21	1 (5%)	18,18,25	1.00	1 (5%)
5	HEM	A	602	1	41,50,50	1.43	8 (19%)	45,82,82	1.89	12 (26%)
7	OLC	C	101	-	23,23,24	1.00	1 (4%)	24,24,25	0.76	0
7	OLC	A	609	-	14,14,24	1.29	1 (7%)	15,15,25	1.00	1 (6%)
7	OLC	A	604	-	22,22,24	1.07	1 (4%)	23,23,25	1.09	2 (8%)
7	OLC	A	606	-	16,16,24	1.26	1 (6%)	17,17,25	1.09	3 (17%)

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	C	103	-	-	7/23/23/24	-
7	OLC	A	613	-	-	2/6/6/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLC	B	202	-	-	7/24/24/24	-
7	OLC	A	611	-	-	6/20/20/24	-
7	OLC	A	612	-	-	8/18/18/24	-
7	OLC	A	605	-	-	7/17/17/24	-
7	OLC	A	607	-	-	8/14/14/24	-
7	OLC	C	102	-	-	7/14/14/24	-
6	HAS	A	603	1	-	6/40/82/82	-
7	OLC	A	610	-	-	9/19/19/24	-
7	OLC	A	614	-	-	3/6/6/24	-
7	OLC	A	608	-	-	8/17/17/24	-
5	HEM	A	602	1	-	1/12/54/54	-
7	OLC	C	101	-	-	12/23/23/24	-
7	OLC	A	609	-	-	8/14/14/24	-
7	OLC	A	604	-	-	5/22/22/24	-
7	OLC	A	606	-	-	4/16/16/24	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHD-C4A	8.67	1.47	1.35
6	A	603	HAS	C3B-C2B	5.52	1.47	1.34
7	A	612	OLC	O20-C1	4.91	1.48	1.33
7	C	102	OLC	O20-C1	4.82	1.47	1.33
7	B	202	OLC	O20-C1	4.79	1.47	1.33
6	A	603	HAS	CHB-C1D	4.79	1.48	1.38
7	A	607	OLC	O20-C1	4.73	1.47	1.33
7	A	606	OLC	O20-C1	4.68	1.47	1.33
7	A	610	OLC	O20-C1	4.68	1.47	1.33
7	A	609	OLC	O20-C1	4.61	1.46	1.33
7	A	608	OLC	O20-C1	4.56	1.46	1.33
7	A	604	OLC	O20-C1	4.55	1.46	1.33
7	A	611	OLC	O20-C1	4.54	1.46	1.33
7	C	103	OLC	O20-C1	4.46	1.46	1.33
7	C	101	OLC	O20-C1	4.40	1.46	1.33
6	A	603	HAS	C3C-C2C	4.39	1.46	1.40
5	A	602	HEM	C1B-NB	-4.36	1.32	1.40
7	A	605	OLC	O20-C1	4.32	1.46	1.33
6	A	603	HAS	C4B-NB	-4.21	1.33	1.40
6	A	603	HAS	C2A-C3A	3.92	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHC-C4B	3.85	1.44	1.35
6	A	603	HAS	C2D-C3D	3.60	1.44	1.36
6	A	603	HAS	CHA-C1A	3.41	1.45	1.38
6	A	603	HAS	FE-NA	3.35	2.08	1.95
6	A	603	HAS	C4B-C3B	3.17	1.49	1.44
6	A	603	HAS	C4A-NA	-2.94	1.34	1.39
6	A	603	HAS	CHB-C1B	2.80	1.45	1.39
5	A	602	HEM	CHB-C1B	2.72	1.41	1.35
5	A	602	HEM	FE-NB	2.70	2.10	1.96
6	A	603	HAS	CHA-C4D	2.68	1.45	1.39
6	A	603	HAS	C1D-ND	-2.67	1.35	1.40
5	A	602	HEM	C4B-NB	-2.64	1.33	1.38
6	A	603	HAS	C1C-CHC	2.60	1.48	1.41
6	A	603	HAS	C1A-NA	-2.54	1.34	1.39
5	A	602	HEM	C4D-C3D	2.43	1.49	1.45
6	A	603	HAS	FE-NB	2.32	2.09	1.97
6	A	603	HAS	C4C-CHD	2.25	1.47	1.41
5	A	602	HEM	C3C-C2C	-2.21	1.37	1.40
6	A	603	HAS	C1B-C2B	2.15	1.48	1.44
5	A	602	HEM	C4D-ND	-2.12	1.36	1.40
5	A	602	HEM	O1D-CGD	2.12	1.29	1.22

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2D-C3D-C4D	-8.30	100.57	106.49
6	A	603	HAS	C2B-C1B-NB	5.98	117.05	109.88
6	A	603	HAS	C2A-C1A-NA	5.91	116.08	110.32
6	A	603	HAS	C3D-C4D-ND	5.79	115.96	110.36
6	A	603	HAS	C3B-C4B-NB	5.47	116.33	109.84
5	A	602	HEM	C1B-NB-C4B	5.35	110.60	105.07
5	A	602	HEM	CHC-C4B-NB	5.04	129.91	124.43
6	A	603	HAS	CAD-C3D-C4D	4.55	132.60	124.66
6	A	603	HAS	C1B-C2B-C3B	-4.53	101.38	106.80
6	A	603	HAS	CAA-CBA-CGA	-4.30	104.35	113.60
6	A	603	HAS	C3C-C4C-NC	4.05	114.45	109.21
5	A	602	HEM	CHD-C1D-ND	3.99	128.76	124.43
6	A	603	HAS	OMD-CMD-C2D	-3.73	117.25	125.69
6	A	603	HAS	C1A-C2A-C3A	-3.66	102.35	107.13
7	A	610	OLC	O20-C1-C2	3.58	123.13	111.91
5	A	602	HEM	O2A-CGA-CBA	3.47	125.17	114.03
6	A	603	HAS	CMB-C2B-C1B	3.44	130.28	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	604	OLC	O20-C1-C2	3.41	122.61	111.91
7	A	612	OLC	C21-O20-C1	3.33	127.09	116.11
7	A	605	OLC	O20-C1-C2	3.22	122.00	111.91
6	A	603	HAS	C3A-C4A-NA	3.21	115.61	109.69
6	A	603	HAS	CAA-C2A-C1A	3.05	130.65	124.89
6	A	603	HAS	CMA-C3A-C4A	2.97	129.95	124.71
7	A	607	OLC	O20-C1-C2	2.96	121.19	111.91
6	A	603	HAS	C4B-C3B-C2B	-2.95	102.38	107.41
7	C	103	OLC	O20-C1-C2	2.93	121.09	111.91
7	A	610	OLC	O20-C1-O19	-2.90	116.28	123.59
6	A	603	HAS	CHB-C1B-C2B	-2.85	120.53	124.98
7	B	202	OLC	O20-C1-C2	2.85	120.85	111.91
6	A	603	HAS	C4A-C3A-C2A	-2.81	102.84	106.94
7	C	102	OLC	O20-C1-C2	2.79	120.66	111.91
5	A	602	HEM	CMA-C3A-C4A	-2.78	124.19	128.46
7	A	606	OLC	O20-C1-C2	2.75	120.55	111.91
6	A	603	HAS	C4B-NB-C1B	-2.75	102.23	105.07
6	A	603	HAS	C32-C30-C31	2.74	120.67	114.60
6	A	603	HAS	C4A-NA-C1A	-2.74	102.67	105.35
6	A	603	HAS	CMC-C2C-C3C	2.71	129.75	124.68
7	A	605	OLC	O20-C1-O19	-2.63	116.94	123.59
6	A	603	HAS	CHA-C4D-C3D	-2.61	121.01	124.84
6	A	603	HAS	CHA-C1A-C2A	-2.61	120.72	124.94
7	A	608	OLC	O20-C1-C2	2.59	120.05	111.91
5	A	602	HEM	CHD-C1D-C2D	-2.58	120.95	124.98
7	A	604	OLC	O20-C1-O19	-2.57	117.11	123.59
5	A	602	HEM	CAD-C3D-C4D	2.56	129.14	124.66
7	A	607	OLC	O20-C1-O19	-2.48	117.34	123.59
5	A	602	HEM	CHA-C4D-C3D	-2.47	120.69	125.33
7	A	611	OLC	O20-C1-C2	2.46	119.64	111.91
5	A	602	HEM	CHA-C4D-ND	2.37	127.31	124.38
7	A	609	OLC	O20-C1-C2	2.37	119.34	111.91
5	A	602	HEM	C4B-CHC-C1C	2.20	125.46	122.56
5	A	602	HEM	O1A-CGA-CBA	-2.18	116.08	123.08
6	A	603	HAS	C27-C19-C20	2.14	118.87	115.27
5	A	602	HEM	C4A-C3A-C2A	2.13	108.48	107.00
7	A	612	OLC	O20-C1-C2	2.08	120.46	112.23
7	A	606	OLC	C21-O20-C1	2.03	124.62	117.12
7	C	102	OLC	C21-O20-C1	2.02	124.61	117.12
7	A	606	OLC	O20-C1-O19	-2.02	118.49	123.59

There are no chirality outliers.

All (108) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	HAS	C3D-C2D-CMD-OMD
7	A	605	OLC	C21-C22-C24-O25
7	A	607	OLC	C21-C22-C24-O25
7	A	608	OLC	C21-C22-C24-O25
7	A	609	OLC	O20-C21-C22-O23
7	A	611	OLC	O20-C21-C22-C24
7	B	202	OLC	C21-C22-C24-O25
7	A	608	OLC	C2-C1-O20-C21
7	A	611	OLC	O20-C21-C22-O23
7	C	102	OLC	C2-C1-O20-C21
7	A	608	OLC	O19-C1-O20-C21
7	C	102	OLC	O19-C1-O20-C21
7	A	612	OLC	C2-C1-O20-C21
7	C	103	OLC	O20-C21-C22-C24
7	C	102	OLC	O20-C21-C22-O23
7	C	103	OLC	O20-C21-C22-O23
7	C	103	OLC	C2-C1-O20-C21
7	A	611	OLC	C1-C2-C3-C4
7	A	605	OLC	O23-C22-C24-O25
7	A	609	OLC	O23-C22-C24-O25
7	C	101	OLC	C1-C2-C3-C4
7	C	103	OLC	O19-C1-O20-C21
7	C	102	OLC	C1-C2-C3-C4
7	A	610	OLC	O20-C21-C22-O23
7	A	612	OLC	O19-C1-O20-C21
7	A	605	OLC	C2-C3-C4-C5
7	A	605	OLC	C4-C5-C6-C7
7	A	610	OLC	C2-C3-C4-C5
7	A	609	OLC	C21-C22-C24-O25
7	C	102	OLC	C21-C22-C24-O25
7	A	610	OLC	C5-C6-C7-C8
7	A	606	OLC	C5-C6-C7-C8
7	C	102	OLC	O23-C22-C24-O25
7	A	614	OLC	C14-C15-C16-C17
7	A	610	OLC	C2-C1-O20-C21
7	B	202	OLC	C6-C7-C8-C9
7	A	608	OLC	C2-C3-C4-C5
7	A	610	OLC	O20-C21-C22-C24
7	A	604	OLC	C2-C3-C4-C5
7	A	610	OLC	O19-C1-O20-C21
7	A	604	OLC	C12-C13-C14-C15
7	C	101	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	A	612	OLC	C14-C15-C16-C17
7	A	608	OLC	O23-C22-C24-O25
7	B	202	OLC	O23-C22-C24-O25
7	C	103	OLC	C10-C11-C12-C13
7	A	608	OLC	C3-C4-C5-C6
7	A	612	OLC	C11-C12-C13-C14
7	C	101	OLC	C2-C1-O20-C21
7	A	613	OLC	C10-C11-C12-C13
7	A	610	OLC	C3-C4-C5-C6
7	C	101	OLC	C11-C12-C13-C14
7	A	609	OLC	C5-C6-C7-C8
7	A	607	OLC	C2-C3-C4-C5
7	C	101	OLC	O19-C1-O20-C21
7	A	607	OLC	O23-C22-C24-O25
7	A	605	OLC	C1-C2-C3-C4
7	A	606	OLC	C3-C4-C5-C6
7	B	202	OLC	C3-C4-C5-C6
7	A	612	OLC	C3-C4-C5-C6
7	A	609	OLC	O20-C21-C22-C24
7	A	611	OLC	C11-C12-C13-C14
7	A	612	OLC	C2-C3-C4-C5
7	A	607	OLC	C1-C2-C3-C4
7	A	614	OLC	C10-C11-C12-C13
7	C	101	OLC	C13-C14-C15-C16
7	A	606	OLC	C2-C1-O20-C21
7	A	606	OLC	O19-C1-O20-C21
7	C	102	OLC	O20-C21-C22-C24
7	A	609	OLC	C1-C2-C3-C4
7	A	612	OLC	C1-C2-C3-C4
7	C	101	OLC	O20-C21-C22-O23
7	A	608	OLC	C4-C5-C6-C7
7	A	604	OLC	C13-C14-C15-C16
7	C	103	OLC	C13-C14-C15-C16
7	A	605	OLC	O20-C21-C22-O23
7	A	612	OLC	C4-C5-C6-C7
7	A	613	OLC	C14-C15-C16-C17
7	A	610	OLC	C7-C8-C9-C10
7	A	604	OLC	C10-C11-C12-C13
6	A	603	HAS	CAD-CBD-CGD-O1D
6	A	603	HAS	C23-C24-C28-C29
7	B	202	OLC	C9-C10-C11-C12
7	C	101	OLC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
7	C	101	OLC	O20-C21-C22-C24
6	A	603	HAS	CAA-CBA-CGA-O1A
6	A	603	HAS	CAD-CBD-CGD-O2D
6	A	603	HAS	CAA-CBA-CGA-O2A
7	C	101	OLC	C9-C10-C11-C12
7	C	103	OLC	C7-C8-C9-C10
7	B	202	OLC	O19-C1-O20-C21
7	A	607	OLC	C2-C1-O20-C21
7	B	202	OLC	C2-C1-O20-C21
7	A	608	OLC	C7-C8-C9-C10
7	A	611	OLC	C7-C8-C9-C10
7	C	101	OLC	C6-C7-C8-C9
7	A	614	OLC	C11-C12-C13-C14
7	A	610	OLC	C9-C10-C11-C12
7	A	604	OLC	C7-C8-C9-C10
7	A	605	OLC	C7-C8-C9-C10
7	C	101	OLC	C7-C8-C9-C10
7	A	607	OLC	O19-C1-O20-C21
5	A	602	HEM	CAD-CBD-CGD-O2D
7	A	607	OLC	O20-C1-C2-C3
7	A	609	OLC	O20-C1-C2-C3
7	A	607	OLC	O19-C1-C2-C3
7	A	609	OLC	O19-C1-C2-C3
7	A	611	OLC	C4-C5-C6-C7

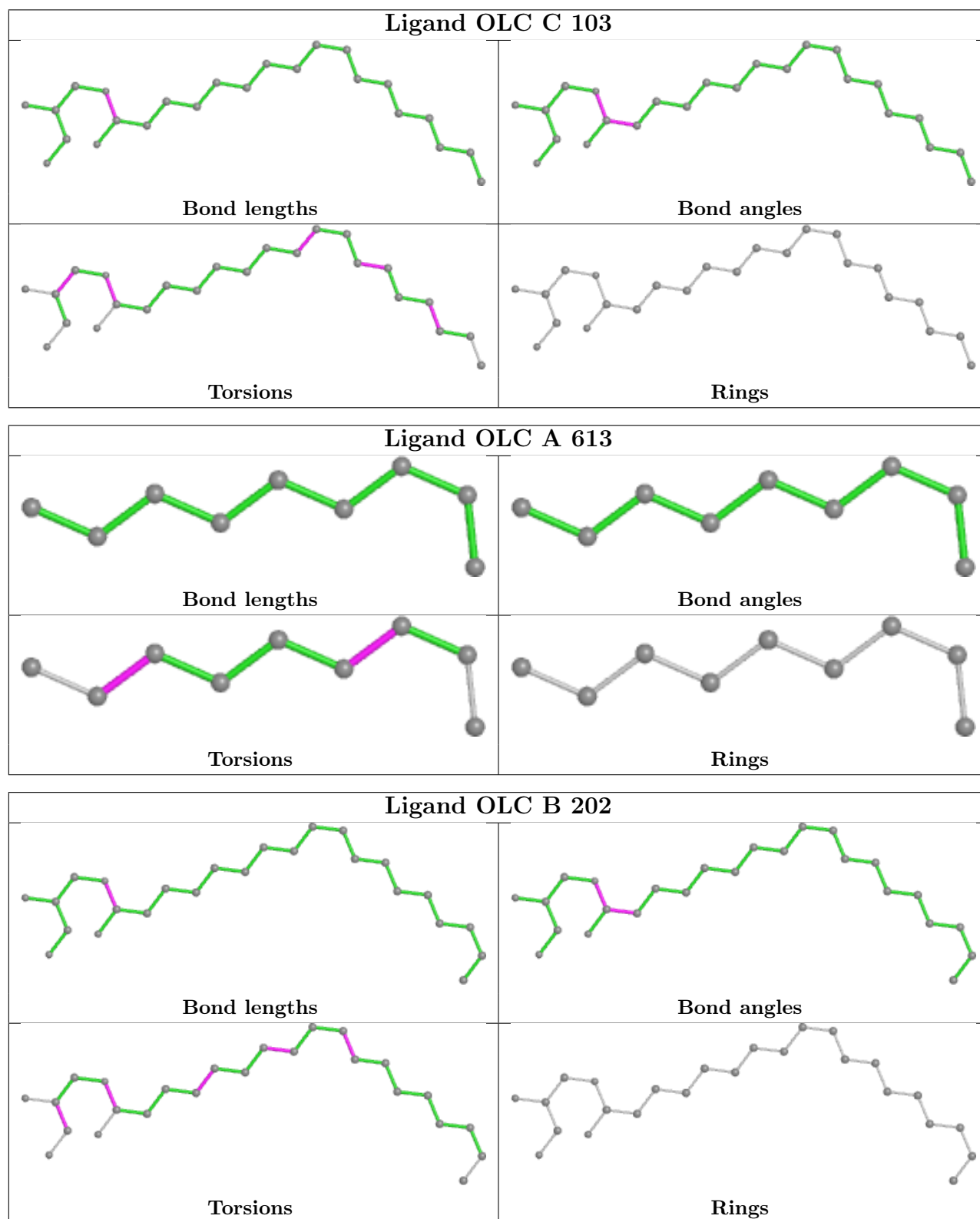
There are no ring outliers.

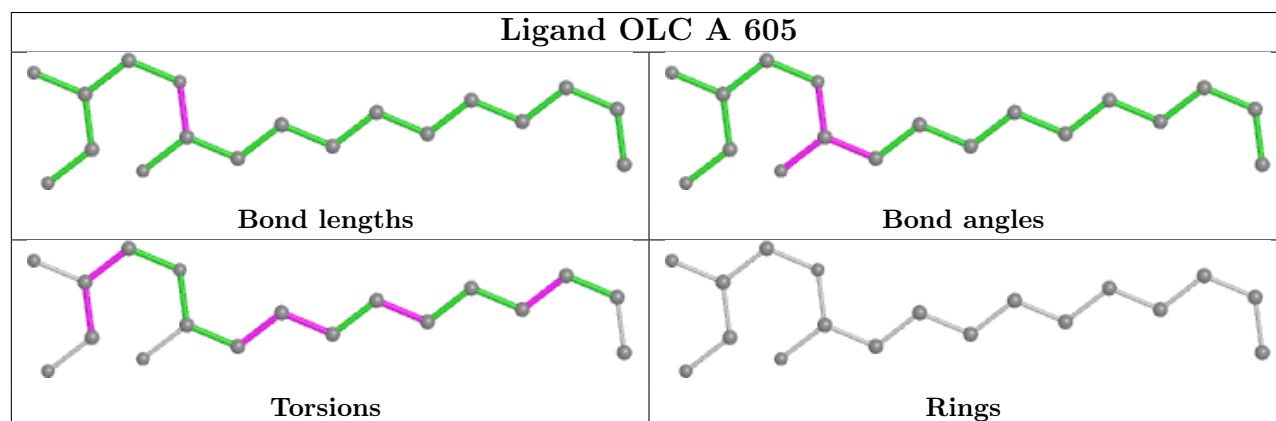
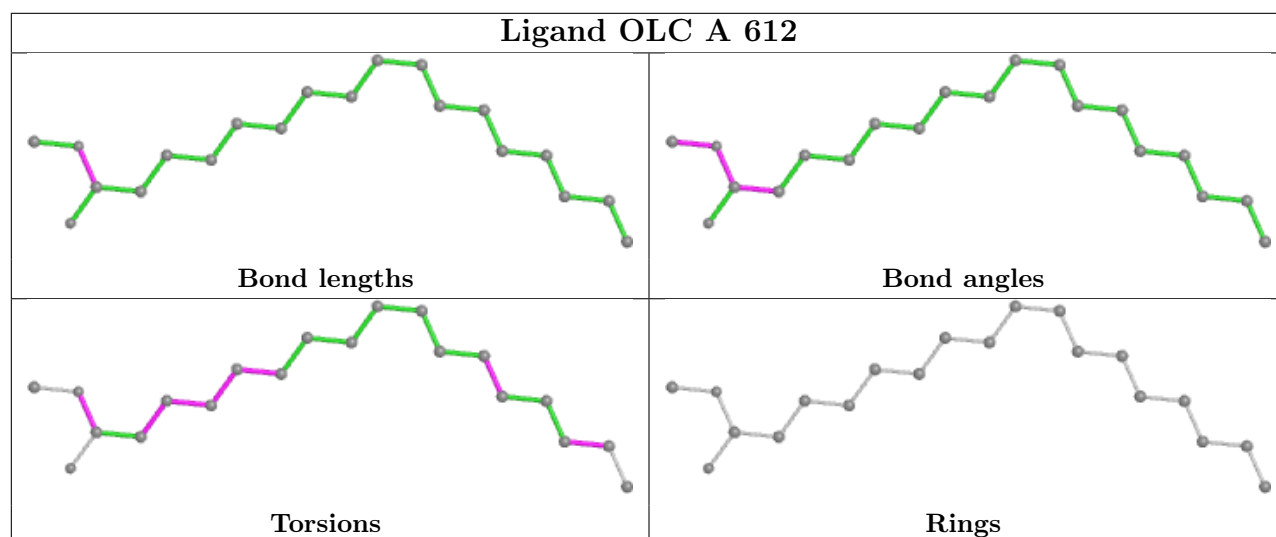
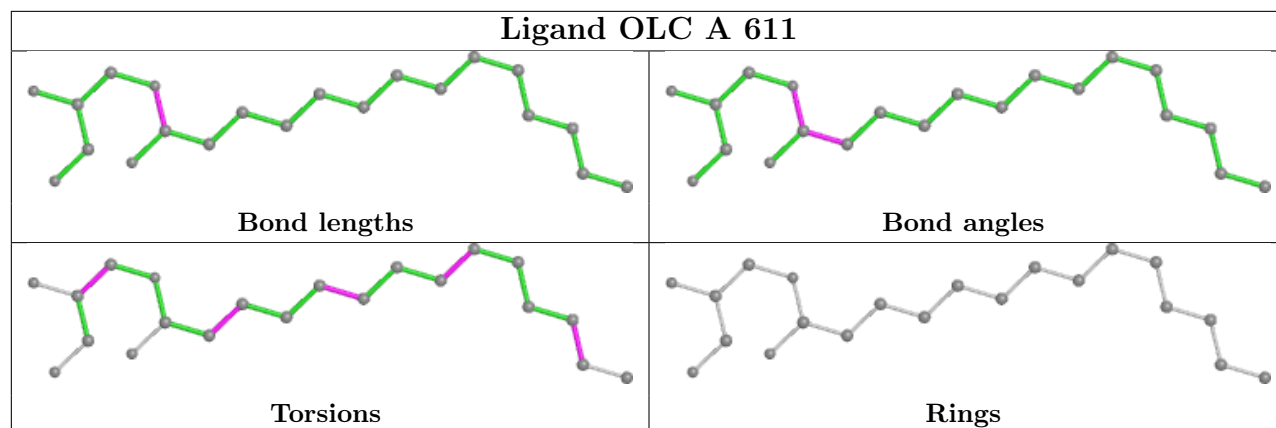
2 monomers are involved in 3 short contacts:

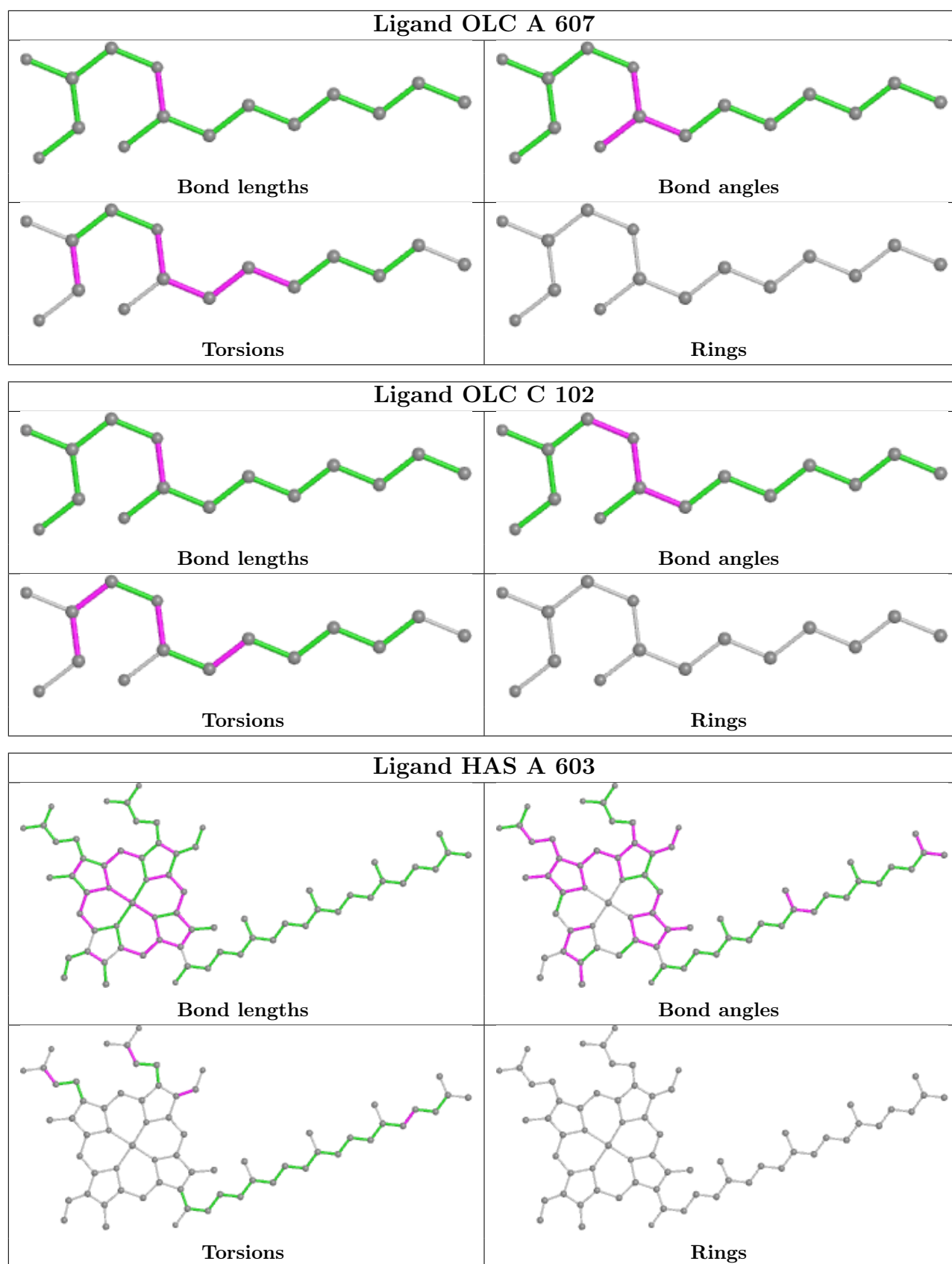
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	HAS	1	0
5	A	602	HEM	2	0

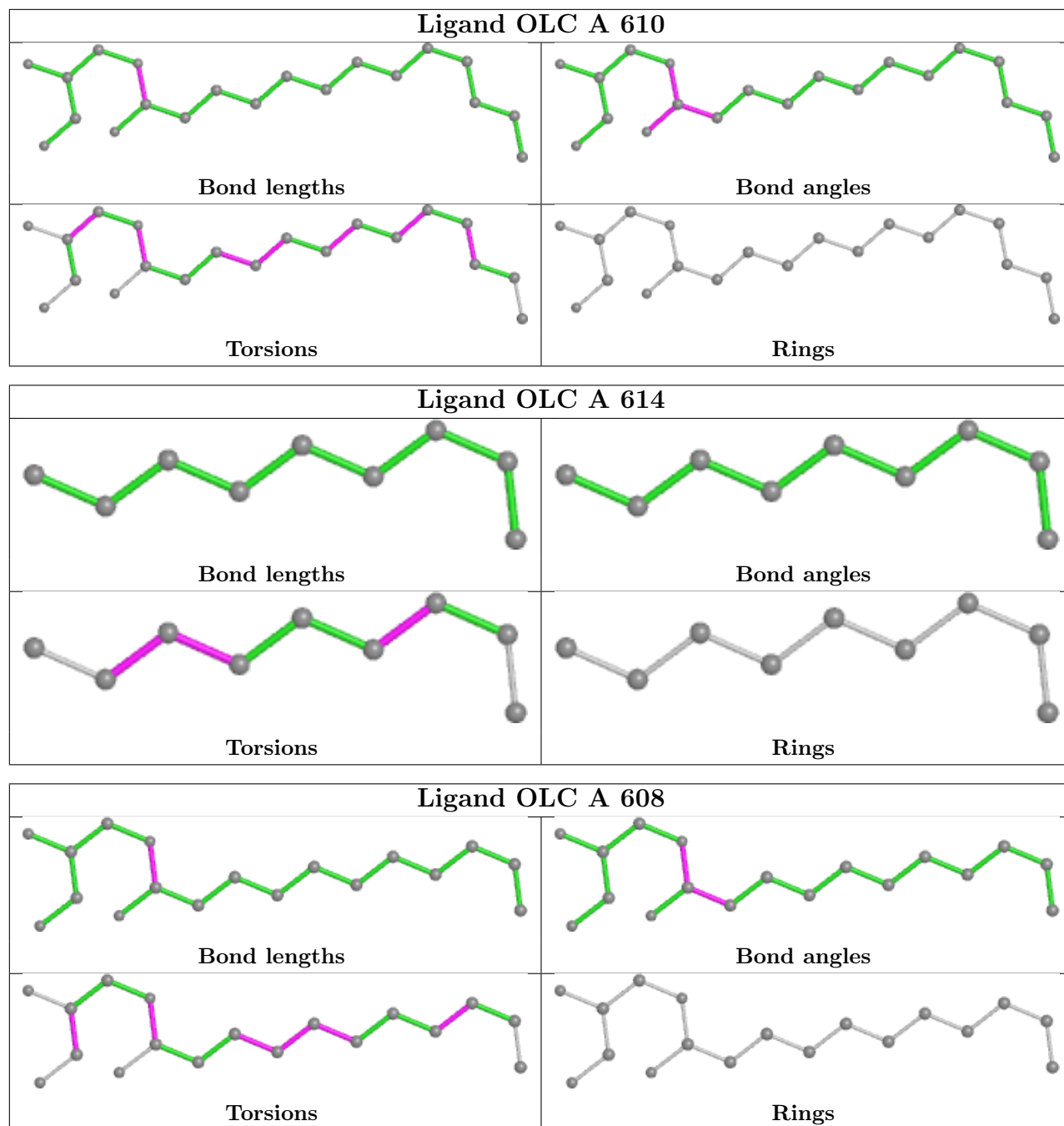
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

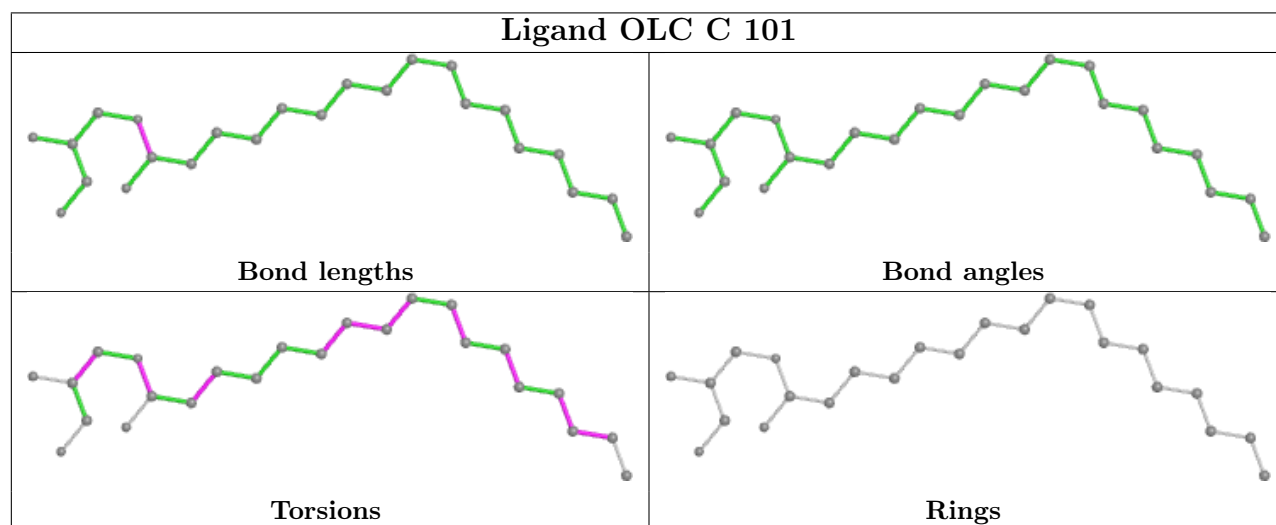
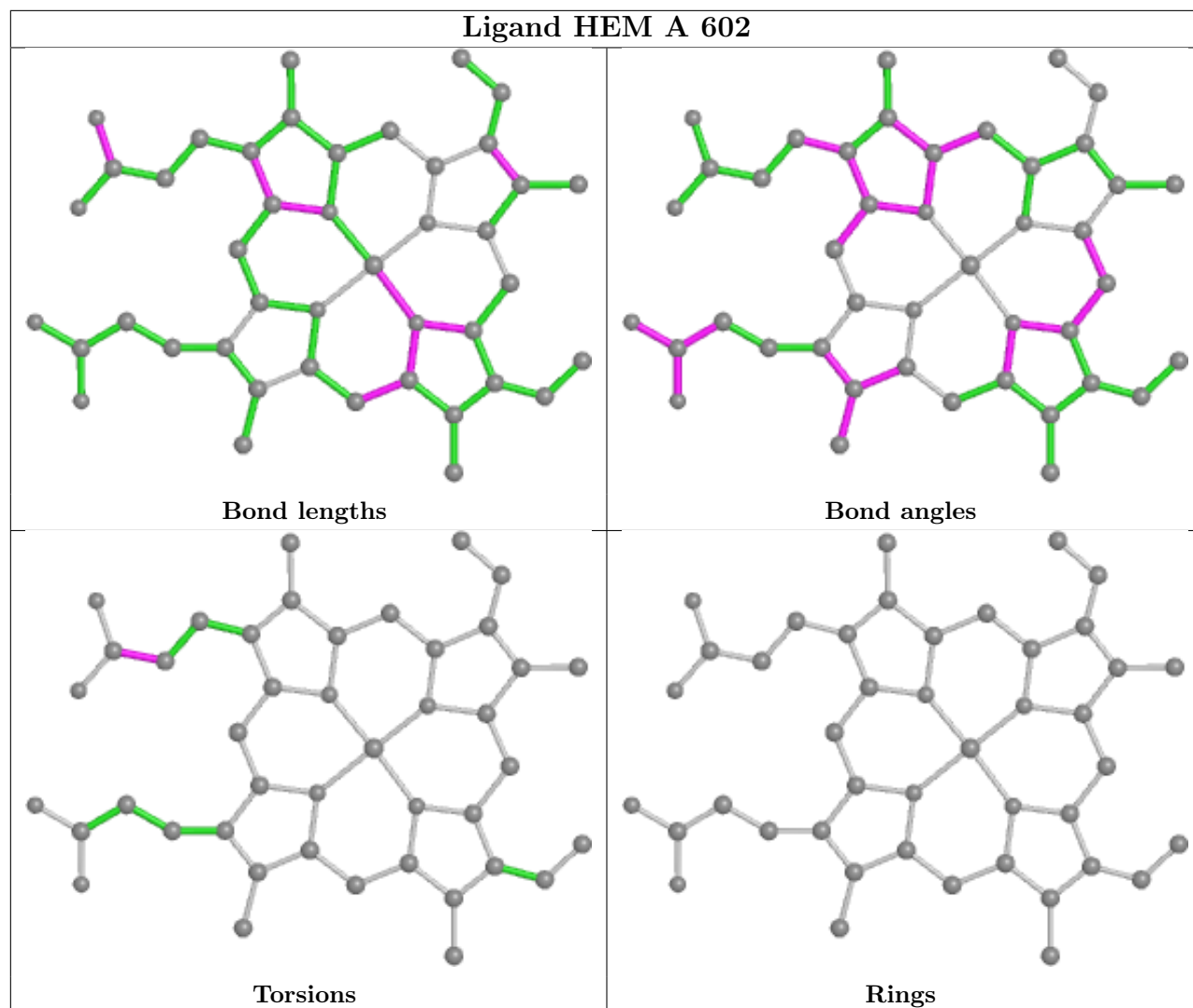


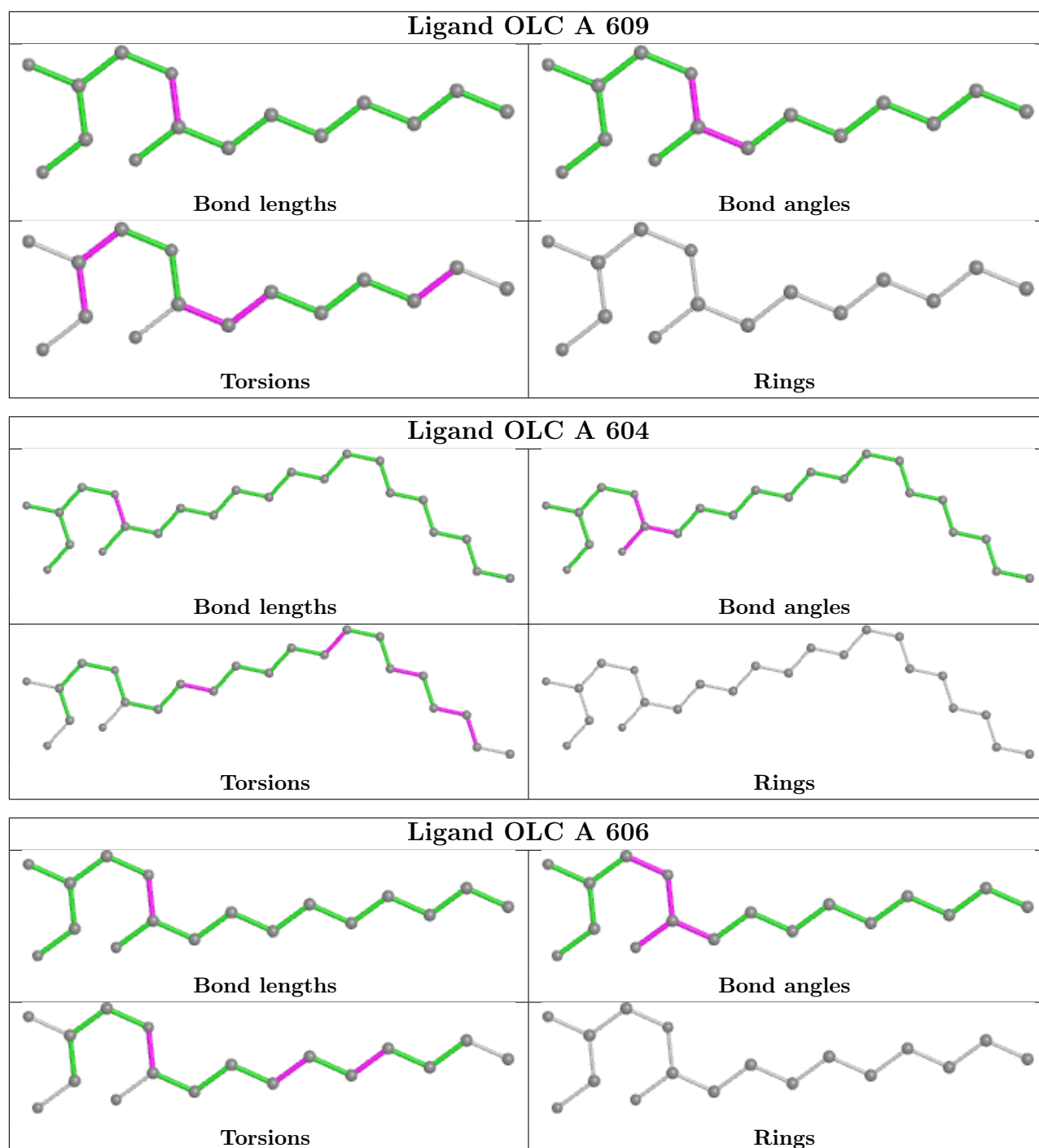












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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%)	0.23	49 (8%) <b>10</b> <b>13</b>	35, 47, 77, 114	0
2	B	167/168 (99%)	-0.12	6 (3%) 42 49	35, 47, 70, 110	0
3	C	31/34 (91%)	-0.57	0 <b>100</b> <b>100</b>	42, 47, 61, 76	0
All	All	752/771 (97%)	0.12	55 (7%) <b>15</b> <b>20</b>	35, 47, 75, 114	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	ARG	6.9
1	A	240	LEU	4.4
1	A	175	PRO	4.3
1	A	494	SER	4.0
1	A	493	LEU	3.7
1	A	393	VAL	3.6
1	A	133	TYR	3.6
1	A	523	ALA	3.6
1	A	57	ARG	3.6
1	A	10	ARG	3.4
1	A	236	VAL	3.4
1	A	389	VAL	3.3
1	A	497	ARG	3.3
1	A	333	PHE	3.3
2	B	76	PRO	3.3
1	A	235	ILE	3.2
2	B	2	VAL	3.0
1	A	174	ASN	3.0
1	A	518	ARG	3.0
1	A	392	LEU	3.0
1	A	241	LEU	3.0
1	A	247	ILE	2.9
1	A	239	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	176	GLY	2.9
1	A	78	ILE	2.9
1	A	244	TYR	2.9
1	A	326	LEU	2.9
2	B	5	HIS	2.8
1	A	337	ARG	2.8
1	A	243	ALA	2.8
1	A	134	THR	2.8
1	A	12	TYR	2.7
1	A	242	PRO	2.7
1	A	547	VAL	2.6
1	A	522	LEU	2.6
1	A	496	GLU	2.5
1	A	74	VAL	2.5
1	A	353	LEU	2.5
1	A	77	ALA	2.4
1	A	172	ALA	2.4
1	A	136	TYR	2.4
1	A	548	GLN	2.4
2	B	168	GLU	2.3
1	A	13	GLU	2.3
2	B	141	ARG	2.2
1	A	11	VAL	2.2
1	A	513	SER	2.2
1	A	84	PHE	2.2
1	A	499	PRO	2.2
2	B	75	GLY	2.2
1	A	88	ILE	2.1
1	A	246	ILE	2.1
1	A	81	THR	2.1
1	A	135	PHE	2.1
1	A	515	PRO	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

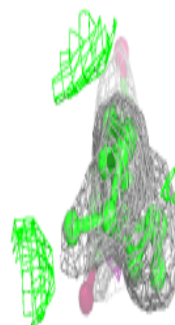
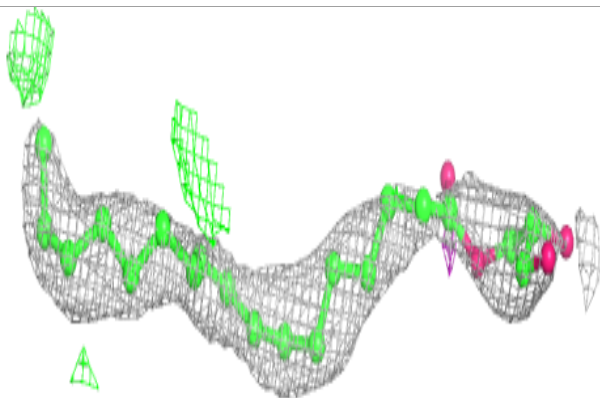
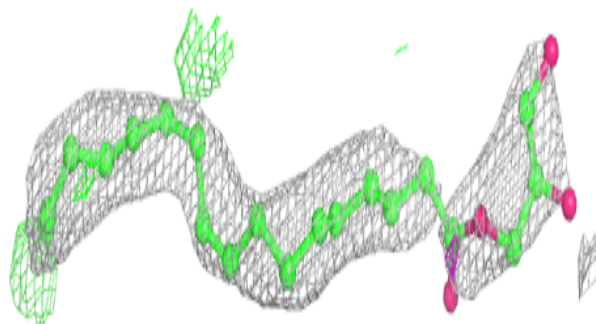
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	C	101	24/25	0.53	0.33	79,87,103,105	0
7	OLC	A	609	15/25	0.60	0.24	77,80,89,90	0
7	OLC	A	606	17/25	0.63	0.23	77,85,100,102	0
7	OLC	A	611	21/25	0.64	0.23	75,82,87,88	0
7	OLC	A	605	18/25	0.66	0.22	74,79,84,90	0
7	OLC	A	610	20/25	0.69	0.29	75,81,90,91	0
7	OLC	A	607	15/25	0.71	0.31	69,79,84,85	0
7	OLC	A	608	18/25	0.72	0.24	65,72,94,94	0
7	OLC	C	102	15/25	0.76	0.27	90,95,99,103	0
7	OLC	C	103	24/25	0.79	0.21	74,83,86,87	0
7	OLC	A	612	20/25	0.83	0.15	72,76,87,87	0
7	OLC	B	202	25/25	0.84	0.17	66,69,90,93	0
7	OLC	A	614	9/25	0.85	0.13	73,75,82,82	0
7	OLC	A	604	23/25	0.88	0.16	49,61,87,88	0
7	OLC	A	613	9/25	0.89	0.14	79,81,85,86	0
5	HEM	A	602	43/43	0.96	0.14	28,33,37,42	0
6	HAS	A	603	65/65	0.97	0.19	29,35,49,53	0
8	CUA	B	201	2/2	0.99	0.05	32,32,32,33	0
4	CU	A	601	1/1	1.00	0.07	35,35,35,35	0

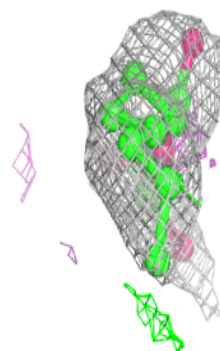
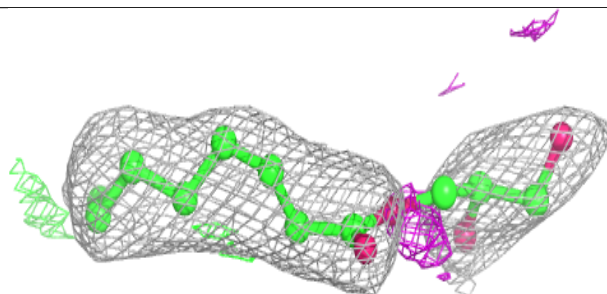
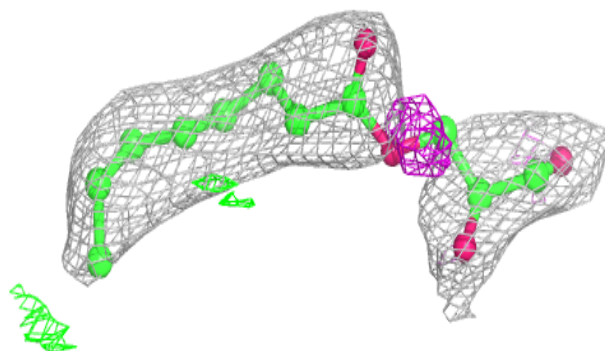
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

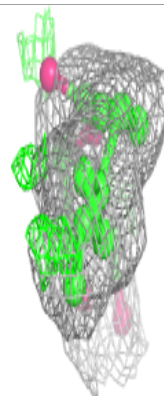
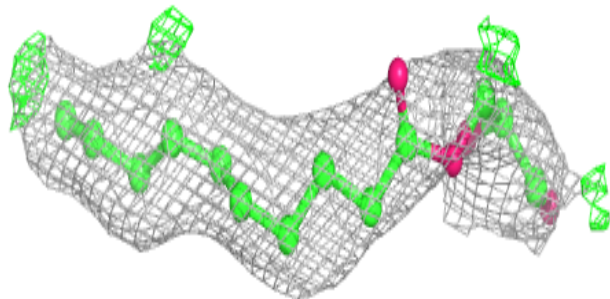
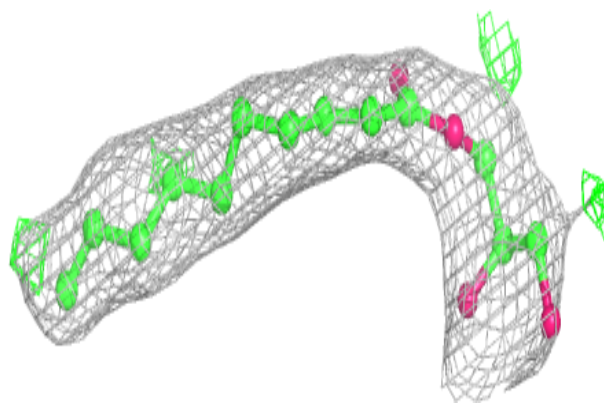
**Electron density around OLC A 609:**

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

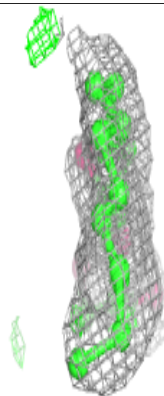
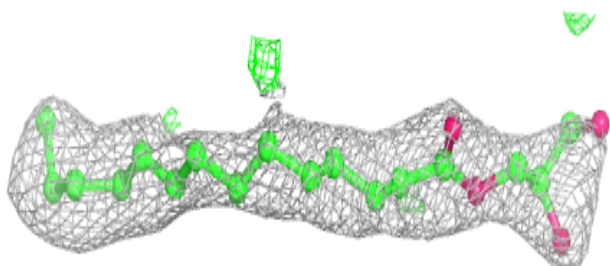
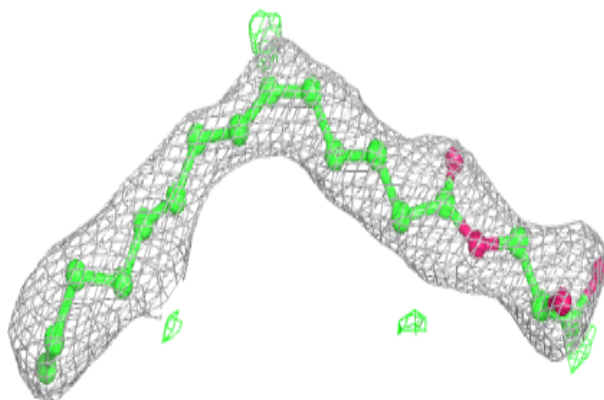


**Electron density around OLC A 606:**

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

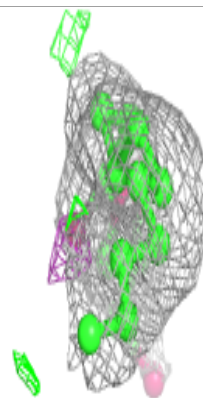
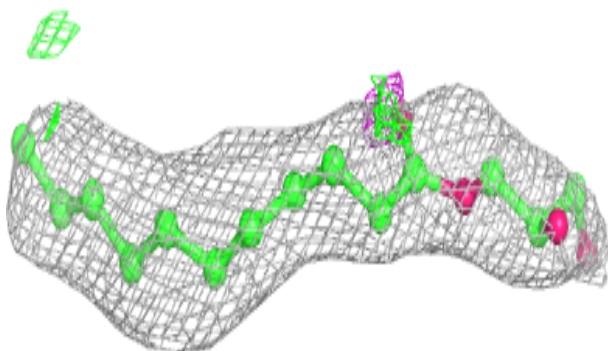
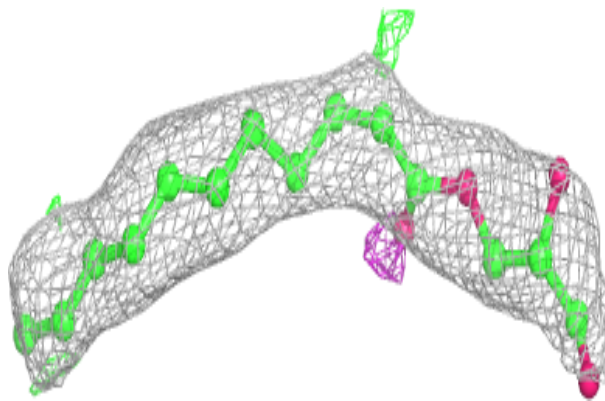
**Electron density around OLC A 611:**

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

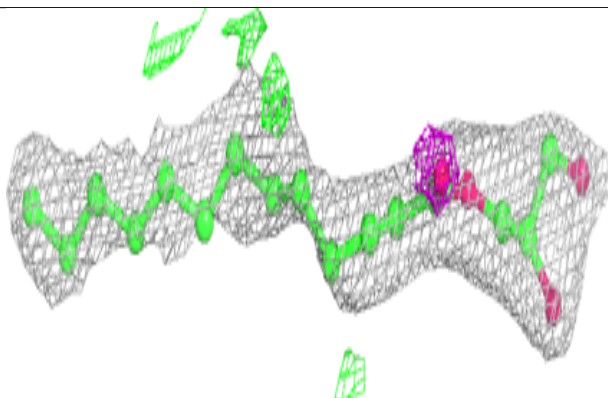
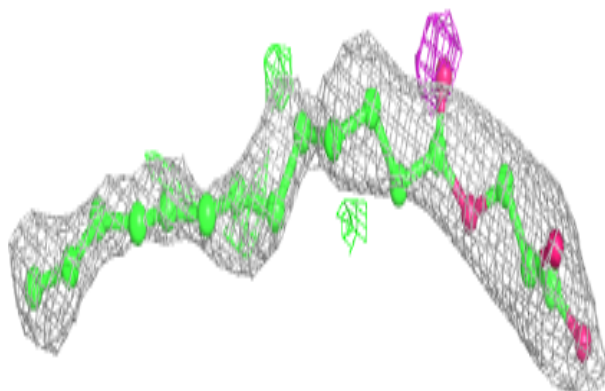


**Electron density around OLC A 605:**

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

**Electron density around OLC A 610:**

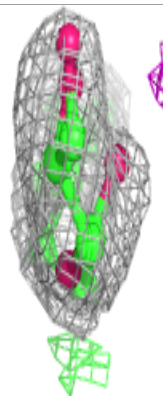
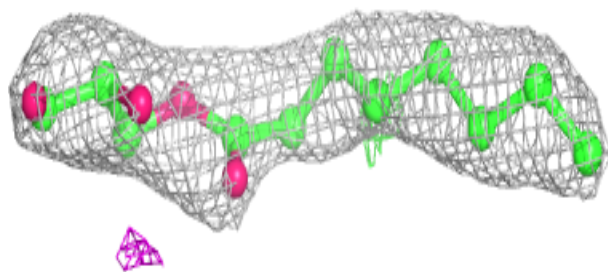
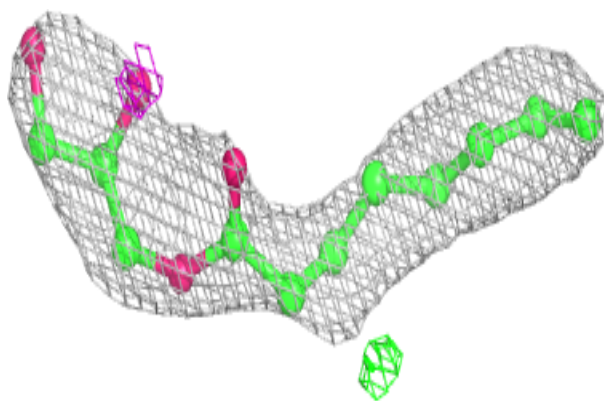
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



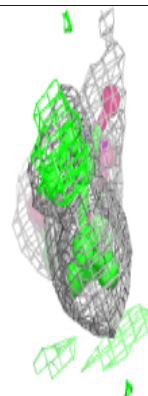
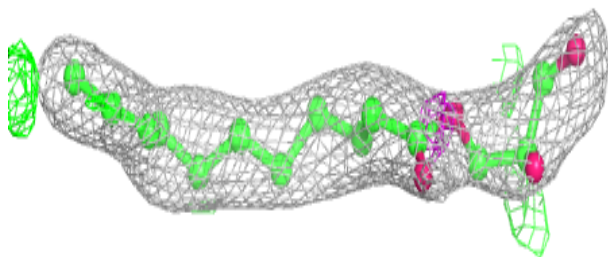
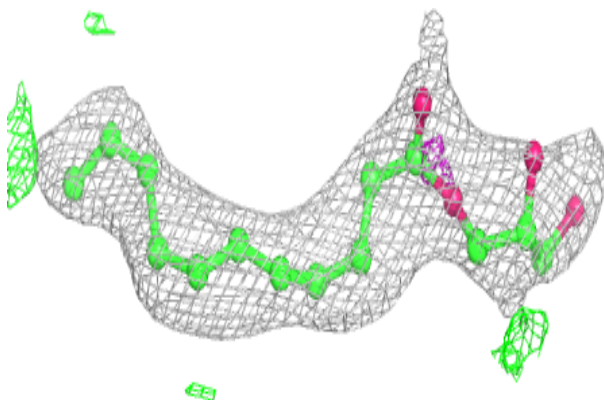


**Electron density around OLC A 607:**

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

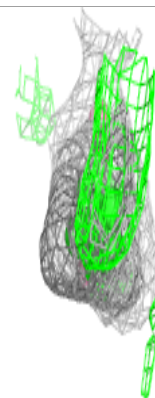
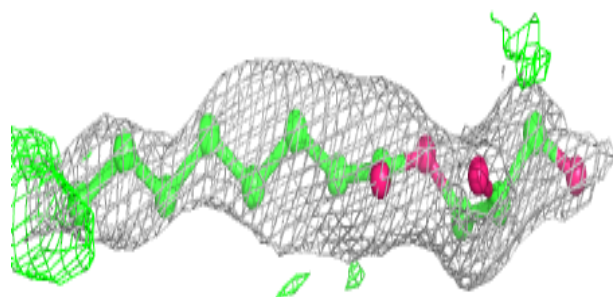
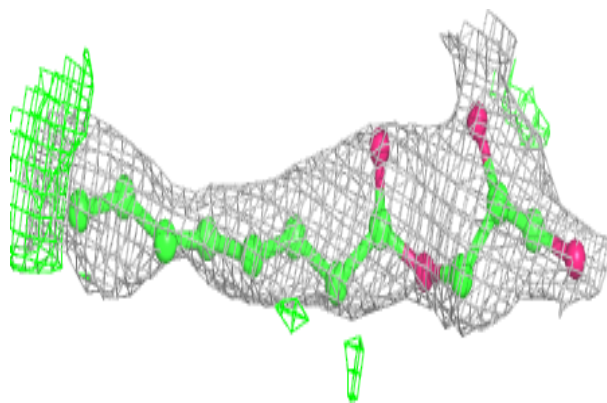
**Electron density around OLC A 608:**

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

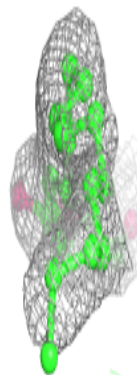
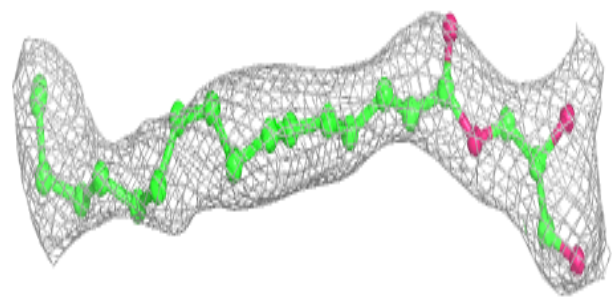
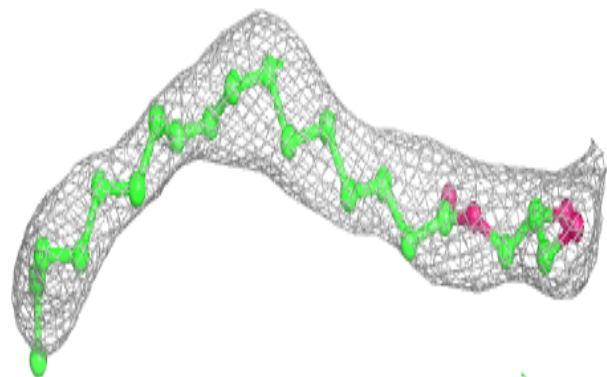


**Electron density around OLC C 102:**

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

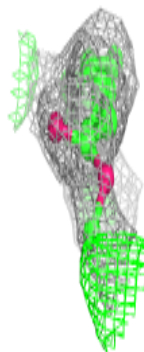
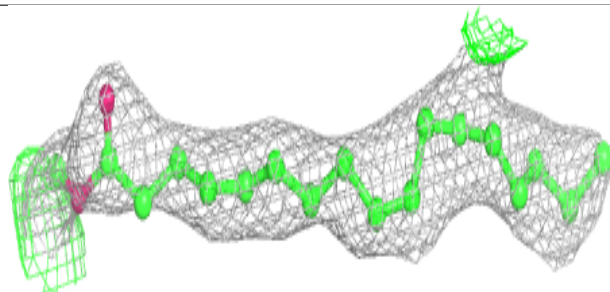
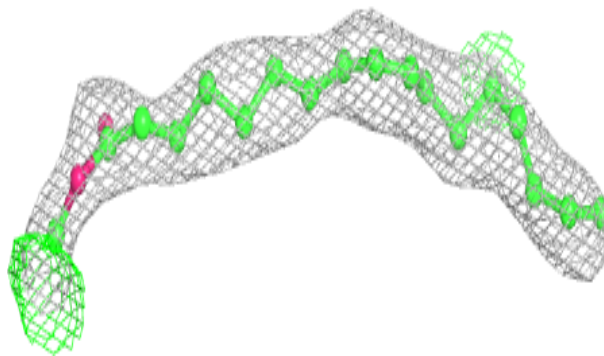
**Electron density around OLC C 103:**

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

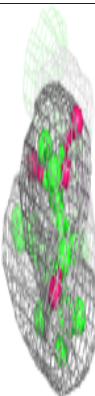
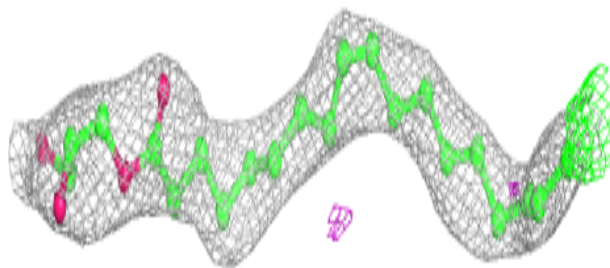
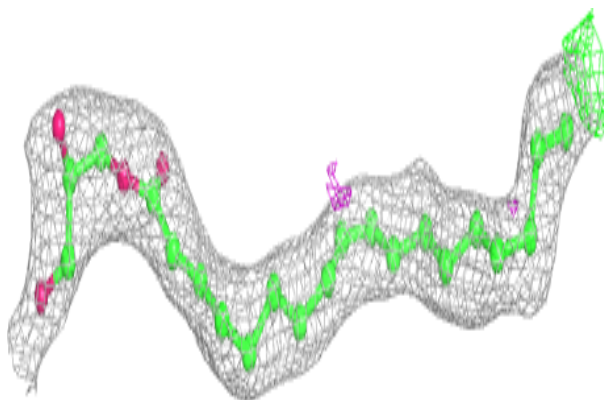


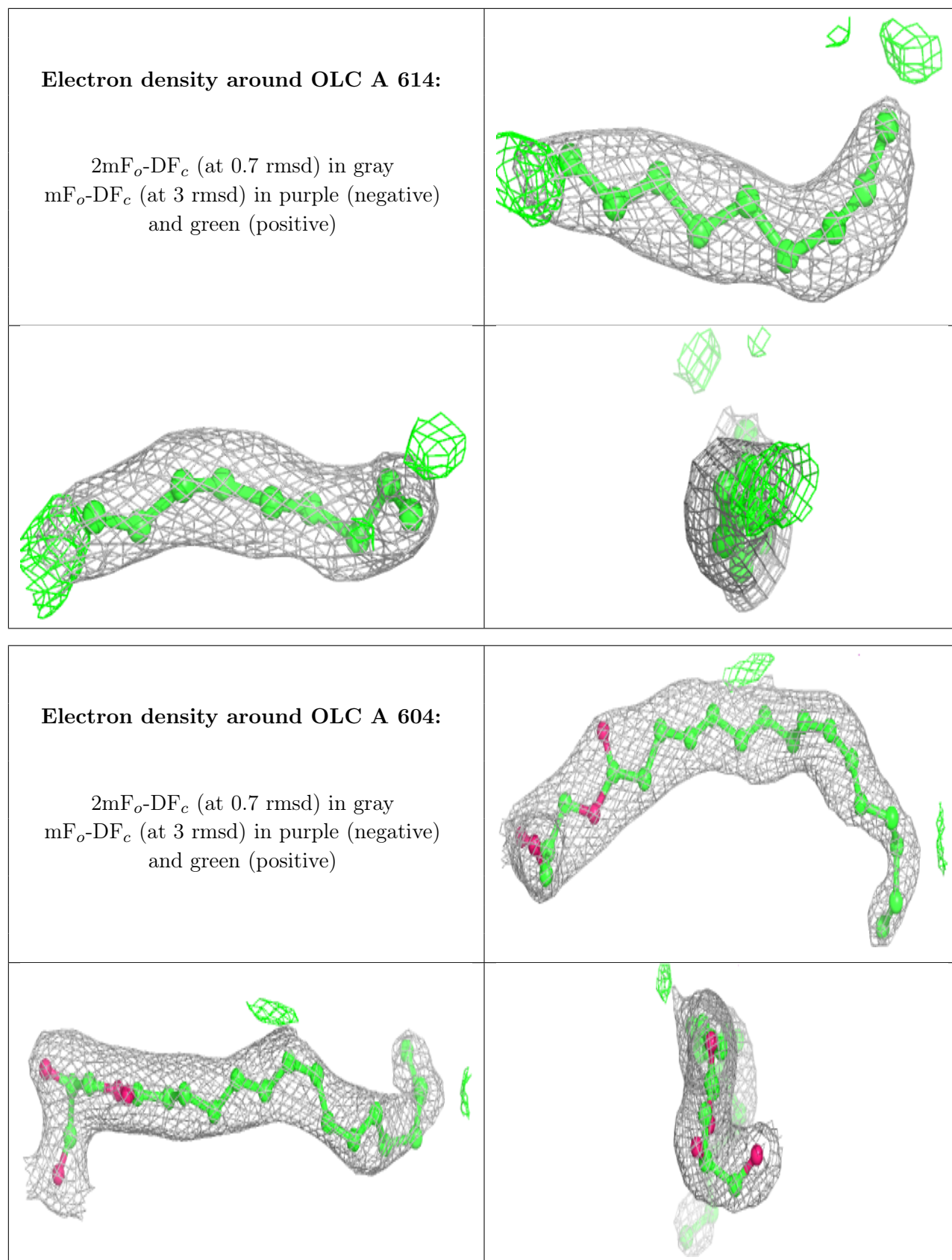
**Electron density around OLC A 612:**

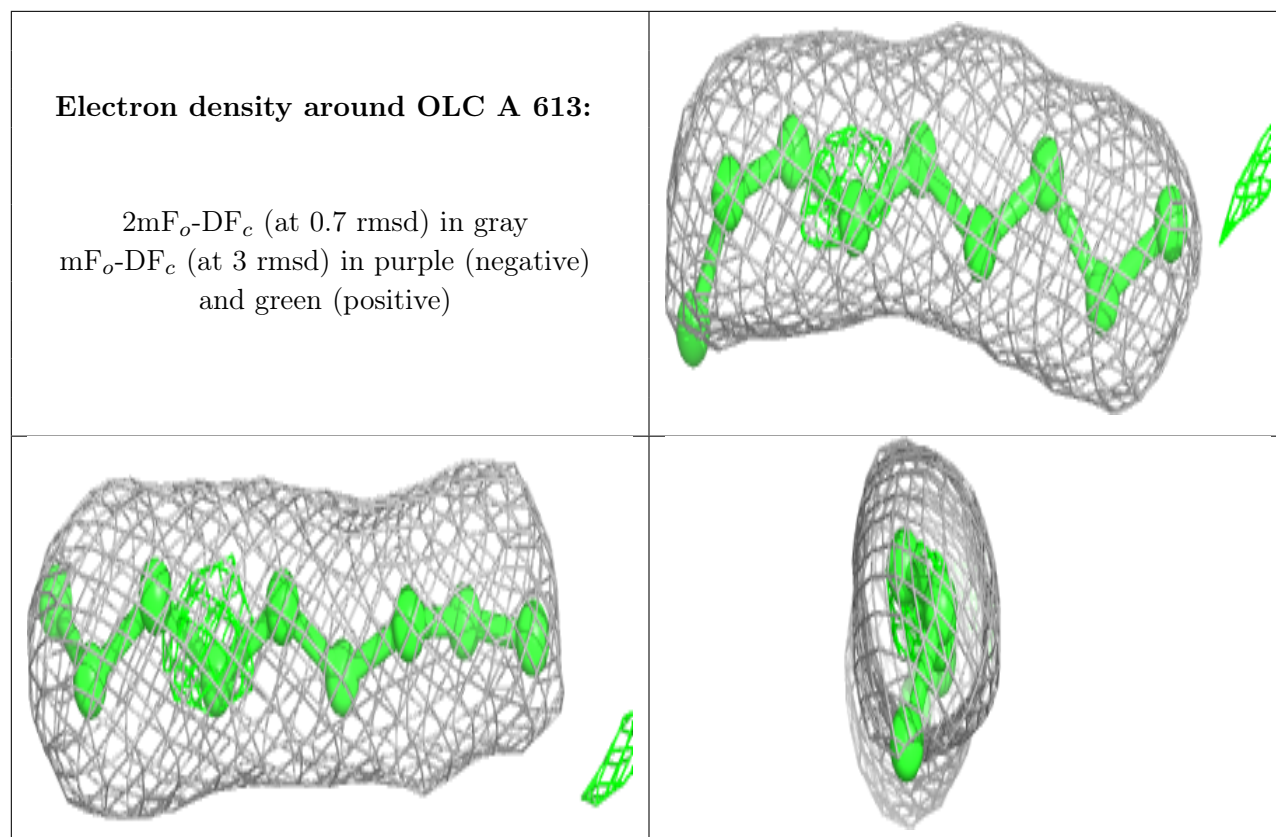
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around OLC B 202:**

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

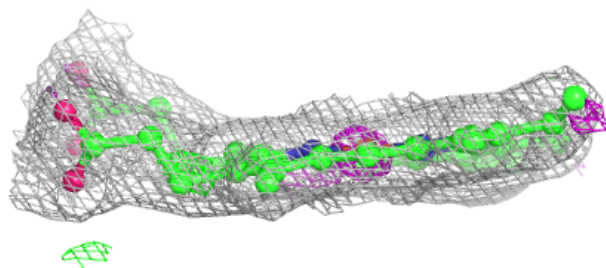
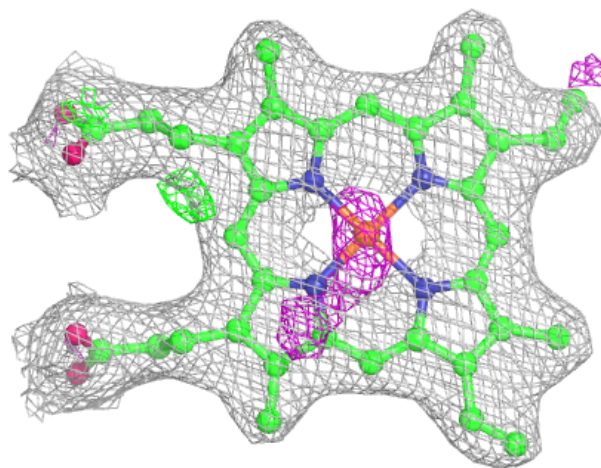


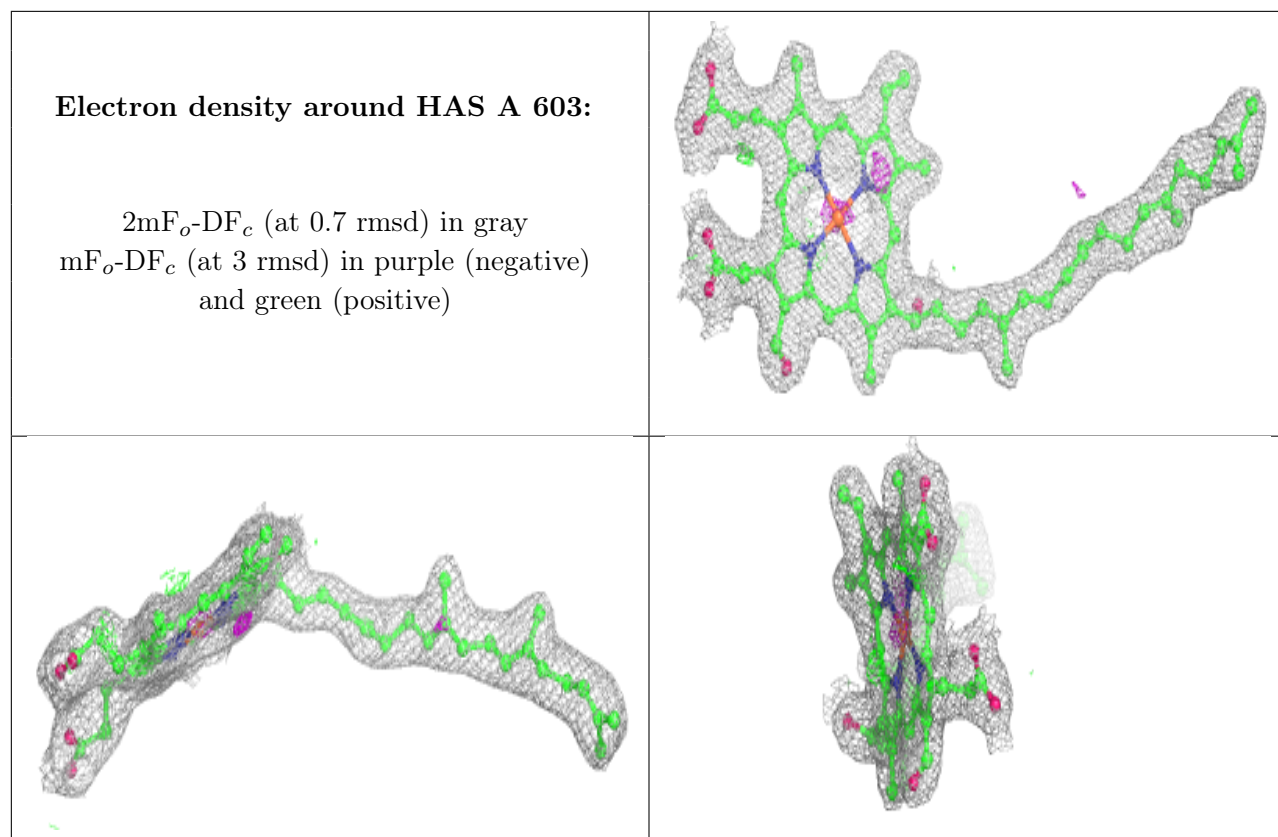




**Electron density around HEM A 602:**

$2mF_o-DF_c$  (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.