wwPDB X-ray Structure Validation Summary Report (i)

Feb 18, 2024 – 03:35 PM EST

PDB ID	:	4G7S
Title	:	Structure of Recombinant Cytochrome ba3 Oxidase mutant V236I from Thermus thermophilus
Authors	:	Li, Y.; Chen, Y.; Stout, C.D.
Deposited on	:	2012-07-20
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

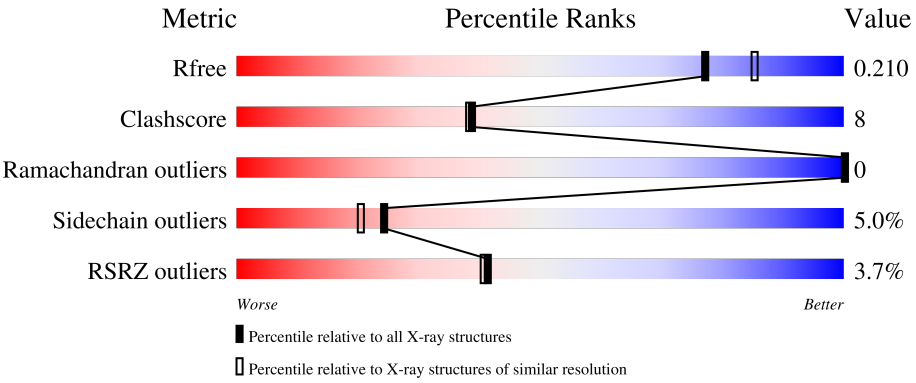
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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 >=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 <=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	4% 81% 14%
2	B	168	2% 88% 11%
3	C	34	65% 21% 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 6475 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	3	0
			4368	2966	695	691	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	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
A	120	PHE	ALA	engineered mutation	UNP Q5SJ79
A	236	ILE	VAL	engineered mutation	UNP Q5SJ79

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

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

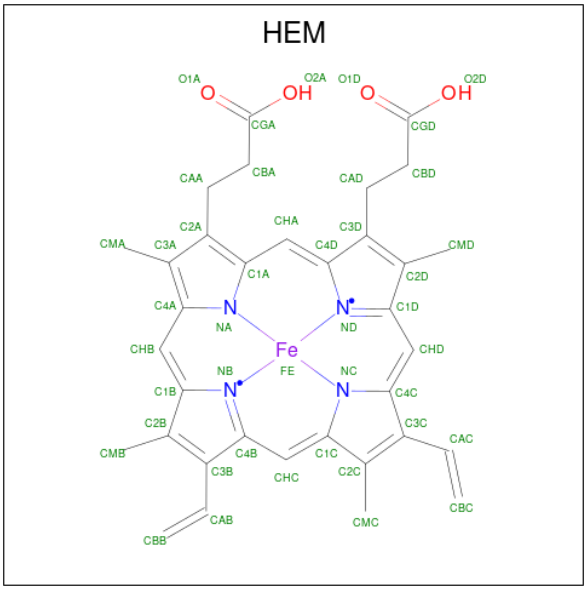
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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

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

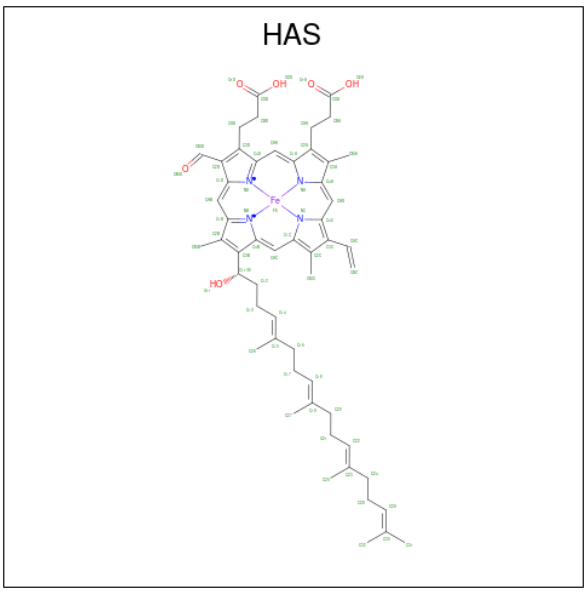
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

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



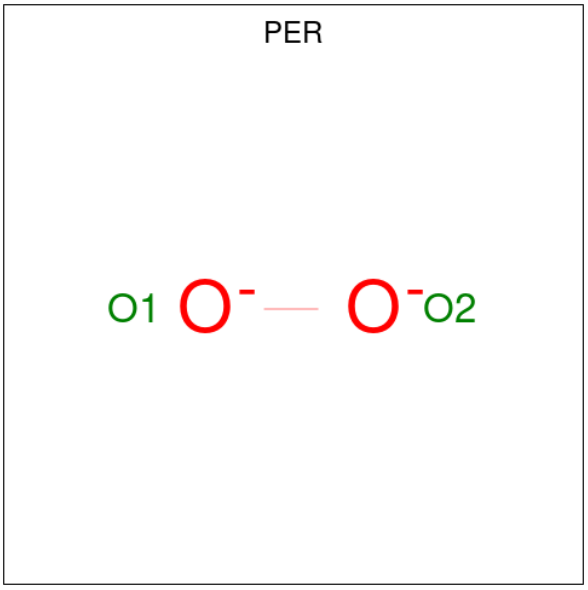
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0

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



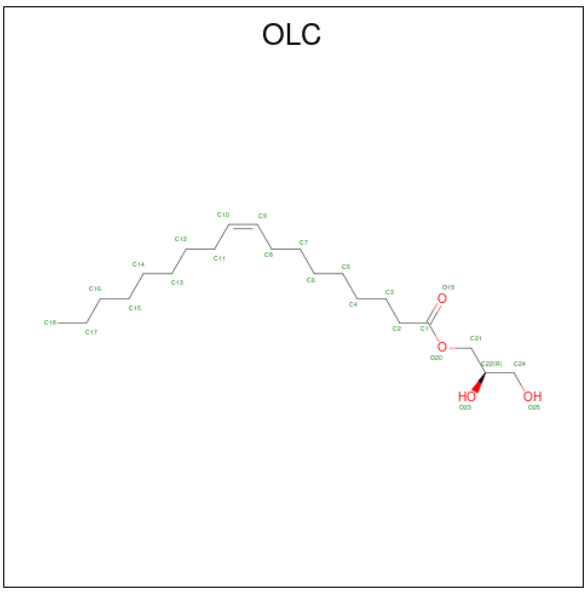
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



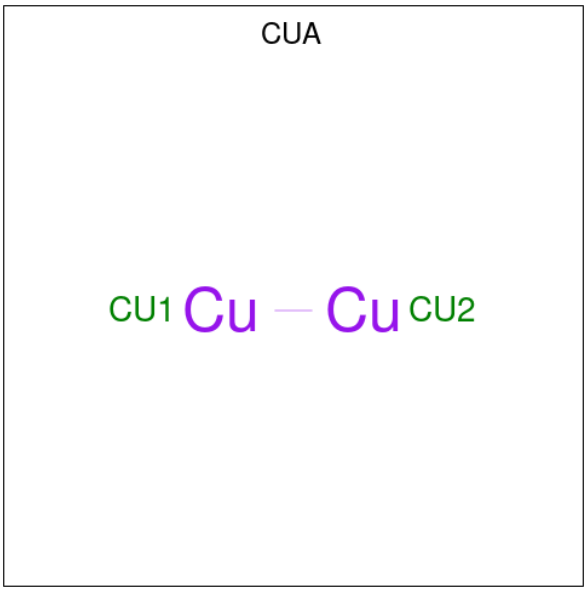
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O		0	0
			2	2			

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 19 17 2	0	0
8	A	1	Total C O 23 19 4	0	0
8	A	1	Total C O 14 12 2	0	0
8	A	1	Total C O 12 10 2	0	0
8	A	1	Total C O 15 11 4	0	0
8	A	1	Total C O 20 16 4	0	0
8	A	1	Total C O 25 21 4	0	0
8	A	1	Total C O 21 17 4	0	0
8	A	1	Total C O 25 21 4	0	0
8	B	1	Total C O 20 18 2	0	0
8	B	1	Total C O 24 20 4	0	0
8	B	1	Total C O 16 12 4	0	0
8	B	1	Total C O 20 18 2	0	0
8	C	1	Total C O 23 19 4	0	0
8	C	1	Total C 9 9	0	0

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

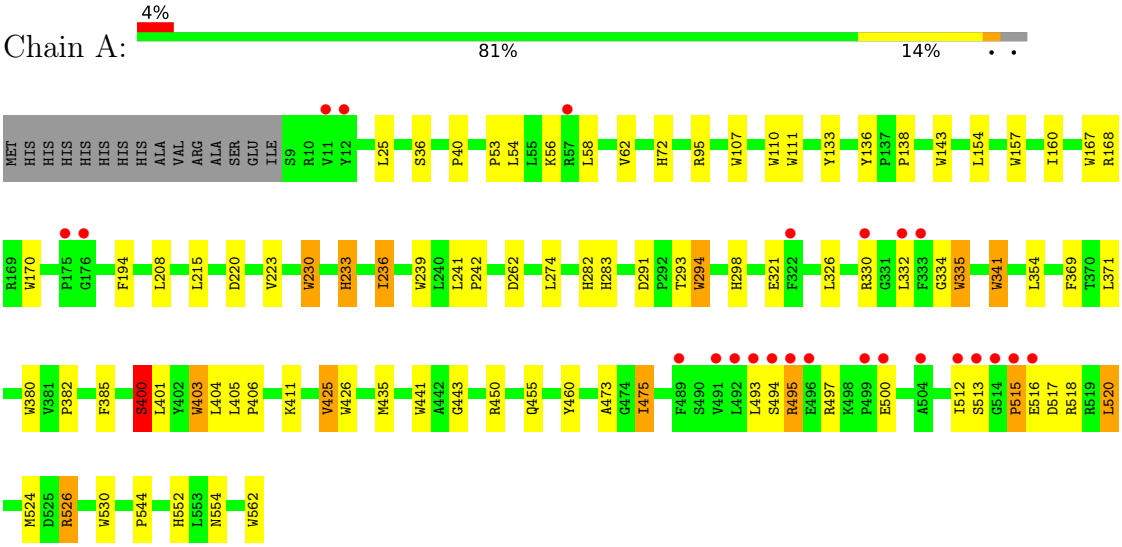
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	106	Total O 106 106	0	0
10	B	67	Total O 67 67	0	0
10	C	6	Total O 6 6	0	0

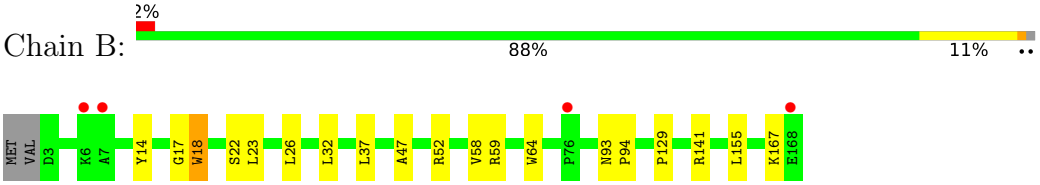
3 Residue-property plots (i)

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 (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.57Å 98.39Å 94.58Å 90.00° 127.64° 90.00°	Depositor
Resolution (Å)	74.89 – 2.00 56.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (74.89-2.00) 93.5 (56.84-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.182 , 0.207 0.183 , 0.210	Depositor DCC
R_{free} test set	3315 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 70.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6475	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, HEM, HAS, CUA, PER, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	1.33	25/4535 (0.6%)	1.05	11/6227 (0.2%)
2	B	1.27	2/1330 (0.2%)	1.03	3/1817 (0.2%)
3	C	1.19	0/247	1.17	2/335 (0.6%)
All	All	1.31	27/6112 (0.4%)	1.05	16/8379 (0.2%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	TRP	CD2-CE2	7.41	1.50	1.41
1	A	400	SER	CB-OG	7.18	1.51	1.42
1	A	341	TRP	CD2-CE2	6.46	1.49	1.41
1	A	460	TYR	CB-CG	6.28	1.61	1.51
1	A	298	HIS	CG-CD2	6.27	1.46	1.35

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	95	ARG	NE-CZ-NH1	-12.15	114.22	120.30
2	B	59	ARG	NE-CZ-NH2	9.41	125.01	120.30
3	C	24	LEU	CB-CG-CD1	8.53	125.50	111.00
1	A	450	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	A	95	ARG	NE-CZ-NH2	7.75	124.17	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	4462	64	0
2	B	1288	0	1260	15	0
3	C	241	0	267	5	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
6	A	65	0	62	5	0
7	A	2	0	0	0	0
8	A	174	0	247	31	0
8	B	80	0	112	12	0
8	C	32	0	50	2	0
9	B	2	0	0	0	0
10	A	106	0	0	3	0
10	B	67	0	0	1	0
10	C	6	0	0	1	0
All	All	6475	0	6490	96	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 8.

The worst 5 of 96 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:168:ARG:HH22	8:A:609:OLC:C2	1.62	1.11
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.67	1.07
1:A:168:ARG:NH1	8:A:609:OLC:H7A	1.77	0.99
1:A:168:ARG:HH12	8:A:609:OLC:H5	1.26	0.99
1:A:330[B]:ARG:HG2	1:A:330[B]:ARG:NH1	1.54	0.94

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	554/569 (97%)	539 (97%)	15 (3%)	0	100	100
2	B	165/168 (98%)	163 (99%)	2 (1%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	748/771 (97%)	731 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/464 (96%)	424 (95%)	23 (5%)	24	19
2	B	134/138 (97%)	130 (97%)	4 (3%)	41	41
3	C	24/27 (89%)	21 (88%)	3 (12%)	4	2
All	All	605/629 (96%)	575 (95%)	30 (5%)	24	20

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

Mol	Chain	Res	Type
1	A	493	LEU
3	C	17	LEU
1	A	500	GLU
3	C	24	LEU
2	B	37	LEU

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

Mol	Chain	Res	Type
2	B	8	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
8	OLC	A	607	-	13,13,24	0.65	0	13,13,25	0.82	0
9	CUA	B	201	2	0,1,1	-	-	-		
8	OLC	B	205	-	19,19,24	0.53	0	19,19,25	0.60	0
8	OLC	A	612	-	20,20,24	0.51	0	21,21,25	0.85	0
8	OLC	B	203	-	23,23,24	0.99	1 (4%)	24,24,25	1.68	4 (16%)
8	OLC	A	608	-	11,11,24	0.76	0	11,11,25	1.00	1 (9%)
5	HEM	A	602	1	41,50,50	2.31	14 (34%)	45,82,82	3.30	24 (53%)
8	OLC	C	101	-	22,22,24	0.58	0	23,23,25	1.05	1 (4%)
6	HAS	A	603	1,7	69,72,72	2.20	17 (24%)	73,109,109	1.75	16 (21%)
8	OLC	A	611	-	24,24,24	0.67	1 (4%)	25,25,25	1.09	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	OLC	A	605	-	18,18,24	0.49	0	18,18,25	1.15	2 (11%)
8	OLC	A	606	-	22,22,24	0.69	0	23,23,25	1.17	2 (8%)
8	OLC	A	610	-	19,19,24	0.40	0	20,20,25	0.84	0
8	OLC	B	202	-	19,19,24	0.64	1 (5%)	19,19,25	0.77	0
8	OLC	A	613	-	24,24,24	0.35	0	25,25,25	1.17	3 (12%)
8	OLC	B	204	-	15,15,24	0.50	0	16,16,25	0.72	0
7	PER	A	604	6,4	0,1,1	-	-	-		
8	OLC	C	102	-	8,8,24	0.11	0	7,7,25	0.39	0
8	OLC	A	609	-	14,14,24	1.19	1 (7%)	15,15,25	1.59	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	B	202	-	-	9/18/18/24	-
8	OLC	A	607	-	-	3/12/12/24	-
8	OLC	A	613	-	-	10/24/24/24	-
8	OLC	A	610	-	-	9/19/19/24	-
8	OLC	B	205	-	-	7/18/18/24	-
6	HAS	A	603	1,7	1/1/8/18	6/40/82/82	-
8	OLC	A	611	-	-	15/24/24/24	-
8	OLC	A	612	-	-	4/20/20/24	-
8	OLC	B	203	-	-	10/23/23/24	-
8	OLC	B	204	-	-	6/15/15/24	-
8	OLC	A	606	-	-	8/22/22/24	-
8	OLC	A	608	-	-	3/9/9/24	-
5	HEM	A	602	1	-	1/12/54/54	-
8	OLC	A	605	-	-	5/16/16/24	-
8	OLC	C	102	-	-	3/6/6/24	-
8	OLC	C	101	-	-	9/22/22/24	-
8	OLC	A	609	-	-	9/14/14/24	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C3C-C2C	7.83	1.51	1.40
6	A	603	HAS	C3C-CAC	-6.78	1.34	1.47
5	A	602	HEM	CHB-C1B	5.53	1.49	1.35
5	A	602	HEM	C1A-NA	5.49	1.47	1.36
6	A	603	HAS	C1D-ND	5.17	1.49	1.40

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	602	HEM	CHC-C4B-NB	9.80	135.07	124.43
5	A	602	HEM	CHD-C1D-ND	7.33	132.40	124.43
5	A	602	HEM	C4D-ND-C1D	7.24	112.55	105.07
5	A	602	HEM	CHA-C4D-ND	6.44	132.34	124.38
5	A	602	HEM	C2C-C3C-C4C	-5.51	103.05	106.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

5 of 117 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	HEM	C2B-C3B-CAB-CBB
8	A	606	OLC	C21-C22-C24-O25
8	A	609	OLC	C21-C22-C24-O25
8	A	610	OLC	O20-C21-C22-O23
8	A	612	OLC	C21-C22-C24-O25

There are no ring outliers.

14 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	205	OLC	1	0
8	A	612	OLC	1	0
8	B	203	OLC	7	0
5	A	602	HEM	2	0
8	C	101	OLC	2	0
6	A	603	HAS	5	0
8	A	611	OLC	9	0
8	A	605	OLC	3	0
8	A	606	OLC	3	0

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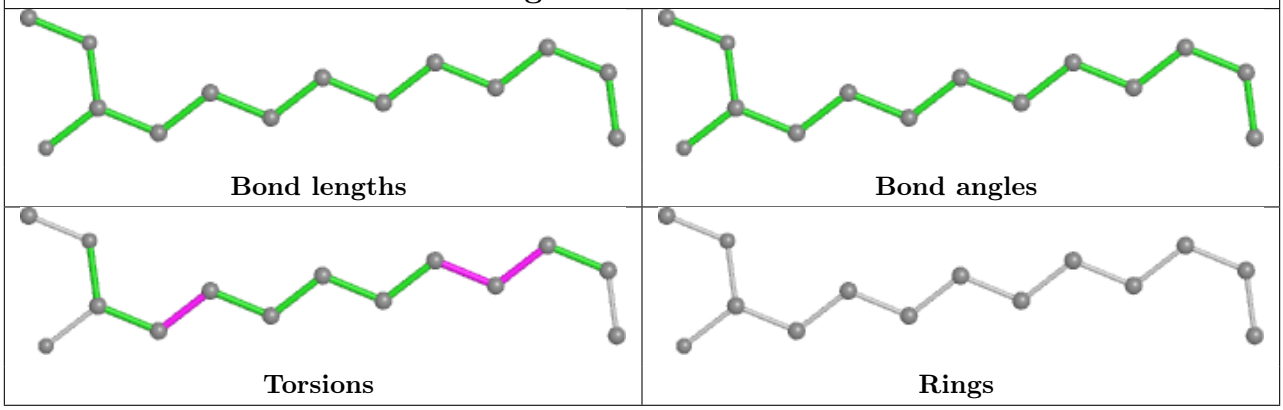
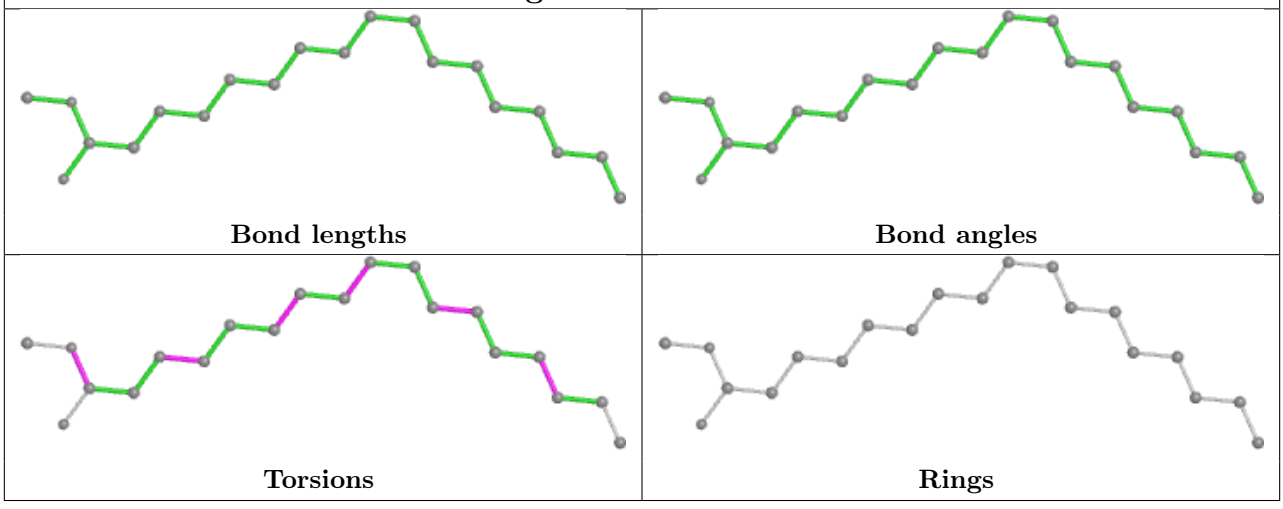
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	610	OLC	1	0
8	B	202	OLC	1	0
8	A	613	OLC	1	0
8	B	204	OLC	3	0
8	A	609	OLC	19	0

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 then 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.

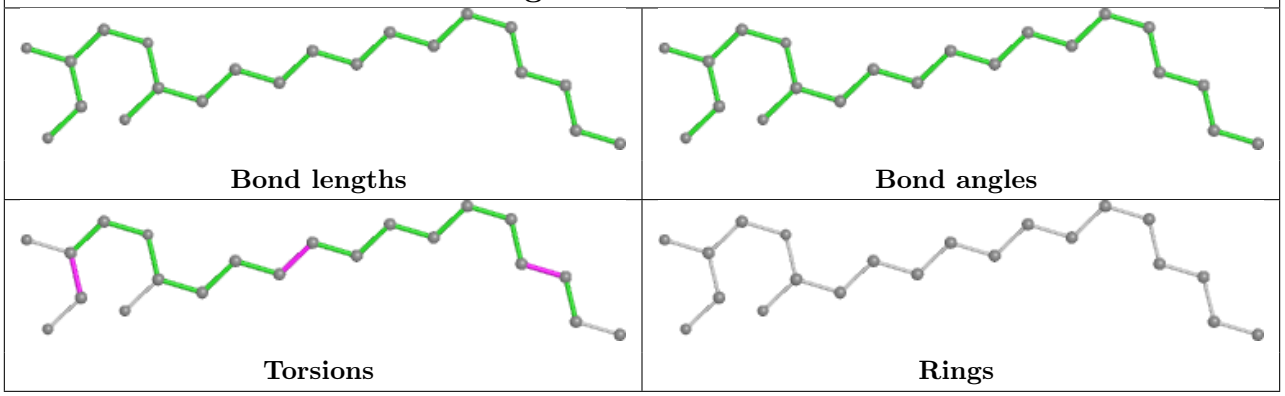
Ligand OLC A 607



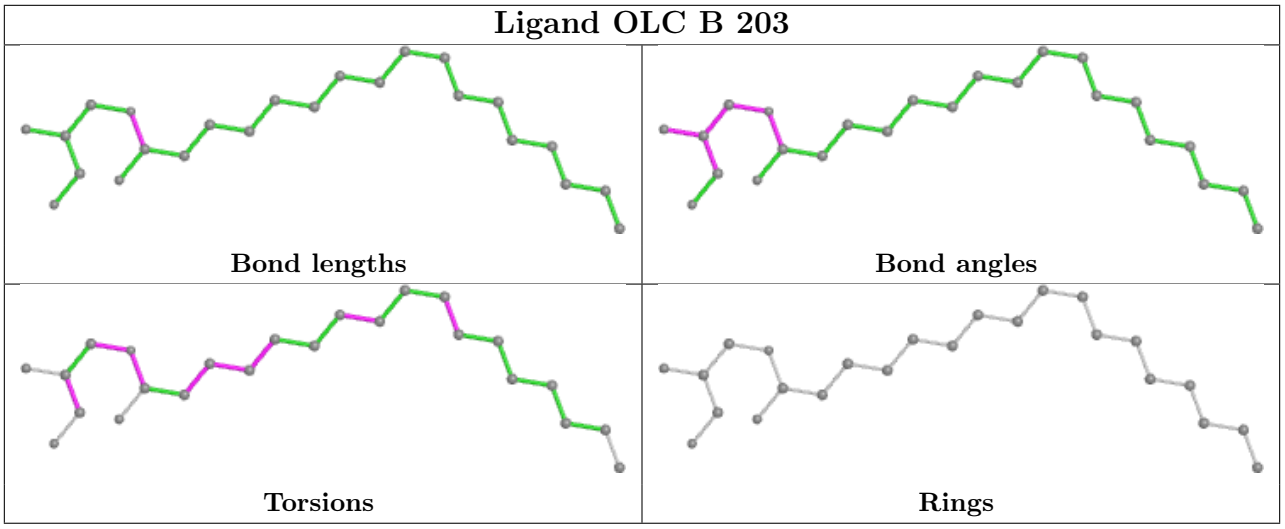
Ligand OLC B 205



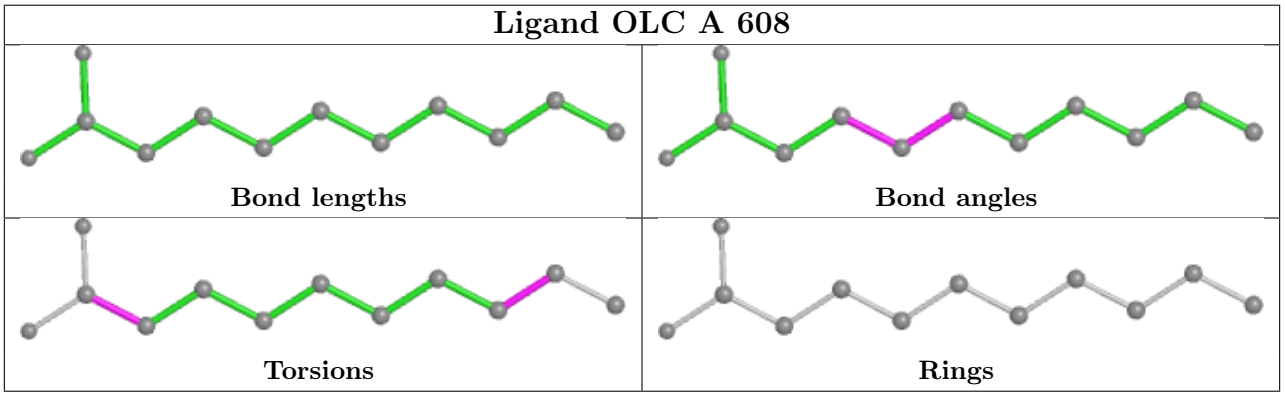
Ligand OLC A 612



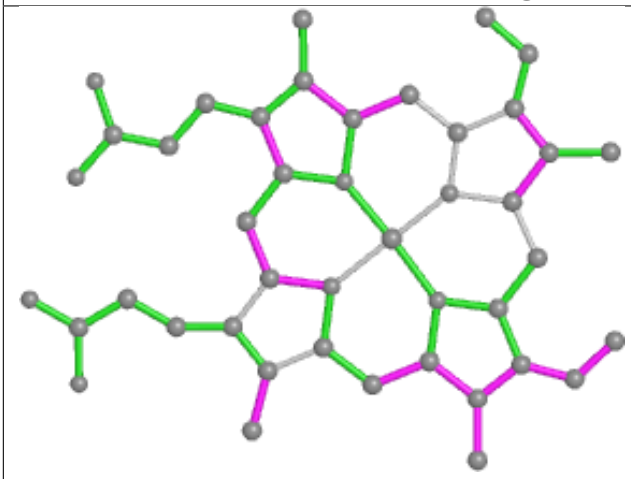
Ligand OLC B 203



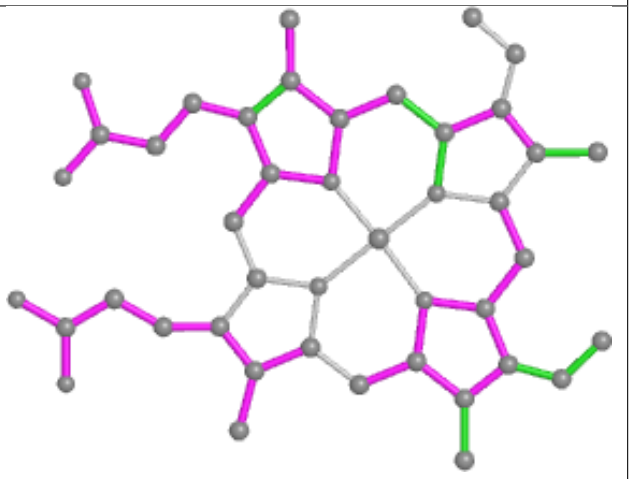
Ligand OLC A 608



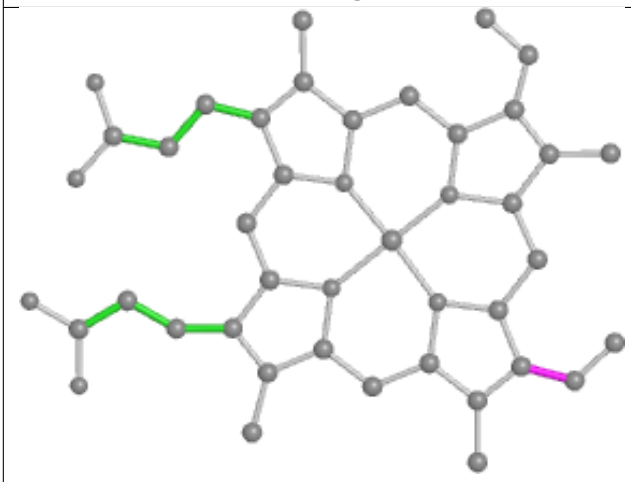
Ligand HEM A 602



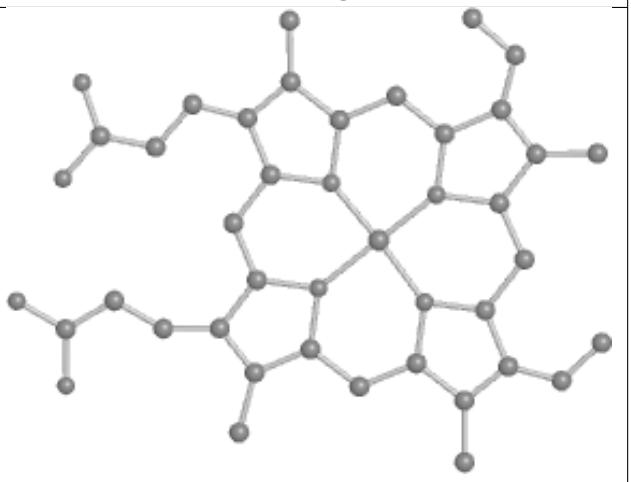
Bond lengths



Bond angles

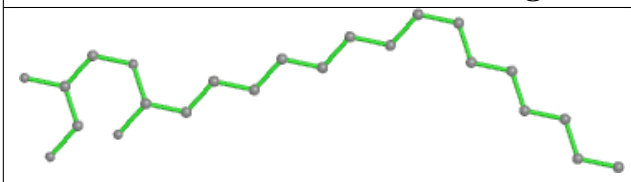


Torsions

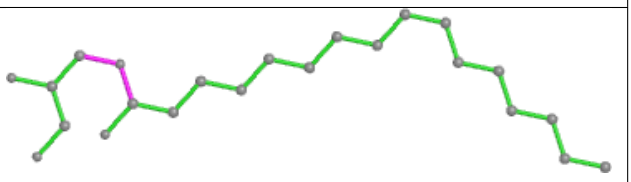


Rings

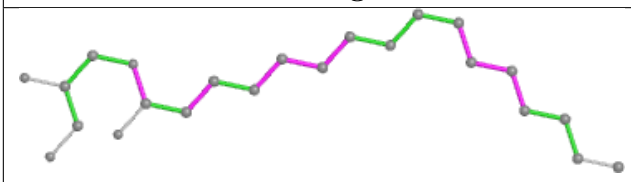
Ligand OLC C 101



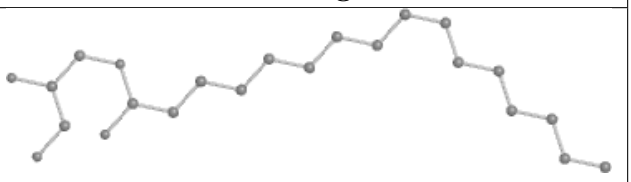
Bond lengths



Bond angles

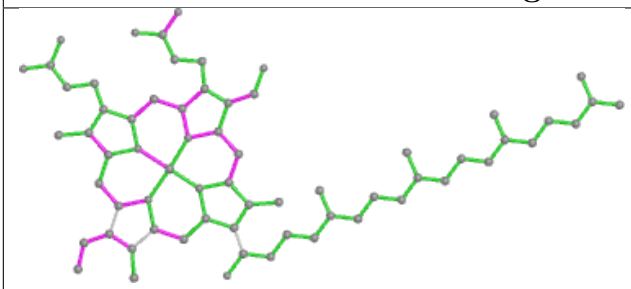


Torsions

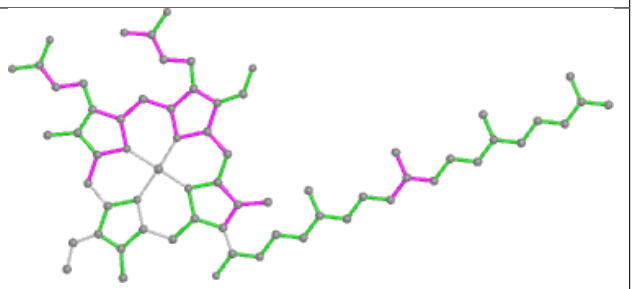


Rings

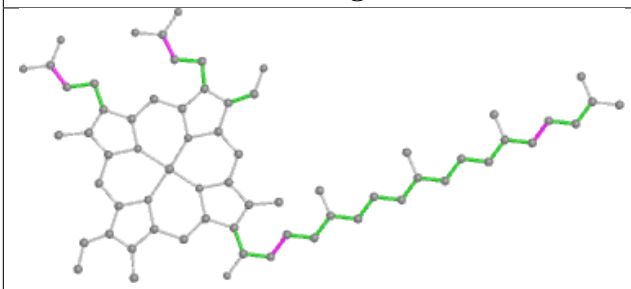
Ligand HAS A 603



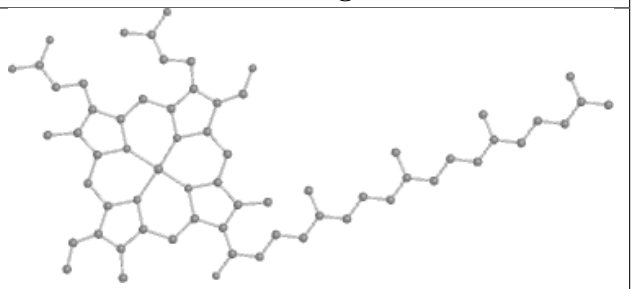
Bond lengths



Bond angles

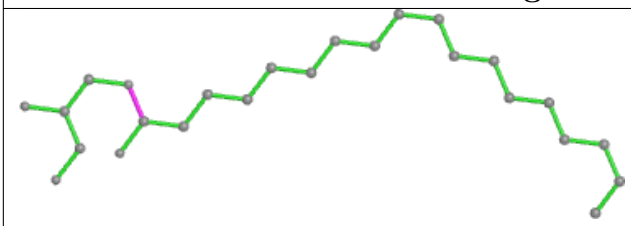


Torsions

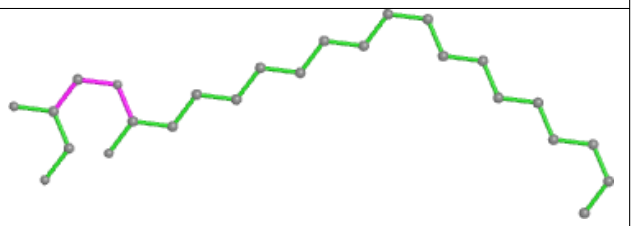


Rings

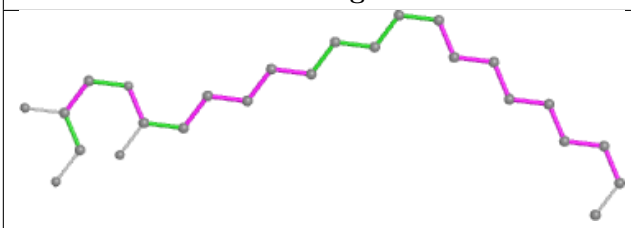
Ligand OLC A 611



Bond lengths



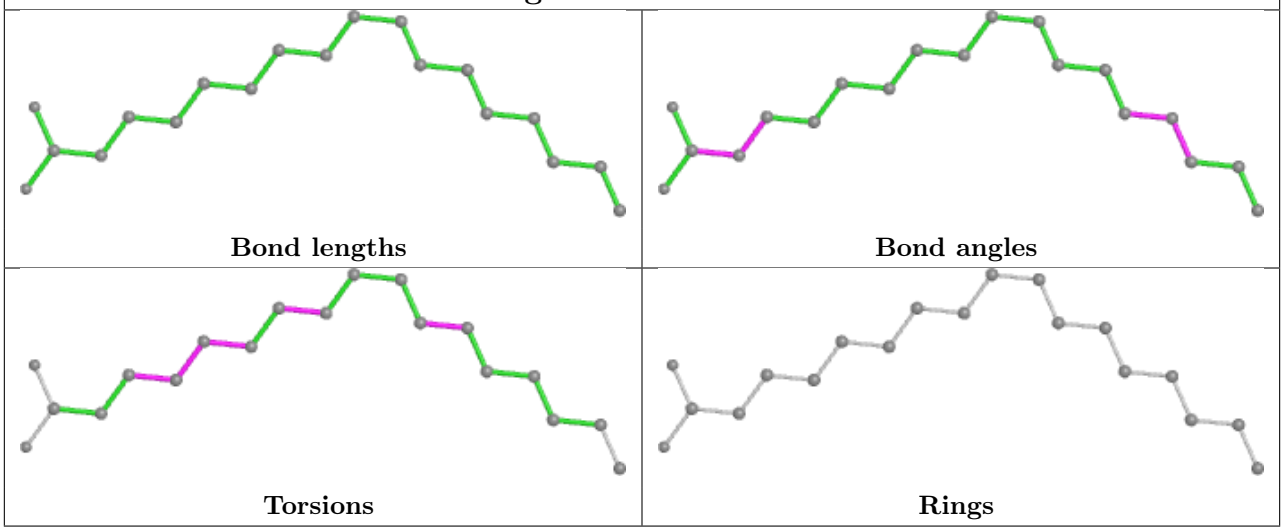
Bond angles



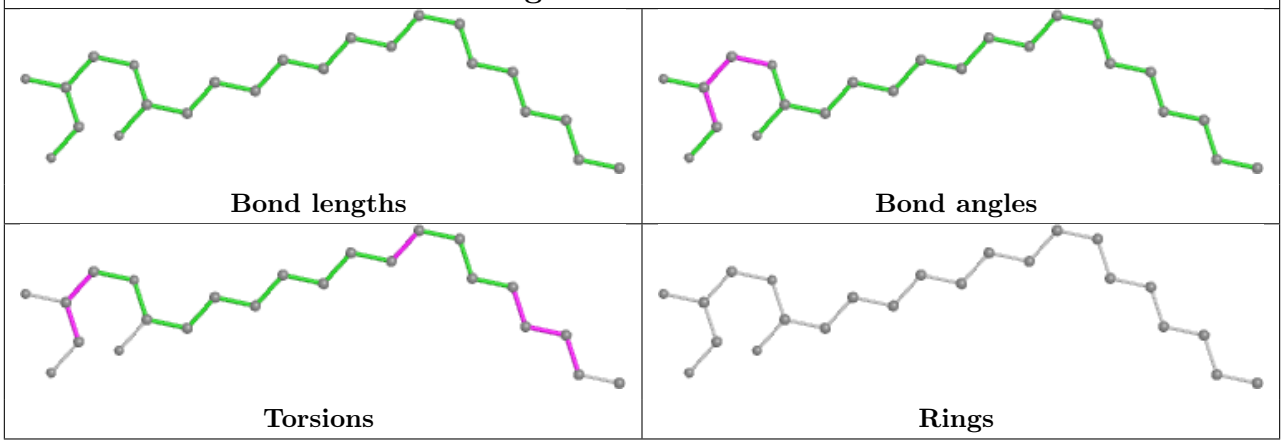
Torsions

Rings

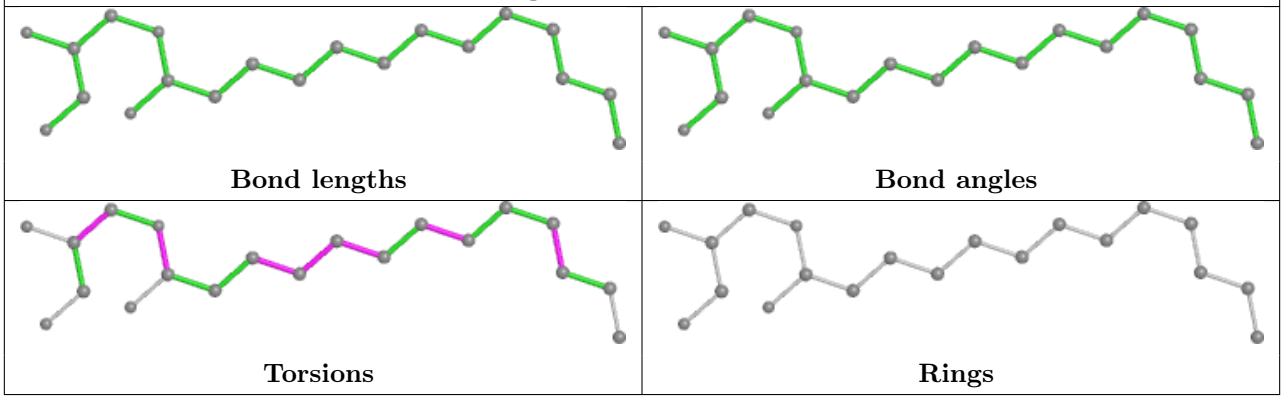
Ligand OLC A 605



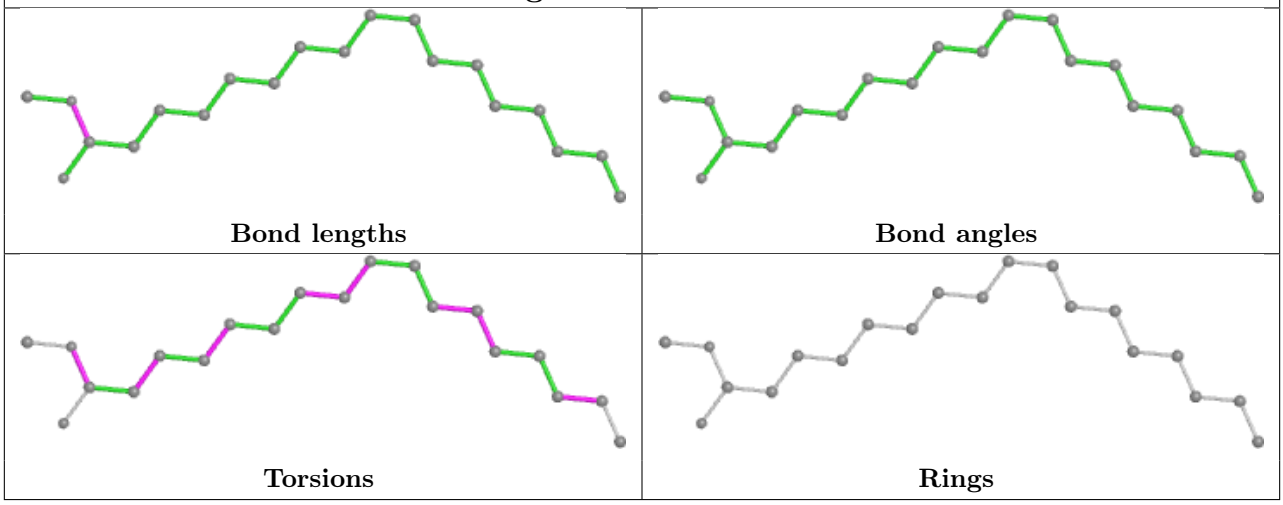
Ligand OLC A 606



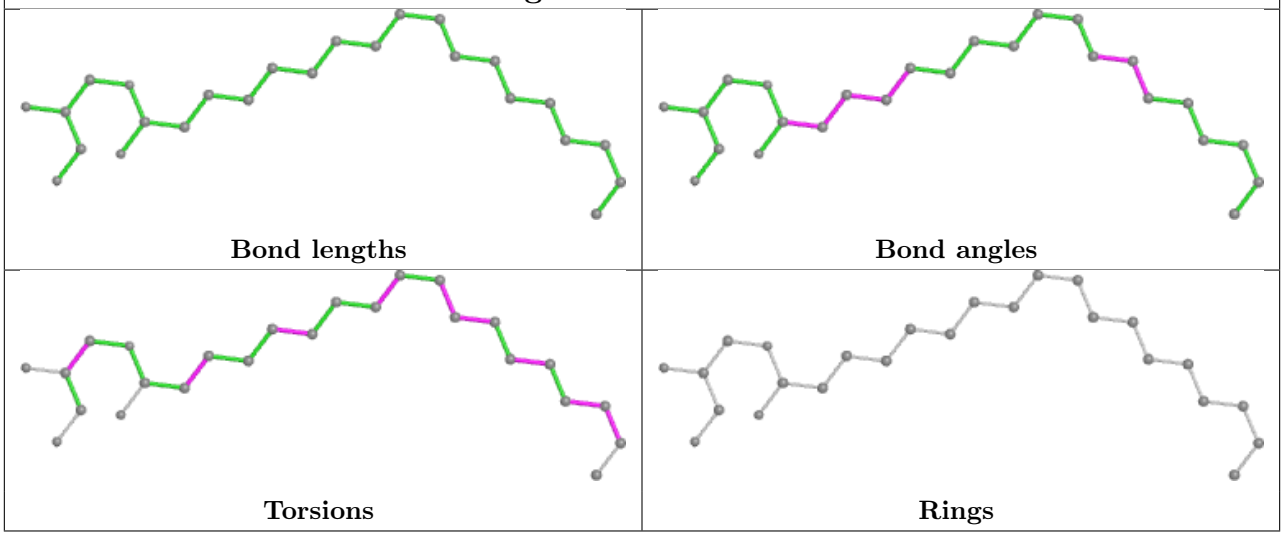
Ligand OLC A 610



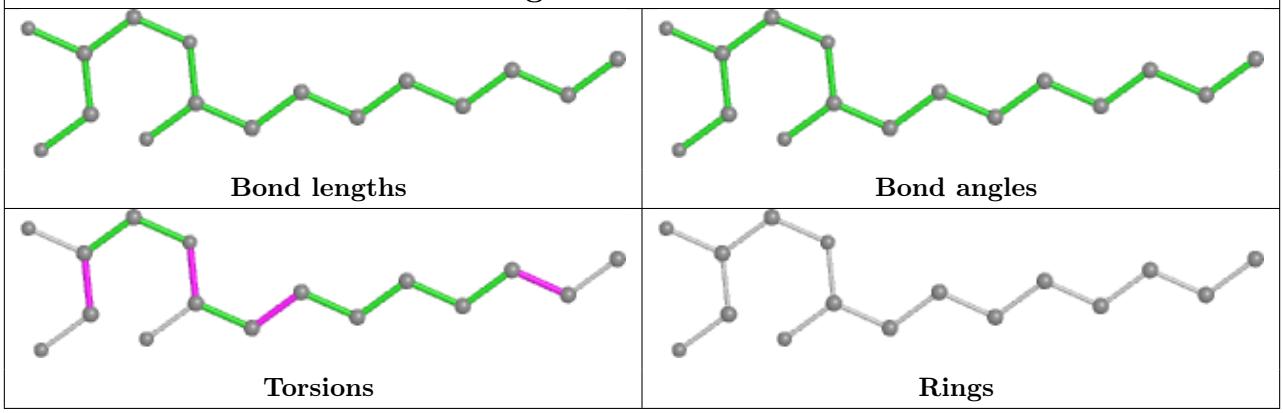
Ligand OLC B 202



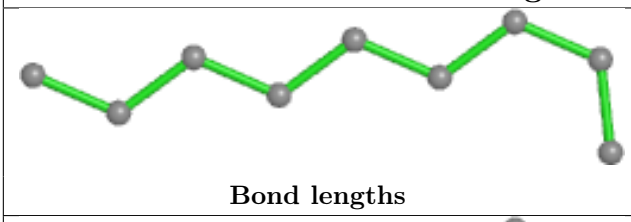
Ligand OLC A 613



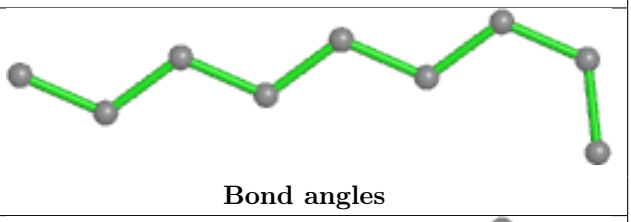
Ligand OLC B 204



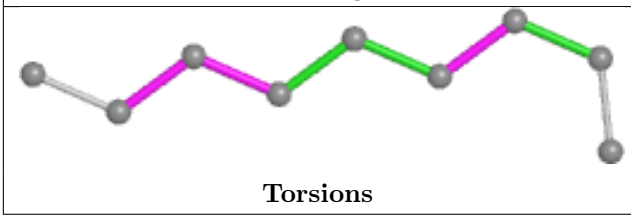
Ligand OLC C 102



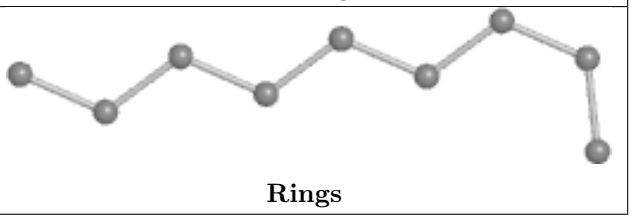
Bond lengths



Bond angles

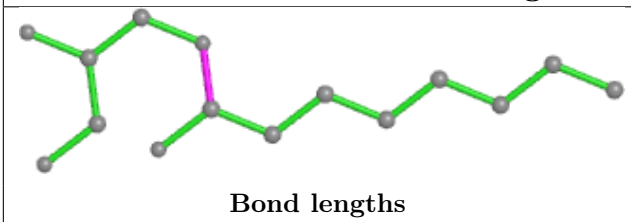


Torsions

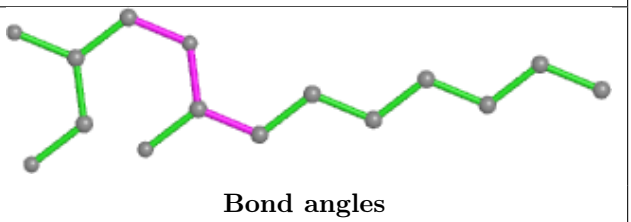


Rings

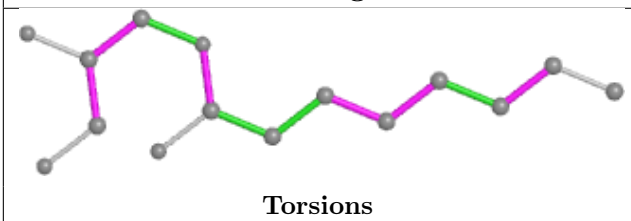
Ligand OLC A 609



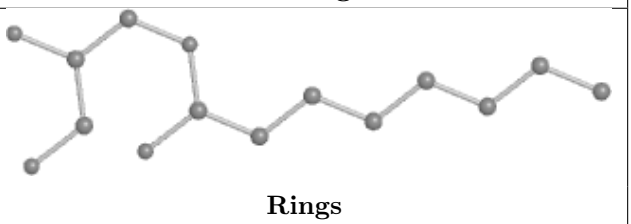
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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^2)	Q<0.9
1	A	554/569 (97%)	-0.32	24 (4%) 35 34	15, 25, 49, 100	0
2	B	166/168 (98%)	-0.44	4 (2%) 59 57	16, 26, 45, 64	0
3	C	31/34 (91%)	-0.66	0 100 100	20, 26, 37, 59	0
All	All	751/771 (97%)	-0.36	28 (3%) 41 41	15, 26, 49, 100	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	ARG	8.1
1	A	494	SER	5.1
1	A	513	SER	5.0
1	A	515	PRO	5.0
1	A	330[A]	ARG	4.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

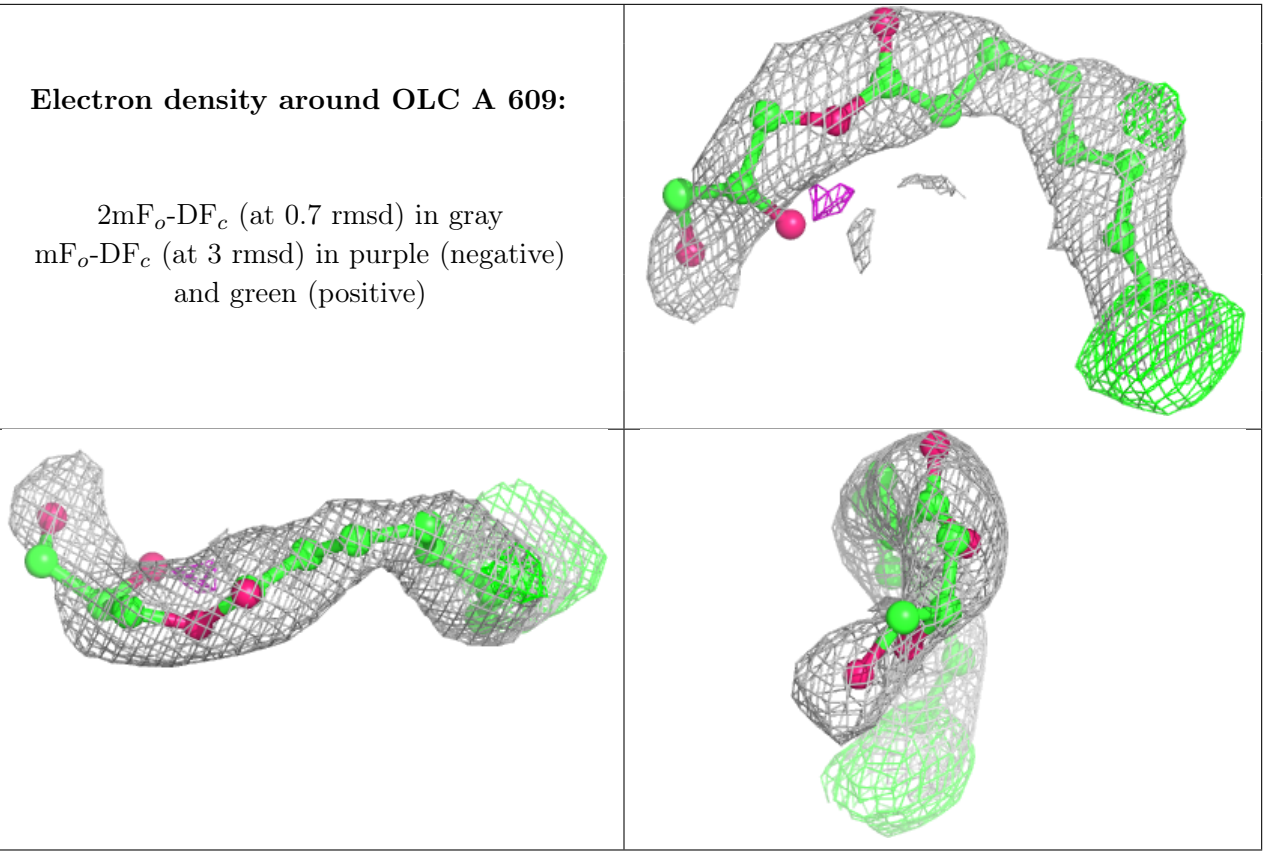
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	OLC	A	609	15/25	0.56	0.24	50,62,84,92	0
8	OLC	B	203	24/25	0.67	0.23	46,62,86,100	0
8	OLC	A	607	14/25	0.77	0.23	46,55,74,79	0
8	OLC	A	611	25/25	0.78	0.19	42,59,71,76	0
8	OLC	B	205	20/25	0.78	0.22	47,55,80,82	0
8	OLC	C	102	9/25	0.78	0.25	56,60,62,66	0
8	OLC	A	613	25/25	0.80	0.18	47,57,69,87	0
8	OLC	A	612	21/25	0.80	0.15	46,57,86,96	0
8	OLC	C	101	23/25	0.81	0.20	37,53,73,79	0
8	OLC	B	204	16/25	0.82	0.20	49,60,80,93	0
8	OLC	B	202	20/25	0.82	0.16	46,57,65,67	0
8	OLC	A	610	20/25	0.83	0.19	46,66,86,87	0
8	OLC	A	608	12/25	0.86	0.14	48,54,71,86	0
8	OLC	A	606	23/25	0.88	0.14	29,40,58,68	0
8	OLC	A	605	19/25	0.88	0.19	43,57,83,84	0
7	PER	A	604	2/2	0.94	0.12	21,21,21,23	0
6	HAS	A	603	65/65	0.98	0.10	14,18,33,36	0
5	HEM	A	602	43/43	0.99	0.07	12,15,18,19	0
4	CU	A	601	1/1	1.00	0.10	21,21,21,21	0
9	CUA	B	201	2/2	1.00	0.09	19,19,19,19	0

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

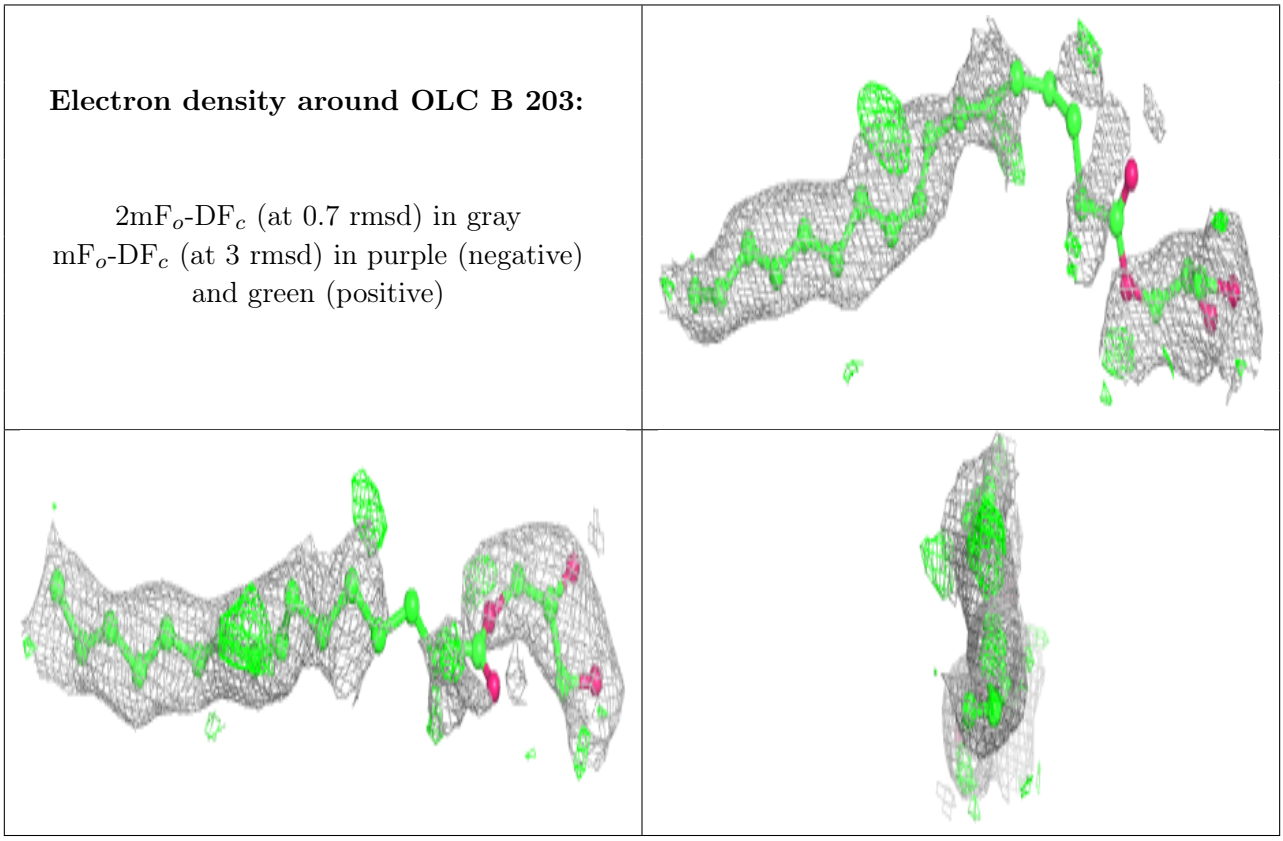
Electron density around OLC A 609:

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



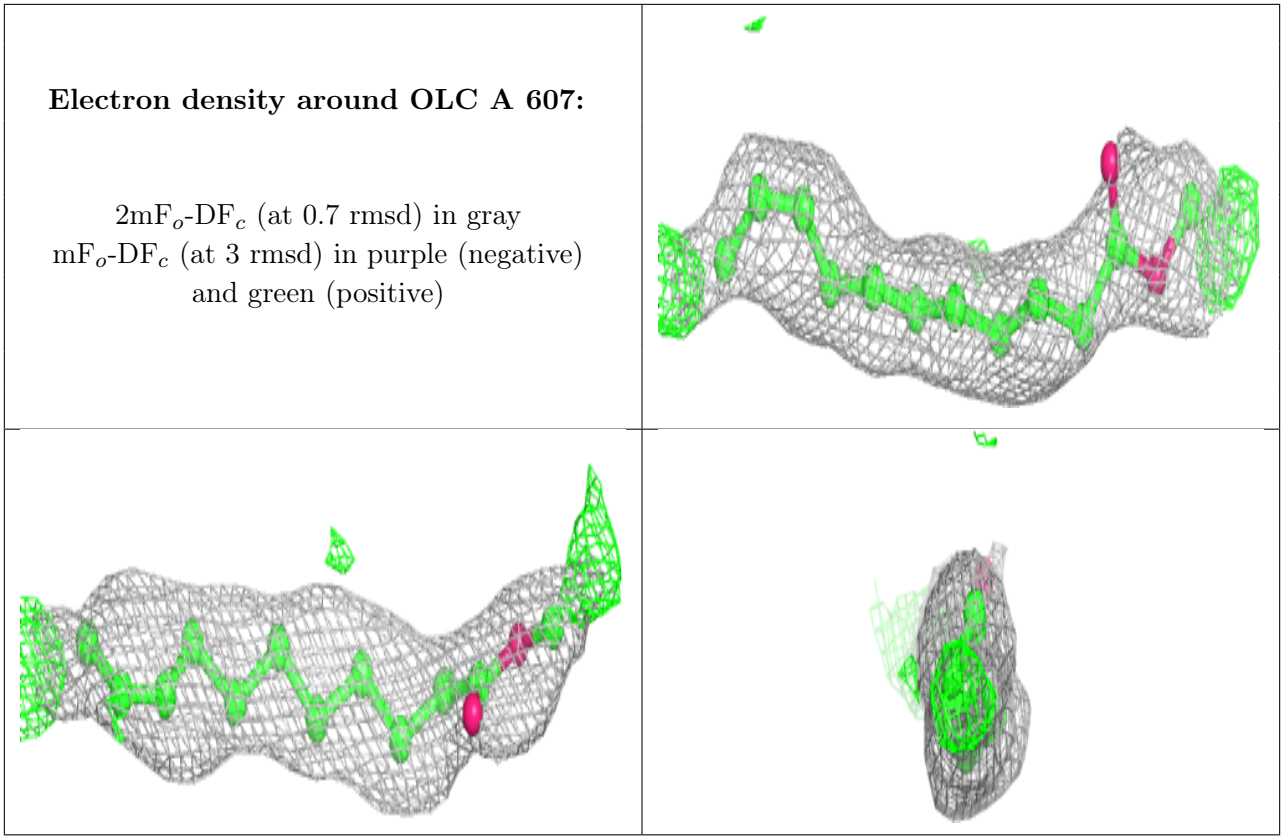
Electron density around OLC B 203:

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



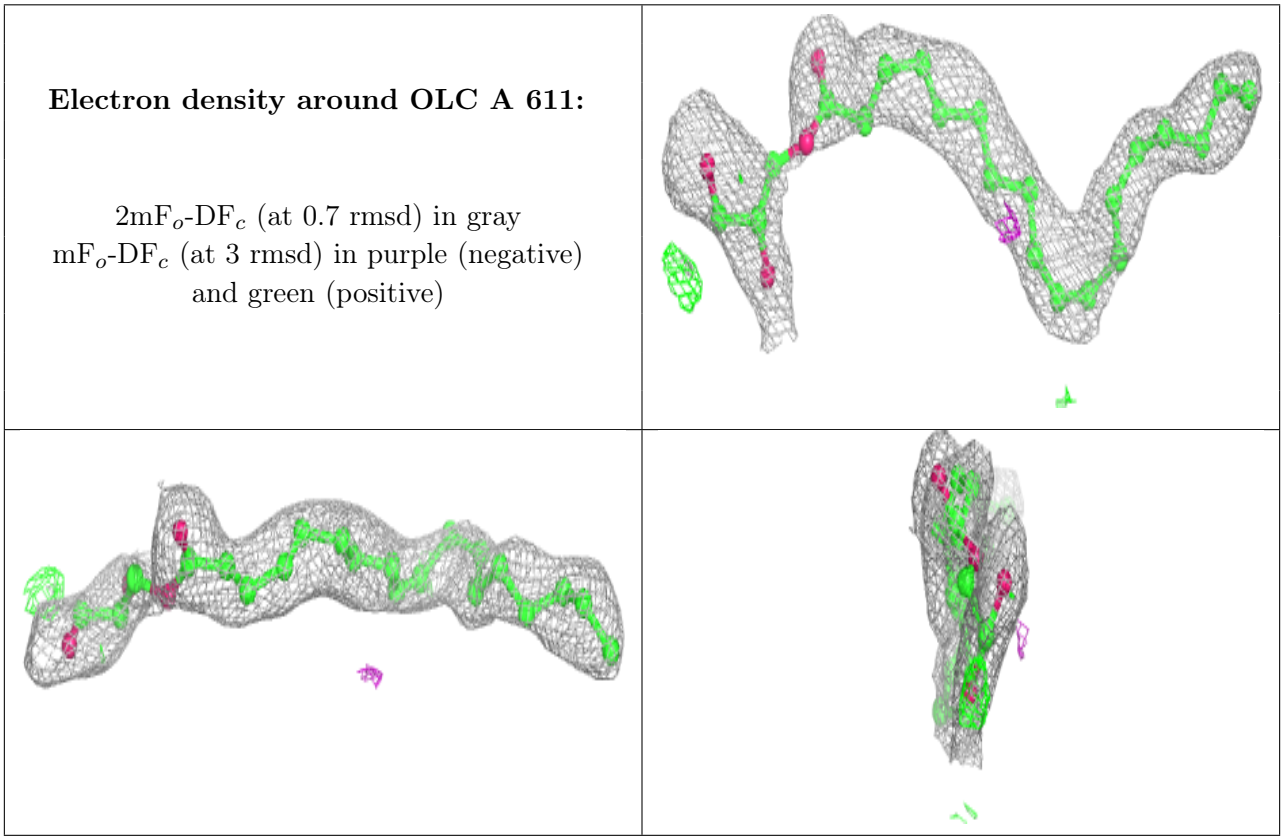
Electron density around OLC A 607:

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



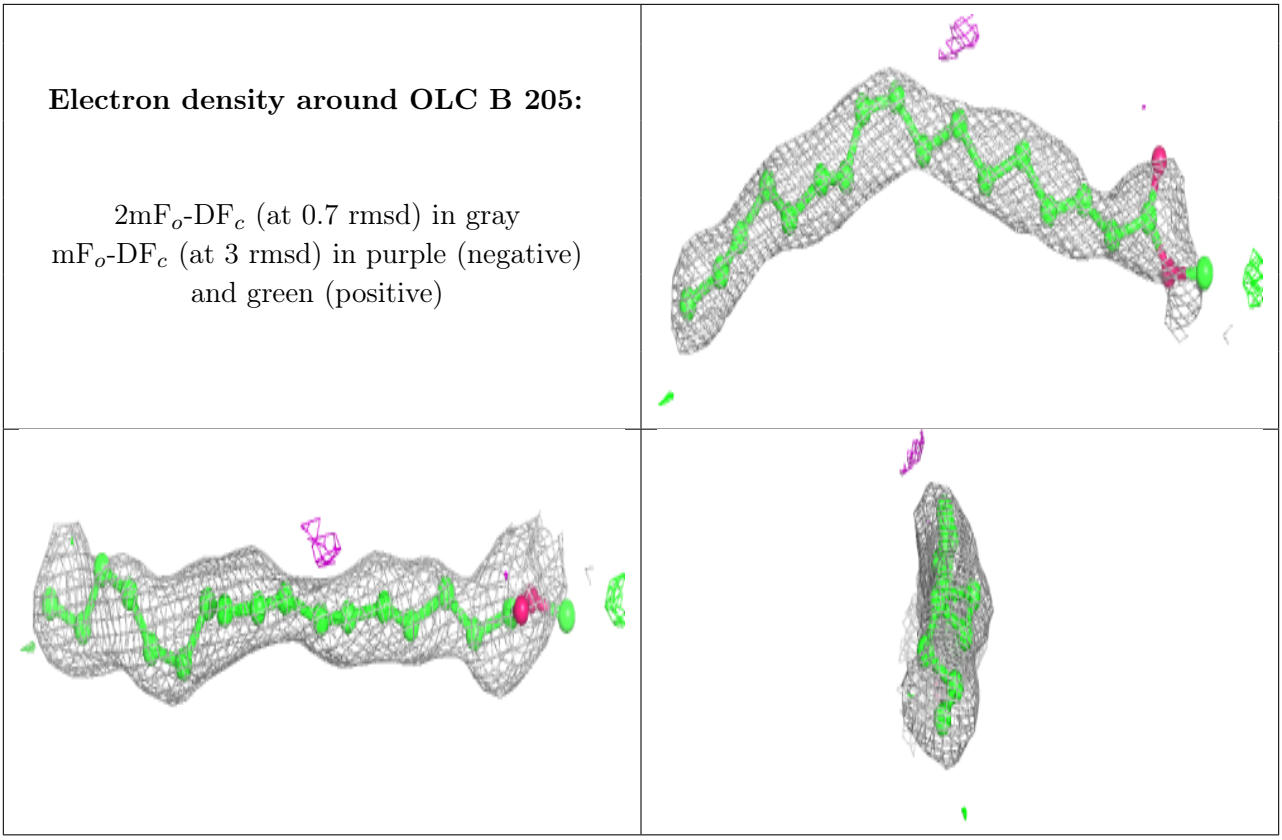
Electron density around OLC A 611:

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



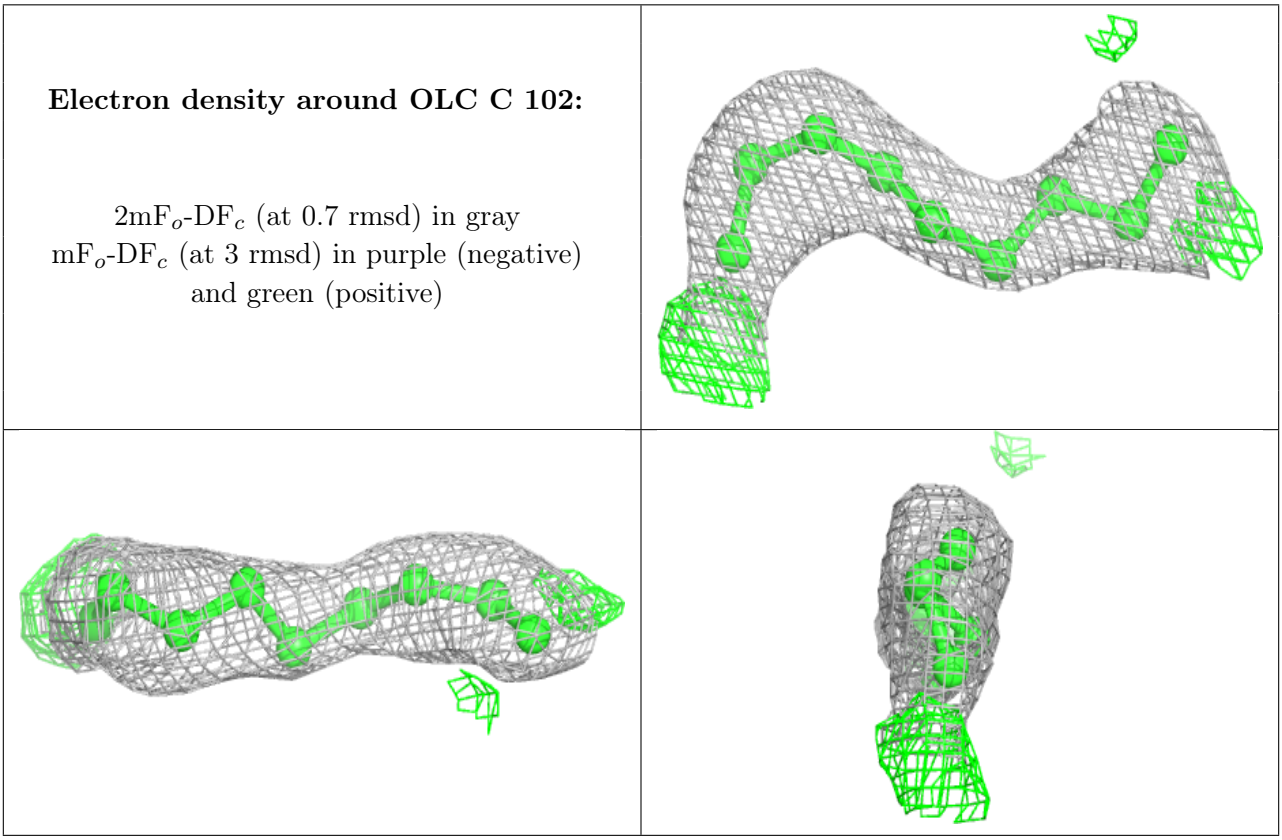
Electron density around OLC B 205:

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



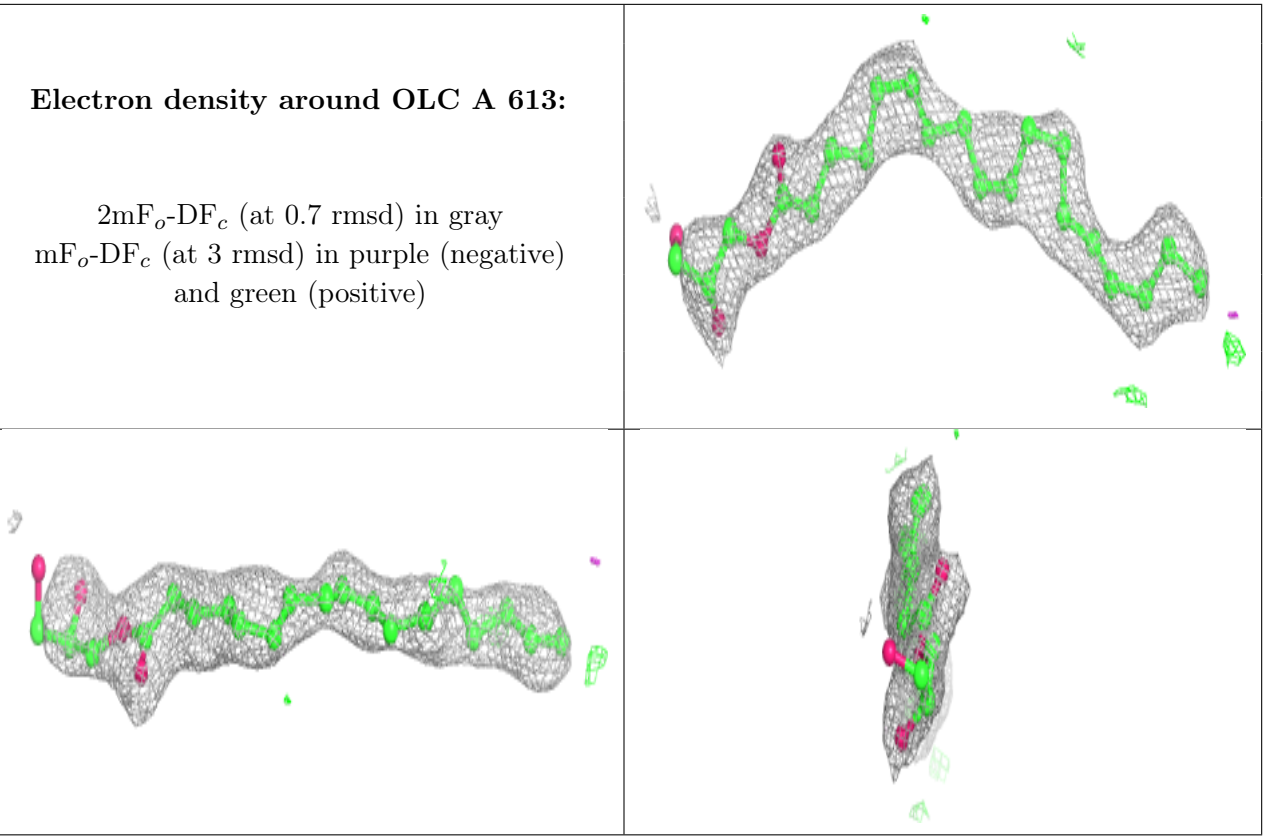
Electron density around OLC C 102:

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



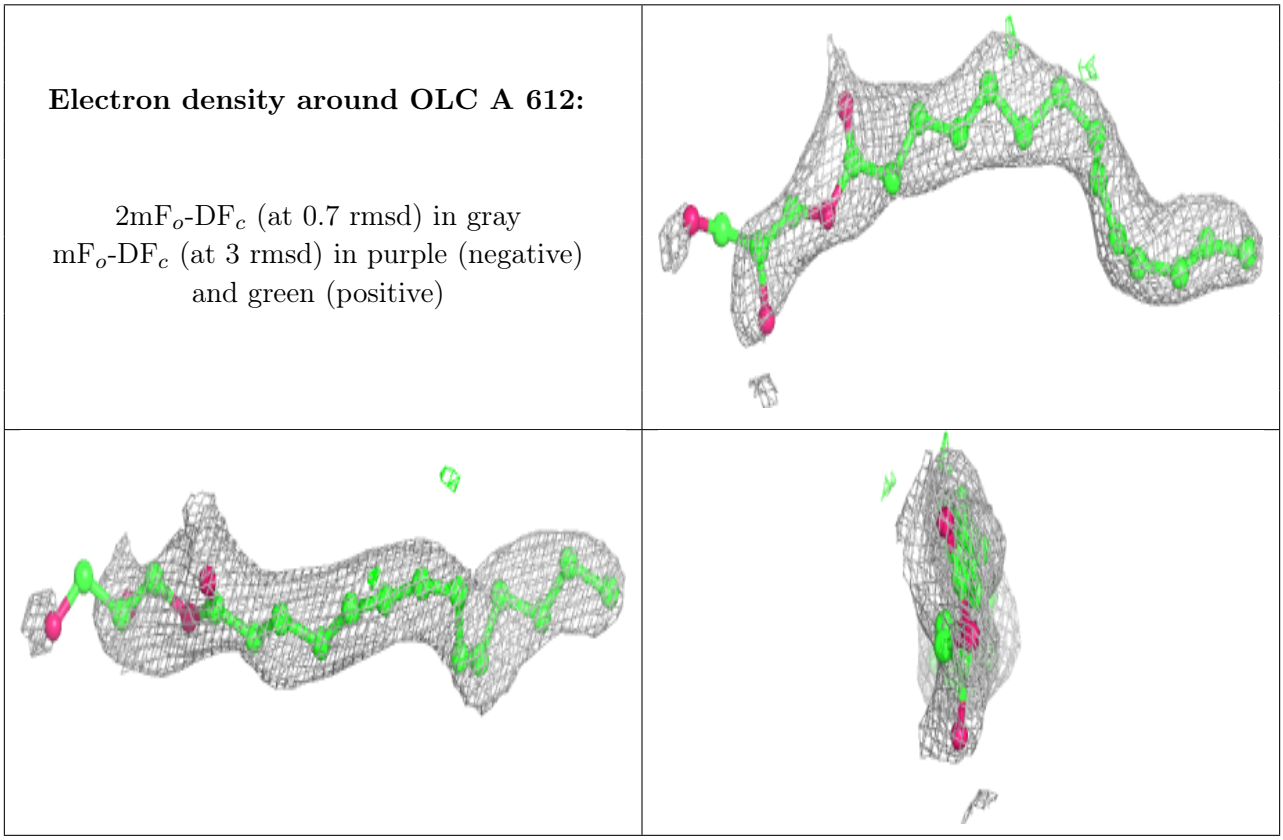
Electron density around OLC A 613:

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



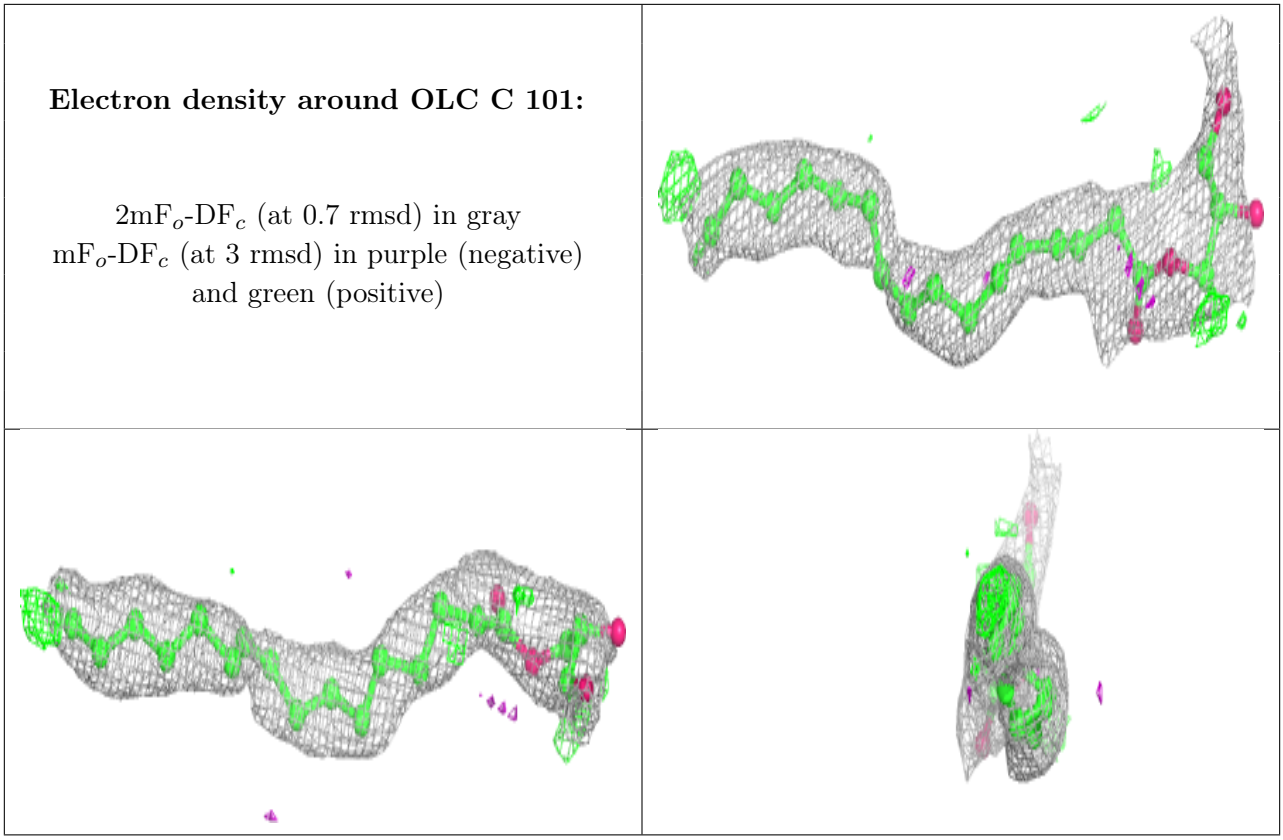
Electron density around OLC A 612:

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



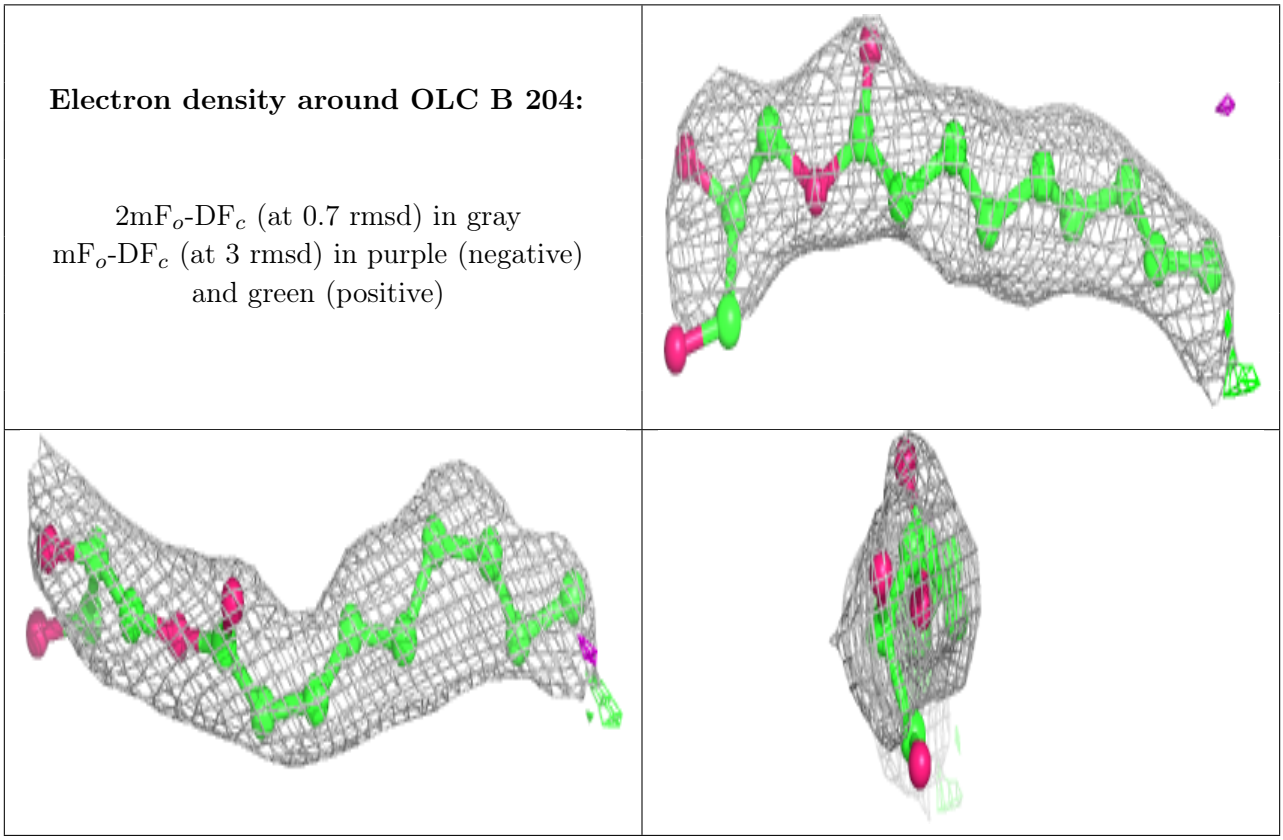
Electron density around OLC C 101:

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



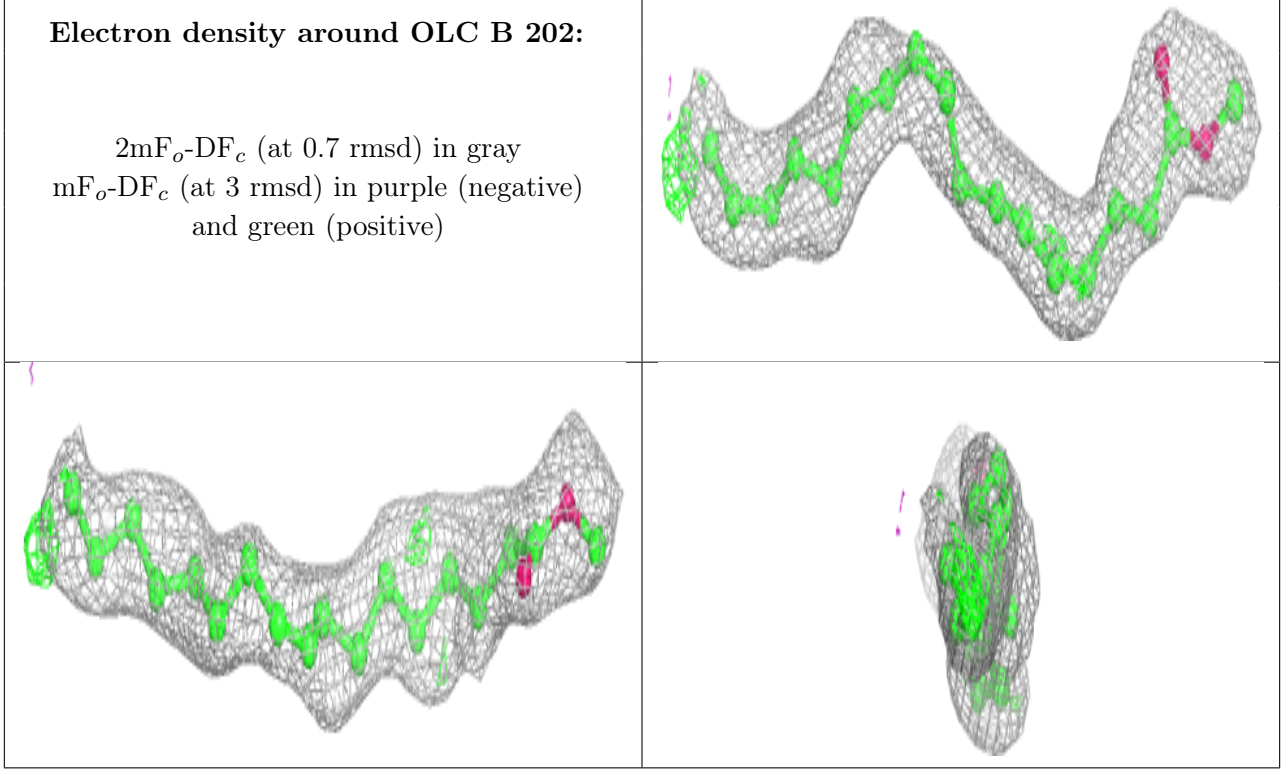
Electron density around OLC B 204:

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



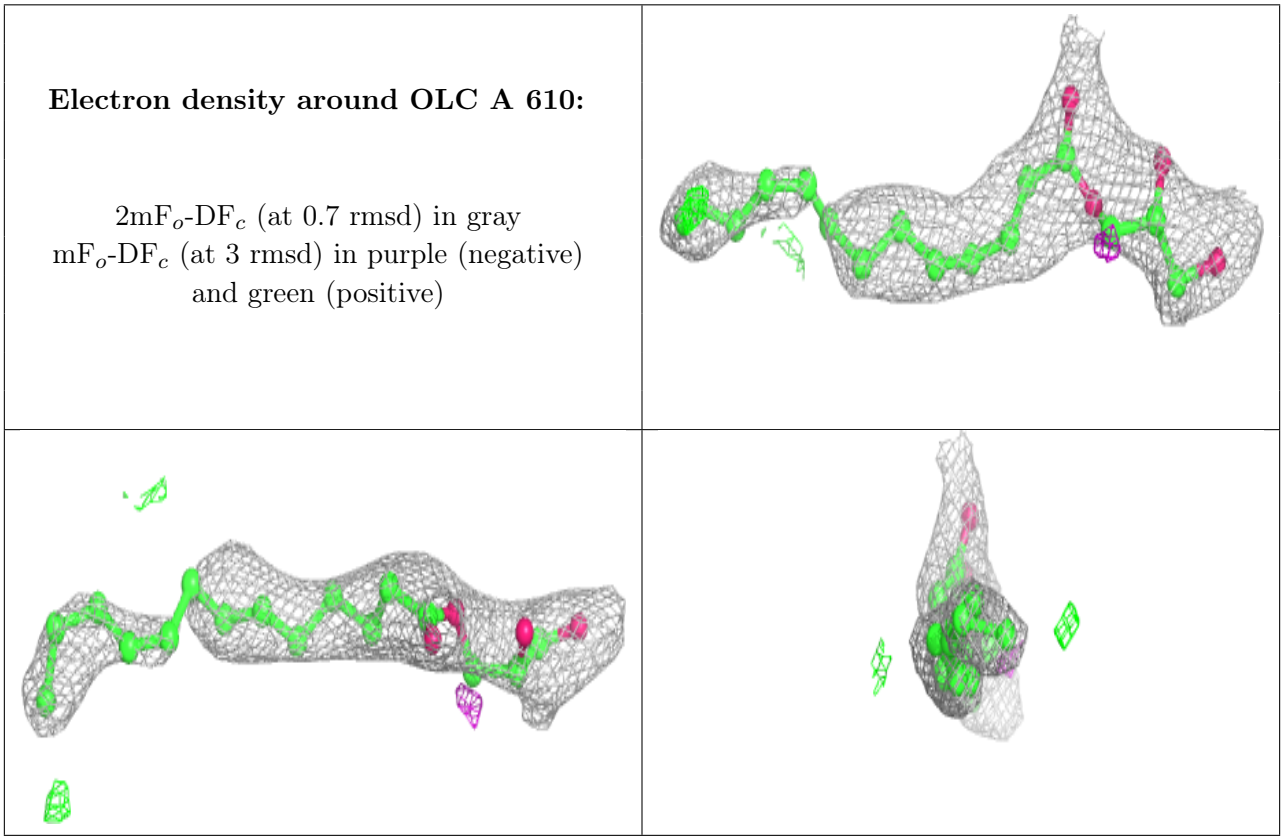
Electron density around OLC B 202:

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



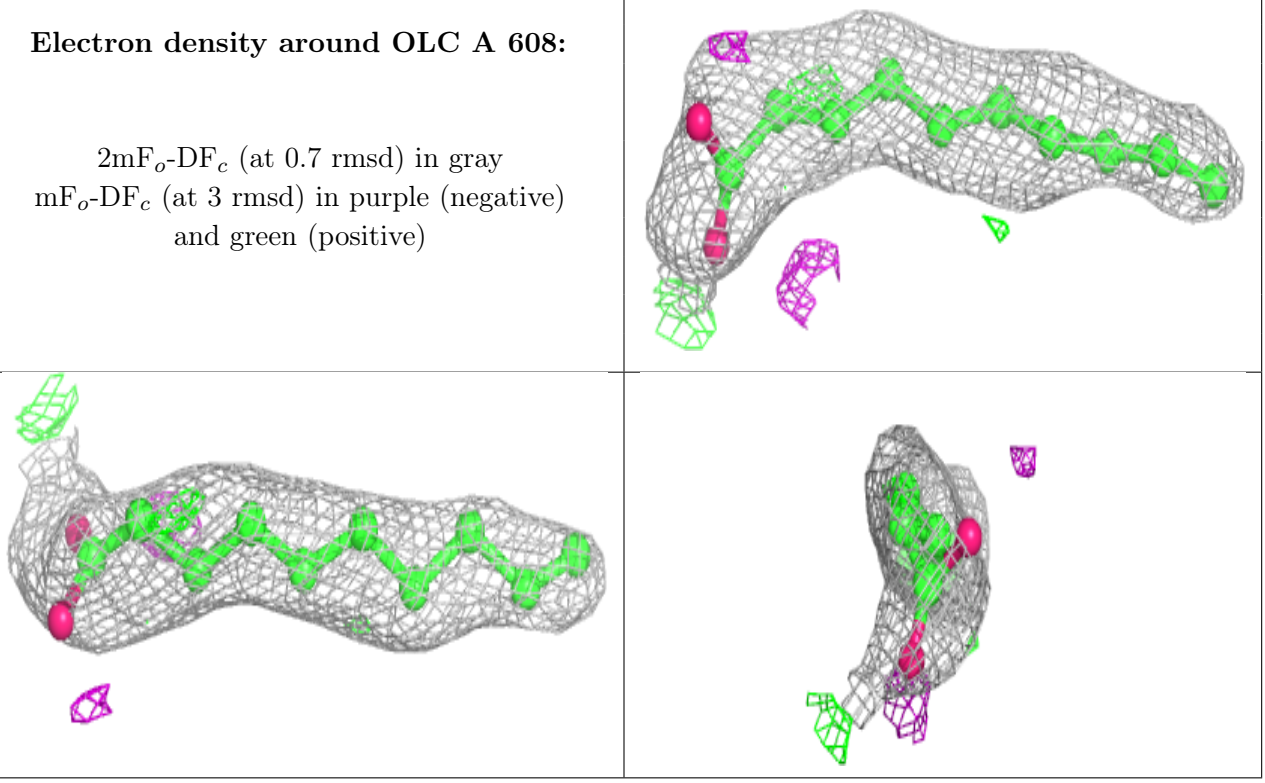
Electron density around OLC A 610:

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



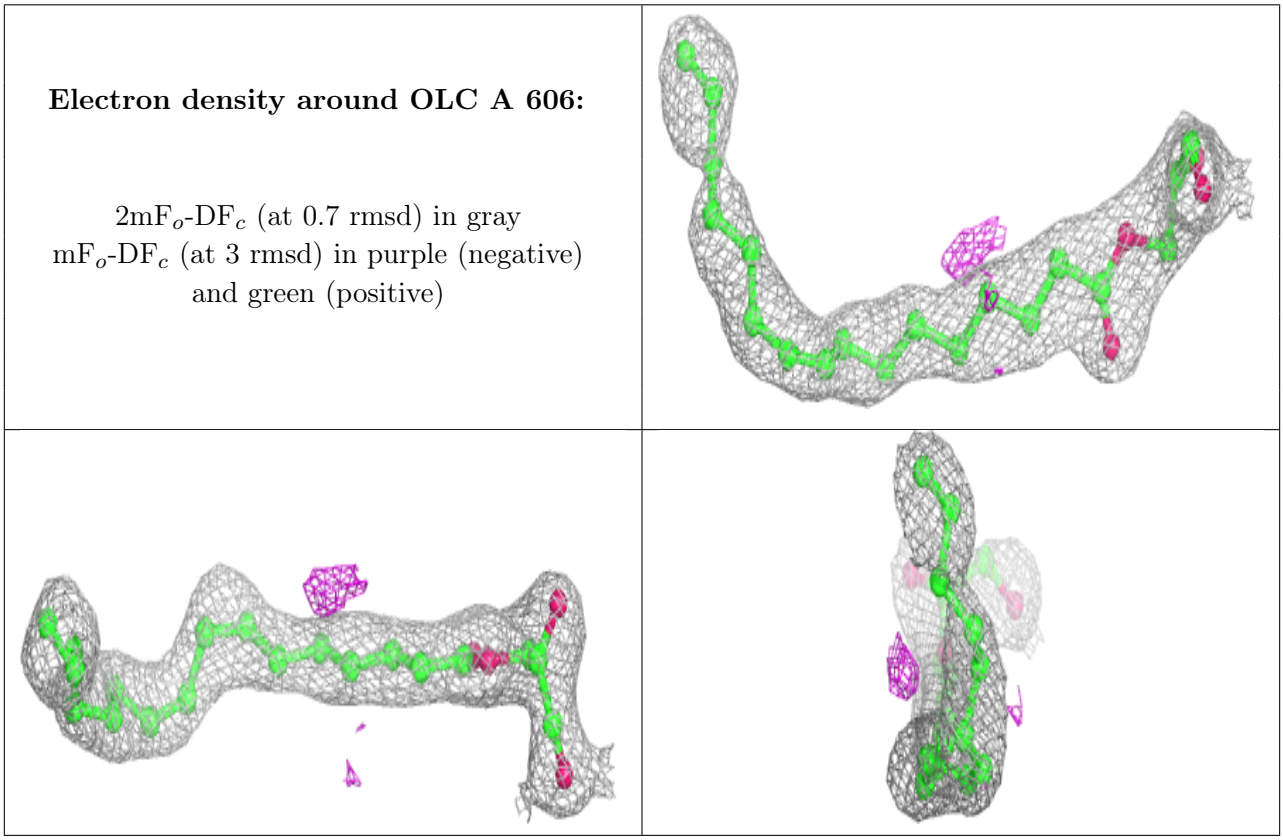
Electron density around OLC A 608:

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



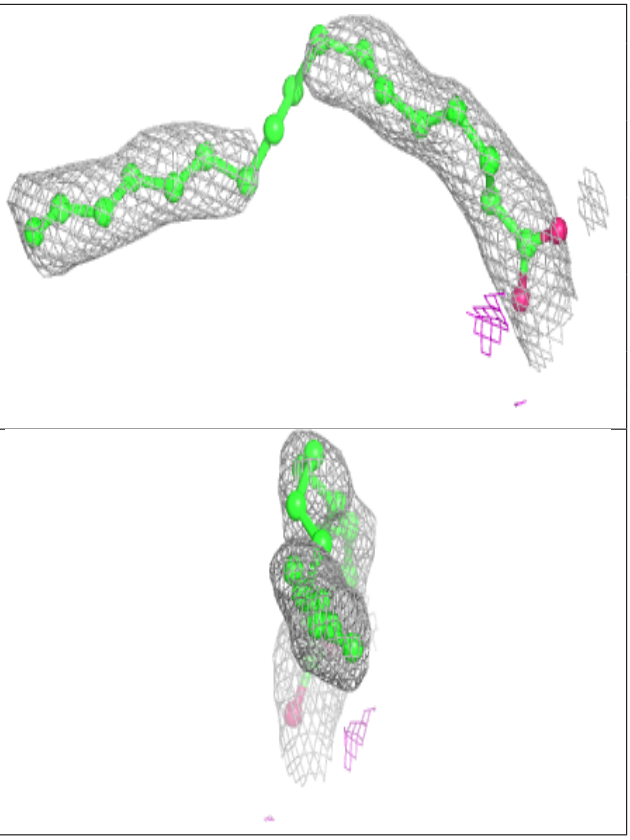
Electron density around OLC A 606:

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



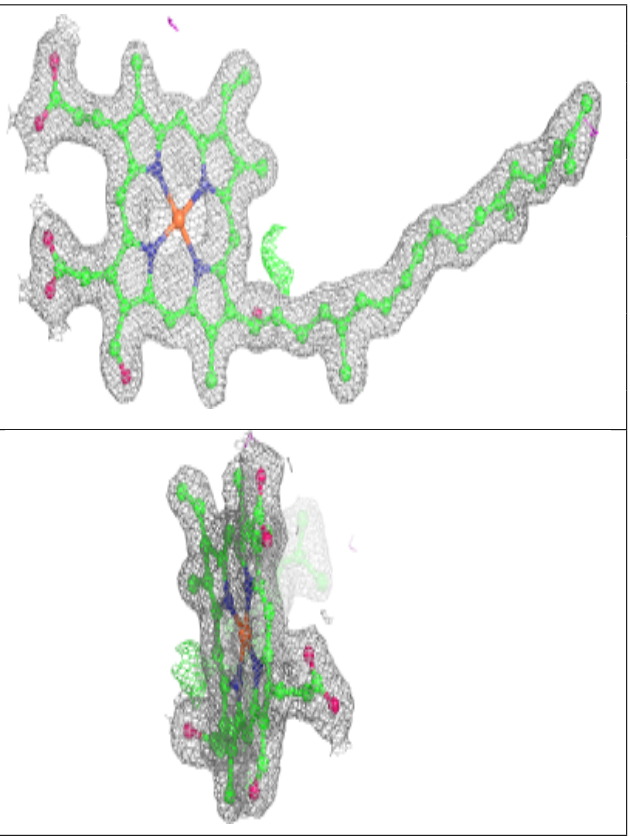
Electron density around OLC A 605:

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



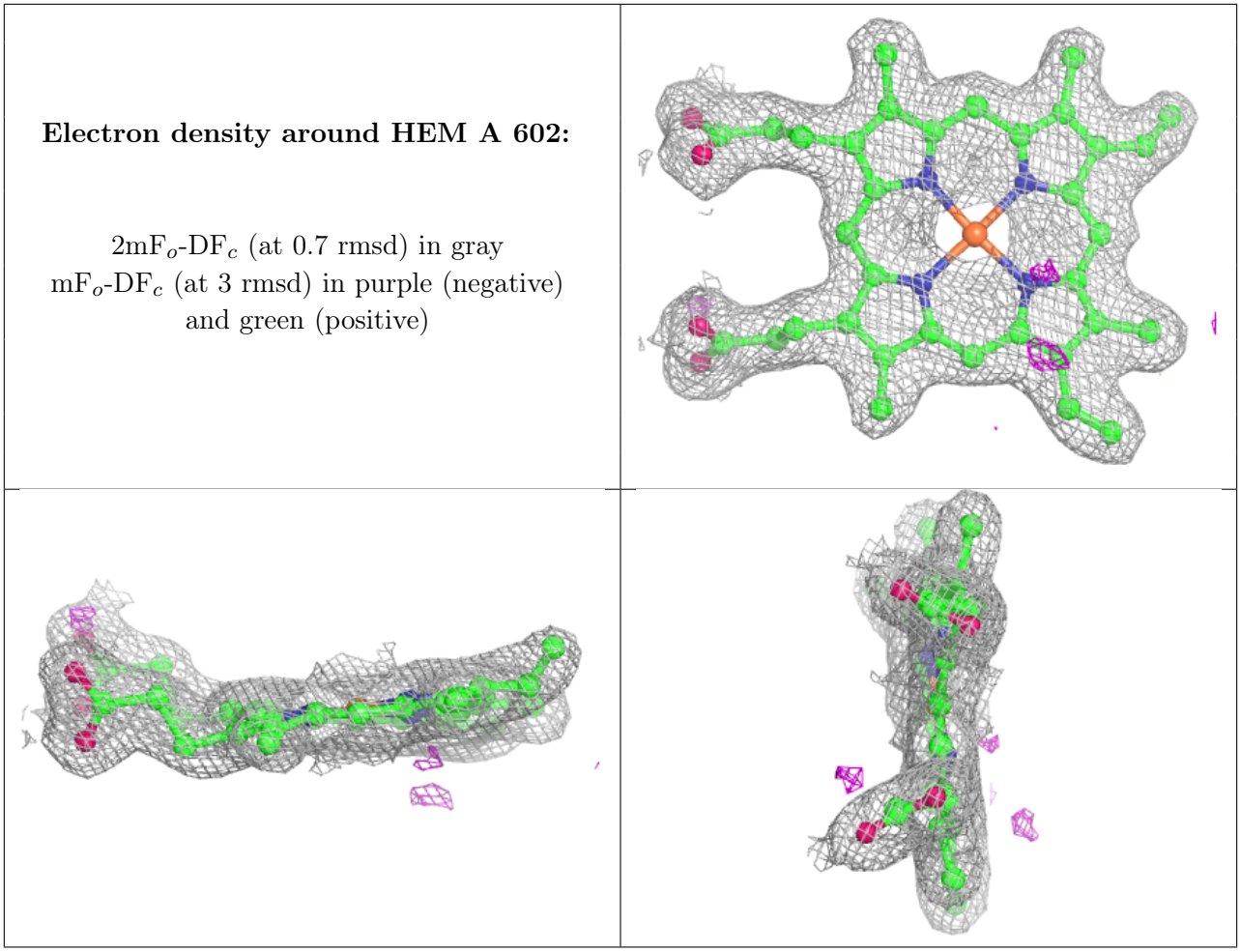
Electron density around HAS A 603:

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



Electron density around 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.