wwPDB X-ray Structure Validation Summary Report (i)

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 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 (1)) were used in the production of this report:

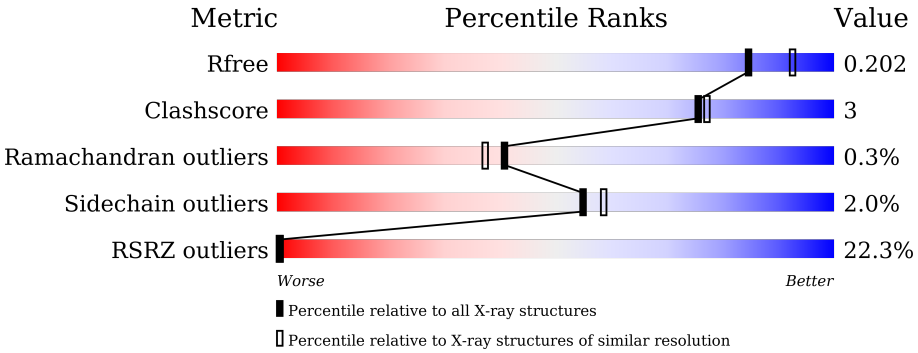
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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	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
1	A	554	Total	C	N	O	S	0	0	0
			4368	2963	698	691	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q5SJ79
A	-5	HIS	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1301	846	216	235	4			

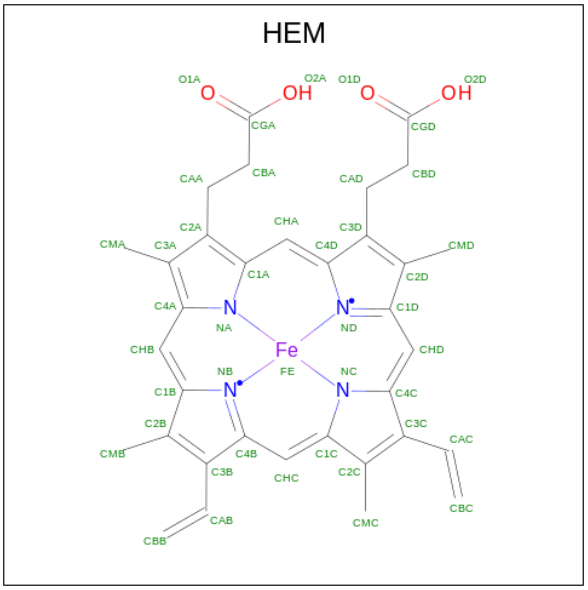
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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) (labeled as "Ligand of Interest" by depositor).

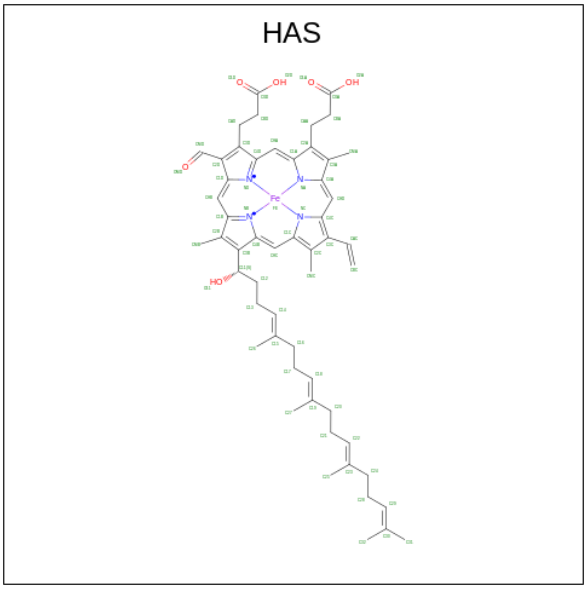
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

- 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).



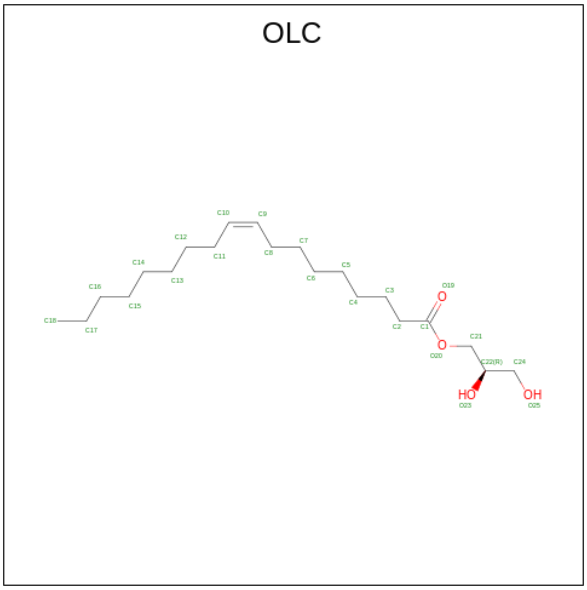
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0

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



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

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$) (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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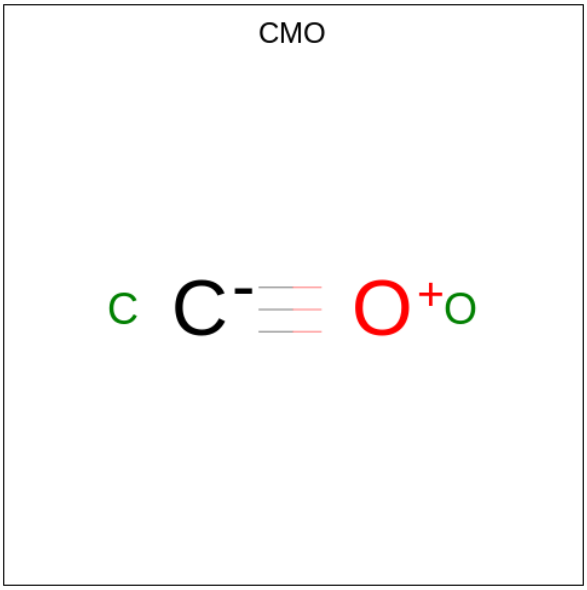
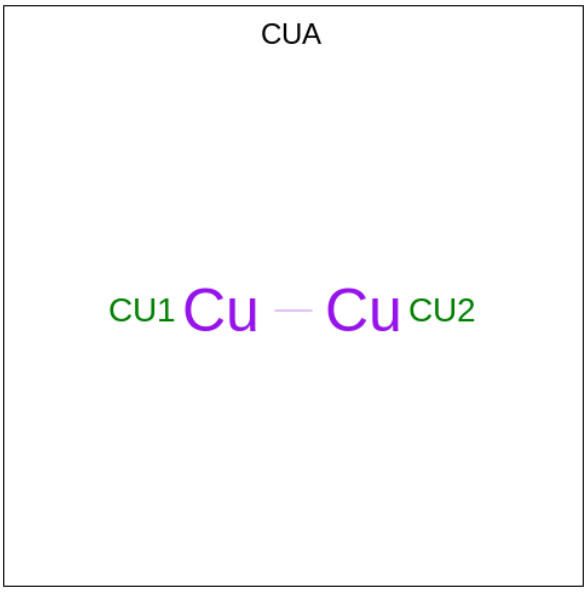
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 20 18 2	0	0
7	B	1	Total C O 25 21 4	0	0
7	B	1	Total C O 24 20 4	0	0
7	C	1	Total C O 24 20 4	0	0
7	C	1	Total C O 15 11 4	0	0

- 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 2 1 1	0	0

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

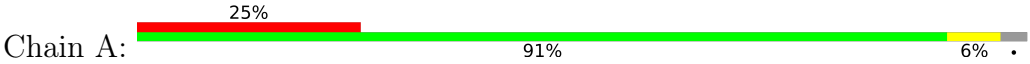
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	99	Total O 100 100	0	1
10	B	88	Total O 88 88	0	0
10	C	3	Total O 3 3	0	0

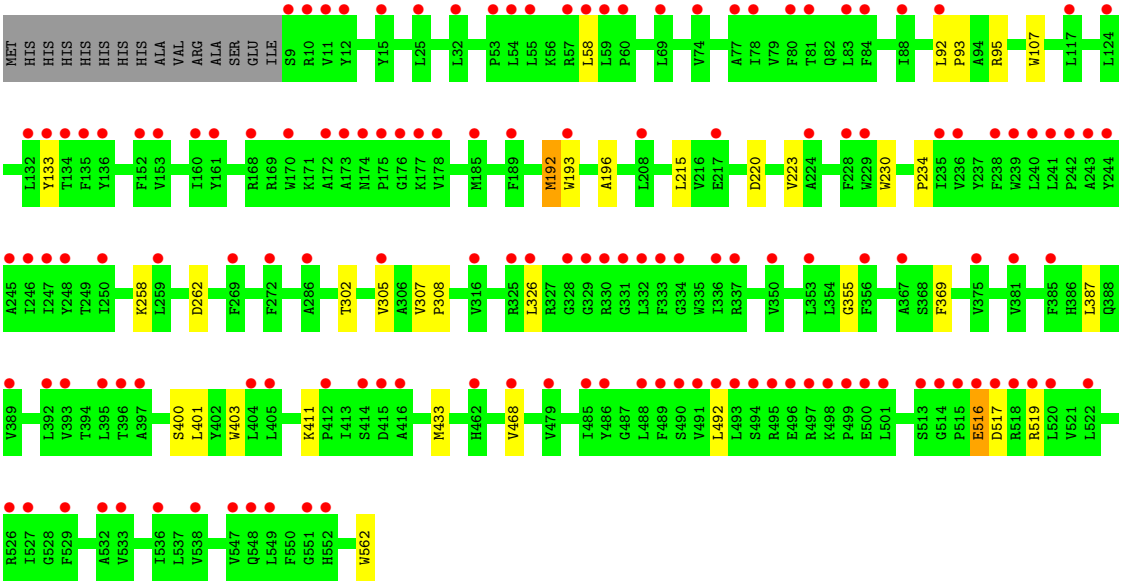
3 Residue-property plots

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

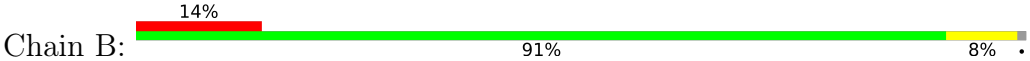
Chain A:

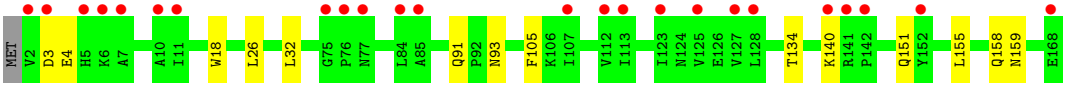




- Molecule 2: Cytochrome c oxidase subunit 2

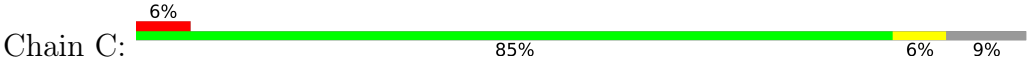
Chain B:





- Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.39 (at 2.00Å)	Xtriage
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^2)	35.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 84.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6487	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage'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.*

[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: 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(^{o})	Ideal(^{o})
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

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.

The worst 5 of 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

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

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	401	LEU
2	B	26	LEU
3	C	17	LEU
2	B	140	LYS
1	A	215	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	99	GLN

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Mol	Chain	Res	Type
2	B	158	GLN
2	B	159	ASN
1	A	446	ASN
1	A	254	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 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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	-

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHC-C4B	4.41	1.46	1.35
6	A	603	HAS	C3B-C2B	4.40	1.44	1.34
6	A	603	HAS	C4B-NB	-4.35	1.32	1.40
6	A	603	HAS	C3C-C2C	4.10	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	603	HAS	NA

5 of 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

There are no ring outliers.

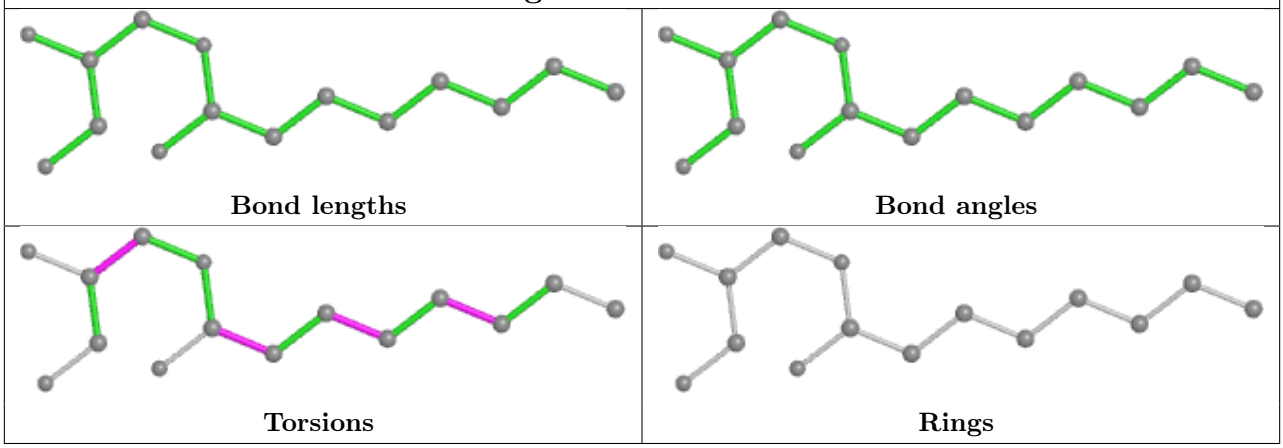
5 monomers are involved in 6 short contacts:

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 then 5% of the Mogul distribution of torsion angles is

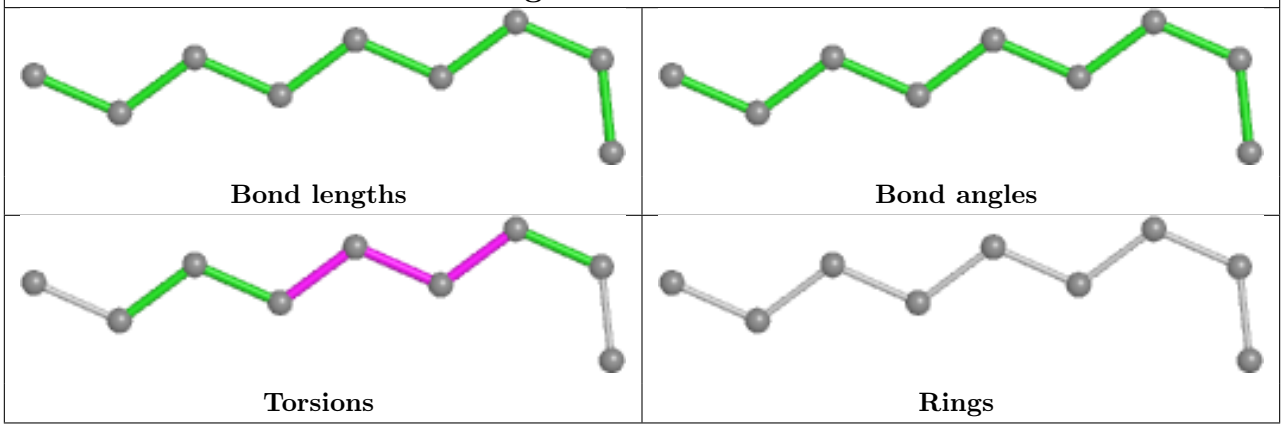
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 609

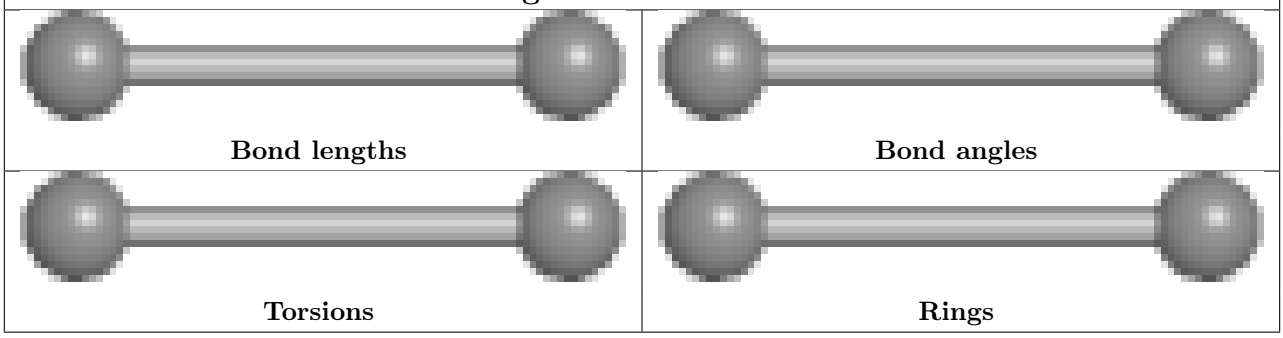


Ligand OLC A 610

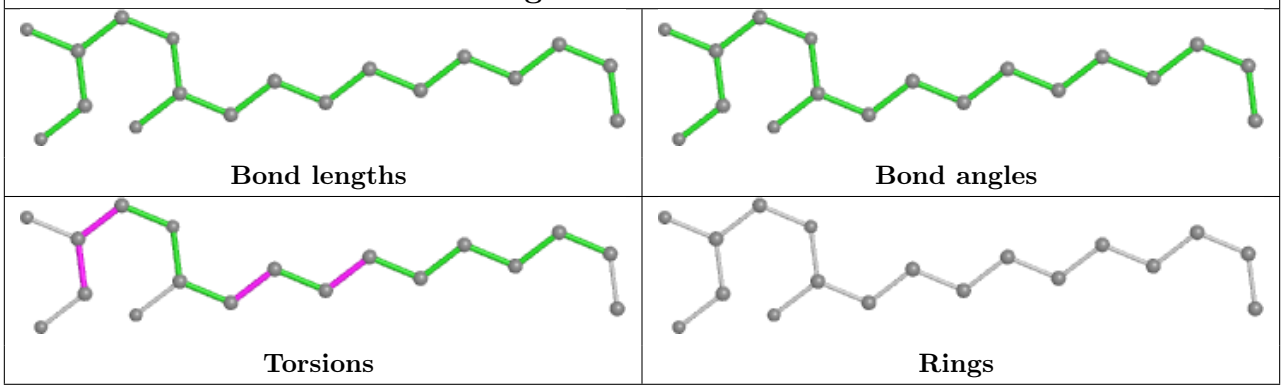
Ligand OLC A 612



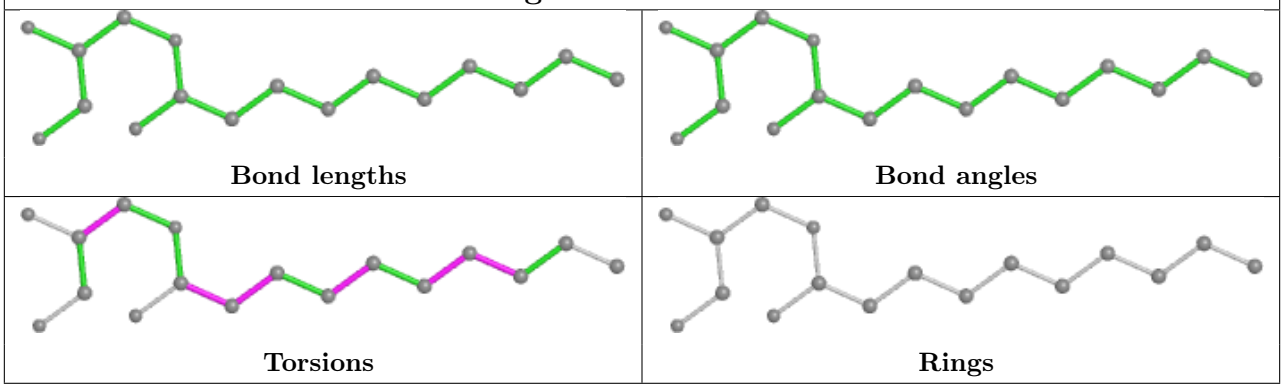
Ligand CUA B 202



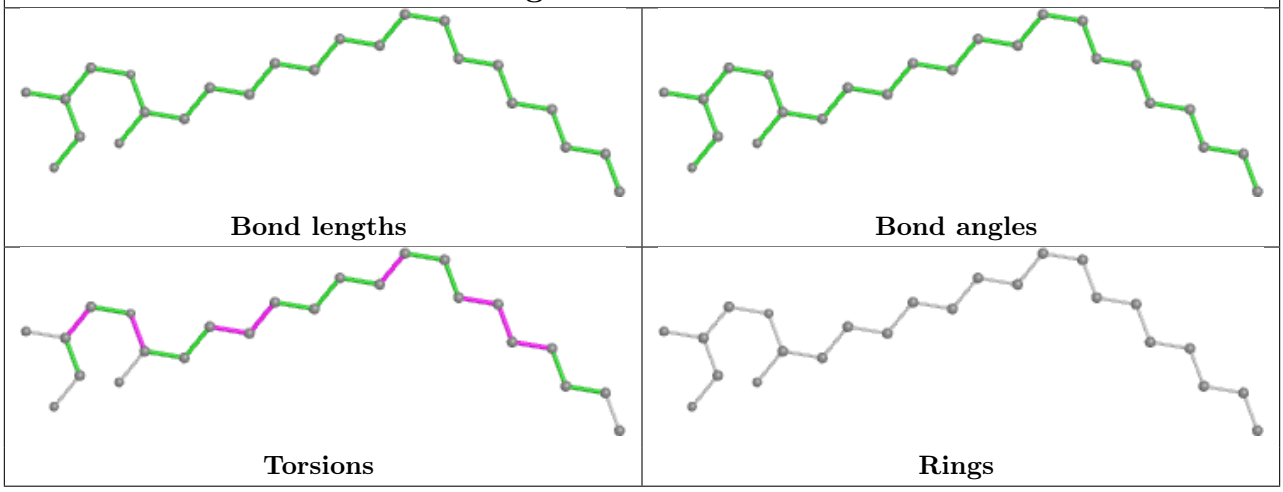
Ligand OLC A 605



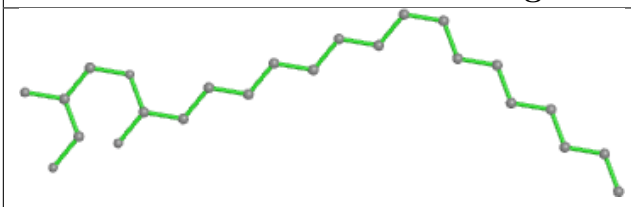
Ligand OLC A 606



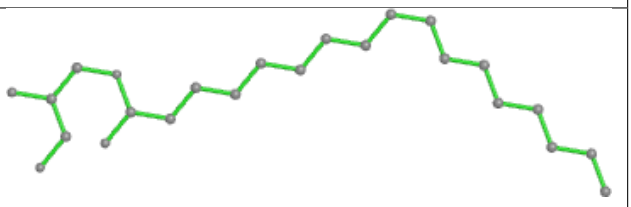
Ligand OLC B 204



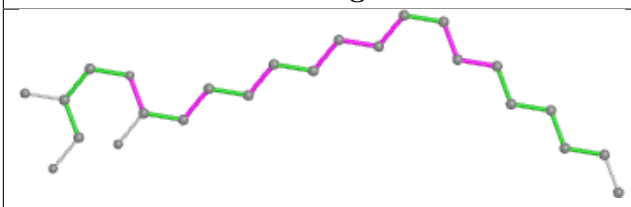
Ligand OLC C 101



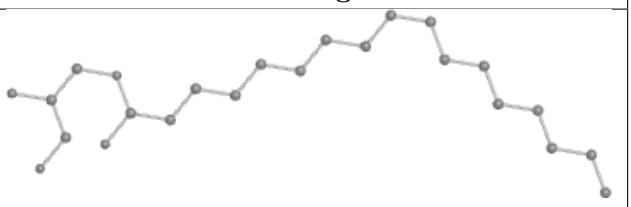
Bond lengths



Bond angles

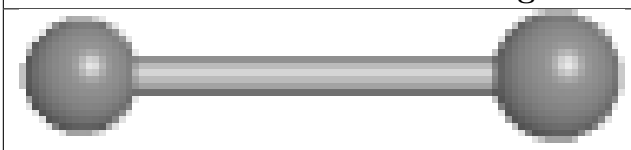


Torsions

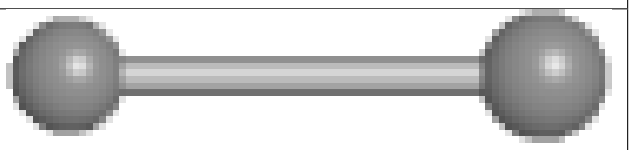


Rings

Ligand CMO A 614



Bond lengths

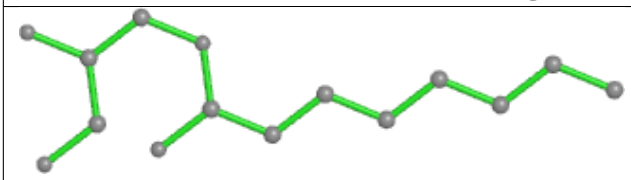


Bond angles

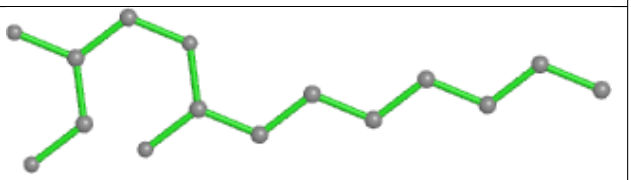
Torsions

Rings

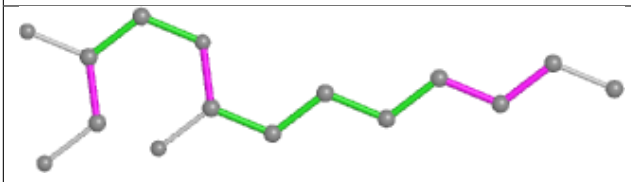
Ligand OLC C 102



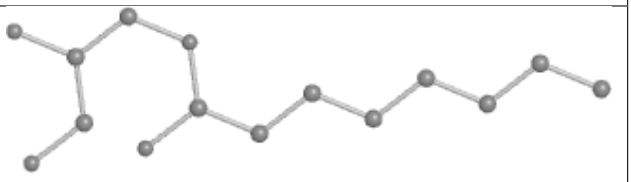
Bond lengths



Bond angles

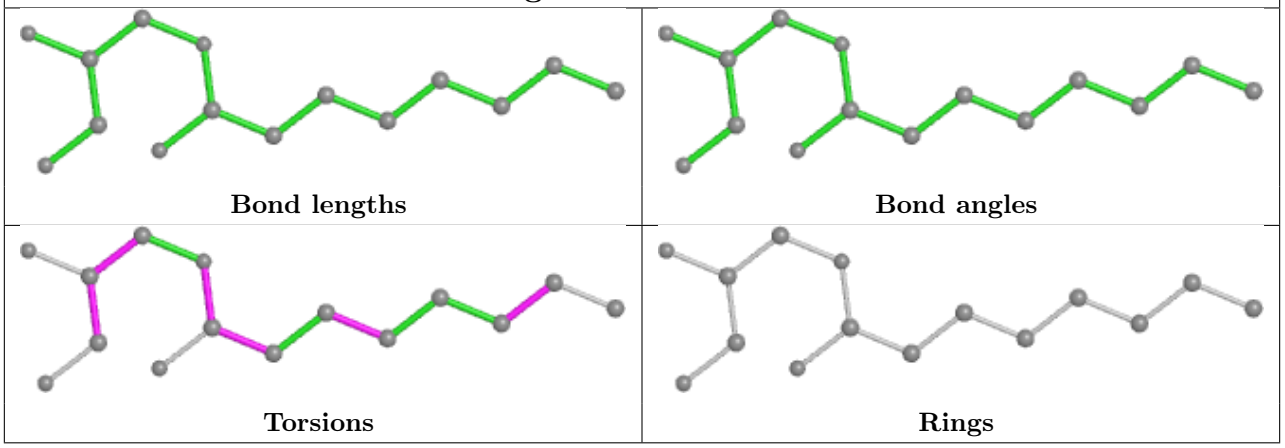


Torsions

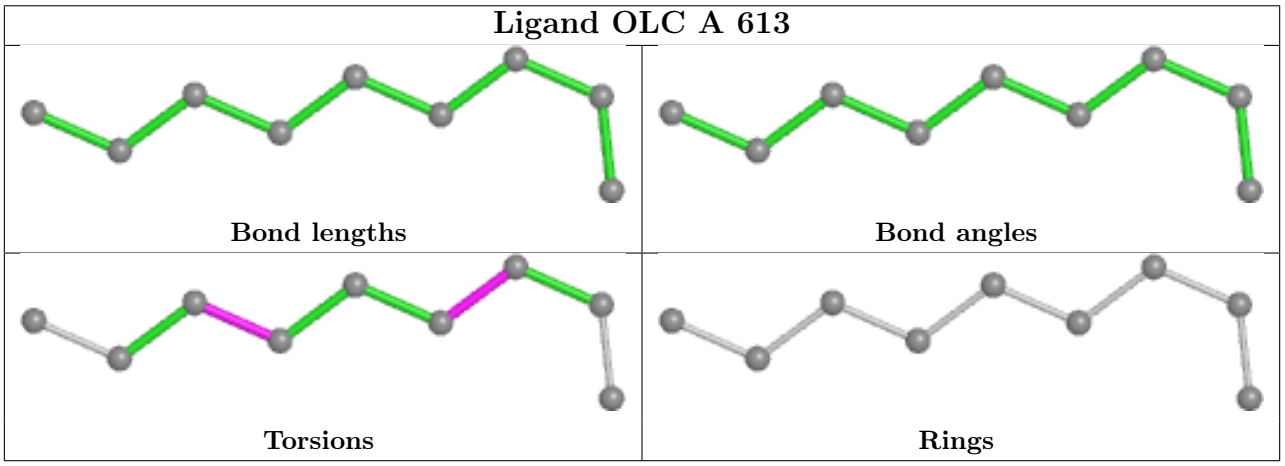


Rings

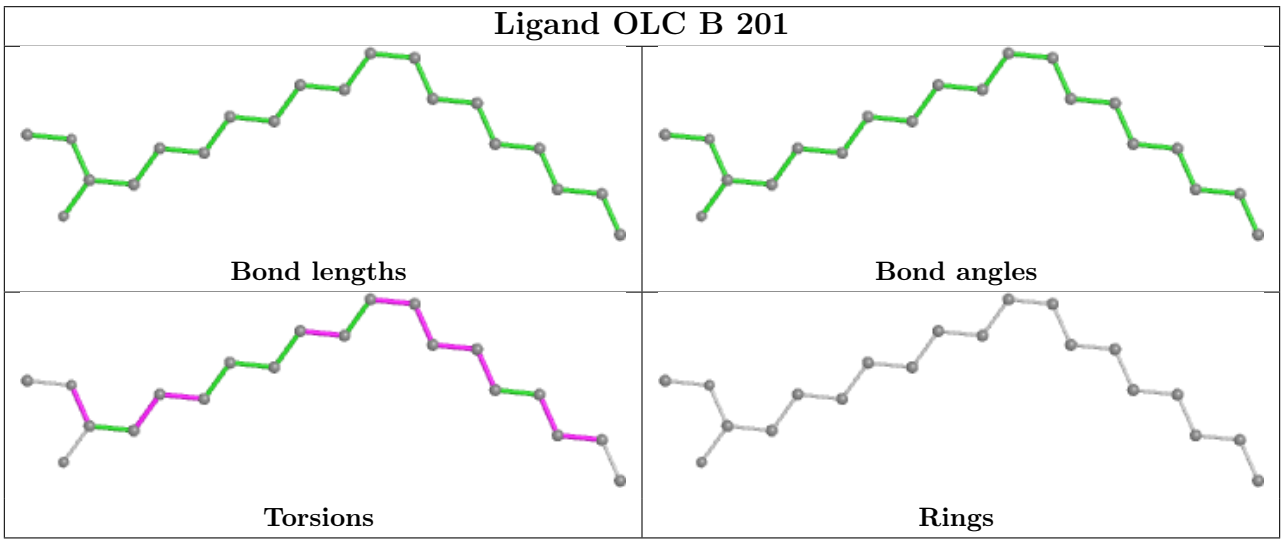
Ligand OLC A 607



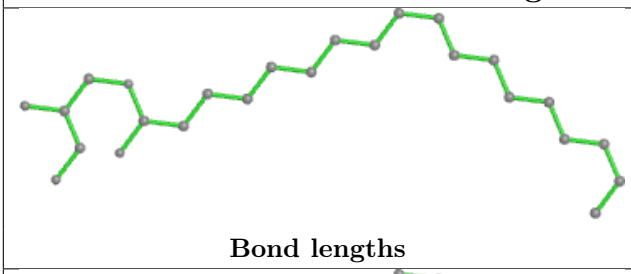
Ligand OLC A 613



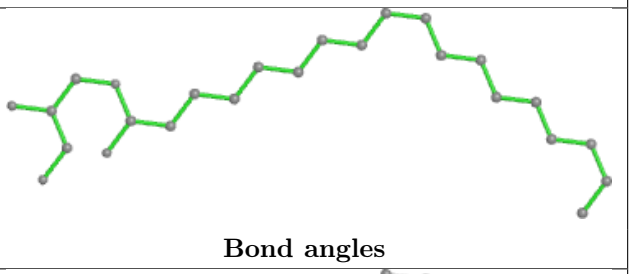
Ligand OLC B 201



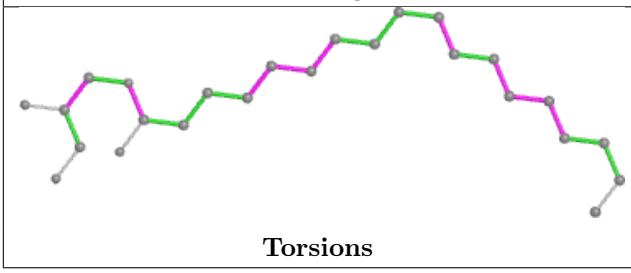
Ligand OLC B 203



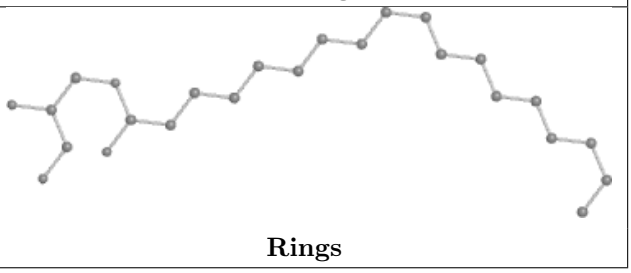
Bond lengths



Bond angles

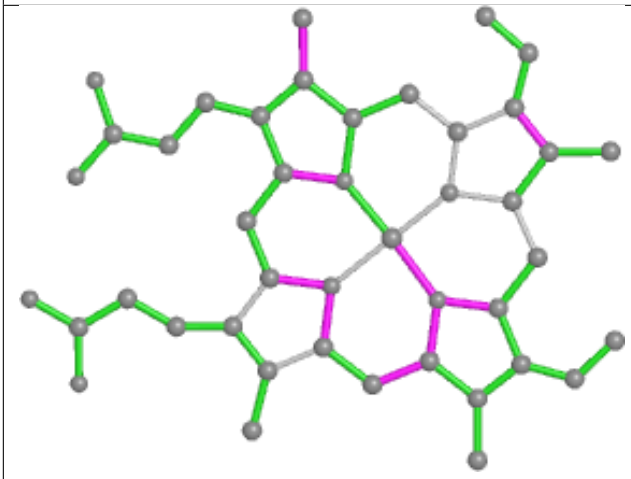


Torsions

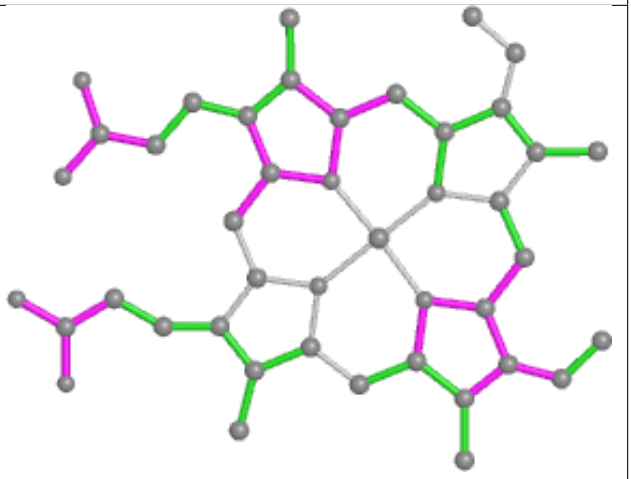


Rings

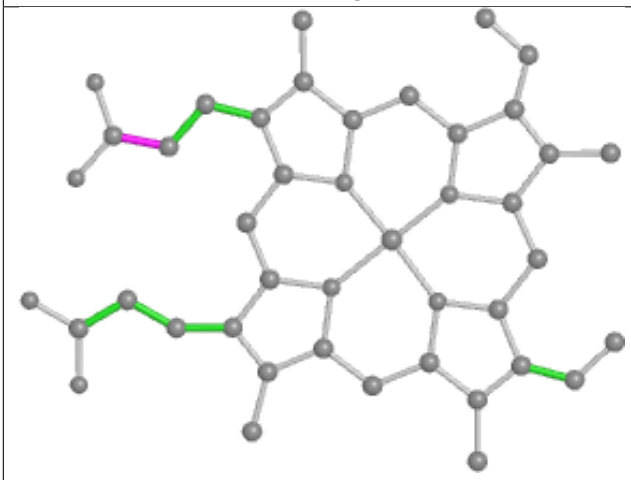
Ligand HEM A 602



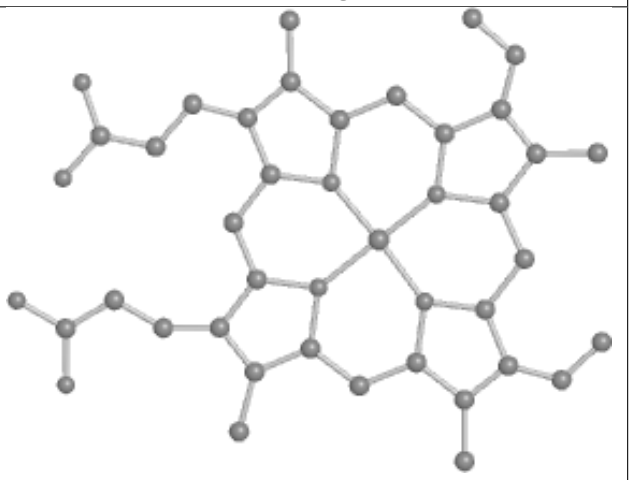
Bond lengths



Bond angles

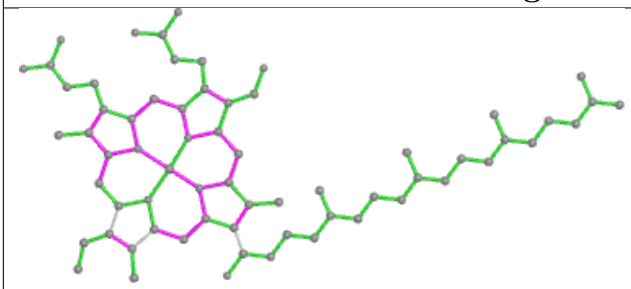


Torsions

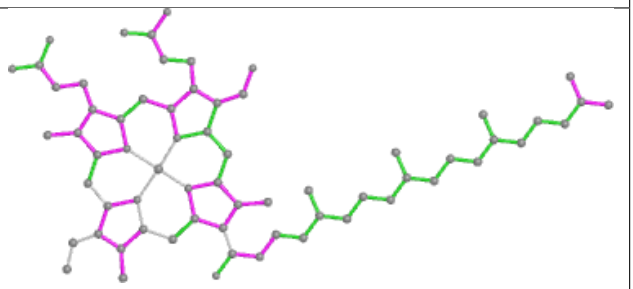


Rings

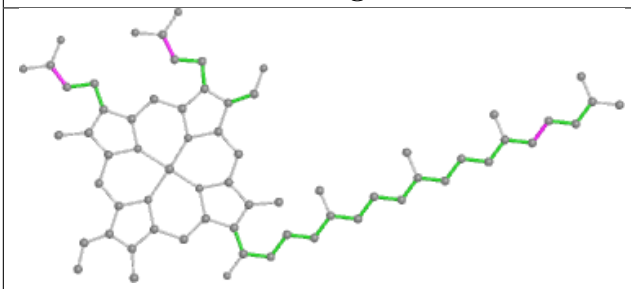
Ligand HAS A 603



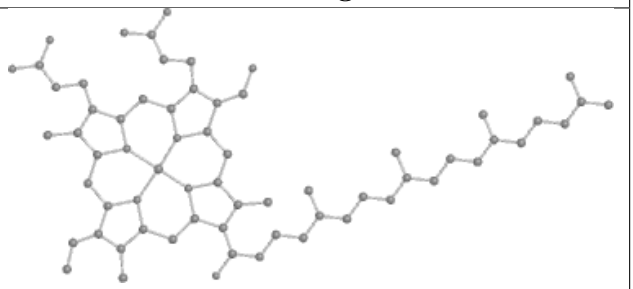
Bond lengths



Bond angles

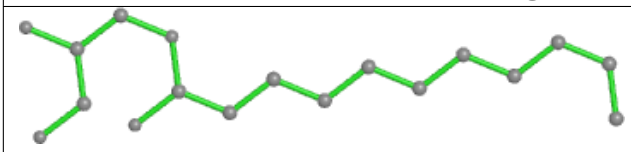


Torsions

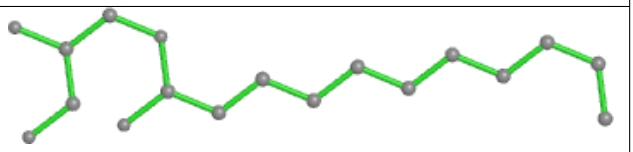


Rings

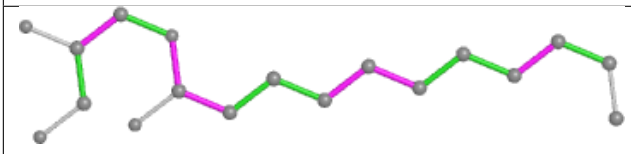
Ligand OLC A 608



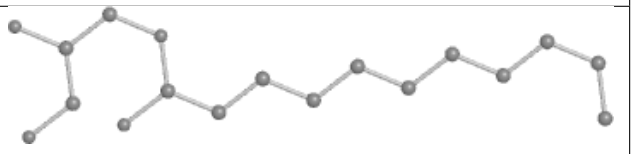
Bond lengths



Bond angles

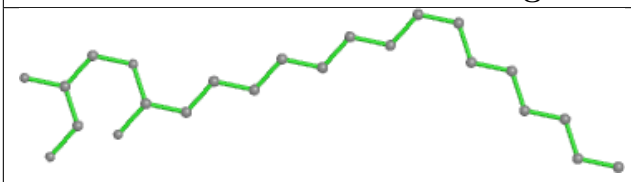


Torsions

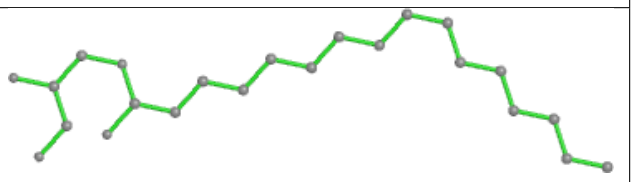


Rings

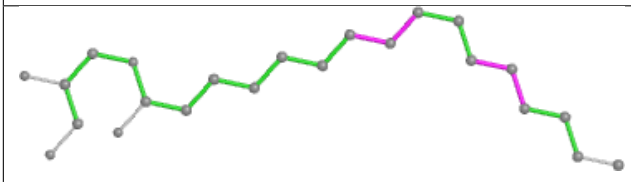
Ligand OLC A 604



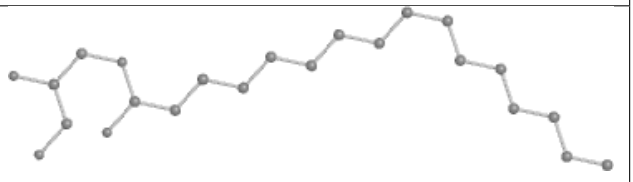
Bond lengths



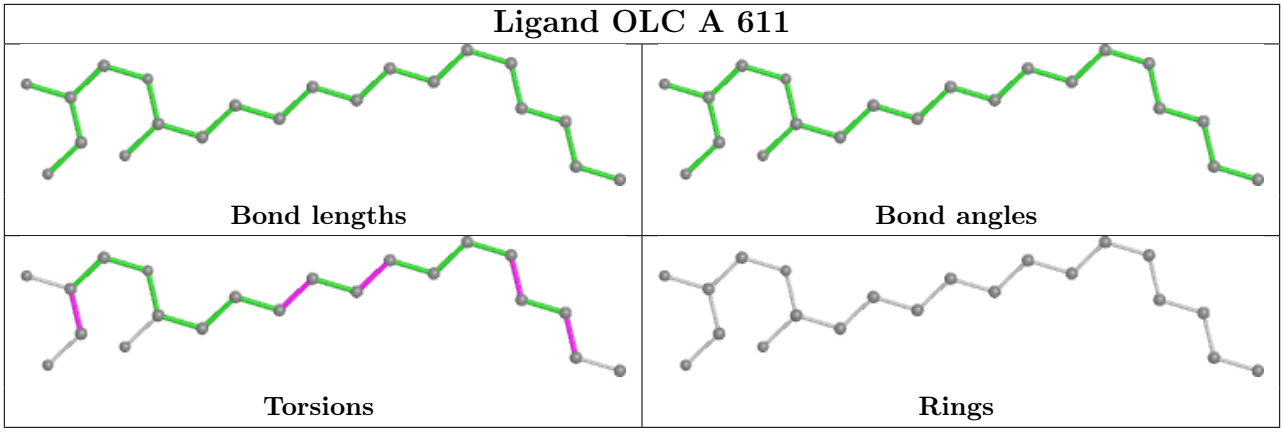
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	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

The worst 5 of 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

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

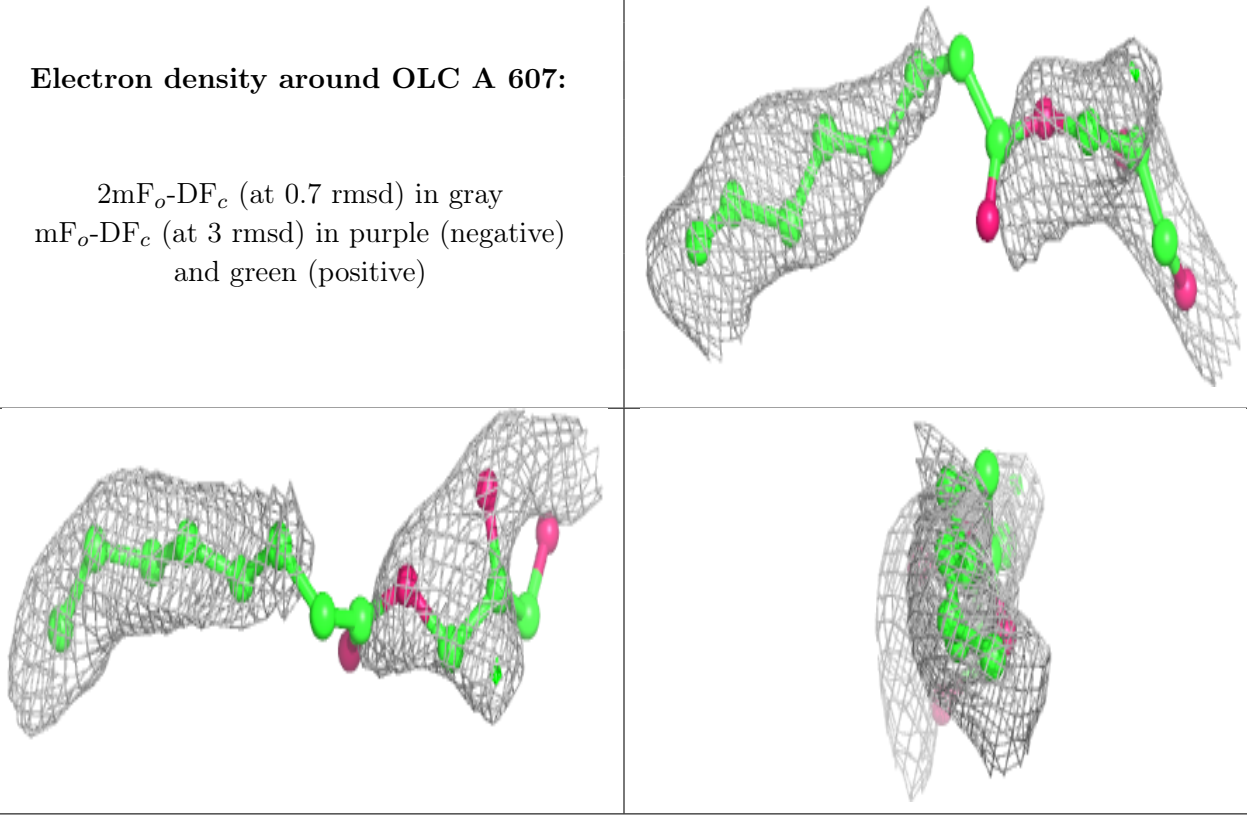
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

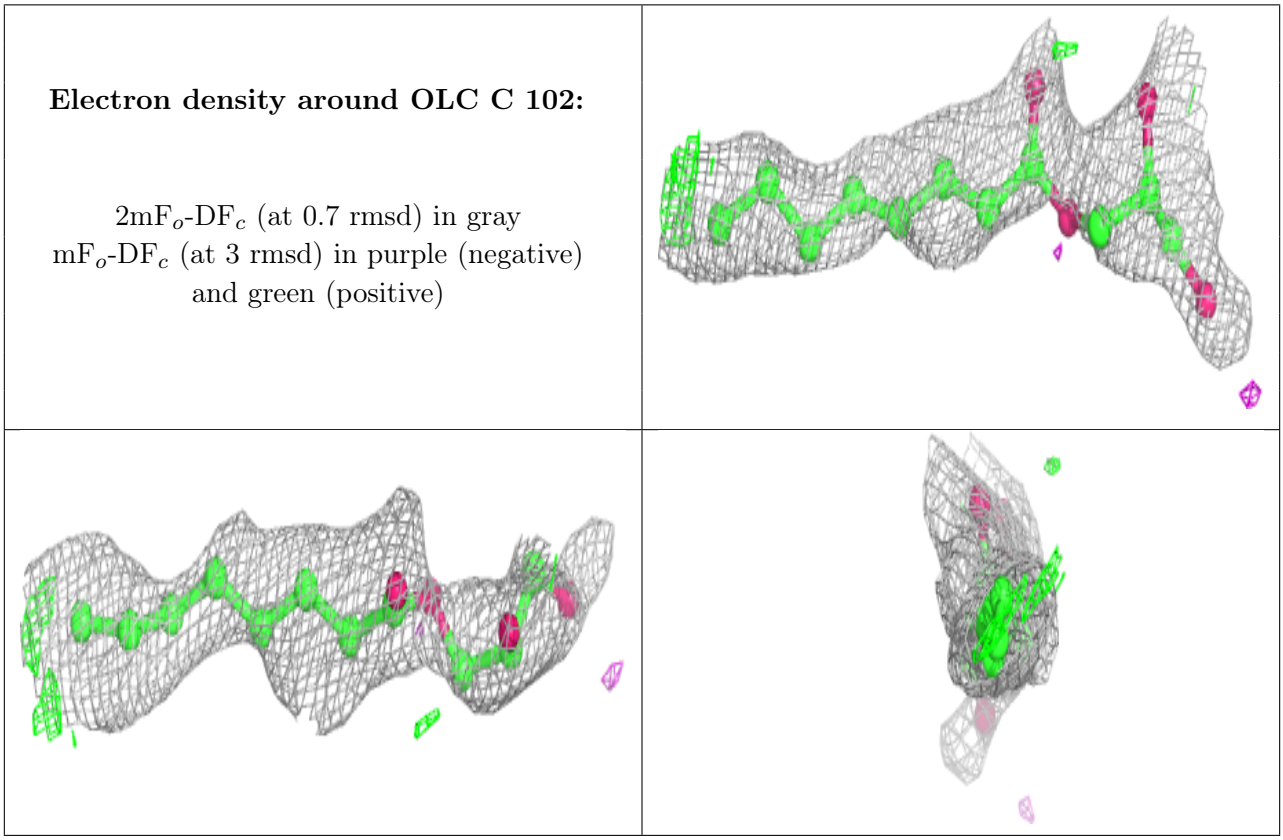
Electron density around OLC A 607:

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



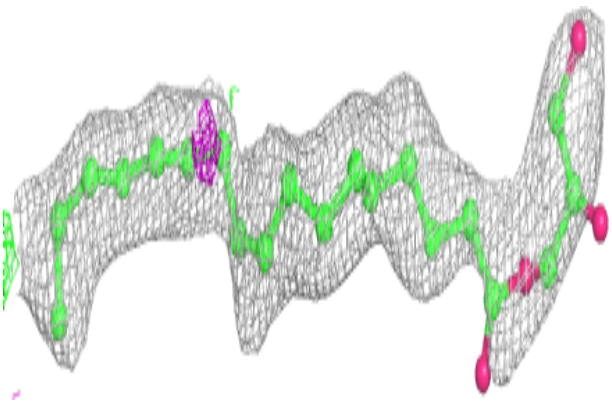
Electron density around OLC C 102:

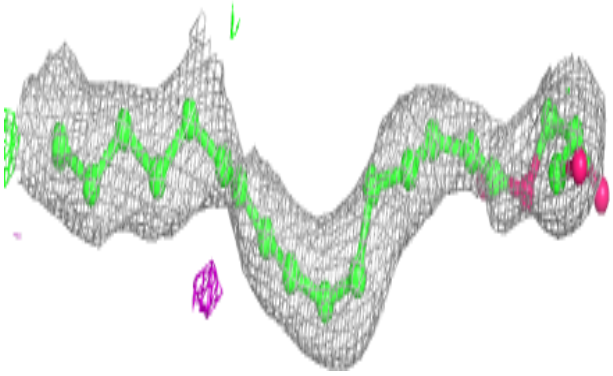
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

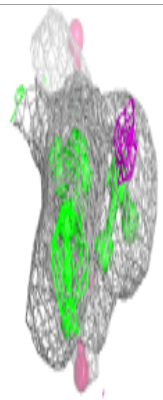


Electron density around OLC C 101:

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

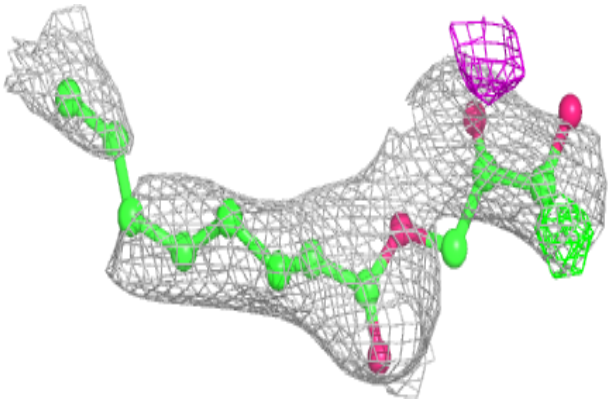


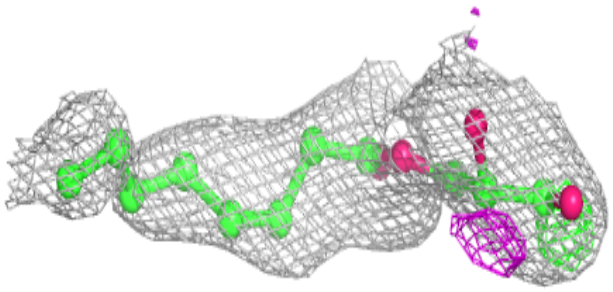


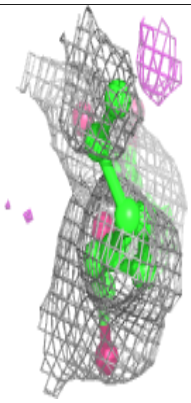


Electron density around OLC A 609:

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

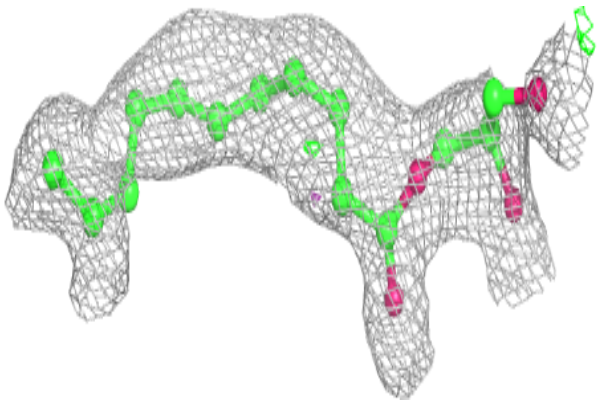


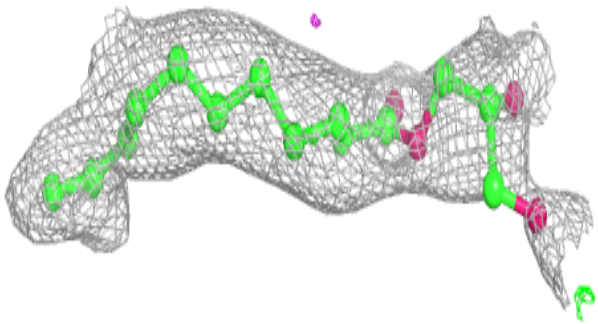


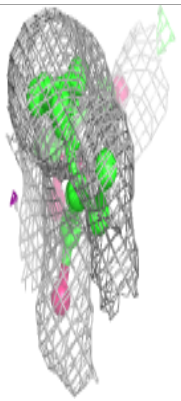


Electron density around OLC A 608:

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

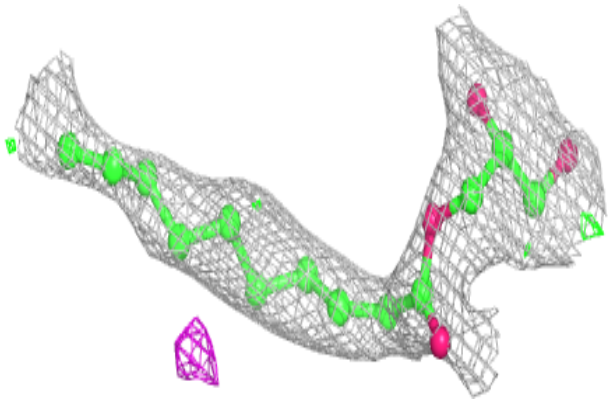


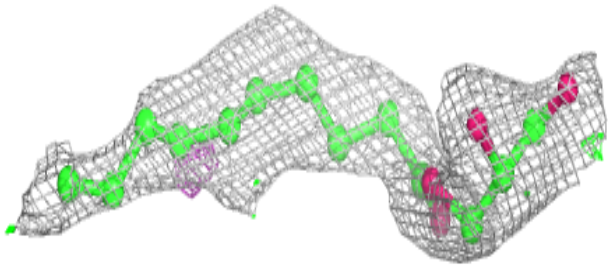


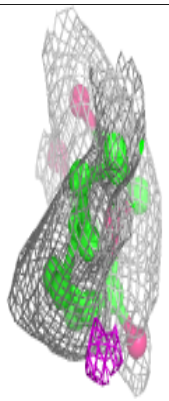


Electron density around OLC A 606:

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

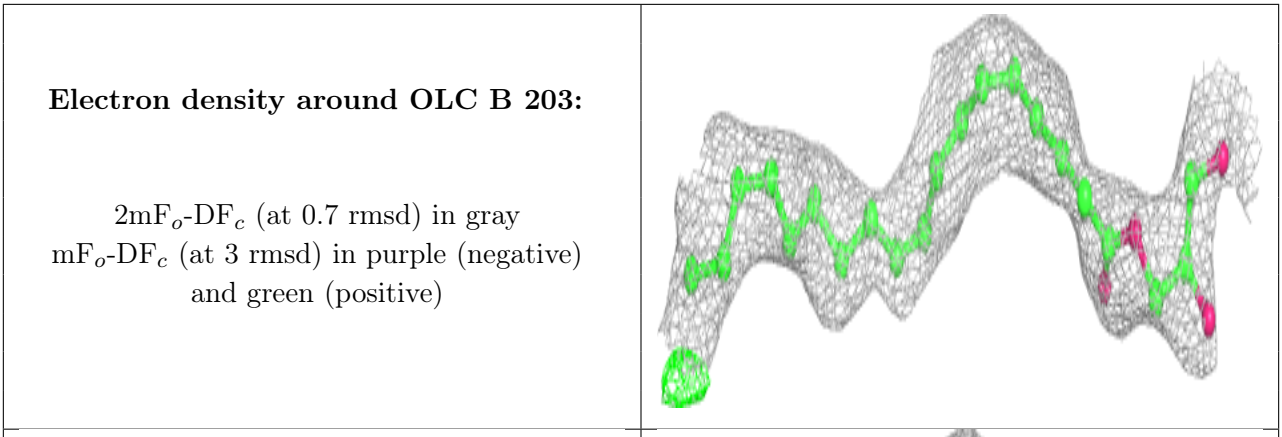






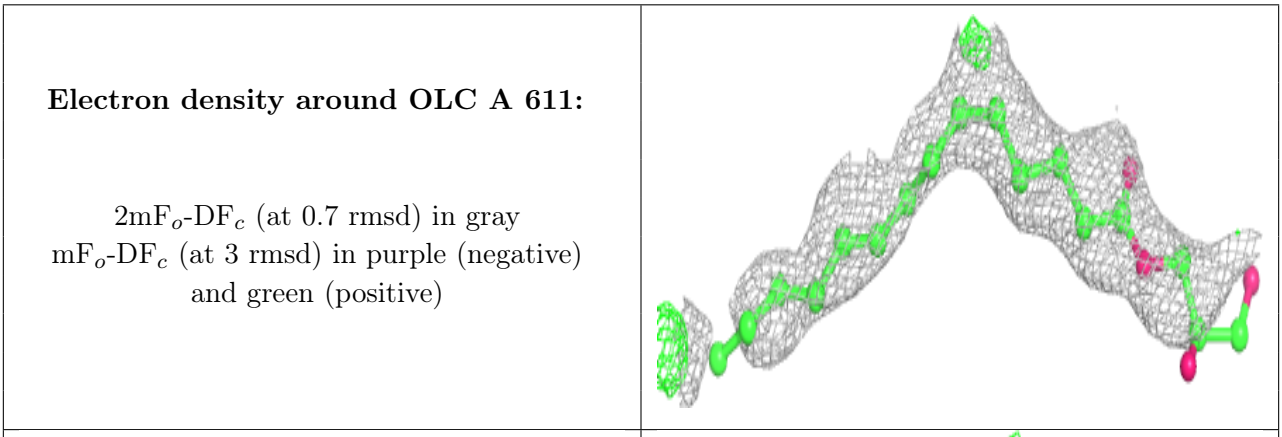
Electron density around OLC B 203:

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



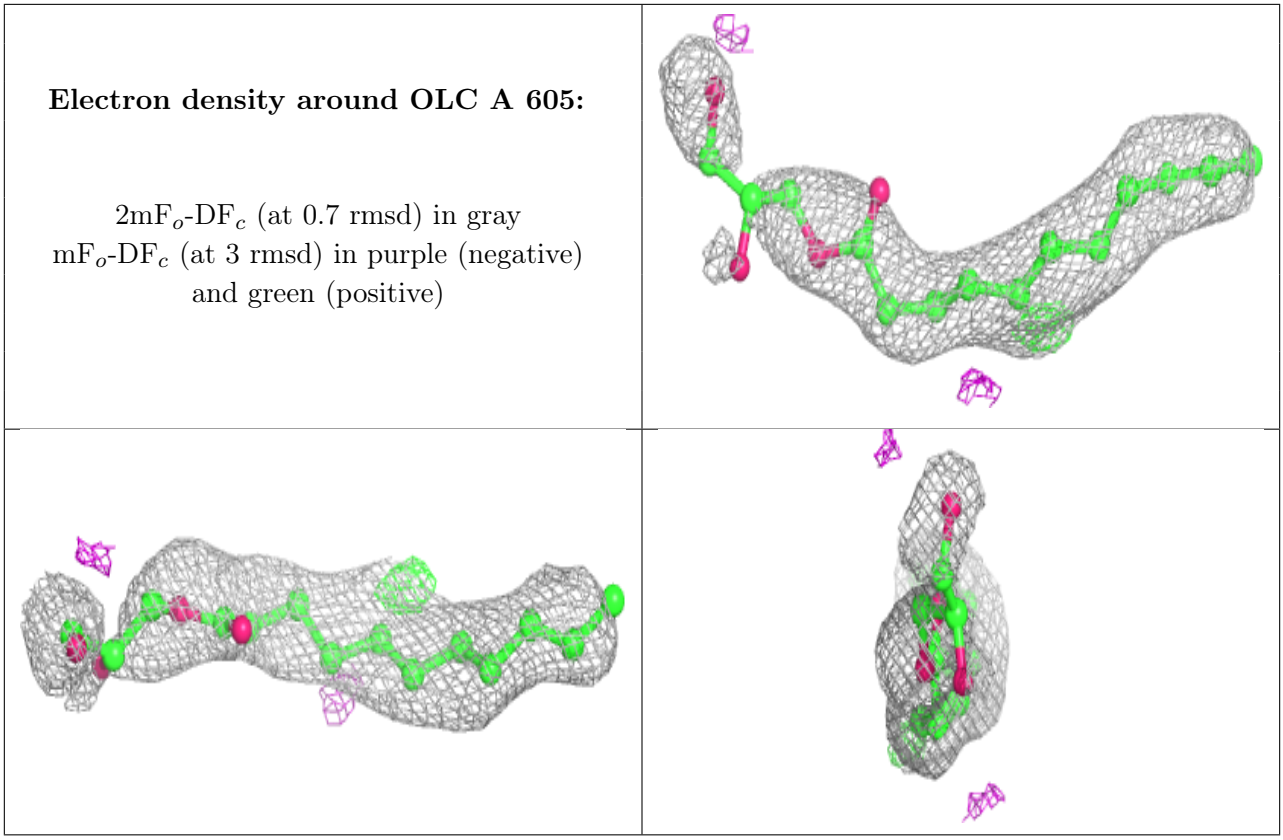
Electron density around OLC A 611:

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



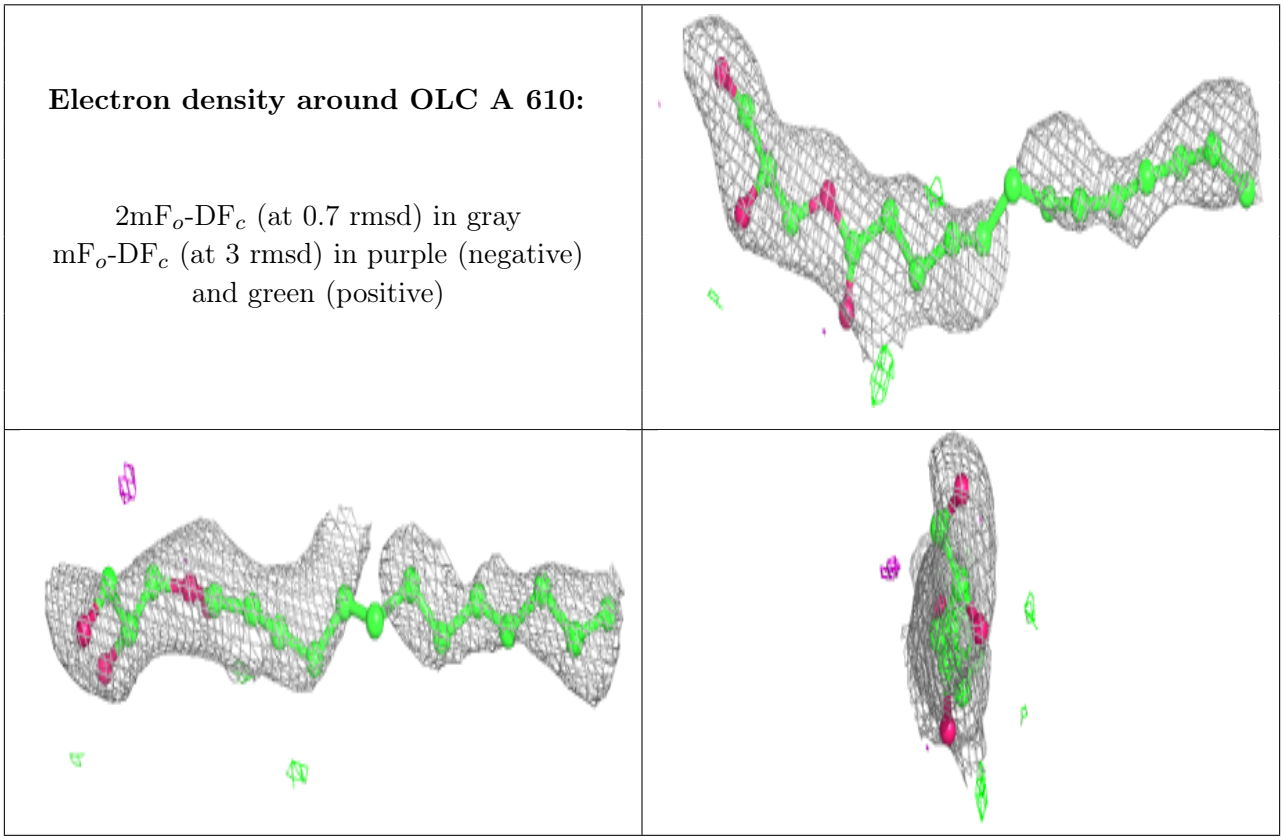
Electron density around OLC A 605:

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



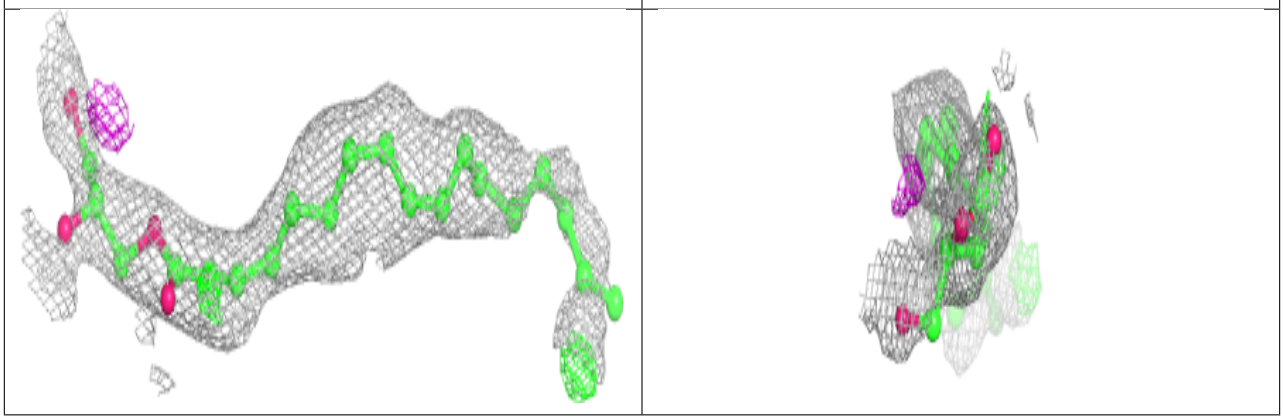
Electron density around OLC A 610:

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



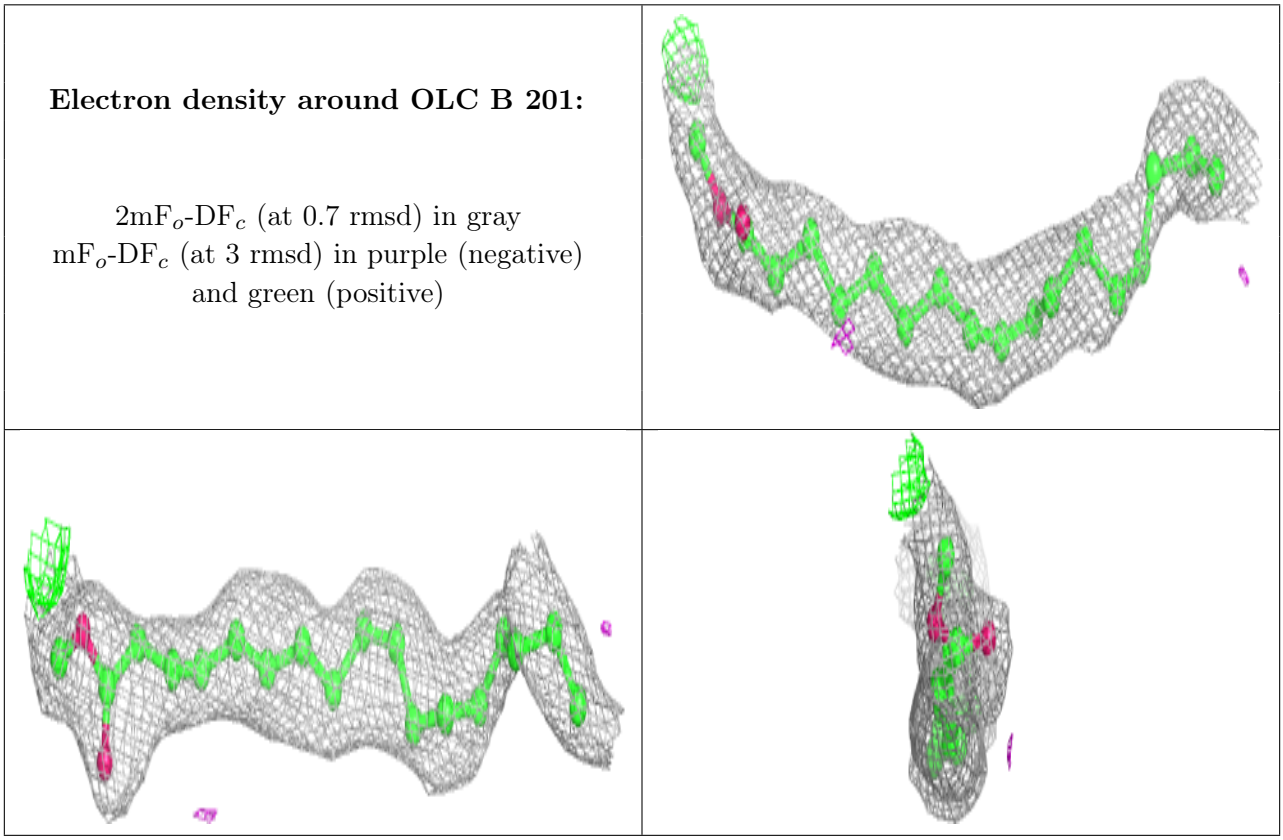
Electron density around OLC B 204:

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



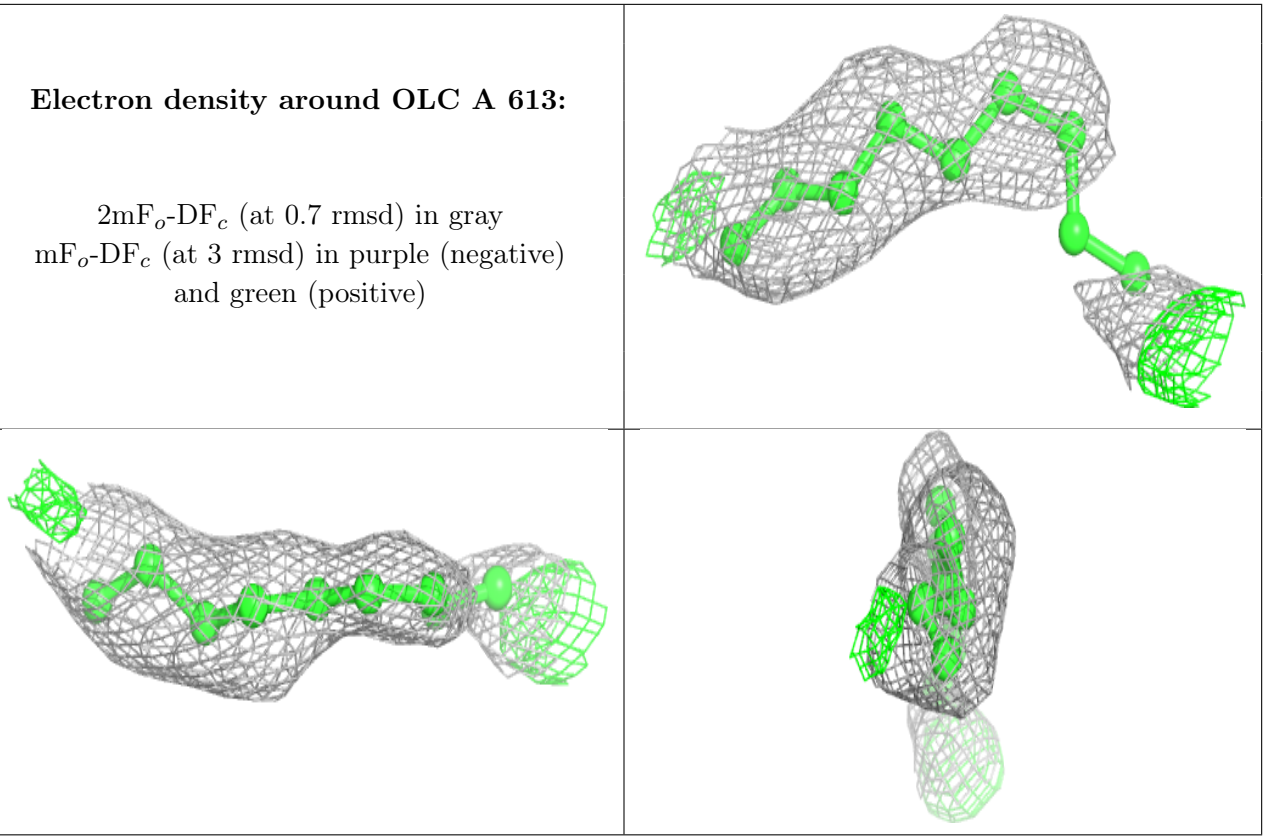
Electron density around OLC B 201:

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



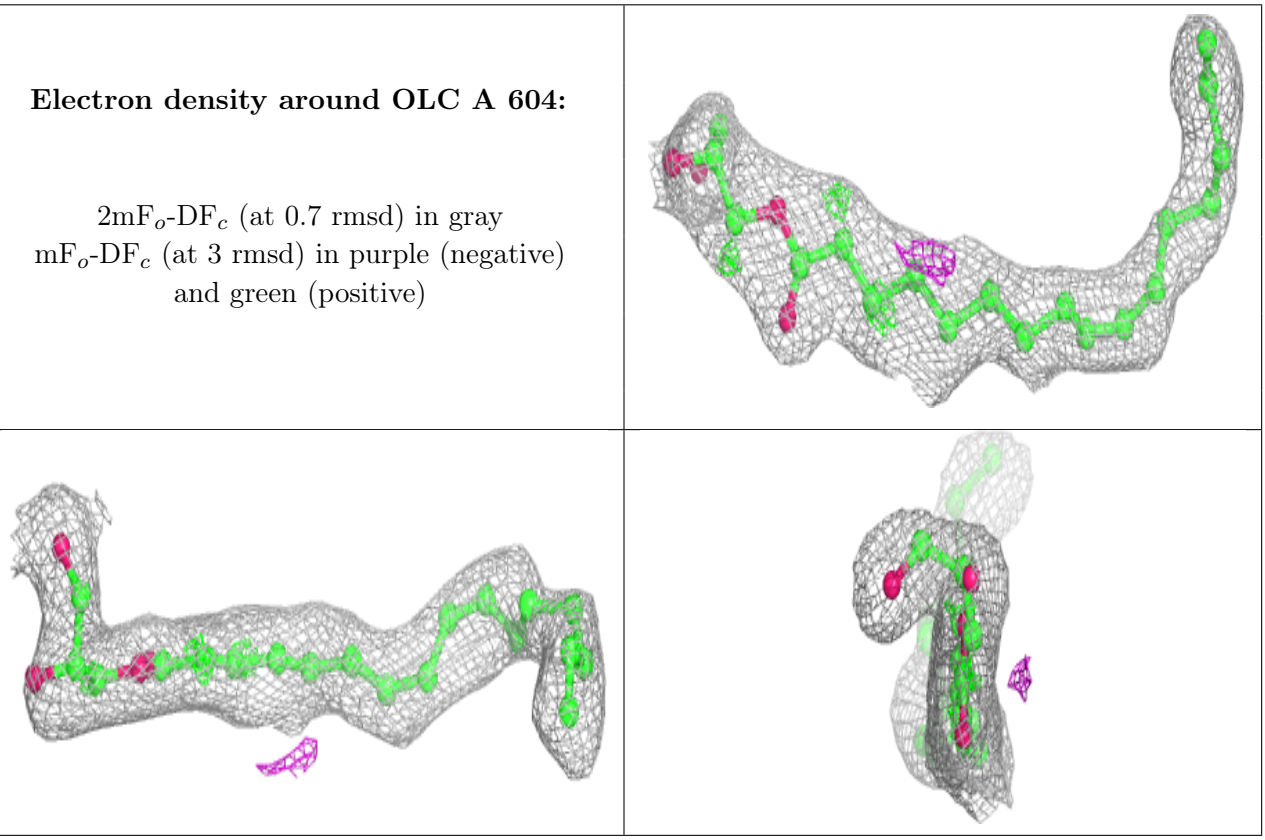
Electron density around OLC A 613:

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



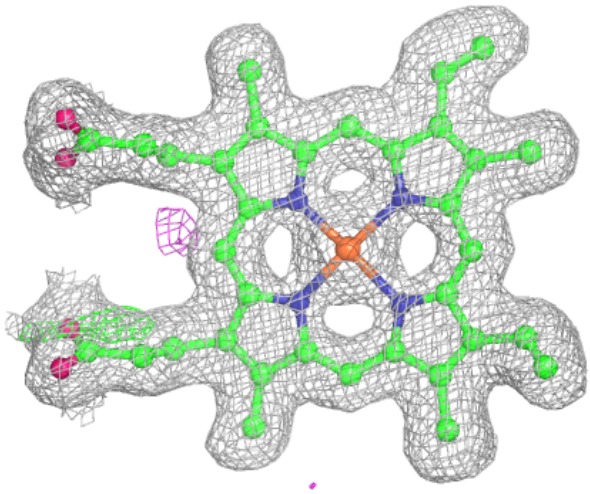
Electron density around OLC A 604:

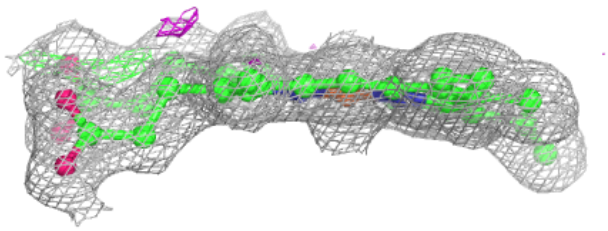
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

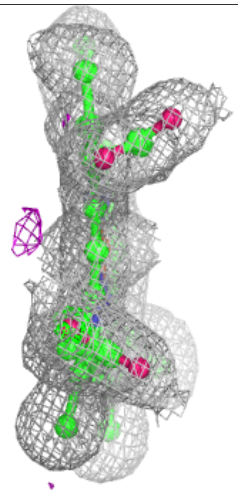


Electron density around HEM A 602:

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

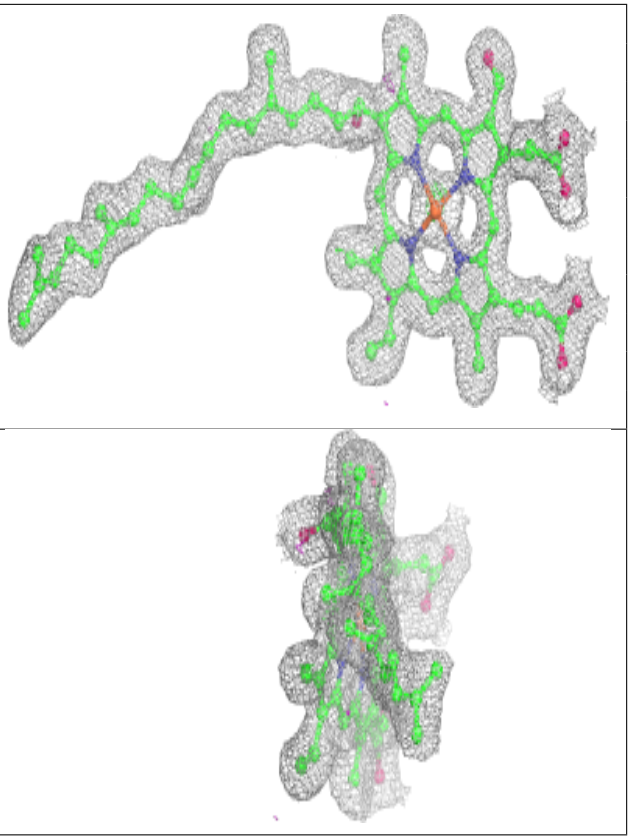


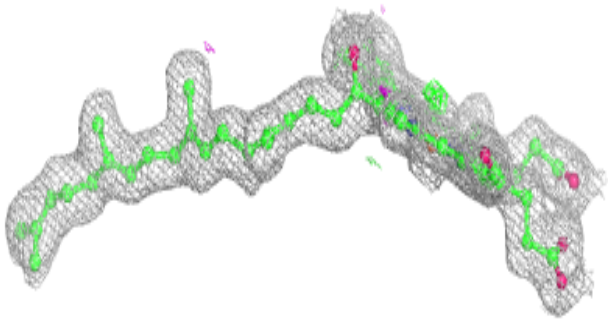




Electron density around HAS A 603:

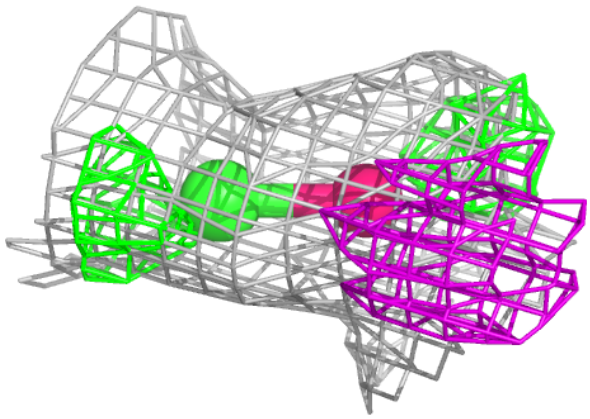
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

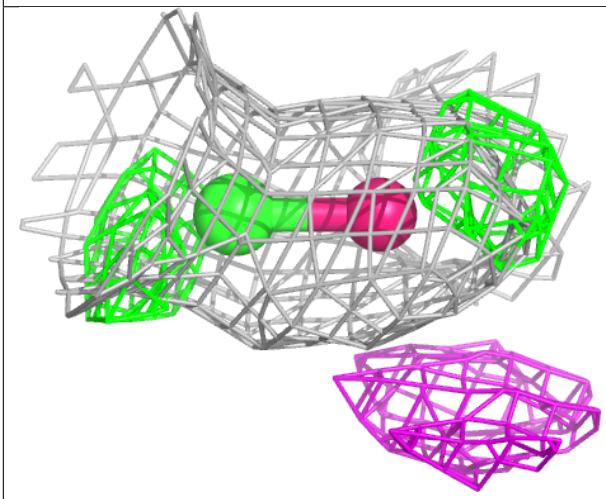


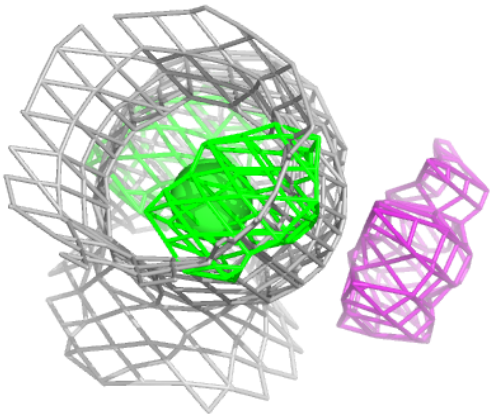


Electron density around CMO A 614:

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

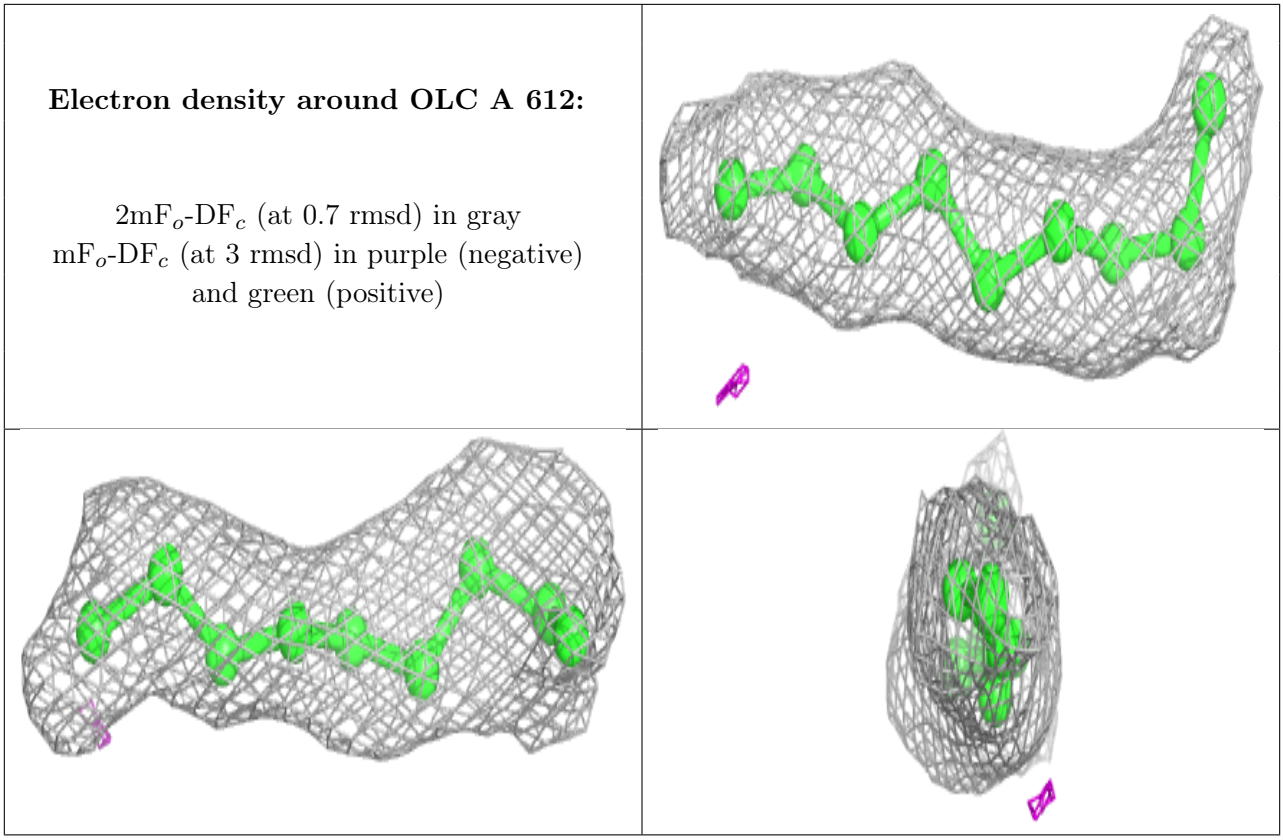






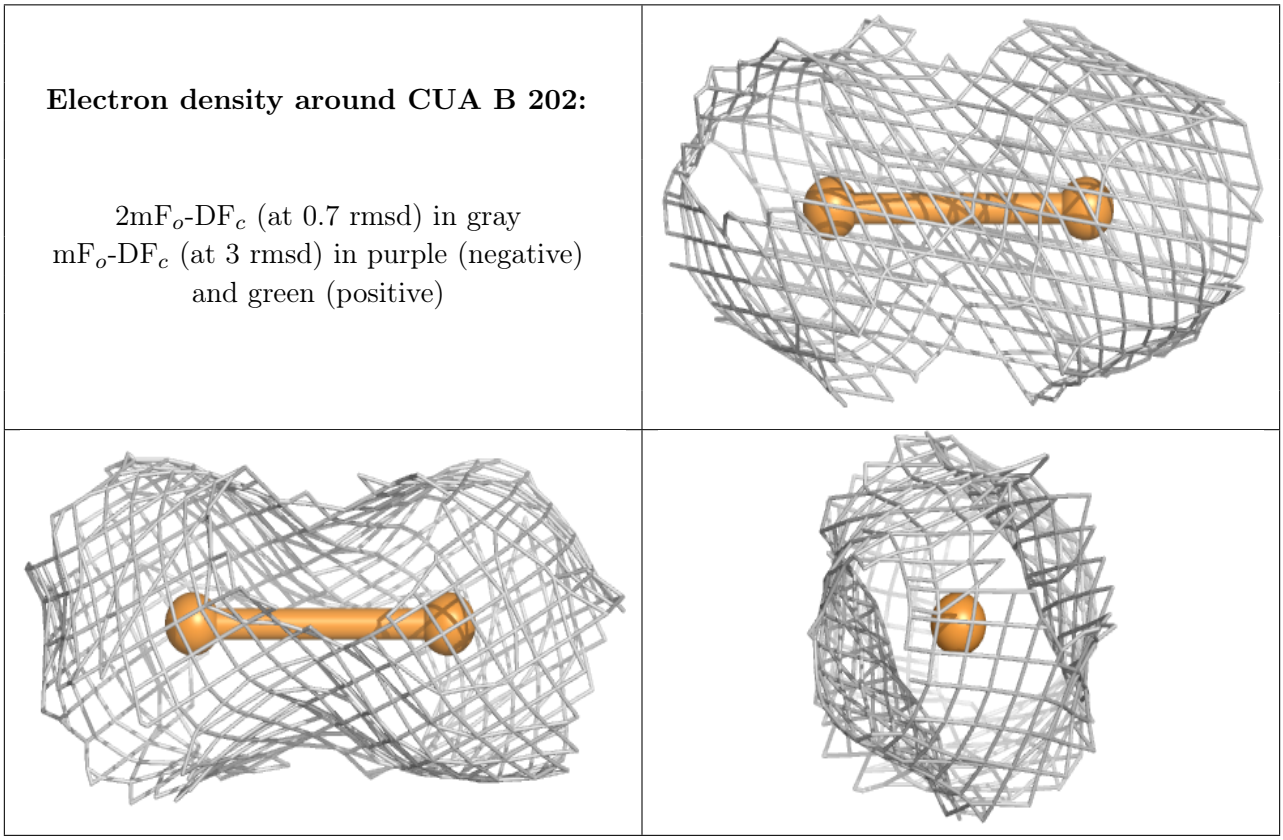
Electron density around OLC A 612:

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



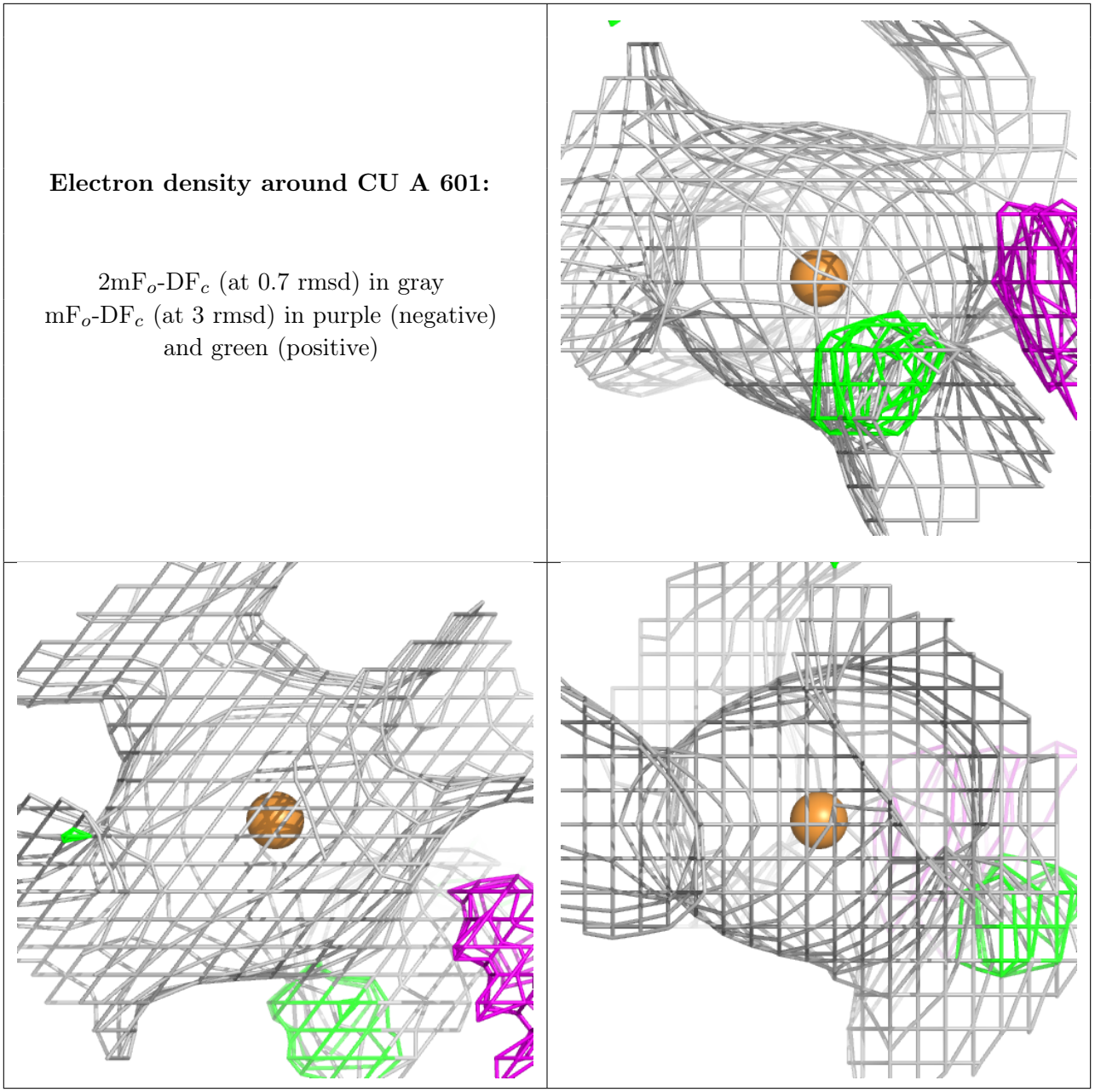
Electron density around CUA B 202:

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



Electron density around CU A 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.