Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 01:21 AM JST

PDB ID	:	6A2J
Title	:	Crystal structure of heme A synthase from Bacillus subtilis
Authors	:	Niwa, S.; Takeda, K.; Kosugi, M.; Tsutsumi, E.; Miki, K.
Deposited on	:	2018-06-12
Resolution	:	2.20 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*
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.

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

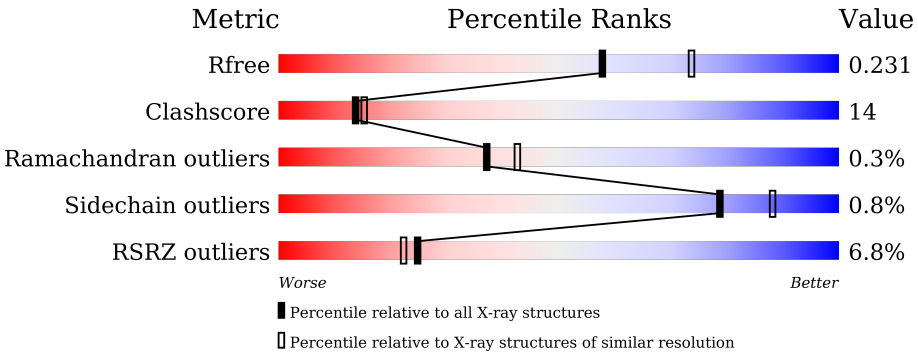
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	309	7%, 71%, 29%, .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2874 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.

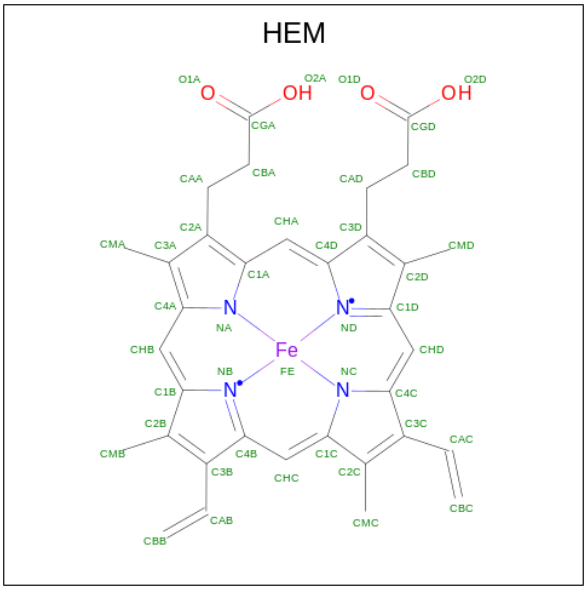
- Molecule 1 is a protein called Heme A synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	309	2431	1628	393	394	16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P12946
A	-4	MET	-	expression tag	UNP P12946
A	-3	LEU	-	expression tag	UNP P12946
A	-2	GLU	-	expression tag	UNP P12946
A	-1	ASP	-	expression tag	UNP P12946
A	0	PRO	-	expression tag	UNP P12946

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

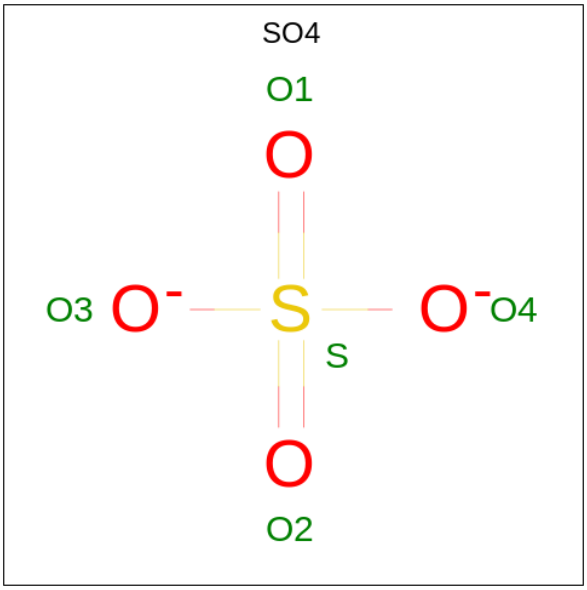


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

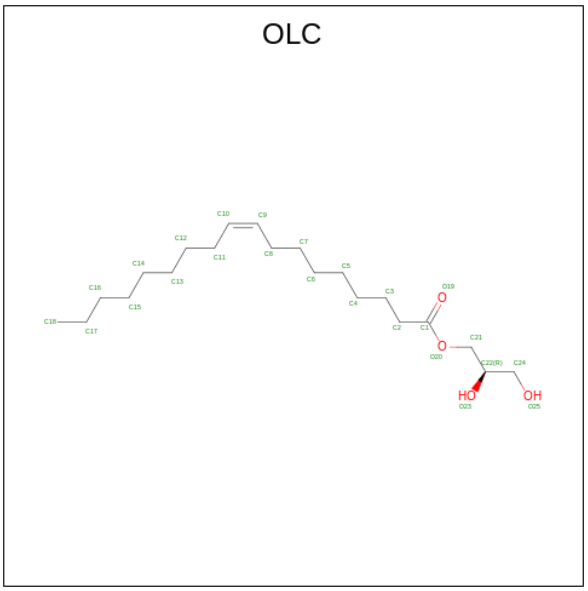
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 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
5	A	1	Total C O 22 18 4	0	0
5	A	1	Total C O 22 18 4	0	0
5	A	1	Total C O 15 11 4	0	0
5	A	1	Total C 11 11	0	0
5	A	1	Total C O 16 12 4	0	0
5	A	1	Total C O 23 19 4	0	0
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C 7 7	0	0
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C O 23 19 4	0	0
5	A	1	Total C O 14 12 2	0	0
5	A	1	Total C O 14 12 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C 13 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 11 11	0	0
5	A	1	Total C O 18 14 4	0	0
5	A	1	Total C O 15 11 4	0	0
5	A	1	Total C O 12 8 4	0	0
5	A	1	Total C O 18 14 4	0	0
5	A	1	Total C O 15 11 4	0	0
5	A	1	Total C O 18 14 4	0	0

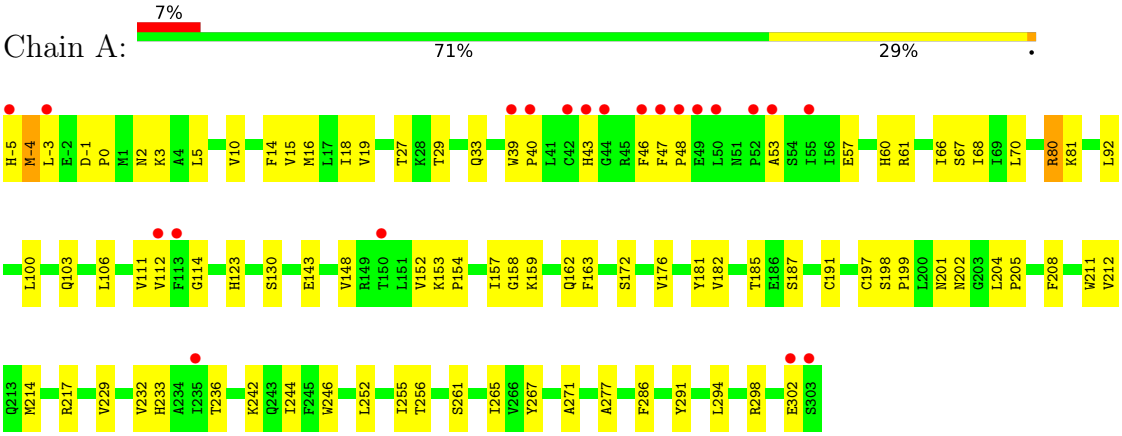
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	32	Total O 32 32	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: Heme A synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	90.47Å 90.47Å 147.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.03 – 2.20 29.03 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.03-2.20) 99.9 (29.03-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.206 , 0.229 0.209 , 0.231	Depositor DCC
R_{free} test set	1150 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.041 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2874	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.15% 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, CU, SO4

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	0.43	0/2498	0.58	0/3396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2431	0	2529	83	0
2	A	43	0	30	0	0
3	A	1	0	0	0	0
4	A	15	0	0	1	0
5	A	352	0	478	26	0
6	A	32	0	0	0	0
All	All	2874	0	3037	84	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 14.

All (84) 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:-3:LEU:HD23	1:A:-3:LEU:O	1.60	1.01
1:A:159:LYS:HD2	5:A:611:OLC:H24	1.58	0.84
1:A:233:HIS:HB2	5:A:621:OLC:H3A	1.60	0.84
1:A:33:GLN:NE2	1:A:111:VAL:HG22	1.95	0.82
1:A:208:PHE:HA	5:A:624:OLC:H2A	1.63	0.78
1:A:80:ARG:HA	1:A:80:ARG:HE	1.48	0.78
1:A:43:HIS:NE2	1:A:61:ARG:NH2	2.33	0.75
1:A:57:GLU:O	1:A:61:ARG:HG2	1.88	0.73
1:A:185:THR:HG23	1:A:187:SER:OG	1.91	0.69
1:A:16:MET:HE3	1:A:67:SER:HB2	1.75	0.69
1:A:-1:ASP:O	1:A:2:ASN:ND2	2.25	0.69
1:A:-3:LEU:O	1:A:-3:LEU:CD2	2.40	0.66
1:A:92:LEU:HD21	5:A:606:OLC:H6	1.77	0.66
1:A:191:CYS:SG	1:A:214:MET:HE3	2.35	0.66
1:A:-3:LEU:HD23	1:A:-3:LEU:C	2.16	0.65
1:A:252:LEU:O	1:A:255:ILE:HG22	1.96	0.65
1:A:148:VAL:HG23	1:A:148:VAL:O	1.95	0.64
1:A:267:TYR:HB3	5:A:623:OLC:H22	1.79	0.64
1:A:0:PRO:O	1:A:3:LYS:HG2	1.97	0.63
1:A:16:MET:CE	1:A:67:SER:HB2	2.28	0.62
1:A:33:GLN:NE2	1:A:111:VAL:CG2	2.63	0.61
1:A:233:HIS:HB2	5:A:621:OLC:C3	2.31	0.60
1:A:39:TRP:HE1	1:A:46:PHE:HE2	1.50	0.59
1:A:185:THR:HG21	1:A:212:VAL:HG11	1.83	0.59
1:A:191:CYS:HB3	1:A:197:CYS:HA	1.84	0.59
1:A:252:LEU:HD21	5:A:614:OLC:H15A	1.84	0.59
1:A:47:PHE:N	1:A:48:PRO:HD2	2.18	0.58
1:A:229:VAL:O	5:A:621:OLC:H2A	2.03	0.57
1:A:15:VAL:HG12	1:A:16:MET:CE	2.34	0.57
1:A:16:MET:HE2	1:A:16:MET:N	2.19	0.57
1:A:112:VAL:HG12	1:A:112:VAL:O	2.04	0.57
1:A:182:VAL:HG22	1:A:212:VAL:HG12	1.87	0.57
1:A:205:PRO:O	5:A:625:OLC:H24A	2.04	0.57
1:A:208:PHE:HD1	5:A:624:OLC:H3A	1.71	0.55
1:A:256:THR:OG1	5:A:614:OLC:H10	2.07	0.55
1:A:271:ALA:HB1	5:A:615:OLC:H22	1.90	0.54
1:A:16:MET:HE3	1:A:67:SER:CB	2.38	0.54
1:A:157:ILE:CD1	1:A:244:ILE:HD11	2.38	0.53
1:A:204:LEU:HB2	5:A:625:OLC:H24	1.89	0.53
1:A:252:LEU:HD23	5:A:614:OLC:H7A	1.90	0.53
1:A:232:VAL:HG12	5:A:621:OLC:O19	2.09	0.52
1:A:5:LEU:HD23	1:A:81:LYS:HD3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HA	1:A:100:LEU:HD21	1.93	0.50
1:A:106:LEU:HD23	1:A:123:HIS:HA	1.92	0.49
1:A:-5:HIS:ND1	1:A:-4:MET:N	2.54	0.49
1:A:261:SER:O	1:A:265:ILE:HG13	2.13	0.49
1:A:302:GLU:OE2	1:A:302:GLU:HA	2.13	0.49
1:A:33:GLN:HE22	1:A:111:VAL:CG2	2.25	0.48
1:A:214:MET:HE1	1:A:217:ARG:NH1	2.28	0.48
1:A:211:TRP:CZ2	5:A:625:OLC:H3	2.49	0.48
1:A:181:TYR:O	1:A:185:THR:HB	2.14	0.48
1:A:158:GLY:HA3	4:A:604:SO4:O2	2.14	0.48
1:A:201:ASN:O	1:A:202:ASN:HB2	2.14	0.47
1:A:185:THR:CG2	1:A:187:SER:OG	2.61	0.46
1:A:153:LYS:HD2	1:A:154:PRO:HD2	1.97	0.46
1:A:172:SER:O	1:A:176:VAL:HG23	2.15	0.46
1:A:204:LEU:HB3	5:A:625:OLC:O25	2.15	0.45
1:A:148:VAL:O	1:A:148:VAL:CG2	2.64	0.45
1:A:158:GLY:O	1:A:162:GLN:HG3	2.16	0.45
1:A:242:LYS:HB2	5:A:607:OLC:O19	2.15	0.45
1:A:198:SER:HB2	1:A:199:PRO:CD	2.46	0.45
1:A:163:PHE:HZ	5:A:611:OLC:H12	1.83	0.44
1:A:66:ILE:HG13	1:A:70:LEU:HG	2.00	0.44
1:A:246:TRP:CD2	5:A:626:OLC:H3	2.52	0.44
1:A:19:VAL:O	1:A:60:HIS:HE1	2.01	0.44
1:A:14:PHE:O	1:A:18:ILE:HG12	2.17	0.43
1:A:16:MET:CE	1:A:67:SER:CB	2.96	0.43
5:A:607:OLC:H13	5:A:619:OLC:H9	2.00	0.43
1:A:232:VAL:O	1:A:236:THR:HG23	2.17	0.43
1:A:291:TYR:CD2	5:A:607:OLC:H10	2.54	0.43
1:A:182:VAL:O	1:A:185:THR:HG22	2.18	0.43
1:A:29:THR:HB	1:A:114:GLY:HA3	2.01	0.42
1:A:143:GLU:HG3	1:A:152:VAL:HG23	2.00	0.42
1:A:103:GLN:NE2	1:A:130:SER:CB	2.83	0.42
1:A:277:ALA:HB2	5:A:615:OLC:H5	2.01	0.42
1:A:294:LEU:O	1:A:298:ARG:HG3	2.20	0.42
1:A:80:ARG:HA	1:A:80:ARG:NE	2.26	0.41
1:A:112:VAL:O	1:A:112:VAL:CG1	2.67	0.41
1:A:204:LEU:CB	5:A:625:OLC:H24	2.51	0.41
1:A:286:PHE:HZ	5:A:606:OLC:H12A	1.85	0.41
1:A:53:ALA:O	1:A:57:GLU:HG3	2.20	0.40
1:A:27:THR:HG22	1:A:29:THR:H	1.86	0.40
1:A:10:VAL:HG11	5:A:612:OLC:H10	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:HA	1:A:143:GLU:OE1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	307/309 (99%)	297 (97%)	9 (3%)	1 (0%)	37 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO

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	260/260 (100%)	258 (99%)	2 (1%)	79 88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	MET
1	A	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	60	HIS
1	A	103	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	$\#\|Z\| > 2$
5	OLC	A	611	-	22,22,24	1.01	1 (4%)	23,23,25	1.18	3 (13%)
5	OLC	A	626	-	17,17,24	1.26	1 (5%)	18,18,25	1.59	4 (22%)
2	HEM	A	601	1	41,50,50	3.31	23 (56%)	45,82,82	3.12	18 (40%)
5	OLC	A	613	-	6,6,24	0.87	0	4,5,25	0.25	0
5	OLC	A	606	-	21,21,24	1.13	1 (4%)	22,22,25	1.23	4 (18%)
5	OLC	A	615	-	22,22,24	0.99	1 (4%)	23,23,25	1.25	4 (17%)
4	SO4	A	603	-	4,4,4	0.27	0	6,6,6	0.15	0
5	OLC	A	619	-	12,12,24	0.63	0	11,11,25	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	OLC	A	620	-	10,10,24	0.64	0	9,9,25	0.50	0
5	OLC	A	622	-	14,14,24	1.10	1 (7%)	15,15,25	1.51	4 (26%)
5	OLC	A	609	-	10,10,24	0.73	0	9,9,25	0.35	0
5	OLC	A	607	-	21,21,24	1.14	1 (4%)	22,22,25	1.37	4 (18%)
5	OLC	A	616	-	13,13,24	1.37	1 (7%)	13,13,25	0.82	0
5	OLC	A	614	-	24,24,24	1.02	1 (4%)	25,25,25	1.21	4 (16%)
4	SO4	A	604	-	4,4,4	0.29	0	6,6,6	0.08	0
5	OLC	A	610	-	15,15,24	1.11	1 (6%)	16,16,25	1.41	4 (25%)
5	OLC	A	612	-	24,24,24	1.04	1 (4%)	25,25,25	1.19	4 (16%)
5	OLC	A	617	-	13,13,24	1.30	1 (7%)	13,13,25	0.81	0
5	OLC	A	608	-	14,14,24	1.28	2 (14%)	15,15,25	1.51	4 (26%)
5	OLC	A	625	-	14,14,24	1.25	1 (7%)	15,15,25	1.76	4 (26%)
4	SO4	A	605	-	4,4,4	0.33	0	6,6,6	0.11	0
5	OLC	A	618	-	14,14,24	1.31	1 (7%)	13,14,25	0.77	0
5	OLC	A	621	-	17,17,24	1.24	1 (5%)	18,18,25	1.43	4 (22%)
5	OLC	A	623	-	11,11,24	1.44	1 (9%)	12,12,25	1.61	4 (33%)
5	OLC	A	624	-	17,17,24	1.09	1 (5%)	18,18,25	1.49	4 (22%)

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	OLC	A	611	-	-	0/22/22/24	-
5	OLC	A	626	-	-	1/17/17/24	-
2	HEM	A	601	1	-	5/12/54/54	-
5	OLC	A	613	-	-	1/4/4/24	-
5	OLC	A	606	-	-	5/21/21/24	-
5	OLC	A	615	-	-	4/22/22/24	-
5	OLC	A	619	-	-	1/10/10/24	-
5	OLC	A	620	-	-	1/8/8/24	-
5	OLC	A	622	-	-	1/14/14/24	-
5	OLC	A	609	-	-	0/8/8/24	-
5	OLC	A	607	-	-	4/21/21/24	-
5	OLC	A	616	-	-	1/12/12/24	-
5	OLC	A	614	-	-	3/24/24/24	-
5	OLC	A	610	-	-	2/15/15/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	612	-	-	4/24/24/24	-
5	OLC	A	617	-	-	2/12/12/24	-
5	OLC	A	608	-	-	1/14/14/24	-
5	OLC	A	625	-	-	3/14/14/24	-
5	OLC	A	618	-	-	0/13/13/24	-
5	OLC	A	621	-	-	5/17/17/24	-
5	OLC	A	623	-	-	0/11/11/24	-
5	OLC	A	624	-	-	0/17/17/24	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3C-C2C	9.68	1.53	1.40
2	A	601	HEM	C3B-C2B	6.72	1.50	1.37
2	A	601	HEM	C4D-C3D	6.71	1.56	1.45
2	A	601	HEM	CMC-C2C	5.45	1.64	1.51
2	A	601	HEM	C1D-C2D	5.32	1.54	1.44
5	A	607	OLC	O20-C1	4.36	1.46	1.33
5	A	626	OLC	O20-C1	4.28	1.45	1.33
2	A	601	HEM	CAB-C3B	4.26	1.59	1.47
5	A	606	OLC	O20-C1	4.14	1.45	1.33
5	A	623	OLC	O20-C1	4.14	1.45	1.33
2	A	601	HEM	CMB-C2B	4.08	1.59	1.50
5	A	625	OLC	O20-C1	4.07	1.45	1.33
5	A	612	OLC	O20-C1	4.05	1.45	1.33
5	A	614	OLC	O20-C1	4.03	1.45	1.33
2	A	601	HEM	O1A-CGA	4.03	1.35	1.22
5	A	615	OLC	O20-C1	4.01	1.45	1.33
5	A	611	OLC	O20-C1	4.00	1.45	1.33
5	A	621	OLC	O20-C1	3.99	1.45	1.33
5	A	616	OLC	O20-C1	3.94	1.45	1.33
5	A	617	OLC	O20-C1	3.91	1.45	1.33
5	A	618	OLC	O20-C1	3.90	1.45	1.33
5	A	610	OLC	O20-C1	3.89	1.44	1.33
5	A	608	OLC	O20-C1	3.89	1.44	1.33
5	A	624	OLC	O20-C1	3.80	1.44	1.33
5	A	622	OLC	O20-C1	3.79	1.44	1.33
2	A	601	HEM	C1A-NA	-3.73	1.28	1.36
2	A	601	HEM	C1A-CHA	3.68	1.51	1.41
2	A	601	HEM	FE-ND	3.57	2.14	1.96
2	A	601	HEM	CHB-C1B	3.13	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	FE-NB	3.00	2.11	1.96
2	A	601	HEM	C1B-NB	-2.97	1.35	1.40
2	A	601	HEM	C3D-C2D	2.96	1.43	1.36
2	A	601	HEM	C3C-CAC	-2.95	1.41	1.47
2	A	601	HEM	C4A-NA	2.77	1.41	1.36
2	A	601	HEM	CMA-C3A	2.56	1.57	1.51
2	A	601	HEM	O1D-CGD	2.54	1.30	1.22
2	A	601	HEM	C1B-C2B	-2.48	1.39	1.44
2	A	601	HEM	C4D-ND	-2.39	1.36	1.40
2	A	601	HEM	CBD-CGD	-2.16	1.45	1.50
2	A	601	HEM	CHD-C1D	-2.09	1.35	1.41
5	A	608	OLC	C2-C1	2.05	1.56	1.50

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	HEM	C4B-CHC-C1C	10.28	136.12	122.56
2	A	601	HEM	C2C-C3C-C4C	-9.20	100.47	106.90
2	A	601	HEM	C3B-C2B-C1B	-5.89	102.12	106.49
2	A	601	HEM	C4C-CHD-C1D	4.86	128.97	122.56
2	A	601	HEM	CHB-C1B-NB	-4.76	118.50	124.38
2	A	601	HEM	C2B-C1B-NB	4.75	115.46	109.84
2	A	601	HEM	C1D-C2D-C3D	-4.03	102.72	106.96
2	A	601	HEM	CBA-CAA-C2A	4.03	119.49	112.62
2	A	601	HEM	C4B-C3B-C2B	-3.66	104.21	107.11
5	A	625	OLC	O20-C21-C22	3.50	122.67	105.77
5	A	607	OLC	O20-C21-C22	3.47	122.55	105.77
5	A	625	OLC	O23-C22-C21	3.46	121.70	109.56
5	A	626	OLC	O20-C21-C22	3.43	122.31	105.77
2	A	601	HEM	CMA-C3A-C4A	-3.39	123.25	128.46
2	A	601	HEM	CHC-C4B-NB	-3.39	120.75	124.43
5	A	608	OLC	O23-C22-C21	3.33	121.22	109.56
5	A	622	OLC	O23-C22-C21	3.31	121.17	109.56
5	A	611	OLC	O23-C22-C21	3.28	121.07	109.56
5	A	626	OLC	O23-C22-C21	3.25	120.95	109.56
5	A	624	OLC	O20-C21-C22	3.24	121.42	105.77
5	A	621	OLC	O23-C22-C21	3.22	120.85	109.56
5	A	612	OLC	O20-C21-C22	3.16	121.02	105.77
5	A	614	OLC	O20-C21-C22	3.13	120.90	105.77
5	A	615	OLC	O23-C22-C21	3.10	120.42	109.56
2	A	601	HEM	CMA-C3A-C2A	3.07	130.73	124.94
5	A	623	OLC	O20-C21-C22	3.06	120.55	105.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	621	OLC	O20-C21-C22	3.06	120.54	105.77
5	A	612	OLC	O23-C22-C21	3.06	120.28	109.56
5	A	606	OLC	O20-C21-C22	3.04	120.47	105.77
5	A	608	OLC	O20-C21-C22	3.00	120.28	105.77
5	A	615	OLC	O20-C21-C22	3.00	120.27	105.77
5	A	610	OLC	O23-C22-C21	3.00	120.08	109.56
5	A	606	OLC	O23-C22-C21	2.92	119.81	109.56
5	A	607	OLC	O23-C22-C21	2.92	119.79	109.56
5	A	610	OLC	O20-C21-C22	2.91	119.84	105.77
5	A	623	OLC	O23-C22-C21	2.83	119.49	109.56
5	A	614	OLC	O23-C22-C21	2.82	119.46	109.56
5	A	625	OLC	O20-C1-C2	2.82	120.75	111.91
5	A	622	OLC	O20-C21-C22	2.81	119.35	105.77
5	A	611	OLC	O20-C21-C22	2.80	119.28	105.77
2	A	601	HEM	CMC-C2C-C3C	2.76	129.84	124.68
5	A	607	OLC	O20-C1-C2	2.75	120.53	111.91
5	A	624	OLC	O23-C22-C21	2.75	119.19	109.56
5	A	626	OLC	O20-C1-C2	2.74	120.51	111.91
2	A	601	HEM	CMB-C2B-C1B	2.68	129.12	125.04
2	A	601	HEM	C2D-C1D-ND	2.65	113.05	109.88
5	A	606	OLC	O25-C24-C22	2.64	122.88	110.20
5	A	624	OLC	O20-C1-C2	2.55	119.91	111.91
5	A	621	OLC	O20-C1-C2	2.40	119.44	111.91
5	A	623	OLC	O25-C24-C22	2.39	121.66	110.20
5	A	614	OLC	O20-C1-C2	2.39	119.40	111.91
5	A	607	OLC	O25-C24-C22	2.39	121.65	110.20
5	A	608	OLC	O25-C24-C22	2.37	121.59	110.20
5	A	624	OLC	O25-C24-C22	2.36	121.51	110.20
5	A	615	OLC	O25-C24-C22	2.32	121.32	110.20
5	A	625	OLC	O25-C24-C22	2.29	121.20	110.20
5	A	611	OLC	O25-C24-C22	2.29	121.18	110.20
5	A	615	OLC	O20-C1-C2	2.26	119.00	111.91
5	A	614	OLC	O25-C24-C22	2.23	120.92	110.20
2	A	601	HEM	O2D-CGD-CBD	2.21	121.14	114.03
5	A	610	OLC	O25-C24-C22	2.21	120.79	110.20
5	A	621	OLC	O25-C24-C22	2.20	120.73	110.20
5	A	612	OLC	O20-C1-C2	2.19	118.77	111.91
5	A	623	OLC	O20-C1-C2	2.15	118.65	111.91
5	A	622	OLC	O20-C1-C2	2.14	118.63	111.91
2	A	601	HEM	CHA-C4D-ND	-2.13	121.75	124.38
5	A	622	OLC	O25-C24-C22	2.10	120.28	110.20
5	A	612	OLC	O25-C24-C22	2.10	120.26	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	610	OLC	O20-C1-C2	2.10	118.49	111.91
5	A	626	OLC	O25-C24-C22	2.05	120.05	110.20
5	A	608	OLC	O20-C1-C2	2.05	118.33	111.91
5	A	606	OLC	O20-C1-C2	2.01	118.22	111.91
2	A	601	HEM	O2A-CGA-CBA	2.01	120.48	114.03

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	606	OLC	O20-C21-C22-O23
5	A	607	OLC	O20-C21-C22-O23
5	A	613	OLC	C9-C10-C11-C12
5	A	615	OLC	C21-C22-C24-O25
5	A	615	OLC	O23-C22-C24-O25
5	A	622	OLC	C21-C22-C24-O25
5	A	607	OLC	O20-C21-C22-C24
5	A	612	OLC	C2-C3-C4-C5
5	A	606	OLC	O20-C21-C22-C24
5	A	606	OLC	C21-C22-C24-O25
5	A	610	OLC	O23-C22-C24-O25
5	A	617	OLC	C6-C7-C8-C9
5	A	625	OLC	O19-C1-O20-C21
2	A	601	HEM	C2B-C3B-CAB-CBB
2	A	601	HEM	C4B-C3B-CAB-CBB
5	A	606	OLC	C10-C11-C12-C13
5	A	625	OLC	C2-C1-O20-C21
5	A	608	OLC	O23-C22-C24-O25
5	A	619	OLC	C4-C5-C6-C7
5	A	607	OLC	C3-C4-C5-C6
5	A	625	OLC	C2-C3-C4-C5
5	A	614	OLC	C12-C13-C14-C15
5	A	621	OLC	C3-C4-C5-C6
5	A	621	OLC	C5-C6-C7-C8
5	A	610	OLC	C21-C22-C24-O25
5	A	626	OLC	C3-C4-C5-C6
5	A	614	OLC	C13-C14-C15-C16
5	A	621	OLC	O20-C1-C2-C3
2	A	601	HEM	CAA-CBA-CGA-O1A
5	A	606	OLC	C7-C8-C9-C10
5	A	614	OLC	C9-C10-C11-C12
5	A	616	OLC	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	612	OLC	C14-C15-C16-C17
5	A	617	OLC	C5-C6-C7-C8
5	A	621	OLC	C7-C8-C9-C10
5	A	607	OLC	C10-C11-C12-C13
5	A	620	OLC	C9-C10-C11-C12
2	A	601	HEM	CAD-CBD-CGD-O2D
5	A	615	OLC	C9-C10-C11-C12
5	A	615	OLC	O20-C21-C22-O23
5	A	621	OLC	O23-C22-C24-O25
2	A	601	HEM	CAA-CBA-CGA-O2A
5	A	612	OLC	O20-C1-C2-C3
5	A	612	OLC	C7-C8-C9-C10

There are no ring outliers.

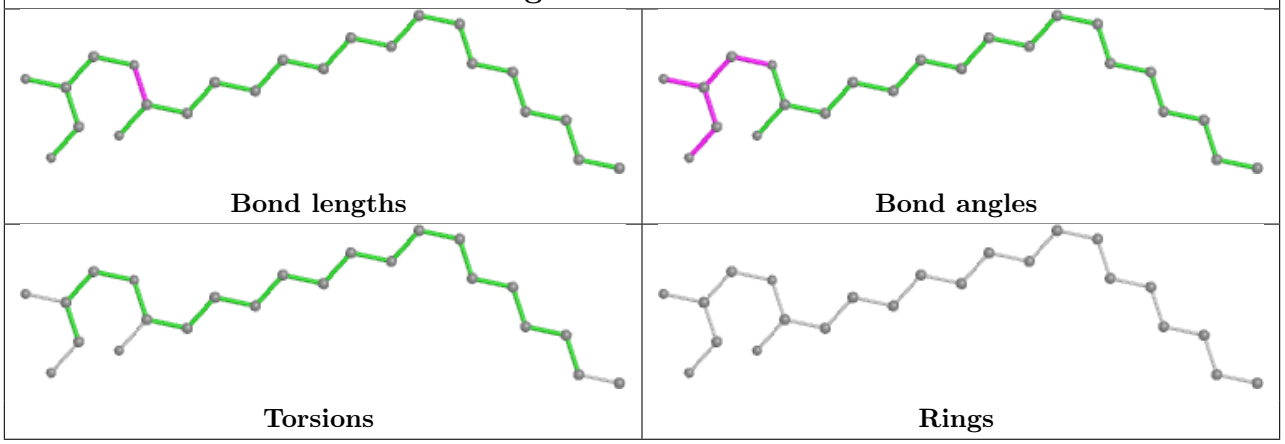
13 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	611	OLC	2	0
5	A	626	OLC	1	0
5	A	606	OLC	2	0
5	A	615	OLC	2	0
5	A	619	OLC	1	0
5	A	607	OLC	3	0
5	A	614	OLC	3	0
4	A	604	SO4	1	0
5	A	612	OLC	1	0
5	A	625	OLC	5	0
5	A	621	OLC	4	0
5	A	623	OLC	1	0
5	A	624	OLC	2	0

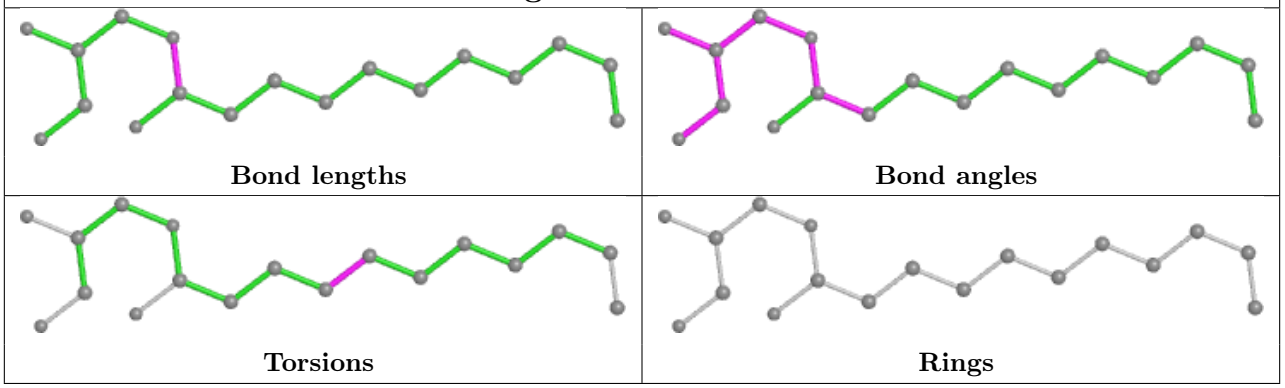
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

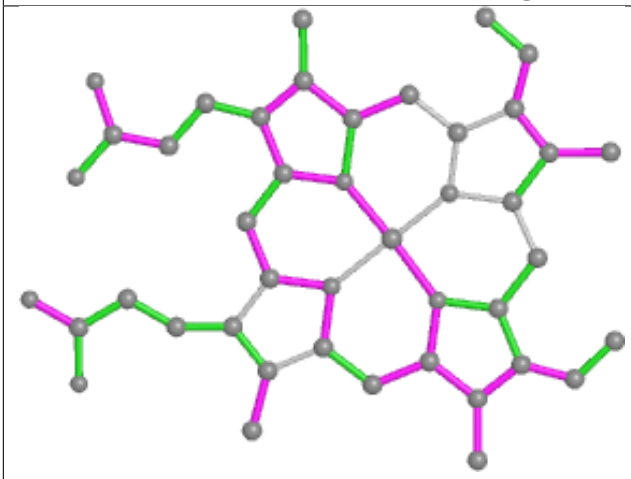
Ligand OLC A 611



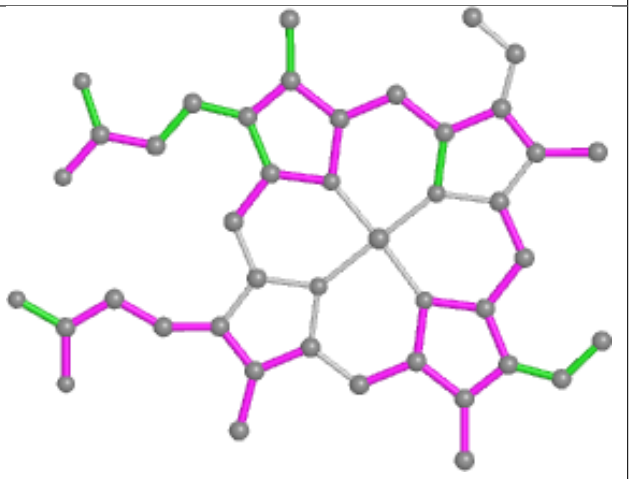
Ligand OLC A 626



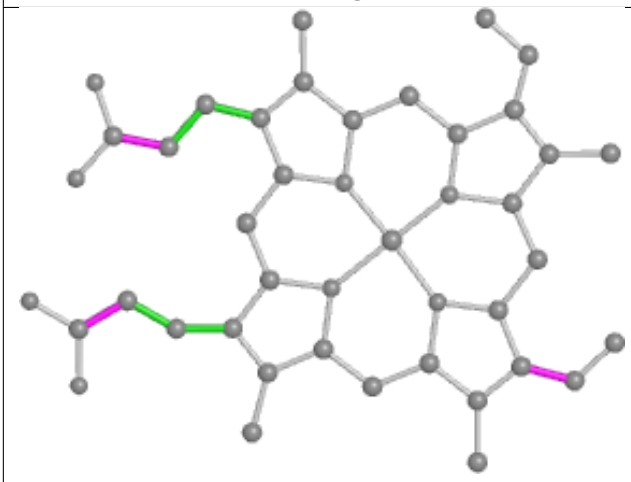
Ligand HEM A 601



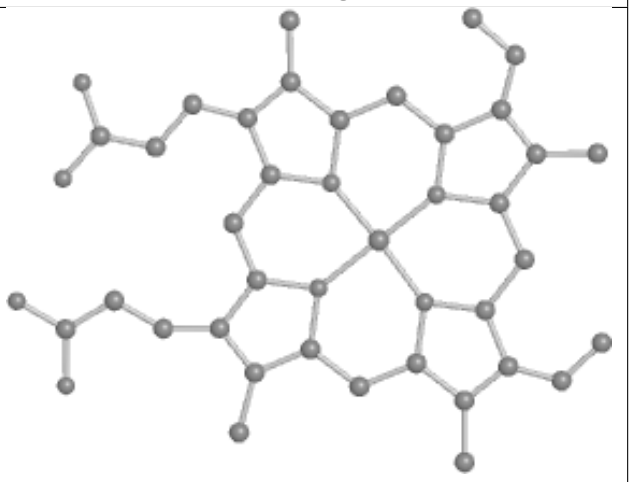
Bond lengths



Bond angles

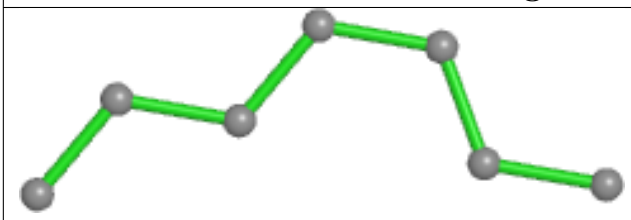


Torsions

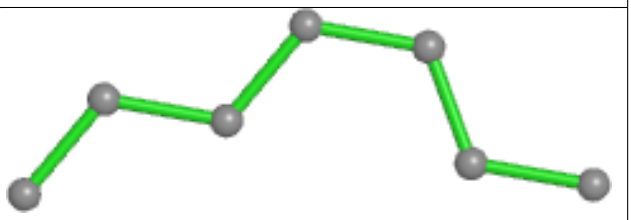


Rings

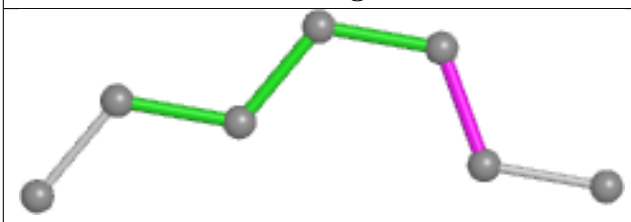
Ligand OLC A 613



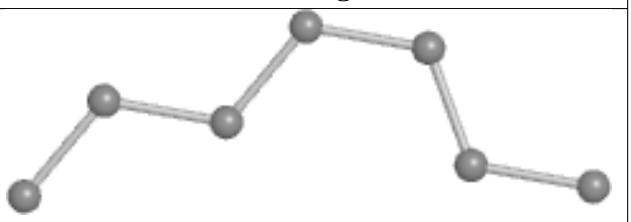
Bond lengths



Bond angles

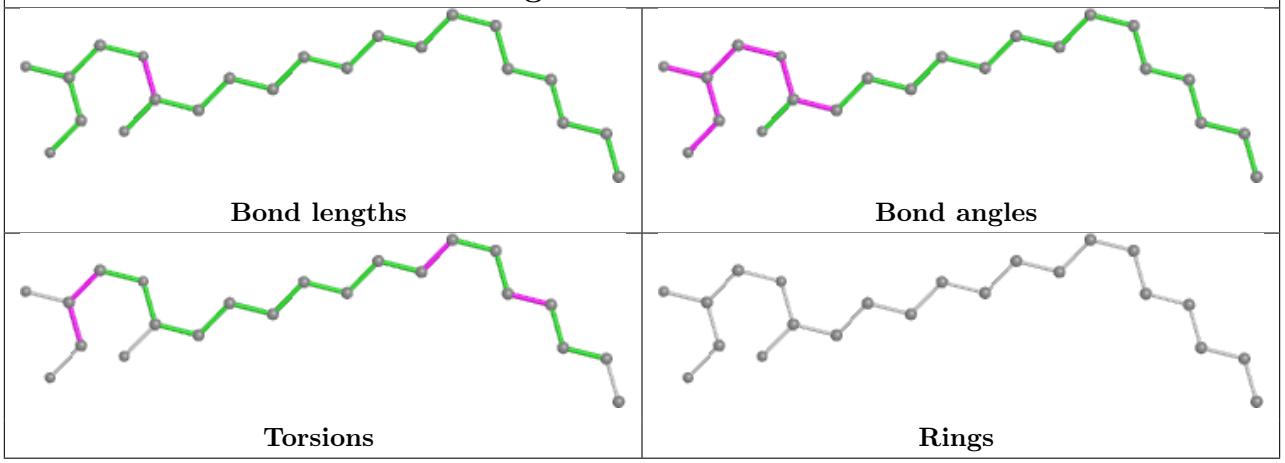


Torsions

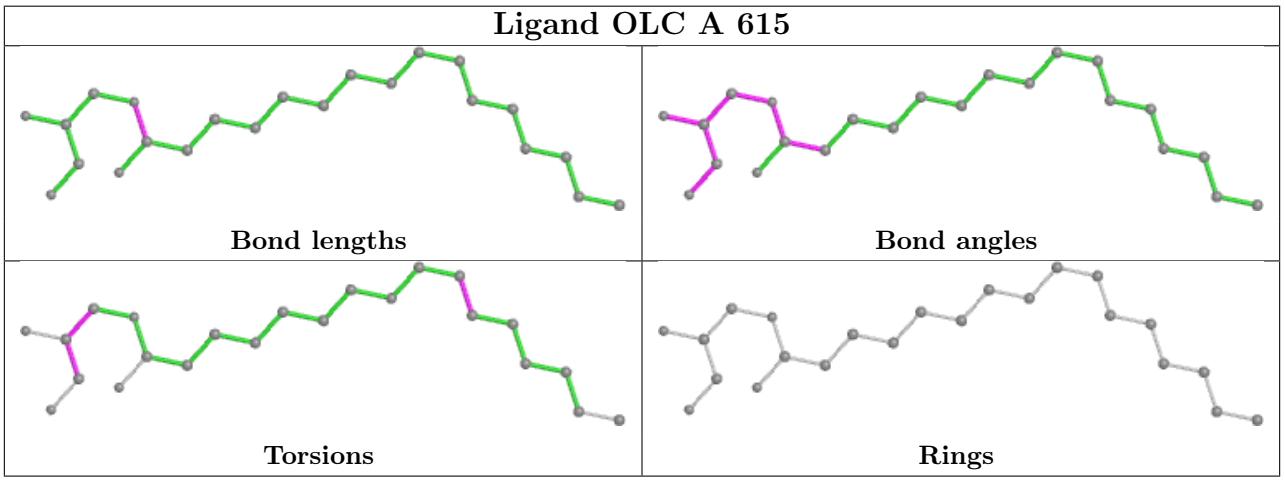


Rings

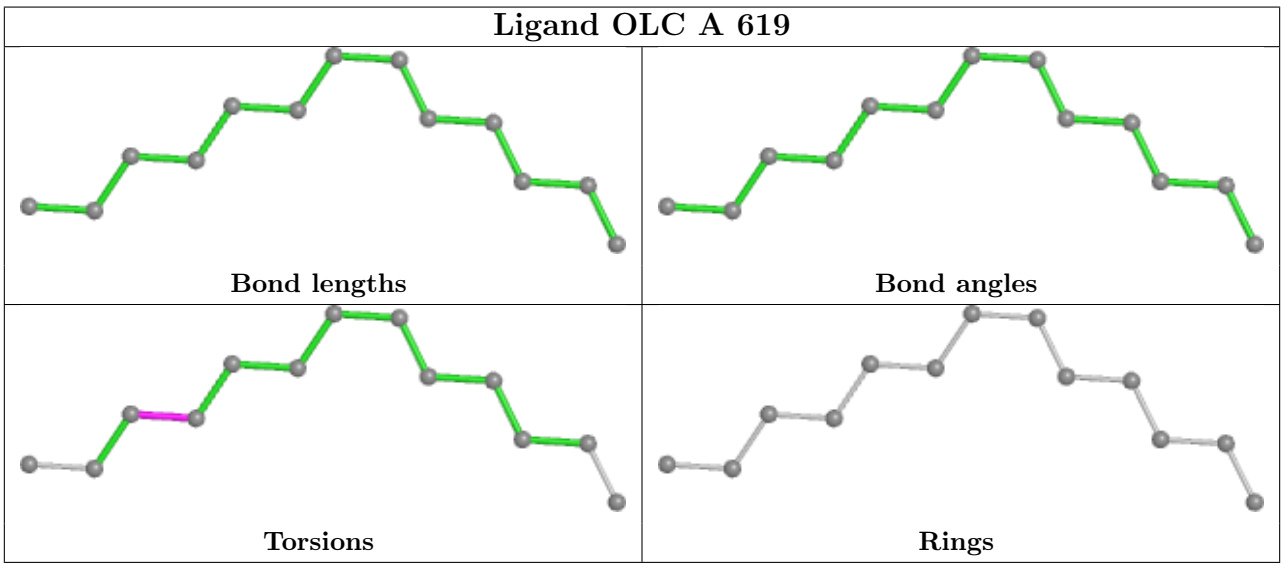
Ligand OLC A 606



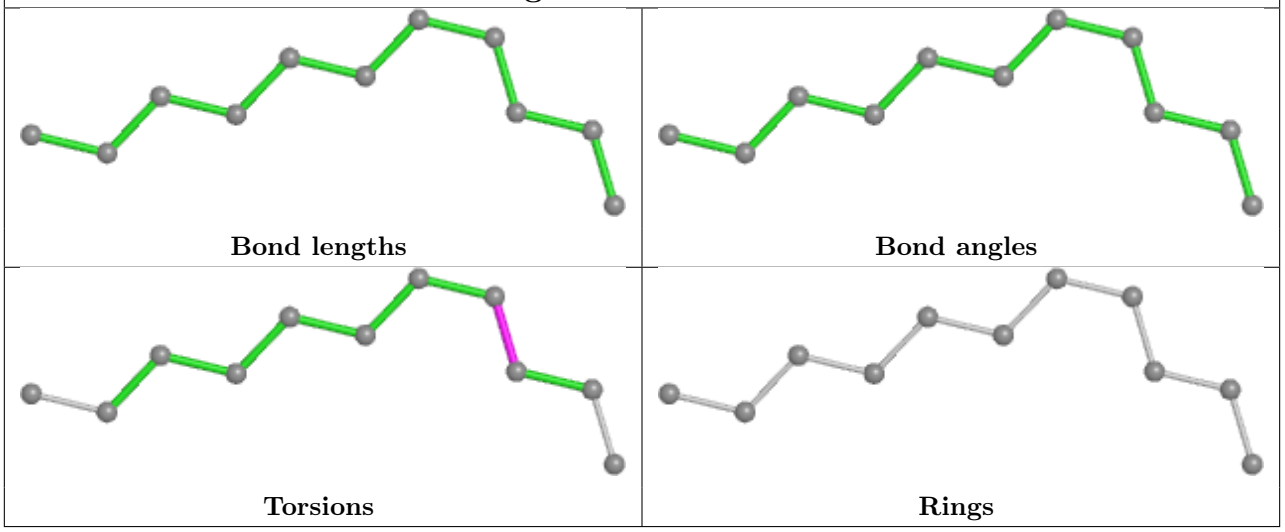
Ligand OLC A 615



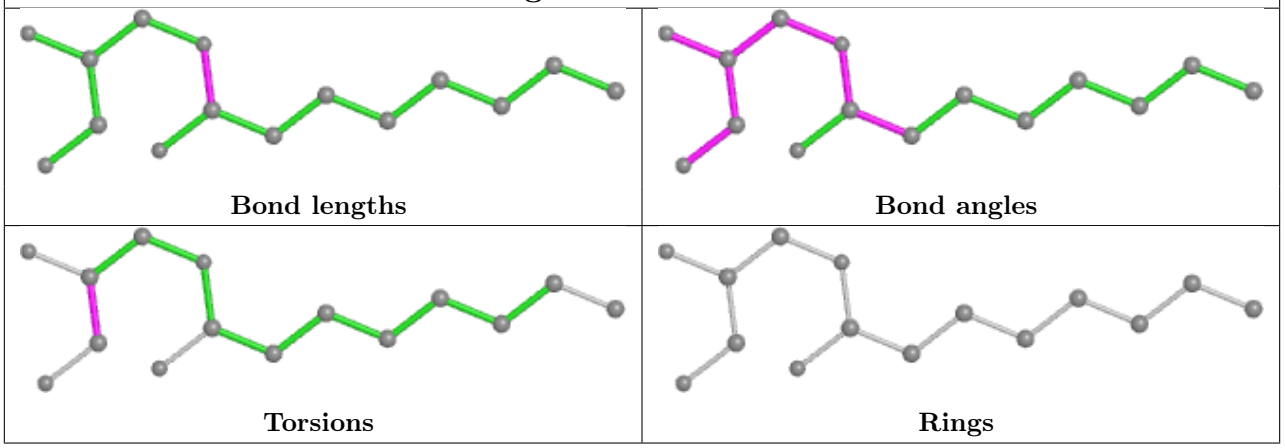
Ligand OLC A 619



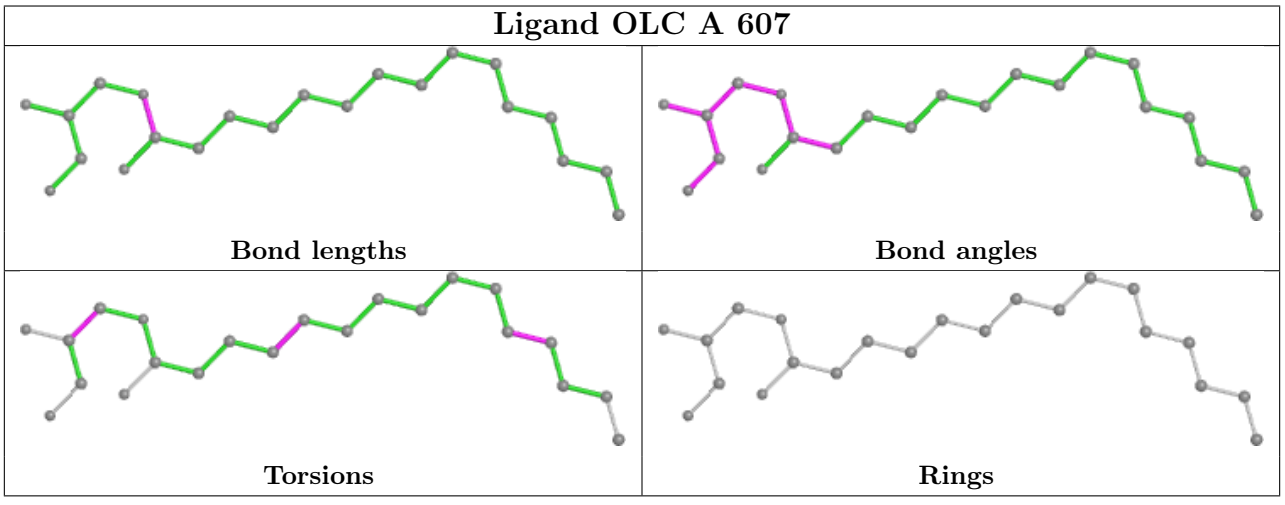
Ligand OLC A 620



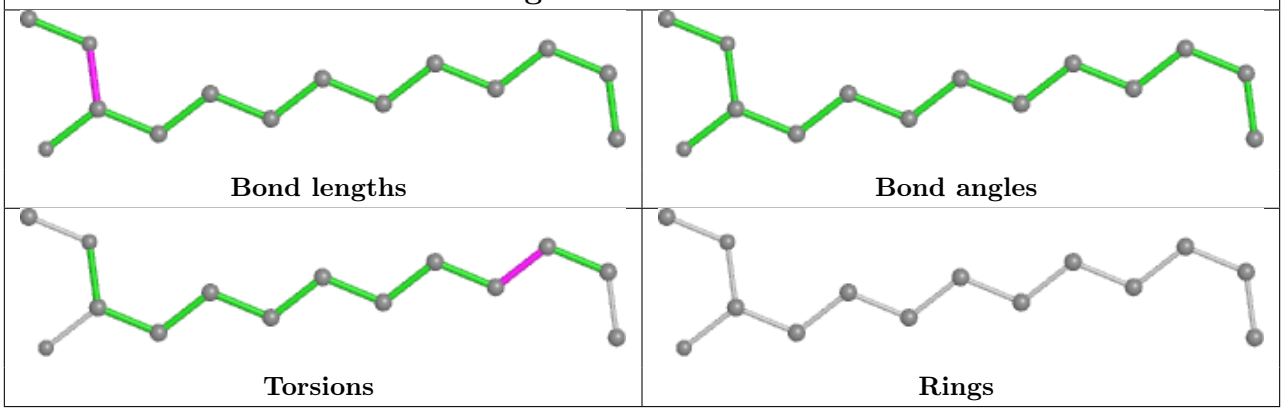
Ligand OLC A 622



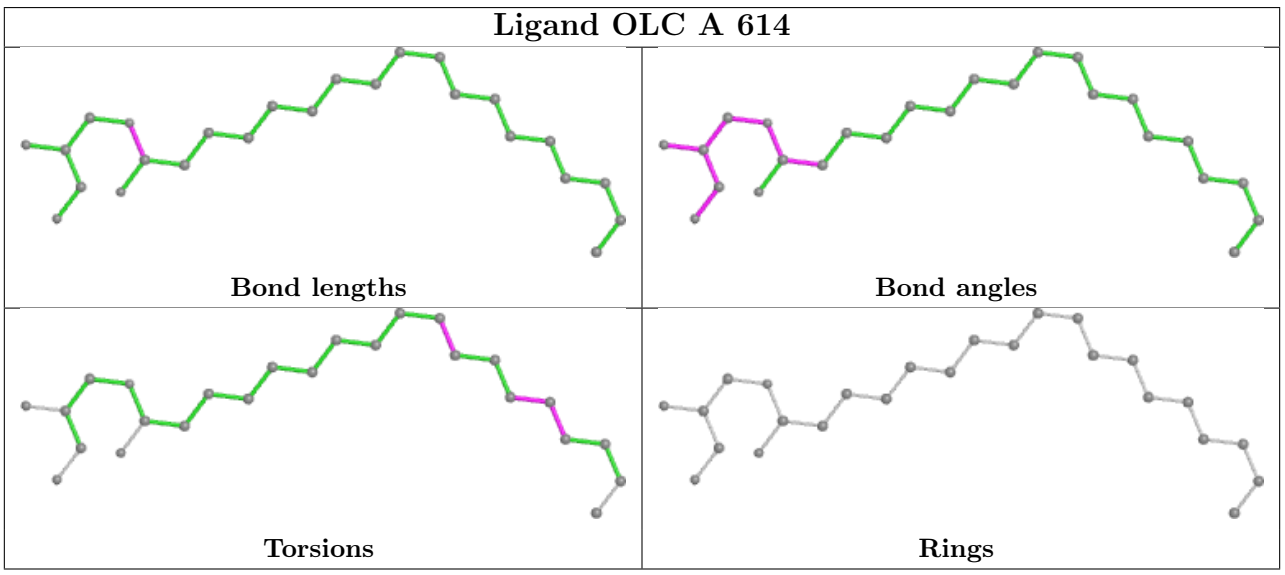
Ligand OLC A 607



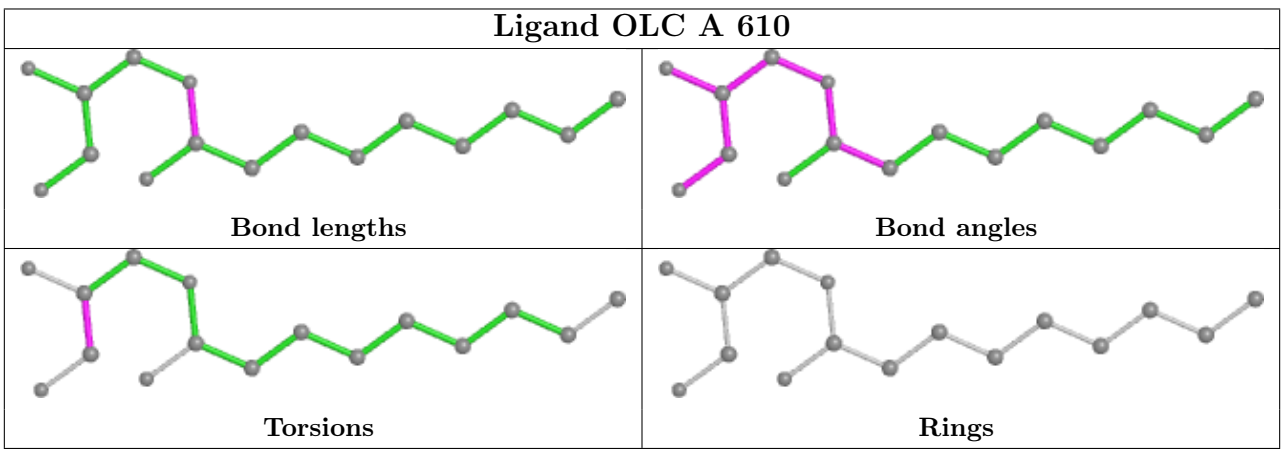
Ligand OLC A 616



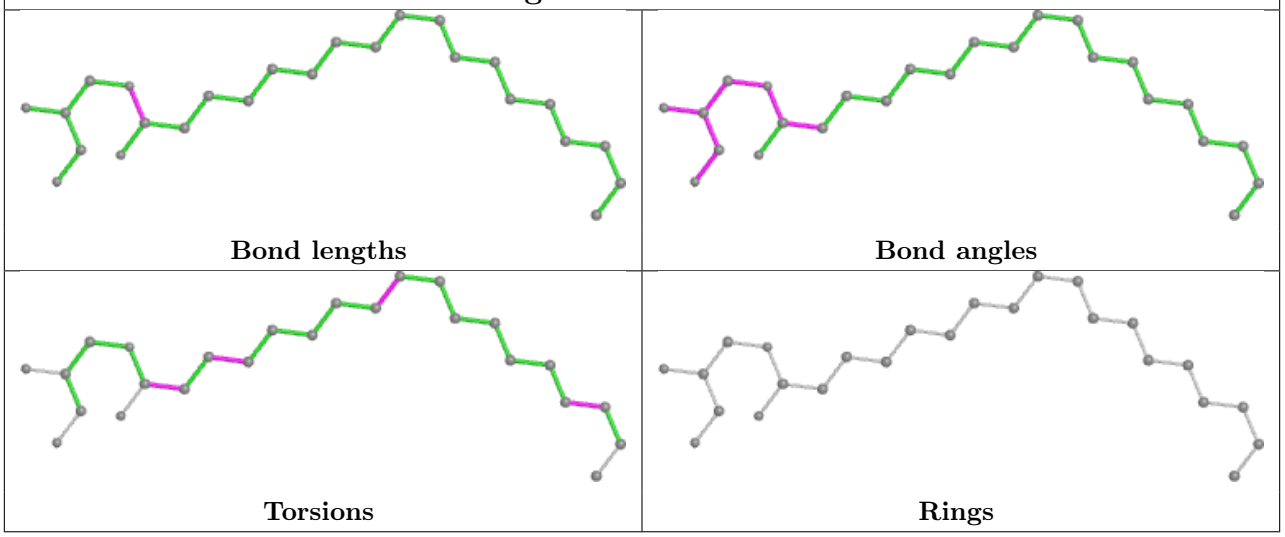
Ligand OLC A 614



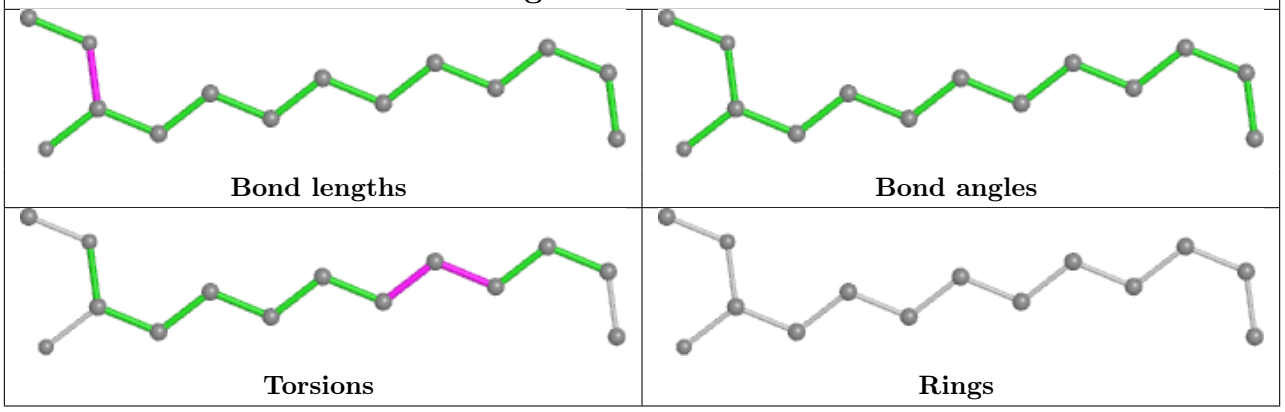
Ligand OLC A 610



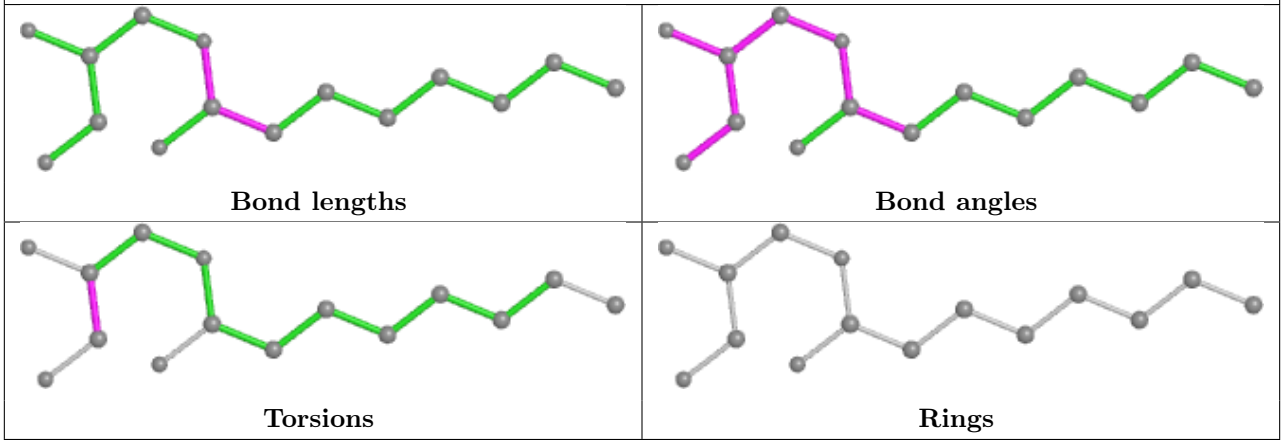
Ligand OLC A 612



Ligand OLC A 617

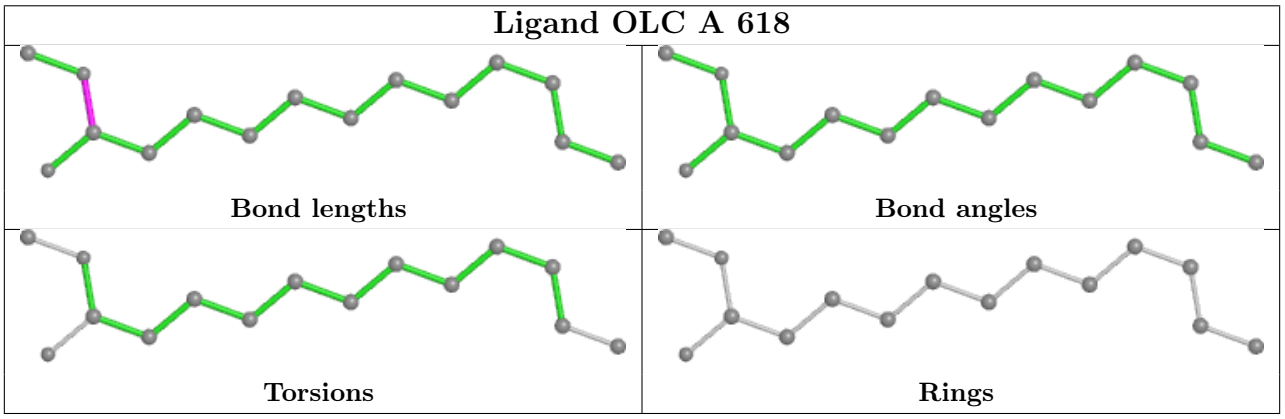


Ligand OLC A 608

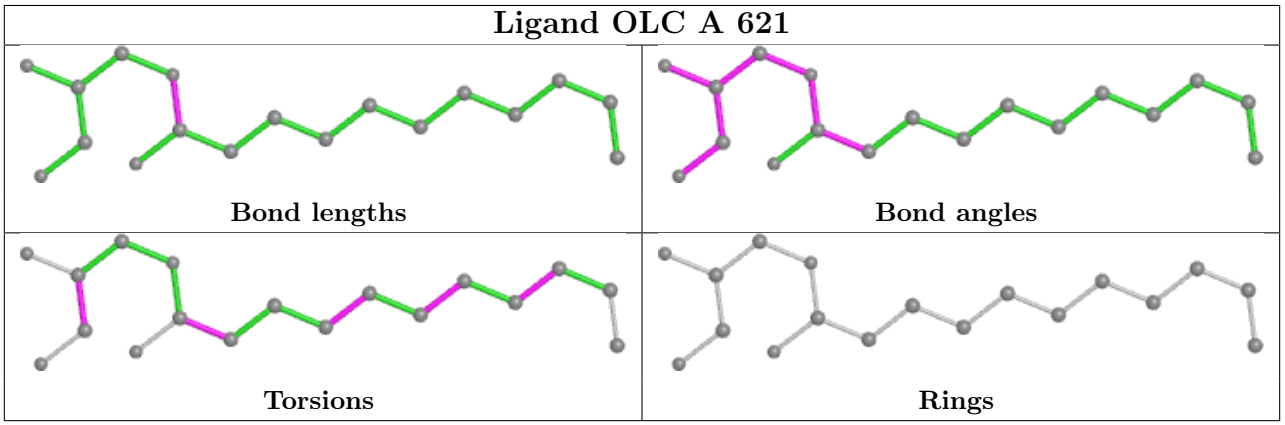


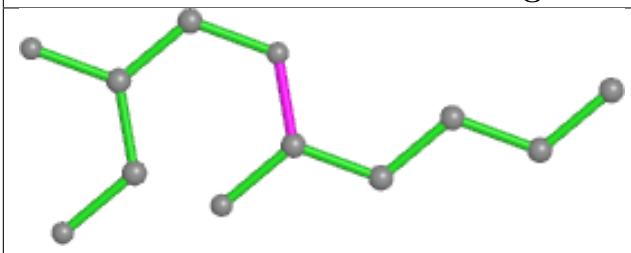
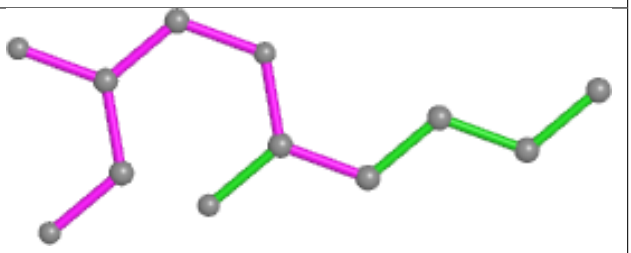
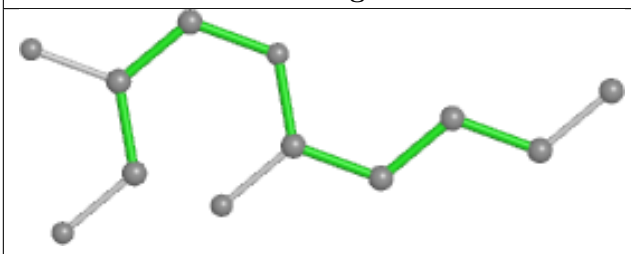
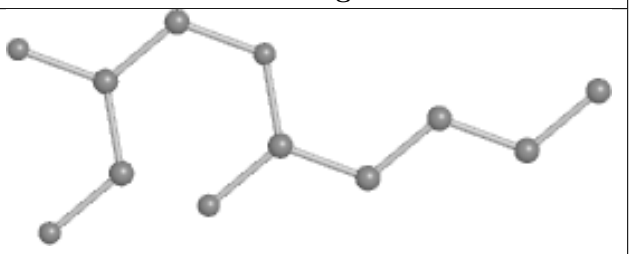
Ligand OLC A 625

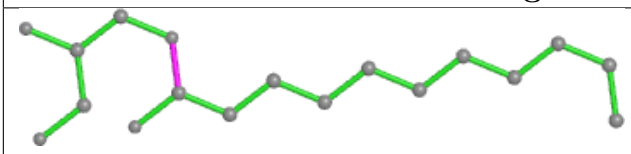
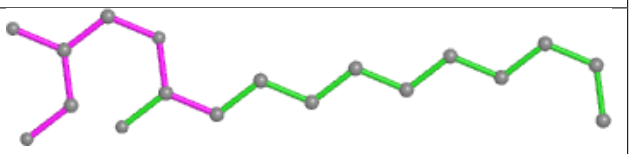
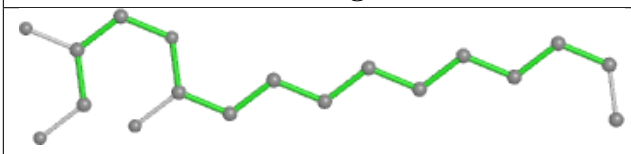
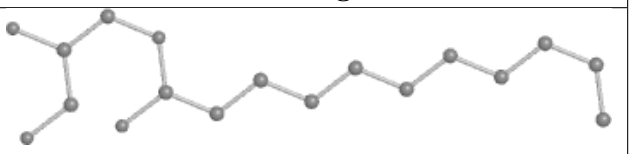
Ligand OLC A 618



Ligand OLC A 621



Ligand OLC A 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLC A 624	
 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	309/309 (100%)	0.24	21 (6%)	25	22	37, 49, 80, 150	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	LEU	4.8
1	A	47	PHE	3.9
1	A	-3	LEU	3.9
1	A	150	THR	3.8
1	A	-5	HIS	3.7
1	A	52	PRO	3.6
1	A	113	PHE	3.2
1	A	46	PHE	3.0
1	A	42	CYS	2.9
1	A	48	PRO	2.8
1	A	39	TRP	2.5
1	A	43	HIS	2.4
1	A	40	PRO	2.3
1	A	55	ILE	2.3
1	A	49	GLU	2.2
1	A	303	SER	2.2
1	A	235	ILE	2.1
1	A	53	ALA	2.1
1	A	112	VAL	2.1
1	A	44	GLY	2.1
1	A	302	GLU	2.0

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

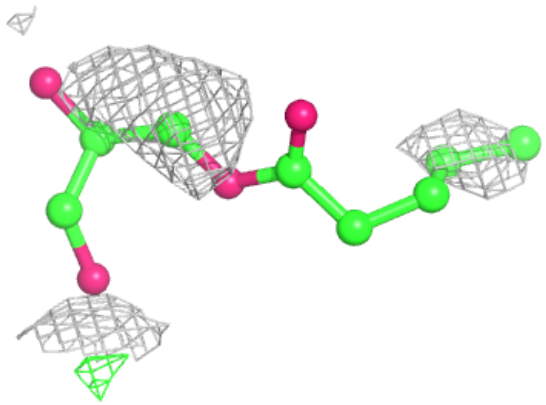
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

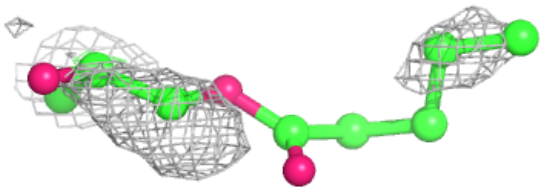
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	OLC	A	623	12/25	0.58	0.27	97,102,106,107	0
5	OLC	A	622	15/25	0.62	0.26	78,90,98,100	0
5	OLC	A	621	18/25	0.67	0.28	101,103,109,110	0
5	OLC	A	617	14/25	0.68	0.26	85,90,95,105	0
5	OLC	A	625	15/25	0.68	0.24	86,102,109,111	0
5	OLC	A	612	25/25	0.69	0.26	88,94,103,113	0
5	OLC	A	616	14/25	0.72	0.21	78,82,96,103	0
5	OLC	A	613	7/25	0.72	0.34	87,89,98,98	0
5	OLC	A	611	23/25	0.75	0.18	62,67,78,81	0
5	OLC	A	626	18/25	0.75	0.22	97,104,112,127	0
5	OLC	A	618	15/25	0.77	0.18	64,69,81,84	0
5	OLC	A	614	25/25	0.77	0.21	76,84,100,102	0
5	OLC	A	615	23/25	0.79	0.23	73,81,91,99	0
4	SO4	A	605	5/5	0.80	0.12	90,91,92,92	0
5	OLC	A	620	11/25	0.81	0.26	75,81,107,107	0
5	OLC	A	610	16/25	0.81	0.15	60,69,79,82	0
5	OLC	A	619	13/25	0.81	0.23	60,66,86,88	0
5	OLC	A	624	18/25	0.82	0.24	89,91,97,102	0
5	OLC	A	609	11/25	0.83	0.20	52,57,66,67	0
5	OLC	A	606	22/25	0.83	0.18	45,56,67,72	0
5	OLC	A	607	22/25	0.86	0.14	45,67,78,85	0
5	OLC	A	608	15/25	0.87	0.14	53,62,68,80	0
4	SO4	A	604	5/5	0.96	0.14	56,63,64,68	0
4	SO4	A	603	5/5	0.97	0.09	41,47,54,57	0
2	HEM	A	601	43/43	0.97	0.08	33,40,48,53	0
3	CU	A	602	1/1	1.00	0.01	50,50,50,50	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 623:

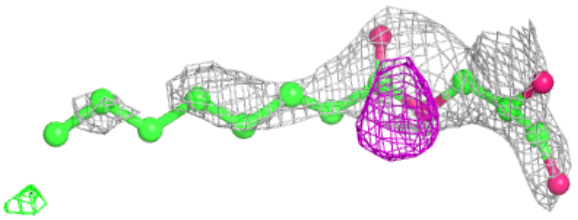
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

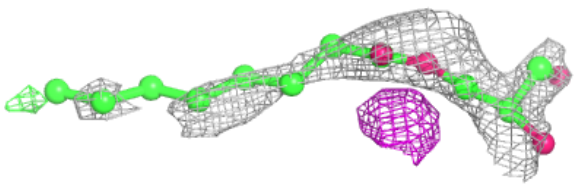


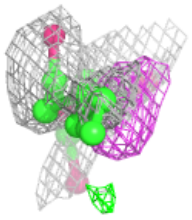


Electron density around OLC A 622:

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

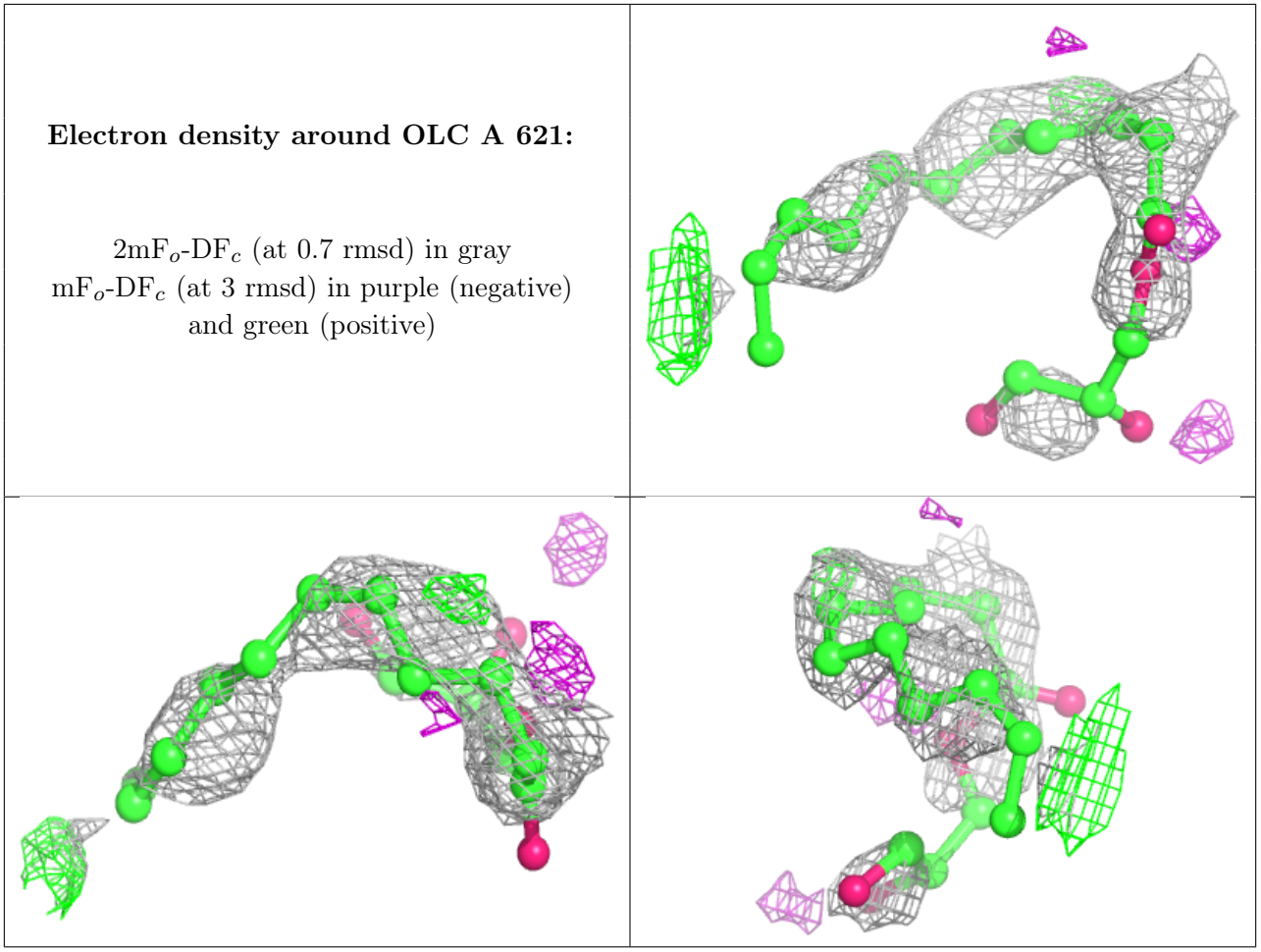






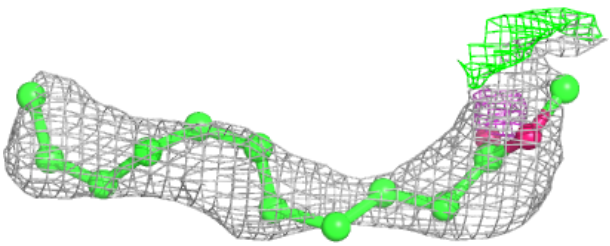
Electron density around OLC A 621:

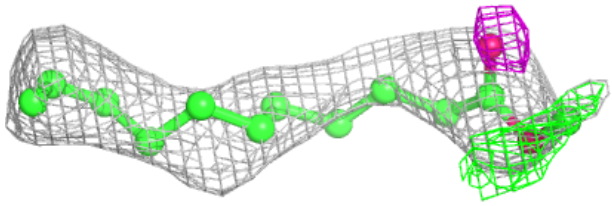
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

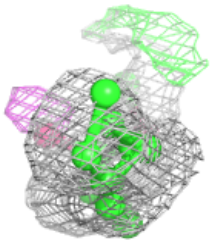


Electron density around OLC A 617:

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

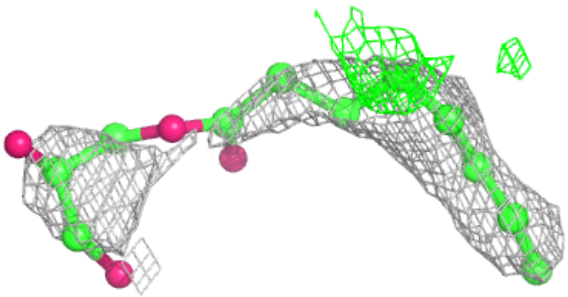


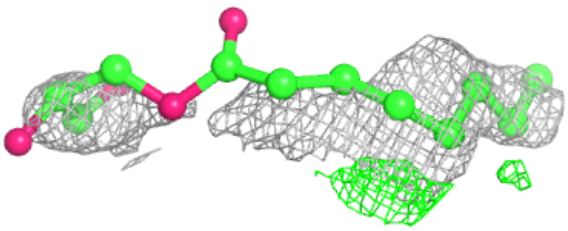


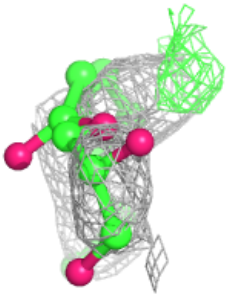


Electron density around OLC A 625:

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

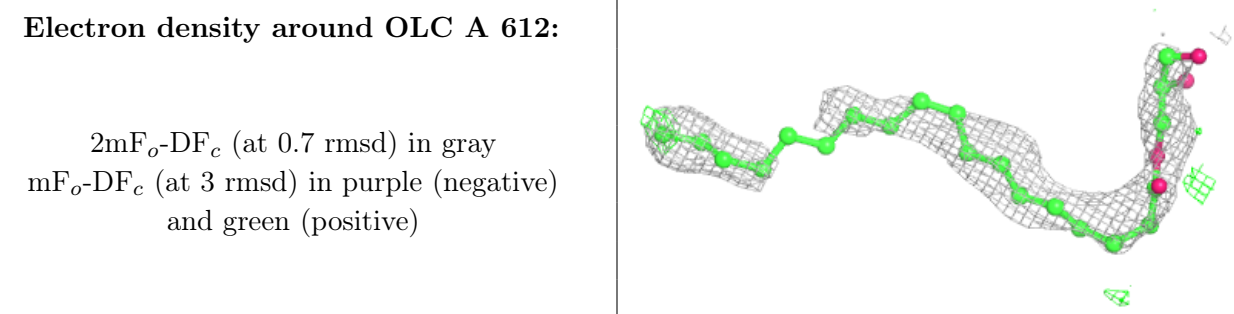


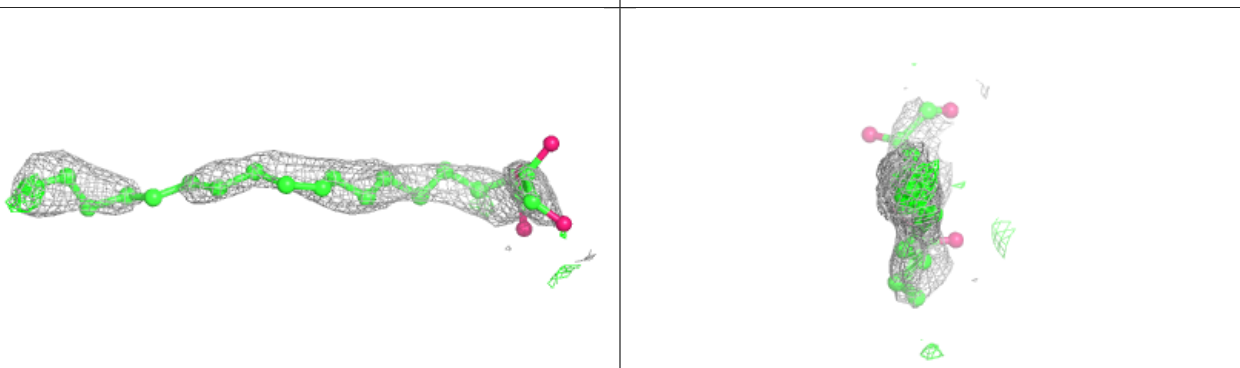




Electron density around OLC A 612:

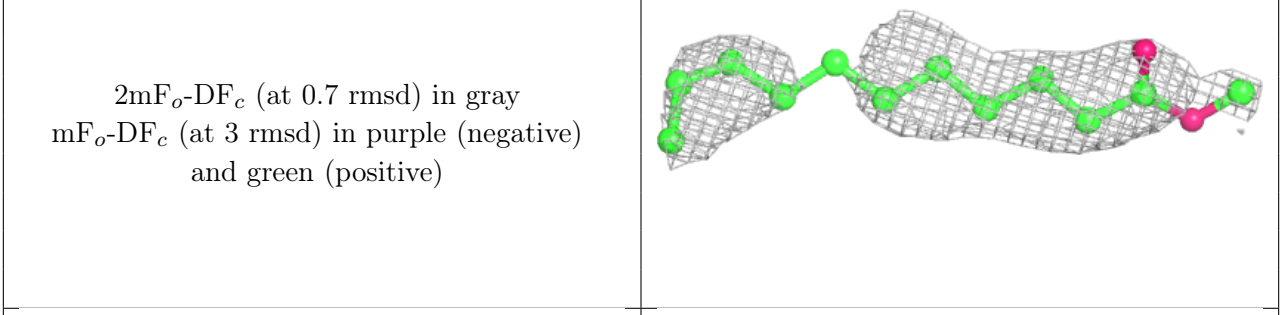
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

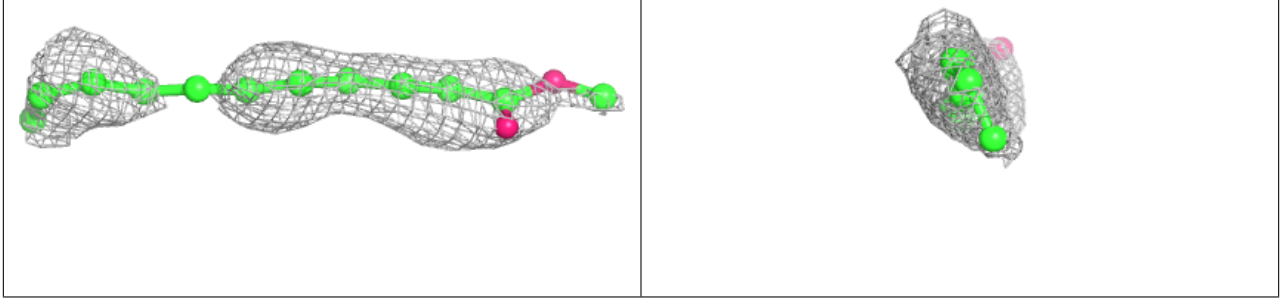




Electron density around OLC A 616:

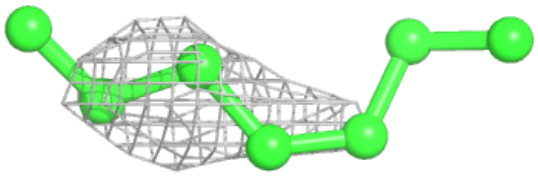
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

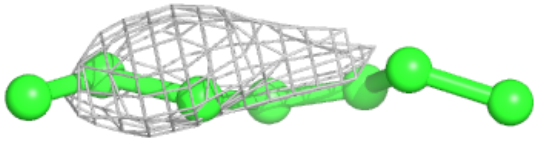


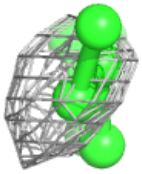


Electron density around OLC A 613:

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

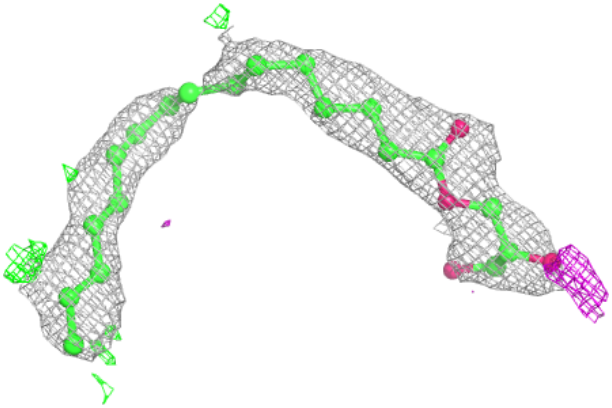


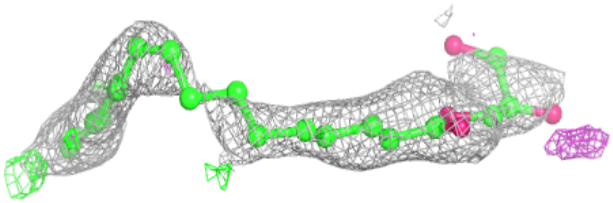


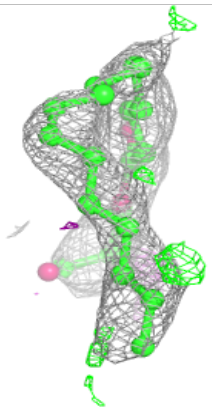


Electron density around OLC A 611:

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

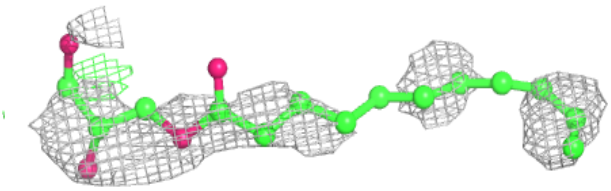


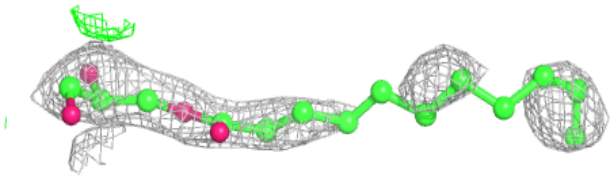


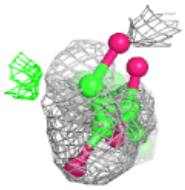


Electron density around OLC A 626:

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

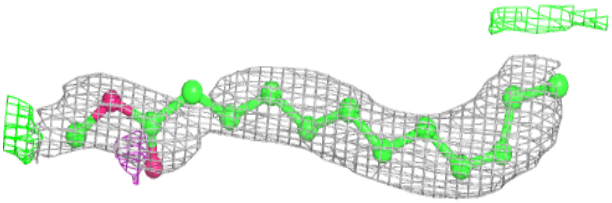


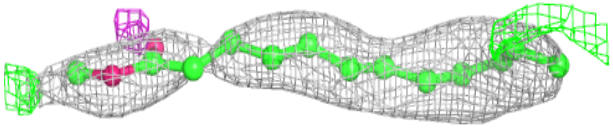


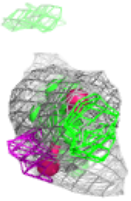


Electron density around OLC A 618:

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

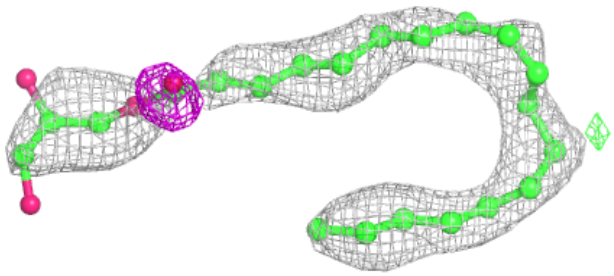


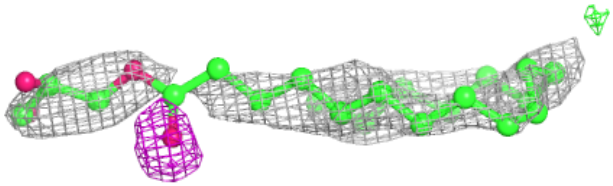


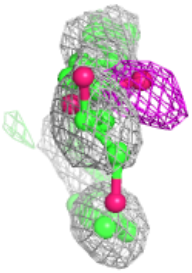


Electron density around OLC A 614:

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

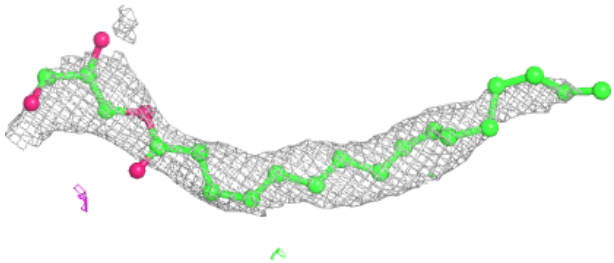


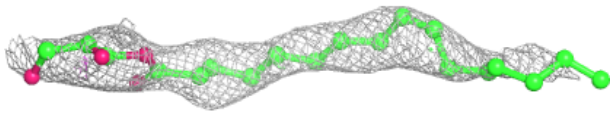


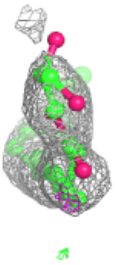


Electron density around OLC A 615:

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

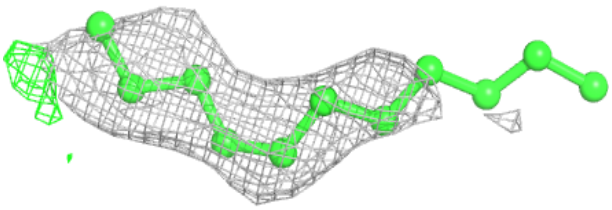


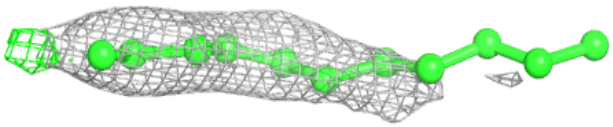


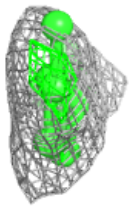


Electron density around OLC A 620:

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

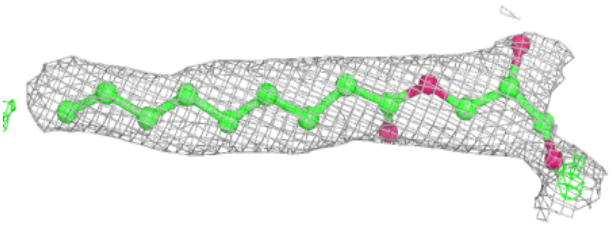


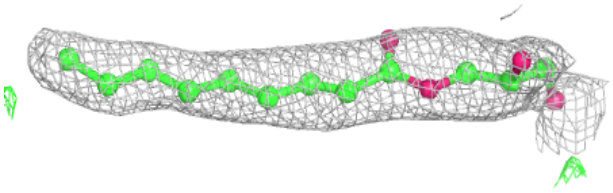


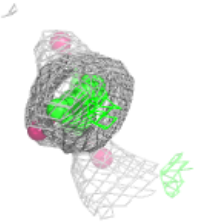


Electron density around OLC A 610:

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

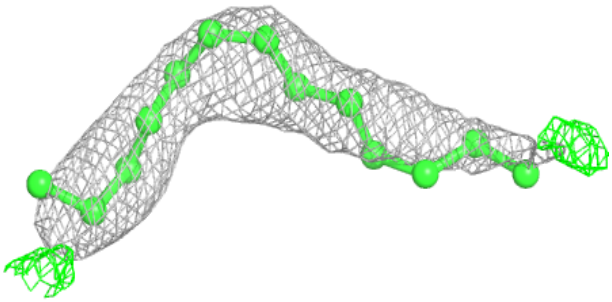


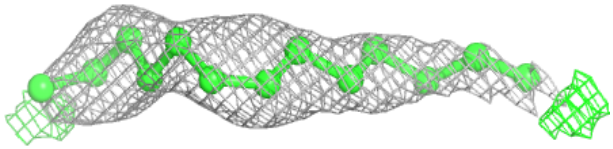


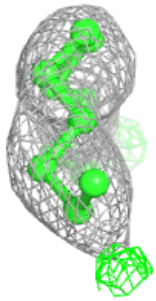


Electron density around OLC A 619:

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

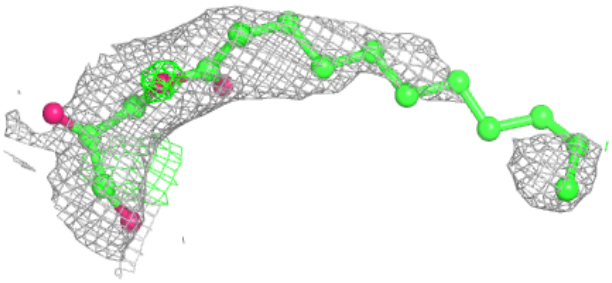


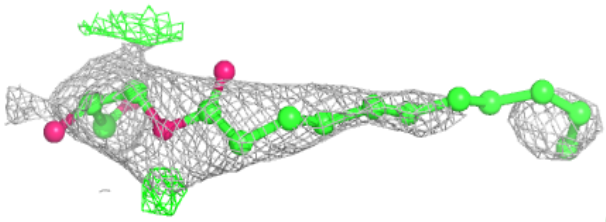


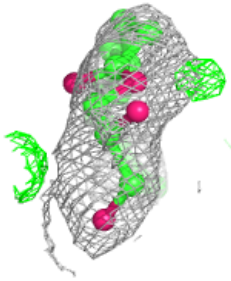


Electron density around OLC A 624:

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

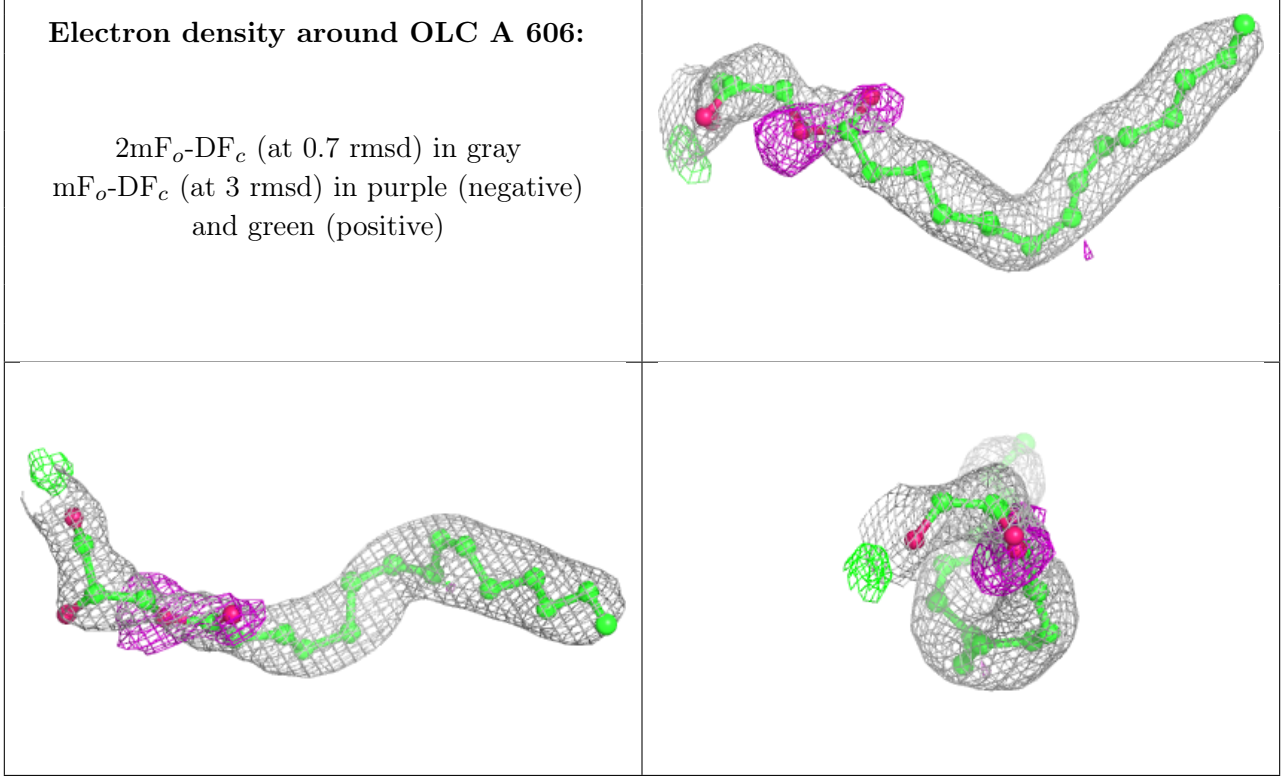






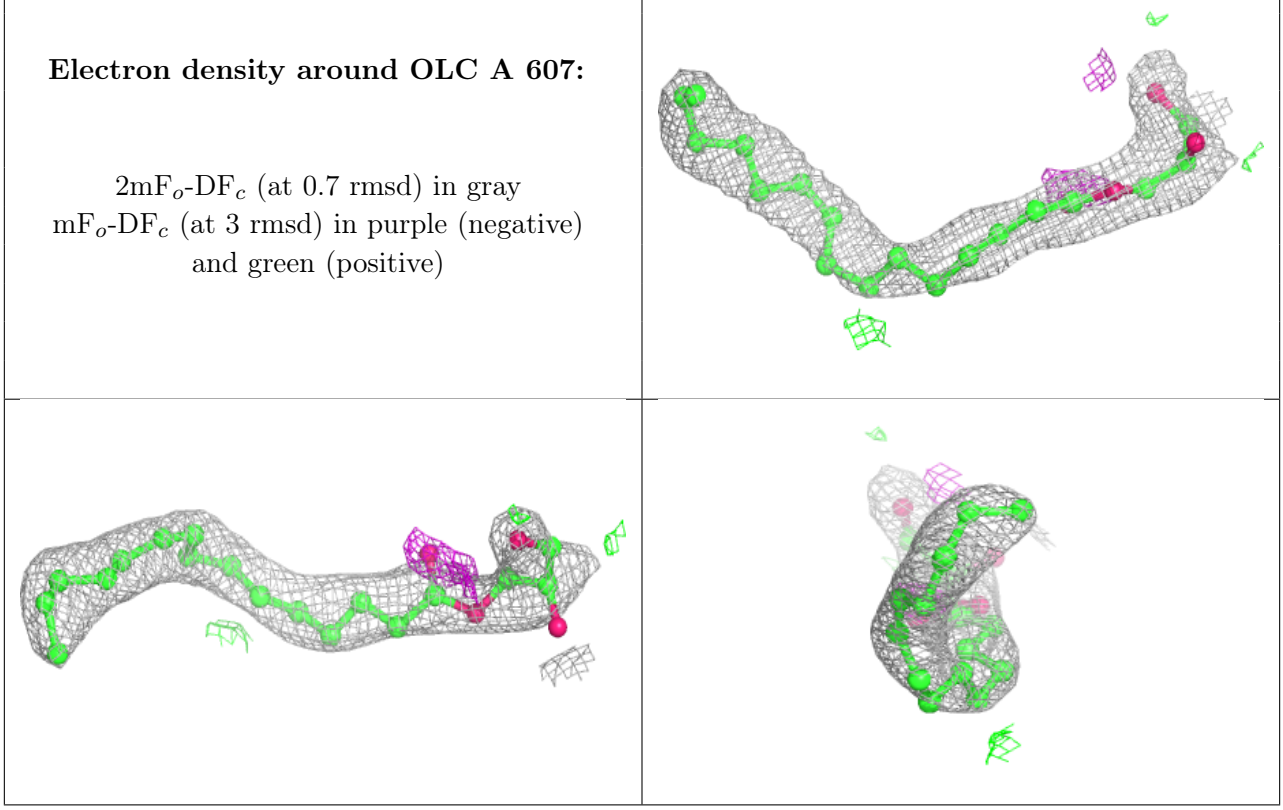
Electron density around OLC A 606:

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



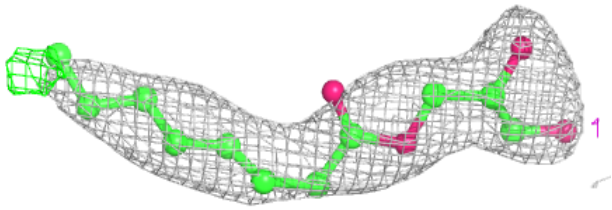
Electron density around OLC A 607:

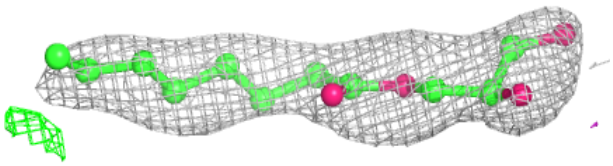
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

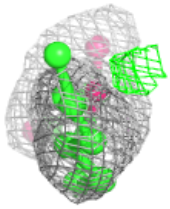


Electron density around OLC A 608:

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

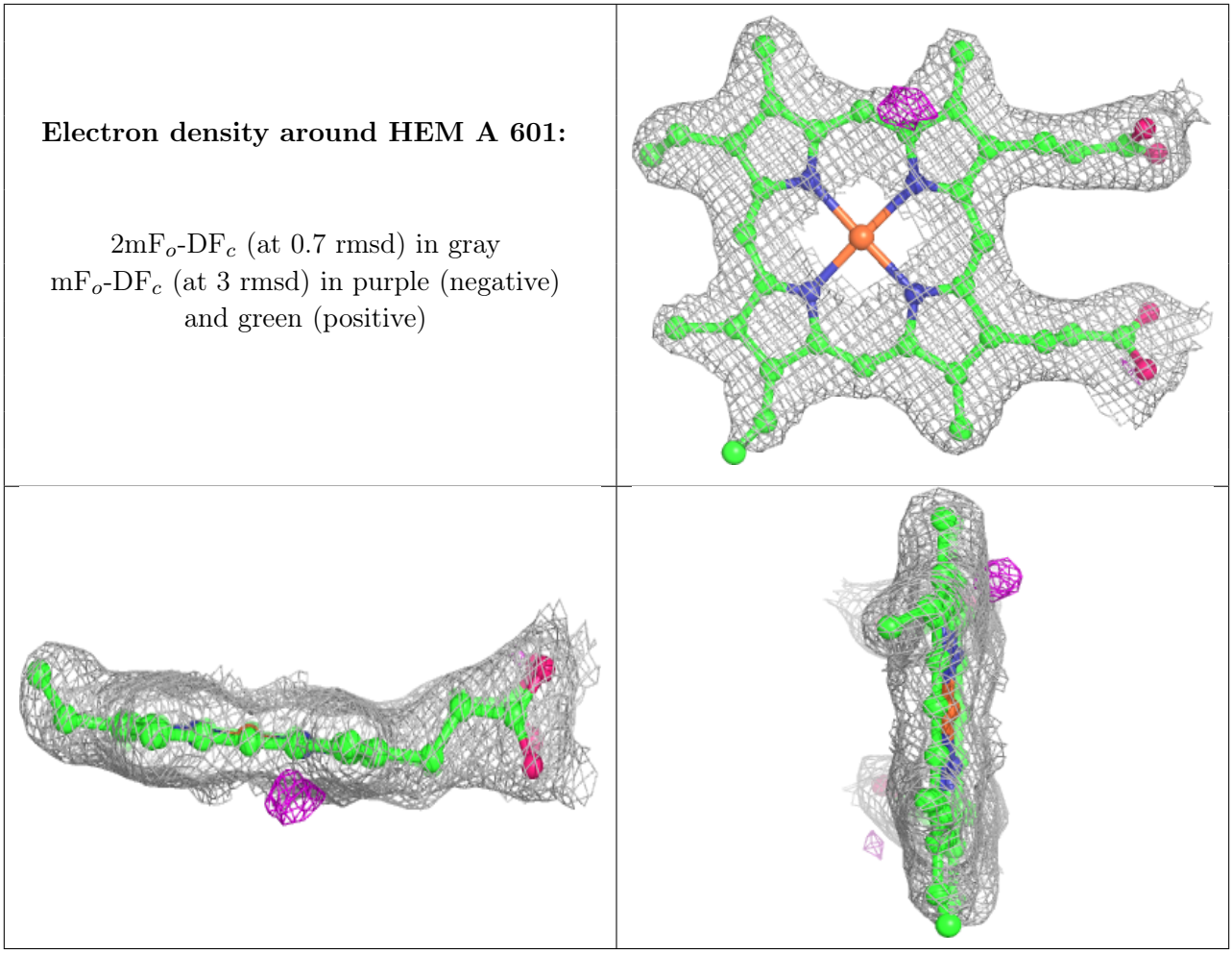






Electron density around HEM A 601:

$2mF_o$-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

There are no such residues in this entry.