Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2023 – 02:55 AM EDT

PDB ID	:	8SG5
Title	:	Cytochrome P450 (CYP) 3A5 crystallized with clotrimazole
Authors	:	Hsu, M.H.; Johnson, E.F.
Deposited on	:	2023-04-11
Resolution	:	2.80 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:

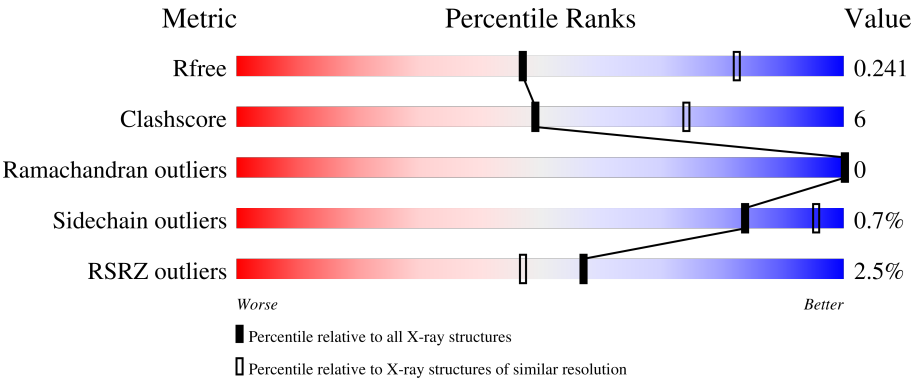
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	480	81% 13% 5%
1	B	480	84% 11% 5%
1	C	480	83% 11% 6%
1	D	480	85% 9% 6%
1	E	480	84% 10% 6%

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Mol	Chain	Length	Quality of chain
1	F	480	2% 85% 9% 6%
1	G	480	3% 80% 14% 6%
1	H	480	6% 78% 14% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30098 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 P450 3A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3635	2366	593	659	17			
1	B	456	Total	C	N	O	S	0	0	0
			3655	2381	598	659	17			
1	C	451	Total	C	N	O	S	0	0	0
			3618	2357	593	651	17			
1	D	453	Total	C	N	O	S	0	0	0
			3630	2363	595	655	17			
1	E	452	Total	C	N	O	S	0	0	0
			3626	2361	594	654	17			
1	F	452	Total	C	N	O	S	0	0	0
			3614	2354	592	651	17			
1	G	449	Total	C	N	O	S	0	0	0
			3601	2347	588	649	17			
1	H	446	Total	C	N	O	S	0	0	0
			3572	2326	585	644	17			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP P20815
A	23	ALA	-	expression tag	UNP P20815
A	498	HIS	-	expression tag	UNP P20815
A	499	HIS	-	expression tag	UNP P20815
A	500	HIS	-	expression tag	UNP P20815
A	501	HIS	-	expression tag	UNP P20815
B	22	MET	-	initiating methionine	UNP P20815
B	23	ALA	-	expression tag	UNP P20815
B	498	HIS	-	expression tag	UNP P20815
B	499	HIS	-	expression tag	UNP P20815
B	500	HIS	-	expression tag	UNP P20815
B	501	HIS	-	expression tag	UNP P20815
C	22	MET	-	initiating methionine	UNP P20815

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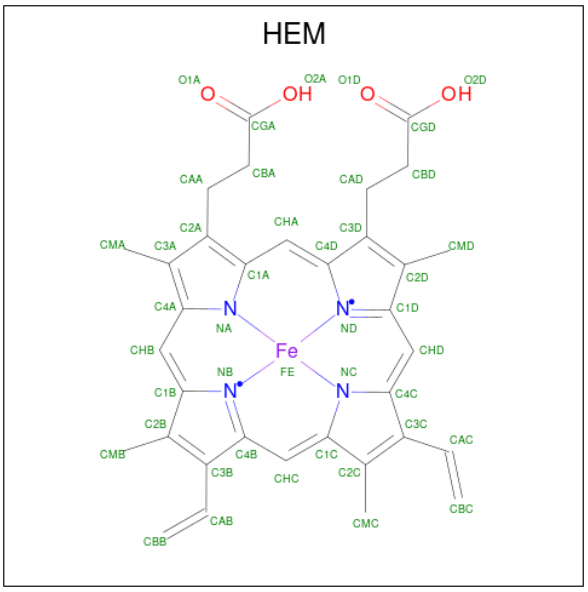
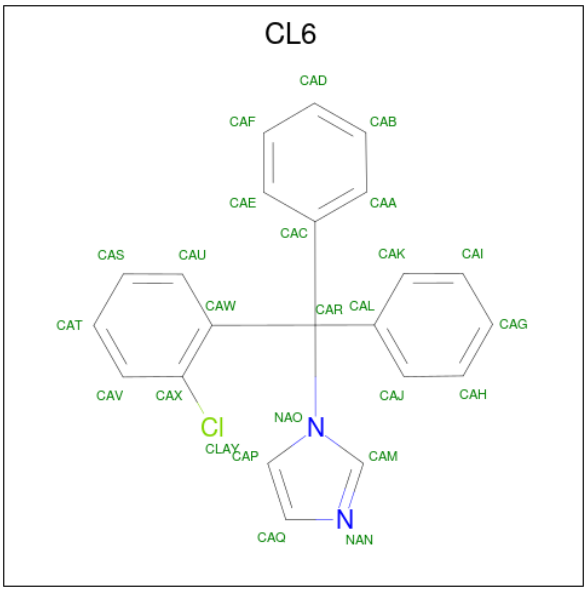
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	ALA	-	expression tag	UNP P20815
C	498	HIS	-	expression tag	UNP P20815
C	499	HIS	-	expression tag	UNP P20815
C	500	HIS	-	expression tag	UNP P20815
C	501	HIS	-	expression tag	UNP P20815
D	22	MET	-	initiating methionine	UNP P20815
D	23	ALA	-	expression tag	UNP P20815
D	498	HIS	-	expression tag	UNP P20815
D	499	HIS	-	expression tag	UNP P20815
D	500	HIS	-	expression tag	UNP P20815
D	501	HIS	-	expression tag	UNP P20815
E	22	MET	-	initiating methionine	UNP P20815
E	23	ALA	-	expression tag	UNP P20815
E	498	HIS	-	expression tag	UNP P20815
E	499	HIS	-	expression tag	UNP P20815
E	500	HIS	-	expression tag	UNP P20815
E	501	HIS	-	expression tag	UNP P20815
F	22	MET	-	initiating methionine	UNP P20815
F	23	ALA	-	expression tag	UNP P20815
F	498	HIS	-	expression tag	UNP P20815
F	499	HIS	-	expression tag	UNP P20815
F	500	HIS	-	expression tag	UNP P20815
F	501	HIS	-	expression tag	UNP P20815
G	22	MET	-	initiating methionine	UNP P20815
G	23	ALA	-	expression tag	UNP P20815
G	498	HIS	-	expression tag	UNP P20815
G	499	HIS	-	expression tag	UNP P20815
G	500	HIS	-	expression tag	UNP P20815
G	501	HIS	-	expression tag	UNP P20815
H	22	MET	-	initiating methionine	UNP P20815
H	23	ALA	-	expression tag	UNP P20815
H	498	HIS	-	expression tag	UNP P20815
H	499	HIS	-	expression tag	UNP P20815
H	500	HIS	-	expression tag	UNP P20815
H	501	HIS	-	expression tag	UNP P20815

- Molecule 2 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1-[(2-CHLOROPHENYL)(DIPHENYL)METHYL]-1H-IMIDAZOLE (three-letter code: CL6) (formula: $C_{22}H_{17}ClN_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	C	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	C	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	C	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	D	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	D	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	D	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	E	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	E	1	Total	C	Cl	N	0	0
			25	22	1	2		

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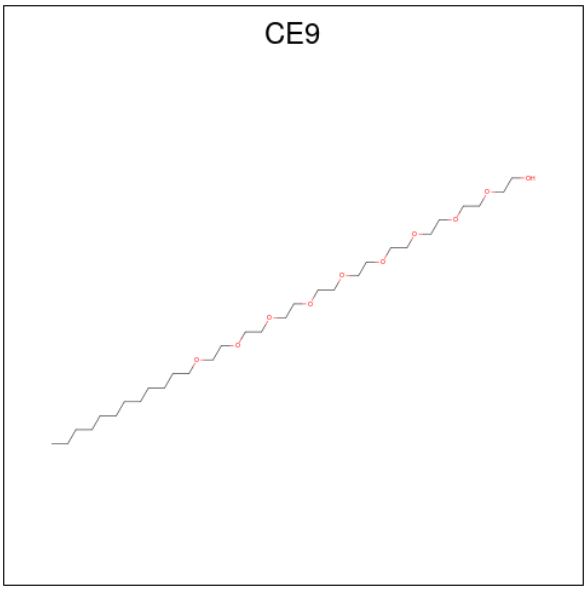
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	F	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	F	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	F	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	G	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	G	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	G	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	H	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	H	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	H	1	Total	C	Cl	N	0	0
			25	22	1	2		

- Molecule 4 is DODECYL NONA ETHYLENE GLYCOL ETHER (three-letter code: CE9) (formula: $C_{30}H_{62}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			40	30	10		

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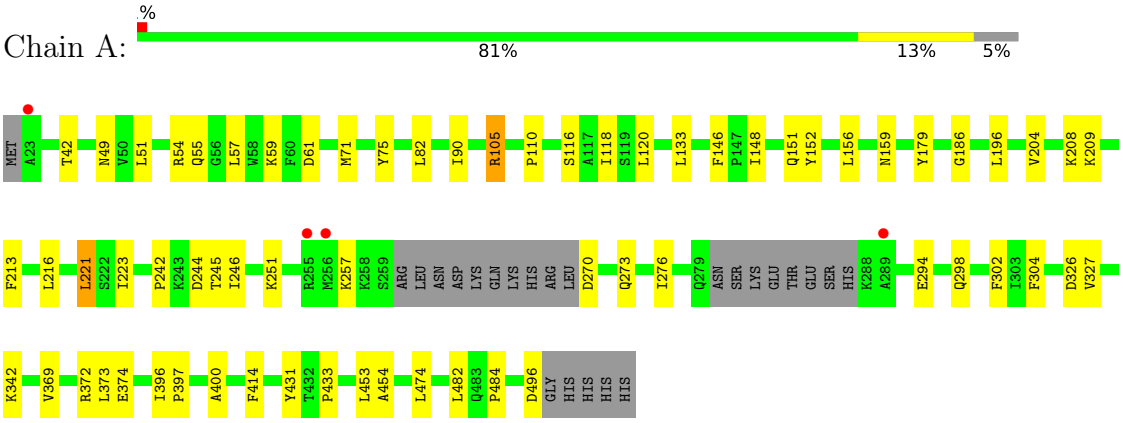
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 34 26 8	0	0
4	C	1	Total C O 24 17 7	0	0
4	D	1	Total C O 24 20 4	0	0
4	E	1	Total C O 22 17 5	0	0
4	F	1	Total C O 29 23 6	0	0
4	G	1	Total C O 30 22 8	0	0

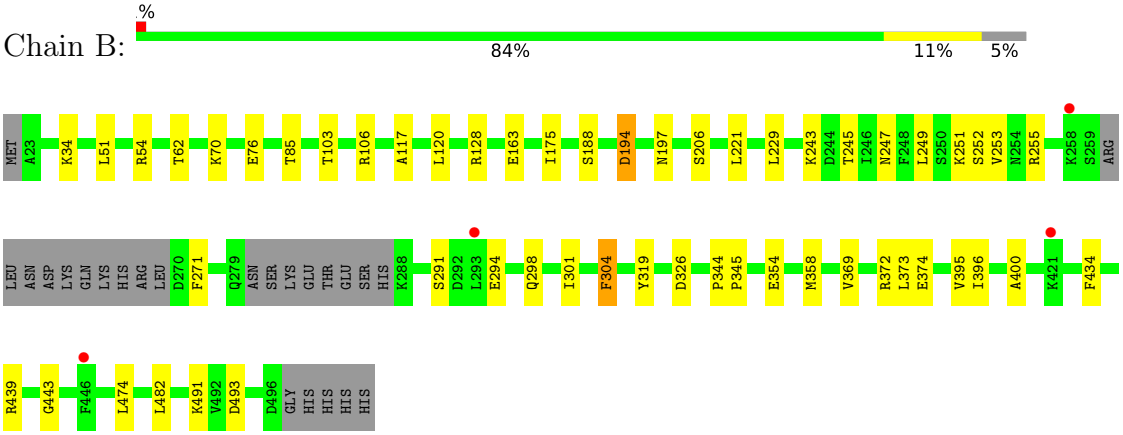
3 Residue-property plots (i)

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

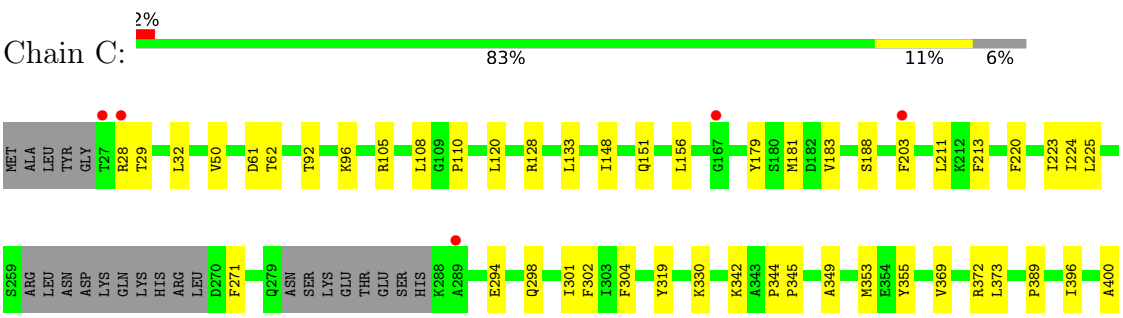
• Molecule 1: Cytochrome P450 3A5

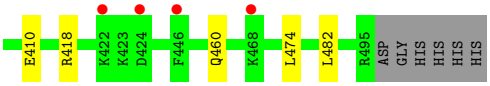


• Molecule 1: Cytochrome P450 3A5



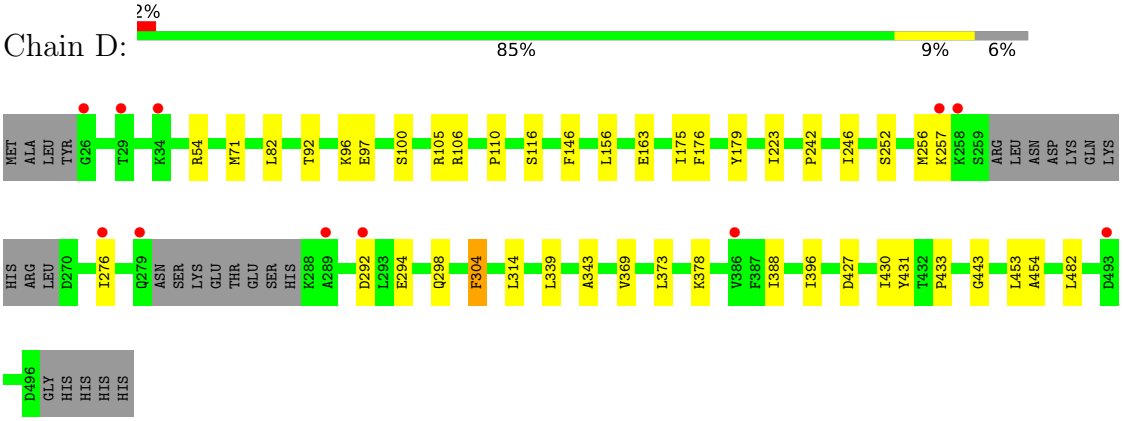
• Molecule 1: Cytochrome P450 3A5





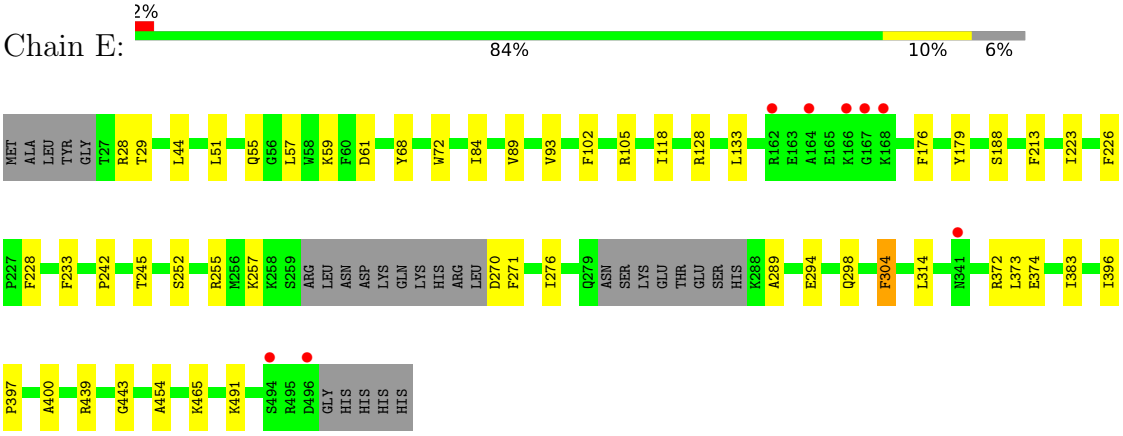
• Molecule 1: Cytochrome P450 3A5

Chain D:



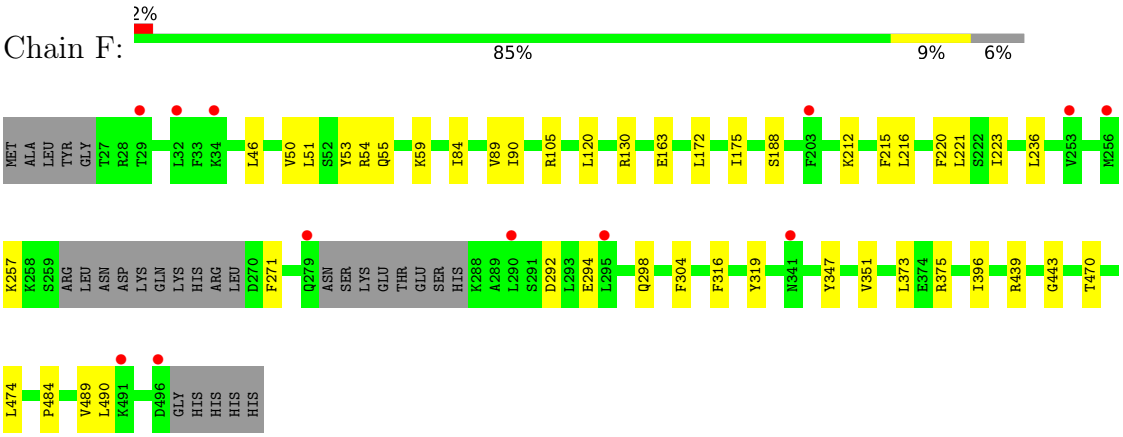
• Molecule 1: Cytochrome P450 3A5

Chain E:



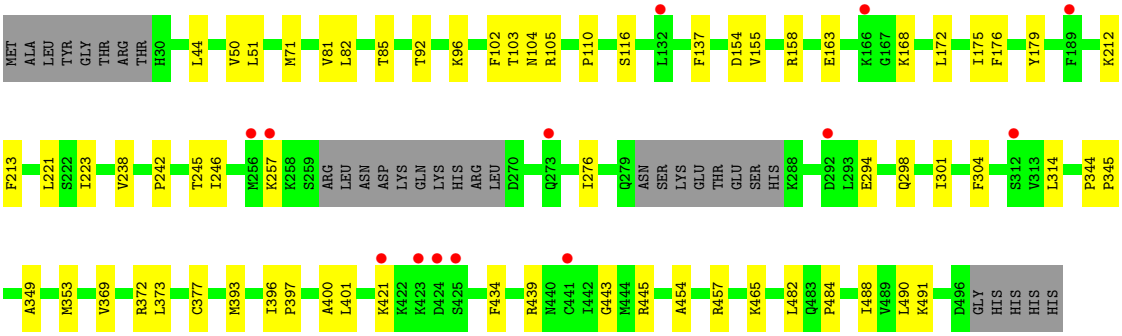
• Molecule 1: Cytochrome P450 3A5

Chain F:



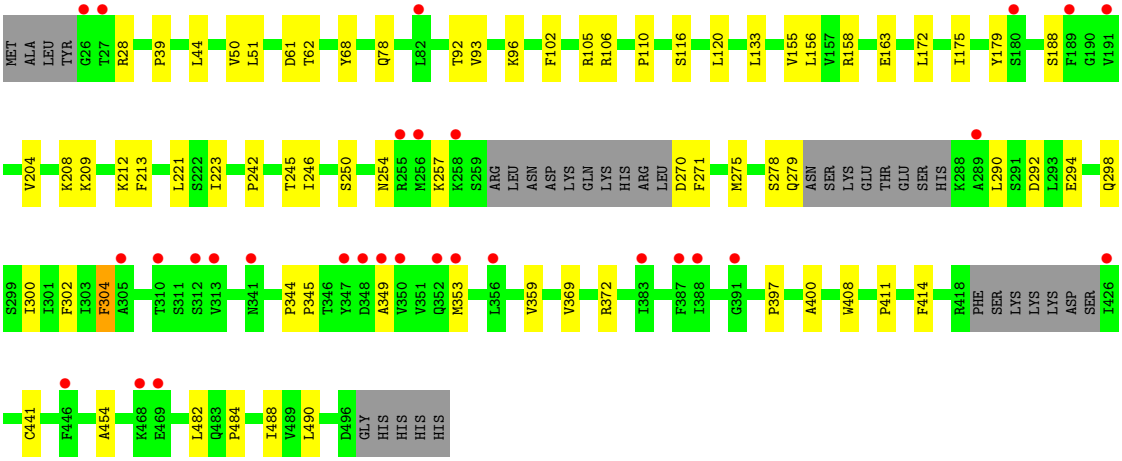
• Molecule 1: Cytochrome P450 3A5

Chain G:



• Molecule 1: Cytochrome P450 3A5

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.13Å 200.68Å 110.82Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	39.10 – 2.80 39.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.10-2.80) 99.2 (39.10-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.241 0.206 , 0.241	Depositor DCC
R_{free} test set	5604 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	30098	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.55% 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: CL6, CE9, 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	0.25	0/3723	0.45	0/5048
1	B	0.25	0/3743	0.45	0/5068
1	C	0.26	0/3705	0.46	0/5016
1	D	0.25	0/3717	0.45	0/5032
1	E	0.25	0/3713	0.45	0/5027
1	F	0.25	0/3701	0.45	0/5014
1	G	0.25	0/3688	0.45	0/4993
1	H	0.25	0/3657	0.45	0/4953
All	All	0.25	0/29647	0.45	0/40151

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	3635	0	3689	40	0
1	B	3655	0	3744	36	0
1	C	3618	0	3712	31	0
1	D	3630	0	3719	27	0
1	E	3626	0	3716	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3614	0	3689	30	0
1	G	3601	0	3689	39	0
1	H	3572	0	3656	44	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
2	E	43	0	30	2	0
2	F	43	0	30	4	0
2	G	43	0	30	3	0
2	H	43	0	30	3	0
3	A	75	0	51	13	0
3	B	75	0	51	12	0
3	C	75	0	51	11	0
3	D	75	0	51	10	0
3	E	75	0	51	15	0
3	F	75	0	51	13	0
3	G	75	0	51	10	0
3	H	75	0	51	16	0
4	A	40	0	62	3	0
4	B	34	0	53	3	0
4	C	24	0	30	0	0
4	D	24	0	39	2	0
4	E	22	0	30	0	0
4	F	29	0	45	4	0
4	G	30	0	42	1	0
All	All	30098	0	30563	358	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 6.

All (358) 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:F:105:ARG:HD3	3:F:602:CL6:HAG	1.62	0.82
1:A:54:ARG:HA	4:A:605:CE9:H202	1.67	0.77
1:B:163:GLU:HG3	1:B:175:ILE:HD11	1.72	0.71
1:F:236:LEU:HD13	1:G:238:VAL:HG21	1.75	0.68
1:E:105:ARG:HD2	3:E:602:CL6:HAG	1.77	0.66
1:E:105:ARG:CD	3:E:602:CL6:HAG	2.26	0.66
1:D:443:GLY:HA3	2:D:601:HEM:HBC2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:OE1	1:B:106:ARG:NH2	2.30	0.65
1:C:32:LEU:HD21	1:C:389:PRO:HG2	1.79	0.65
1:B:54:ARG:HA	4:B:605:CE9:H202	1.79	0.64
1:A:221:LEU:HD11	4:A:605:CE9:H151	1.77	0.64
1:H:120:LEU:HD21	3:H:603:CL6:HAM	1.80	0.64
1:G:443:GLY:HA3	2:G:601:HEM:HBC2	1.80	0.63
1:D:373:LEU:HB2	1:D:396:ILE:HB	1.79	0.63
1:F:443:GLY:HA3	2:F:601:HEM:HBC2	1.81	0.62
1:F:50:VAL:HG11	1:F:221:LEU:HD11	1.82	0.61
3:G:603:CL6:HAE	3:G:603:CL6:CAP	2.30	0.61
1:D:105:ARG:HH12	2:D:601:HEM:HAD2	1.64	0.61
1:F:54:ARG:HA	4:F:605:CE9:H202	1.83	0.61
1:H:397:PRO:HB2	1:H:400:ALA:HB3	1.82	0.61
1:H:156:LEU:HD13	1:H:179:TYR:HB2	1.82	0.60
3:D:603:CL6:HAE	3:D:603:CL6:CAP	2.32	0.59
1:C:50:VAL:HG21	1:C:225:LEU:HD21	1.84	0.59
1:H:304:PHE:CD2	3:H:602:CL6:HAT	2.37	0.59
1:F:188:SER:HA	1:F:271:PHE:HB2	1.85	0.59
3:B:603:CL6:HAE	3:B:603:CL6:CAP	2.33	0.58
3:E:603:CL6:CAP	3:E:603:CL6:HAE	2.33	0.58
1:D:92:THR:HA	1:D:96:LYS:HB3	1.84	0.58
1:H:369:VAL:HA	1:H:482:LEU:HB2	1.85	0.58
3:A:603:CL6:HAE	3:A:603:CL6:CAP	2.34	0.58
1:F:470:THR:OG1	1:F:489:VAL:O	2.18	0.58
1:G:116:SER:O	1:G:298:GLN:NE2	2.35	0.58
1:E:373:LEU:HB2	1:E:396:ILE:HB	1.86	0.58
3:F:603:CL6:HAE	3:F:603:CL6:CAP	2.34	0.58
1:E:128:ARG:NH1	1:E:289:ALA:O	2.37	0.58
1:C:188:SER:HA	1:C:271:PHE:HB2	1.86	0.58
1:C:120:LEU:HD21	3:C:603:CL6:HAM	1.86	0.57
1:A:342:LYS:NZ	1:A:496:ASP:OD2	2.33	0.57
1:H:188:SER:HA	1:H:271:PHE:HB2	1.85	0.57
1:C:92:THR:HG23	1:C:96:LYS:HD3	1.87	0.57
1:H:279:GLN:NE2	1:H:290:LEU:O	2.29	0.56
3:C:603:CL6:HAE	3:C:603:CL6:CAP	2.34	0.56
1:C:28:ARG:HG3	1:C:29:THR:HG23	1.88	0.56
3:G:604:CL6:HAU	3:G:604:CL6:CAJ	2.34	0.56
1:A:110:PRO:HD2	1:A:223:ILE:HD13	1.88	0.56
1:G:369:VAL:HA	1:G:482:LEU:HB2	1.87	0.56
3:A:604:CL6:CAJ	3:A:604:CL6:HAU	2.36	0.56
1:D:257:LYS:HG2	1:D:276:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:163:GLU:HG3	1:H:175:ILE:HD11	1.88	0.55
1:A:242:PRO:HB2	1:A:245:THR:HB	1.87	0.55
1:C:344:PRO:HG2	1:G:154:ASP:HB3	1.88	0.55
1:D:339:LEU:HB3	1:D:343:ALA:HB3	1.88	0.55
3:H:603:CL6:HAE	3:H:603:CL6:CAP	2.35	0.55
1:F:212:LYS:HA	1:F:215:PHE:CD1	2.42	0.54
1:G:373:LEU:HB2	1:G:396:ILE:HB	1.89	0.54
1:F:55:GLN:HB2	1:F:59:LYS:HD3	1.88	0.54
1:C:62:THR:HG22	1:C:400:ALA:HA	1.89	0.54
1:E:443:GLY:HA3	2:E:601:HEM:HBC2	1.87	0.54
1:B:188:SER:HA	1:B:271:PHE:HB2	1.90	0.54
1:B:221:LEU:HD11	4:B:605:CE9:H151	1.88	0.54
1:H:257:LYS:NZ	1:H:292:ASP:OD1	2.41	0.54
1:C:133:LEU:HD13	1:C:302:PHE:HZ	1.73	0.54
1:H:105:ARG:NH1	2:H:601:HEM:O2D	2.34	0.53
1:H:110:PRO:HD2	1:H:223:ILE:HD13	1.90	0.53
1:A:55:GLN:HB2	1:A:59:LYS:HD3	1.89	0.53
3:A:603:CL6:HAJ	3:A:603:CL6:CAA	2.38	0.53
1:B:369:VAL:HA	1:B:482:LEU:HB2	1.91	0.53
1:C:369:VAL:HA	1:C:482:LEU:HB2	1.90	0.53
1:D:294:GLU:O	1:D:298:GLN:HG2	2.09	0.53
1:E:223:ILE:HD11	1:E:233:PHE:HD2	1.74	0.53
1:H:275:MET:O	1:H:278:SER:OG	2.25	0.53
3:F:604:CL6:CAJ	3:F:604:CL6:HAU	2.39	0.52
1:H:92:THR:HG23	1:H:96:LYS:HD3	1.91	0.52
1:A:369:VAL:HA	1:A:482:LEU:HB2	1.92	0.52
1:E:188:SER:HA	1:E:271:PHE:HB2	1.92	0.52
1:F:105:ARG:NH2	1:F:439:ARG:HG2	2.24	0.52
1:B:128:ARG:NH2	1:B:294:GLU:OE2	2.42	0.52
3:H:603:CL6:HAJ	3:H:603:CL6:CAA	2.39	0.52
1:A:133:LEU:HD13	1:A:302:PHE:HZ	1.74	0.52
1:G:110:PRO:HD2	1:G:223:ILE:HD13	1.90	0.52
1:D:179:TYR:CZ	1:D:454:ALA:HB2	2.44	0.52
1:A:209:LYS:NZ	1:A:244:ASP:OD2	2.38	0.52
1:D:82:LEU:HD22	1:D:388:ILE:HD11	1.92	0.52
1:D:369:VAL:HA	1:D:482:LEU:HB2	1.90	0.52
3:E:602:CL6:CAJ	3:E:602:CL6:HAM	2.40	0.52
3:C:604:CL6:CAJ	3:C:604:CL6:HAU	2.40	0.52
1:F:120:LEU:HD21	3:F:603:CL6:HAM	1.92	0.51
1:G:44:LEU:HD12	1:G:51:LEU:HD12	1.92	0.51
1:H:133:LEU:HD13	1:H:302:PHE:HZ	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:LEU:HB2	1:C:396:ILE:HB	1.91	0.51
1:G:242:PRO:HB2	1:G:245:THR:HB	1.91	0.51
1:H:250:SER:O	1:H:254:ASN:ND2	2.40	0.51
1:B:491:LYS:NZ	1:B:493:ASP:OD1	2.44	0.51
1:E:105:ARG:HG3	1:E:374:GLU:O	2.11	0.51
1:H:304:PHE:CG	3:H:602:CL6:HAT	2.46	0.51
1:G:103:THR:O	1:G:439:ARG:NH1	2.39	0.51
1:H:408:TRP:HB2	1:H:411:PRO:HB3	1.91	0.51
3:C:603:CL6:HAJ	3:C:603:CL6:CAA	2.39	0.50
1:G:257:LYS:HG2	1:G:276:ILE:HD11	1.91	0.50
1:H:61:ASP:OD1	1:H:372:ARG:NH2	2.45	0.50
1:B:206:SER:HB3	1:B:245:THR:HG23	1.92	0.50
1:F:294:GLU:O	1:F:298:GLN:HG2	2.11	0.50
2:H:601:HEM:C1A	3:H:602:CL6:HAM	2.47	0.50
1:F:257:LYS:NZ	1:F:292:ASP:OD1	2.45	0.49
1:B:117:ALA:HB3	1:B:120:LEU:HD13	1.94	0.49
1:E:61:ASP:OD1	1:E:372:ARG:NH2	2.46	0.49
3:E:604:CL6:CAJ	3:E:604:CL6:HAU	2.43	0.49
1:E:128:ARG:NH2	1:E:294:GLU:OE2	2.44	0.49
1:F:84:ILE:HD12	1:F:89:VAL:HG12	1.94	0.49
3:B:602:CL6:CAJ	3:B:602:CL6:HAM	2.42	0.49
3:B:604:CL6:HAU	3:B:604:CL6:CAJ	2.41	0.49
1:C:211:LEU:C	1:C:213:PHE:H	2.14	0.49
3:G:602:CL6:CAJ	3:G:602:CL6:HAM	2.42	0.49
1:H:62:THR:HG22	1:H:400:ALA:HA	1.95	0.49
1:F:373:LEU:HB2	1:F:396:ILE:HB	1.94	0.49
1:B:62:THR:HG22	1:B:400:ALA:HA	1.94	0.49
1:C:110:PRO:HD2	1:C:223:ILE:HD13	1.95	0.49
1:E:397:PRO:HB2	1:E:400:ALA:HB3	1.95	0.49
1:F:163:GLU:HG3	1:F:175:ILE:HD11	1.94	0.49
3:A:602:CL6:CAJ	3:A:602:CL6:HAM	2.43	0.49
1:H:92:THR:HA	1:H:96:LYS:HB3	1.94	0.49
1:D:116:SER:HB3	1:D:294:GLU:HG2	1.94	0.48
1:E:44:LEU:HD12	1:E:51:LEU:HD12	1.94	0.48
1:C:211:LEU:O	1:C:213:PHE:N	2.44	0.48
3:D:604:CL6:HAU	3:D:604:CL6:CAJ	2.42	0.48
1:E:252:SER:HA	1:E:255:ARG:HG2	1.95	0.48
1:B:70:LYS:HA	1:B:85:THR:OG1	2.13	0.48
1:D:163:GLU:HG3	1:D:175:ILE:HD11	1.94	0.48
1:A:474:LEU:HD11	1:A:484:PRO:HB3	1.96	0.48
1:D:156:LEU:HD13	1:D:179:TYR:HB2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:603:CL6:CAA	3:F:603:CL6:HAJ	2.44	0.48
1:B:194:ASP:HB3	1:B:197:ASN:HB2	1.95	0.48
1:H:359:VAL:HG13	1:H:414:PHE:HZ	1.79	0.48
1:D:252:SER:O	1:D:256:MET:HG2	2.14	0.48
1:E:304:PHE:CG	3:E:602:CL6:HAT	2.49	0.47
1:E:213:PHE:CZ	3:E:604:CL6:HAG	2.49	0.47
1:G:298:GLN:HA	1:G:301:ILE:HG22	1.96	0.47
1:H:294:GLU:O	1:H:298:GLN:HG2	2.13	0.47
1:A:373:LEU:HB2	1:A:396:ILE:HB	1.97	0.47
2:A:601:HEM:C1A	3:A:602:CL6:HAM	2.49	0.47
1:H:116:SER:HB3	1:H:294:GLU:HG2	1.97	0.47
1:E:294:GLU:O	1:E:298:GLN:HG2	2.15	0.47
1:E:304:PHE:CD2	3:E:602:CL6:HAT	2.49	0.47
3:F:603:CL6:CAC	3:F:603:CL6:CLAY	2.99	0.47
1:F:130:ARG:NH1	2:F:601:HEM:O1D	2.48	0.47
1:H:39:PRO:HB2	1:H:68:TYR:CD1	2.49	0.47
3:H:602:CL6:HAM	3:H:602:CL6:CAJ	2.44	0.47
1:B:304:PHE:CG	3:B:602:CL6:HAT	2.50	0.47
1:D:146:PHE:CZ	1:D:453:LEU:HD21	2.50	0.47
1:A:146:PHE:CZ	1:A:453:LEU:HD21	2.50	0.46
1:B:319:TYR:CZ	1:B:474:LEU:HB2	2.50	0.46
1:E:118:ILE:HD12	1:E:133:LEU:HD12	1.97	0.46
1:F:216:LEU:HB2	4:F:605:CE9:H242	1.96	0.46
3:H:604:CL6:CAJ	3:H:604:CL6:HAU	2.44	0.46
1:E:84:ILE:HD12	1:E:89:VAL:HG12	1.97	0.46
1:H:50:VAL:HG11	1:H:221:LEU:HD11	1.97	0.46
3:C:602:CL6:CAX	3:C:602:CL6:HAK	2.46	0.46
4:D:605:CE9:H151	4:D:605:CE9:H121	1.58	0.46
1:F:347:TYR:O	1:F:351:VAL:HG23	2.16	0.46
1:F:375:ARG:HH22	2:F:601:HEM:CGA	2.26	0.46
1:G:163:GLU:HG3	1:G:175:ILE:HD11	1.98	0.46
1:A:120:LEU:HD21	3:A:603:CL6:HAM	1.97	0.46
1:E:179:TYR:CE2	1:E:454:ALA:HB2	2.51	0.46
2:G:601:HEM:C1A	3:G:602:CL6:HAM	2.51	0.46
1:B:106:ARG:NH1	3:B:604:CL6:HAS	2.31	0.46
3:D:602:CL6:CAJ	3:D:602:CL6:HAM	2.46	0.46
1:G:242:PRO:O	1:G:246:ILE:HG12	2.16	0.46
1:A:179:TYR:CZ	1:A:454:ALA:HB2	2.52	0.45
3:G:602:CL6:CAP	3:G:602:CL6:HAA	2.45	0.45
1:H:39:PRO:HB2	1:H:68:TYR:HD1	1.82	0.45
3:B:603:CL6:HAJ	3:B:603:CL6:CAA	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:PHE:O	1:C:224:ILE:HG12	2.17	0.45
1:D:54:ARG:HA	4:D:605:CE9:H212	1.97	0.45
1:A:327:VAL:HG11	1:A:414:PHE:HE2	1.82	0.45
3:D:603:CL6:CAC	3:D:603:CL6:CLAY	3.02	0.45
3:E:602:CL6:CAX	3:E:602:CL6:HAK	2.47	0.45
3:E:603:CL6:HAJ	3:E:603:CL6:CAA	2.45	0.45
1:F:220:PHE:O	1:F:223:ILE:HG12	2.16	0.45
1:G:213:PHE:CZ	3:G:604:CL6:HAG	2.52	0.45
3:C:602:CL6:HAA	3:C:602:CL6:CAP	2.47	0.45
1:D:71:MET:HG2	1:D:82:LEU:HD11	1.97	0.45
1:D:92:THR:HG23	1:D:97:GLU:HG3	1.96	0.45
1:E:28:ARG:HG3	1:E:29:THR:HG23	1.99	0.45
3:D:603:CL6:HAJ	3:D:603:CL6:CAA	2.45	0.45
1:H:209:LYS:O	1:H:212:LYS:HG2	2.16	0.45
1:A:71:MET:HG2	1:A:82:LEU:HD11	1.98	0.45
1:D:110:PRO:HD2	1:D:223:ILE:HD13	1.99	0.45
1:G:179:TYR:CZ	1:G:454:ALA:HB2	2.51	0.45
3:G:603:CL6:CAA	3:G:603:CL6:HAJ	2.47	0.45
4:A:605:CE9:H231	4:A:605:CE9:H261	1.79	0.45
1:C:344:PRO:HA	1:C:345:PRO:HD3	1.87	0.45
1:H:44:LEU:HD22	1:H:51:LEU:HD12	1.99	0.45
1:A:51:LEU:HD22	1:A:54:ARG:CZ	2.47	0.45
3:B:602:CL6:CAP	3:B:602:CL6:HAA	2.47	0.45
1:C:61:ASP:OD1	1:C:372:ARG:NH2	2.50	0.45
3:C:602:CL6:CAJ	3:C:602:CL6:HAM	2.47	0.45
1:A:116:SER:O	1:A:298:GLN:NE2	2.45	0.44
1:D:431:TYR:CZ	1:D:433:PRO:HG3	2.52	0.44
1:C:105:ARG:HH21	2:C:601:HEM:HAD2	1.82	0.44
1:D:106:ARG:NH2	3:D:604:CL6:HAT	2.32	0.44
1:H:106:ARG:HB2	3:H:603:CL6:HAS	1.99	0.44
1:H:484:PRO:HG2	1:H:488:ILE:HG13	1.98	0.44
2:B:601:HEM:C1A	3:B:602:CL6:HAM	2.52	0.44
1:F:172:LEU:HD11	1:F:490:LEU:HD12	1.98	0.44
3:G:604:CL6:CAX	3:G:604:CL6:HAA	2.47	0.44
1:A:148:ILE:O	1:A:151:GLN:HG2	2.18	0.44
1:A:270:ASP:HB3	1:A:273:GLN:H	1.82	0.44
3:C:603:CL6:CLAY	3:C:603:CL6:CAC	3.03	0.44
1:E:257:LYS:HG2	1:E:276:ILE:HD11	1.99	0.44
1:G:81:VAL:HG22	1:G:393:MET:HB3	1.99	0.44
2:C:601:HEM:C1A	3:C:602:CL6:HAM	2.53	0.44
1:G:85:THR:HB	1:G:401:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:603:CL6:CLAY	3:G:603:CL6:CAC	3.03	0.44
1:A:159:ASN:HB3	1:A:196:LEU:HD23	1.99	0.44
1:C:319:TYR:CZ	1:C:474:LEU:HB2	2.53	0.44
1:E:176:PHE:HD2	1:E:314:LEU:HD13	1.83	0.44
1:G:102:PHE:HE1	1:G:377:CYS:HG	1.66	0.44
1:A:397:PRO:HB2	1:A:400:ALA:HB3	2.00	0.44
3:B:603:CL6:CLAY	3:B:603:CL6:CAC	3.03	0.44
1:C:105:ARG:NH1	2:C:601:HEM:O2A	2.50	0.44
1:C:410:GLU:O	1:C:418:ARG:NH2	2.49	0.44
1:H:179:TYR:CZ	1:H:454:ALA:HB2	2.53	0.44
1:B:243:LYS:HE2	1:B:243:LYS:HB3	1.78	0.44
1:F:50:VAL:HG12	4:F:605:CE9:H152	1.98	0.44
1:G:294:GLU:O	1:G:298:GLN:HG2	2.18	0.44
1:G:349:ALA:O	1:G:353:MET:HG3	2.17	0.44
3:H:602:CL6:CAX	3:H:602:CL6:HAK	2.48	0.44
1:E:242:PRO:HB2	1:E:245:THR:HB	1.99	0.44
1:F:105:ARG:HH21	1:F:439:ARG:HG2	1.81	0.44
1:G:172:LEU:HD11	1:G:490:LEU:HD12	2.00	0.44
1:H:204:VAL:O	1:H:208:LYS:HB2	2.18	0.44
1:G:71:MET:HG2	1:G:82:LEU:HD11	2.00	0.43
3:H:602:CL6:HAA	3:H:602:CL6:CAP	2.47	0.43
3:A:602:CL6:CAX	3:A:602:CL6:HAK	2.49	0.43
3:F:602:CL6:CAE	3:F:602:CL6:HAU	2.48	0.43
3:H:604:CL6:HAA	3:H:604:CL6:CAX	2.48	0.43
1:A:61:ASP:OD1	1:A:372:ARG:NH2	2.42	0.43
1:A:152:TYR:OH	1:A:186:GLY:HA3	2.18	0.43
1:A:251:LYS:HA	1:A:251:LYS:HD3	1.86	0.43
1:B:294:GLU:O	1:B:298:GLN:HG2	2.18	0.43
1:D:242:PRO:O	1:D:246:ILE:HG12	2.18	0.43
3:E:602:CL6:CAP	3:E:602:CL6:HAA	2.48	0.43
1:H:155:VAL:HG13	1:H:158:ARG:HH21	1.83	0.43
1:H:441:CYS:HB2	2:H:601:HEM:NA	2.33	0.43
1:A:156:LEU:HD13	1:A:179:TYR:HB2	2.00	0.43
1:D:304:PHE:CG	3:D:602:CL6:HAT	2.53	0.43
1:F:51:LEU:HD23	4:F:605:CE9:H141	2.01	0.43
1:H:242:PRO:HB2	1:H:245:THR:HB	2.00	0.43
3:C:604:CL6:HAM	3:C:604:CL6:CAE	2.49	0.43
3:A:603:CL6:CAC	3:A:603:CL6:CLAY	3.04	0.43
3:A:604:CL6:CAX	3:A:604:CL6:HAA	2.49	0.43
3:G:604:CL6:CLAY	3:G:604:CL6:NAO	2.88	0.43
1:H:172:LEU:HD11	1:H:490:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:603:CL6:CLAY	3:H:603:CL6:CAC	3.03	0.43
3:A:602:CL6:CAP	3:A:602:CL6:HAA	2.49	0.43
1:B:373:LEU:HB2	1:B:396:ILE:HB	2.00	0.43
1:F:212:LYS:HA	1:F:215:PHE:HD1	1.82	0.43
1:A:294:GLU:O	1:A:298:GLN:HG2	2.18	0.43
1:C:330:LYS:HD3	1:C:355:TYR:CZ	2.53	0.43
1:D:176:PHE:HD2	1:D:314:LEU:HD13	1.83	0.43
3:D:602:CL6:CAE	3:D:602:CL6:HAU	2.49	0.43
1:F:90:ILE:HG23	1:F:396:ILE:HG12	2.01	0.43
4:G:605:CE9:H262	4:G:605:CE9:H231	1.76	0.43
1:H:28:ARG:HG2	1:H:78:GLN:NE2	2.34	0.43
1:H:344:PRO:HA	1:H:345:PRO:HD3	1.93	0.43
1:B:326:ASP:OD1	1:B:326:ASP:N	2.51	0.43
1:G:155:VAL:HG13	1:G:158:ARG:HH21	1.84	0.43
1:A:90:ILE:HG23	1:A:396:ILE:HG12	2.00	0.42
3:D:604:CL6:HAM	3:D:604:CL6:CAE	2.49	0.42
1:H:349:ALA:O	1:H:353:MET:HG3	2.20	0.42
1:A:105:ARG:HG2	1:A:374:GLU:O	2.19	0.42
1:H:257:LYS:HB3	1:H:257:LYS:HE2	1.82	0.42
1:H:482:LEU:HD23	1:H:482:LEU:HA	1.89	0.42
3:H:604:CL6:HAM	3:H:604:CL6:CAE	2.50	0.42
1:A:118:ILE:HD12	1:A:133:LEU:HD12	2.01	0.42
1:B:51:LEU:HD22	1:B:54:ARG:CZ	2.49	0.42
3:B:604:CL6:HAM	3:B:604:CL6:CAE	2.50	0.42
1:E:89:VAL:HG13	1:E:383:ILE:HD11	2.01	0.42
1:F:319:TYR:CZ	1:F:474:LEU:HB2	2.55	0.42
2:F:601:HEM:C1A	3:F:602:CL6:HAM	2.54	0.42
1:G:92:THR:HA	1:G:96:LYS:HB2	2.01	0.42
1:A:326:ASP:OD1	1:A:326:ASP:N	2.52	0.42
1:A:431:TYR:CZ	1:A:433:PRO:HG3	2.55	0.42
1:B:103:THR:O	1:B:439:ARG:NH1	2.46	0.42
1:C:301:ILE:HD12	1:C:301:ILE:HA	1.92	0.42
3:E:604:CL6:CAE	3:E:604:CL6:HAM	2.50	0.42
1:A:244:ASP:OD1	1:A:245:THR:N	2.53	0.42
1:B:304:PHE:CD2	3:B:602:CL6:HAT	2.54	0.42
1:C:294:GLU:O	1:C:298:GLN:HG2	2.20	0.42
3:D:604:CL6:CAX	3:D:604:CL6:HAA	2.49	0.42
3:F:602:CL6:HAM	3:F:602:CL6:CAJ	2.50	0.42
1:A:49:ASN:OD1	1:A:75:TYR:N	2.48	0.42
1:B:344:PRO:HA	1:B:345:PRO:HD3	1.91	0.42
1:E:105:ARG:NH2	1:E:439:ARG:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:604:CL6:CAX	3:F:604:CL6:HAA	2.50	0.42
1:G:168:LYS:HE2	1:G:168:LYS:HB3	1.89	0.42
3:A:604:CL6:CLAY	3:A:604:CL6:NAO	2.90	0.41
1:B:252:SER:HA	1:B:255:ARG:HG2	2.02	0.41
1:E:55:GLN:HB2	1:E:59:LYS:HD3	2.01	0.41
2:E:601:HEM:C1A	3:E:602:CL6:HAM	2.55	0.41
1:A:257:LYS:HG2	1:A:276:ILE:HD11	2.01	0.41
1:E:465:LYS:HG3	1:E:491:LYS:HB3	2.01	0.41
1:G:50:VAL:HG11	1:G:221:LEU:HD11	2.03	0.41
1:A:204:VAL:O	1:A:208:LYS:HB2	2.20	0.41
1:G:154:ASP:OD1	1:G:457:ARG:NH2	2.49	0.41
1:H:213:PHE:CZ	3:H:604:CL6:HAG	2.55	0.41
1:H:246:ILE:HD13	1:H:300:ILE:HG21	2.02	0.41
3:F:602:CL6:CAX	3:F:602:CL6:HAK	2.50	0.41
1:G:484:PRO:HG2	1:G:488:ILE:HG13	2.03	0.41
1:A:242:PRO:O	1:A:246:ILE:HG12	2.20	0.41
1:B:34:LYS:HB3	1:B:34:LYS:HE2	1.85	0.41
1:C:349:ALA:O	1:C:353:MET:HG3	2.20	0.41
1:F:53:TYR:HB3	3:F:604:CL6:HAB	2.01	0.41
3:F:604:CL6:CLAY	3:F:604:CL6:NAO	2.90	0.41
1:G:105:ARG:NH2	1:G:439:ARG:HG2	2.34	0.41
1:A:213:PHE:CE1	3:A:602:CL6:HAU	2.56	0.41
1:B:249:LEU:O	1:B:253:VAL:HG23	2.20	0.41
1:C:128:ARG:NH2	1:C:294:GLU:OE2	2.53	0.41
1:C:156:LEU:HD13	1:C:179:TYR:HB2	2.02	0.41
3:C:604:CL6:CAX	3:C:604:CL6:HAA	2.51	0.41
1:E:68:TYR:HB2	1:E:72:TRP:HB3	2.03	0.41
1:G:344:PRO:HA	1:G:345:PRO:HD3	1.90	0.41
1:D:427:ASP:HB3	1:D:430:ILE:HB	2.02	0.41
1:E:93:VAL:HG13	1:E:102:PHE:CG	2.56	0.41
1:G:434:PHE:CE1	2:G:601:HEM:HBB2	2.56	0.41
1:B:434:PHE:CZ	2:B:601:HEM:HBB2	2.55	0.41
1:B:443:GLY:HA3	2:B:601:HEM:HBC2	2.03	0.41
1:C:342:LYS:HE2	1:C:460:GLN:O	2.21	0.41
1:D:257:LYS:NZ	1:D:292:ASP:OD1	2.54	0.41
1:E:57:LEU:HD22	1:E:372:ARG:NH2	2.36	0.41
3:E:604:CL6:CLAY	3:E:604:CL6:NAO	2.90	0.41
1:F:316:PHE:CE1	1:F:484:PRO:HG3	2.56	0.41
3:A:604:CL6:HAM	3:A:604:CL6:CAE	2.51	0.41
1:B:229:LEU:HD11	4:B:605:CE9:H21	2.02	0.41
3:B:602:CL6:CAX	3:B:602:CL6:HAK	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:MET:HB2	1:C:181:MET:HE3	1.93	0.41
1:G:482:LEU:HA	1:G:482:LEU:HD12	1.86	0.41
1:A:57:LEU:HD13	1:A:372:ARG:HD2	2.02	0.40
1:B:194:ASP:OD2	1:B:197:ASN:ND2	2.49	0.40
1:B:247:ASN:O	1:B:251:LYS:HG2	2.21	0.40
1:B:374:GLU:HG2	1:B:395:VAL:HG22	2.02	0.40
1:C:179:TYR:CZ	1:C:183:VAL:HG21	2.56	0.40
1:G:137:PHE:O	1:G:445:ARG:NH2	2.55	0.40
3:H:603:CL6:CAK	3:H:603:CL6:HAU	2.50	0.40
1:B:482:LEU:HD23	1:B:482:LEU:HA	1.90	0.40
1:C:148:ILE:O	1:C:151:GLN:HG2	2.20	0.40
1:G:104:ASN:HA	1:G:439:ARG:NH1	2.36	0.40
1:G:397:PRO:HB2	1:G:400:ALA:HB3	2.03	0.40
1:G:421:LYS:HD2	1:G:421:LYS:HA	1.96	0.40
1:A:116:SER:HB2	1:A:294:GLU:HG2	2.03	0.40
3:E:603:CL6:CAC	3:E:603:CL6:CLAY	3.06	0.40
1:G:176:PHE:HD2	1:G:314:LEU:HD13	1.87	0.40
1:G:465:LYS:HG3	1:G:491:LYS:HB3	2.02	0.40
1:H:93:VAL:HG13	1:H:102:PHE:CG	2.56	0.40
1:B:298:GLN:HA	1:B:301:ILE:HG22	2.04	0.40
1:B:354:GLU:O	1:B:358:MET:HG3	2.22	0.40
1:D:100:SER:O	1:D:378:LYS:HE2	2.22	0.40
1:E:226:PHE:HB3	1:E:228:PHE:CE2	2.56	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	450/480 (94%)	430 (96%)	20 (4%)	0	100	100
1	B	450/480 (94%)	436 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	445/480 (93%)	427 (96%)	18 (4%)	0	100	100
1	D	447/480 (93%)	429 (96%)	18 (4%)	0	100	100
1	E	446/480 (93%)	433 (97%)	13 (3%)	0	100	100
1	F	446/480 (93%)	426 (96%)	20 (4%)	0	100	100
1	G	443/480 (92%)	428 (97%)	15 (3%)	0	100	100
1	H	438/480 (91%)	418 (95%)	20 (5%)	0	100	100
All	All	3565/3840 (93%)	3427 (96%)	138 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/434 (94%)	401 (99%)	5 (1%)	71	92
1	B	411/434 (95%)	407 (99%)	4 (1%)	76	93
1	C	408/434 (94%)	405 (99%)	3 (1%)	84	95
1	D	409/434 (94%)	408 (100%)	1 (0%)	93	98
1	E	409/434 (94%)	407 (100%)	2 (0%)	88	96
1	F	405/434 (93%)	403 (100%)	2 (0%)	88	96
1	G	406/434 (94%)	403 (99%)	3 (1%)	84	95
1	H	402/434 (93%)	400 (100%)	2 (0%)	88	96
All	All	3256/3472 (94%)	3234 (99%)	22 (1%)	84	95

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	105	ARG
1	A	216	LEU
1	A	221	LEU

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Mol	Chain	Res	Type
1	A	304	PHE
1	B	194	ASP
1	B	291	SER
1	B	304	PHE
1	B	372	ARG
1	C	108	LEU
1	C	203	PHE
1	C	304	PHE
1	D	304	PHE
1	E	270	ASP
1	E	304	PHE
1	F	46	LEU
1	F	304	PHE
1	G	212	LYS
1	G	304	PHE
1	G	372	ARG
1	H	270	ASP
1	H	304	PHE

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

Mol	Chain	Res	Type
1	E	483	GLN
1	G	159	ASN
1	G	197	ASN
1	H	78	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)

39 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	CL6	C	602	2	26,28,28	0.51	0	35,39,39	1.25	4 (11%)
3	CL6	G	602	2	26,28,28	0.50	0	35,39,39	1.21	3 (8%)
2	HEM	H	601	3,1	41,50,50	1.28	4 (9%)	45,82,82	1.81	7 (15%)
2	HEM	B	601	3,1	41,50,50	1.30	4 (9%)	45,82,82	1.81	6 (13%)
4	CE9	A	605	-	39,39,39	0.14	0	38,38,38	0.14	0
2	HEM	F	601	3,1	41,50,50	1.28	4 (9%)	45,82,82	1.79	9 (20%)
3	CL6	D	602	2	26,28,28	0.50	0	35,39,39	1.34	5 (14%)
2	HEM	E	601	3,1	41,50,50	1.29	5 (12%)	45,82,82	1.77	9 (20%)
3	CL6	E	602	2	26,28,28	0.46	0	35,39,39	1.18	3 (8%)
3	CL6	G	603	-	26,28,28	0.50	0	35,39,39	1.82	6 (17%)
3	CL6	C	603	-	26,28,28	0.50	0	35,39,39	1.77	6 (17%)
4	CE9	E	605	-	21,21,39	0.17	0	20,20,38	0.09	0
4	CE9	B	605	-	33,33,39	0.13	0	32,32,38	0.16	0
3	CL6	C	604	-	26,28,28	0.58	0	35,39,39	1.44	6 (17%)
3	CL6	H	604	-	26,28,28	0.53	0	35,39,39	1.30	3 (8%)
4	CE9	C	605	-	23,23,39	0.17	0	22,22,38	0.10	0
4	CE9	G	605	-	29,29,39	0.18	0	28,28,38	0.09	0
2	HEM	A	601	3,1	41,50,50	1.28	5 (12%)	45,82,82	1.81	9 (20%)
3	CL6	B	604	-	26,28,28	0.53	0	35,39,39	1.33	4 (11%)
3	CL6	G	604	-	26,28,28	0.49	0	35,39,39	1.37	4 (11%)
3	CL6	B	602	2	26,28,28	0.49	0	35,39,39	1.19	3 (8%)
4	CE9	D	605	-	23,23,39	0.18	0	22,22,38	0.10	0
3	CL6	H	602	2	26,28,28	0.47	0	35,39,39	1.08	1 (2%)
3	CL6	E	604	-	26,28,28	0.49	0	35,39,39	1.37	5 (14%)
3	CL6	D	603	-	26,28,28	0.48	0	35,39,39	1.81	6 (17%)
3	CL6	F	602	2	26,28,28	0.52	0	35,39,39	1.37	4 (11%)
3	CL6	E	603	-	26,28,28	0.50	0	35,39,39	1.80	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CL6	A	602	2	26,28,28	0.51	0	35,39,39	1.33	2 (5%)
3	CL6	A	604	-	26,28,28	0.51	0	35,39,39	1.27	3 (8%)
2	HEM	D	601	3,1	41,50,50	1.29	4 (9%)	45,82,82	1.81	9 (20%)
3	CL6	F	603	-	26,28,28	0.47	0	35,39,39	1.79	6 (17%)
3	CL6	B	603	-	26,28,28	0.49	0	35,39,39	1.92	7 (20%)
2	HEM	C	601	3,1	41,50,50	1.29	4 (9%)	45,82,82	1.79	8 (17%)
3	CL6	H	603	-	26,28,28	0.48	0	35,39,39	1.67	5 (14%)
4	CE9	F	605	-	28,28,39	0.13	0	27,27,38	0.14	0
3	CL6	F	604	-	26,28,28	0.48	0	35,39,39	1.32	5 (14%)
3	CL6	A	603	-	26,28,28	0.52	0	35,39,39	1.78	6 (17%)
3	CL6	D	604	-	26,28,28	0.50	0	35,39,39	1.34	5 (14%)
2	HEM	G	601	3,1	41,50,50	1.30	4 (9%)	45,82,82	1.84	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CL6	C	602	2	-	0/18/24/24	0/4/4/4
3	CL6	G	602	2	-	2/18/24/24	0/4/4/4
2	HEM	H	601	3,1	-	4/12/54/54	-
2	HEM	B	601	3,1	-	4/12/54/54	-
4	CE9	A	605	-	-	15/37/37/37	-
2	HEM	F	601	3,1	-	2/12/54/54	-
3	CL6	D	602	2	-	0/18/24/24	0/4/4/4
2	HEM	E	601	3,1	-	4/12/54/54	-
3	CL6	E	602	2	-	1/18/24/24	0/4/4/4
3	CL6	G	603	-	-	5/18/24/24	0/4/4/4
3	CL6	C	603	-	-	3/18/24/24	0/4/4/4
4	CE9	E	605	-	-	7/19/19/37	-
4	CE9	B	605	-	-	10/31/31/37	-
3	CL6	C	604	-	-	0/18/24/24	0/4/4/4
3	CL6	H	604	-	-	0/18/24/24	0/4/4/4
4	CE9	C	605	-	-	8/21/21/37	-
4	CE9	G	605	-	-	11/27/27/37	-
2	HEM	A	601	3,1	-	6/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CL6	B	604	-	-	0/18/24/24	0/4/4/4
3	CL6	G	604	-	-	0/18/24/24	0/4/4/4
3	CL6	B	602	2	-	0/18/24/24	0/4/4/4
4	CE9	D	605	-	-	3/21/21/37	-
3	CL6	H	602	2	-	0/18/24/24	0/4/4/4
3	CL6	E	604	-	-	0/18/24/24	0/4/4/4
3	CL6	D	603	-	-	3/18/24/24	0/4/4/4
3	CL6	F	602	2	-	0/18/24/24	0/4/4/4
3	CL6	E	603	-	-	0/18/24/24	0/4/4/4
3	CL6	A	602	2	-	0/18/24/24	0/4/4/4
3	CL6	A	604	-	-	0/18/24/24	0/4/4/4
2	HEM	D	601	3,1	-	4/12/54/54	-
3	CL6	F	603	-	-	3/18/24/24	0/4/4/4
3	CL6	B	603	-	-	2/18/24/24	0/4/4/4
2	HEM	C	601	3,1	-	4/12/54/54	-
3	CL6	H	603	-	-	3/18/24/24	0/4/4/4
4	CE9	F	605	-	-	6/26/26/37	-
3	CL6	F	604	-	-	0/18/24/24	0/4/4/4
3	CL6	A	603	-	-	3/18/24/24	0/4/4/4
3	CL6	D	604	-	-	0/18/24/24	0/4/4/4
2	HEM	G	601	3,1	-	6/12/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C1B-NB	-3.44	1.34	1.40
2	G	601	HEM	C1B-NB	-3.42	1.34	1.40
2	D	601	HEM	C1B-NB	-3.40	1.34	1.40
2	C	601	HEM	C1B-NB	-3.37	1.34	1.40
2	E	601	HEM	C1B-NB	-3.34	1.34	1.40
2	H	601	HEM	C1B-NB	-3.34	1.34	1.40
2	F	601	HEM	C1B-NB	-3.33	1.34	1.40
2	A	601	HEM	C1B-NB	-3.27	1.34	1.40
2	D	601	HEM	C4D-ND	-3.05	1.35	1.40
2	E	601	HEM	C4D-ND	-3.00	1.35	1.40
2	B	601	HEM	C4D-ND	-2.99	1.35	1.40
2	F	601	HEM	C4D-ND	-2.95	1.35	1.40
2	H	601	HEM	C4D-ND	-2.95	1.35	1.40
2	G	601	HEM	C4D-ND	-2.93	1.35	1.40
2	B	601	HEM	FE-NB	2.91	2.11	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C4D-ND	-2.89	1.35	1.40
2	F	601	HEM	FE-NB	2.87	2.11	1.96
2	H	601	HEM	FE-NB	2.86	2.11	1.96
2	A	601	HEM	FE-NB	2.85	2.11	1.96
2	A	601	HEM	C4D-ND	-2.82	1.35	1.40
2	E	601	HEM	FE-NB	2.81	2.10	1.96
2	G	601	HEM	FE-NB	2.80	2.10	1.96
2	C	601	HEM	FE-NB	2.76	2.10	1.96
2	D	601	HEM	FE-NB	2.75	2.10	1.96
2	D	601	HEM	CHB-C1B	2.21	1.40	1.35
2	H	601	HEM	CHB-C1B	2.16	1.40	1.35
2	C	601	HEM	CHB-C1B	2.15	1.40	1.35
2	F	601	HEM	CHB-C1B	2.14	1.40	1.35
2	A	601	HEM	CHB-C1B	2.13	1.40	1.35
2	E	601	HEM	CHB-C1B	2.12	1.40	1.35
2	G	601	HEM	CHB-C1B	2.11	1.40	1.35
2	B	601	HEM	CHB-C1B	2.07	1.40	1.35
2	E	601	HEM	C3B-C4B	2.03	1.48	1.44
2	A	601	HEM	C3B-C4B	2.02	1.48	1.44

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	HEM	CHC-C4B-NB	5.38	130.28	124.43
2	G	601	HEM	CHC-C4B-NB	5.31	130.20	124.43
2	H	601	HEM	CHC-C4B-NB	5.28	130.17	124.43
3	C	604	CL6	CAP-NAO-CAM	-5.17	104.96	108.25
3	A	602	CL6	CAP-NAO-CAM	-5.16	104.97	108.25
3	B	603	CL6	CAW-CAR-NAO	5.15	113.97	106.11
2	F	601	HEM	CHC-C4B-NB	5.14	130.01	124.43
2	D	601	HEM	CHC-C4B-NB	5.14	130.01	124.43
3	B	603	CL6	CAL-CAR-CAW	-5.14	105.16	112.00
3	G	603	CL6	CAL-CAR-CAW	-5.10	105.20	112.00
2	C	601	HEM	CHC-C4B-NB	5.10	129.97	124.43
3	G	603	CL6	CAP-NAO-CAR	5.08	130.95	124.95
3	B	602	CL6	CAP-NAO-CAM	-5.07	105.02	108.25
2	A	601	HEM	CHC-C4B-NB	5.07	129.94	124.43
3	B	604	CL6	CAP-NAO-CAM	-5.05	105.04	108.25
3	F	602	CL6	CAP-NAO-CAM	-5.04	105.04	108.25
3	D	603	CL6	CAP-NAO-CAR	5.03	130.89	124.95
3	G	602	CL6	CAP-NAO-CAM	-5.00	105.06	108.25
3	D	602	CL6	CAP-NAO-CAM	-4.95	105.10	108.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	603	CL6	CAP-NAO-CAM	-4.93	105.11	108.25
3	E	603	CL6	CAP-NAO-CAM	-4.91	105.12	108.25
3	A	603	CL6	CAP-NAO-CAM	-4.91	105.12	108.25
3	D	603	CL6	CAP-NAO-CAM	-4.89	105.14	108.25
3	D	604	CL6	CAP-NAO-CAM	-4.88	105.15	108.25
3	F	603	CL6	CAP-NAO-CAR	4.87	130.71	124.95
3	B	603	CL6	CAP-NAO-CAM	-4.87	105.15	108.25
2	E	601	HEM	CHC-C4B-NB	4.86	129.71	124.43
3	C	602	CL6	CAP-NAO-CAM	-4.85	105.16	108.25
3	H	603	CL6	CAP-NAO-CAR	4.85	130.68	124.95
3	H	604	CL6	CAP-NAO-CAM	-4.80	105.19	108.25
3	E	602	CL6	CAP-NAO-CAM	-4.79	105.20	108.25
3	D	603	CL6	CAL-CAR-CAW	-4.79	105.62	112.00
3	C	603	CL6	CAP-NAO-CAM	-4.77	105.21	108.25
3	G	603	CL6	CAP-NAO-CAM	-4.77	105.21	108.25
3	A	604	CL6	CAP-NAO-CAM	-4.76	105.22	108.25
3	E	604	CL6	CAP-NAO-CAM	-4.74	105.23	108.25
3	C	603	CL6	CAL-CAR-CAW	-4.73	105.69	112.00
3	F	603	CL6	CAL-CAR-CAW	-4.73	105.70	112.00
3	C	603	CL6	CAP-NAO-CAR	4.72	130.53	124.95
3	F	604	CL6	CAP-NAO-CAM	-4.70	105.26	108.25
3	A	603	CL6	CAP-NAO-CAR	4.70	130.50	124.95
3	H	602	CL6	CAP-NAO-CAM	-4.68	105.27	108.25
2	C	601	HEM	CHD-C1D-ND	4.68	129.51	124.43
3	H	603	CL6	CAP-NAO-CAM	-4.68	105.27	108.25
2	G	601	HEM	CHD-C1D-ND	4.65	129.49	124.43
3	A	603	CL6	CAL-CAR-CAW	-4.63	105.83	112.00
2	F	601	HEM	CHD-C1D-ND	4.58	129.41	124.43
3	E	603	CL6	CAW-CAR-NAO	4.55	113.06	106.11
3	E	603	CL6	CAL-CAR-CAW	-4.54	105.95	112.00
3	E	603	CL6	CAP-NAO-CAR	4.52	130.29	124.95
2	B	601	HEM	CHD-C1D-ND	4.52	129.34	124.43
3	G	604	CL6	CAP-NAO-CAM	-4.51	105.38	108.25
2	A	601	HEM	CHD-C1D-ND	4.50	129.31	124.43
2	H	601	HEM	CHD-C1D-ND	4.49	129.31	124.43
3	H	603	CL6	CAL-CAR-CAW	-4.46	106.06	112.00
3	A	603	CL6	CAW-CAR-NAO	4.39	112.81	106.11
3	B	603	CL6	CAP-NAO-CAR	4.39	130.13	124.95
3	G	604	CL6	CAR-CAW-CAX	-4.32	119.91	122.65
3	C	603	CL6	CAW-CAR-NAO	4.28	112.64	106.11
2	D	601	HEM	C1B-NB-C4B	4.26	109.47	105.07
2	E	601	HEM	CHD-C1D-ND	4.23	129.03	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	603	CL6	CAW-CAR-NAO	4.20	112.52	106.11
2	D	601	HEM	CHD-C1D-ND	4.14	128.93	124.43
2	C	601	HEM	C1B-NB-C4B	4.14	109.35	105.07
2	E	601	HEM	C1B-NB-C4B	4.10	109.31	105.07
2	G	601	HEM	C1B-NB-C4B	4.06	109.27	105.07
3	G	603	CL6	CAW-CAR-NAO	4.06	112.31	106.11
2	H	601	HEM	C1B-NB-C4B	4.03	109.23	105.07
3	E	604	CL6	CAR-CAW-CAX	-3.99	120.12	122.65
2	A	601	HEM	C1B-NB-C4B	3.97	109.17	105.07
2	F	601	HEM	C1B-NB-C4B	3.87	109.07	105.07
3	D	603	CL6	CAW-CAR-NAO	3.78	111.88	106.11
2	B	601	HEM	C1B-NB-C4B	3.73	108.92	105.07
3	H	603	CL6	CAW-CAR-NAO	3.63	111.65	106.11
3	A	602	CL6	CAR-CAW-CAX	-3.57	120.39	122.65
2	E	601	HEM	CHB-C1B-NB	3.56	128.78	124.38
3	G	603	CL6	CAM-NAO-CAR	-3.56	123.75	126.71
2	D	601	HEM	CHB-C1B-NB	3.55	128.77	124.38
3	C	604	CL6	CAR-CAW-CAX	-3.52	120.42	122.65
3	D	603	CL6	CAM-NAO-CAR	-3.45	123.85	126.71
2	A	601	HEM	CHA-C4D-ND	3.43	128.62	124.38
2	G	601	HEM	CHB-C1B-NB	3.42	128.60	124.38
3	B	604	CL6	CAR-CAW-CAX	-3.39	120.50	122.65
2	H	601	HEM	CHA-C4D-ND	3.38	128.56	124.38
3	D	604	CL6	CAR-CAW-CAX	-3.37	120.52	122.65
3	H	603	CL6	CAM-NAO-CAR	-3.32	123.95	126.71
3	F	604	CL6	CAR-CAW-CAX	-3.31	120.55	122.65
2	C	601	HEM	CHB-C1B-NB	3.31	128.47	124.38
2	H	601	HEM	CHB-C1B-NB	3.30	128.46	124.38
2	E	601	HEM	CHA-C4D-ND	3.30	128.46	124.38
2	A	601	HEM	CHB-C1B-NB	3.27	128.42	124.38
3	H	604	CL6	CAR-CAW-CAX	-3.25	120.59	122.65
2	B	601	HEM	CHA-C4D-ND	3.25	128.39	124.38
2	D	601	HEM	CHA-C4D-ND	3.24	128.38	124.38
2	B	601	HEM	CHB-C1B-NB	3.23	128.37	124.38
2	F	601	HEM	CHA-C4D-ND	3.23	128.37	124.38
3	B	603	CL6	CAR-CAW-CAX	-3.22	120.61	122.65
2	G	601	HEM	CHA-C4D-ND	3.21	128.35	124.38
2	F	601	HEM	CHB-C1B-NB	3.20	128.34	124.38
2	G	601	HEM	CHD-C1D-C2D	-3.20	119.99	124.98
2	C	601	HEM	CHD-C1D-C2D	-3.18	120.01	124.98
3	F	602	CL6	CAC-CAR-CAW	3.17	116.22	112.00
3	F	603	CL6	CAM-NAO-CAR	-3.15	124.10	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	HEM	CHA-C4D-ND	3.12	128.23	124.38
3	C	603	CL6	CAM-NAO-CAR	-3.11	124.12	126.71
2	F	601	HEM	CHD-C1D-C2D	-3.11	120.12	124.98
2	A	601	HEM	CHD-C1D-C2D	-3.08	120.17	124.98
2	B	601	HEM	CHD-C1D-C2D	-3.06	120.21	124.98
3	A	604	CL6	CAR-CAW-CAX	-3.03	120.73	122.65
3	A	603	CL6	CAM-NAO-CAR	-3.01	124.21	126.71
3	F	602	CL6	CAR-CAW-CAX	-2.98	120.76	122.65
3	D	602	CL6	CAC-CAR-CAW	2.98	115.96	112.00
2	H	601	HEM	CHD-C1D-C2D	-2.92	120.41	124.98
3	D	602	CL6	CAL-CAR-CAC	-2.91	101.90	110.14
2	D	601	HEM	CHD-C1D-C2D	-2.90	120.44	124.98
2	E	601	HEM	CHD-C1D-C2D	-2.89	120.46	124.98
3	G	604	CL6	CAU-CAW-CAR	2.88	123.13	121.05
3	E	603	CL6	CAM-NAO-CAR	-2.75	124.43	126.71
3	C	602	CL6	CAR-CAW-CAX	-2.68	120.95	122.65
3	B	603	CL6	CAC-CAR-CAW	-2.66	108.45	112.00
3	F	602	CL6	CAL-CAR-CAC	-2.65	102.62	110.14
3	H	604	CL6	CAL-CAR-CAW	-2.65	108.47	112.00
3	E	603	CL6	CAC-CAR-CAW	-2.64	108.48	112.00
3	D	602	CL6	CAR-CAW-CAX	-2.62	120.99	122.65
3	C	604	CL6	CAL-CAR-CAW	-2.57	108.57	112.00
3	D	604	CL6	CAL-CAR-CAW	-2.57	108.58	112.00
3	A	604	CL6	CAP-NAO-CAR	2.55	127.97	124.95
3	B	603	CL6	CAM-NAO-CAR	-2.55	124.59	126.71
3	E	604	CL6	CAU-CAW-CAR	2.49	122.85	121.05
3	E	603	CL6	CAR-CAW-CAX	-2.40	121.13	122.65
3	F	604	CL6	CAP-NAO-CAR	2.38	127.77	124.95
3	G	604	CL6	CAP-NAO-CAR	2.37	127.76	124.95
2	D	601	HEM	CHA-C4D-C3D	-2.37	120.87	125.33
2	D	601	HEM	CAA-CBA-CGA	-2.36	107.15	113.76
3	F	604	CL6	CAL-CAR-CAW	-2.35	108.87	112.00
3	G	602	CL6	CAL-CAR-CAW	-2.34	108.89	112.00
3	E	602	CL6	CAL-CAR-CAW	-2.33	108.89	112.00
3	D	603	CL6	CAR-CAW-CAX	-2.31	121.19	122.65
3	C	604	CL6	CAP-NAO-CAR	2.30	127.67	124.95
3	C	604	CL6	CAC-CAR-CAW	2.28	115.04	112.00
3	F	603	CL6	CAR-CAW-CAX	-2.27	121.21	122.65
2	E	601	HEM	CHA-C4D-C3D	-2.24	121.11	125.33
2	F	601	HEM	O2D-CGD-CBD	2.22	121.17	114.03
3	A	603	CL6	CAR-CAW-CAX	-2.20	121.25	122.65
2	H	601	HEM	CHA-C4D-C3D	-2.20	121.20	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	604	CL6	CAU-CAW-CAR	2.20	122.64	121.05
2	A	601	HEM	CAD-CBD-CGD	-2.19	108.88	113.60
3	B	602	CL6	CAR-CAW-CAX	-2.19	121.26	122.65
3	C	603	CL6	CAR-CAW-CAX	-2.17	121.27	122.65
3	B	604	CL6	CAP-NAO-CAR	2.15	127.49	124.95
3	B	602	CL6	CAM-NAO-CAR	2.14	128.48	126.71
2	C	601	HEM	CHA-C4D-C3D	-2.13	121.33	125.33
2	F	601	HEM	CHA-C4D-C3D	-2.13	121.34	125.33
3	C	602	CL6	CAL-CAR-CAW	-2.12	109.17	112.00
3	C	602	CL6	CAL-CAR-CAC	-2.11	104.15	110.14
3	E	604	CL6	CAP-NAO-CAR	2.11	127.45	124.95
2	A	601	HEM	CHA-C4D-C3D	-2.10	121.38	125.33
2	D	601	HEM	O2D-CGD-CBD	2.09	120.75	114.03
3	D	602	CL6	CAM-NAO-CAR	2.09	128.44	126.71
2	A	601	HEM	O2A-CGA-CBA	2.08	120.71	114.03
2	G	601	HEM	CAD-C3D-C4D	2.07	128.28	124.66
3	F	604	CL6	CAC-CAR-CAW	2.07	114.75	112.00
3	B	604	CL6	CAU-CAW-CAR	2.05	122.53	121.05
3	E	602	CL6	CAL-CAR-CAC	-2.05	104.34	110.14
3	G	602	CL6	CAL-CAR-CAC	-2.04	104.36	110.14
3	G	603	CL6	CAR-CAW-CAX	-2.03	121.36	122.65
2	G	601	HEM	CHA-C4D-C3D	-2.03	121.52	125.33
2	E	601	HEM	O2D-CGD-CBD	2.03	120.54	114.03
3	E	604	CL6	CAC-CAR-CAW	2.02	114.69	112.00
2	E	601	HEM	CHB-C1B-C2B	-2.02	121.13	126.72
3	D	604	CL6	CAC-CAR-CAW	2.02	114.69	112.00
3	D	604	CL6	CAP-NAO-CAR	2.01	127.33	124.95
2	F	601	HEM	O2A-CGA-CBA	2.01	120.48	114.03
2	C	601	HEM	CAD-C3D-C4D	2.01	128.16	124.66

There are no chirality outliers.

All (119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	CE9	O31-C32-C33-O34
4	F	605	CE9	O25-C26-C27-O28
4	B	605	CE9	C20-C21-O22-C23
4	E	605	CE9	O13-C14-C15-O16
4	D	605	CE9	C15-C14-O13-C12
4	A	605	CE9	O22-C23-C24-O25
4	C	605	CE9	C10-C11-C12-O13
4	A	605	CE9	O25-C26-C27-O28

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Mol	Chain	Res	Type	Atoms
4	C	605	CE9	O25-C26-C27-O28
4	B	605	CE9	C9-C10-C11-C12
4	A	605	CE9	C11-C10-C9-C8
2	F	601	HEM	C2B-C3B-CAB-CBB
4	A	605	CE9	C20-C21-O22-C23
4	F	605	CE9	O22-C23-C24-O25
4	G	605	CE9	C23-C24-O25-C26
4	C	605	CE9	O16-C17-C18-O19
4	D	605	CE9	C3-C4-C5-C6
2	A	601	HEM	C2B-C3B-CAB-CBB
2	B	601	HEM	C2B-C3B-CAB-CBB
2	C	601	HEM	C2B-C3B-CAB-CBB
2	D	601	HEM	C2B-C3B-CAB-CBB
2	E	601	HEM	C2B-C3B-CAB-CBB
2	G	601	HEM	C2B-C3B-CAB-CBB
2	H	601	HEM	C2B-C3B-CAB-CBB
4	A	605	CE9	C23-C24-O25-C26
4	C	605	CE9	C15-C14-O13-C12
4	G	605	CE9	C33-C32-O31-C30
4	C	605	CE9	C23-C24-O25-C26
4	D	605	CE9	O13-C14-C15-O16
4	B	605	CE9	O25-C26-C27-O28
4	A	605	CE9	O28-C29-C30-O31
4	C	605	CE9	C14-C15-O16-C17
4	E	605	CE9	C20-C21-O22-C23
4	G	605	CE9	C24-C23-O22-C21
4	A	605	CE9	C39-C38-O37-C36
4	B	605	CE9	C21-C20-O19-C18
4	C	605	CE9	C11-C12-O13-C14
4	F	605	CE9	C14-C15-O16-C17
4	F	605	CE9	C17-C18-O19-C20
3	A	603	CL6	CAK-CAL-CAR-NAO
3	C	603	CL6	CAK-CAL-CAR-NAO
3	D	603	CL6	CAK-CAL-CAR-NAO
3	D	603	CL6	CAJ-CAL-CAR-NAO
3	F	603	CL6	CAK-CAL-CAR-NAO
3	G	603	CL6	CAK-CAL-CAR-NAO
3	G	603	CL6	CAJ-CAL-CAR-NAO
3	H	603	CL6	CAK-CAL-CAR-NAO
4	F	605	CE9	C27-C26-O25-C24
4	A	605	CE9	C27-C26-O25-C24
4	B	605	CE9	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	B	605	CE9	C23-C24-O25-C26
4	A	605	CE9	C32-C33-O34-C35
4	B	605	CE9	C33-C32-O31-C30
4	E	605	CE9	C17-C18-O19-C20
4	A	605	CE9	C24-C23-O22-C21
4	E	605	CE9	O16-C17-C18-O19
4	C	605	CE9	C30-C29-O28-C27
4	G	605	CE9	C11-C12-O13-C14
4	A	605	CE9	C26-C27-O28-C29
4	G	605	CE9	C27-C26-O25-C24
3	G	603	CL6	CAK-CAL-CAR-CAC
2	E	601	HEM	C4B-C3B-CAB-CBB
2	F	601	HEM	C4B-C3B-CAB-CBB
2	H	601	HEM	C4B-C3B-CAB-CBB
4	B	605	CE9	O16-C17-C18-O19
4	A	605	CE9	C15-C14-O13-C12
3	A	603	CL6	CAK-CAL-CAR-CAC
4	G	605	CE9	C18-C17-O16-C15
4	G	605	CE9	O16-C17-C18-O19
3	H	603	CL6	CAK-CAL-CAR-CAC
4	A	605	CE9	C14-C15-O16-C17
4	B	605	CE9	C29-C30-O31-C32
4	G	605	CE9	C17-C18-O19-C20
4	E	605	CE9	C15-C14-O13-C12
2	E	601	HEM	CAD-CBD-CGD-O1D
3	C	603	CL6	CAK-CAL-CAR-CAC
3	D	603	CL6	CAK-CAL-CAR-CAC
3	F	603	CL6	CAK-CAL-CAR-CAC
4	B	605	CE9	C5-C6-C7-C8
4	F	605	CE9	C11-C12-O13-C14
2	A	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAD-CBD-CGD-O1D
3	G	603	CL6	CAJ-CAL-CAR-CAC
4	G	605	CE9	C29-C30-O31-C32
2	A	601	HEM	C4B-C3B-CAB-CBB
2	B	601	HEM	C4B-C3B-CAB-CBB
2	C	601	HEM	C4B-C3B-CAB-CBB
2	D	601	HEM	C4B-C3B-CAB-CBB
2	G	601	HEM	C4B-C3B-CAB-CBB
2	A	601	HEM	CAA-CBA-CGA-O2A
2	H	601	HEM	CAD-CBD-CGD-O1D
2	H	601	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	B	603	CL6	CAK-CAL-CAR-CAC
2	C	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAD-CBD-CGD-O2D
2	E	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
4	E	605	CE9	C24-C23-O22-C21
2	G	601	HEM	CAA-CBA-CGA-O2A
2	G	601	HEM	CAD-CBD-CGD-O2D
4	G	605	CE9	C20-C21-O22-C23
3	A	603	CL6	CAJ-CAL-CAR-NAO
3	B	603	CL6	CAK-CAL-CAR-NAO
3	C	603	CL6	CAJ-CAL-CAR-NAO
3	E	602	CL6	CAA-CAC-CAR-NAO
3	F	603	CL6	CAJ-CAL-CAR-NAO
3	G	602	CL6	CAE-CAC-CAR-NAO
3	G	602	CL6	CAA-CAC-CAR-NAO
3	G	603	CL6	CAA-CAC-CAR-NAO
3	H	603	CL6	CAJ-CAL-CAR-NAO
4	A	605	CE9	C35-C36-O37-C38
2	C	601	HEM	CAA-CBA-CGA-O1A
2	G	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAD-CBD-CGD-O2D
2	D	601	HEM	CAA-CBA-CGA-O2A
2	D	601	HEM	CAA-CBA-CGA-O1A
2	G	601	HEM	CAD-CBD-CGD-O1D
4	E	605	CE9	C14-C15-O16-C17
4	G	605	CE9	O19-C20-C21-O22

There are no ring outliers.

37 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	CL6	4	0
3	G	602	CL6	3	0
2	H	601	HEM	3	0
2	B	601	HEM	3	0
4	A	605	CE9	3	0
2	F	601	HEM	4	0
3	D	602	CL6	3	0
2	E	601	HEM	2	0
3	E	602	CL6	8	0
3	G	603	CL6	3	0

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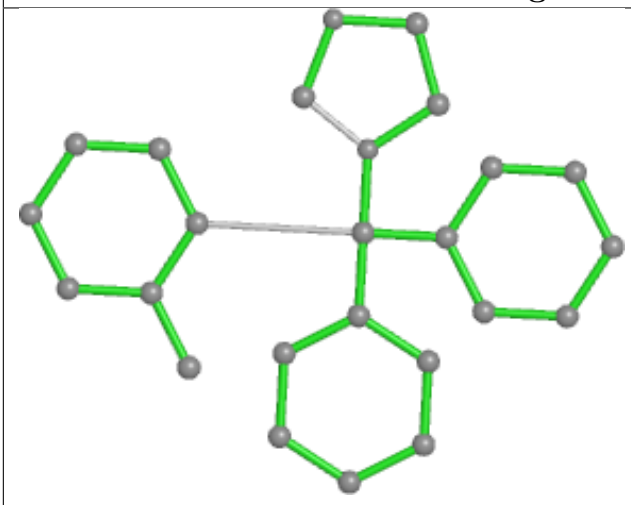
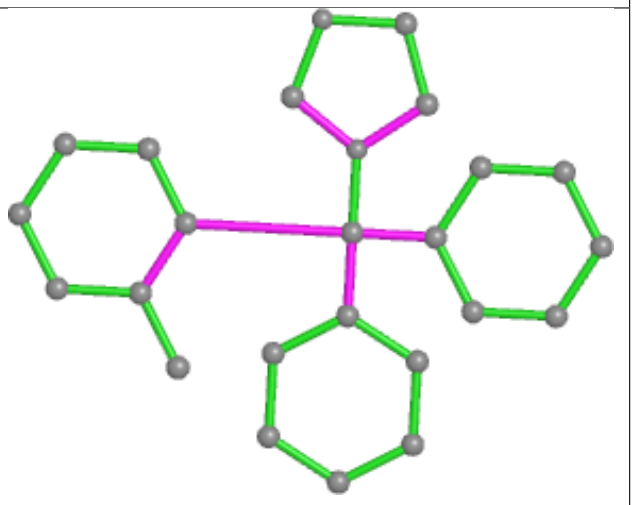
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	603	CL6	4	0
4	B	605	CE9	3	0
3	C	604	CL6	3	0
3	H	604	CL6	4	0
4	G	605	CE9	1	0
2	A	601	HEM	1	0
3	B	604	CL6	3	0
3	G	604	CL6	4	0
3	B	602	CL6	6	0
4	D	605	CE9	2	0
3	H	602	CL6	6	0
3	E	604	CL6	4	0
3	D	603	CL6	3	0
3	F	602	CL6	5	0
3	E	603	CL6	3	0
3	A	602	CL6	5	0
3	A	604	CL6	4	0
2	D	601	HEM	2	0
3	F	603	CL6	4	0
3	B	603	CL6	3	0
2	C	601	HEM	3	0
3	H	603	CL6	6	0
4	F	605	CE9	4	0
3	F	604	CL6	4	0
3	A	603	CL6	4	0
3	D	604	CL6	4	0
2	G	601	HEM	3	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.

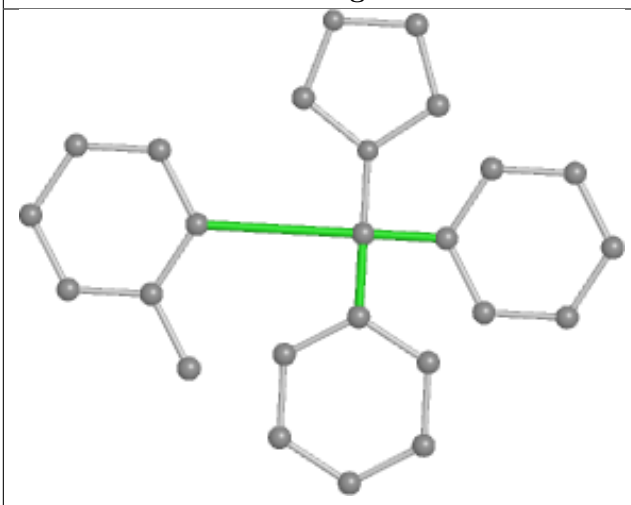
Ligand CL6 C 602



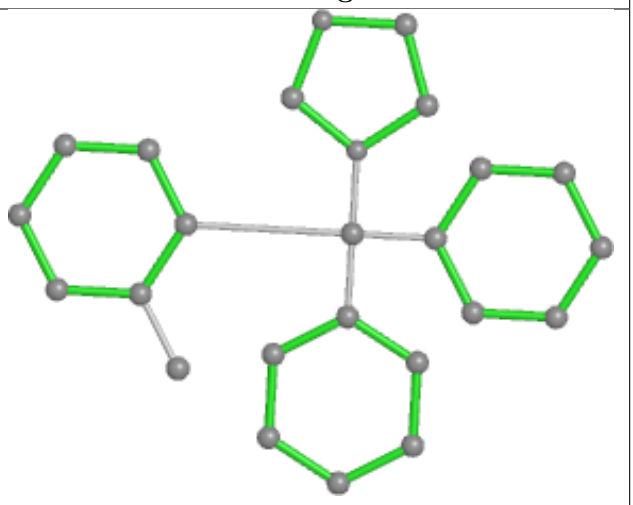
Bond lengths



Bond angles

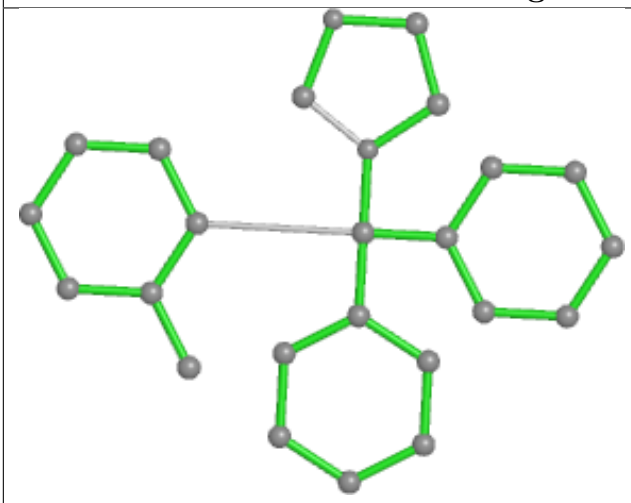


Torsions



Rings

Ligand CL6 G 602



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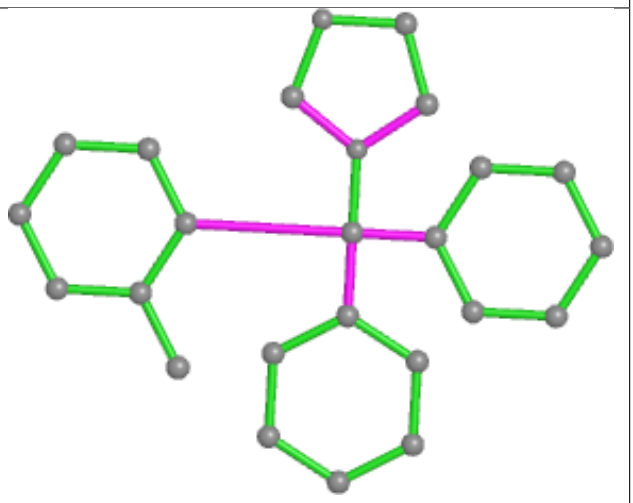
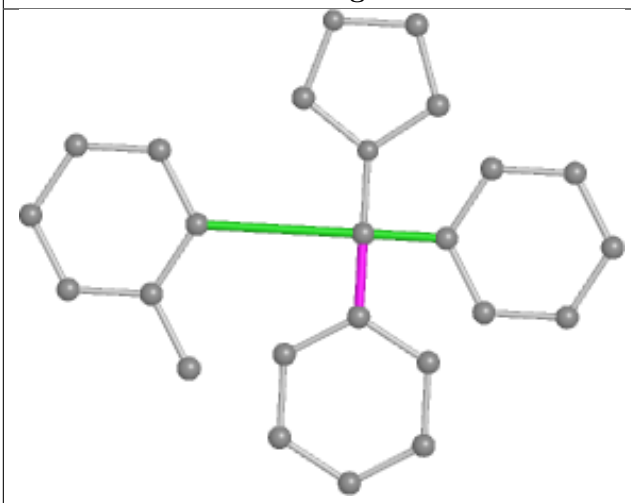


Bond angles



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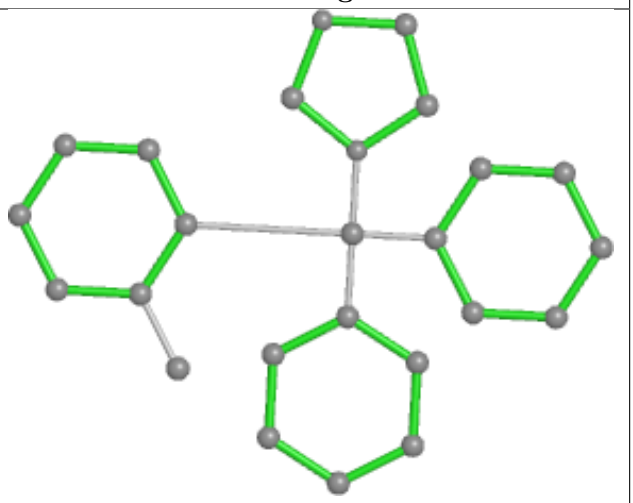
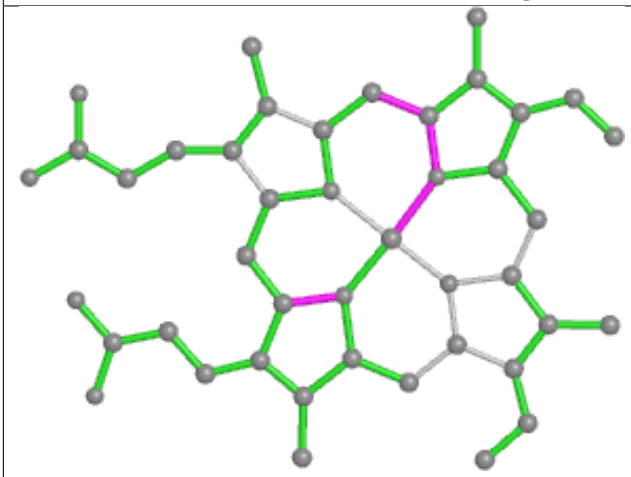
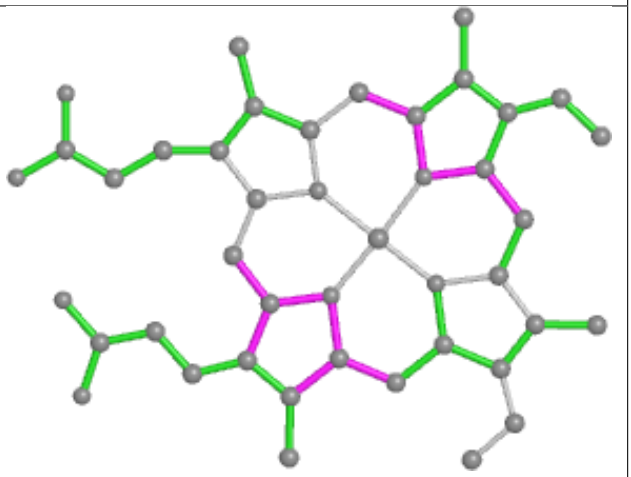


Rings

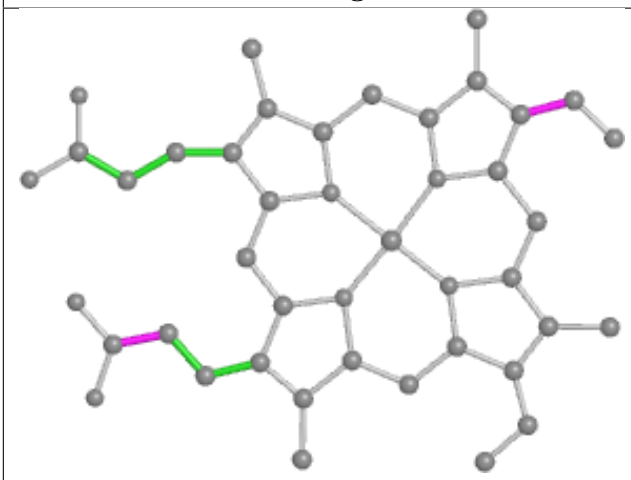
Ligand HEM H 601



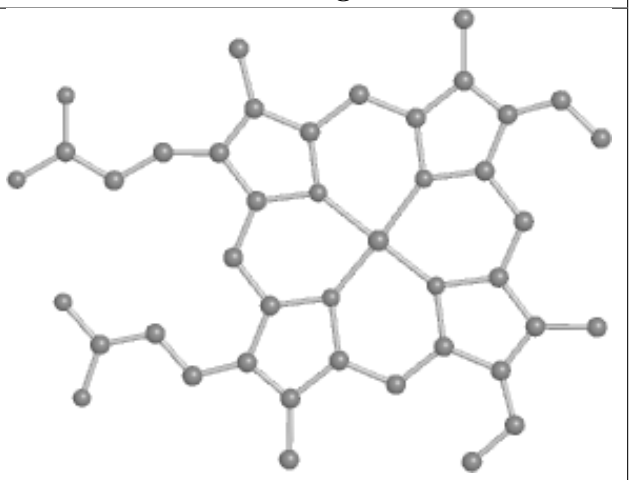
Bond lengths



Bond angles

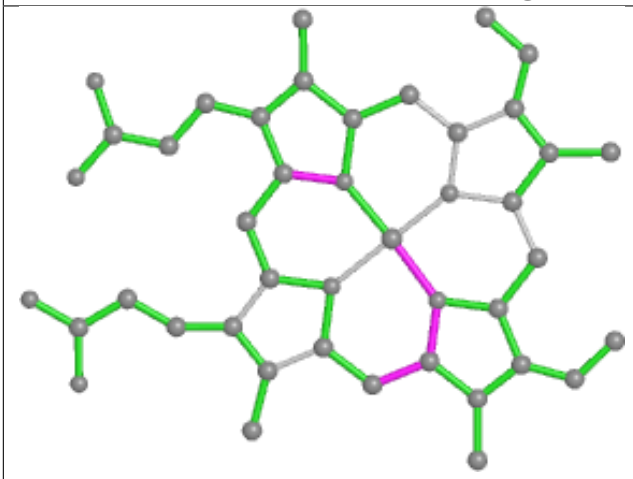


Torsions



Rings

Ligand HEM B 601



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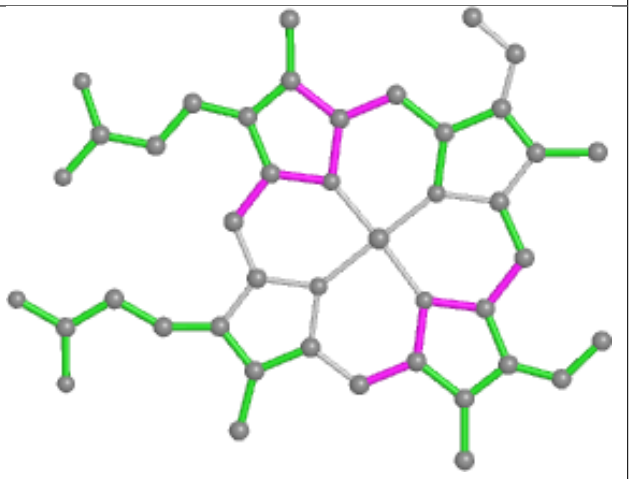
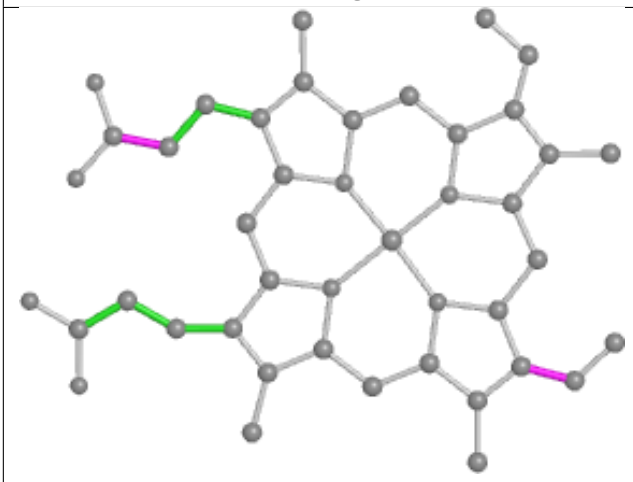


Bond angles



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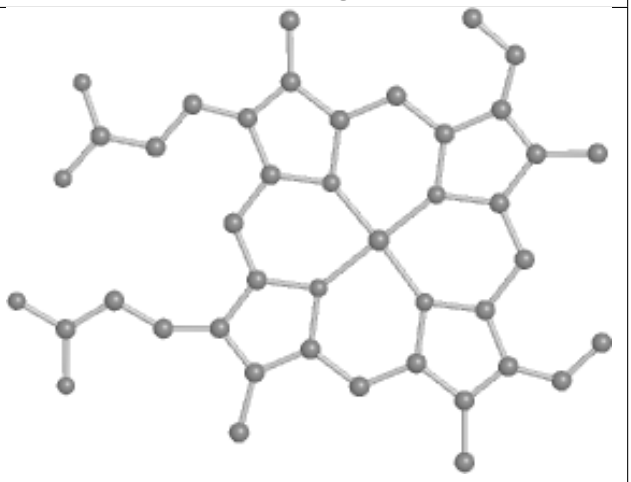
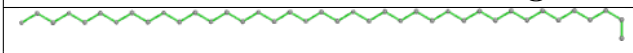


Rings

Ligand CE9 A 605



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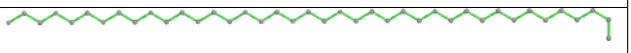
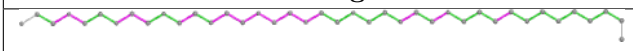


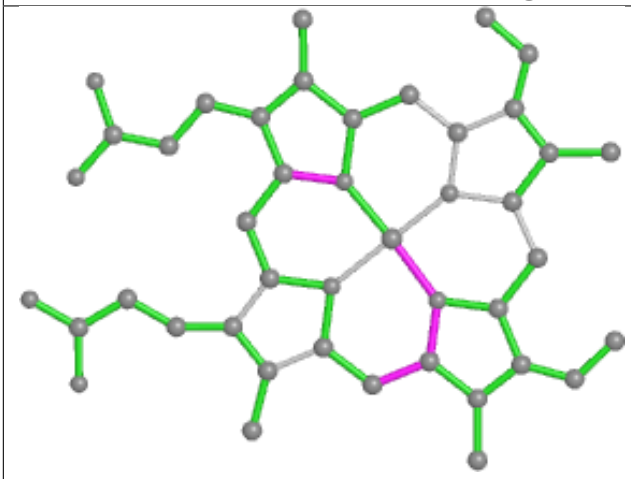
Bond angles



Torsions

Rings

Ligand HEM F 601



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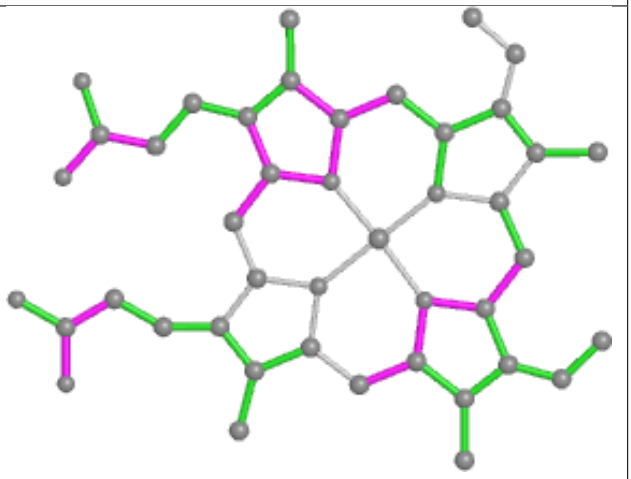

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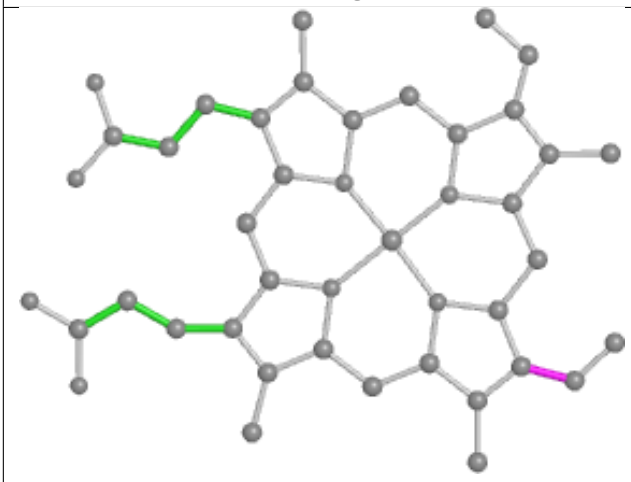

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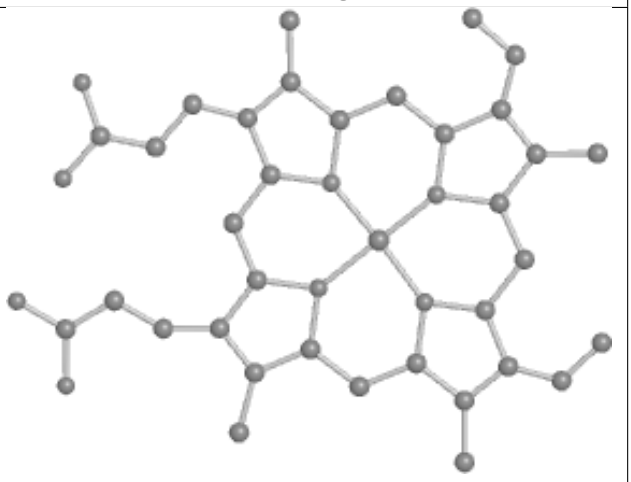
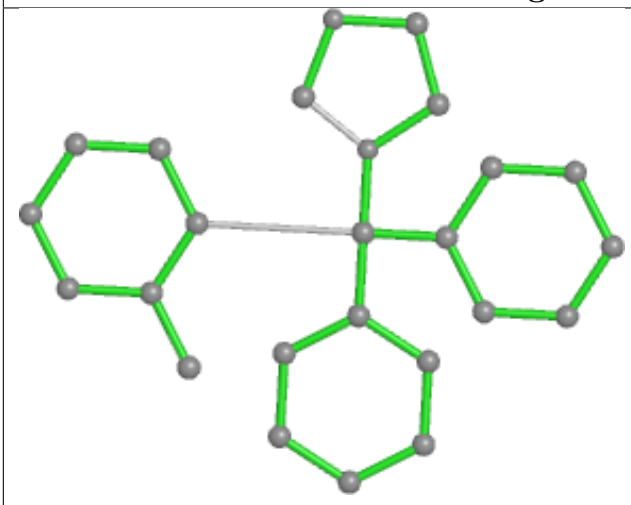


Rings

Ligand CL6 D 602



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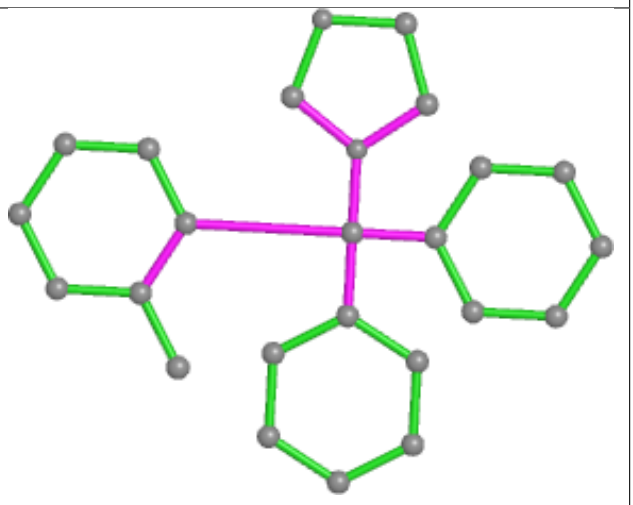

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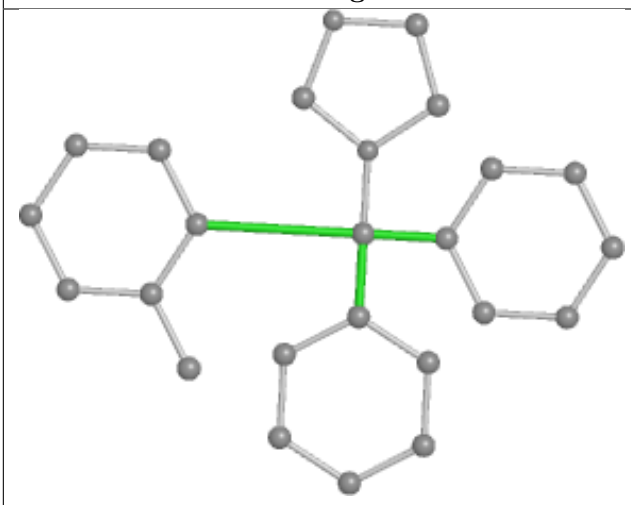

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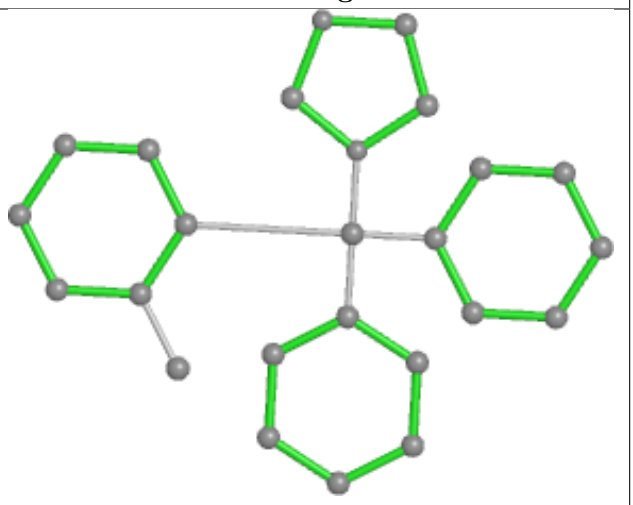
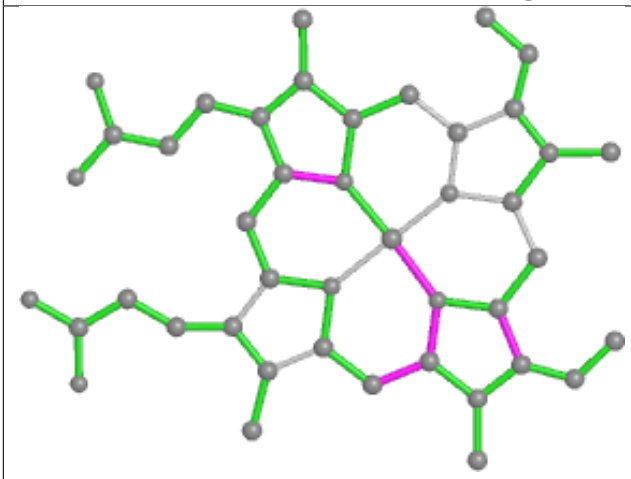


Rings

Ligand HEM E 601



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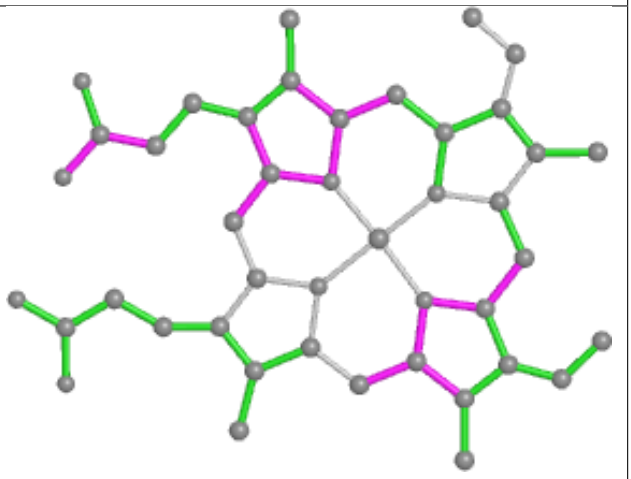

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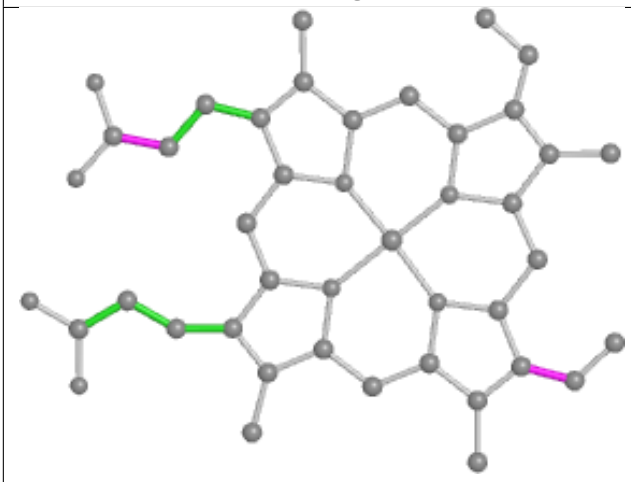

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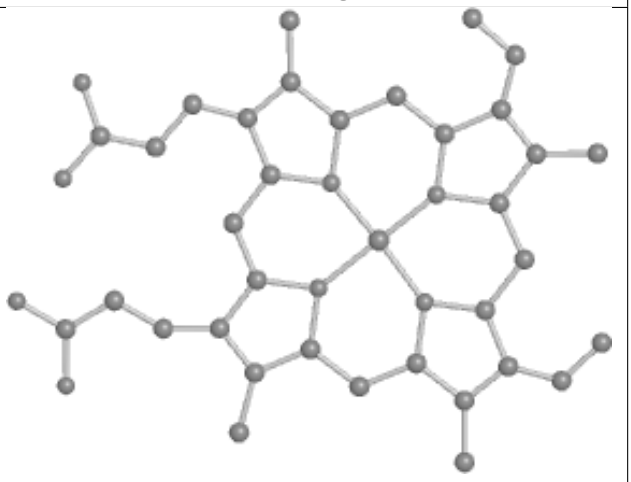
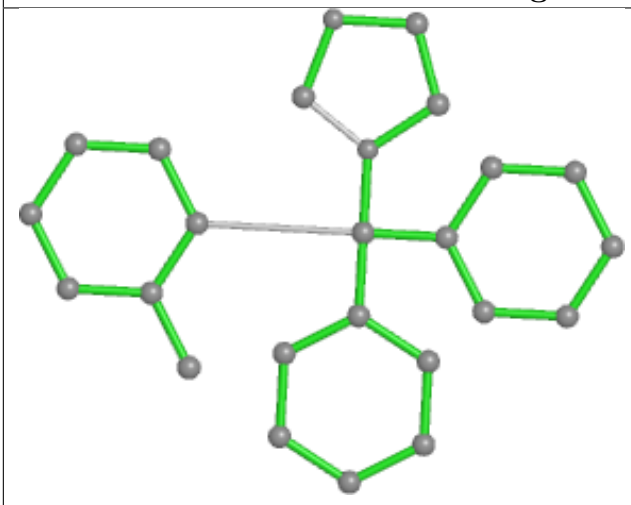


Rings

Ligand CL6 E 602



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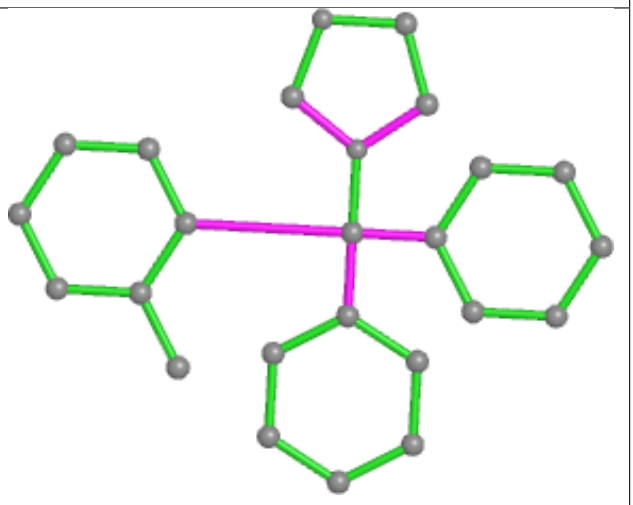
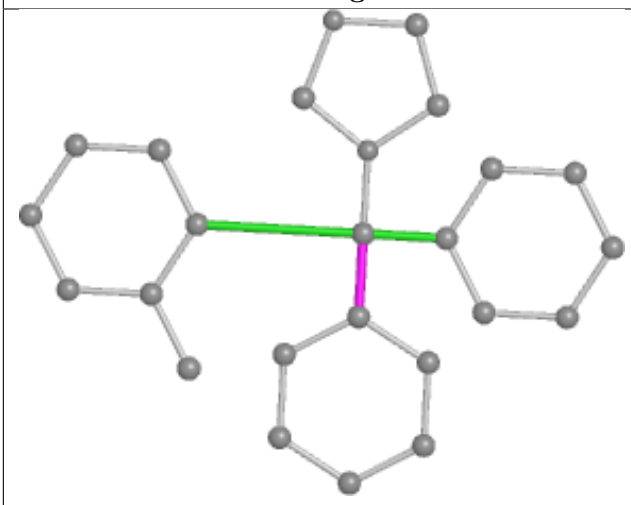


Bond angles



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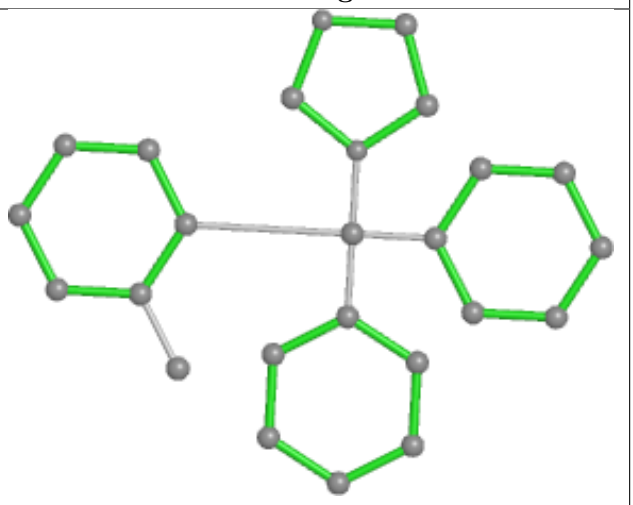
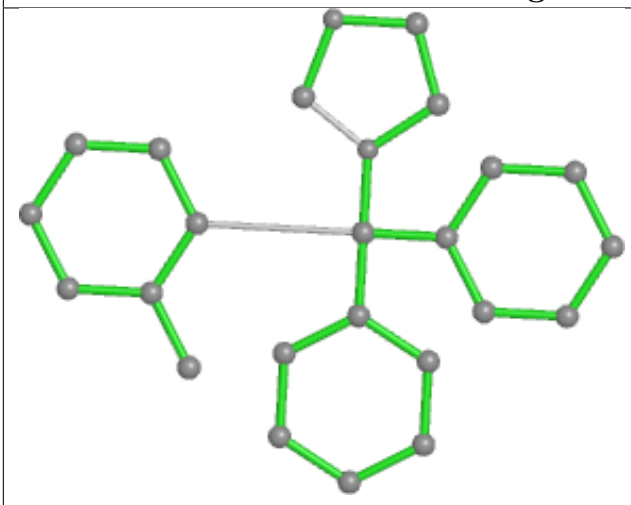


Rings

Ligand CL6 G 603



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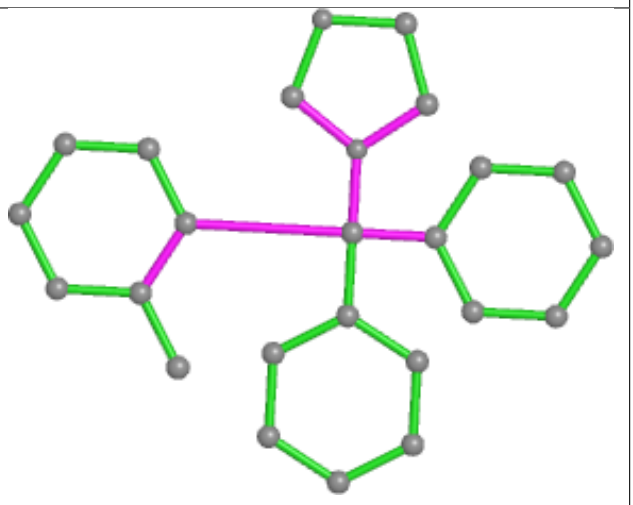
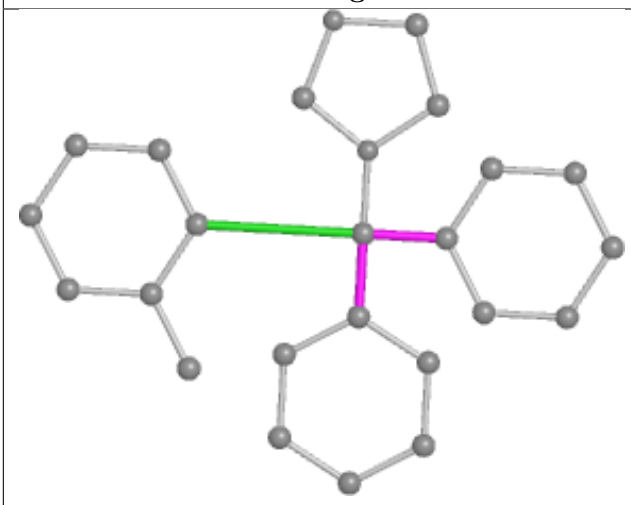


Bond angles



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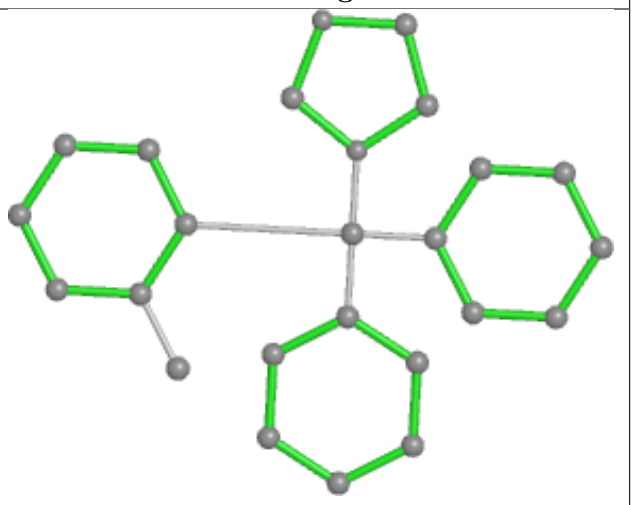
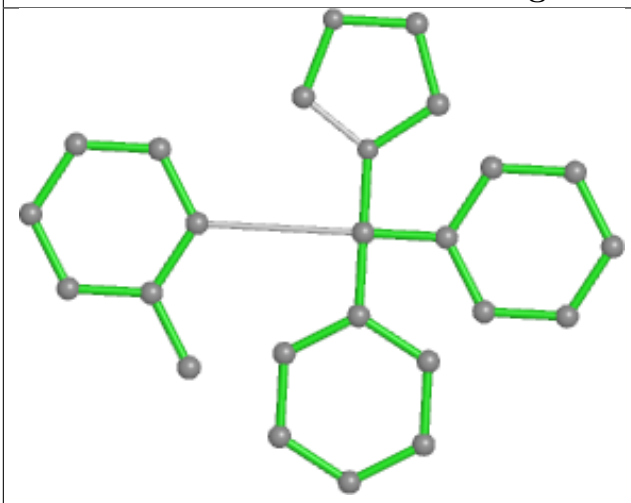


Rings

Ligand CL6 C 603



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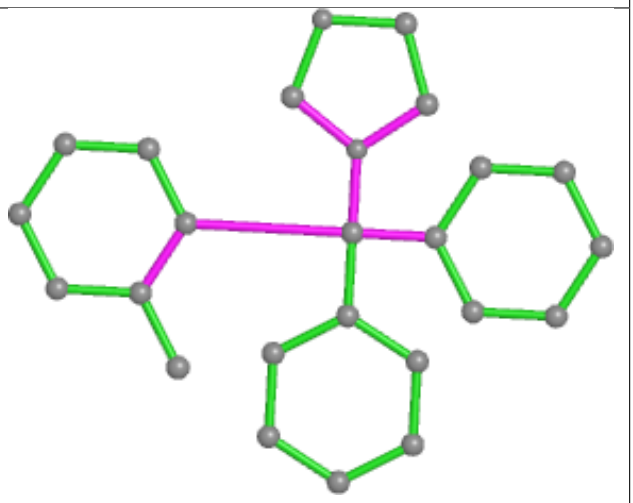
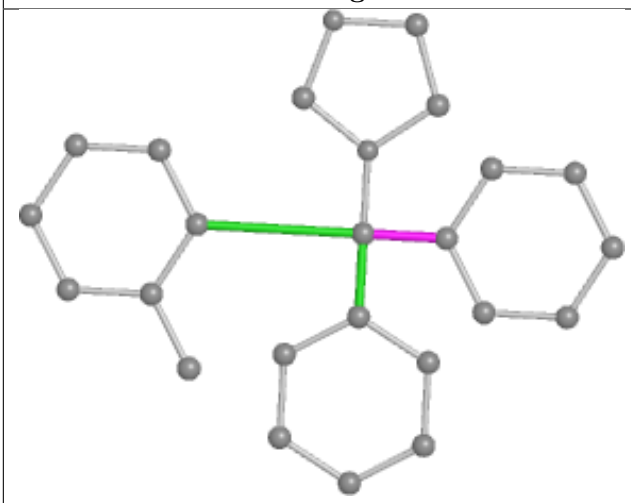


Bond angles



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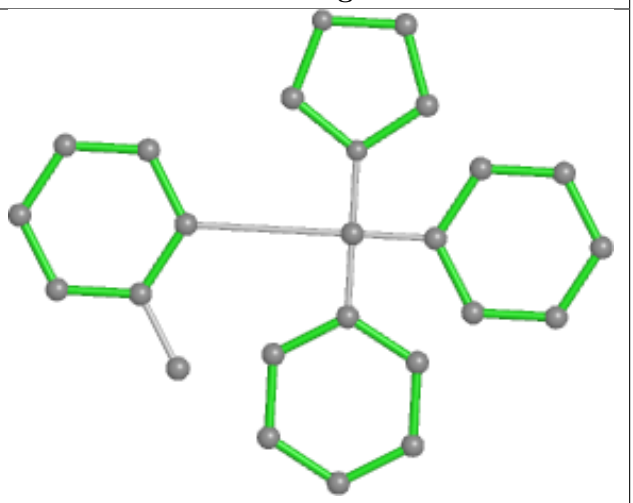
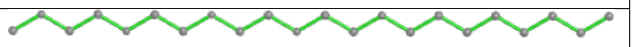


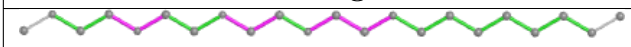
Rings

Ligand CE9 E 605

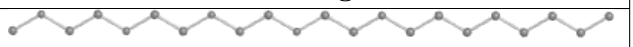
Bond lengths



Bond angles

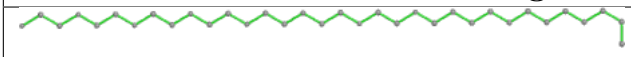


Torsions

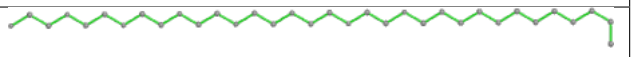


Rings

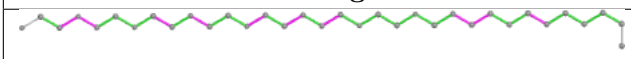
Ligand CE9 B 605



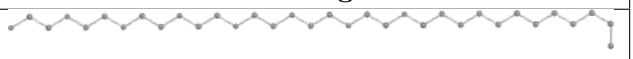
Bond lengths



Bond angles

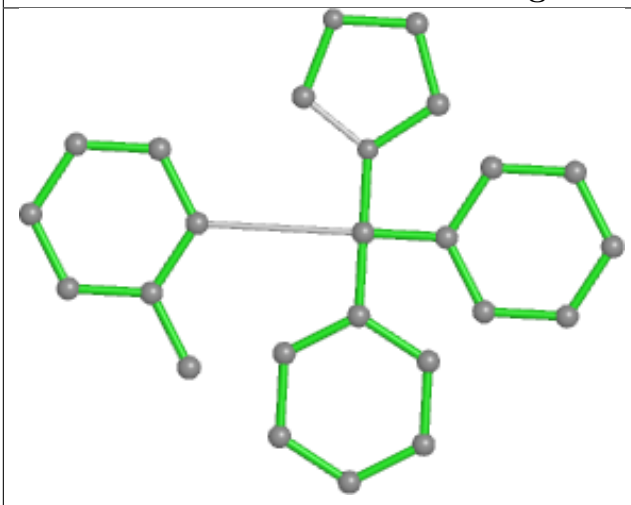


Torsions

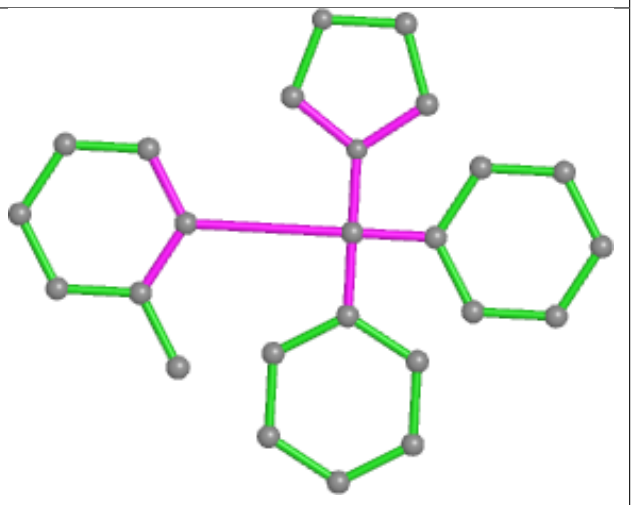


Rings

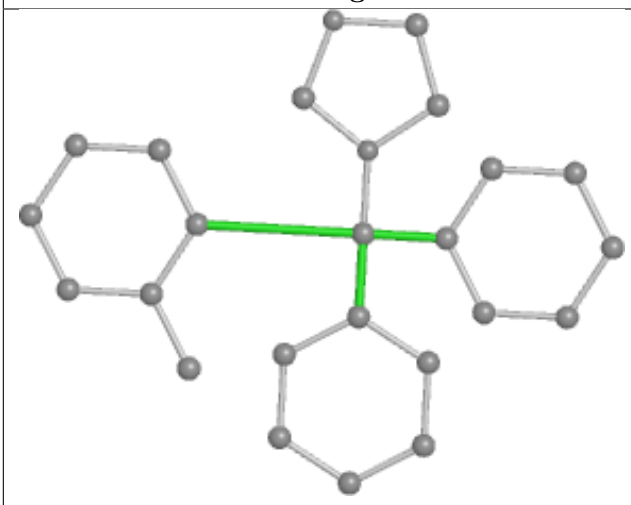
Ligand CL6 C 604



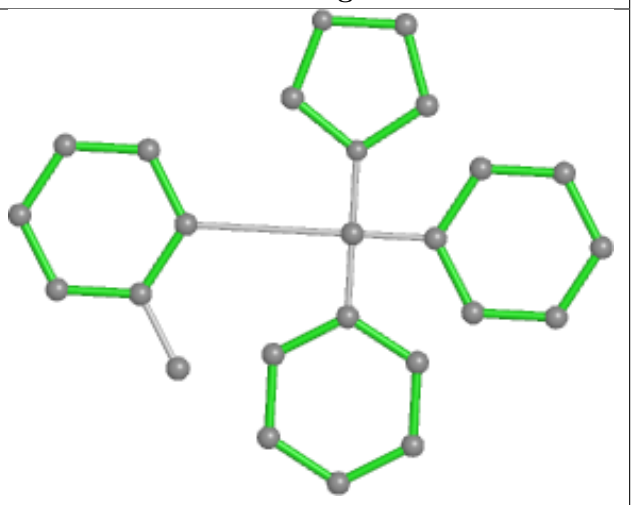
Bond lengths



Bond angles

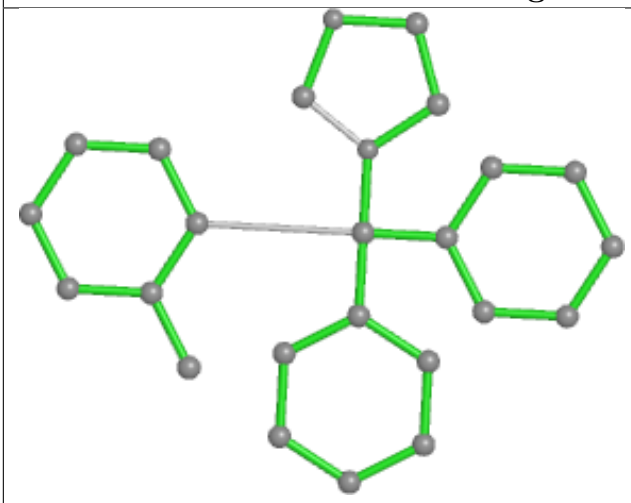


Torsions



Rings

Ligand CL6 H 604



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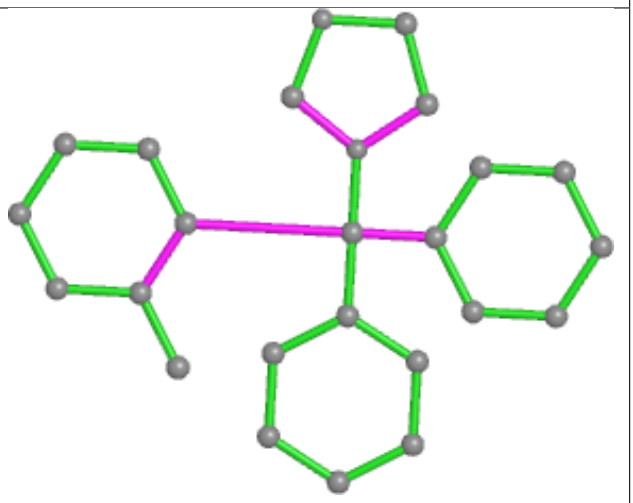

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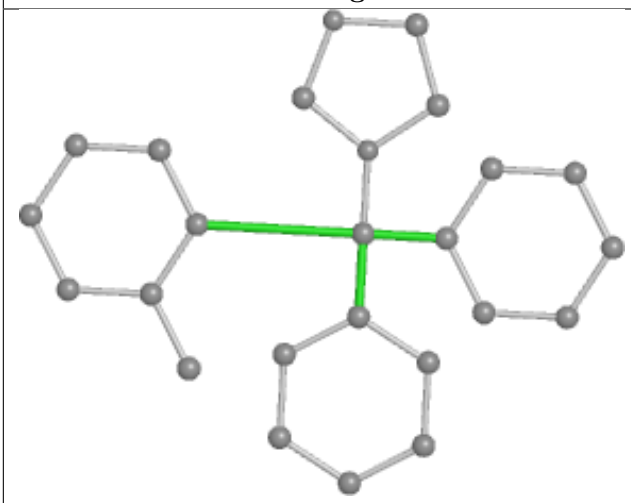
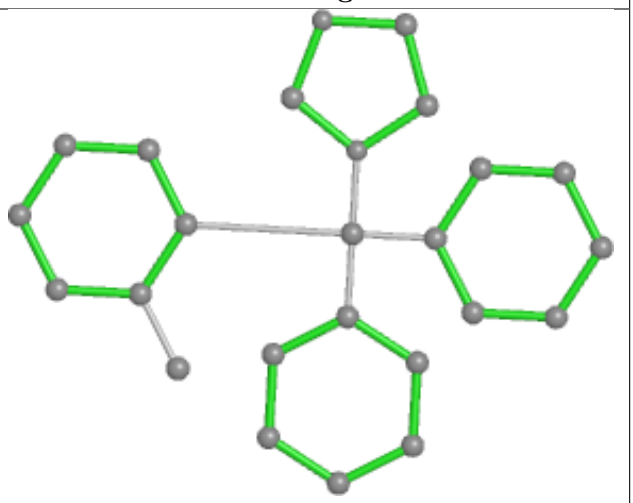
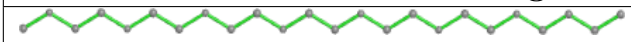


Torsions



Rings

Ligand CE9 C 605



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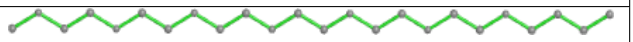

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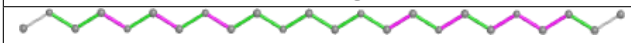


Torsions

Rings

Ligand CE9 G 605

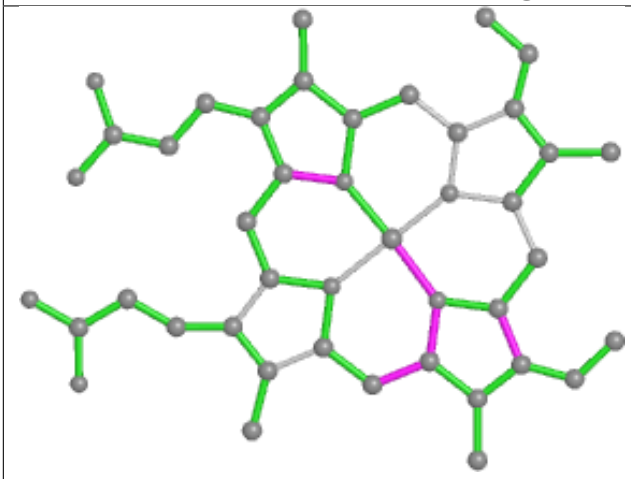
Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 601



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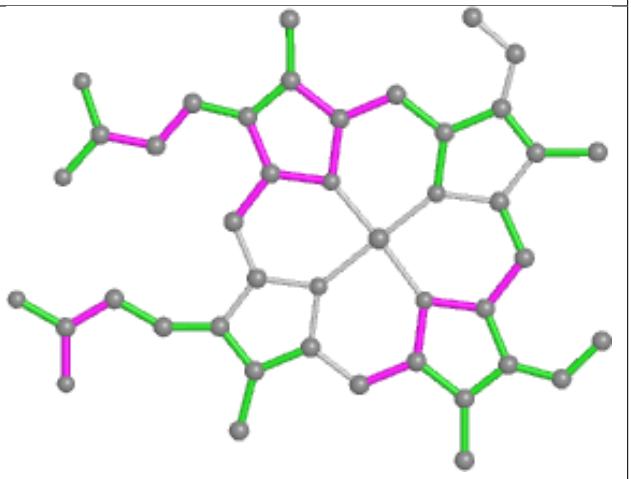
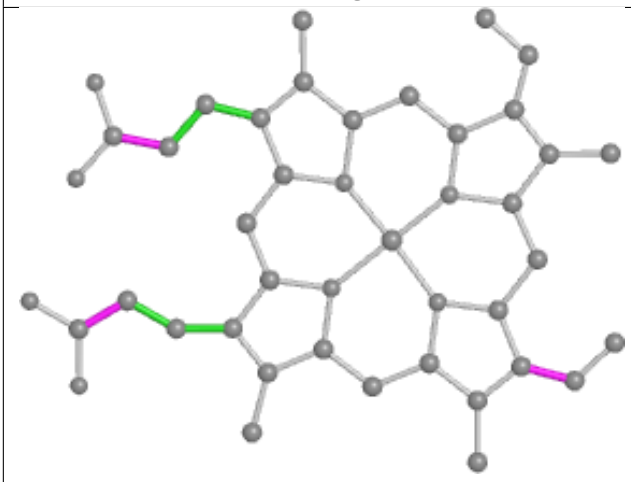


Bond angles



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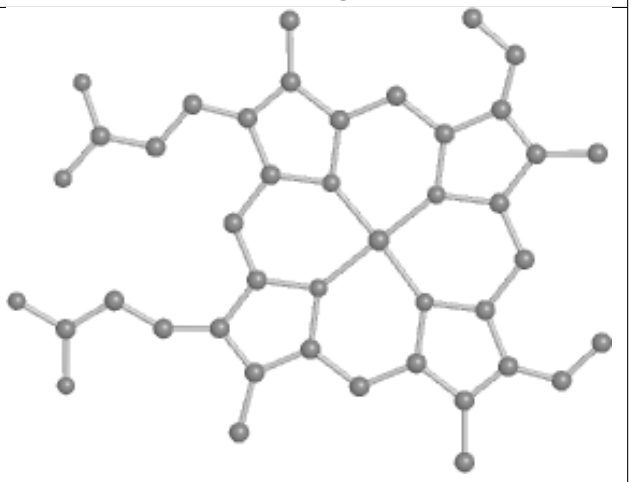
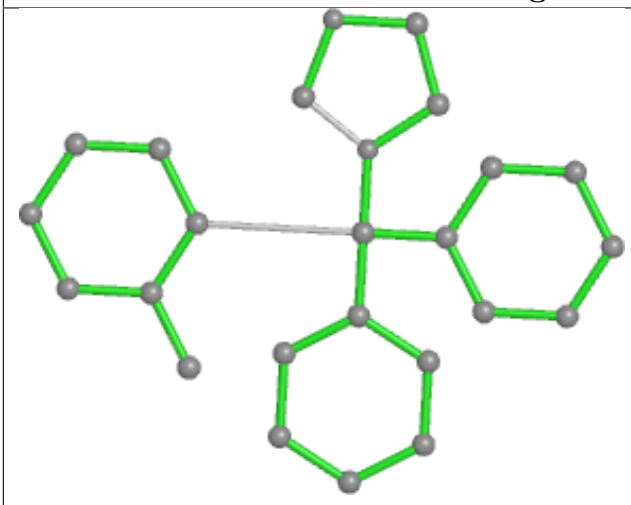


Rings

Ligand CL6 B 604



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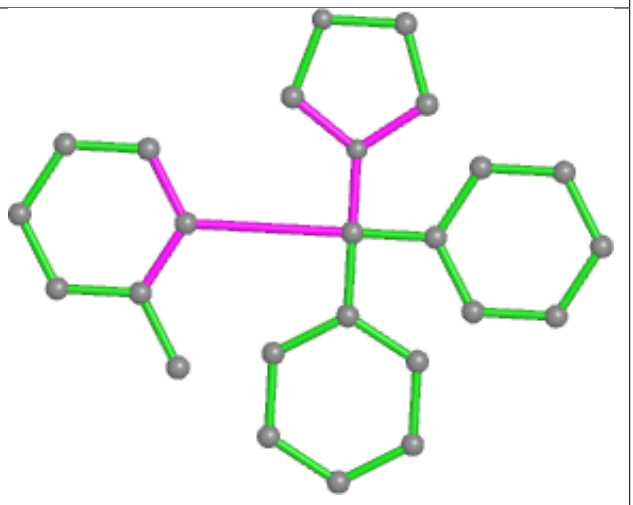
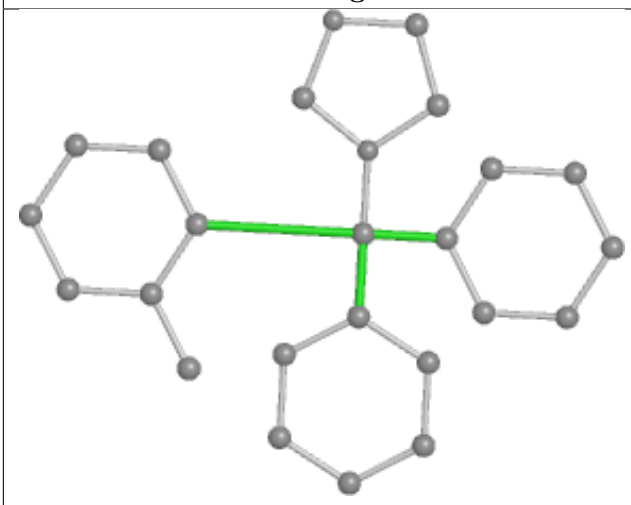


Bond angles



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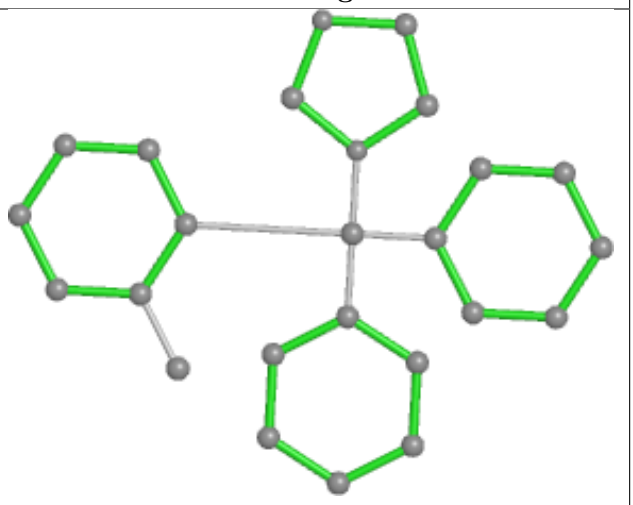
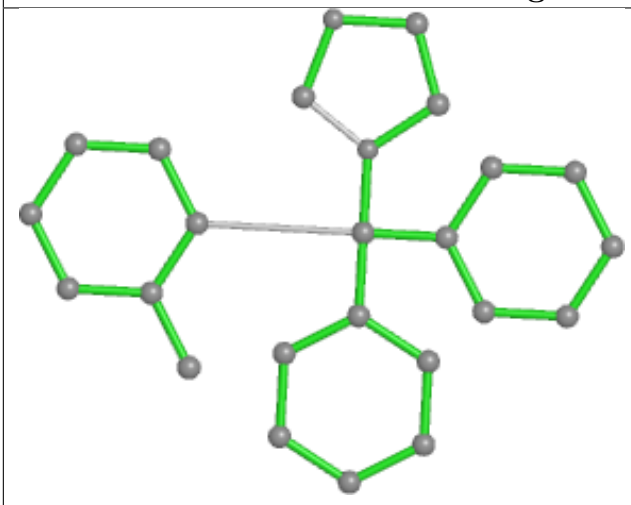


Rings

Ligand CL6 G 604



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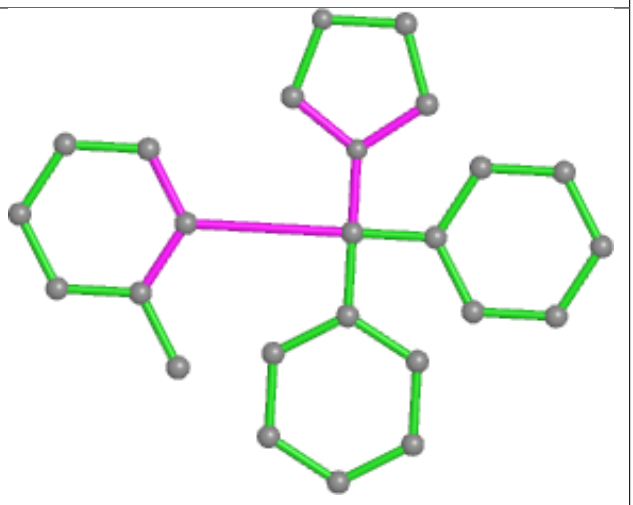

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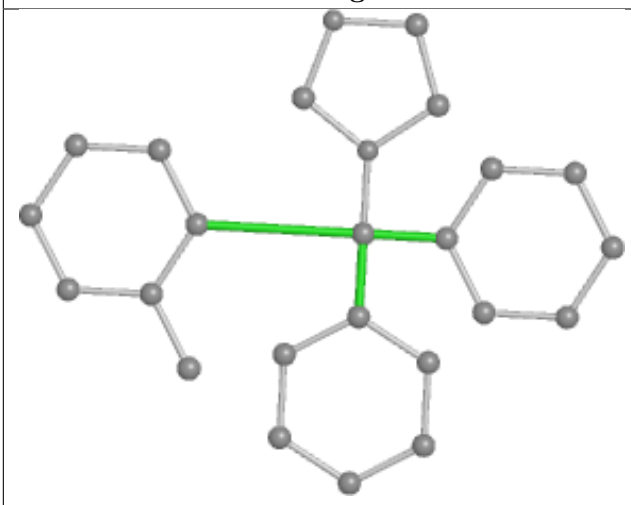

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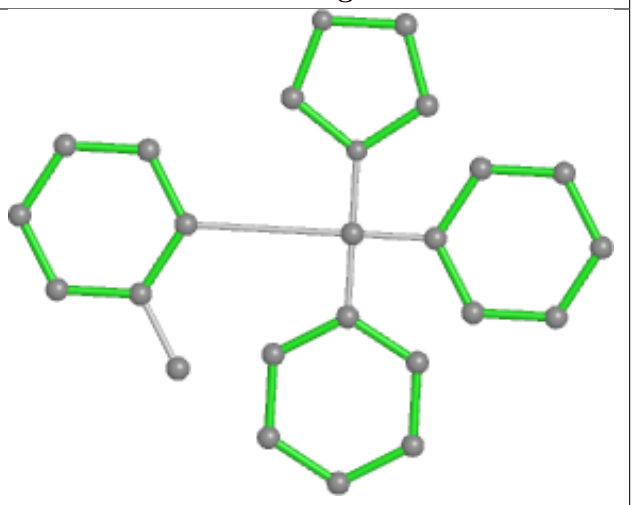
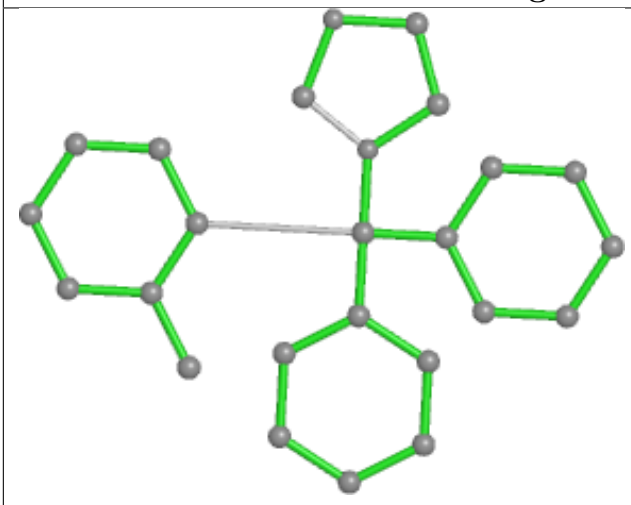


Rings

Ligand CL6 B 602



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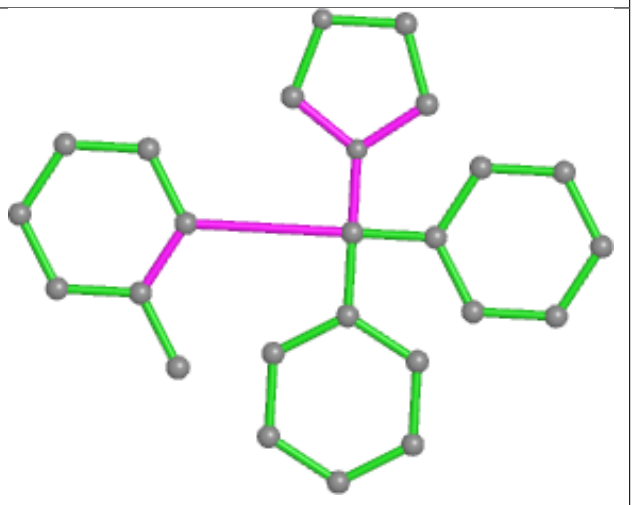

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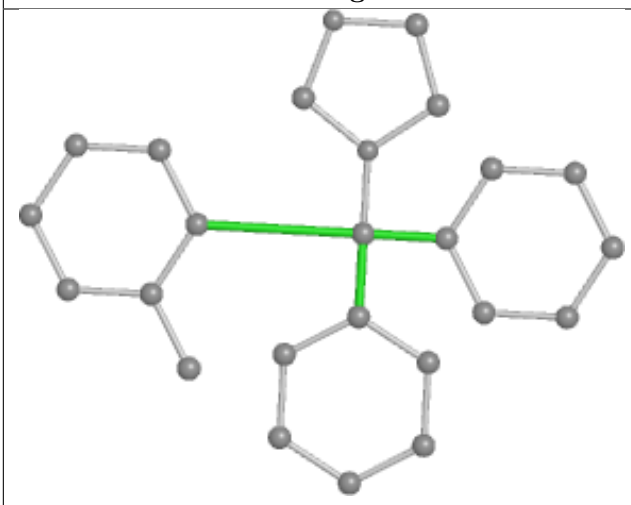

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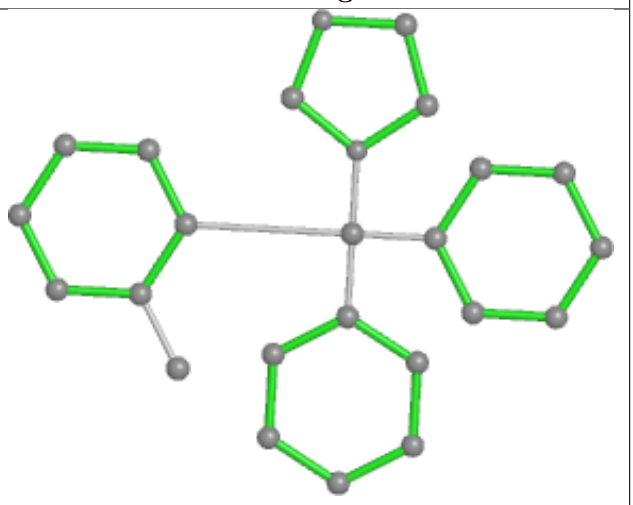
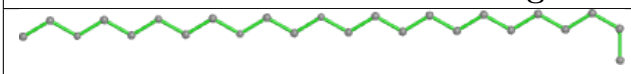


Rings

Ligand CE9 D 605



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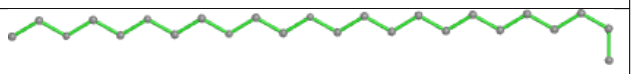
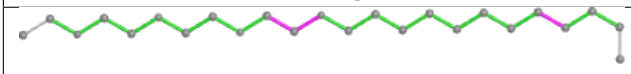


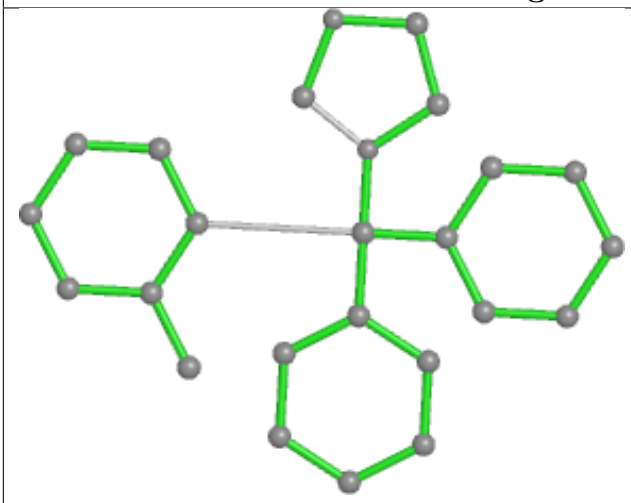
Bond angles



Torsions

Rings

Ligand CL6 H 602



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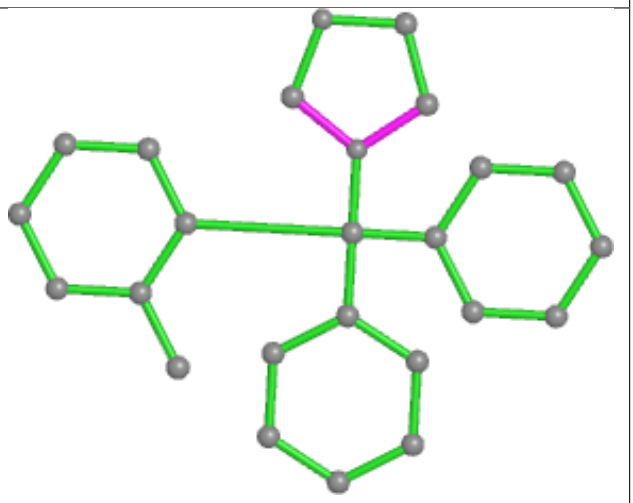
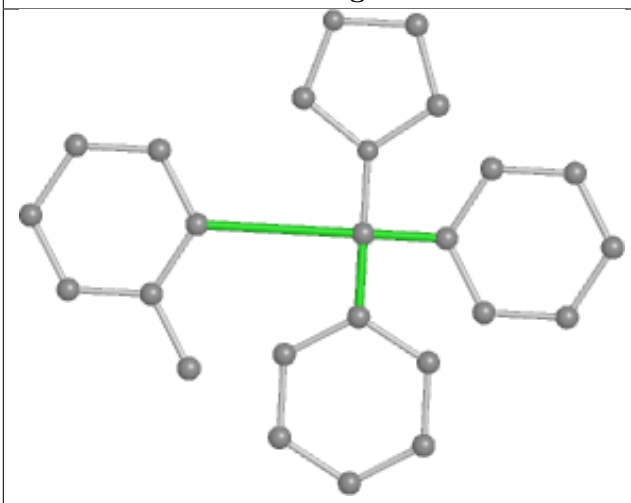


Bond angles



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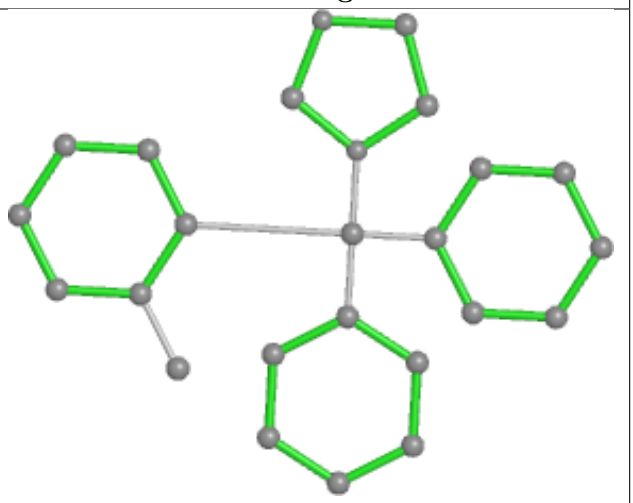
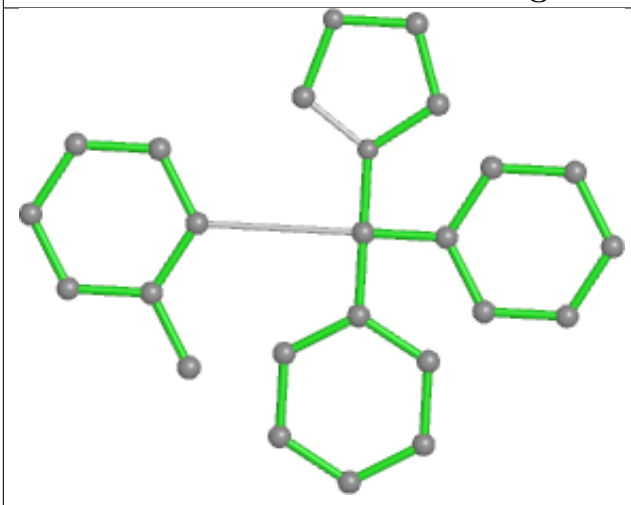


Rings

Ligand CL6 E 604



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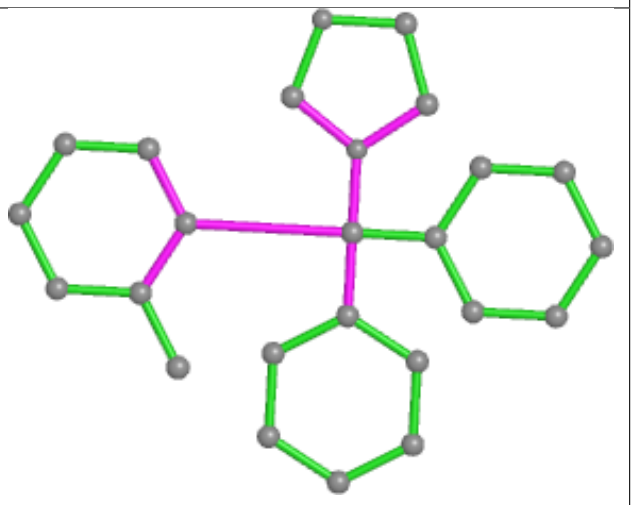
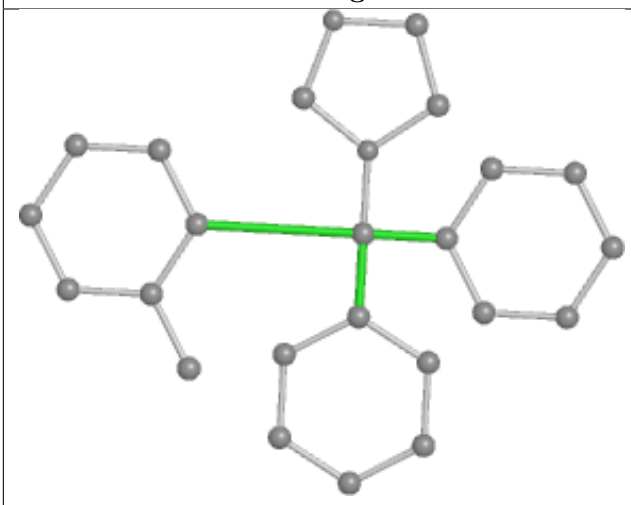


Bond angles



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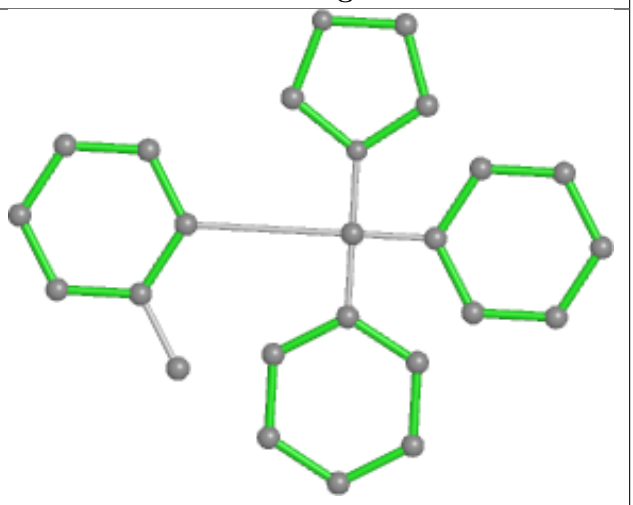
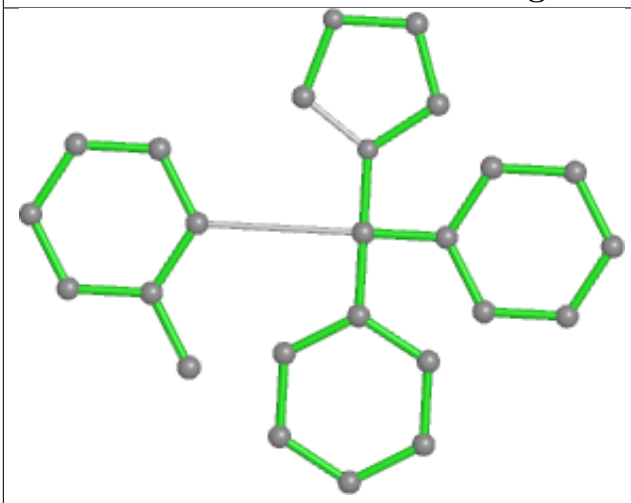
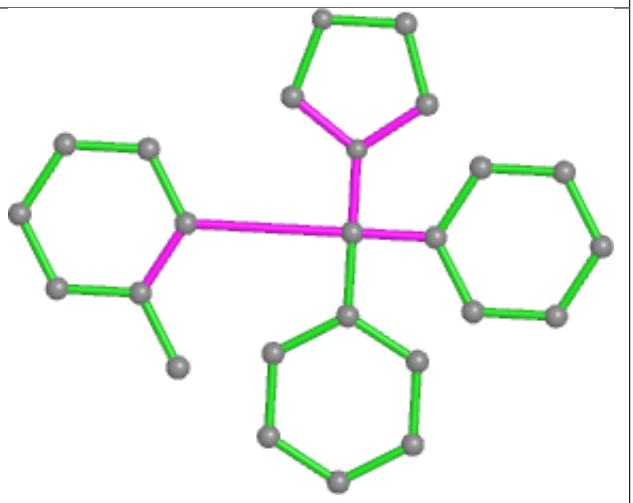


Rings

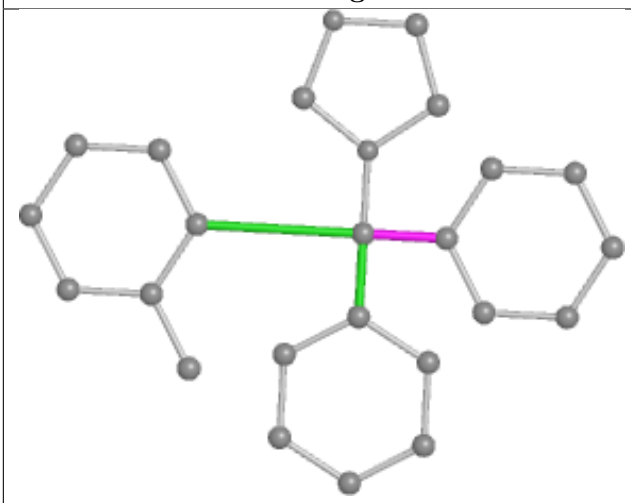
Ligand CL6 D 603



Bond lengths



Bond angles



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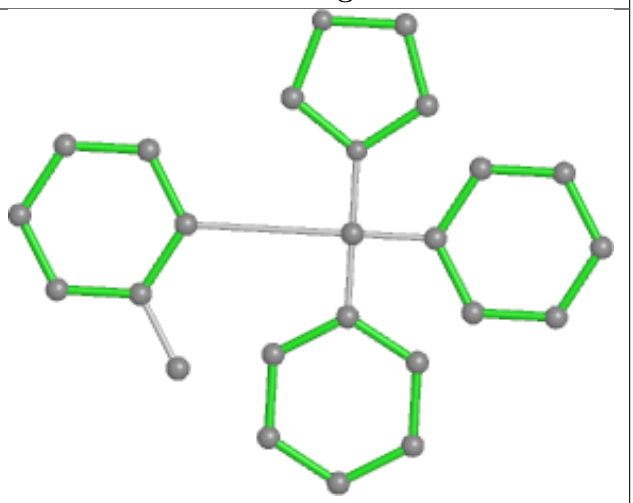
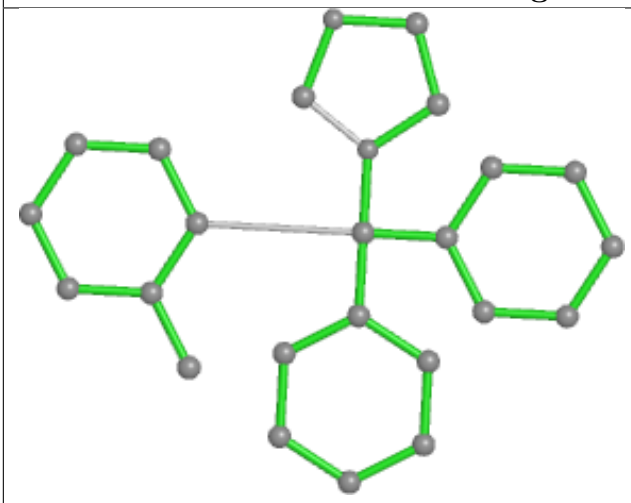


Rings

Ligand CL6 F 602



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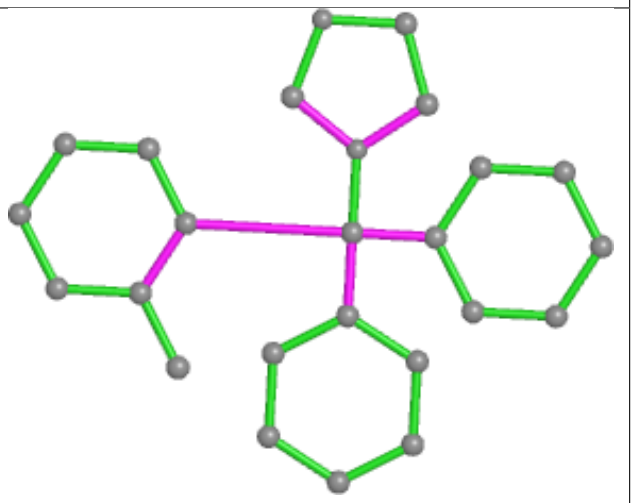
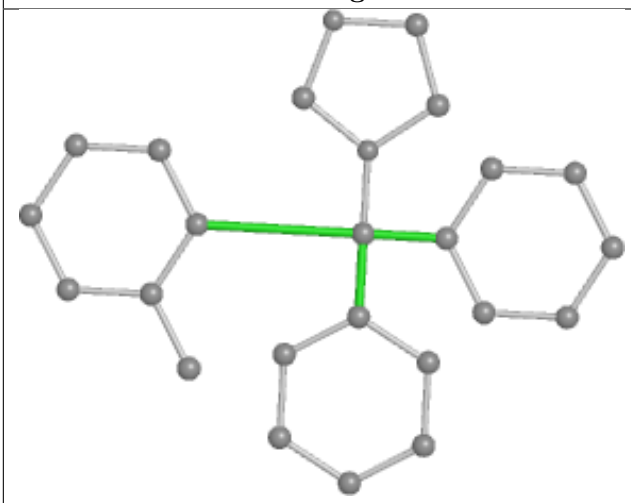
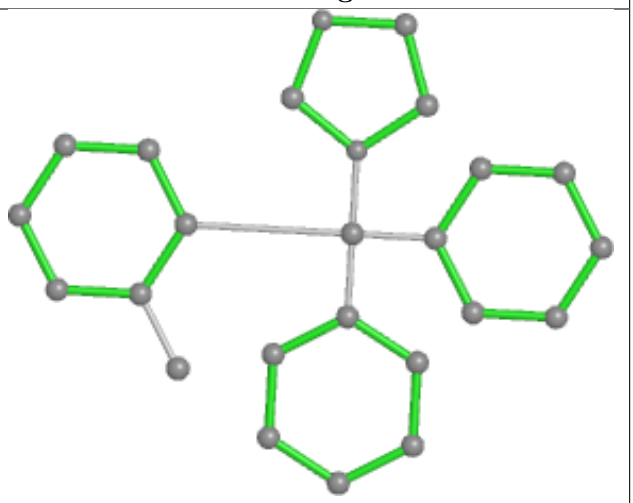


Bond angles

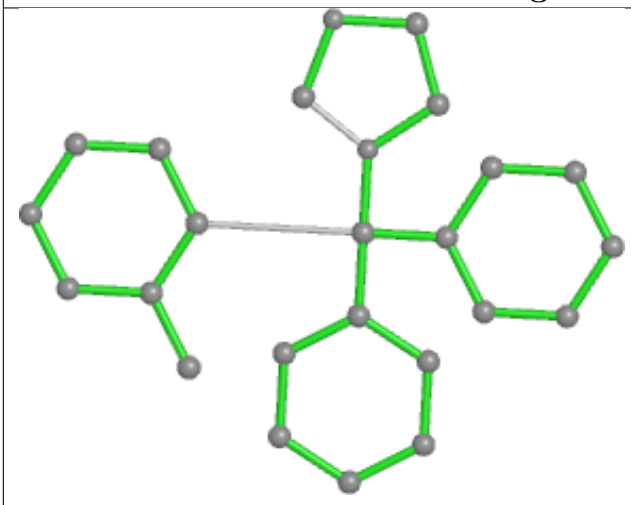


Torsions

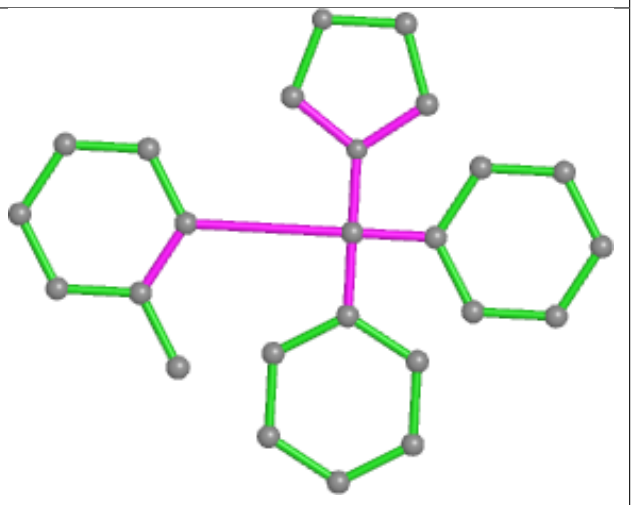


Rings

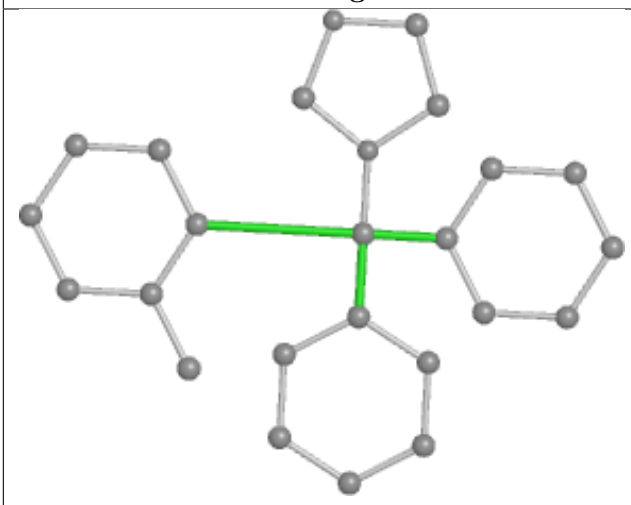
Ligand CL6 E 603



Bond lengths



Bond angles



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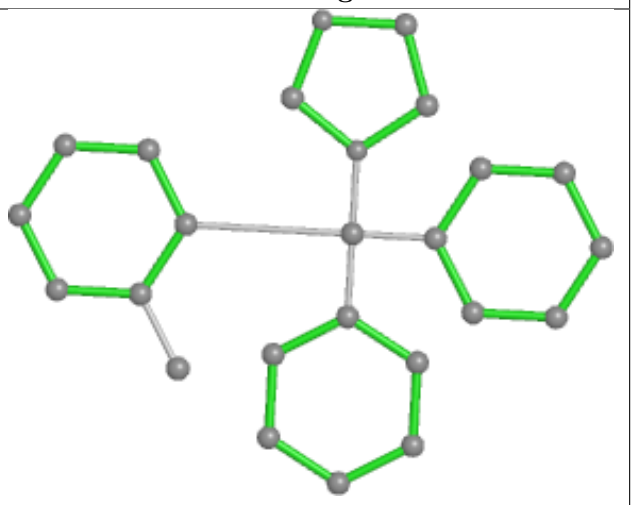
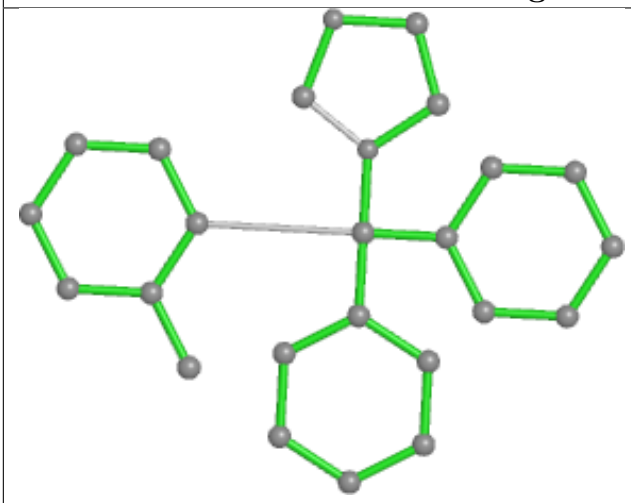


Rings

Ligand CL6 A 602



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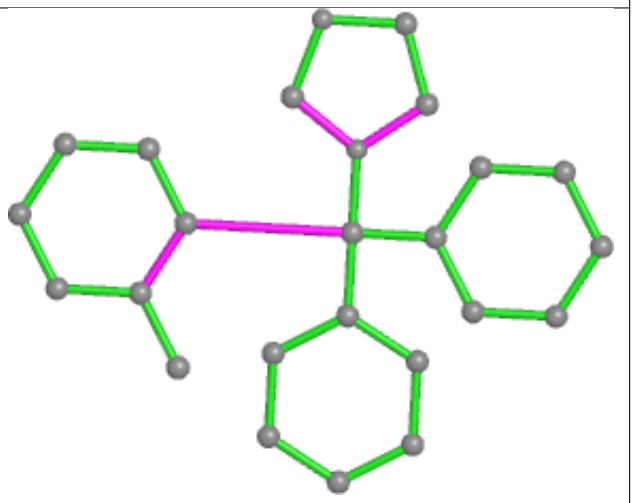
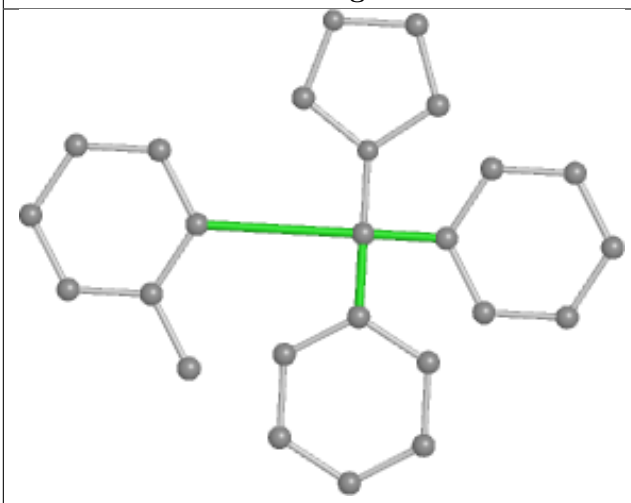


Bond angles



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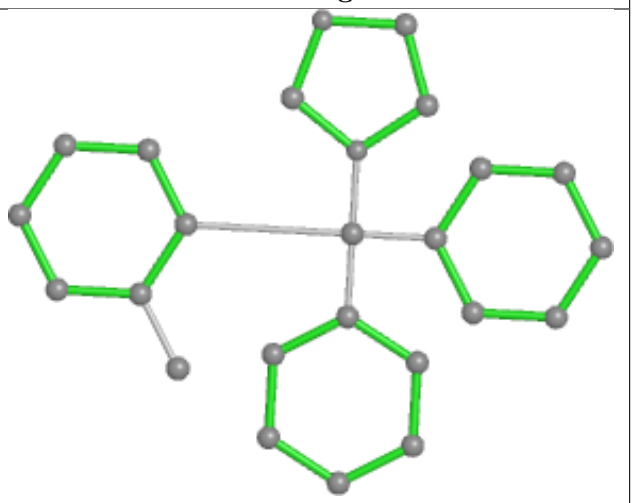
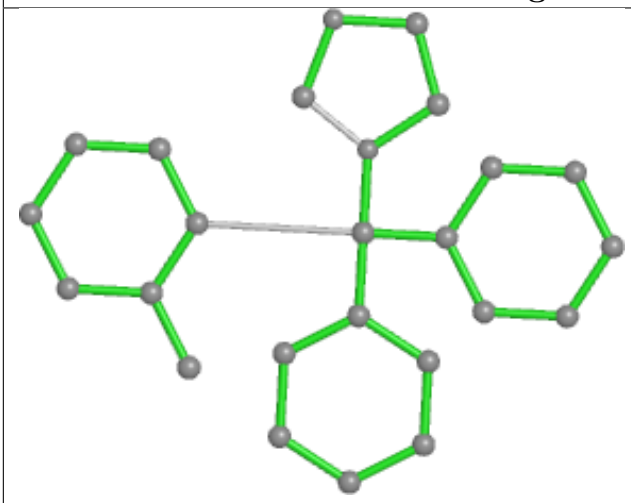
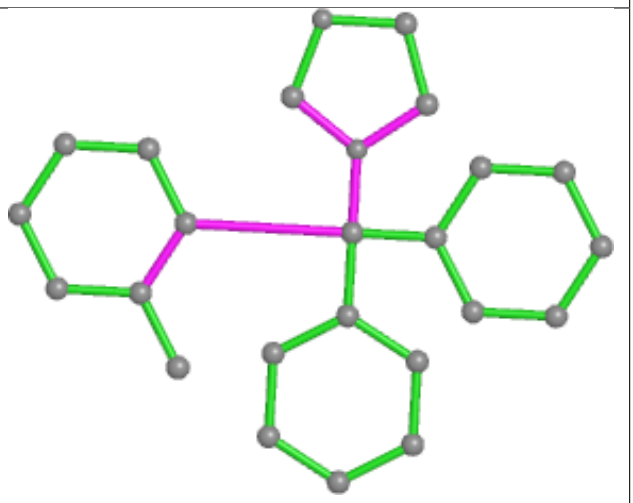


Rings

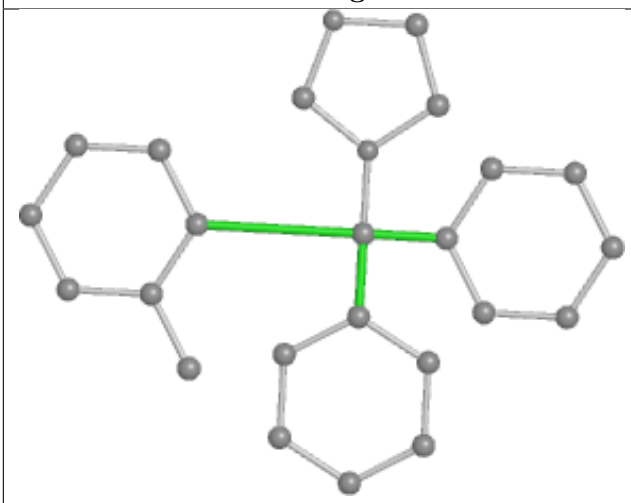
Ligand CL6 A 604



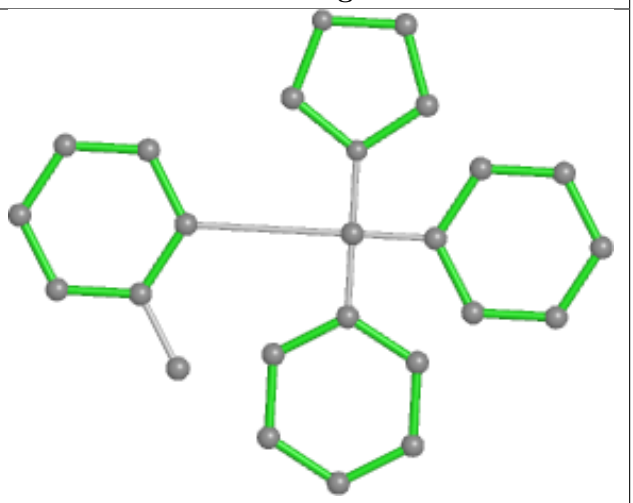
Bond lengths



Bond angles

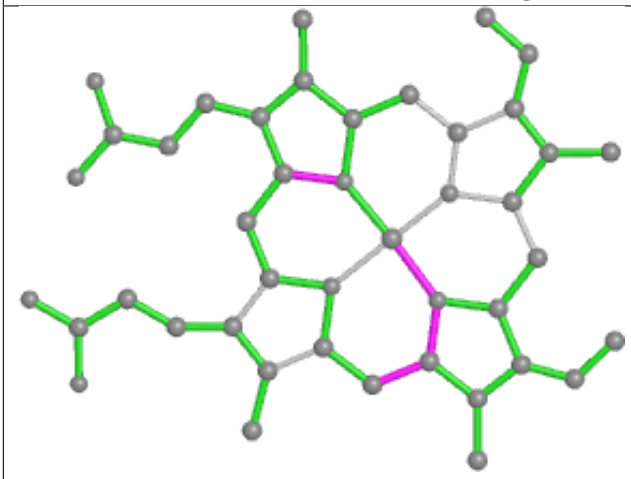


Torsions

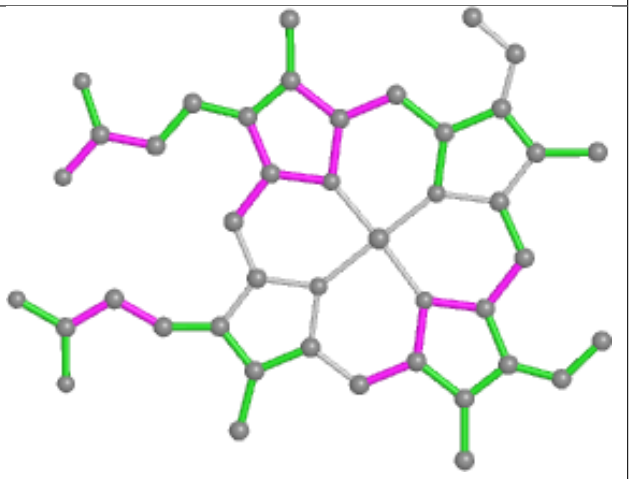


Rings

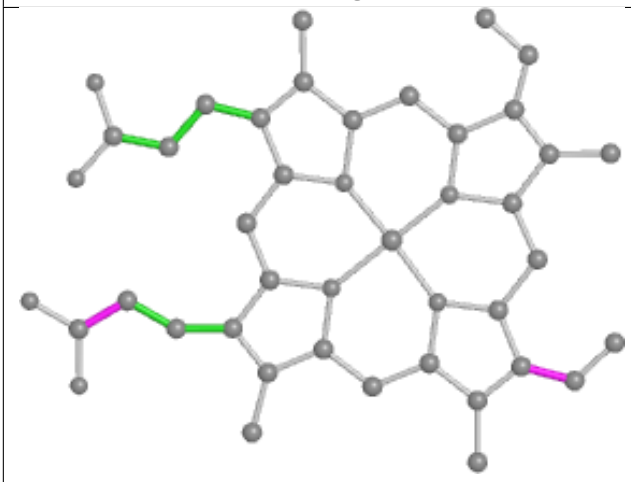
Ligand HEM D 601



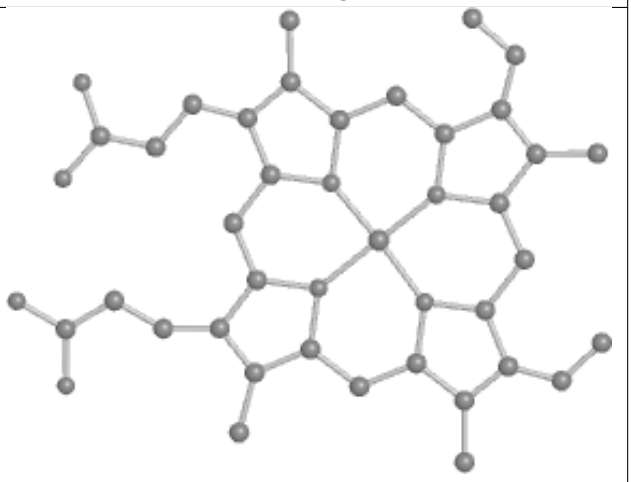
Bond lengths



Bond angles

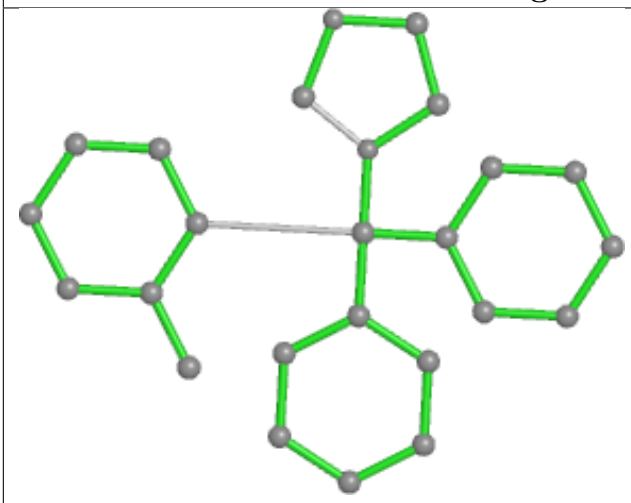


Torsions

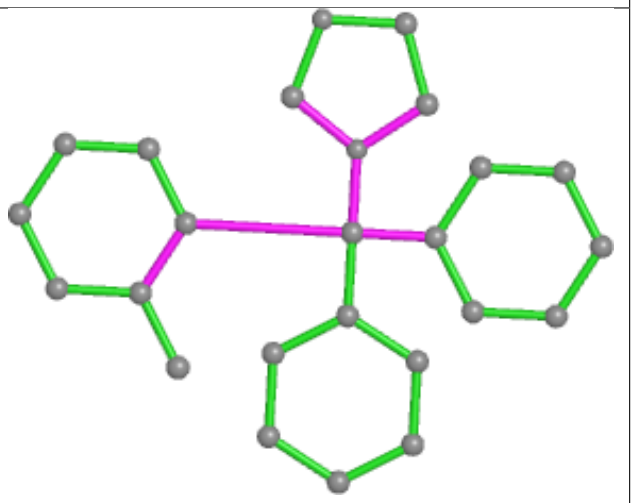


Rings

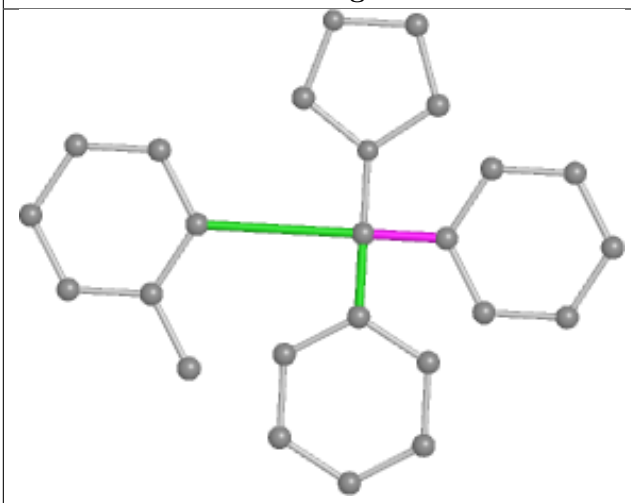
Ligand CL6 F 603



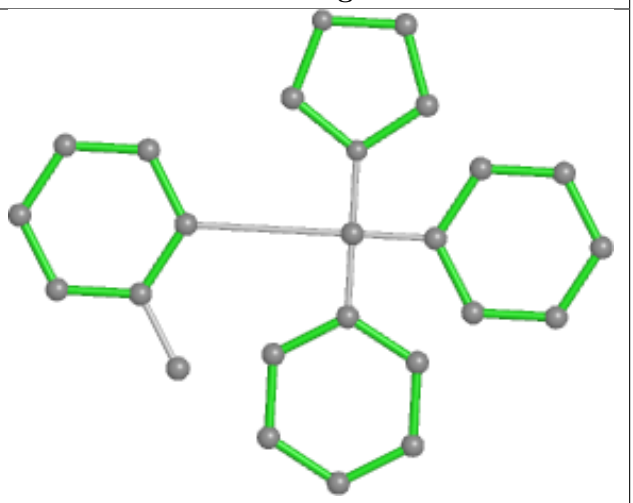
Bond lengths



Bond angles

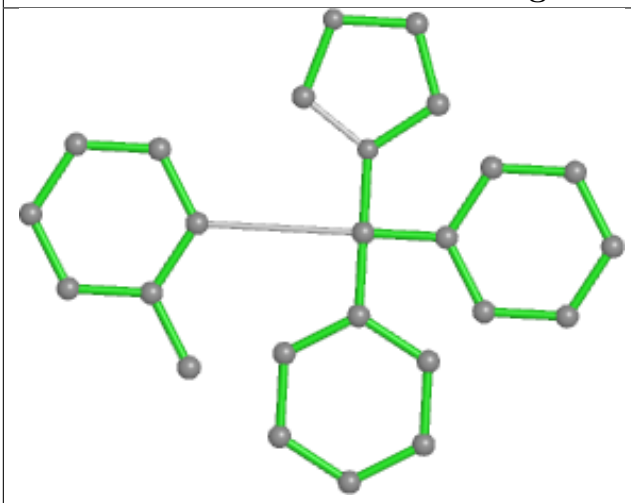


Torsions

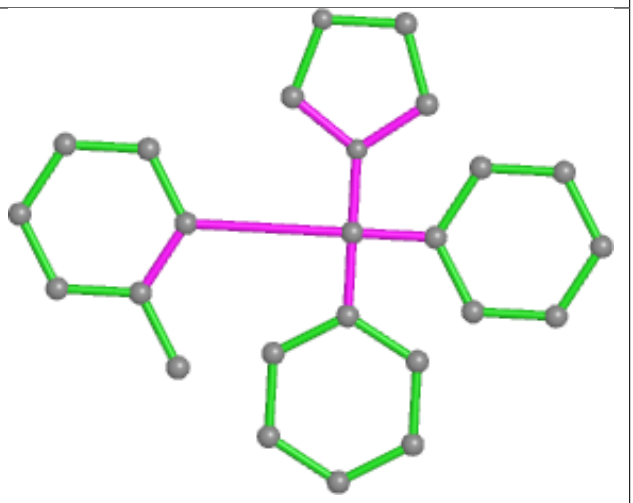


Rings

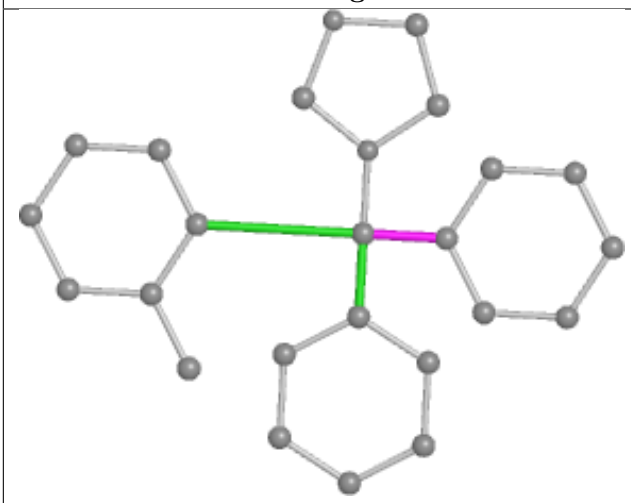
Ligand CL6 B 603



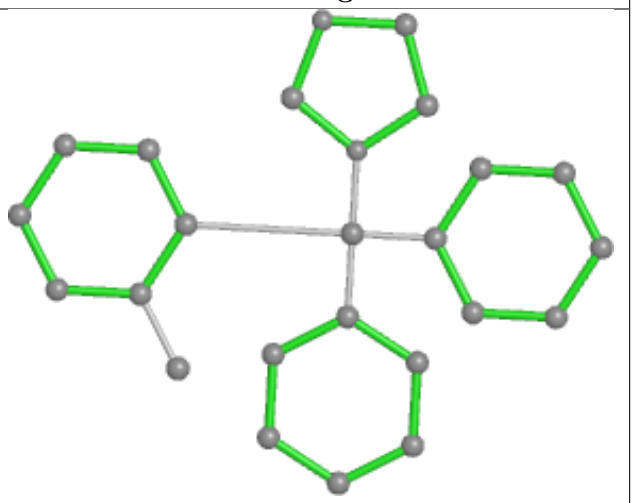
Bond lengths



Bond angles

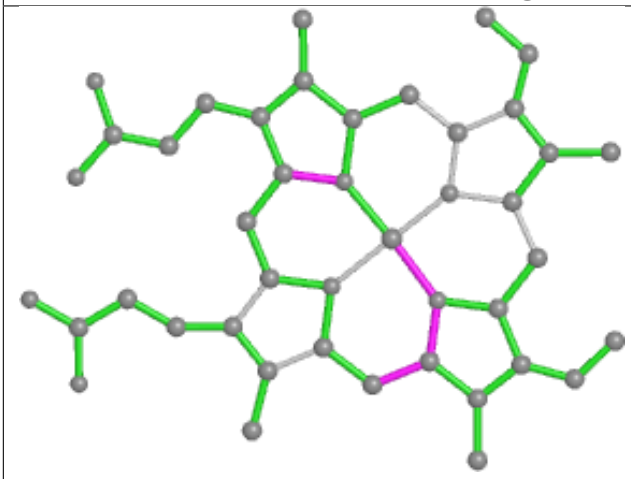


Torsions

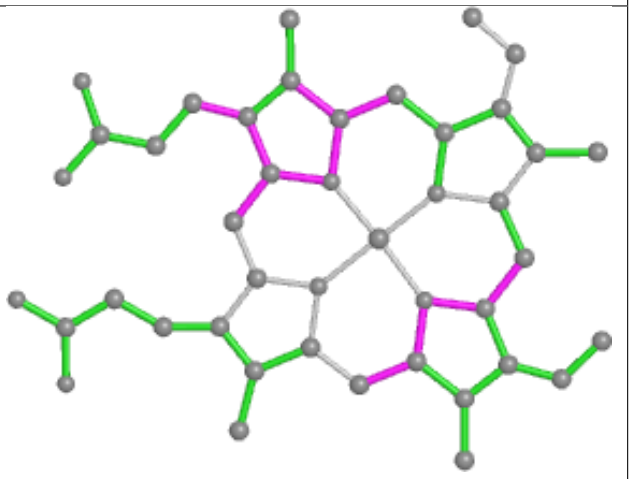


Rings

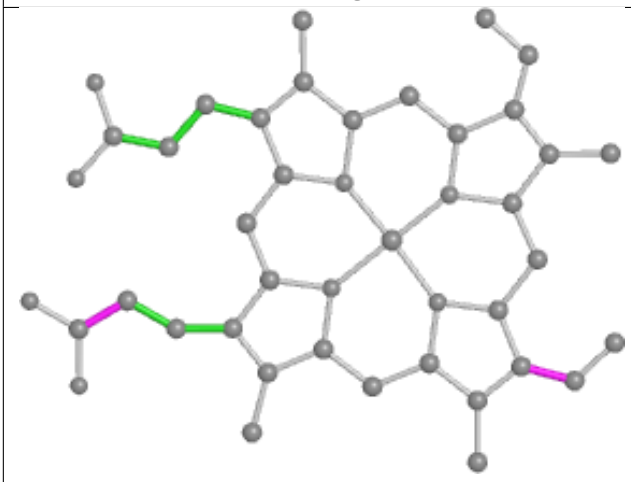
Ligand HEM C 601



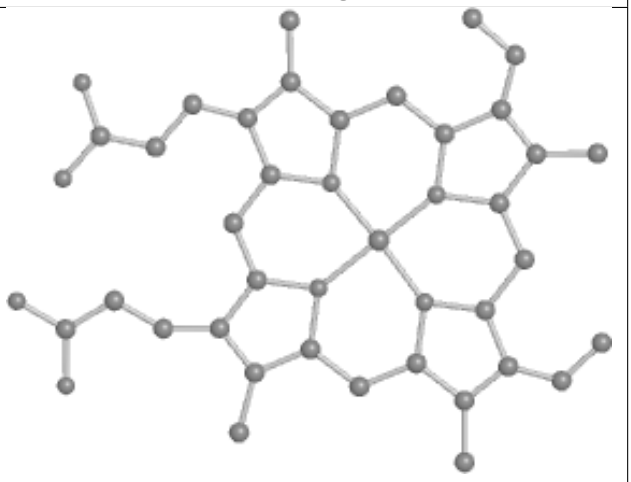
Bond lengths



Bond angles

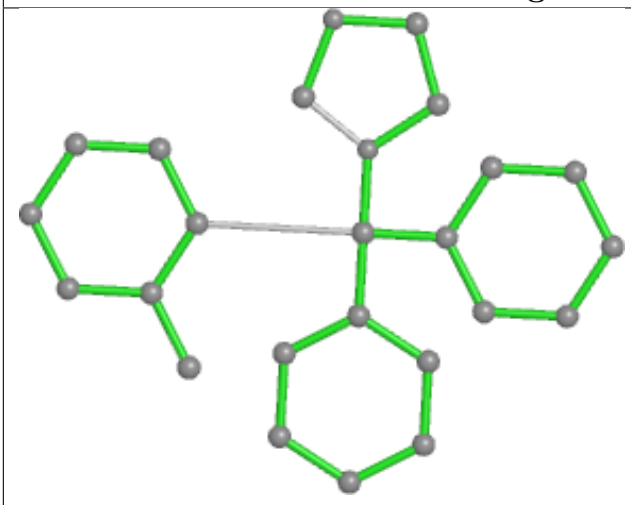


Torsions

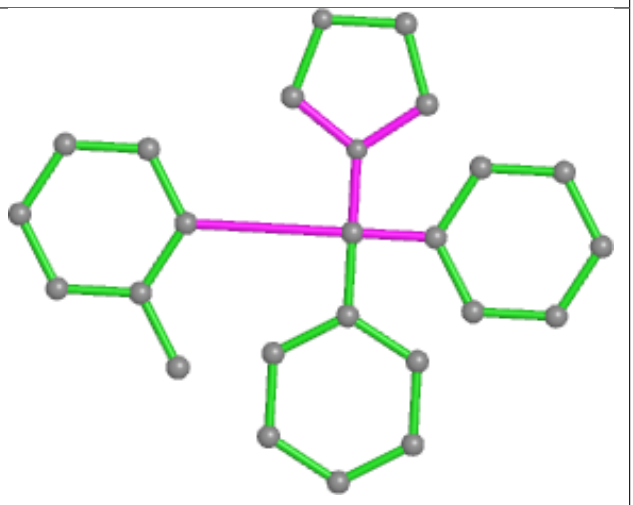


Rings

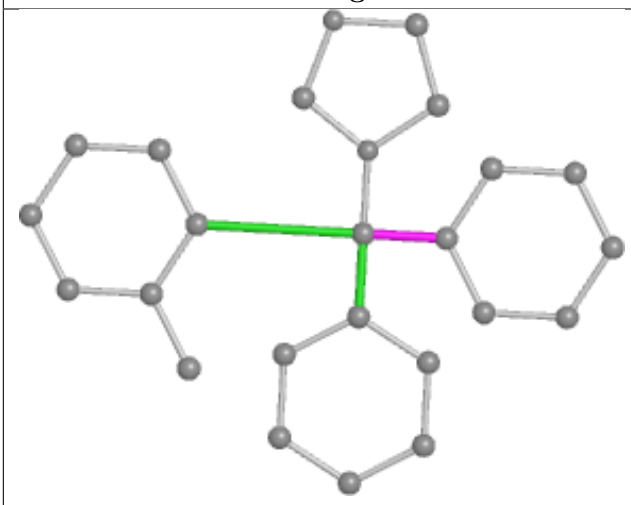
Ligand CL6 H 603



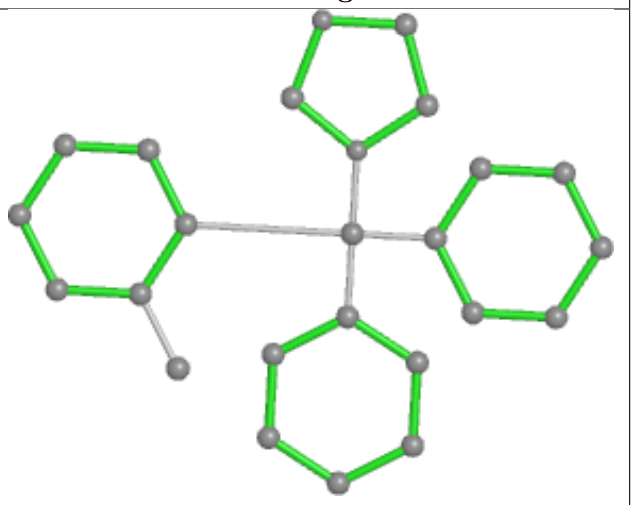
Bond lengths



Bond angles

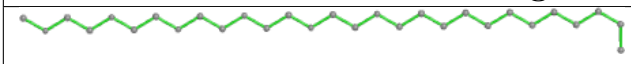


Torsions

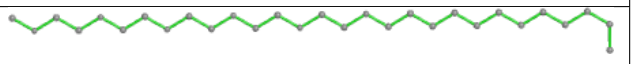


Rings

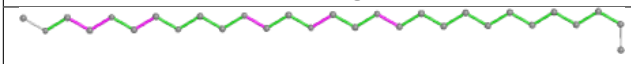
Ligand CE9 F 605



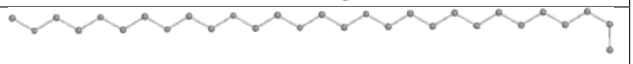
Bond lengths



Bond angles

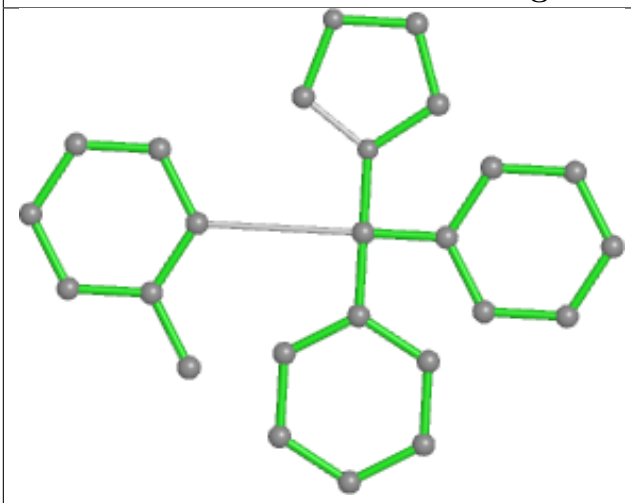


Torsions

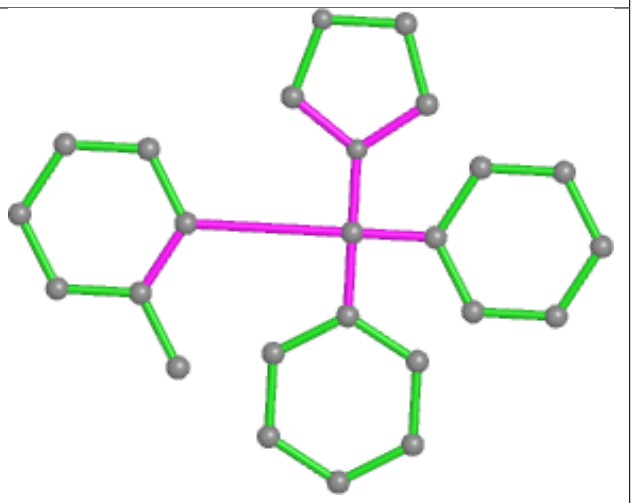


Rings

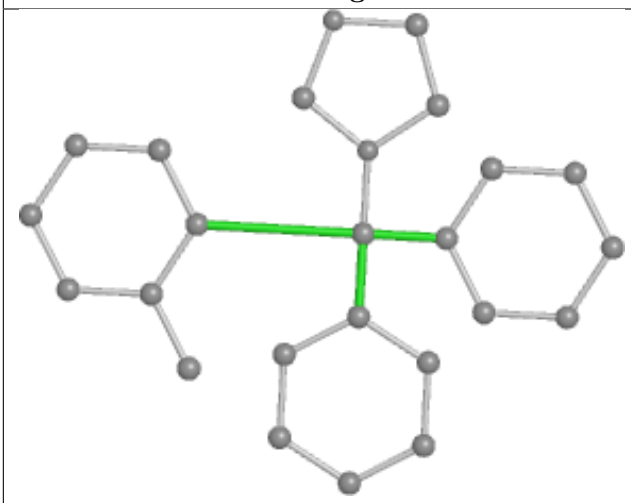
Ligand CL6 F 604



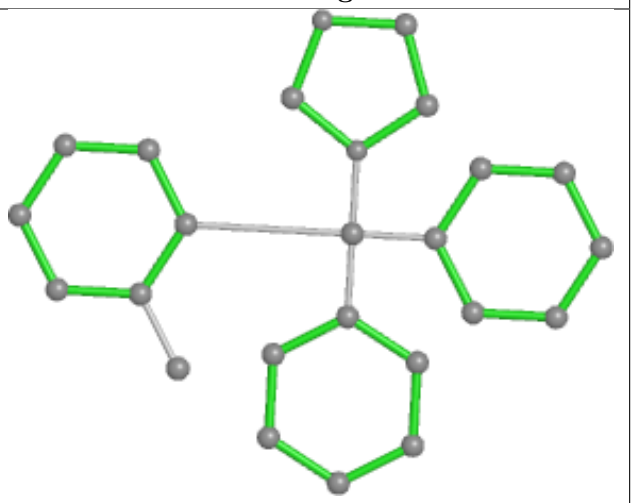
Bond lengths



Bond angles

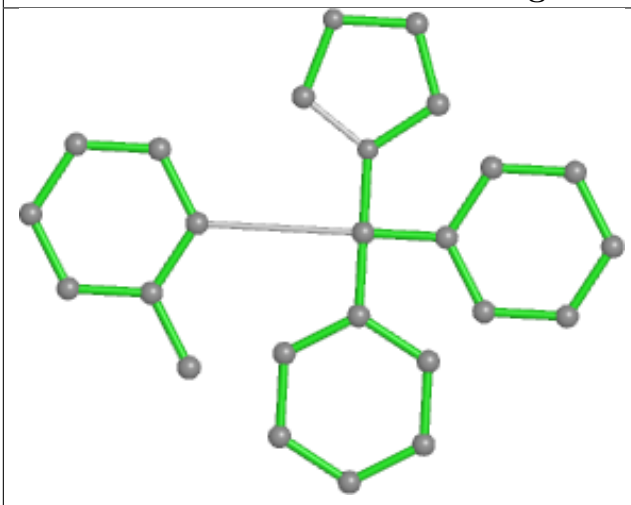


Torsions

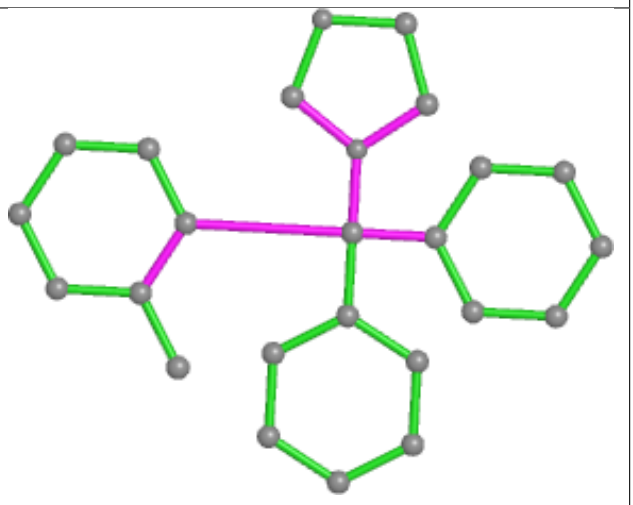


Rings

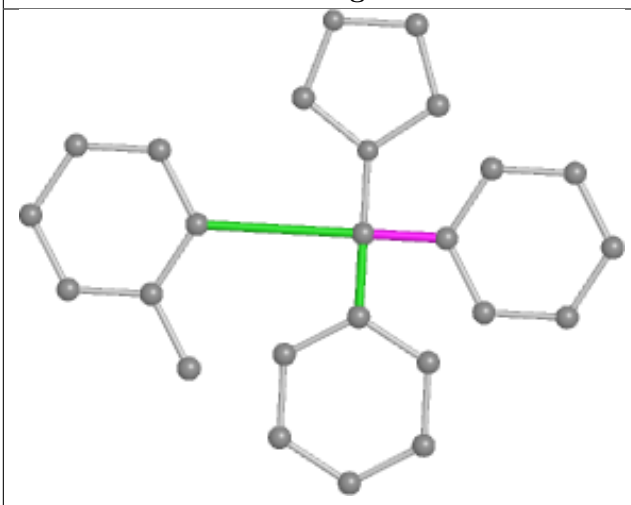
Ligand CL6 A 603



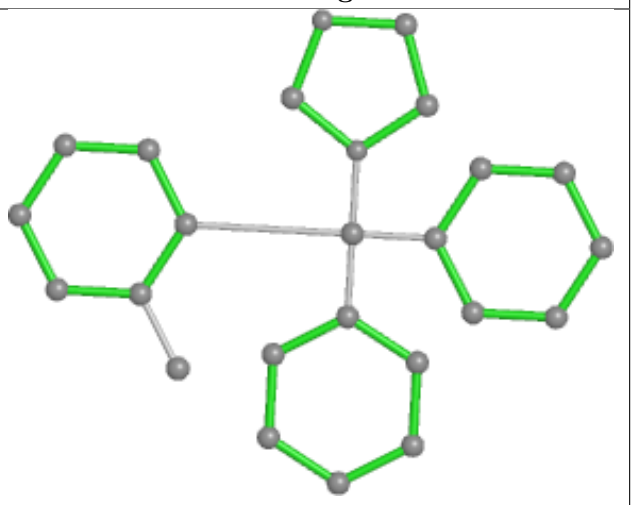
Bond lengths



Bond angles

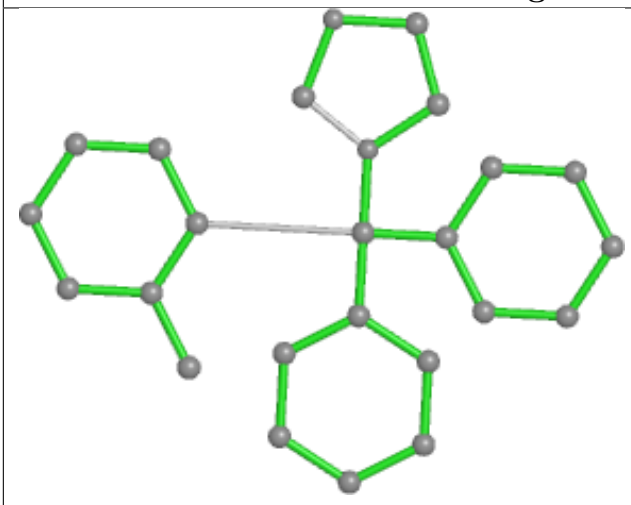


Torsions

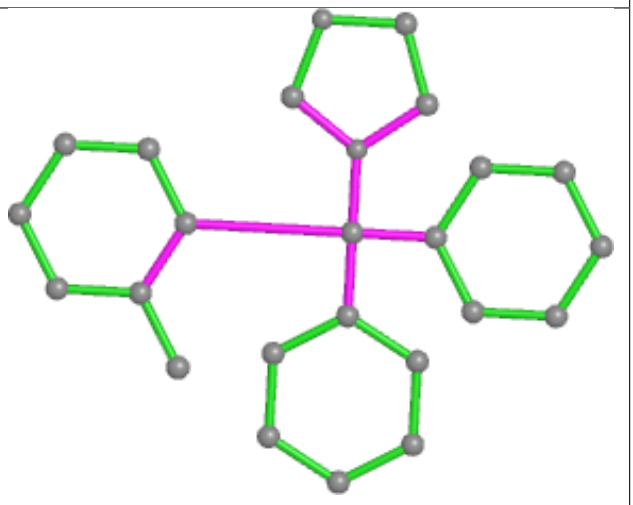


Rings

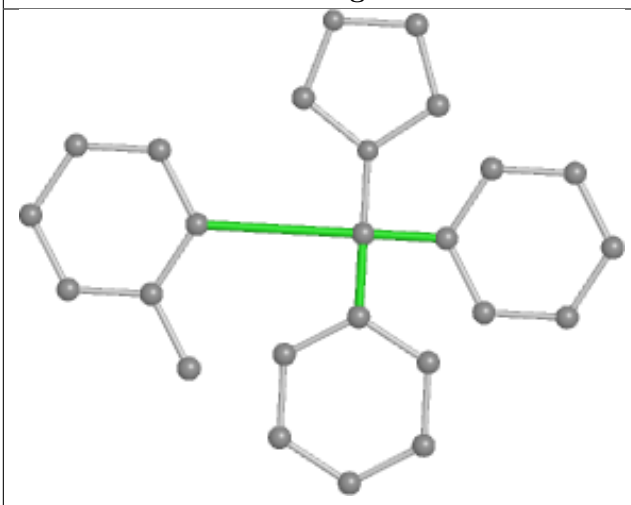
Ligand CL6 D 604



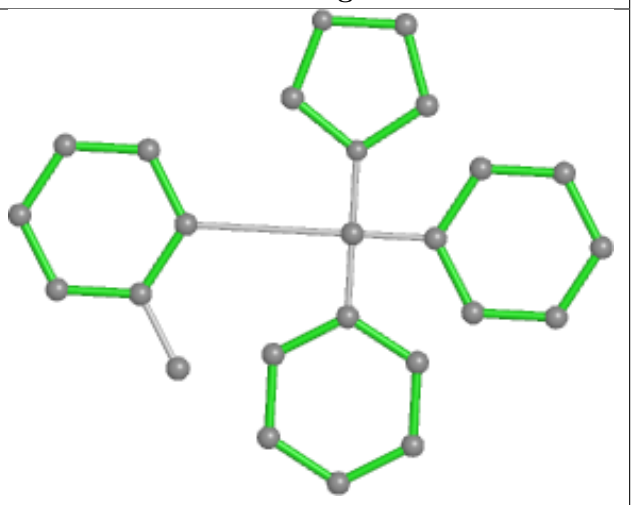
Bond lengths



Bond angles

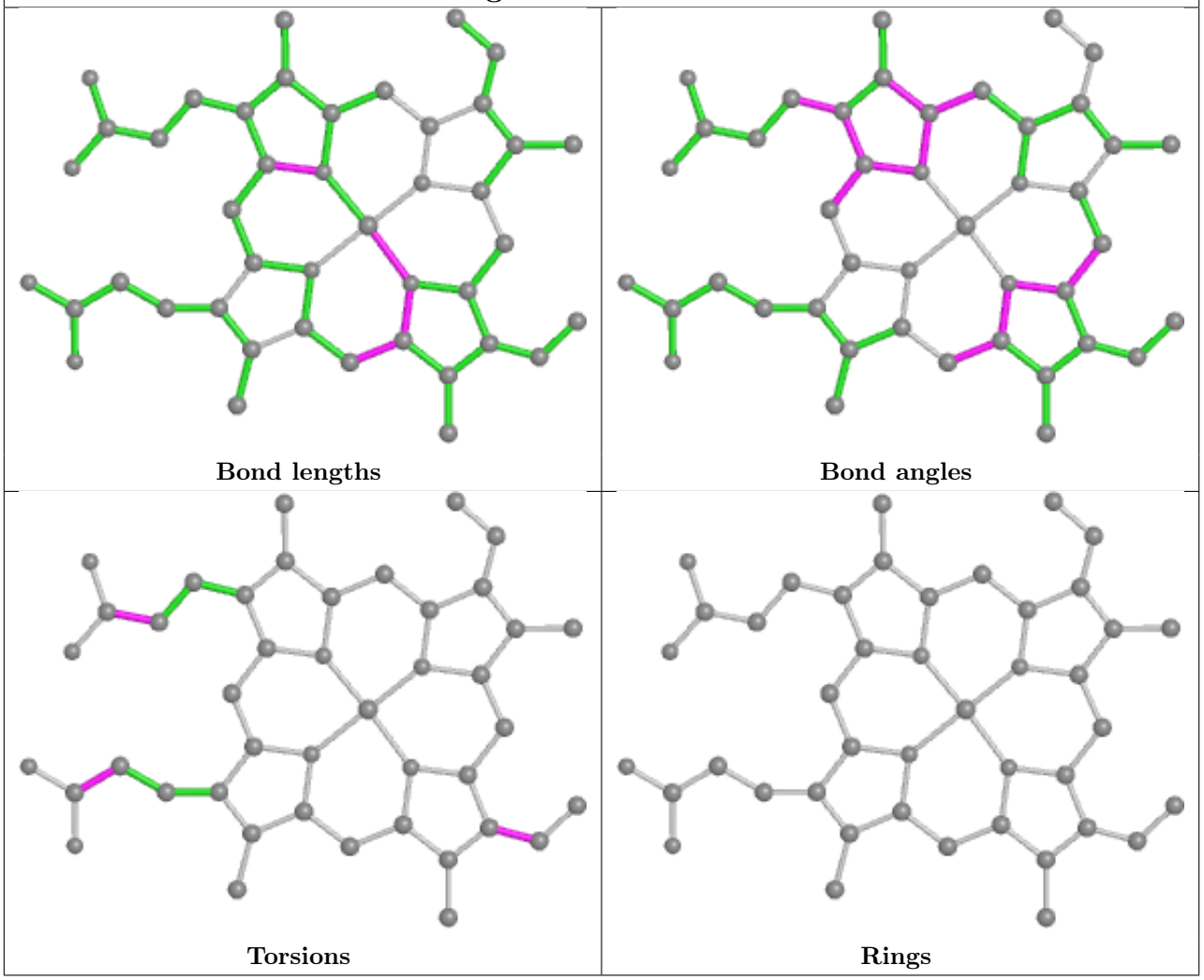


Torsions



Rings

Ligand HEM G 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	456/480 (95%)	-0.25	4 (0%)	84	80	54, 78, 113, 181	0
1	B	456/480 (95%)	-0.17	4 (0%)	84	80	53, 80, 113, 151	0
1	C	451/480 (93%)	-0.17	9 (1%)	65	56	60, 80, 119, 199	0
1	D	453/480 (94%)	-0.12	11 (2%)	59	49	52, 77, 122, 183	0
1	E	452/480 (94%)	0.01	8 (1%)	68	61	59, 83, 117, 170	0
1	F	452/480 (94%)	-0.07	12 (2%)	54	44	60, 87, 127, 180	0
1	G	449/480 (93%)	0.05	13 (2%)	51	41	58, 87, 130, 163	0
1	H	446/480 (92%)	0.17	30 (6%)	17	10	56, 107, 155, 222	0
All	All	3615/3840 (94%)	-0.07	91 (2%)	57	47	52, 84, 130, 222	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	ALA	4.6
1	F	279	GLN	4.5
1	G	257	LYS	4.4
1	G	424	ASP	4.1
1	H	189	PHE	4.1
1	C	424	ASP	3.9
1	D	289	ALA	3.8
1	H	258	LYS	3.5
1	H	350	VAL	3.4
1	H	348	ASP	3.3
1	F	256	MET	3.3
1	E	167	GLY	3.3
1	H	388	ILE	3.3
1	E	494	SER	3.2
1	H	352	GLN	3.2
1	H	347	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	255	ARG	3.1
1	H	349	ALA	3.1
1	D	279	GLN	3.0
1	H	26	GLY	3.0
1	H	468	LYS	2.9
1	D	257	LYS	2.9
1	E	162	ARG	2.9
1	B	293	LEU	2.9
1	E	496	ASP	2.9
1	D	493	ASP	2.9
1	F	203	PHE	2.9
1	G	189	PHE	2.8
1	H	391	GLY	2.8
1	G	425	SER	2.8
1	H	191	VAL	2.8
1	H	356	LEU	2.8
1	A	289	ALA	2.8
1	F	29	THR	2.7
1	E	164	ALA	2.7
1	H	27	THR	2.7
1	H	305	ALA	2.7
1	H	312	SER	2.6
1	F	32	LEU	2.6
1	F	496	ASP	2.6
1	H	353	MET	2.6
1	D	29	THR	2.6
1	H	289	ALA	2.6
1	H	387	PHE	2.6
1	D	26	GLY	2.6
1	G	166	LYS	2.5
1	F	295	LEU	2.5
1	D	292	ASP	2.5
1	F	253	VAL	2.5
1	B	258	LYS	2.5
1	H	383	ILE	2.5
1	H	341	ASN	2.4
1	H	469	GLU	2.4
1	C	27	THR	2.4
1	H	426	ILE	2.4
1	E	341	ASN	2.4
1	H	82	LEU	2.4
1	F	341	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	166	LYS	2.3
1	C	468	LYS	2.3
1	E	168	LYS	2.3
1	A	255	ARG	2.3
1	B	446	PHE	2.3
1	G	256	MET	2.3
1	G	423	LYS	2.3
1	C	446	PHE	2.3
1	H	446	PHE	2.3
1	C	203	PHE	2.3
1	D	34	LYS	2.2
1	C	28	ARG	2.2
1	G	292	ASP	2.2
1	G	132	LEU	2.2
1	B	421	LYS	2.2
1	D	258	LYS	2.2
1	C	167	GLY	2.2
1	G	441	CYS	2.2
1	F	34	LYS	2.2
1	D	276	ILE	2.1
1	C	422	LYS	2.1
1	C	289	ALA	2.1
1	D	386	VAL	2.1
1	F	290	LEU	2.1
1	G	421	LYS	2.1
1	H	310	THR	2.1
1	G	273	GLN	2.0
1	G	312	SER	2.0
1	A	256	MET	2.0
1	H	256	MET	2.0
1	H	313	VAL	2.0
1	H	180	SER	2.0
1	F	491	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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
4	CE9	C	605	24/40	0.84	0.29	73,79,99,105	0
4	CE9	D	605	24/40	0.89	0.21	60,76,81,83	0
4	CE9	G	605	30/40	0.89	0.22	60,70,94,94	0
4	CE9	A	605	40/40	0.90	0.20	60,73,106,107	0
4	CE9	F	605	29/40	0.90	0.25	65,76,90,103	0
3	CL6	D	604	25/25	0.90	0.22	72,75,79,98	0
3	CL6	H	604	25/25	0.91	0.24	75,80,84,106	0
4	CE9	B	605	34/40	0.91	0.22	63,70,95,101	0
3	CL6	C	604	25/25	0.92	0.21	61,70,74,93	0
4	CE9	E	605	22/40	0.93	0.23	50,65,71,73	0
3	CL6	E	604	25/25	0.93	0.21	62,67,74,88	0
3	CL6	B	604	25/25	0.93	0.19	57,65,68,93	0
3	CL6	B	603	25/25	0.94	0.18	59,64,67,80	0
3	CL6	A	603	25/25	0.94	0.17	57,61,64,72	0
3	CL6	F	604	25/25	0.94	0.21	70,77,80,104	0
3	CL6	G	604	25/25	0.94	0.19	65,70,75,94	0
3	CL6	C	603	25/25	0.94	0.20	62,65,69,80	0
3	CL6	A	604	25/25	0.94	0.19	59,65,68,84	0
3	CL6	H	603	25/25	0.95	0.20	68,73,80,80	0
3	CL6	G	603	25/25	0.95	0.18	65,69,74,76	0
3	CL6	F	603	25/25	0.95	0.21	70,72,75,89	0
3	CL6	D	603	25/25	0.96	0.20	66,70,73,84	0
2	HEM	H	601	43/43	0.96	0.22	85,91,95,97	0
3	CL6	H	602	25/25	0.96	0.21	78,82,87,87	0
3	CL6	E	602	25/25	0.96	0.28	61,68,70,73	0
2	HEM	G	601	43/43	0.97	0.26	68,73,83,87	0
3	CL6	E	603	25/25	0.97	0.16	62,68,72,79	0
3	CL6	G	602	25/25	0.97	0.29	65,68,71,71	0
3	CL6	B	602	25/25	0.97	0.20	56,61,63,65	0
3	CL6	F	602	25/25	0.97	0.23	64,68,72,74	0
2	HEM	F	601	43/43	0.98	0.19	62,69,74,75	0
2	HEM	A	601	43/43	0.98	0.21	58,62,65,69	0
3	CL6	C	602	25/25	0.98	0.22	58,63,66,68	0
2	HEM	B	601	43/43	0.98	0.22	57,64,68,70	0
3	CL6	A	602	25/25	0.98	0.22	52,56,58,61	0
3	CL6	D	602	25/25	0.98	0.18	59,63,67,68	0
2	HEM	C	601	43/43	0.98	0.21	62,66,68,70	0

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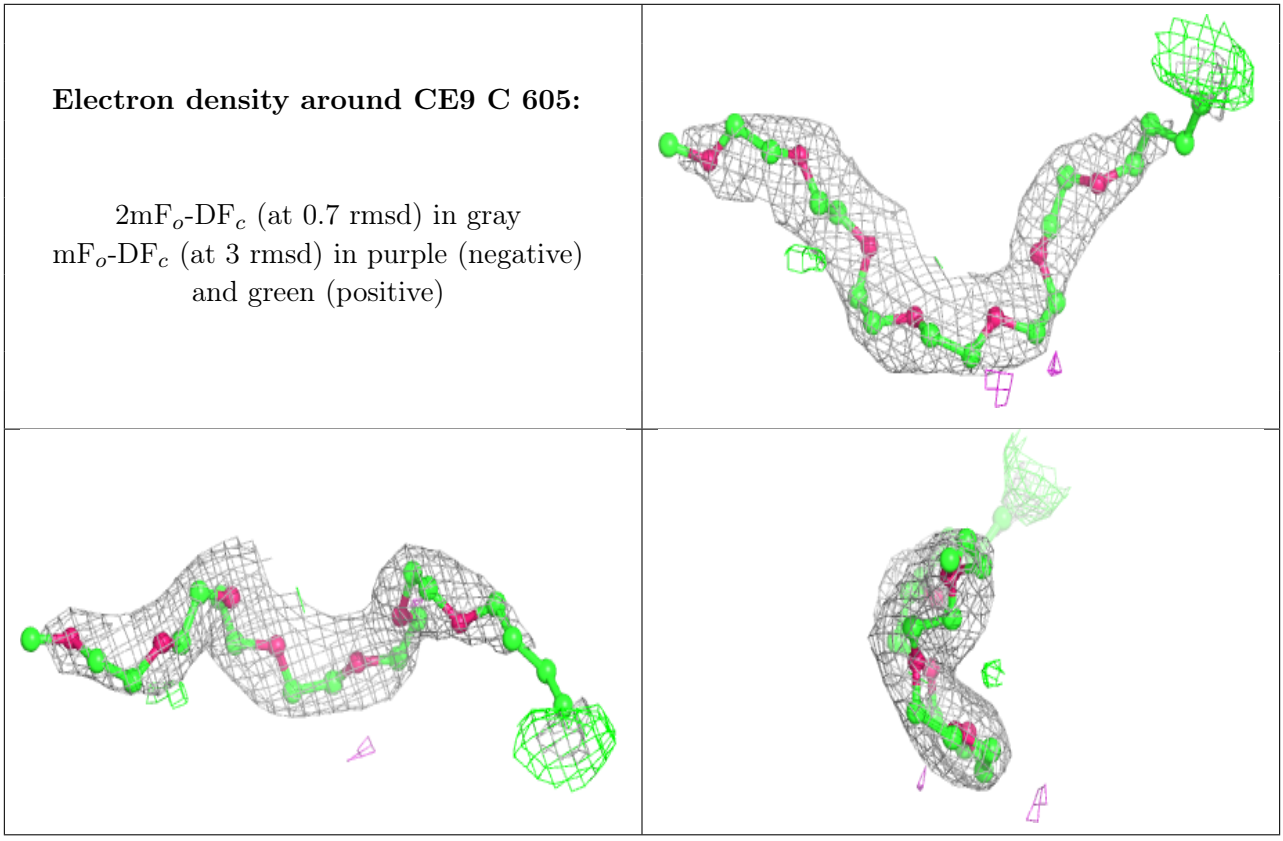
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	D	601	43/43	0.98	0.21	51,62,67,69	0
2	HEM	E	601	43/43	0.98	0.23	66,71,75,76	0

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.

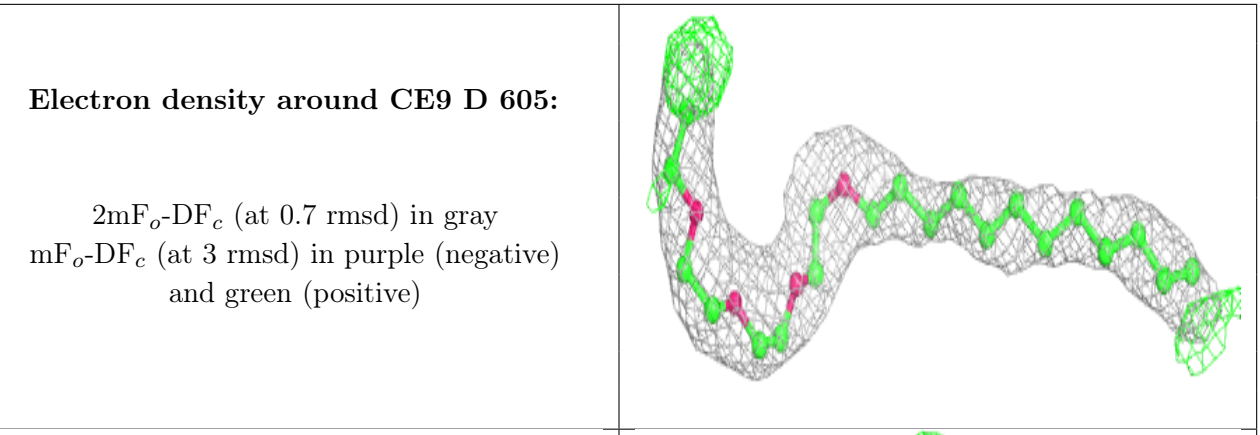
Electron density around CE9 C 605:

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



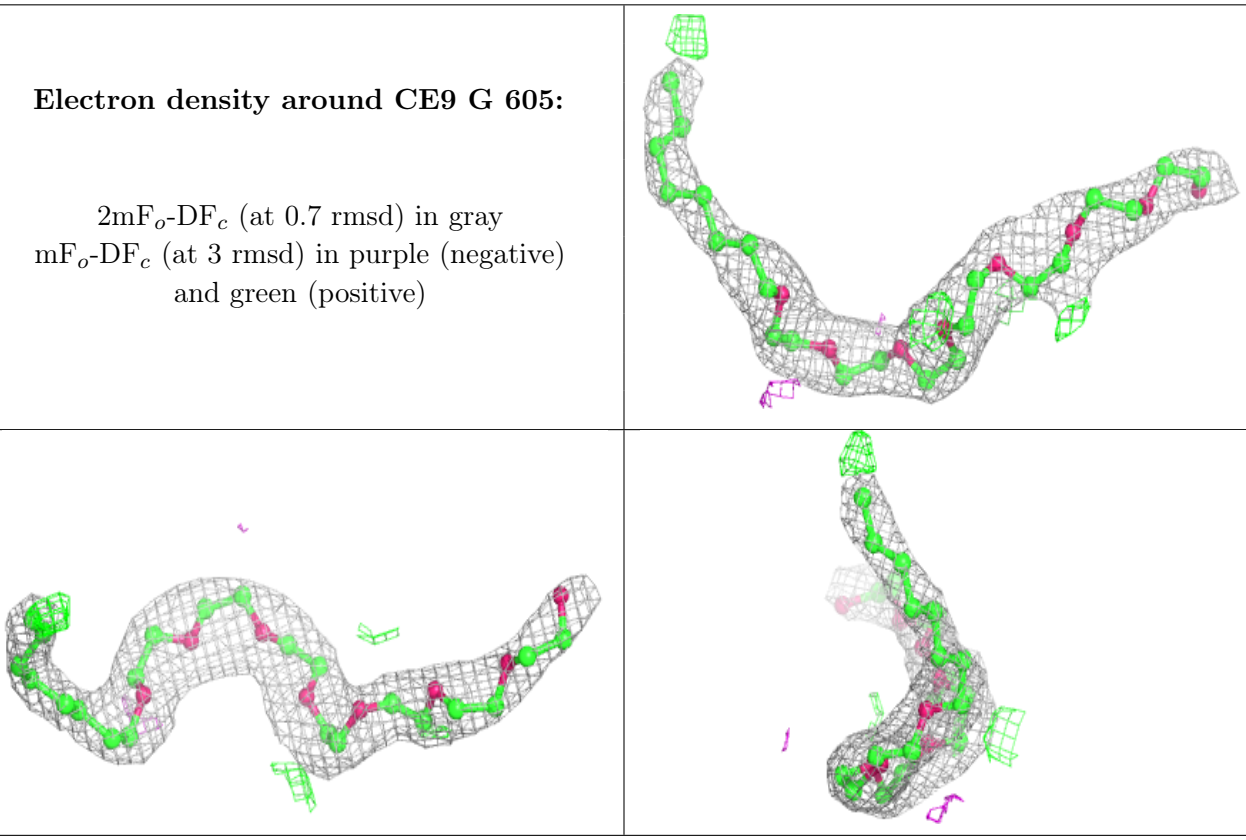
Electron density around CE9 D 605:

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



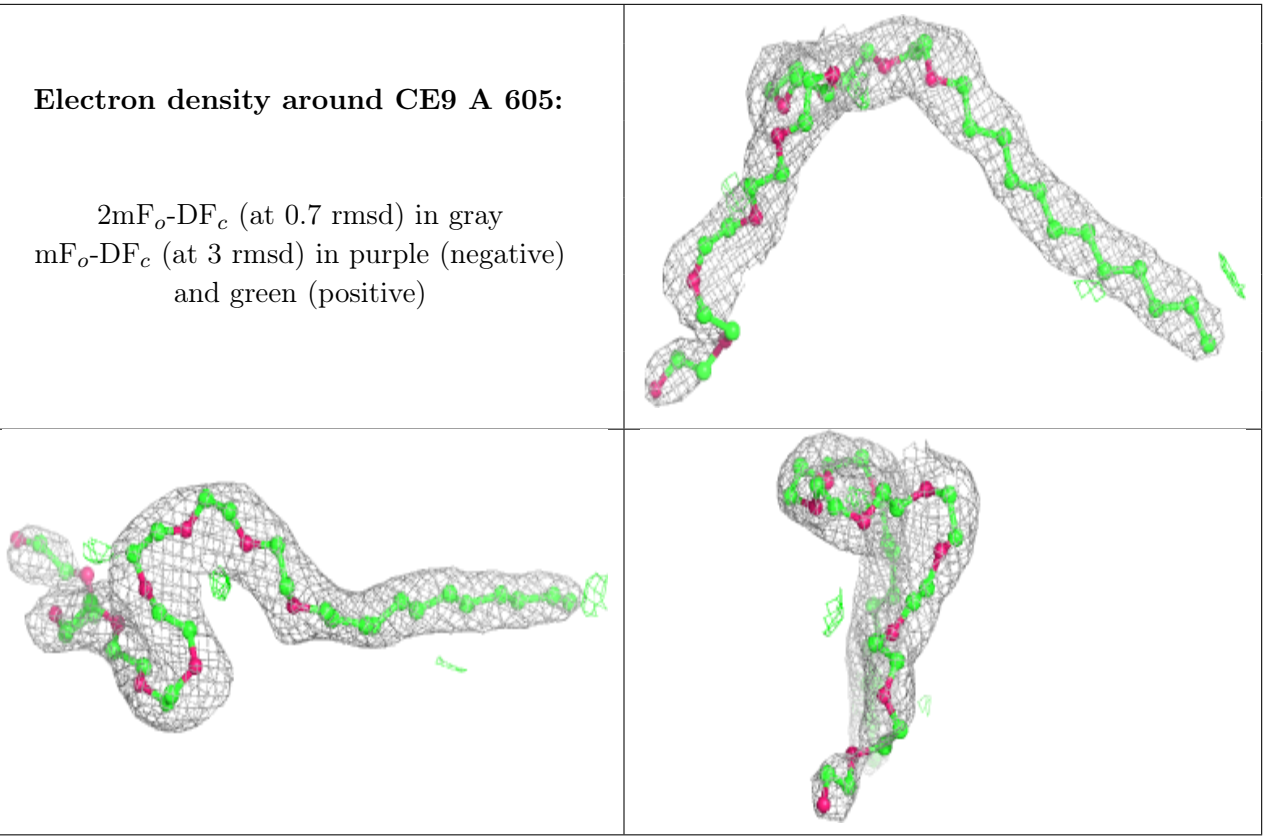
Electron density around CE9 G 605:

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



Electron density around CE9 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 CE9 F 605:

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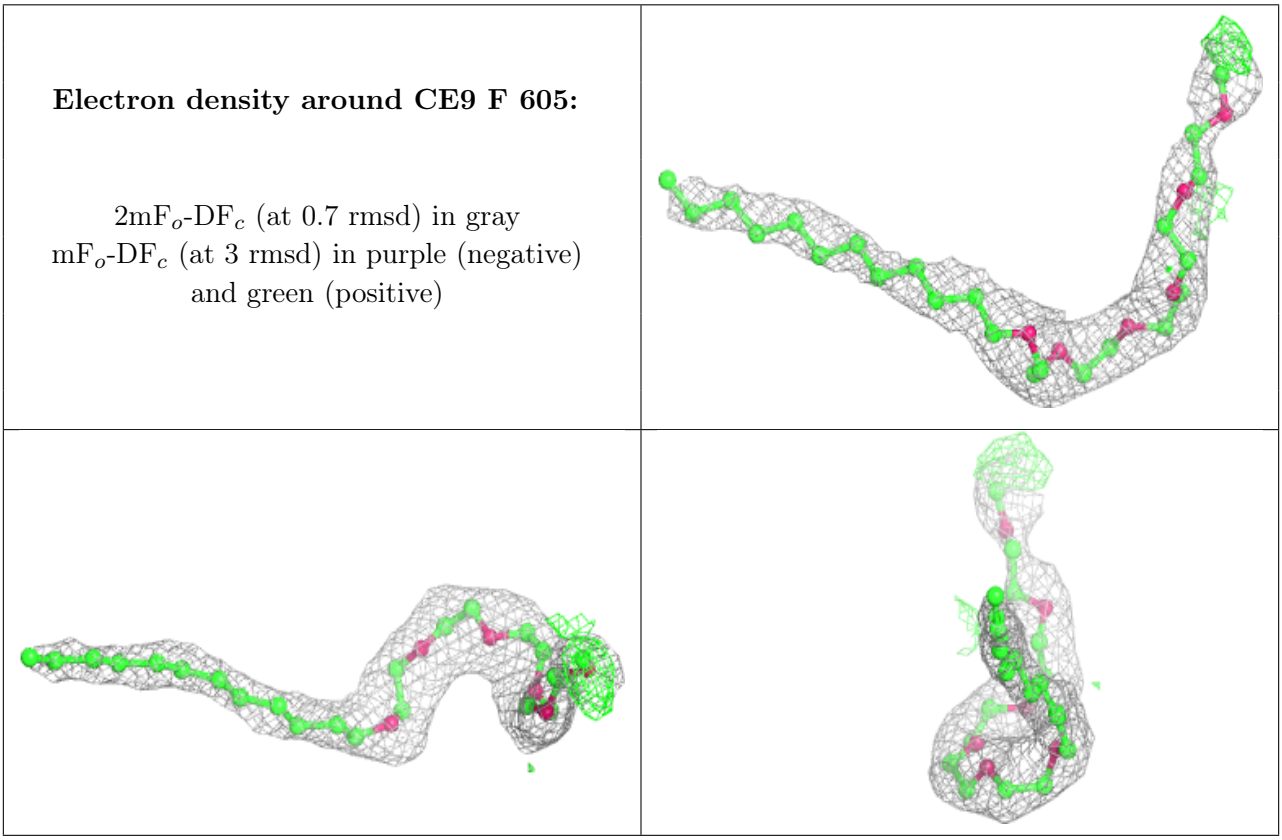
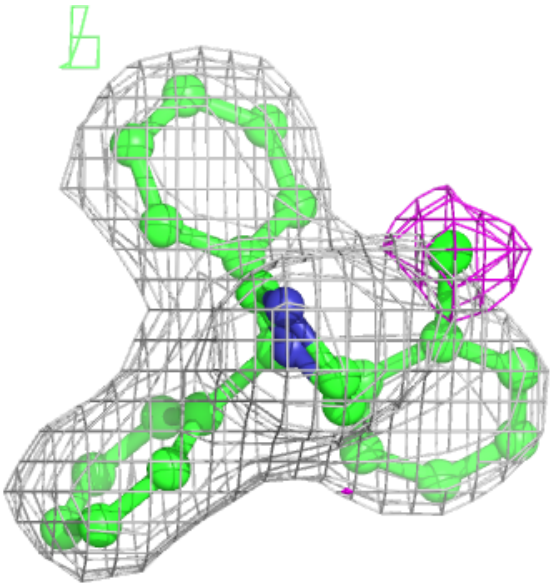
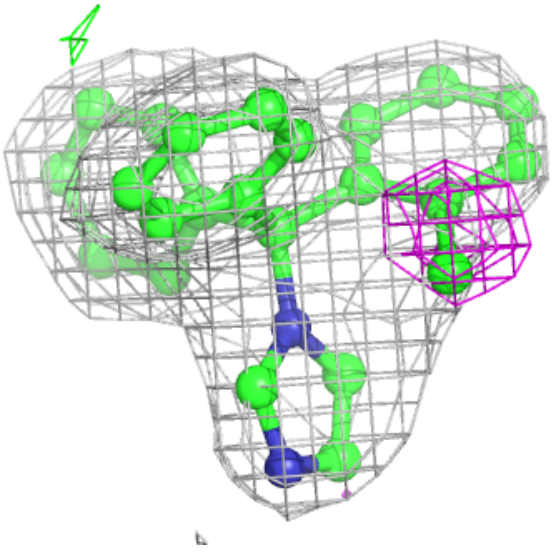
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

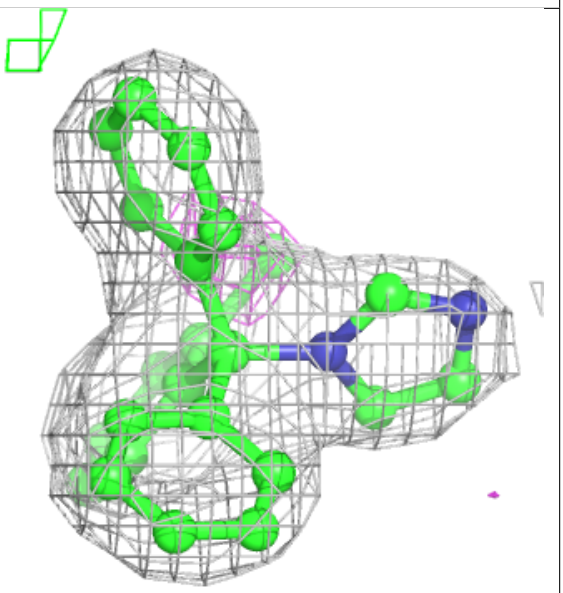


Electron density around CL6 D 604:

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

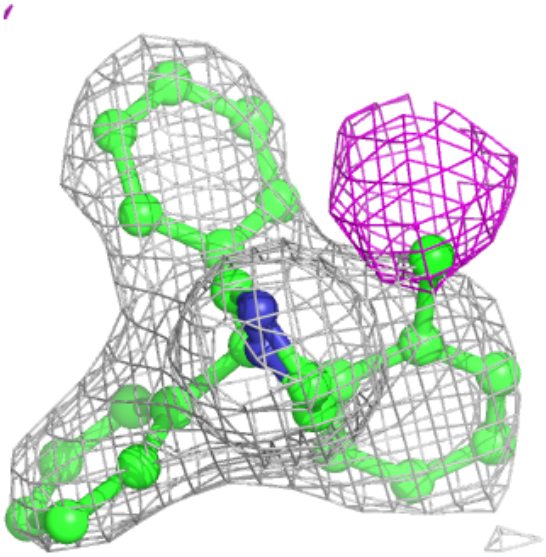


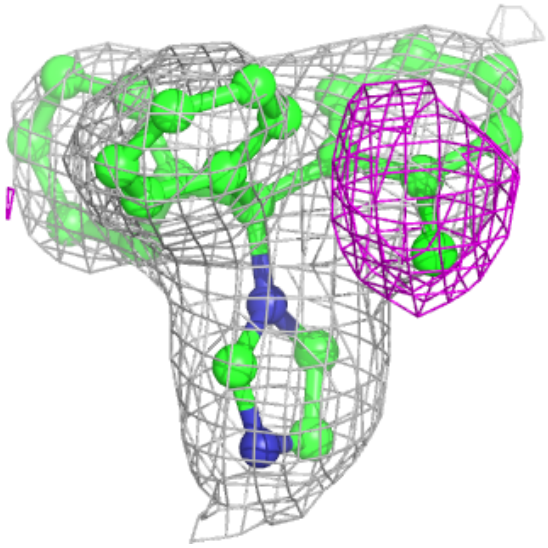


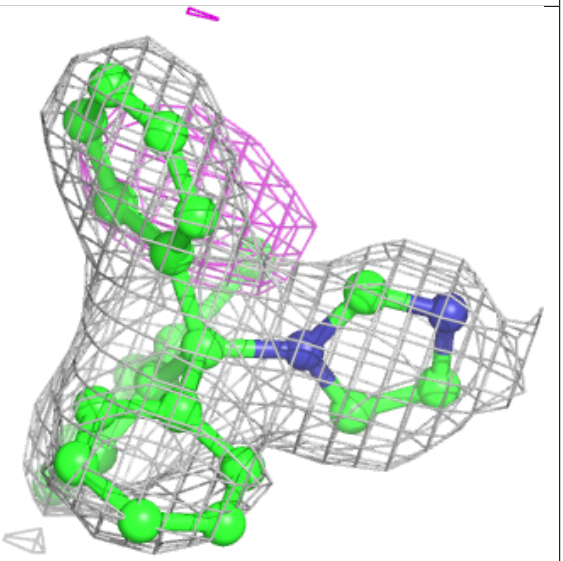


Electron density around CL6 H 604:

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

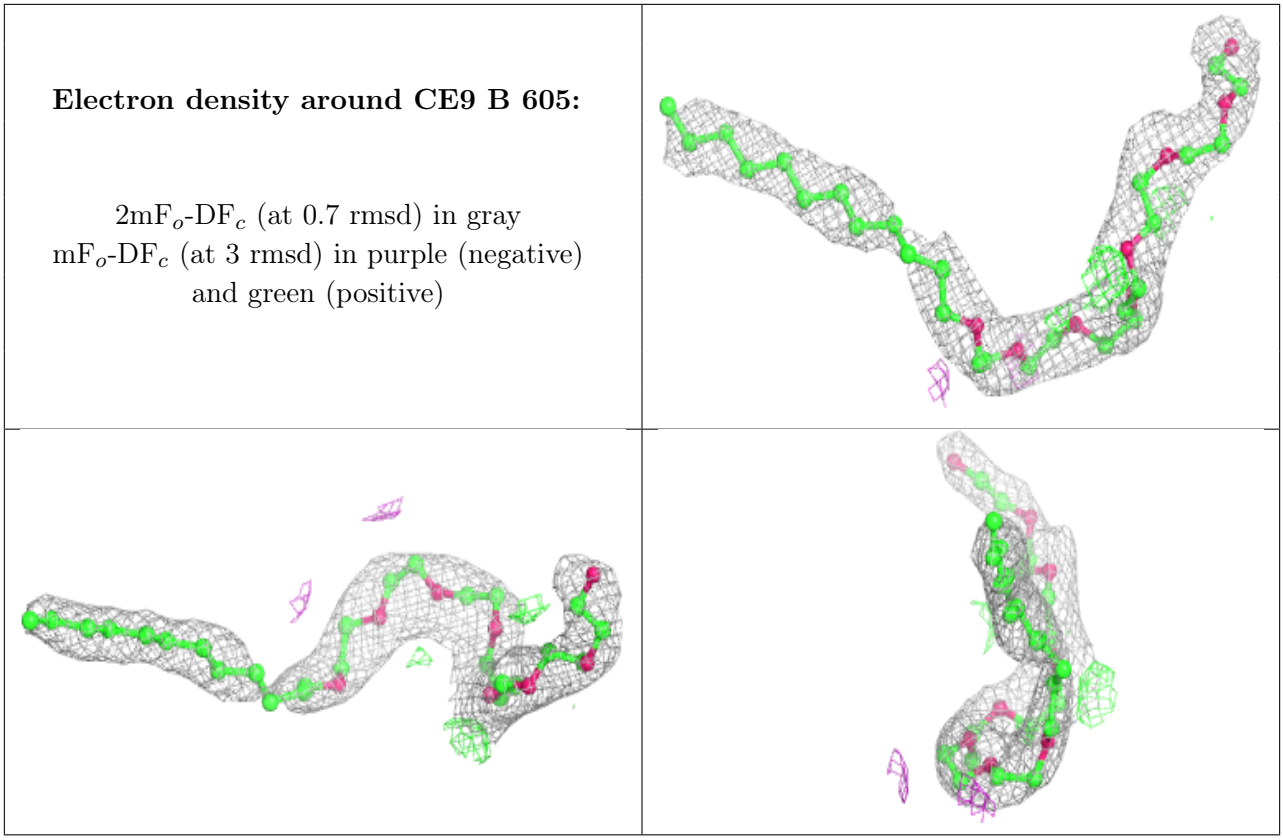






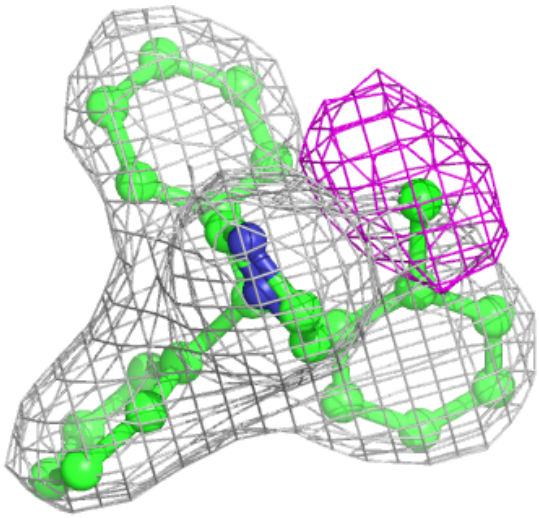
Electron density around CE9 B 605:

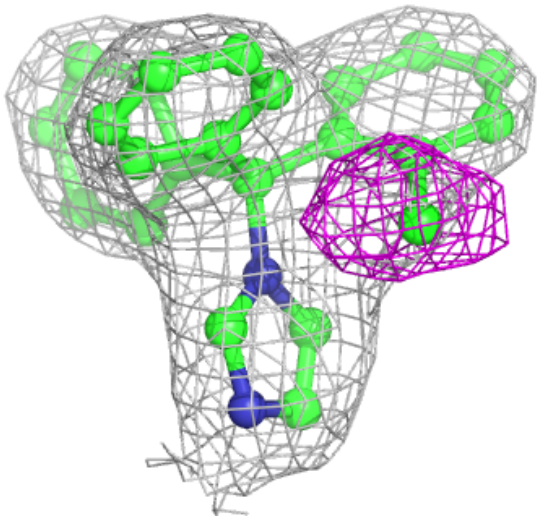
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

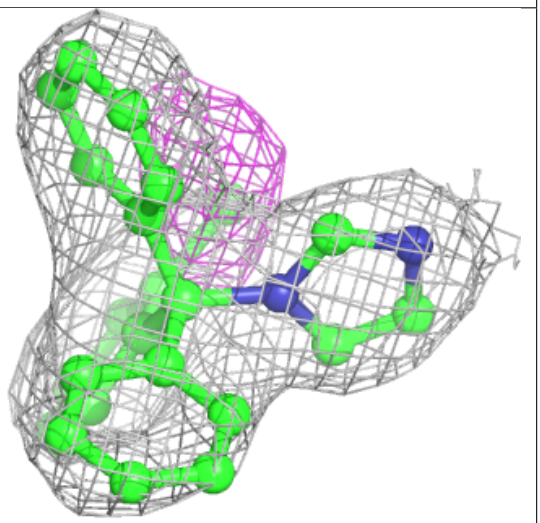


Electron density around CL6 C 604:

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

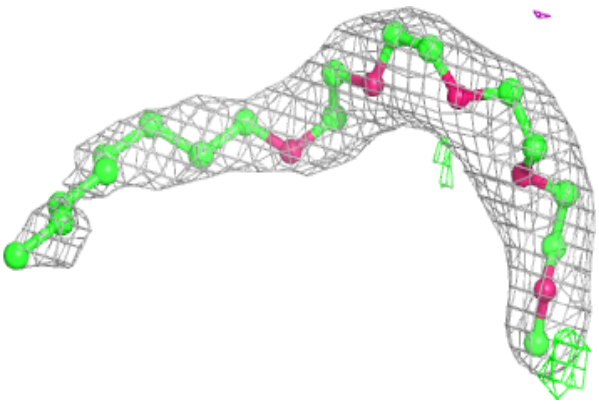


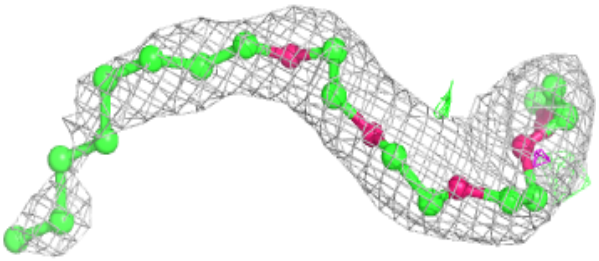


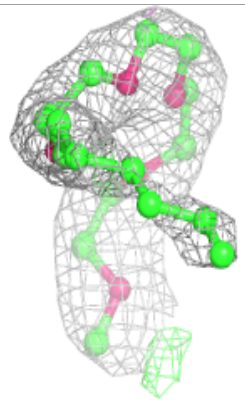


Electron density around CE9 E 605:

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

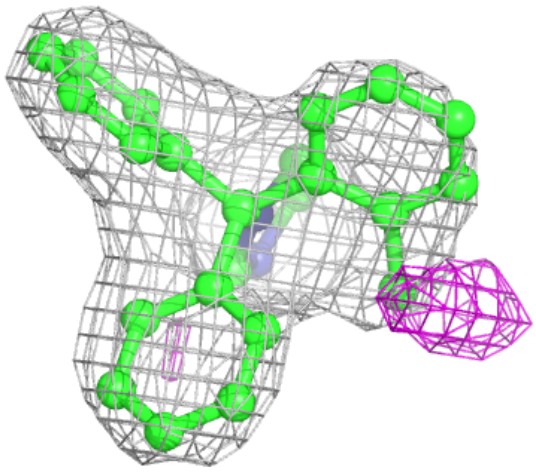


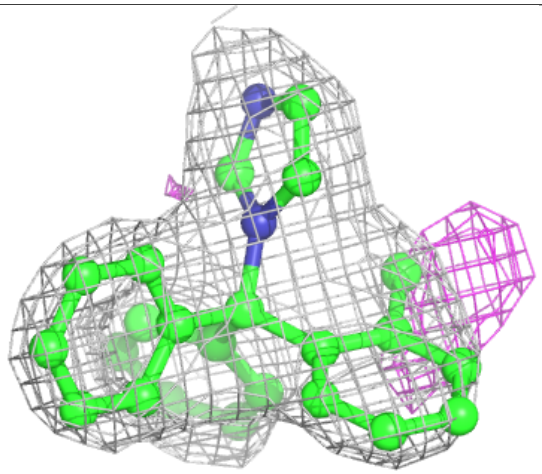


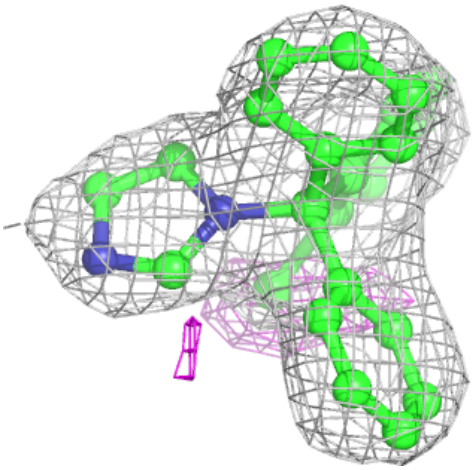


Electron density around CL6 E 604:

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

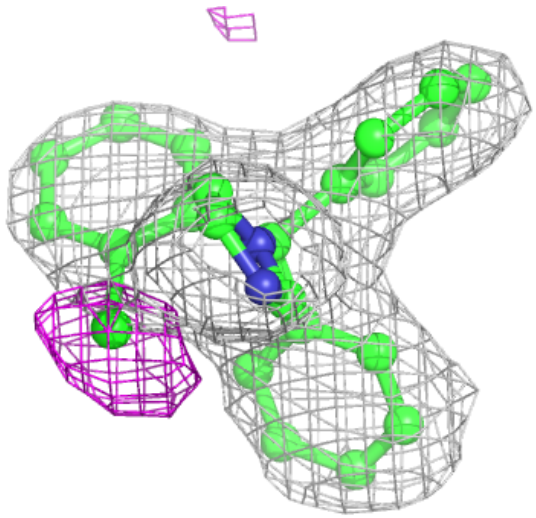


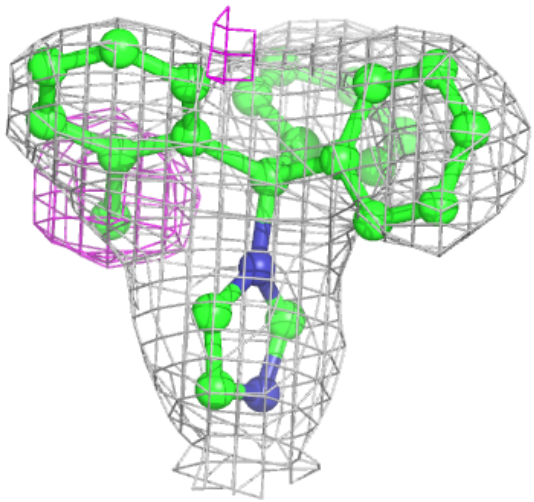


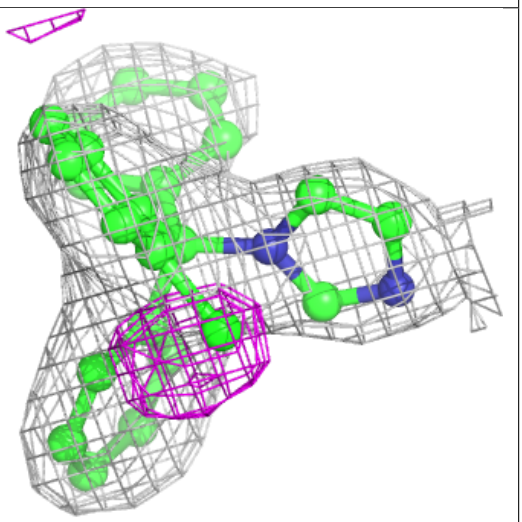


Electron density around CL6 B 604:

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

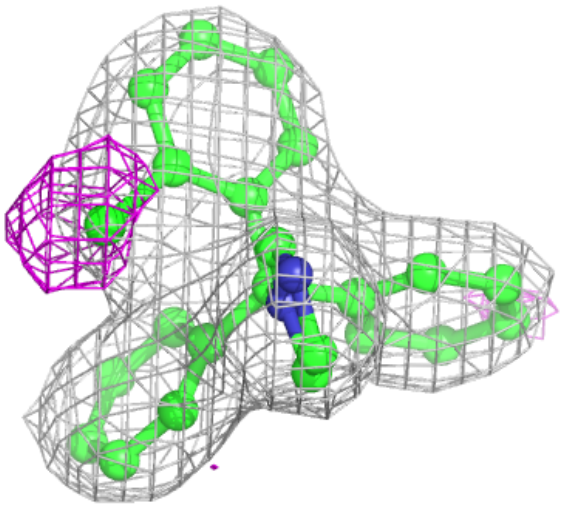


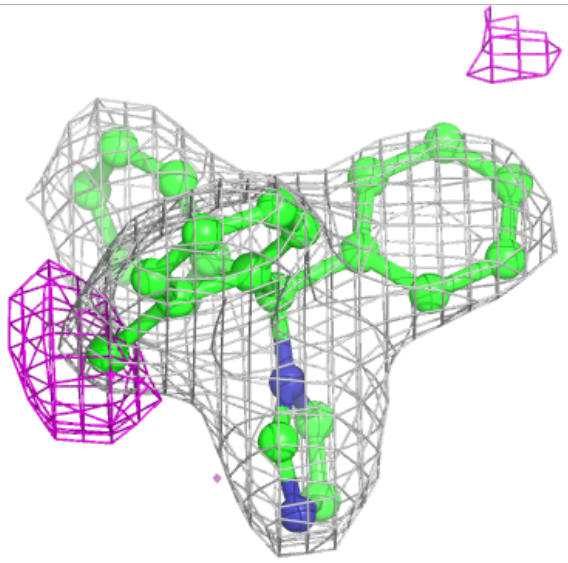


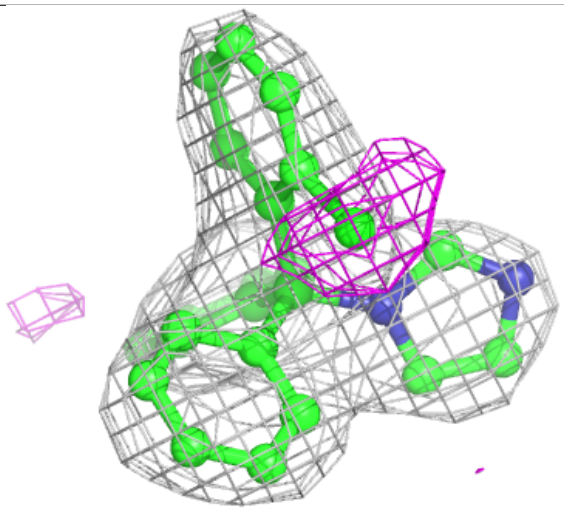


Electron density around CL6 B 603:

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

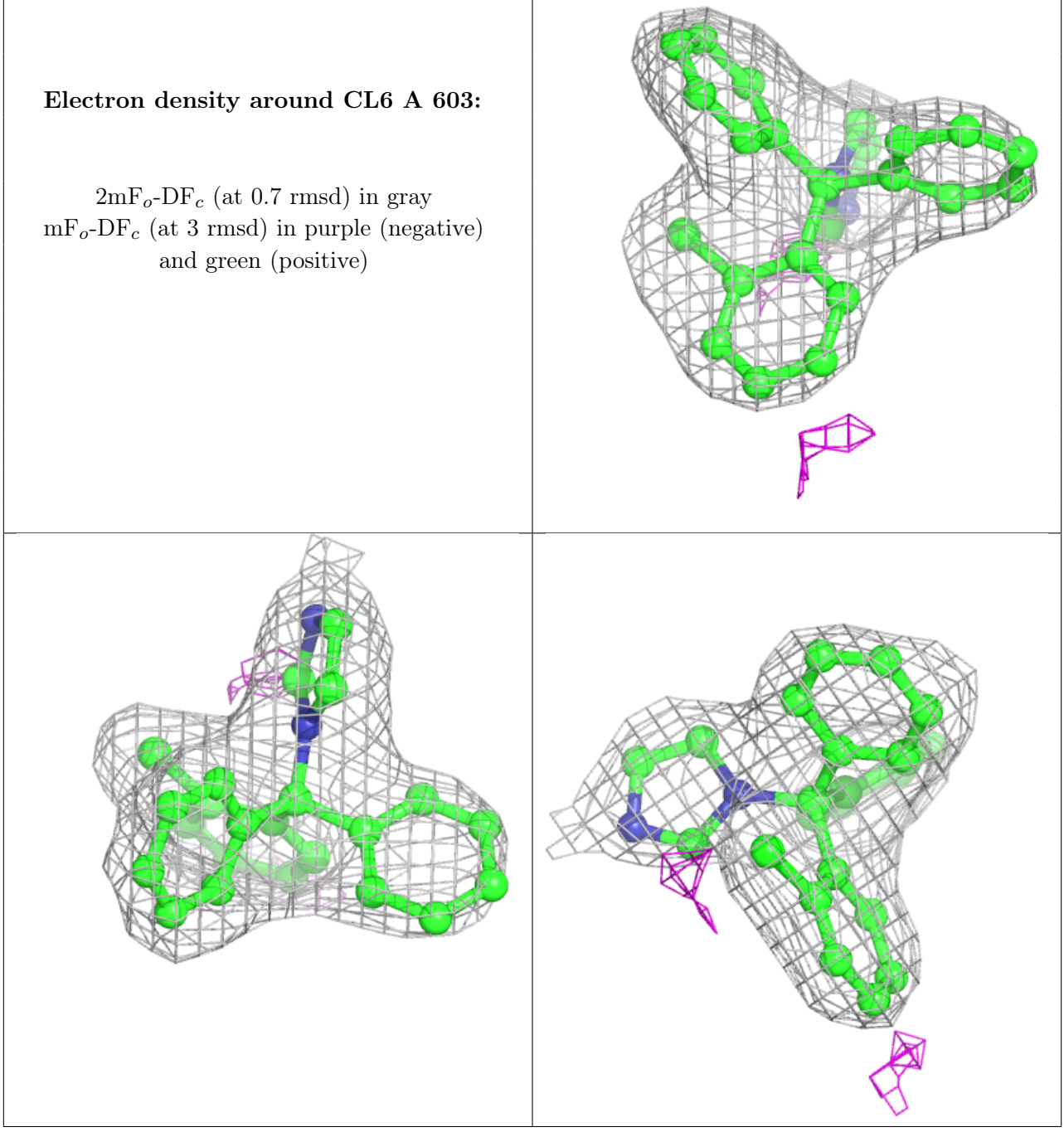






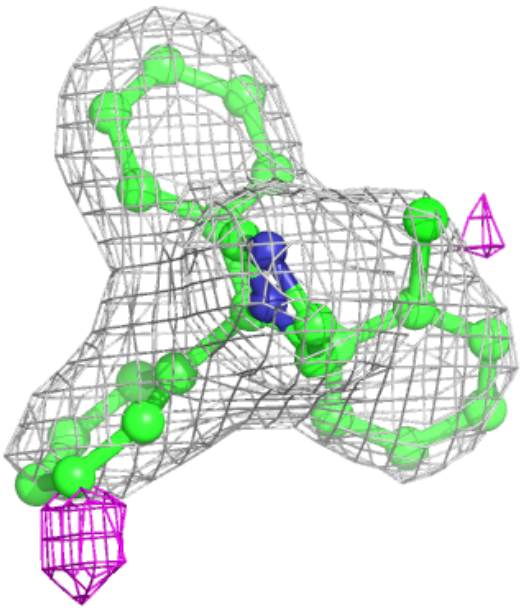
Electron density around CL6 A 603:

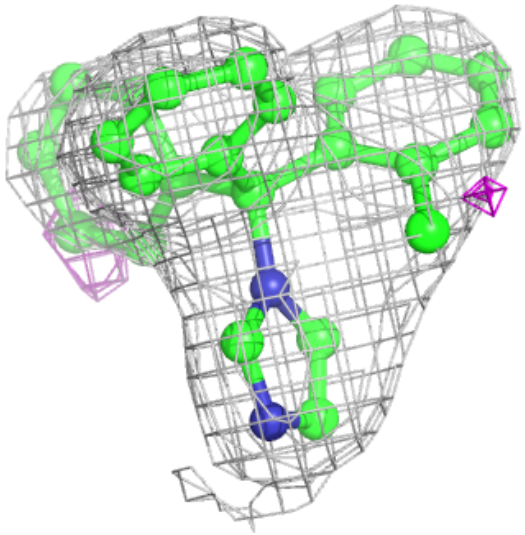
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

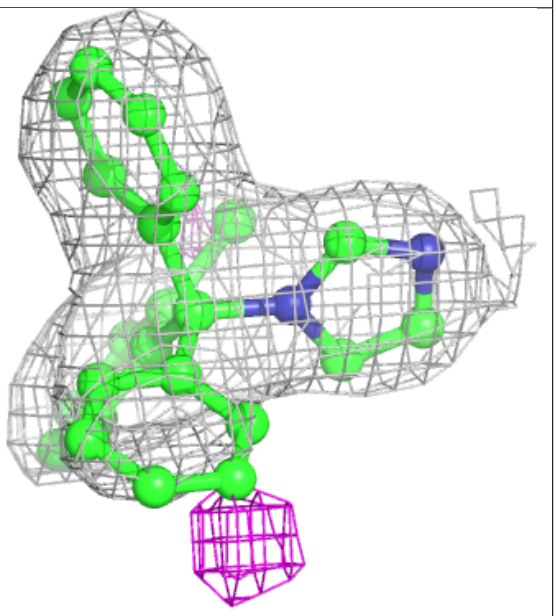


Electron density around CL6 F 604:

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

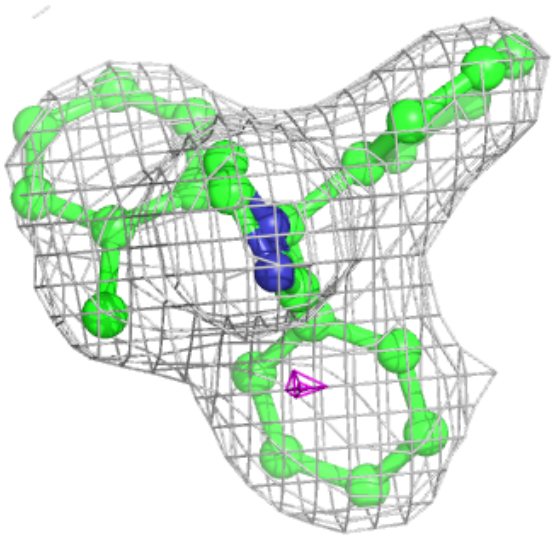


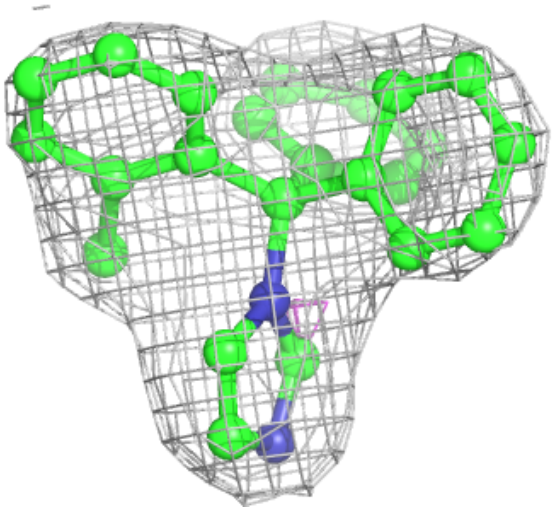


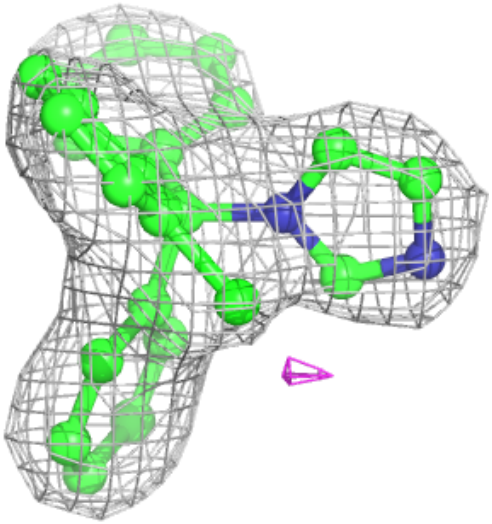


Electron density around CL6 G 604:

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

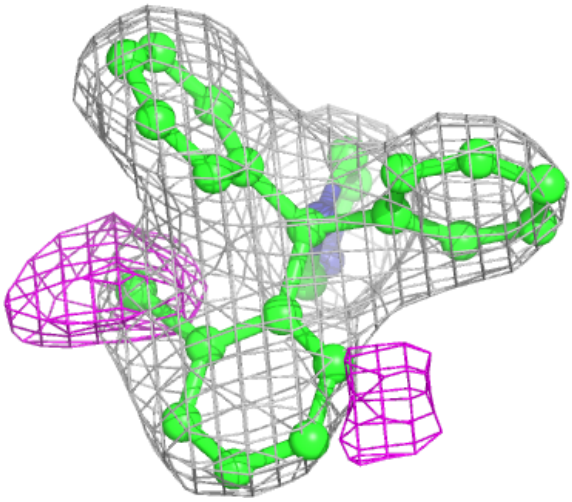


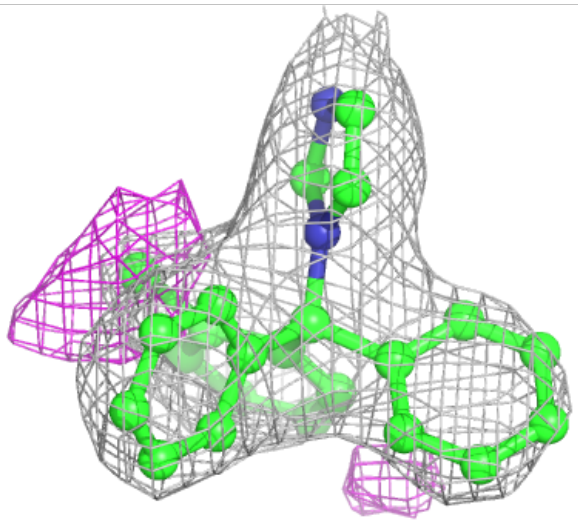


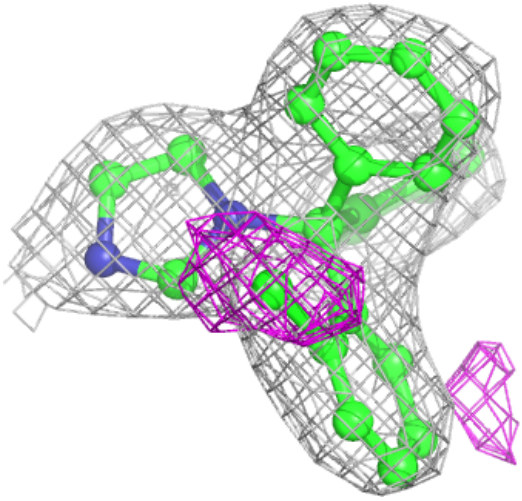


Electron density around CL6 C 603:

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

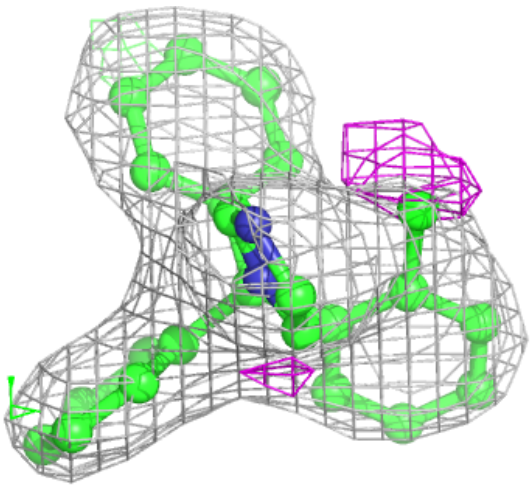


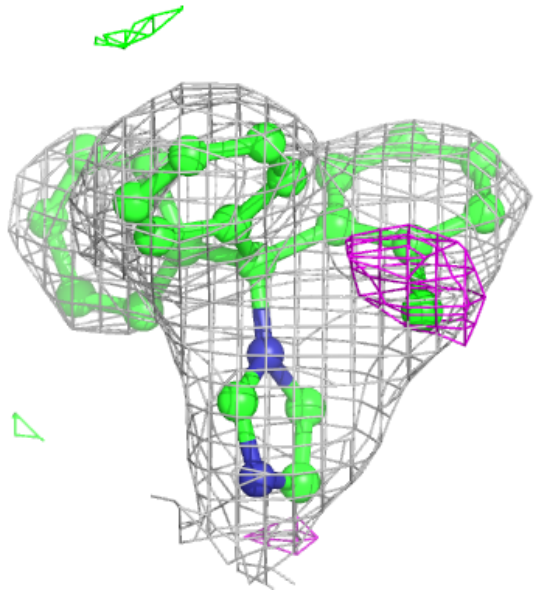


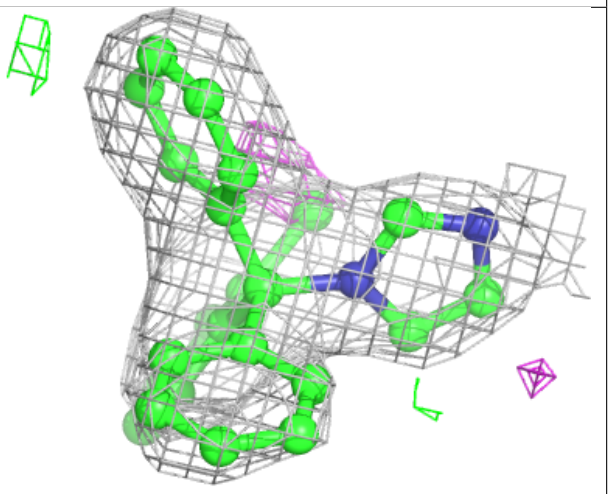


Electron density around CL6 A 604:

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

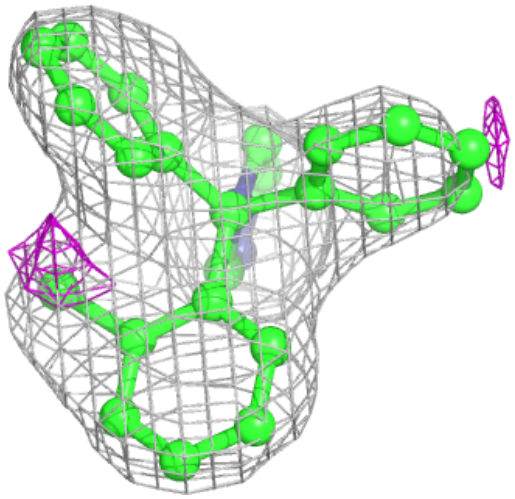


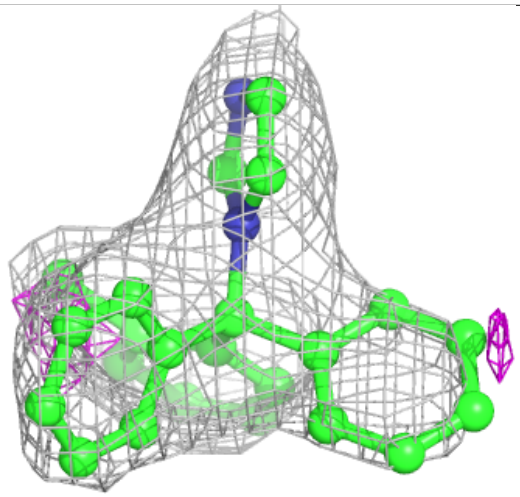


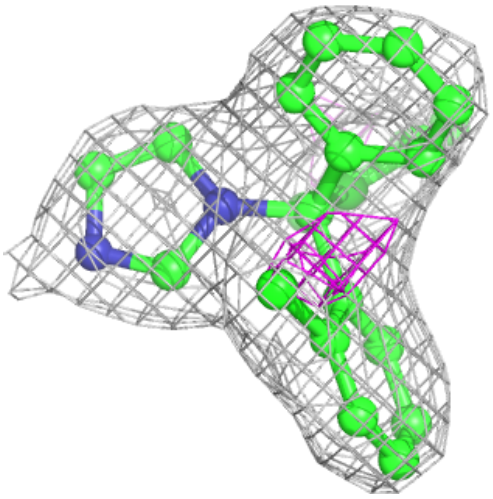


Electron density around CL6 H 603:

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

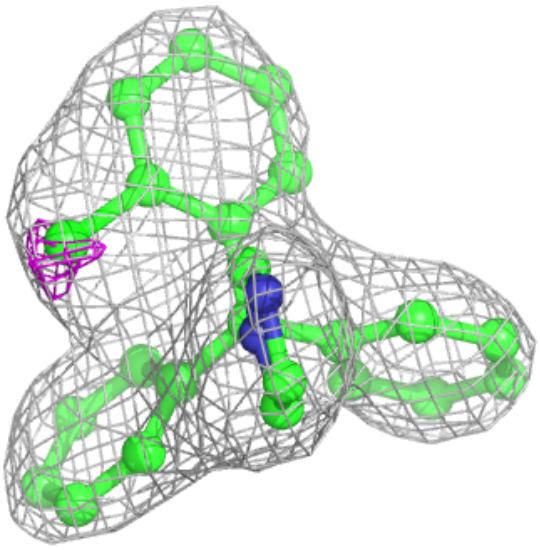


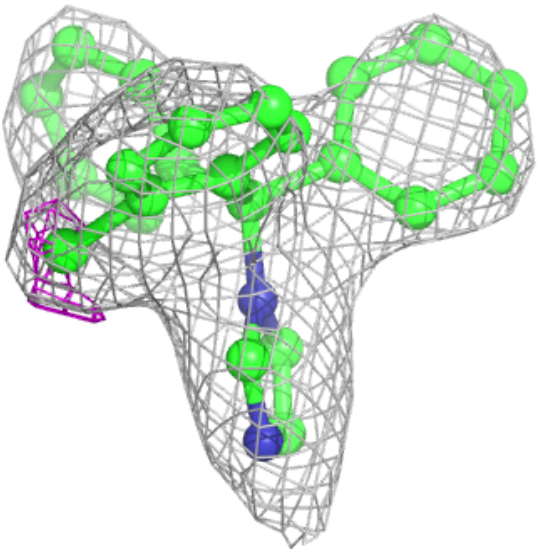


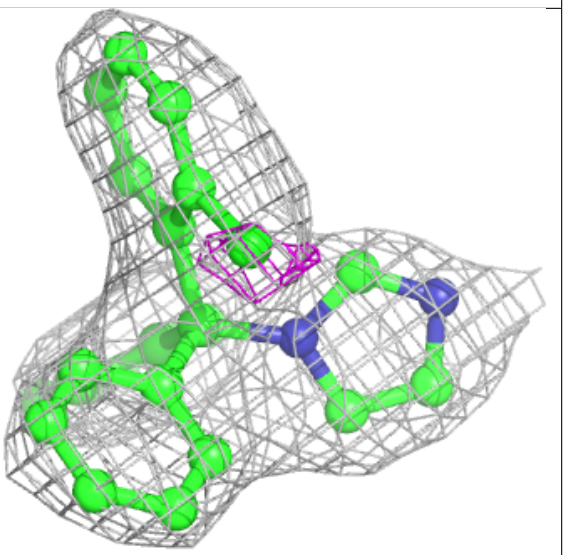


Electron density around CL6 G 603:

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

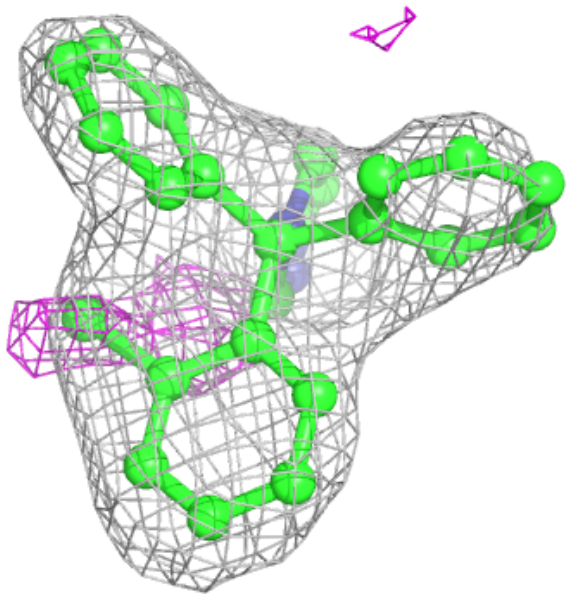


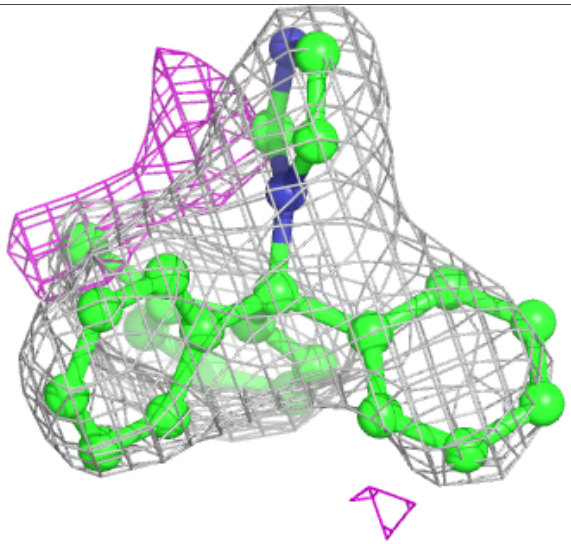


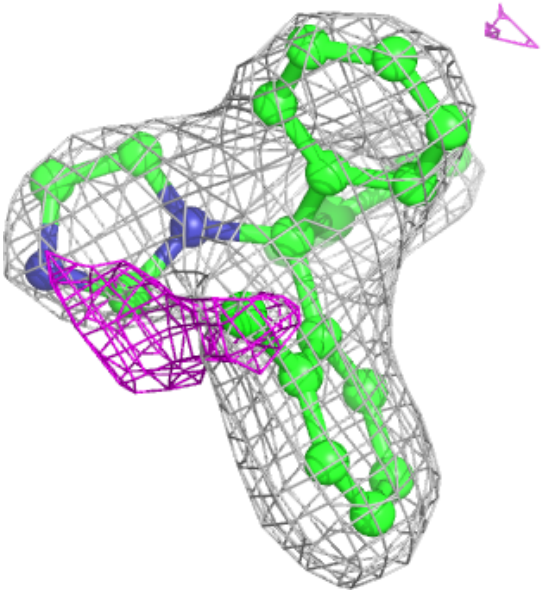


Electron density around CL6 F 603:

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

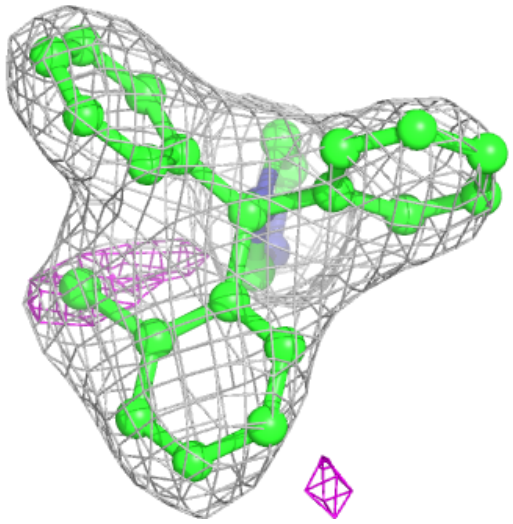


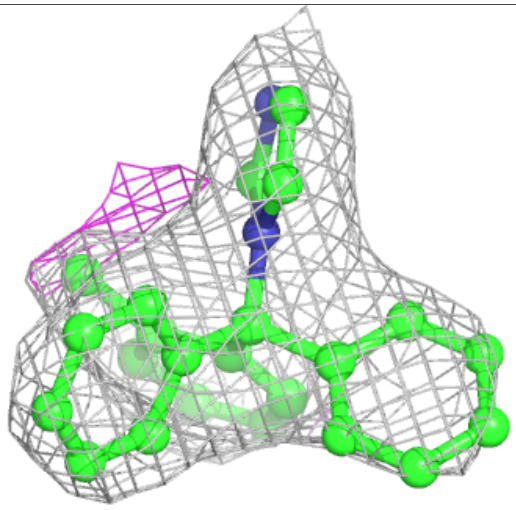


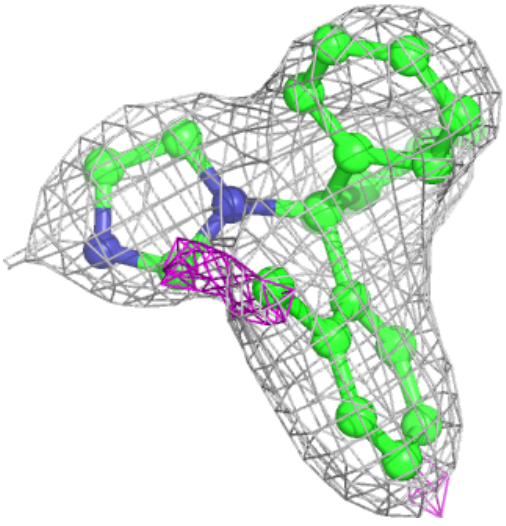


Electron density around CL6 D 603:

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

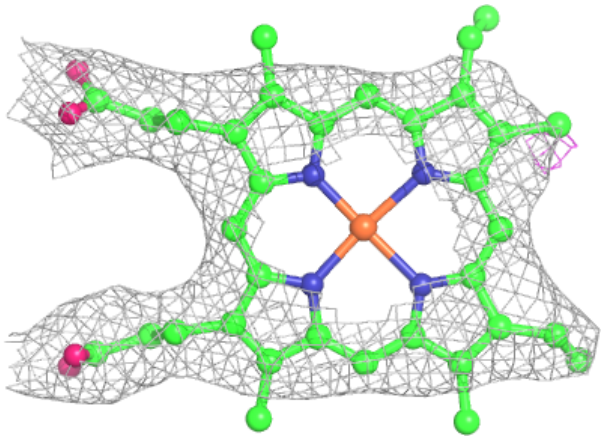


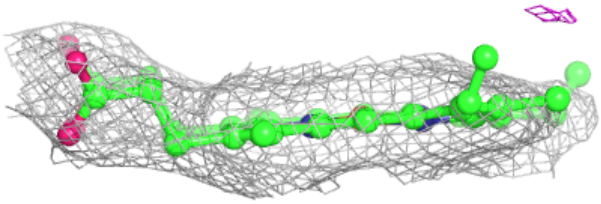


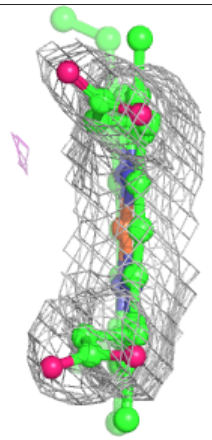


Electron density around HEM H 601:

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

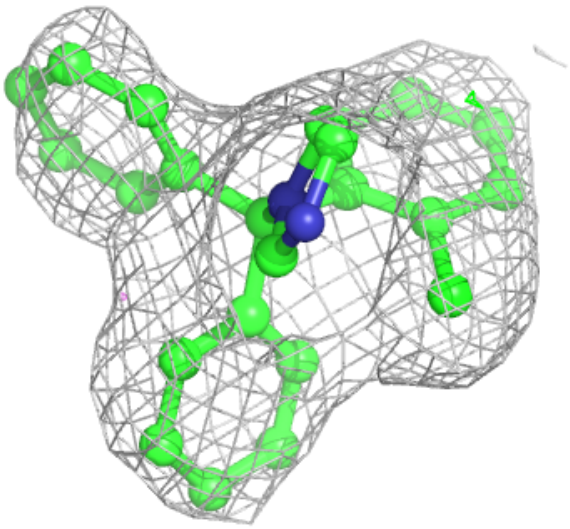


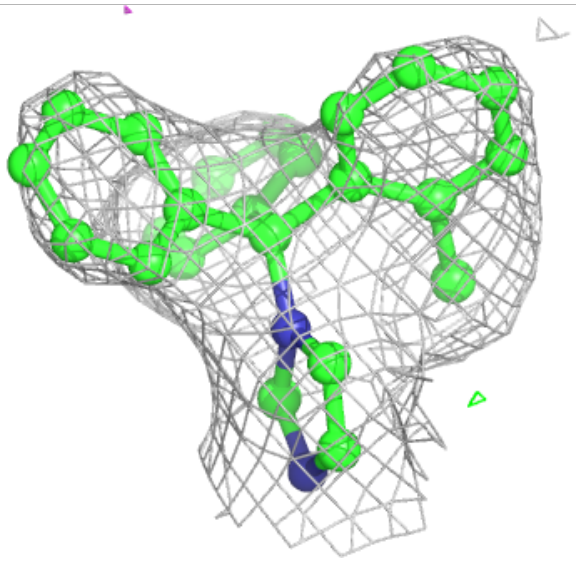


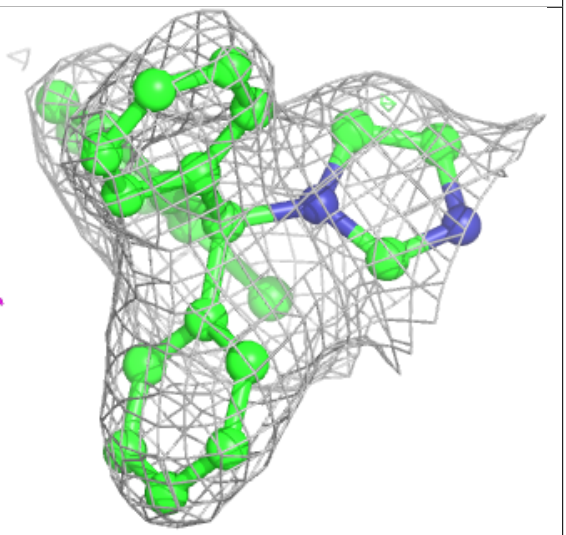


Electron density around CL6 H 602:

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

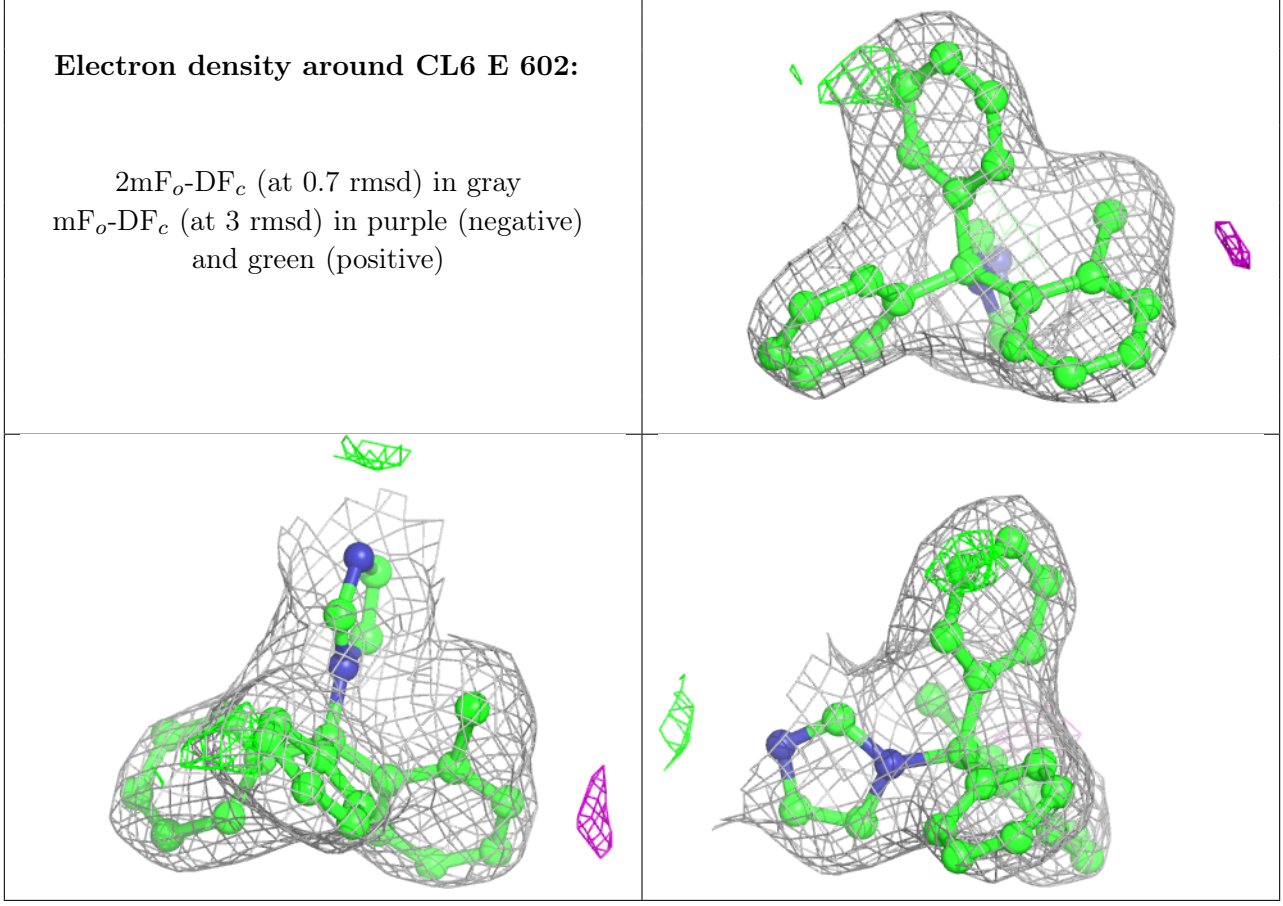






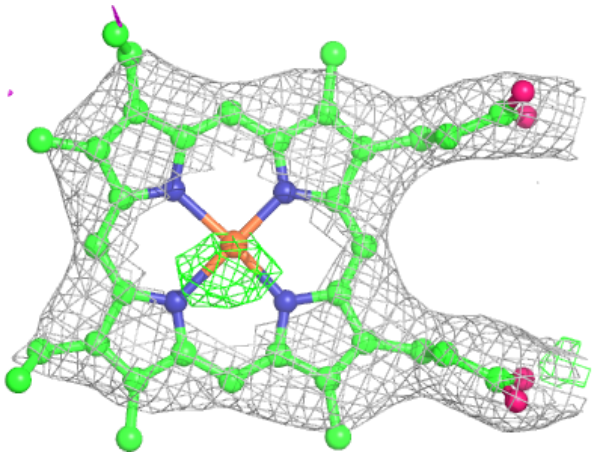
Electron density around CL6 E 602:

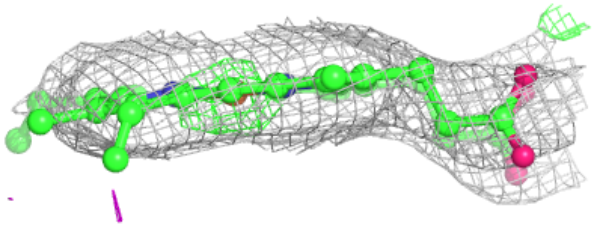
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

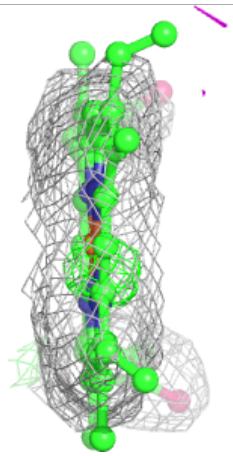


Electron density around HEM G 601:

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

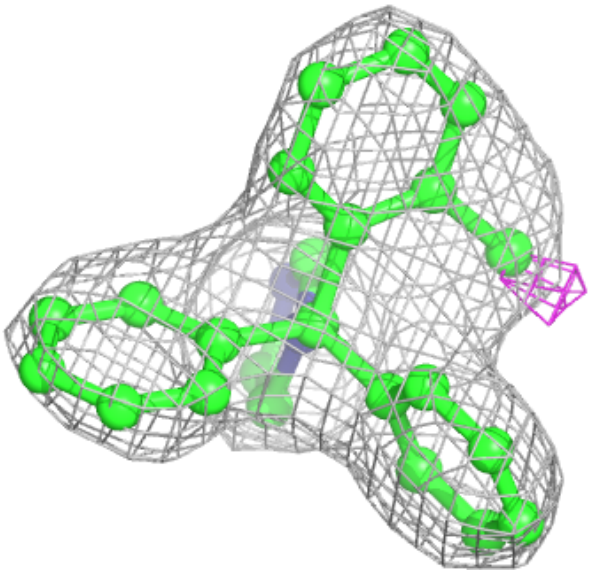


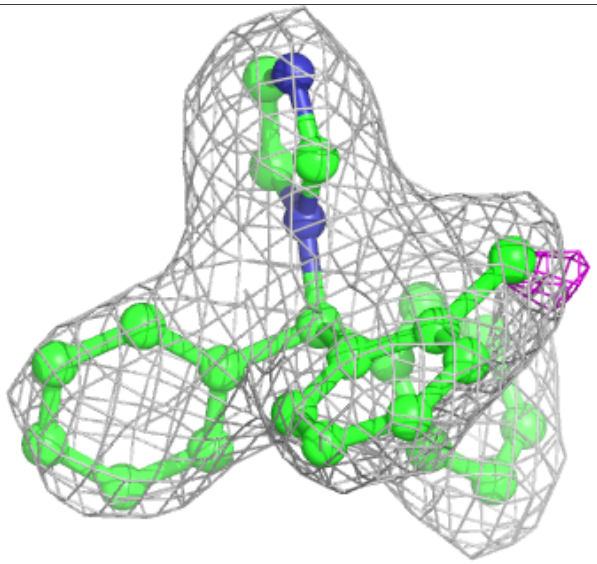


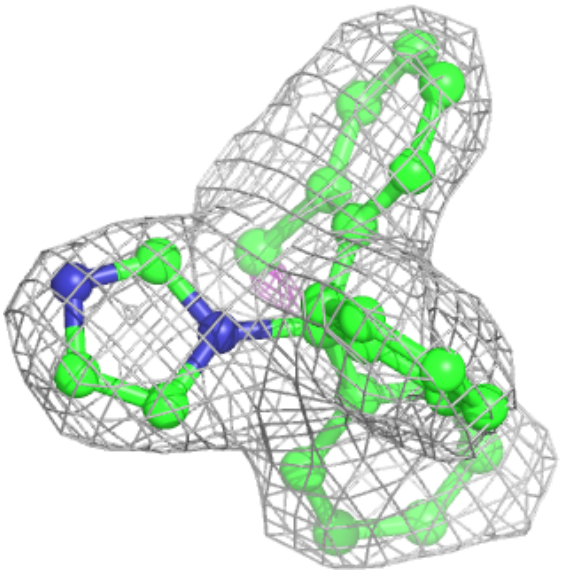


Electron density around CL6 E 603:

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

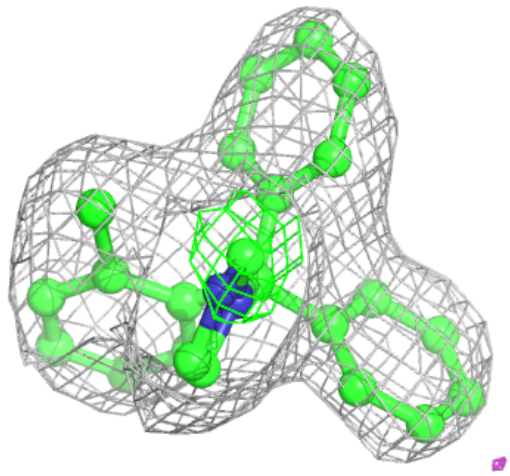


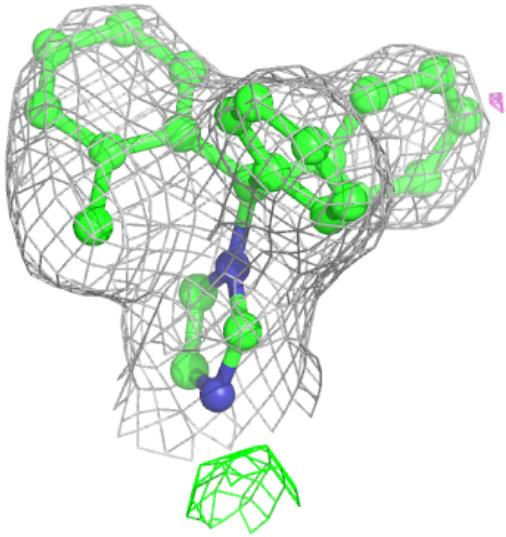


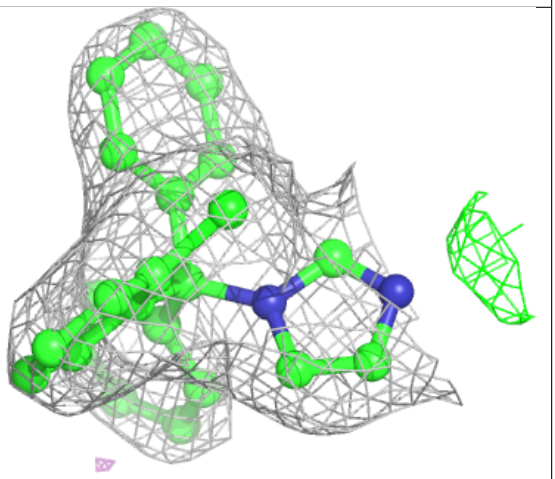


Electron density around CL6 G 602:

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

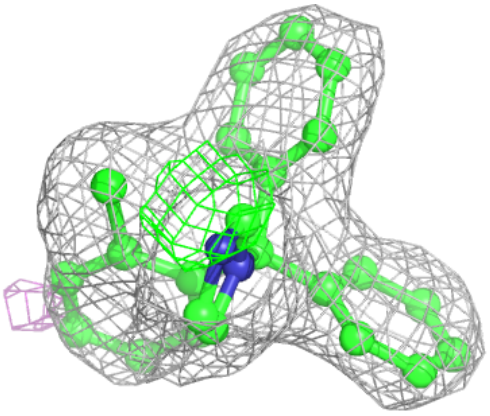


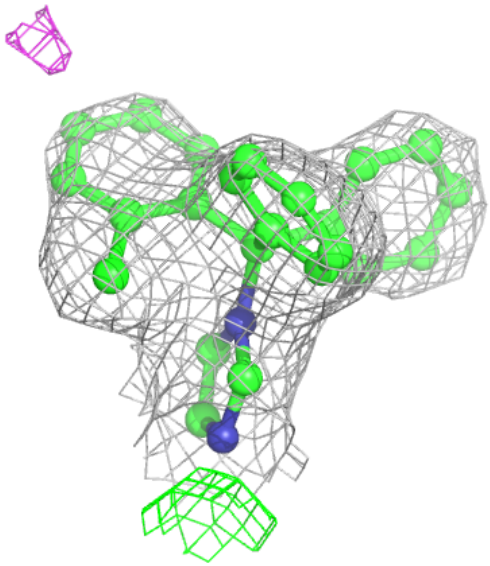


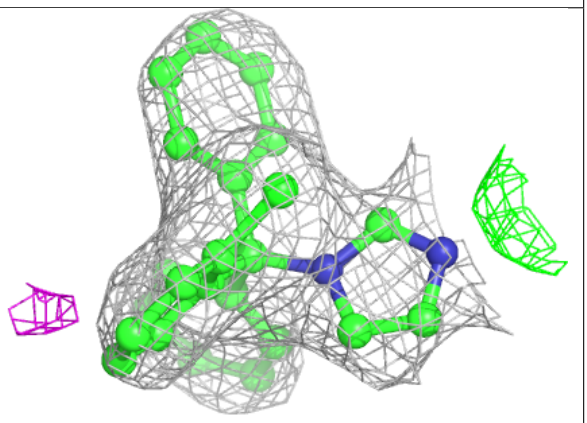


Electron density around CL6 B 602:

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

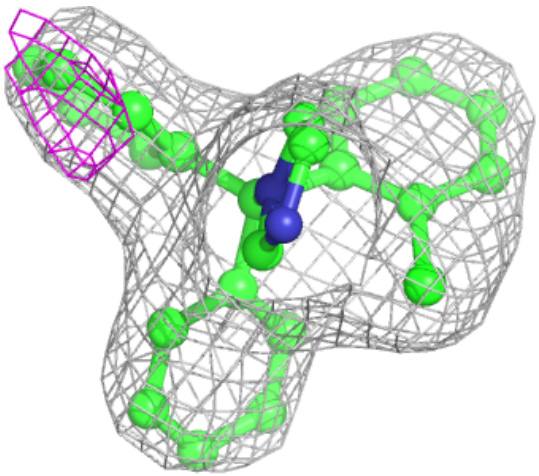


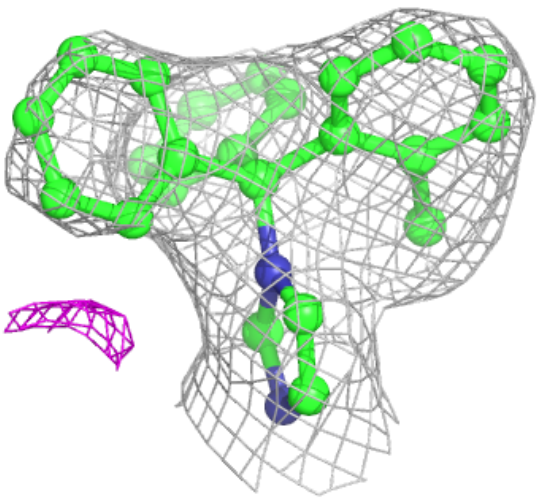


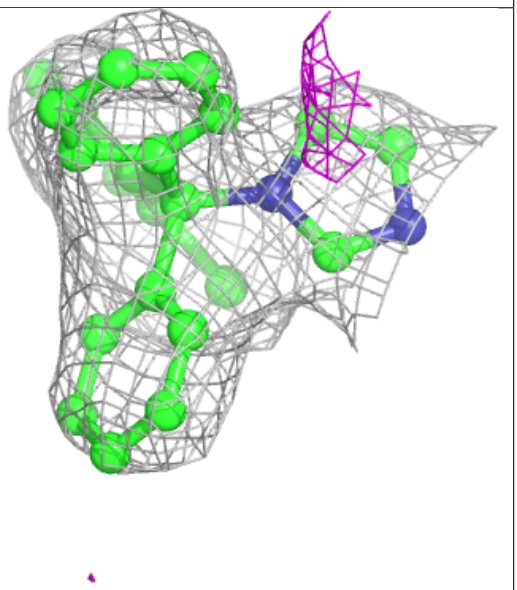


Electron density around CL6 F 602:

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

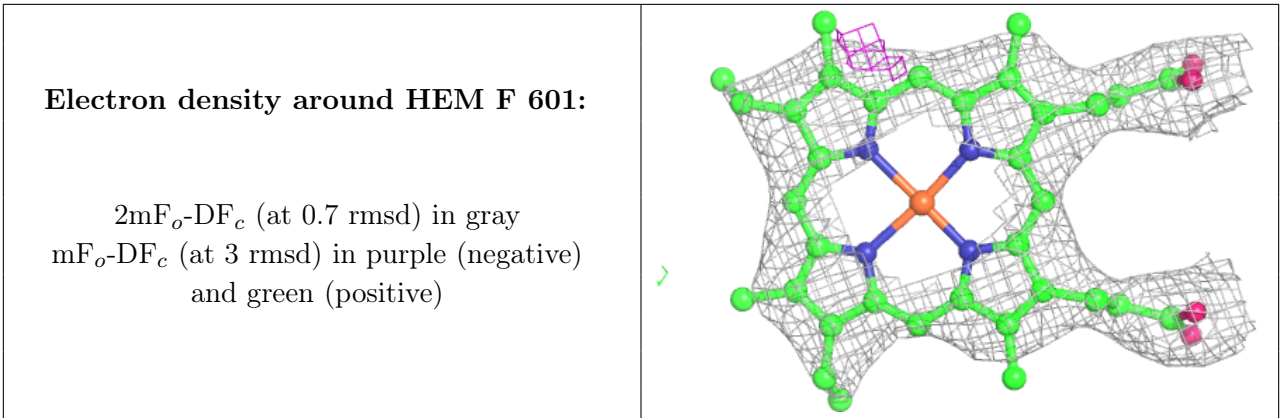


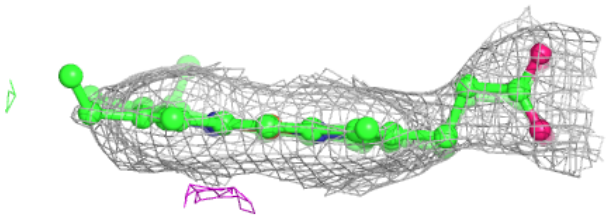


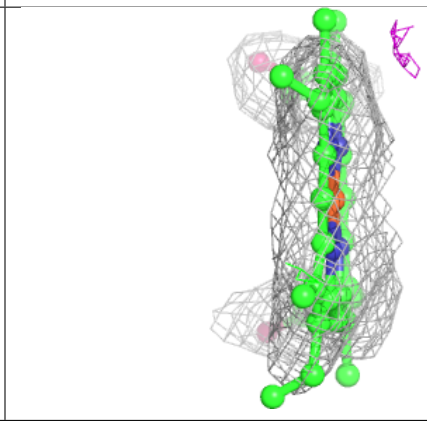


Electron density around HEM F 601:

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

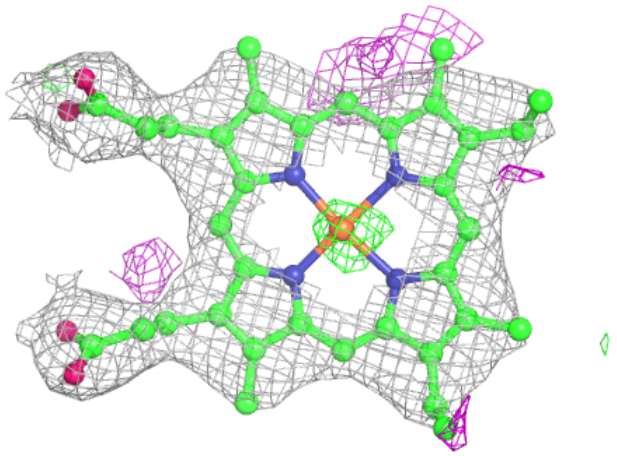


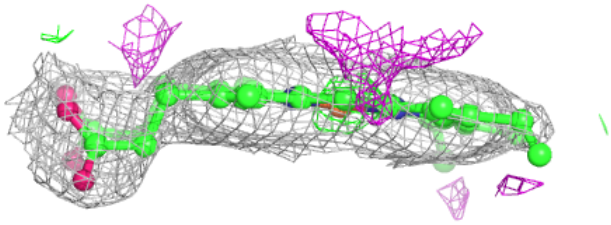


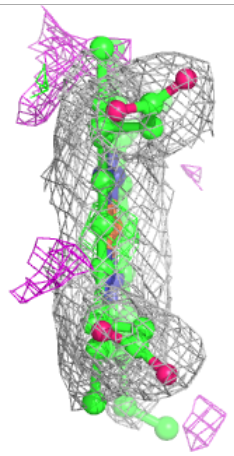


Electron density around HEM A 601:

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

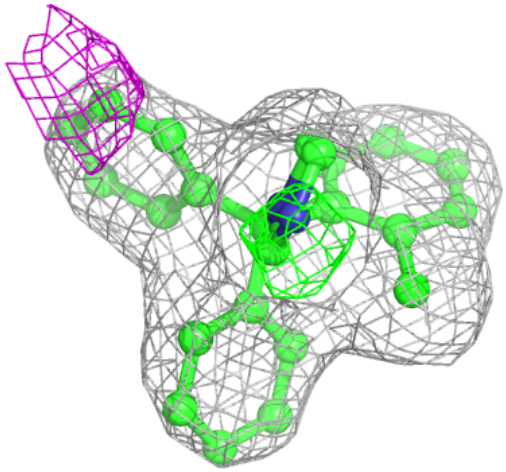


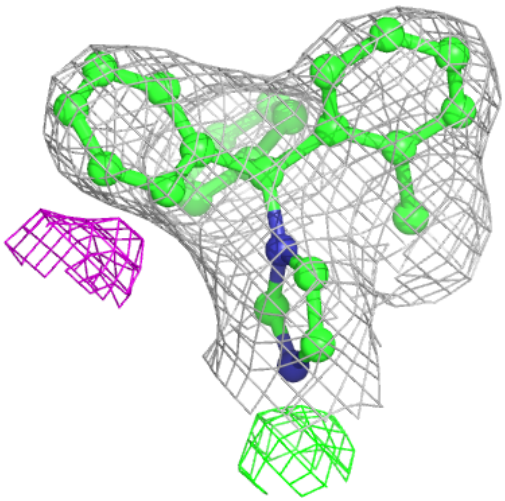


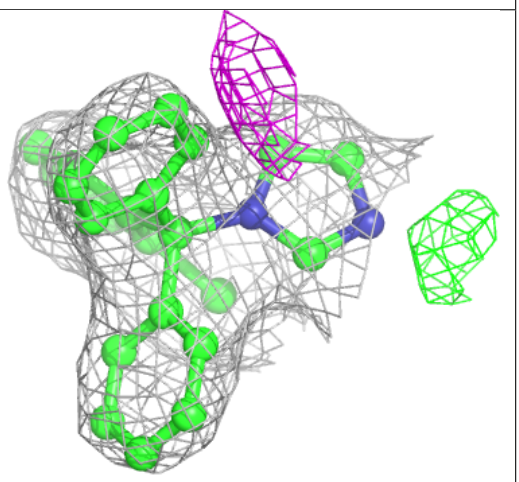


Electron density around CL6 C 602:

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

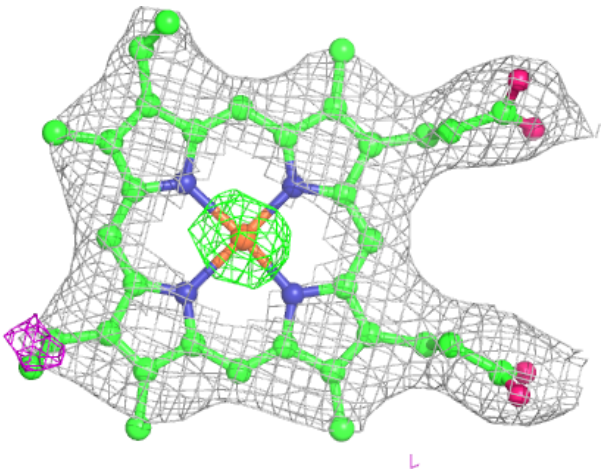


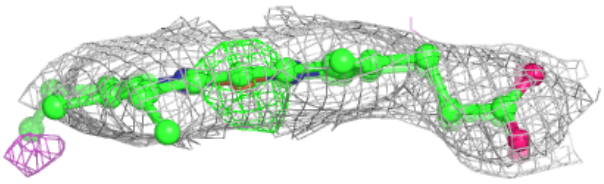


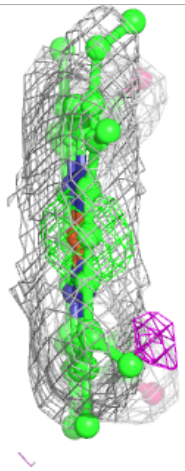


Electron density around HEM B 601:

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

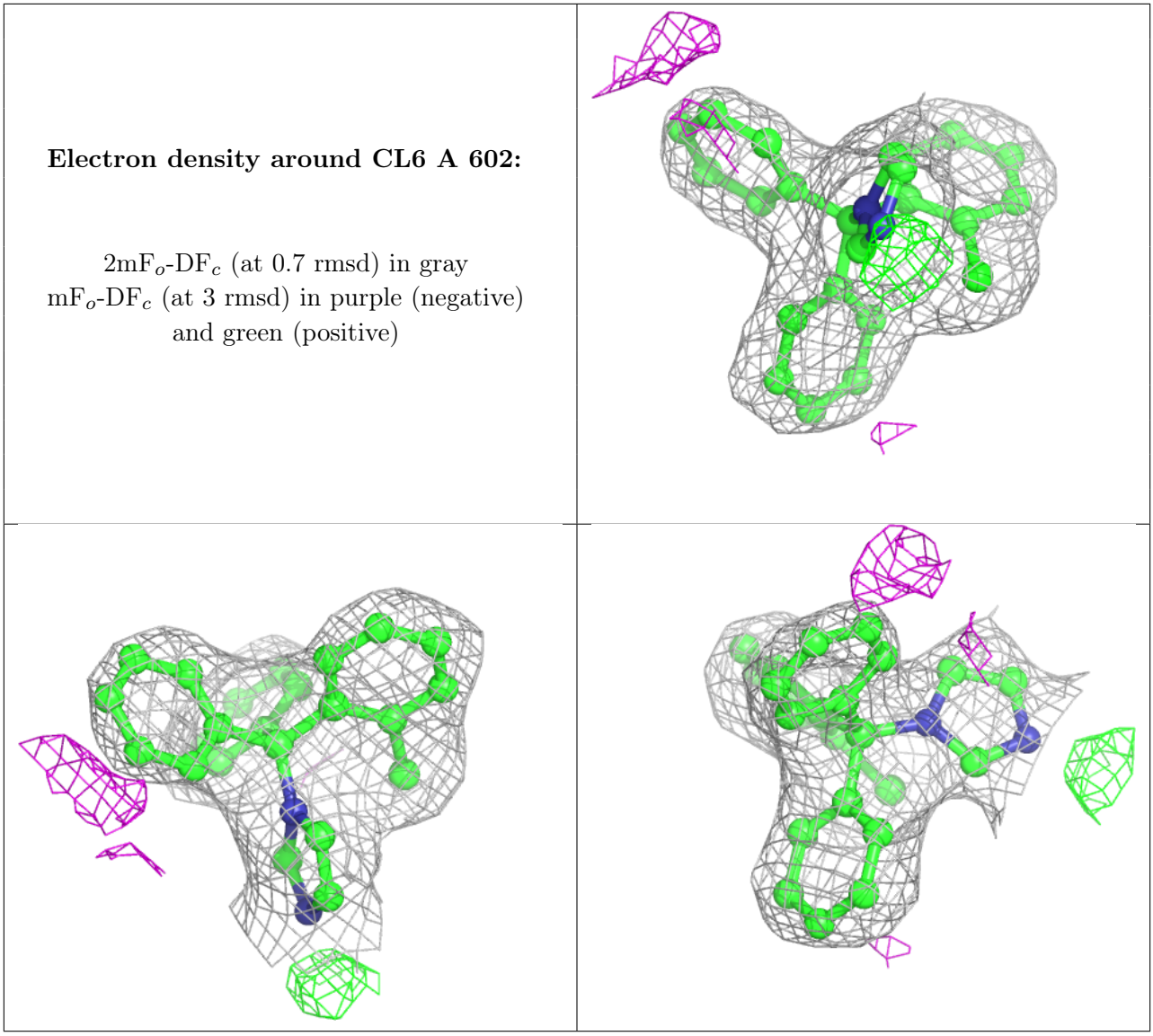






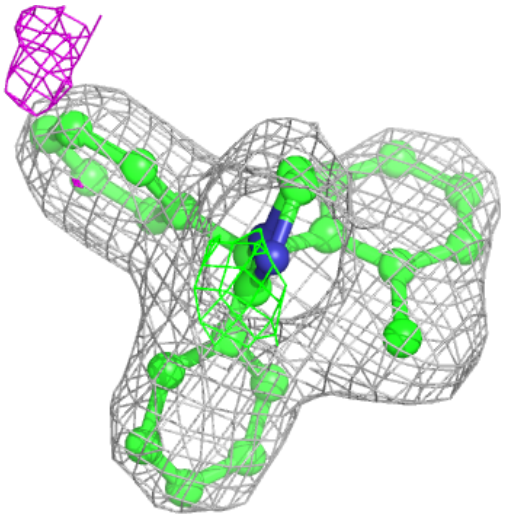
Electron density around CL6 A 602:

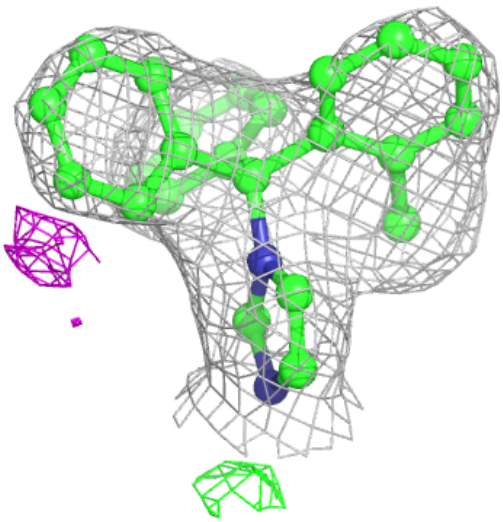
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

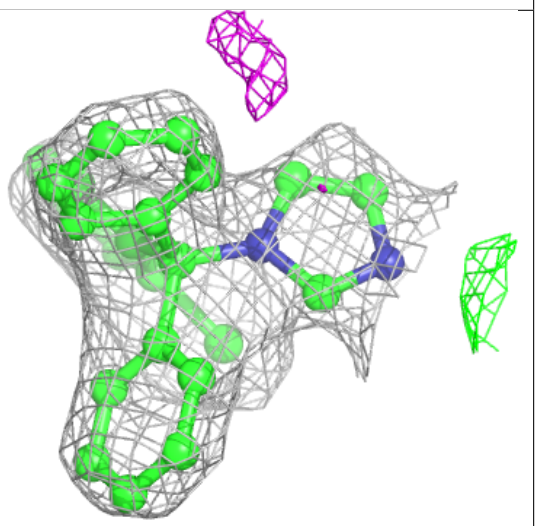


Electron density around CL6 D 602:

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

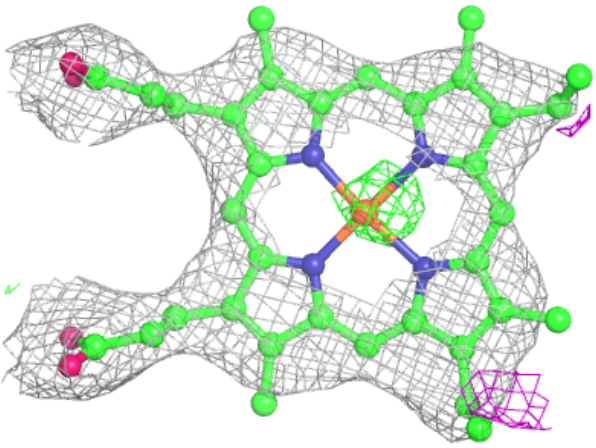


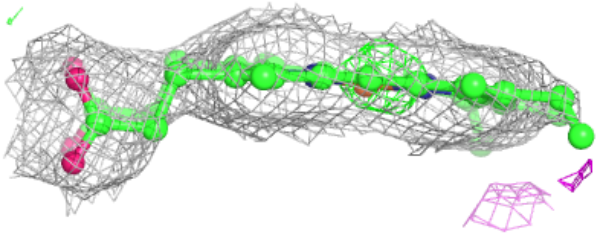


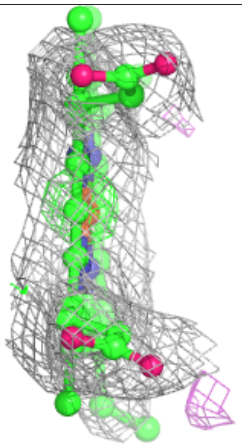


Electron density around HEM C 601:

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

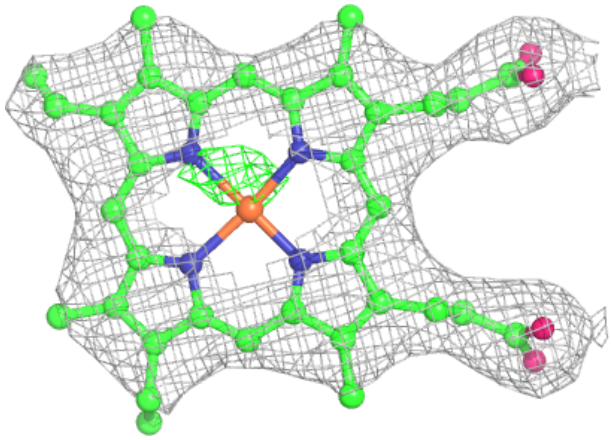


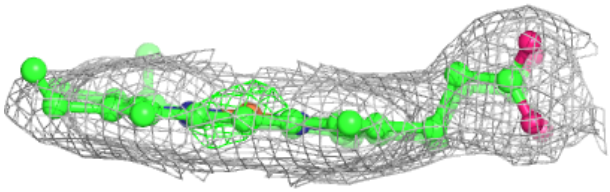


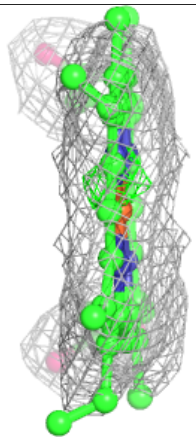


Electron density around HEM D 601:

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

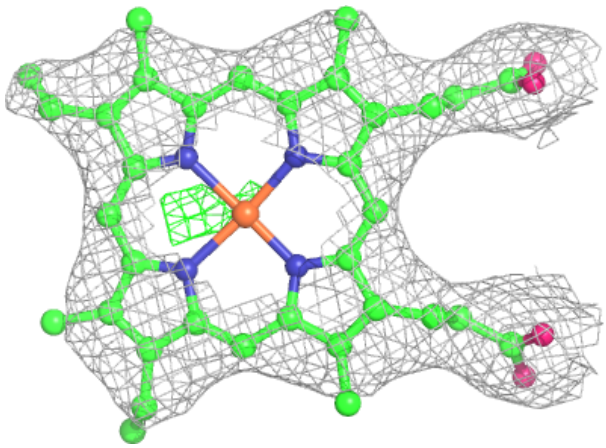


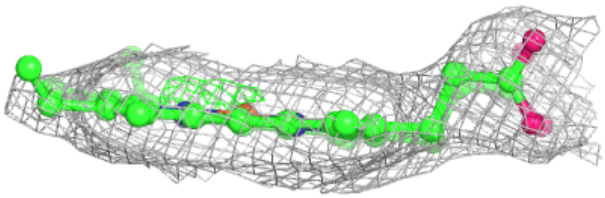


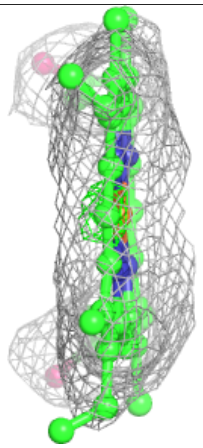


Electron density around HEM E 601:

$2mF_o$-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.