



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 07:58 PM UTC

PDB ID : 8SG5 / pdb_00008sg5
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:

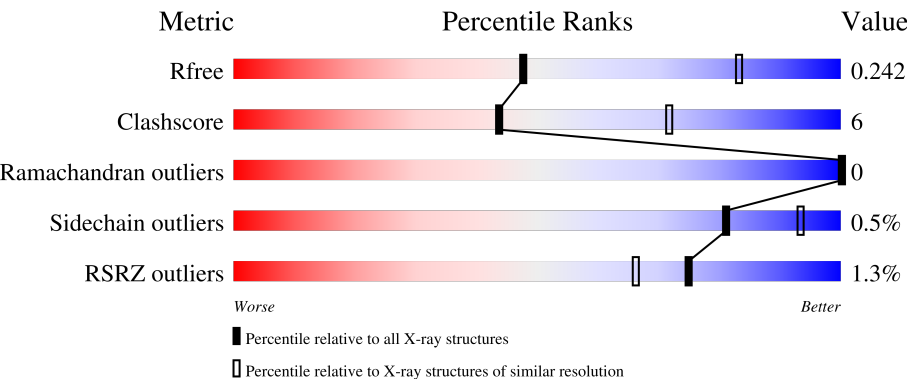
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	480	% 81%14%5%
1	B	480	% 83%12%5%
1	C	480	% 82%11%6%
1	D	480	% 85%9%6%
1	E	480	% 83%11%6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	480	% 84% 10% 6%
1	G	480	% 80% 14% 6%
1	H	480	2% 78% 15% 7%

2 Entry composition

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:

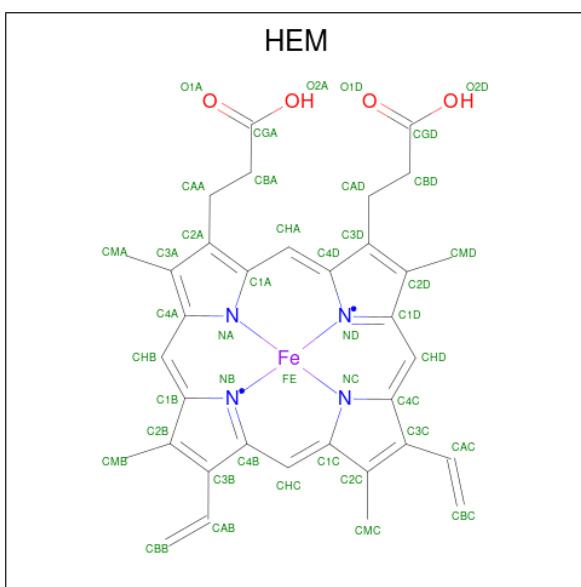
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP P20815
A	23	ALA	-	expression tag	UNP P20815
A	498	HIS	-	expression tag	UNP P20815
A	499	HIS	-	expression tag	UNP P20815
A	500	HIS	-	expression tag	UNP P20815
A	501	HIS	-	expression tag	UNP P20815
B	22	MET	-	initiating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

Continued on next page...

Continued from previous page...

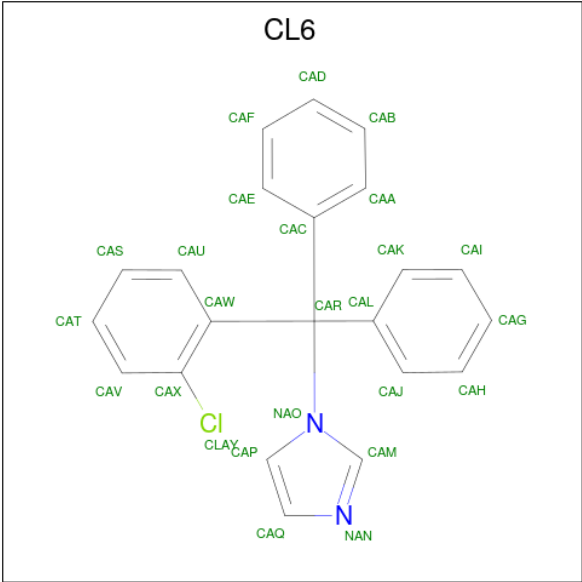
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	ALA	-	expression tag	UNP P20815
C	498	HIS	-	expression tag	UNP P20815
C	499	HIS	-	expression tag	UNP P20815
C	500	HIS	-	expression tag	UNP P20815
C	501	HIS	-	expression tag	UNP P20815
D	22	MET	-	initiating methionine	UNP P20815
D	23	ALA	-	expression 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 (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 1-[(2-CHLOROPHENYL)(DIPHENYL)METHYL]-1H-IMIDAZOLE (CCD ID: CL6) (formula: C₂₂H₁₇ClN₂) (labeled as "Ligand of Interest" by depositor).



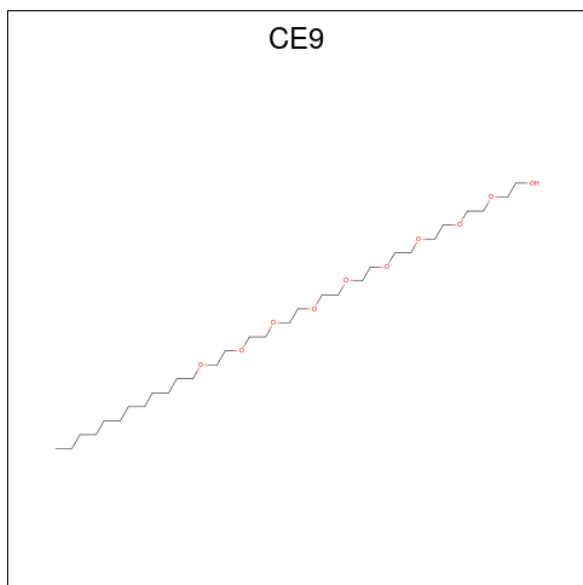
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	C	1	Total	C	Cl	N	0	0
			25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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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		

Continued on next page...

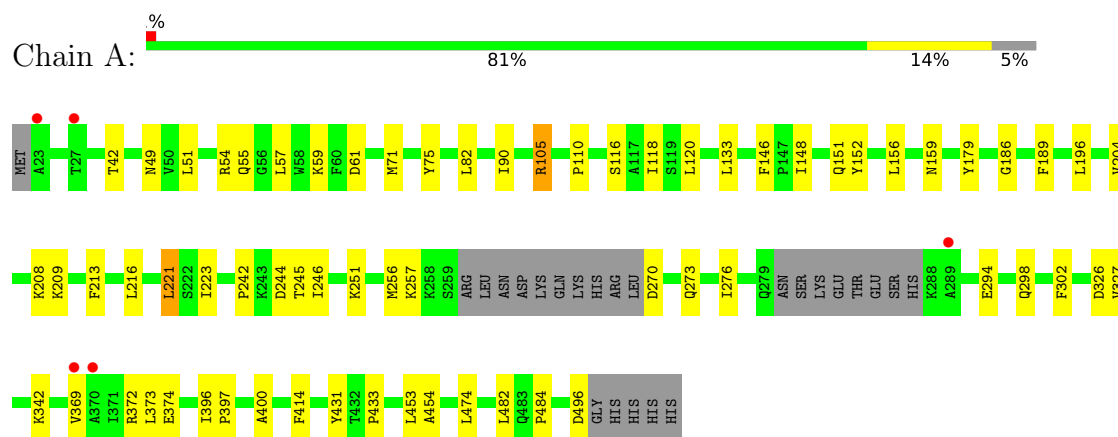
Continued from previous page...

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

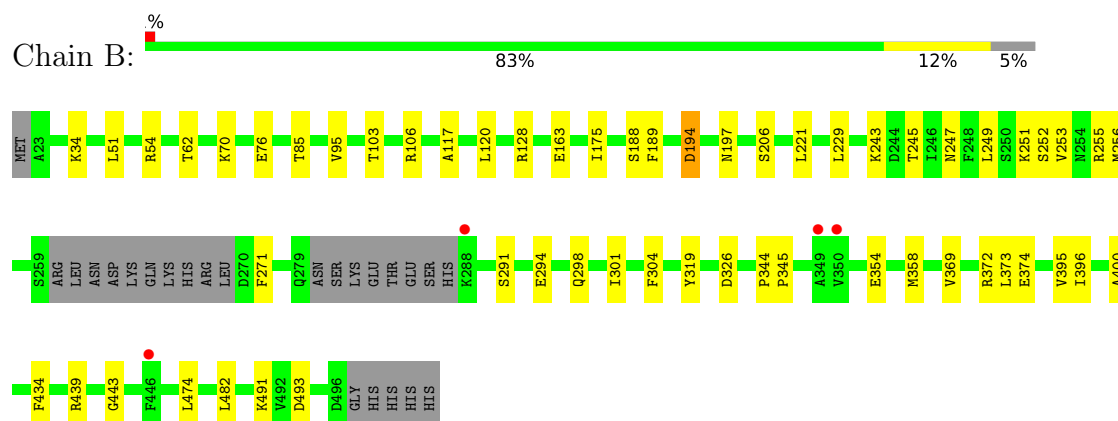
3 Residue-property plots [i](#)

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.

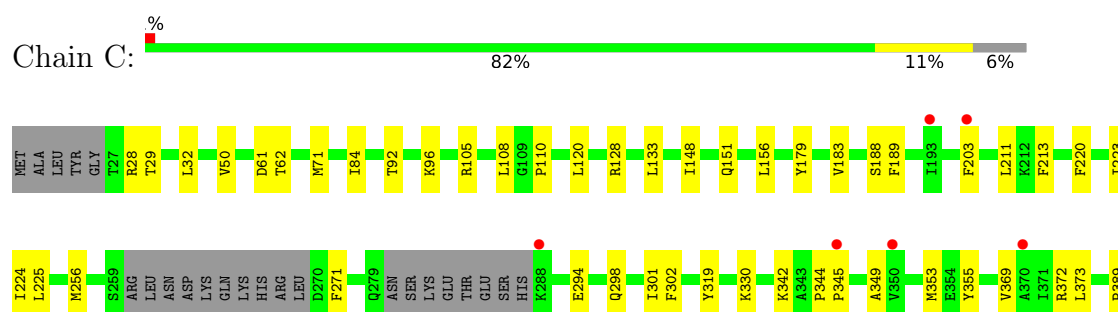
• Molecule 1: Cytochrome P450 3A5



• Molecule 1: Cytochrome P450 3A5

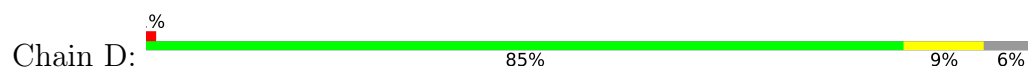


• Molecule 1: Cytochrome P450 3A5

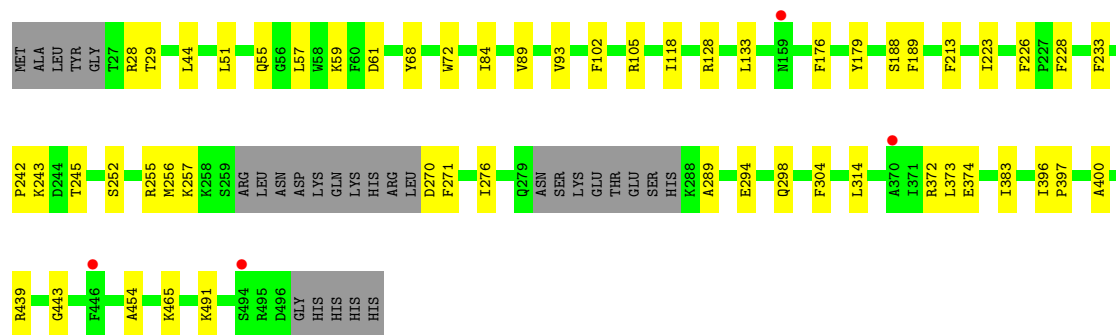
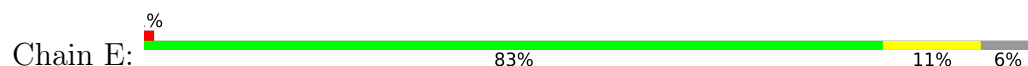




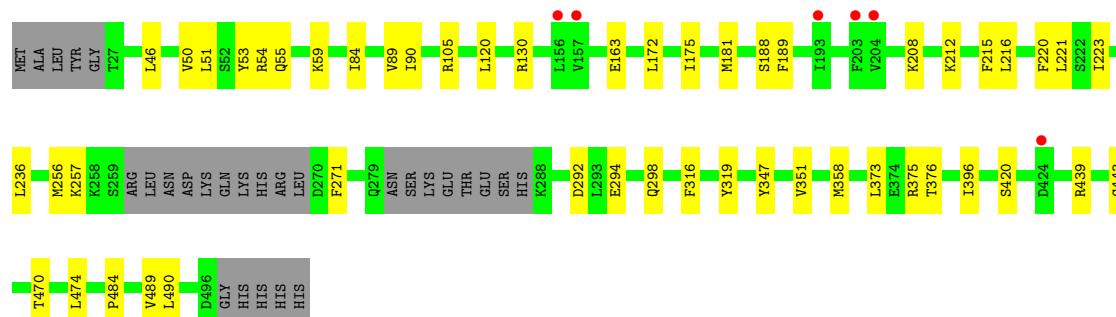
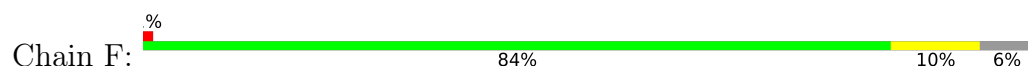
- Molecule 1: Cytochrome P450 3A5



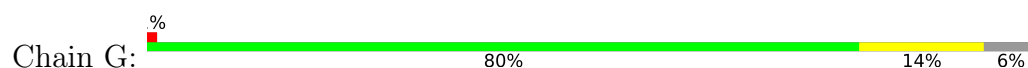
- Molecule 1: Cytochrome P450 3A5

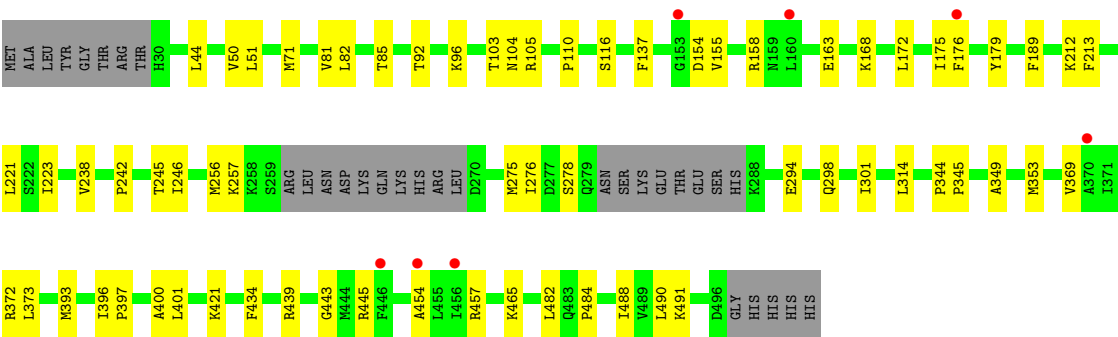


- Molecule 1: Cytochrome P450 3A5

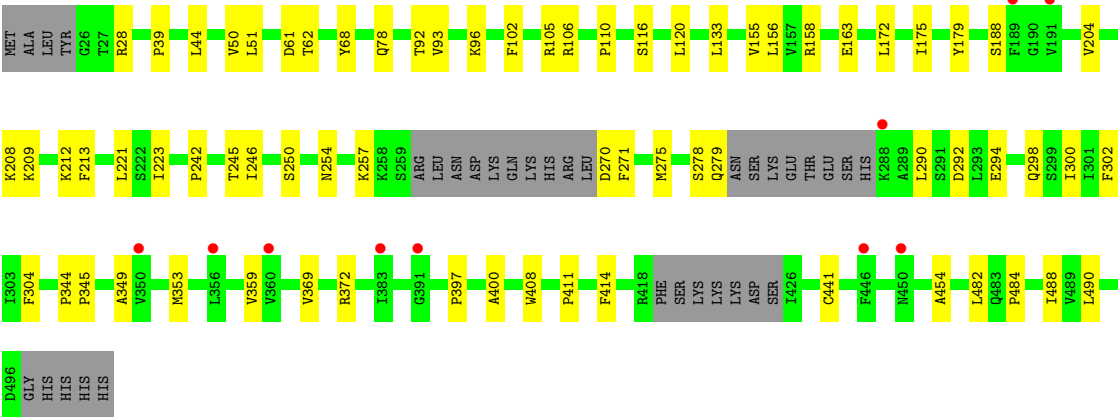
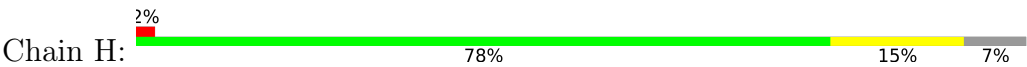


- Molecule 1: Cytochrome P450 3A5





● Molecule 1: Cytochrome P450 3A5



4 Data and refinement statistics

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) 99.1 (39.10-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.203 , 0.241 0.203 , 0.242	Depositor DCC
R_{free} test set	5604 reflections (5.02%)	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 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CE9, CL6

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	0.10	0/3723	0.26	0/5048
1	B	0.10	0/3743	0.26	0/5068
1	C	0.11	0/3705	0.27	0/5016
1	D	0.11	0/3717	0.27	0/5032
1	E	0.11	0/3713	0.27	0/5027
1	F	0.10	0/3701	0.26	0/5014
1	G	0.11	0/3688	0.27	0/4993
1	H	0.09	0/3657	0.25	0/4953
All	All	0.10	0/29647	0.26	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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3635	0	3689	42	0
1	B	3655	0	3744	37	0
1	C	3618	0	3712	33	0
1	D	3630	0	3719	28	0
1	E	3626	0	3716	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3614	0	3689	33	0
1	G	3601	0	3689	40	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	369	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 (369) 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

Continued on next page...

Continued from previous page...

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: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:F:470:THR:OG1	1:F:489:VAL:O	2.18	0.56
1:D:257:LYS:HG2	1:D:276:ILE:HD11	1.88	0.56

Continued on next page...

Continued from previous page...

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:C:211:LEU:C	1:C:213:PHE:H	2.14	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:LEU:HD13	1:H:302:PHE:HZ	1.74	0.51
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
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

Continued on next page...

Continued from previous page...

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:E:189:PHE:CG	1:E:256:MET:HE1	2.50	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:603:CL6:HAJ	3:B:603:CL6:CAA	2.45	0.45
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
1:C:211:LEU:C	1:C:213:PHE:N	2.74	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:61:ASP:CG	1:A:372:ARG:HH21	2.24	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:D:145:MET:HE2	1:D:145:MET:HB3	1.90	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
1:C:71:MET:HE2	1:C:84:ILE:HG22	1.99	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:F:189:PHE:CG	1:F:256:MET:HE1	2.53	0.43
1:H:242:PRO:HB2	1:H:245:THR:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:189:PHE:CG	1:G:256:MET:HE1	2.53	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
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:G:275:MET:O	1:G:278:SER:OG	2.35	0.43
1:A:90:ILE:HG23	1:A:396:ILE:HG12	2.00	0.42
1:A:189:PHE:CG	1:A:256:MET:HE1	2.54	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:F:358:MET:HE2	1:F:420:SER:HA	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:189:PHE:CG	1:B:256:MET:HE1	2.54	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:181:MET:HE1	1:F:208:LYS:HG3	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
1:C:189:PHE:CG	1:C:256:MET:HE1	2.56	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

5.3.1 Protein backbone

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
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

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%)	402 (99%)	4 (1%)	68	88
1	B	411/434 (95%)	407 (99%)	4 (1%)	68	88
1	C	408/434 (94%)	406 (100%)	2 (0%)	81	93
1	D	409/434 (94%)	409 (100%)	0	100	100
1	E	409/434 (94%)	407 (100%)	2 (0%)	81	93
1	F	405/434 (93%)	403 (100%)	2 (0%)	81	93

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	406/434 (94%)	404 (100%)	2 (0%)	81	93
1	H	402/434 (93%)	401 (100%)	1 (0%)	87	96
All	All	3256/3472 (94%)	3239 (100%)	17 (0%)	81	93

All (17) 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
1	B	95	VAL
1	B	194	ASP
1	B	291	SER
1	B	372	ARG
1	C	108	LEU
1	C	203	PHE
1	E	243	LYS
1	E	270	ASP
1	F	46	LEU
1	F	376	THR
1	G	212	LYS
1	G	372	ARG
1	H	270	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	HIS
1	B	198	ASN
1	B	384	ASN
1	D	198	ASN
1	E	198	ASN
1	E	483	GLN
1	G	159	ASN
1	G	197	ASN
1	G	198	ASN
1	G	332	GLN
1	G	450	ASN
1	G	483	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	78	GLN
1	H	384	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
4	CE9	C	605	-	23,23,39	0.16	0	22,22,38	0.09	0
3	CL6	C	604	-	28,28,28	0.81	2 (7%)	39,39,39	0.97	3 (7%)
3	CL6	H	604	-	28,28,28	0.58	1 (3%)	39,39,39	0.84	2 (5%)
3	CL6	E	603	-	28,28,28	0.43	0	39,39,39	1.28	3 (7%)
4	CE9	E	605	-	21,21,39	0.17	0	20,20,38	0.09	0
2	HEM	H	601	1,3	50,50,50	1.52	6 (12%)	67,82,82	1.64	11 (16%)
3	CL6	B	604	-	28,28,28	0.64	2 (7%)	39,39,39	0.84	1 (2%)
3	CL6	G	603	-	28,28,28	0.57	1 (3%)	39,39,39	1.22	3 (7%)
2	HEM	F	601	1,3	50,50,50	1.51	7 (14%)	67,82,82	1.64	13 (19%)
3	CL6	G	602	2	28,28,28	0.44	1 (3%)	39,39,39	0.77	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CL6	G	604	-	28,28,28	0.53	0	39,39,39	0.87	2 (5%)
3	CL6	D	603	-	28,28,28	0.40	0	39,39,39	1.21	3 (7%)
2	HEM	A	601	1,3	50,50,50	1.52	8 (16%)	67,82,82	1.66	11 (16%)
3	CL6	B	603	-	28,28,28	0.43	0	39,39,39	1.42	4 (10%)
3	CL6	D	602	2	28,28,28	0.60	2 (7%)	39,39,39	0.87	3 (7%)
4	CE9	F	605	-	28,28,39	0.12	0	27,27,38	0.14	0
3	CL6	B	602	2	28,28,28	0.38	0	39,39,39	0.72	0
3	CL6	D	604	-	28,28,28	0.45	1 (3%)	39,39,39	0.87	2 (5%)
3	CL6	E	604	-	28,28,28	0.51	1 (3%)	39,39,39	0.89	2 (5%)
2	HEM	C	601	1,3	50,50,50	1.53	9 (18%)	67,82,82	1.63	11 (16%)
4	CE9	D	605	-	23,23,39	0.17	0	22,22,38	0.10	0
2	HEM	E	601	1,3	50,50,50	1.54	8 (16%)	67,82,82	1.63	14 (20%)
3	CL6	F	604	-	28,28,28	0.45	0	39,39,39	0.84	3 (7%)
2	HEM	D	601	1,3	50,50,50	1.54	6 (12%)	67,82,82	1.66	14 (20%)
4	CE9	B	605	-	33,33,39	0.12	0	32,32,38	0.15	0
3	CL6	F	603	-	28,28,28	0.43	0	39,39,39	1.22	2 (5%)
2	HEM	B	601	1,3	50,50,50	1.55	6 (12%)	67,82,82	1.64	10 (14%)
3	CL6	A	603	-	28,28,28	0.52	1 (3%)	39,39,39	1.24	2 (5%)
3	CL6	F	602	2	28,28,28	0.66	2 (7%)	39,39,39	0.90	3 (7%)
2	HEM	G	601	1,3	50,50,50	1.53	9 (18%)	67,82,82	1.67	13 (19%)
3	CL6	H	602	2	28,28,28	0.25	0	39,39,39	0.63	0
3	CL6	A	602	2	28,28,28	0.49	1 (3%)	39,39,39	0.85	1 (2%)
3	CL6	C	603	-	28,28,28	0.49	1 (3%)	39,39,39	1.22	2 (5%)
4	CE9	G	605	-	29,29,39	0.17	0	28,28,38	0.09	0
3	CL6	H	603	-	28,28,28	0.46	0	39,39,39	1.08	2 (5%)
4	CE9	A	605	-	39,39,39	0.13	0	38,38,38	0.13	0
3	CL6	C	602	2	28,28,28	0.48	1 (3%)	39,39,39	0.80	1 (2%)
3	CL6	A	604	-	28,28,28	0.73	2 (7%)	39,39,39	0.78	1 (2%)
3	CL6	E	602	2	28,28,28	0.29	0	39,39,39	0.74	1 (2%)

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
4	CE9	C	605	-	-	8/21/21/37	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CL6	C	604	-	-	0/24/24/24	0/4/4/4
3	CL6	H	604	-	-	0/24/24/24	0/4/4/4
3	CL6	E	603	-	-	0/24/24/24	0/4/4/4
4	CE9	E	605	-	-	7/19/19/37	-
2	HEM	H	601	1,3	-	6/14/54/54	-
3	CL6	B	604	-	-	0/24/24/24	0/4/4/4
3	CL6	G	603	-	-	1/24/24/24	0/4/4/4
2	HEM	F	601	1,3	-	4/14/54/54	-
3	CL6	G	602	2	-	0/24/24/24	0/4/4/4
3	CL6	G	604	-	-	0/24/24/24	0/4/4/4
3	CL6	D	603	-	-	0/24/24/24	0/4/4/4
2	HEM	A	601	1,3	-	7/14/54/54	-
3	CL6	B	603	-	-	0/24/24/24	0/4/4/4
3	CL6	D	602	2	-	0/24/24/24	0/4/4/4
4	CE9	F	605	-	-	6/26/26/37	-
3	CL6	B	602	2	-	0/24/24/24	0/4/4/4
3	CL6	D	604	-	-	0/24/24/24	0/4/4/4
3	CL6	E	604	-	-	0/24/24/24	0/4/4/4
2	HEM	C	601	1,3	-	6/14/54/54	-
4	CE9	D	605	-	-	3/21/21/37	-
2	HEM	E	601	1,3	-	6/14/54/54	-
3	CL6	F	604	-	-	0/24/24/24	0/4/4/4
2	HEM	D	601	1,3	-	5/14/54/54	-
4	CE9	B	605	-	-	10/31/31/37	-
3	CL6	F	603	-	-	1/24/24/24	0/4/4/4
2	HEM	B	601	1,3	-	6/14/54/54	-
3	CL6	A	603	-	-	0/24/24/24	0/4/4/4
3	CL6	F	602	2	-	0/24/24/24	0/4/4/4
2	HEM	G	601	1,3	-	7/14/54/54	-
3	CL6	H	602	2	-	0/24/24/24	0/4/4/4
3	CL6	A	602	2	-	0/24/24/24	0/4/4/4
3	CL6	C	603	-	-	0/24/24/24	0/4/4/4
4	CE9	G	605	-	-	10/27/27/37	-
3	CL6	H	603	-	-	1/24/24/24	0/4/4/4
4	CE9	A	605	-	-	15/37/37/37	-
3	CL6	C	602	2	-	0/24/24/24	0/4/4/4
3	CL6	A	604	-	-	0/24/24/24	0/4/4/4
3	CL6	E	602	2	-	0/24/24/24	0/4/4/4

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	FE-NB	5.31	2.11	1.94
2	F	601	HEM	FE-NB	5.24	2.11	1.94
2	H	601	HEM	FE-NB	5.23	2.11	1.94
2	A	601	HEM	FE-NB	5.22	2.11	1.94
2	E	601	HEM	FE-NB	5.15	2.10	1.94
2	G	601	HEM	FE-NB	5.14	2.10	1.94
2	C	601	HEM	FE-NB	5.07	2.10	1.94
2	D	601	HEM	FE-NB	5.05	2.10	1.94
2	D	601	HEM	FE-NC	4.40	2.09	1.95
2	H	601	HEM	FE-NC	4.35	2.09	1.95
2	B	601	HEM	FE-NC	4.34	2.09	1.95
2	E	601	HEM	FE-NC	4.27	2.09	1.95
2	G	601	HEM	FE-NC	4.26	2.09	1.95
2	C	601	HEM	FE-NC	4.23	2.09	1.95
2	F	601	HEM	FE-NC	4.20	2.09	1.95
2	A	601	HEM	FE-NC	4.18	2.08	1.95
2	B	601	HEM	C1B-NB	-3.39	1.34	1.40
2	G	601	HEM	C1B-NB	-3.37	1.34	1.40
2	D	601	HEM	C1B-NB	-3.35	1.34	1.40
2	C	601	HEM	C1B-NB	-3.32	1.34	1.40
2	E	601	HEM	C1B-NB	-3.29	1.34	1.40
2	H	601	HEM	C1B-NB	-3.29	1.34	1.40
2	F	601	HEM	C1B-NB	-3.28	1.34	1.40
2	A	601	HEM	C1B-NB	-3.22	1.34	1.40
3	C	604	CL6	CAR-NAO	3.12	1.53	1.50
3	A	604	CL6	CAR-CAW	3.02	1.57	1.54
2	D	601	HEM	C4D-ND	-3.00	1.35	1.40
2	E	601	HEM	C4D-ND	-2.95	1.35	1.40
2	B	601	HEM	C4D-ND	-2.94	1.35	1.40
2	F	601	HEM	C4D-ND	-2.90	1.35	1.40
2	H	601	HEM	C4D-ND	-2.90	1.35	1.40
2	G	601	HEM	C4D-ND	-2.88	1.35	1.40
2	C	601	HEM	C4D-ND	-2.84	1.35	1.40
3	C	604	CL6	CAR-CAW	2.81	1.57	1.54
2	A	601	HEM	C4D-ND	-2.77	1.35	1.40
3	F	602	CL6	CAR-NAO	2.63	1.53	1.50
3	H	604	CL6	CAR-NAO	2.58	1.53	1.50
3	B	604	CL6	CAR-NAO	2.58	1.53	1.50
3	A	602	CL6	CAR-NAO	2.45	1.53	1.50
3	A	603	CL6	CAR-NAO	2.37	1.53	1.50
3	C	602	CL6	CAR-NAO	2.30	1.52	1.50
2	B	601	HEM	FE-ND	-2.29	1.87	1.94
3	A	604	CL6	CAR-NAO	2.29	1.52	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C1C-C2C	-2.29	1.40	1.45
3	D	602	CL6	CAR-NAO	2.25	1.52	1.50
2	A	601	HEM	FE-ND	-2.23	1.88	1.94
3	C	603	CL6	CAR-NAO	2.19	1.52	1.50
2	A	601	HEM	C3C-C4C	-2.18	1.42	1.46
2	E	601	HEM	C3C-C4C	-2.18	1.42	1.46
3	G	602	CL6	CAR-NAO	2.17	1.52	1.50
2	H	601	HEM	C1C-C2C	-2.17	1.41	1.45
3	G	603	CL6	CAR-NAO	2.17	1.52	1.50
3	F	602	CL6	CAR-CAW	2.16	1.57	1.54
2	C	601	HEM	FE-ND	-2.16	1.88	1.94
2	F	601	HEM	FE-ND	-2.15	1.88	1.94
3	D	602	CL6	CAR-CAW	2.15	1.57	1.54
2	G	601	HEM	C1C-C2C	-2.15	1.41	1.45
2	G	601	HEM	FE-ND	-2.14	1.88	1.94
2	D	601	HEM	C1C-C2C	-2.14	1.41	1.45
2	H	601	HEM	FE-ND	-2.14	1.88	1.94
2	C	601	HEM	C1C-C2C	-2.13	1.41	1.45
2	D	601	HEM	C3C-C4C	-2.11	1.42	1.46
2	F	601	HEM	C1C-C2C	-2.09	1.41	1.45
2	C	601	HEM	C3C-C4C	-2.09	1.42	1.46
2	E	601	HEM	FE-ND	-2.08	1.88	1.94
2	E	601	HEM	C3B-C4B	2.06	1.48	1.44
3	B	604	CL6	CAR-CAW	2.06	1.56	1.54
3	E	604	CL6	CAR-NAO	2.06	1.52	1.50
2	A	601	HEM	C3B-C4B	2.06	1.48	1.44
2	E	601	HEM	C1C-C2C	-2.05	1.41	1.45
2	G	601	HEM	C3C-C4C	-2.05	1.42	1.46
2	G	601	HEM	C4B-NB	-2.04	1.34	1.38
2	A	601	HEM	C1C-C2C	-2.04	1.41	1.45
2	C	601	HEM	C4B-NB	-2.03	1.34	1.38
2	C	601	HEM	C1D-ND	-2.02	1.34	1.38
2	G	601	HEM	C1D-ND	-2.01	1.34	1.38
3	D	604	CL6	CAR-NAO	2.01	1.52	1.50
2	F	601	HEM	C3C-C4C	-2.00	1.42	1.46

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	CHC-C4B-NB	5.44	130.28	124.42
2	G	601	HEM	CHC-C4B-NB	5.37	130.20	124.42
3	B	603	CL6	CAW-CAR-NAO	5.34	113.96	106.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	HEM	CHC-C4B-NB	5.34	130.17	124.42
2	F	601	HEM	CHC-C4B-NB	5.19	130.01	124.42
2	D	601	HEM	CHC-C4B-NB	5.19	130.01	124.42
2	C	601	HEM	CHC-C4B-NB	5.15	129.97	124.42
2	A	601	HEM	CHC-C4B-NB	5.13	129.94	124.42
2	E	601	HEM	CHC-C4B-NB	4.92	129.72	124.42
2	C	601	HEM	CHD-C1D-ND	4.73	129.51	124.42
3	E	603	CL6	CAW-CAR-NAO	4.71	113.06	106.35
2	G	601	HEM	CHD-C1D-ND	4.71	129.49	124.42
3	B	603	CL6	CAL-CAR-CAW	-4.69	105.16	111.85
3	G	603	CL6	CAL-CAR-CAW	-4.67	105.20	111.85
2	F	601	HEM	CHD-C1D-ND	4.64	129.41	124.42
2	B	601	HEM	CHD-C1D-ND	4.57	129.34	124.42
2	A	601	HEM	CHD-C1D-ND	4.55	129.31	124.42
2	H	601	HEM	CHD-C1D-ND	4.54	129.31	124.42
3	A	603	CL6	CAW-CAR-NAO	4.53	112.81	106.35
3	C	603	CL6	CAW-CAR-NAO	4.41	112.64	106.35
3	D	603	CL6	CAL-CAR-CAW	-4.37	105.62	111.85
3	F	603	CL6	CAW-CAR-NAO	4.33	112.52	106.35
3	C	603	CL6	CAL-CAR-CAW	-4.32	105.69	111.85
3	F	603	CL6	CAL-CAR-CAW	-4.31	105.70	111.85
2	E	601	HEM	CHD-C1D-ND	4.28	129.03	124.42
3	A	603	CL6	CAL-CAR-CAW	-4.22	105.83	111.85
2	D	601	HEM	CHD-C1D-ND	4.19	128.93	124.42
3	G	603	CL6	CAW-CAR-NAO	4.18	112.31	106.35
3	E	603	CL6	CAL-CAR-CAW	-4.14	105.95	111.85
3	H	603	CL6	CAL-CAR-CAW	-4.07	106.06	111.85
3	D	603	CL6	CAW-CAR-NAO	3.88	111.88	106.35
3	H	603	CL6	CAW-CAR-NAO	3.72	111.65	106.35
2	D	601	HEM	C1B-NB-C4B	3.60	109.47	105.21
2	E	601	HEM	CHB-C1B-NB	3.57	128.78	124.37
2	D	601	HEM	CHB-C1B-NB	3.56	128.77	124.37
2	C	601	HEM	C1B-NB-C4B	3.50	109.35	105.21
2	E	601	HEM	C1B-NB-C4B	3.47	109.31	105.21
2	A	601	HEM	CHA-C4D-ND	3.44	128.62	124.37
2	G	601	HEM	C1B-NB-C4B	3.43	109.27	105.21
2	G	601	HEM	CHB-C1B-NB	3.43	128.61	124.37
3	G	604	CL6	CAR-CAW-CAX	-3.41	119.91	122.74
2	H	601	HEM	C1B-NB-C4B	3.40	109.23	105.21
2	H	601	HEM	CHA-C4D-ND	3.39	128.56	124.37
2	A	601	HEM	C1B-NB-C4B	3.35	109.17	105.21
2	C	601	HEM	CHB-C1B-NB	3.31	128.47	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	HEM	CHB-C1B-NB	3.31	128.47	124.37
2	E	601	HEM	CHA-C4D-ND	3.30	128.46	124.37
2	A	601	HEM	CHB-C1B-NB	3.27	128.41	124.37
2	F	601	HEM	C1B-NB-C4B	3.26	109.07	105.21
2	B	601	HEM	CHA-C4D-ND	3.25	128.39	124.37
2	D	601	HEM	CHA-C4D-ND	3.25	128.38	124.37
2	B	601	HEM	CHB-C1B-NB	3.24	128.37	124.37
2	F	601	HEM	CHA-C4D-ND	3.23	128.37	124.37
2	G	601	HEM	CHA-C4D-ND	3.22	128.35	124.37
2	F	601	HEM	CHB-C1B-NB	3.21	128.34	124.37
2	G	601	HEM	CHD-C1D-C2D	-3.19	119.99	125.03
2	C	601	HEM	CHD-C1D-C2D	-3.18	120.01	125.03
3	E	604	CL6	CAR-CAW-CAX	-3.15	120.12	122.74
2	B	601	HEM	C1B-NB-C4B	3.14	108.93	105.21
2	C	601	HEM	CHA-C4D-ND	3.12	128.23	124.37
2	F	601	HEM	CHD-C1D-C2D	-3.11	120.12	125.03
2	A	601	HEM	CHD-C1D-C2D	-3.08	120.17	125.03
3	F	602	CL6	CAC-CAR-CAW	3.06	116.22	111.85
2	B	601	HEM	CHD-C1D-C2D	-3.05	120.21	125.03
2	E	601	HEM	CHD-C4C-NC	2.98	127.70	124.45
2	A	601	HEM	CHD-C4C-NC	2.98	127.69	124.45
2	D	601	HEM	CHD-C4C-NC	2.93	127.65	124.45
2	H	601	HEM	CHD-C1D-C2D	-2.92	120.42	125.03
2	D	601	HEM	CHD-C1D-C2D	-2.90	120.44	125.03
2	E	601	HEM	CHD-C1D-C2D	-2.89	120.46	125.03
3	D	602	CL6	CAC-CAR-CAW	2.88	115.96	111.85
3	A	602	CL6	CAR-CAW-CAX	-2.83	120.39	122.74
3	C	604	CL6	CAR-CAW-CAX	-2.79	120.42	122.74
2	C	601	HEM	CHD-C4C-NC	2.75	127.44	124.45
2	A	601	HEM	C3B-C4B-NB	-2.73	107.51	109.47
2	G	601	HEM	CHD-C4C-NC	2.73	127.42	124.45
2	F	601	HEM	CHD-C4C-NC	2.71	127.40	124.45
3	B	604	CL6	CAR-CAW-CAX	-2.69	120.50	122.74
2	E	601	HEM	C3B-C4B-NB	-2.69	107.54	109.47
3	D	604	CL6	CAR-CAW-CAX	-2.68	120.51	122.74
3	F	604	CL6	CAR-CAW-CAX	-2.63	120.55	122.74
2	C	601	HEM	C3B-C4B-NB	-2.62	107.58	109.47
2	D	601	HEM	C3B-C4B-NB	-2.62	107.58	109.47
3	H	604	CL6	CAR-CAW-CAX	-2.59	120.59	122.74
3	B	603	CL6	CAR-CAW-CAX	-2.55	120.62	122.74
2	H	601	HEM	CHD-C4C-NC	2.51	127.19	124.45
2	D	601	HEM	CAA-CBA-CGA	-2.46	107.15	113.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	HEM	C3B-C4B-NB	-2.44	107.72	109.47
2	A	601	HEM	C1A-CHA-C4D	-2.42	120.56	126.25
3	A	604	CL6	CAR-CAW-CAX	-2.42	120.73	122.74
3	G	604	CL6	CAU-CAW-CAR	2.40	123.13	120.97
3	B	603	CL6	CAC-CAR-CAW	-2.39	108.45	111.85
3	F	602	CL6	CAR-CAW-CAX	-2.38	120.76	122.74
2	F	601	HEM	C3B-C4B-NB	-2.38	107.76	109.47
3	H	604	CL6	CAL-CAR-CAW	-2.37	108.47	111.85
3	E	603	CL6	CAC-CAR-CAW	-2.36	108.48	111.85
2	D	601	HEM	CHA-C4D-C3D	-2.36	120.87	125.23
2	D	601	HEM	CHA-C1A-NA	2.34	128.11	123.86
2	G	601	HEM	C3B-C4B-NB	-2.32	107.81	109.47
3	D	602	CL6	CAL-CAR-CAC	-2.31	101.90	110.34
3	C	604	CL6	CAL-CAR-CAW	-2.30	108.57	111.85
3	D	604	CL6	CAL-CAR-CAW	-2.30	108.58	111.85
2	D	601	HEM	C1A-CHA-C4D	-2.29	120.85	126.25
2	B	601	HEM	CHD-C4C-NC	2.28	126.93	124.45
2	F	601	HEM	C1A-CHA-C4D	-2.27	120.90	126.25
2	F	601	HEM	O2D-CGD-CBD	2.27	121.17	114.00
2	H	601	HEM	C1A-CHA-C4D	-2.26	120.92	126.25
2	B	601	HEM	C1A-CHA-C4D	-2.24	120.97	126.25
2	G	601	HEM	C1A-CHA-C4D	-2.24	120.97	126.25
3	C	604	CL6	CAC-CAR-CAW	2.24	115.04	111.85
2	E	601	HEM	CHA-C4D-C3D	-2.23	121.12	125.23
2	C	601	HEM	C1A-CHA-C4D	-2.19	121.10	126.25
2	H	601	HEM	CHA-C4D-C3D	-2.19	121.20	125.23
2	E	601	HEM	C1A-CHA-C4D	-2.18	121.11	126.25
3	C	602	CL6	CAR-CAW-CAX	-2.15	120.95	122.74
2	D	601	HEM	O2D-CGD-CBD	2.14	120.75	114.00
2	A	601	HEM	O2A-CGA-CBA	2.12	120.71	114.00
2	H	601	HEM	CHA-C1A-NA	2.12	127.70	123.86
2	C	601	HEM	CHA-C4D-C3D	-2.11	121.33	125.23
3	F	602	CL6	CAL-CAR-CAC	-2.11	102.62	110.34
3	D	602	CL6	CAR-CAW-CAX	-2.11	120.99	122.74
2	F	601	HEM	CHA-C4D-C3D	-2.11	121.34	125.23
2	F	601	HEM	CHA-C1A-NA	2.10	127.66	123.86
3	F	604	CL6	CAL-CAR-CAW	-2.09	108.87	111.85
2	B	601	HEM	CHA-C1A-NA	2.09	127.65	123.86
3	E	604	CL6	CAU-CAW-CAR	2.09	122.85	120.97
2	A	601	HEM	CHA-C4D-C3D	-2.09	121.38	125.23
3	G	602	CL6	CAL-CAR-CAW	-2.08	108.89	111.85
3	E	602	CL6	CAL-CAR-CAW	-2.08	108.89	111.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	C3B-C4B-NB	-2.07	107.98	109.47
2	E	601	HEM	CHA-C1A-NA	2.07	127.62	123.86
2	E	601	HEM	O2D-CGD-CBD	2.07	120.54	114.00
3	G	603	CL6	CAR-NAO-CAP	2.07	130.95	125.63
2	G	601	HEM	CHA-C1A-NA	2.06	127.60	123.86
2	G	601	HEM	CAD-C3D-C4D	2.06	128.28	124.70
2	F	601	HEM	O2A-CGA-CBA	2.05	120.48	114.00
2	E	601	HEM	CHB-C1B-C2B	-2.05	121.13	126.95
3	D	603	CL6	CAR-NAO-CAP	2.05	130.89	125.63
3	F	604	CL6	CAC-CAR-CAW	2.03	114.75	111.85
2	C	601	HEM	C4C-CHD-C1D	-2.03	121.71	126.02
2	G	601	HEM	O2D-CGD-CBD	2.01	120.36	114.00
2	G	601	HEM	CHA-C4D-C3D	-2.01	121.52	125.23
2	D	601	HEM	CHB-C1B-C2B	-2.01	121.25	126.95
2	E	601	HEM	O2A-CGA-CBA	2.01	120.34	114.00

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEM	C2C-C3C-CAC-CBC
2	C	601	HEM	C2C-C3C-CAC-CBC
2	D	601	HEM	C2C-C3C-CAC-CBC
2	D	601	HEM	C4C-C3C-CAC-CBC
2	E	601	HEM	C2C-C3C-CAC-CBC
2	F	601	HEM	C2C-C3C-CAC-CBC
2	F	601	HEM	C4C-C3C-CAC-CBC
2	G	601	HEM	C2C-C3C-CAC-CBC
2	H	601	HEM	C2C-C3C-CAC-CBC
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	A	605	CE9	O25-C26-C27-O28
4	C	605	CE9	C10-C11-C12-O13
4	B	605	CE9	C9-C10-C11-C12
4	C	605	CE9	O25-C26-C27-O28
2	B	601	HEM	C2C-C3C-CAC-CBC
2	F	601	HEM	C2B-C3B-CAB-CBB
2	A	601	HEM	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	601	HEM	C4C-C3C-CAC-CBC
2	E	601	HEM	C4C-C3C-CAC-CBC
2	G	601	HEM	C4C-C3C-CAC-CBC
2	H	601	HEM	C4C-C3C-CAC-CBC
4	A	605	CE9	C11-C10-C9-C8
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
4	G	605	CE9	C33-C32-O31-C30
4	C	605	CE9	C23-C24-O25-C26
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	C	605	CE9	C15-C14-O13-C12
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	D	605	CE9	O13-C14-C15-O16
4	F	605	CE9	C14-C15-O16-C17
4	B	605	CE9	C21-C20-O19-C18
4	A	605	CE9	C23-C24-O25-C26
4	C	605	CE9	C11-C12-O13-C14
4	A	605	CE9	O28-C29-C30-O31
4	B	605	CE9	O25-C26-C27-O28
4	F	605	CE9	C17-C18-O19-C20
4	B	605	CE9	C23-C24-O25-C26
4	F	605	CE9	C27-C26-O25-C24
4	A	605	CE9	C32-C33-O34-C35
4	B	605	CE9	C11-C10-C9-C8
4	B	605	CE9	C33-C32-O31-C30
4	E	605	CE9	C17-C18-O19-C20
4	A	605	CE9	C27-C26-O25-C24
4	G	605	CE9	C11-C12-O13-C14
4	A	605	CE9	C24-C23-O22-C21
4	E	605	CE9	O16-C17-C18-O19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	605	CE9	C30-C29-O28-C27
4	G	605	CE9	C27-C26-O25-C24
4	A	605	CE9	C26-C27-O28-C29
2	B	601	HEM	C4C-C3C-CAC-CBC
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
4	G	605	CE9	O16-C17-C18-O19
4	G	605	CE9	C18-C17-O16-C15
4	B	605	CE9	C29-C30-O31-C32
4	G	605	CE9	C17-C18-O19-C20
4	A	605	CE9	C14-C15-O16-C17
4	F	605	CE9	C11-C12-O13-C14
4	E	605	CE9	C15-C14-O13-C12
4	G	605	CE9	C29-C30-O31-C32
4	B	605	CE9	C5-C6-C7-C8
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	E	601	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAA-CBA-CGA-O1A
4	E	605	CE9	C24-C23-O22-C21
2	A	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAD-CBD-CGD-O1D
2	C	601	HEM	CAA-CBA-CGA-O2A
2	H	601	HEM	CAD-CBD-CGD-O1D
2	E	601	HEM	CAD-CBD-CGD-O2D
4	G	605	CE9	C20-C21-O22-C23
2	B	601	HEM	CAD-CBD-CGD-O2D
2	H	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
3	F	603	CL6	NAO-CAR-CAW-CAX
3	G	603	CL6	NAO-CAR-CAW-CAX
3	H	603	CL6	NAO-CAR-CAW-CAX
2	C	601	HEM	CAA-CBA-CGA-O1A
2	G	601	HEM	CAA-CBA-CGA-O2A
2	G	601	HEM	CAD-CBD-CGD-O2D
4	A	605	CE9	C35-C36-O37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	605	CE9	C14-C15-O16-C17
2	G	601	HEM	CAA-CBA-CGA-O1A
2	D	601	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

37 monomers are involved in 127 short contacts:

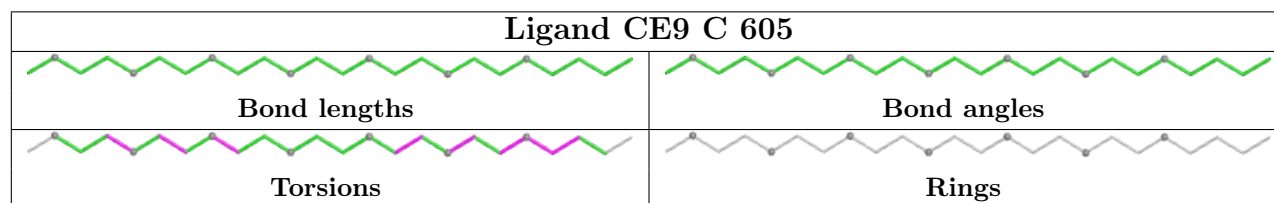
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	604	CL6	3	0
3	H	604	CL6	4	0
3	E	603	CL6	3	0
2	H	601	HEM	3	0
3	B	604	CL6	3	0
3	G	603	CL6	3	0
2	F	601	HEM	4	0
3	G	602	CL6	3	0
3	G	604	CL6	4	0
3	D	603	CL6	3	0
2	A	601	HEM	1	0
3	B	603	CL6	3	0
3	D	602	CL6	3	0
4	F	605	CE9	4	0
3	B	602	CL6	6	0
3	D	604	CL6	4	0
3	E	604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

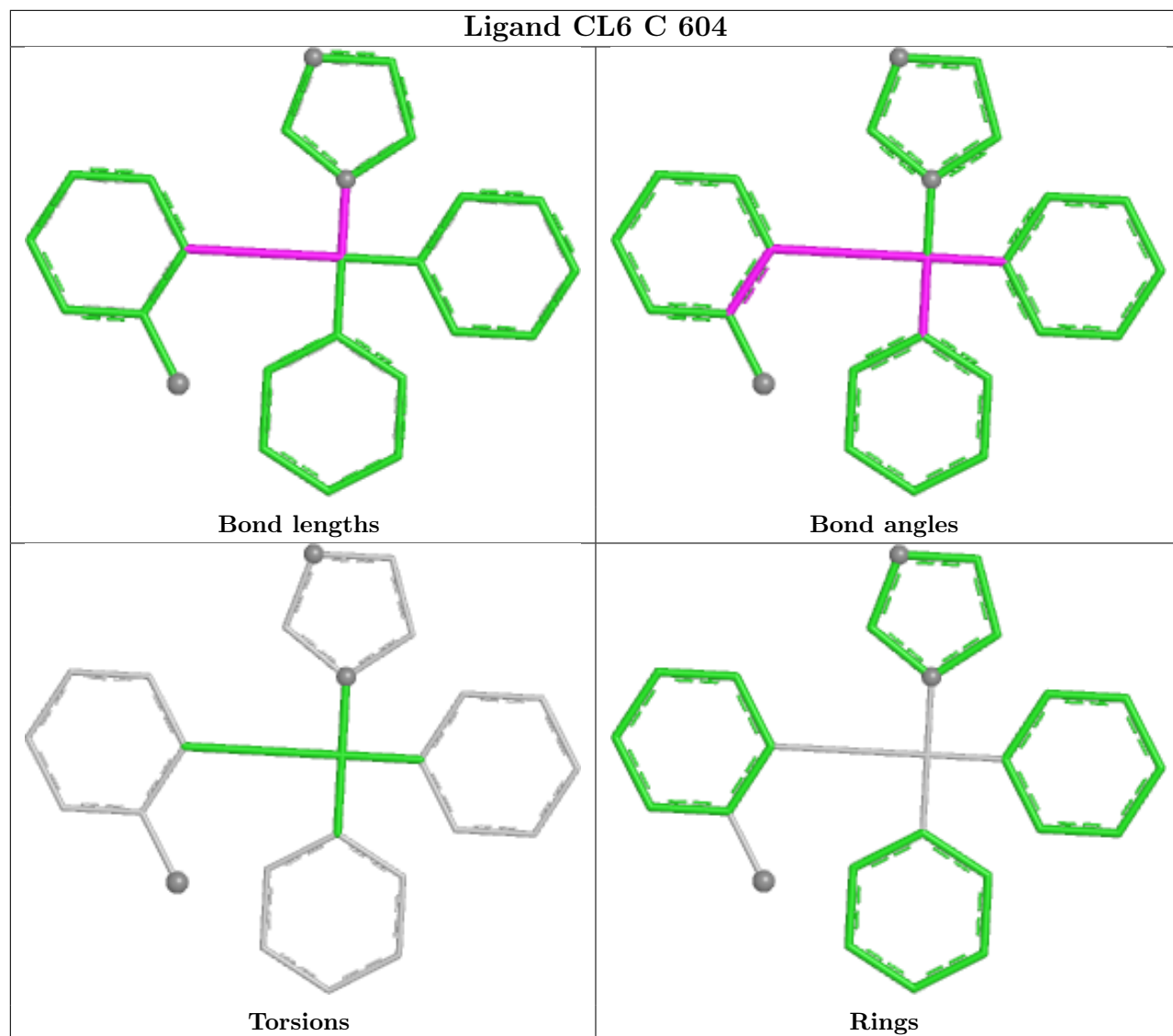
Continued on next page...

Continued from previous page...

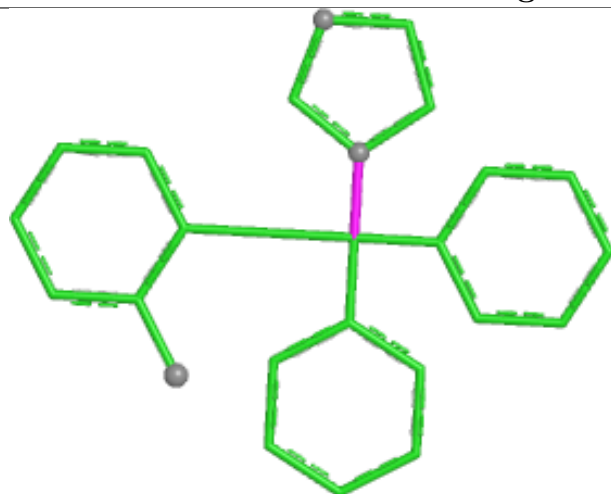
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	CL6	4	0
3	A	604	CL6	4	0
3	E	602	CL6	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

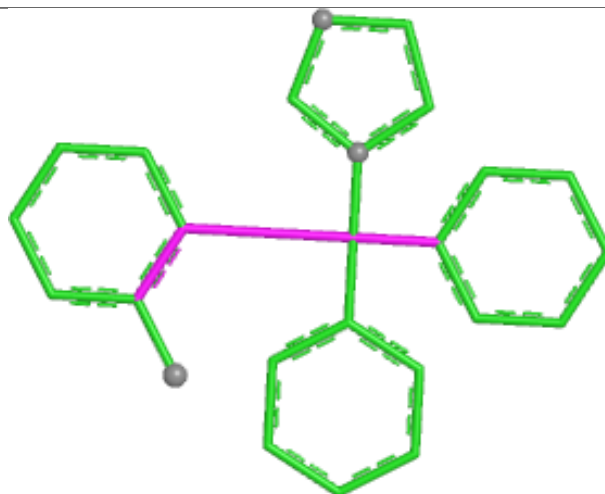




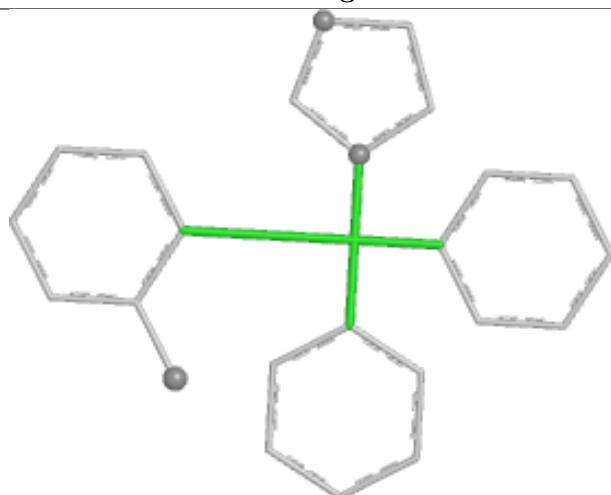
Ligand CL6 H 604



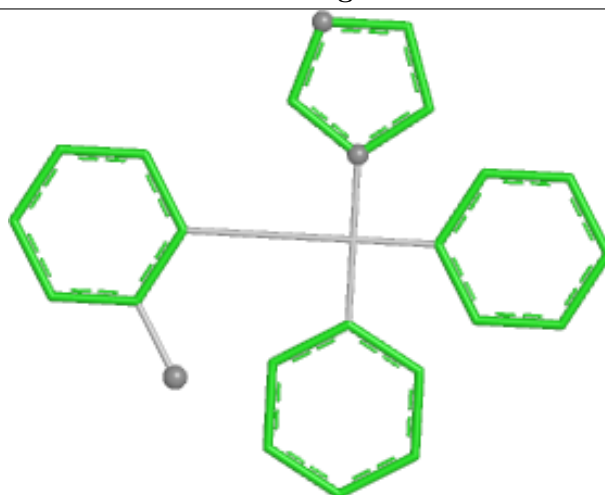
Bond lengths



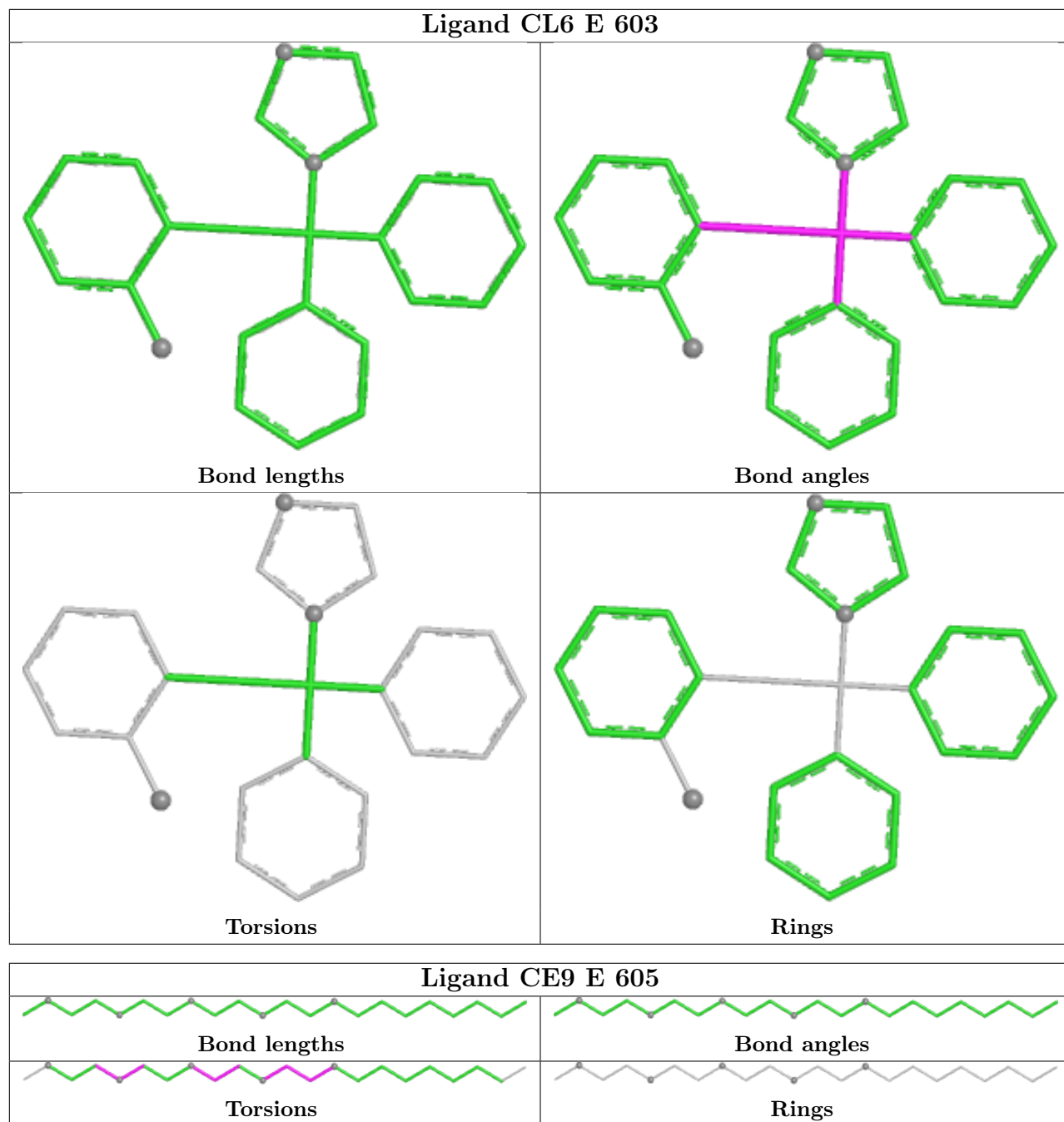
Bond angles

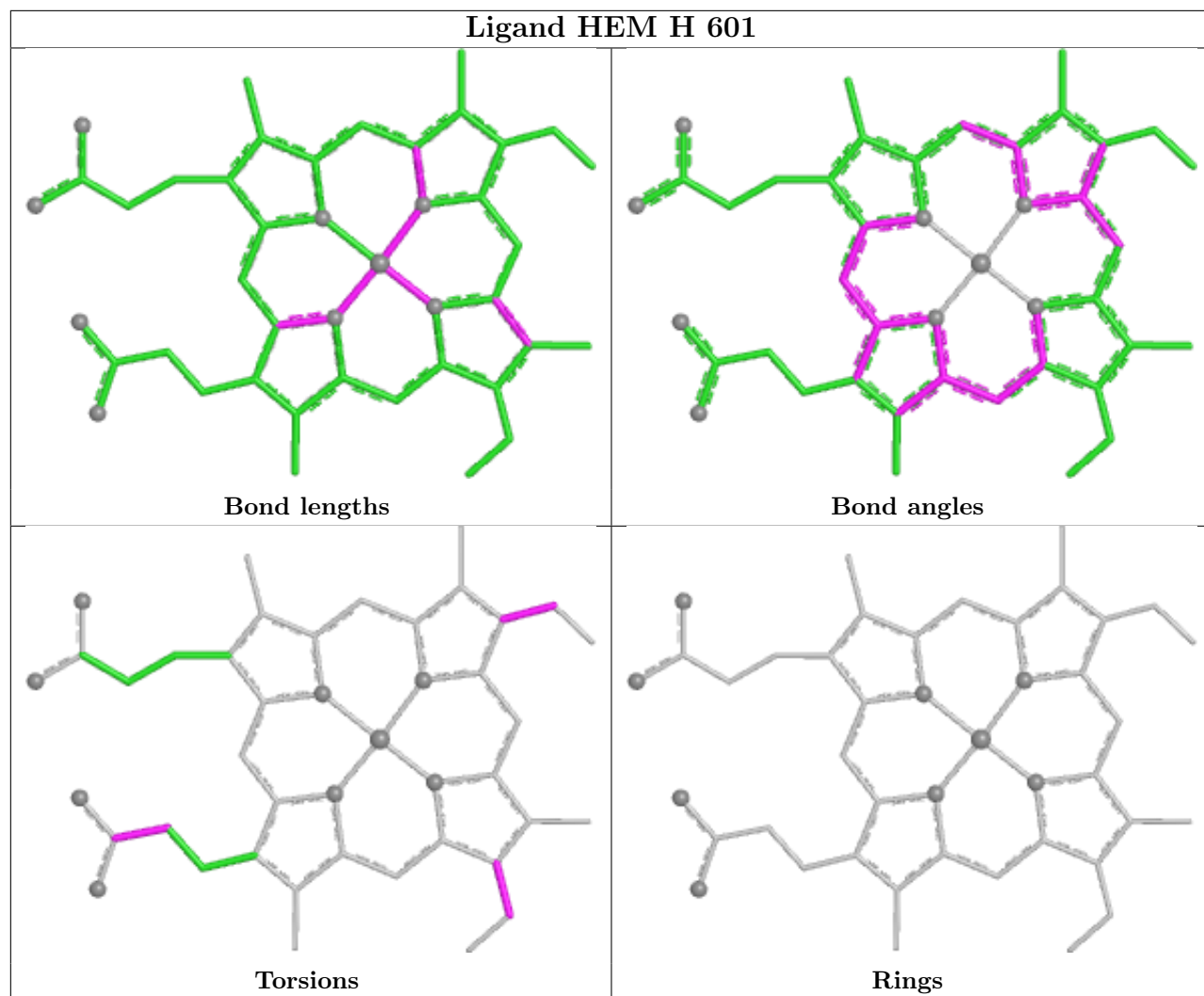


Torsions

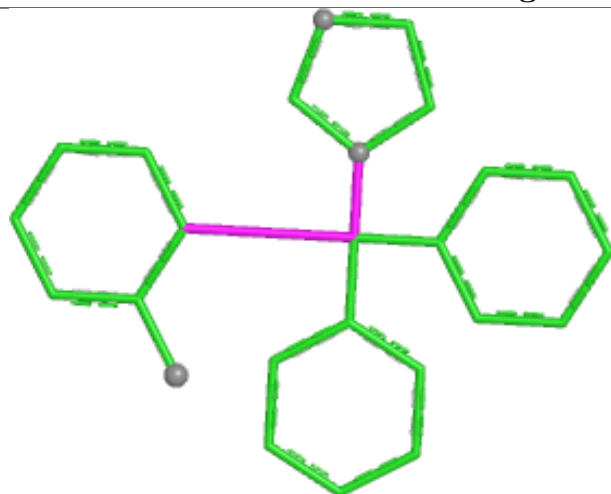


Rings

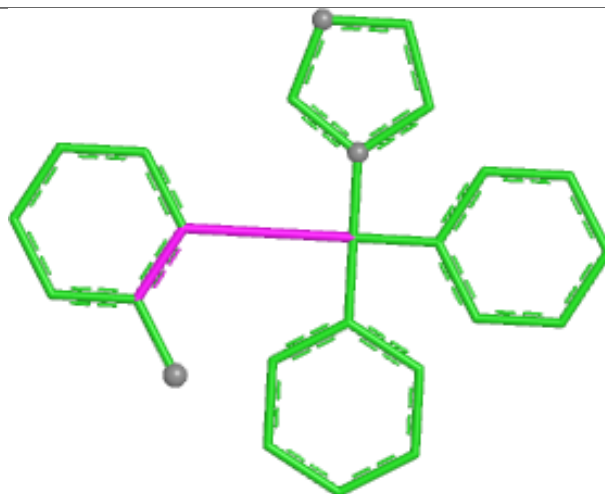




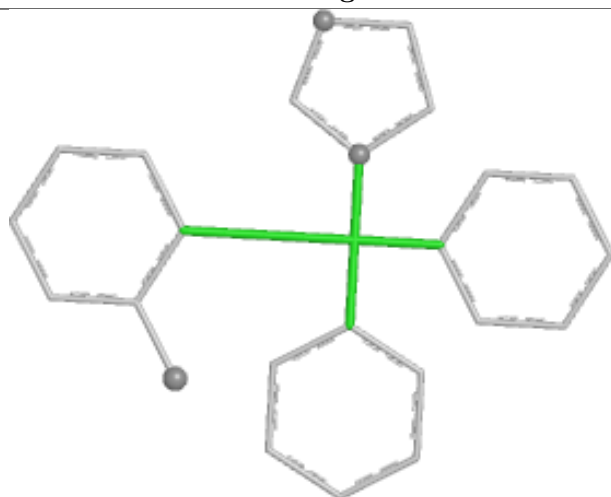
Ligand CL6 B 604



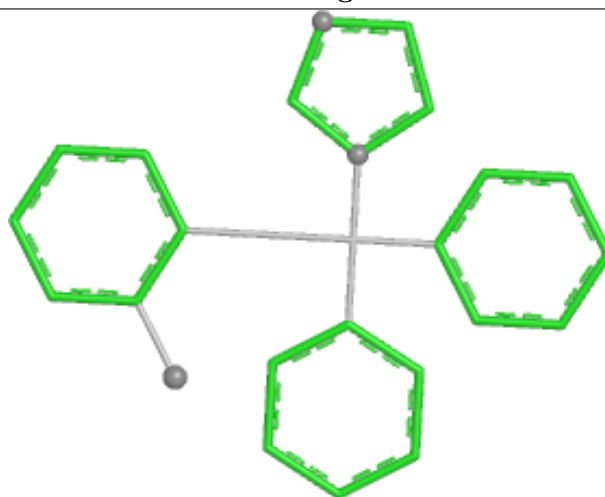
Bond lengths



Bond angles

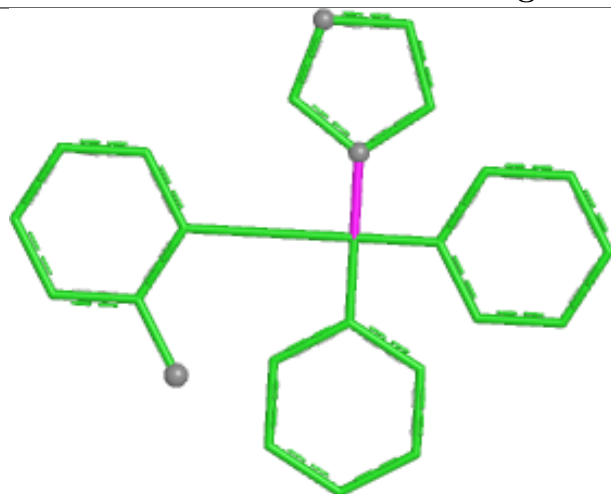


Torsions

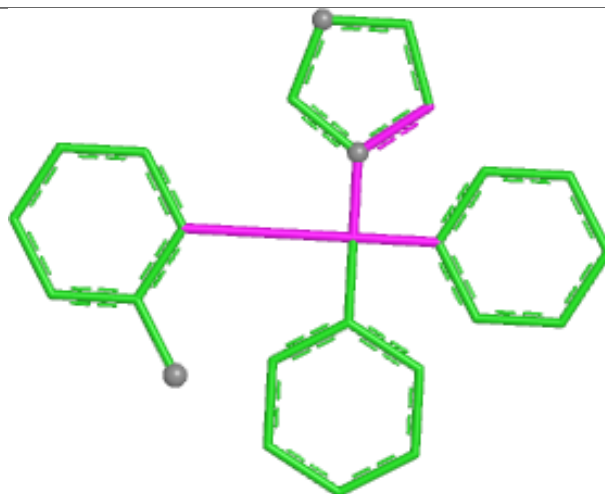


Rings

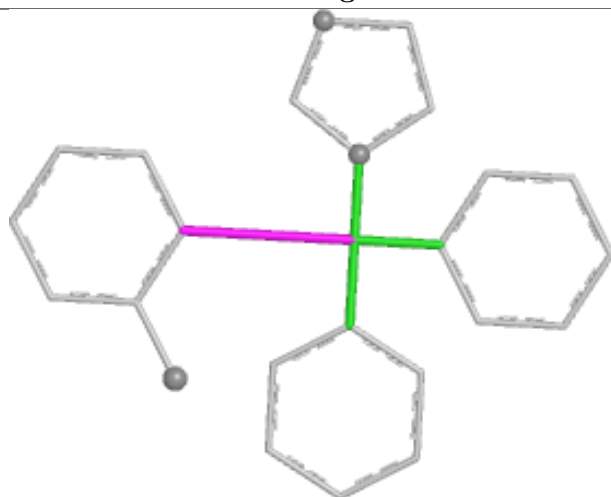
Ligand CL6 G 603



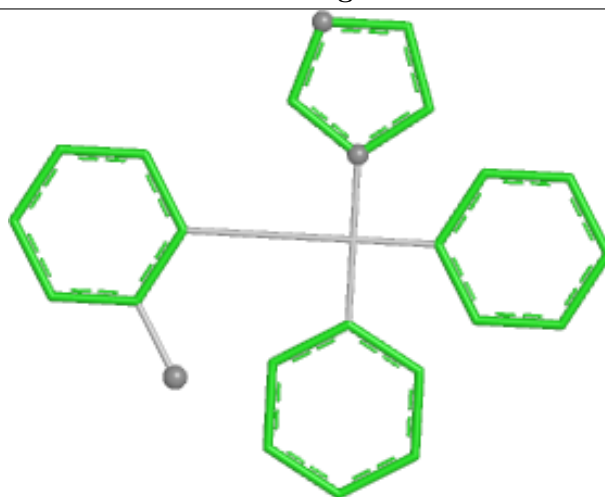
Bond lengths



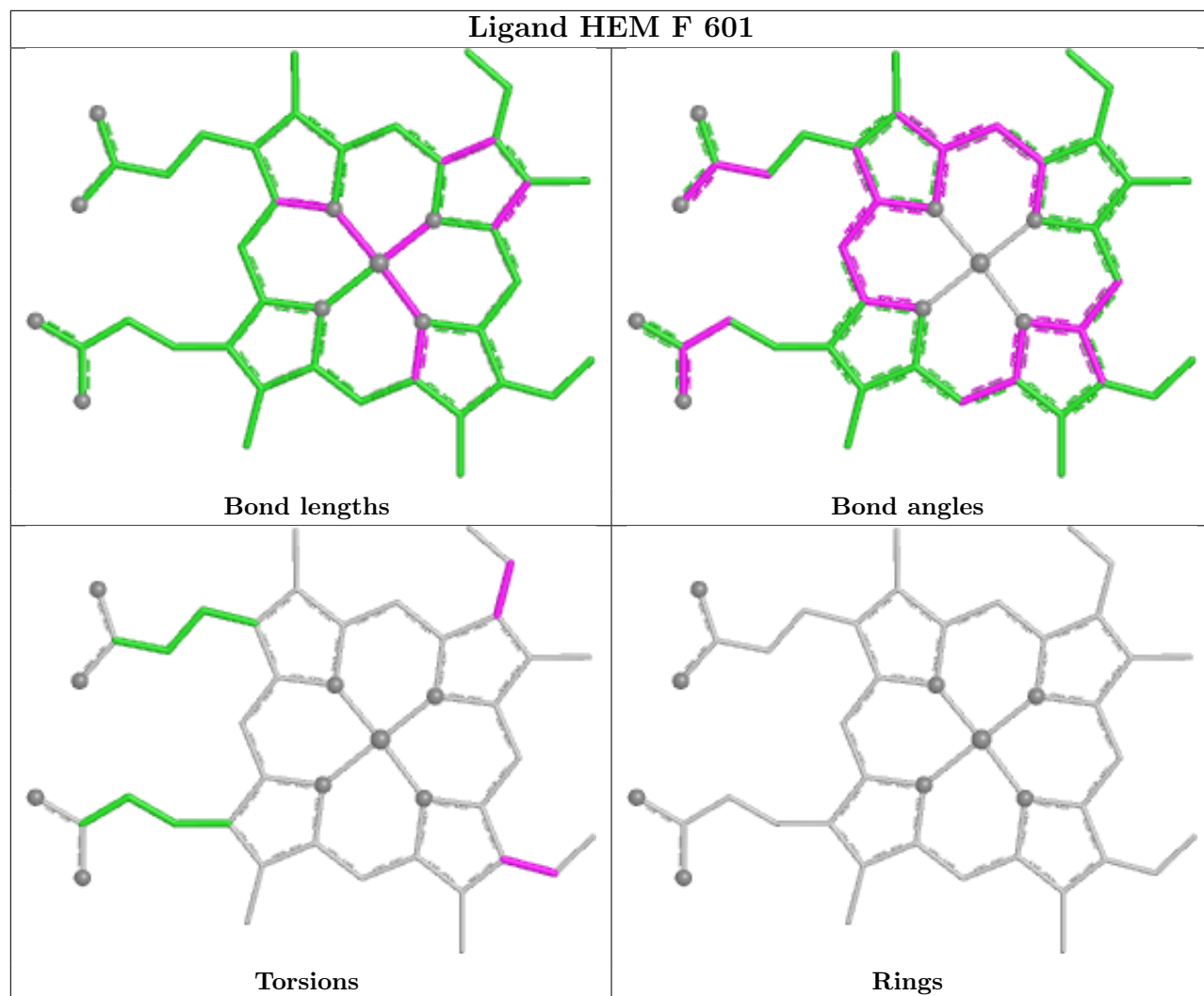
Bond angles



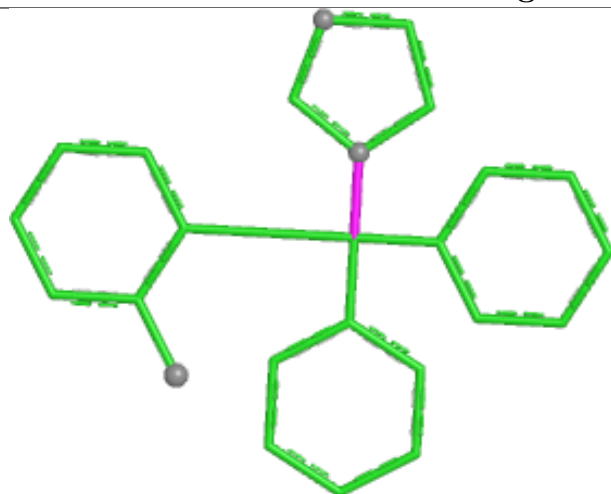
Torsions



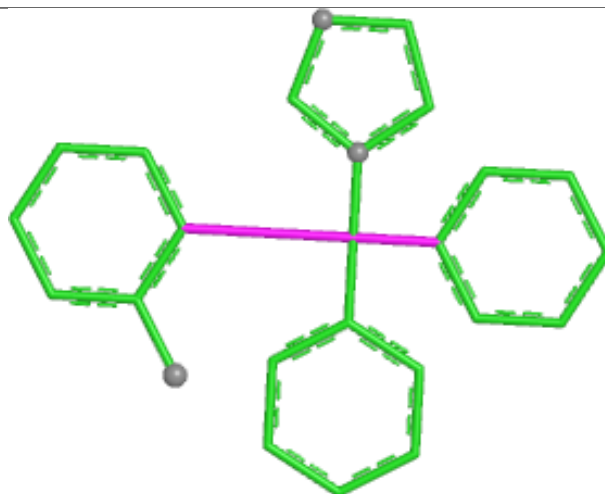
Rings



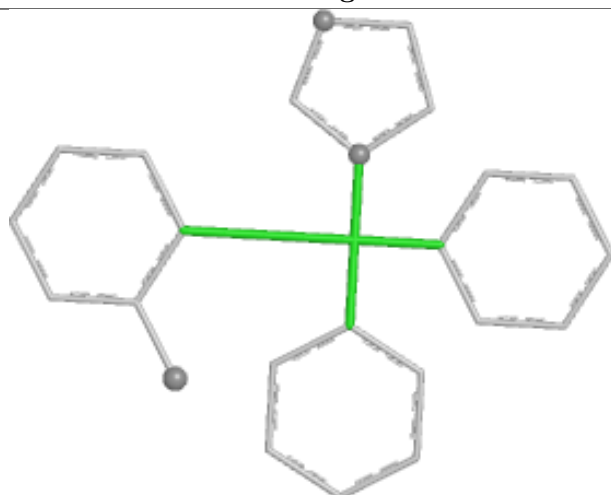
Ligand CL6 G 602



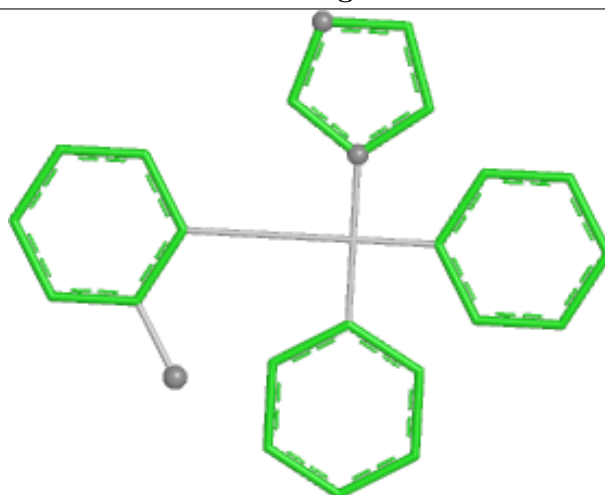
Bond lengths



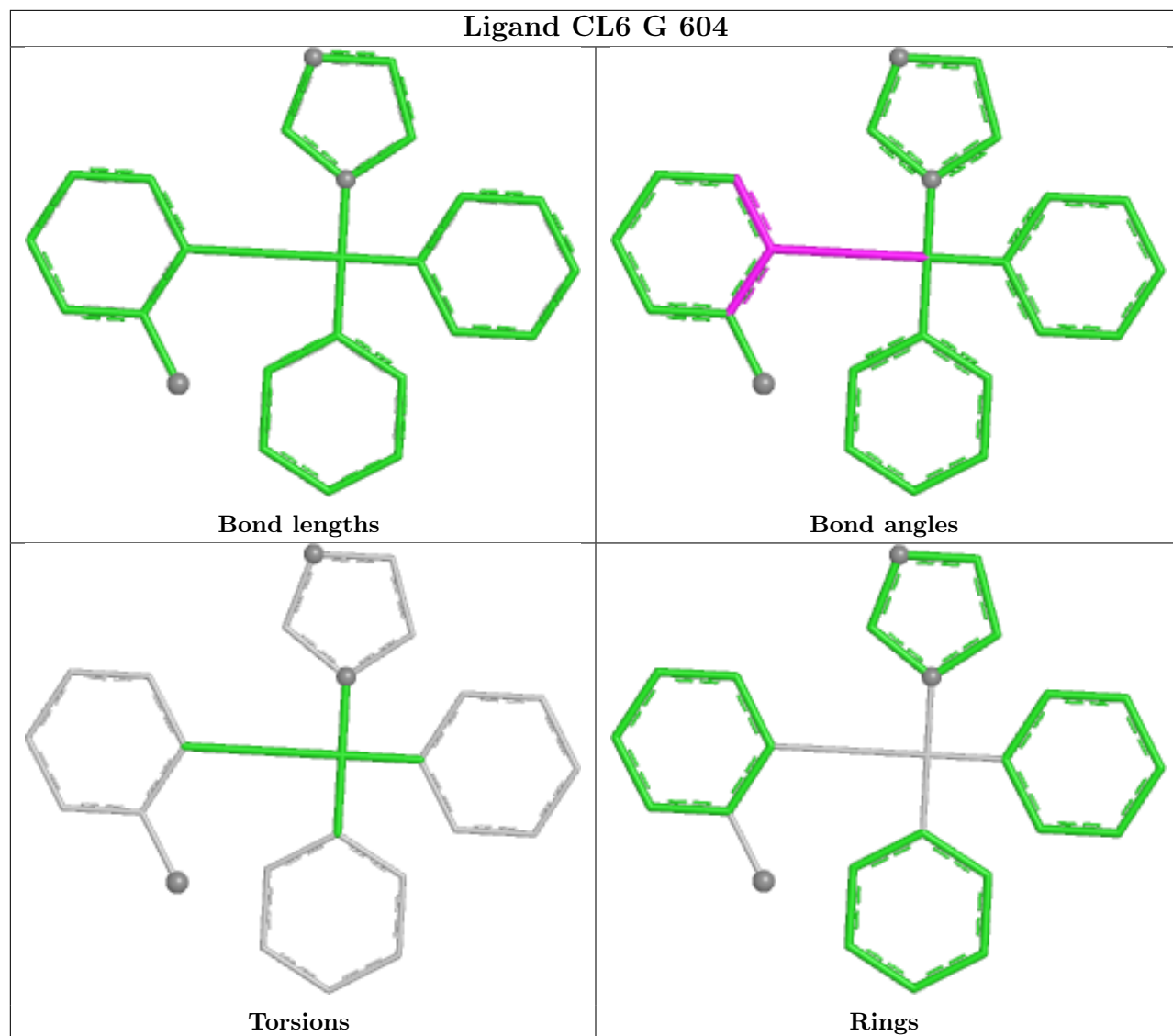
Bond angles



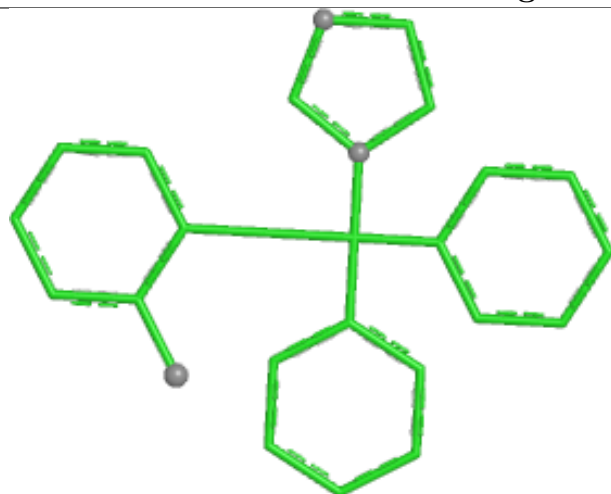
Torsions



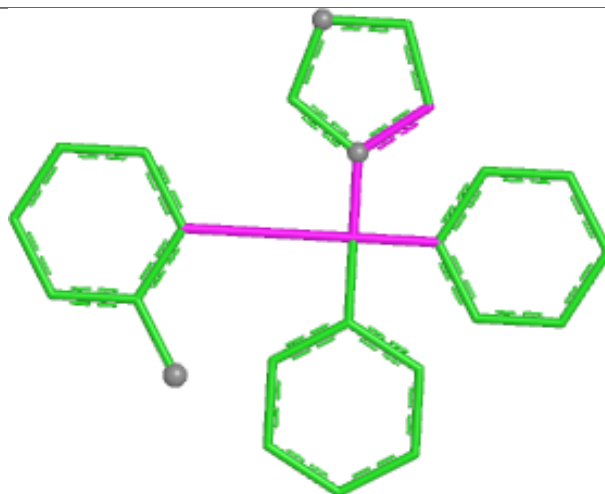
Rings



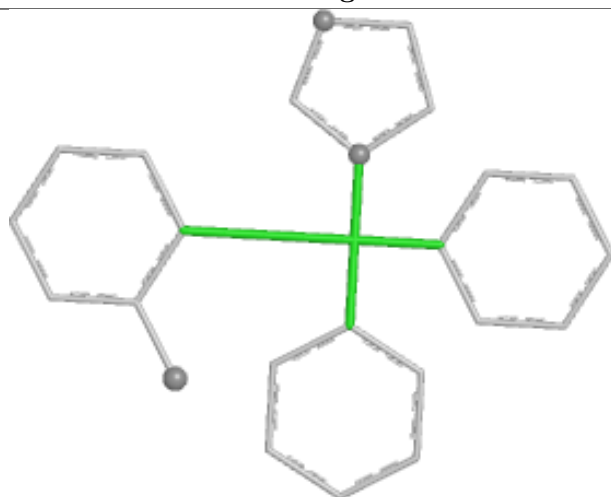
Ligand CL6 D 603



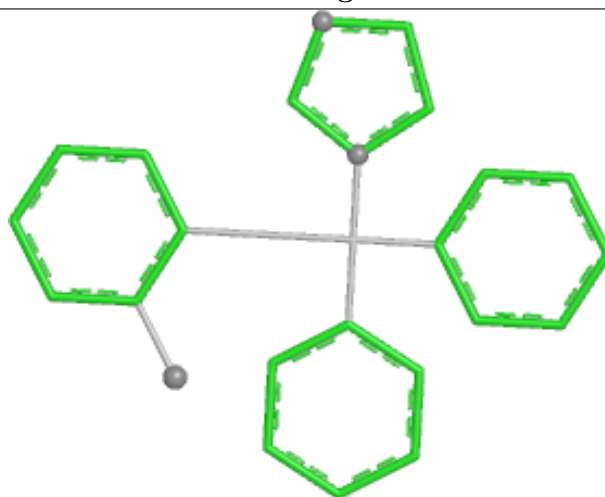
Bond lengths



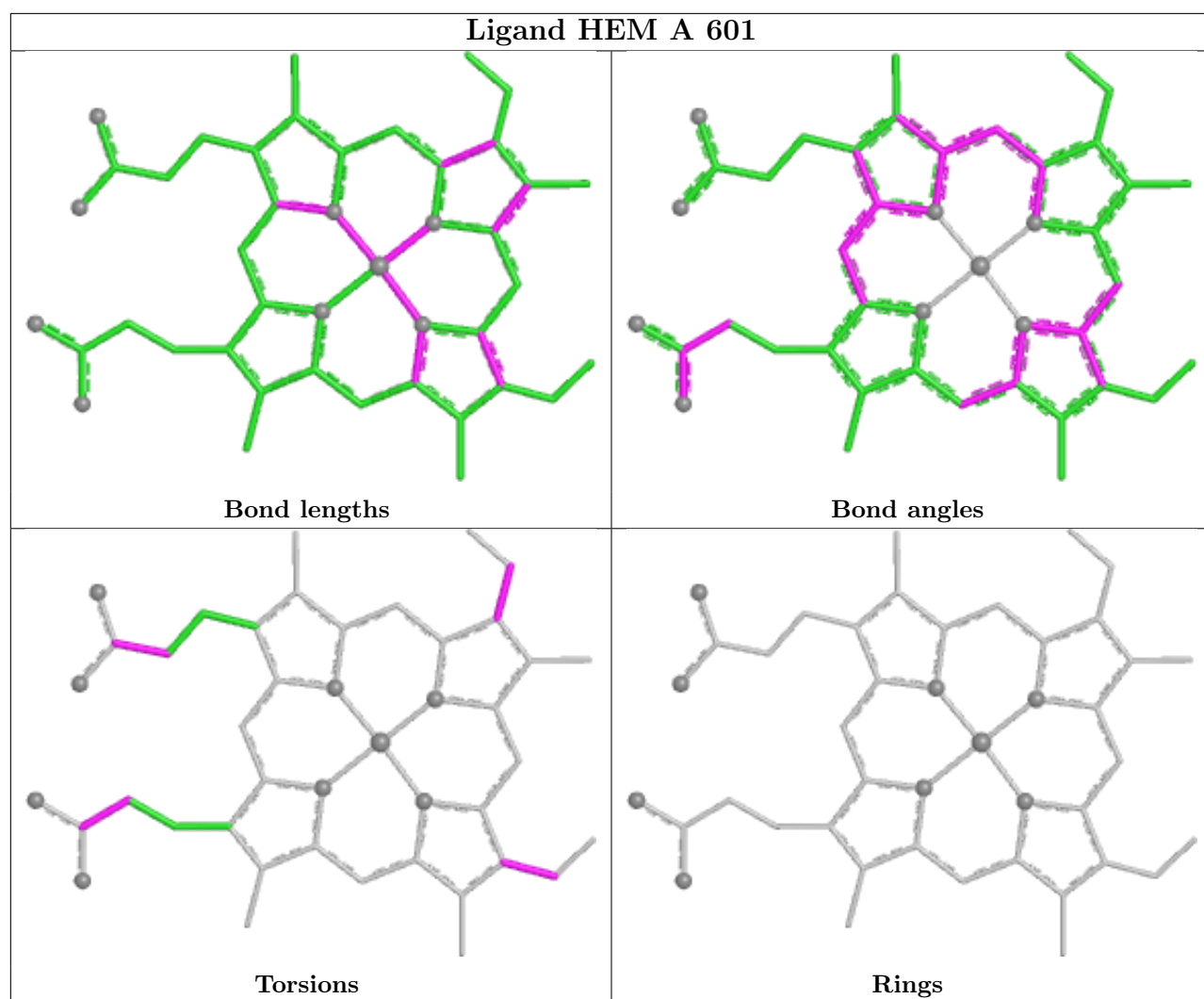
Bond angles



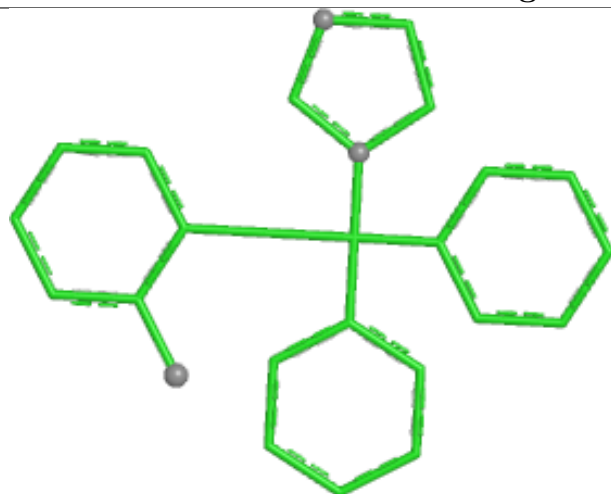
Torsions



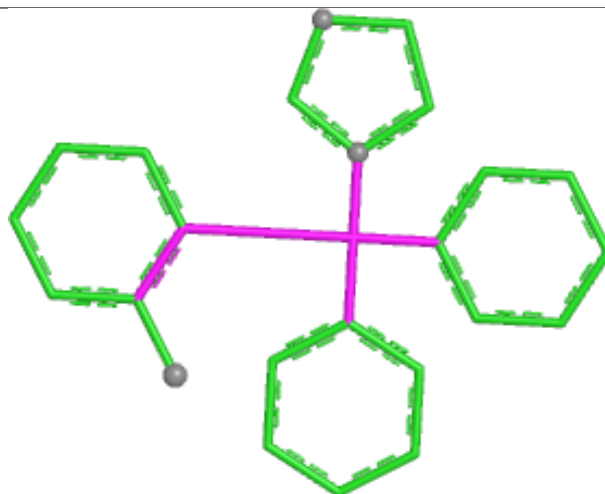
Rings



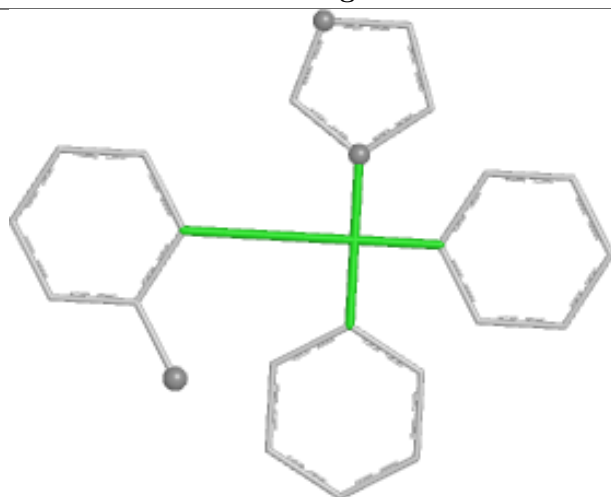
Ligand CL6 B 603



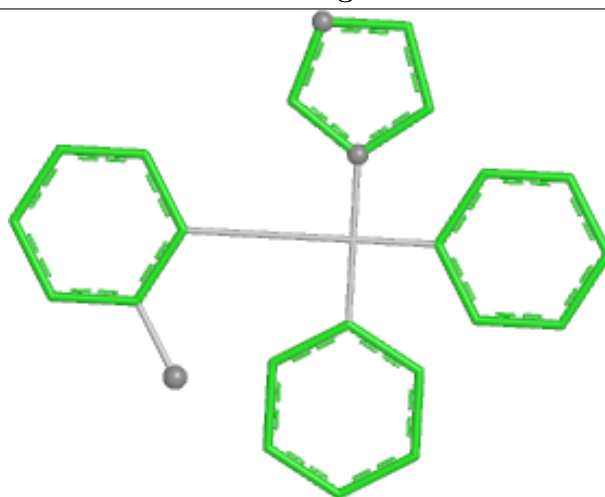
Bond lengths



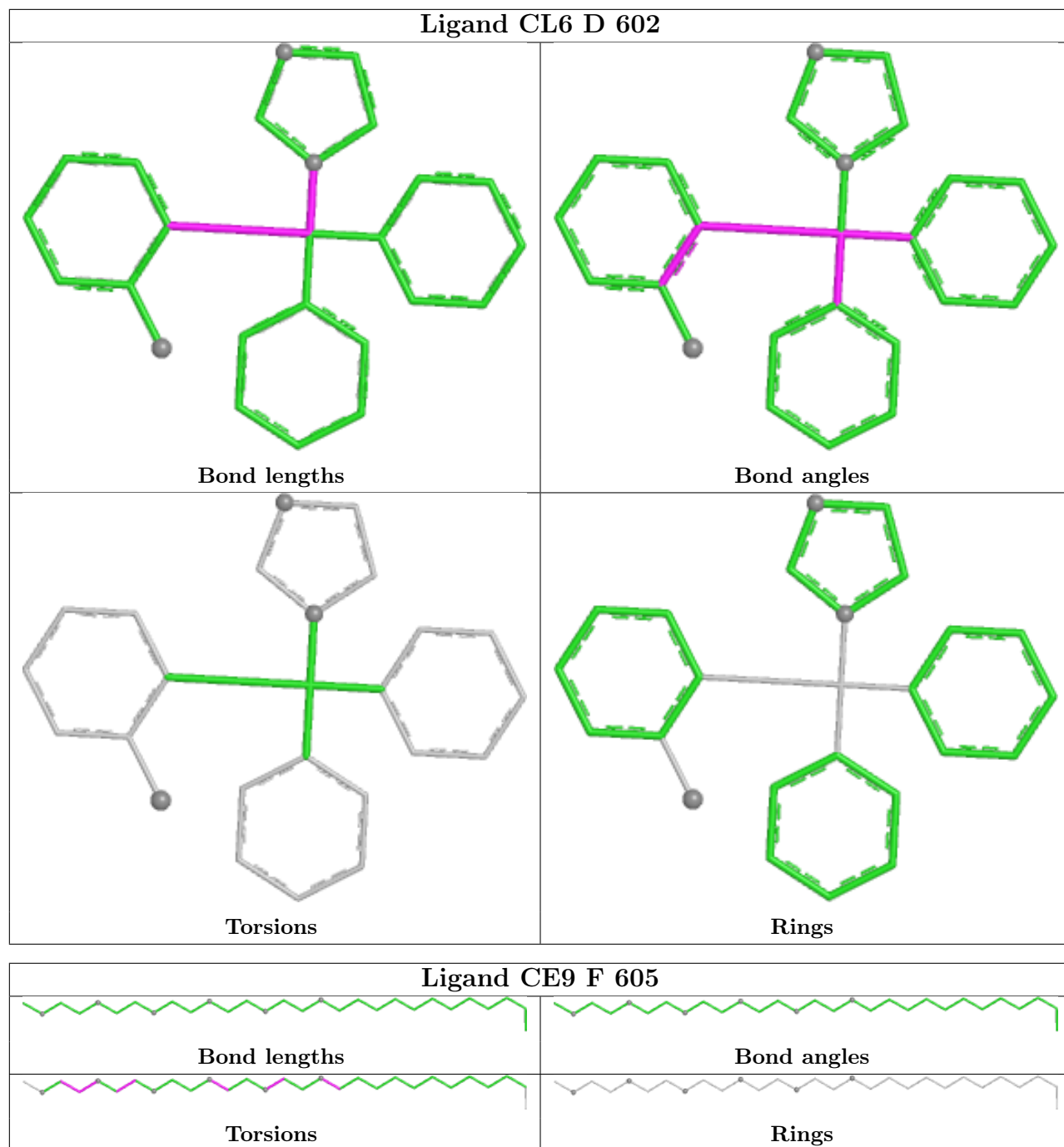
Bond angles



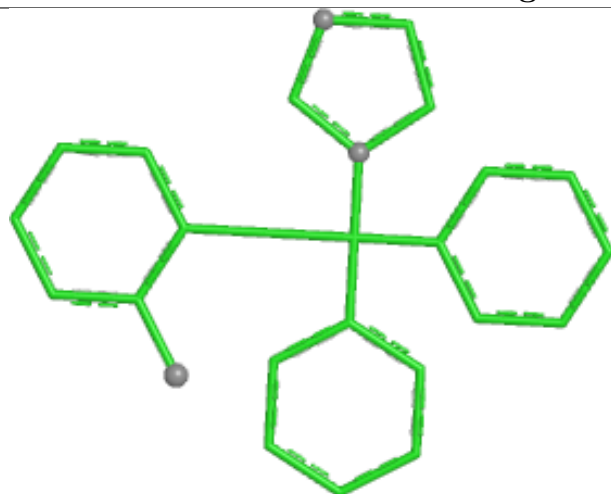
Torsions



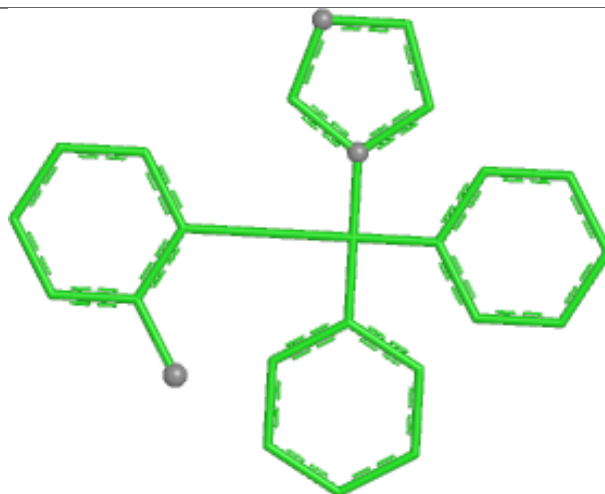
Rings



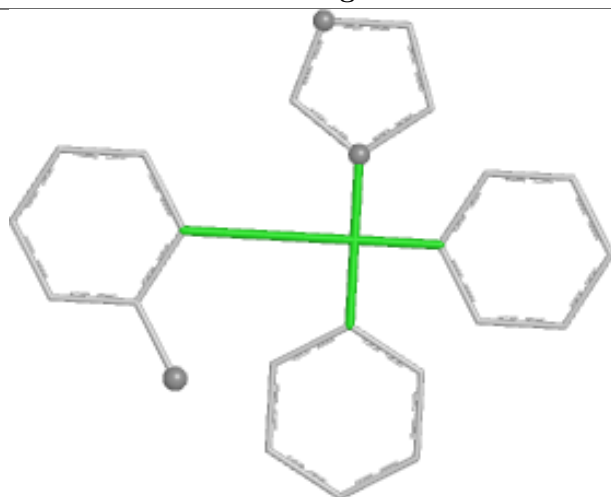
Ligand CL6 B 602



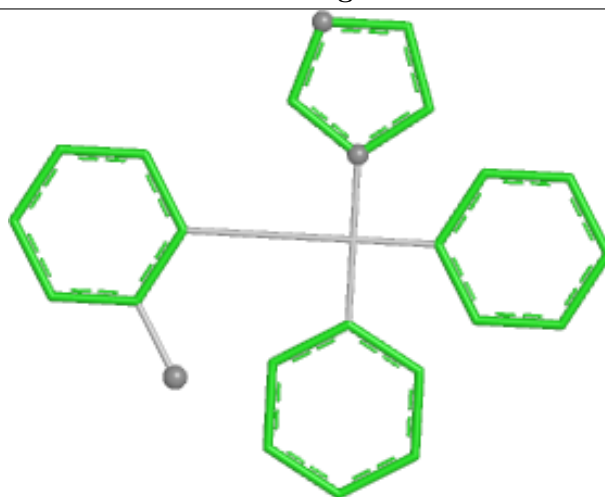
Bond lengths



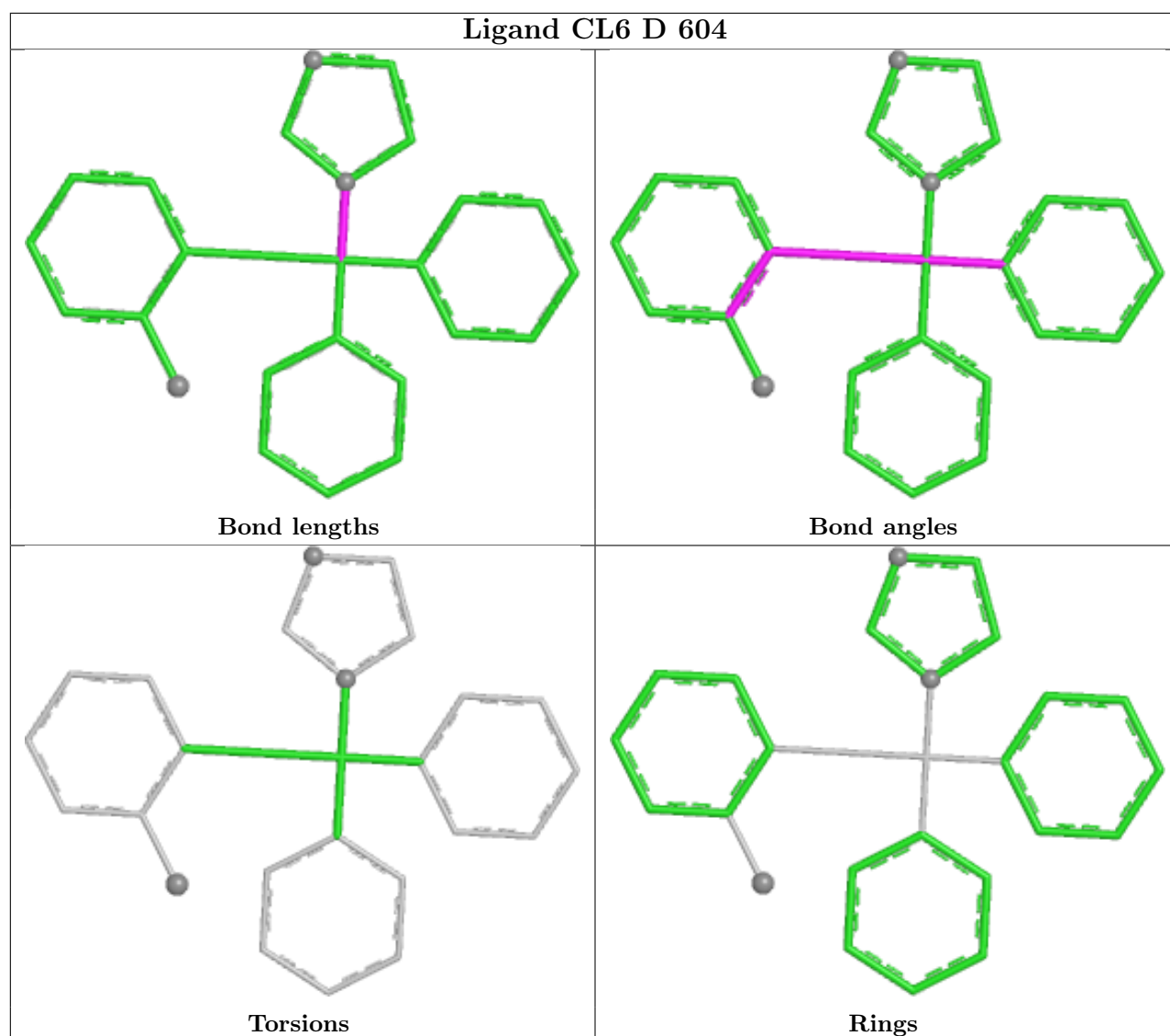
Bond angles



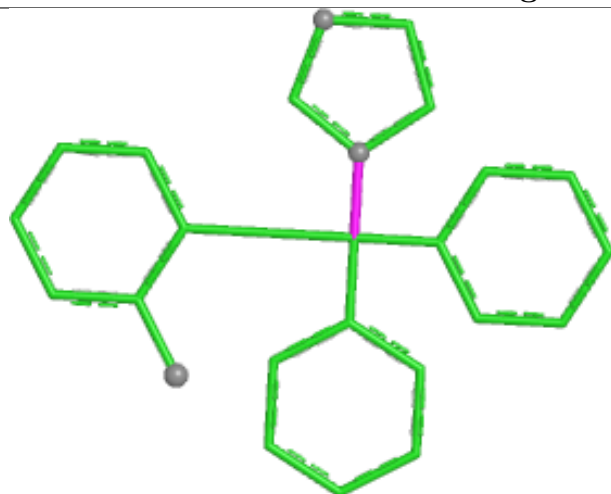
Torsions



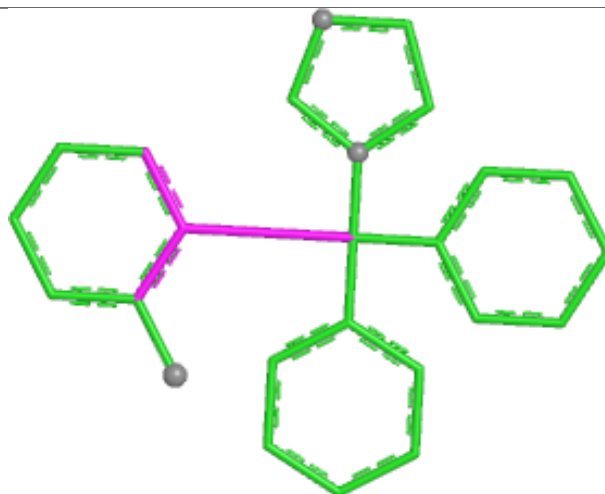
Rings



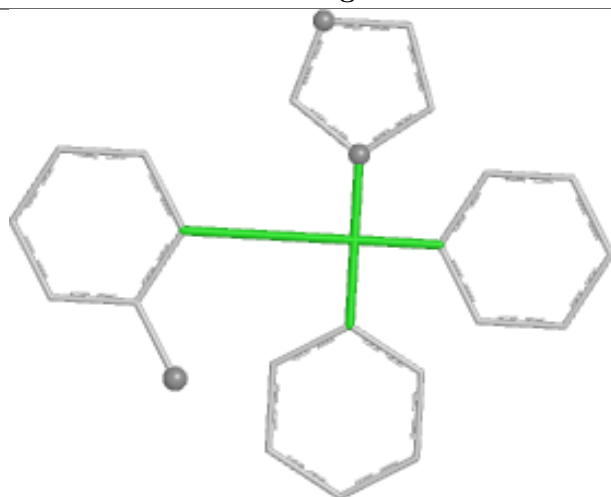
Ligand CL6 E 604



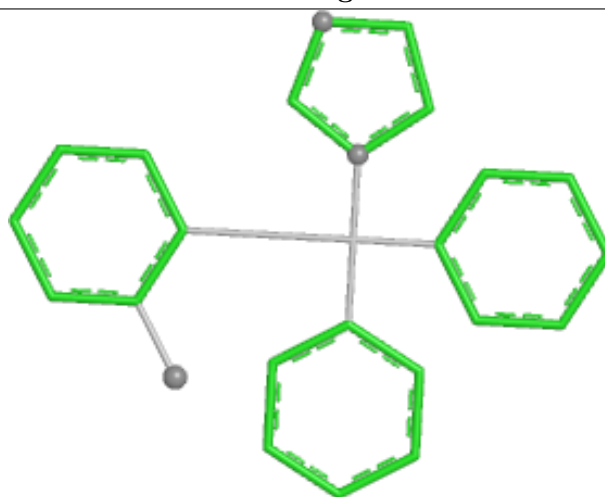
Bond lengths



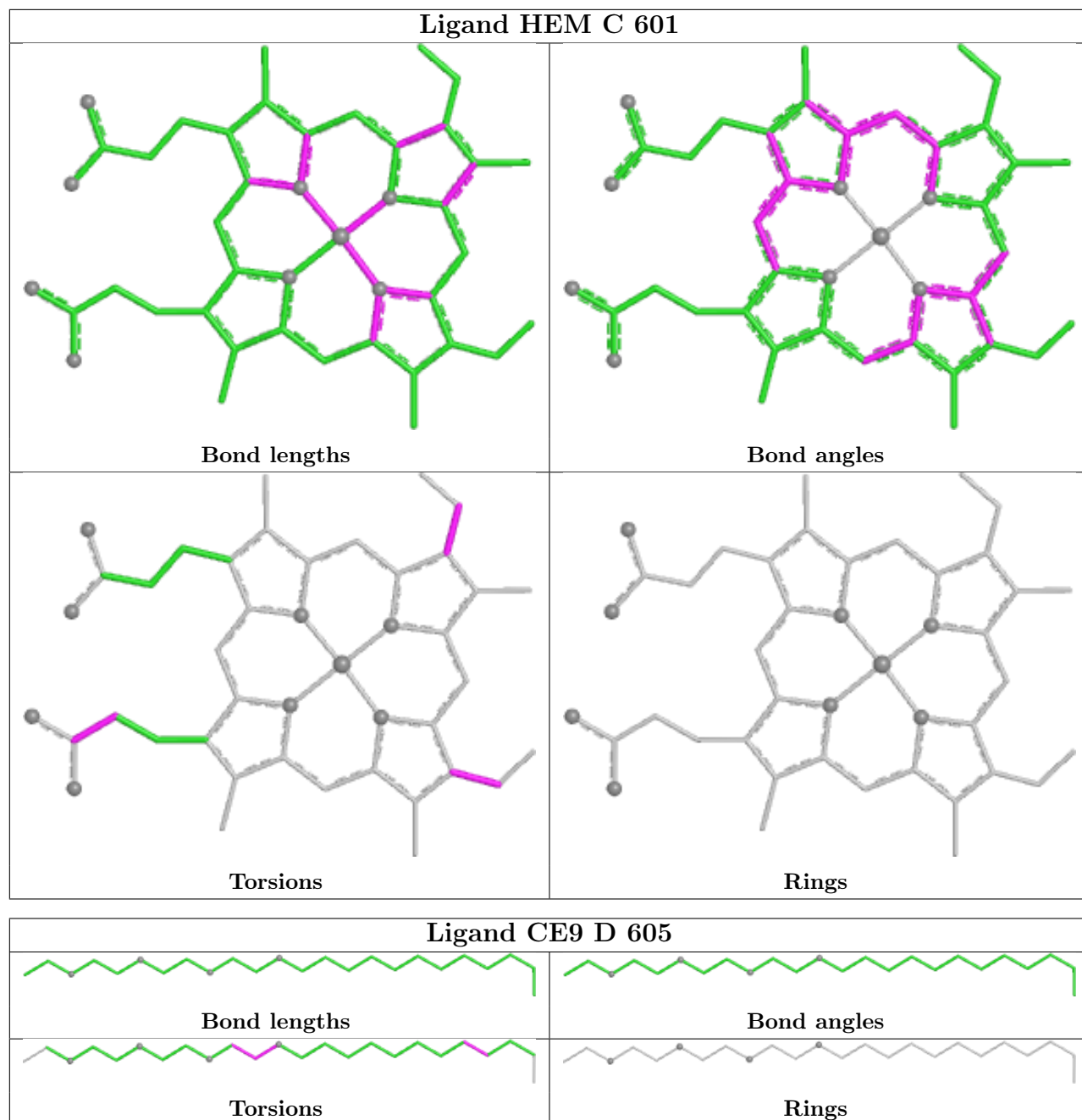
Bond angles

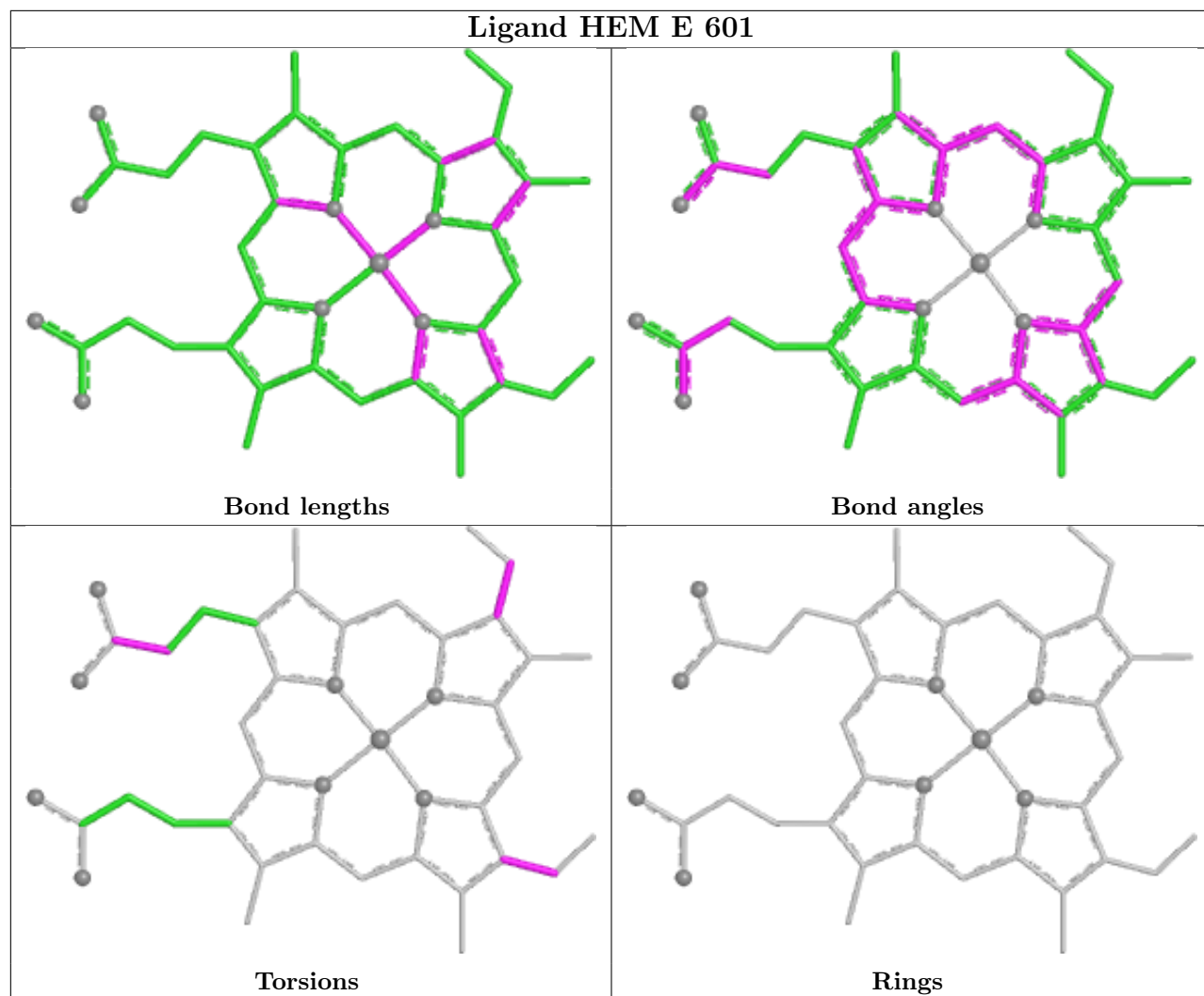


Torsions

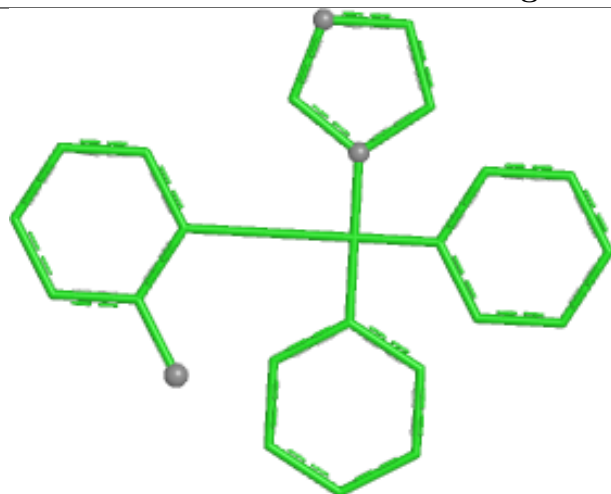


Rings

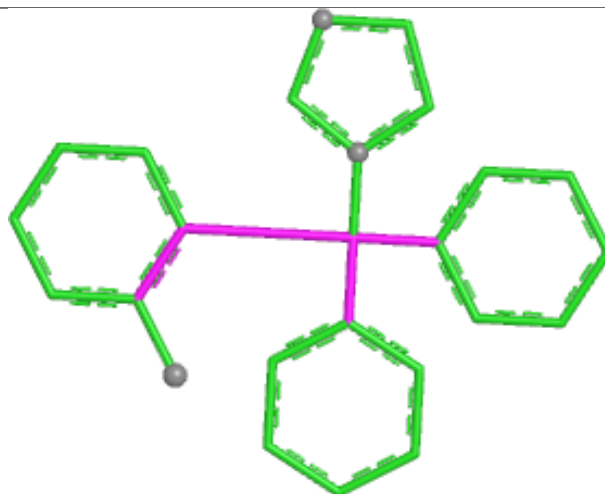




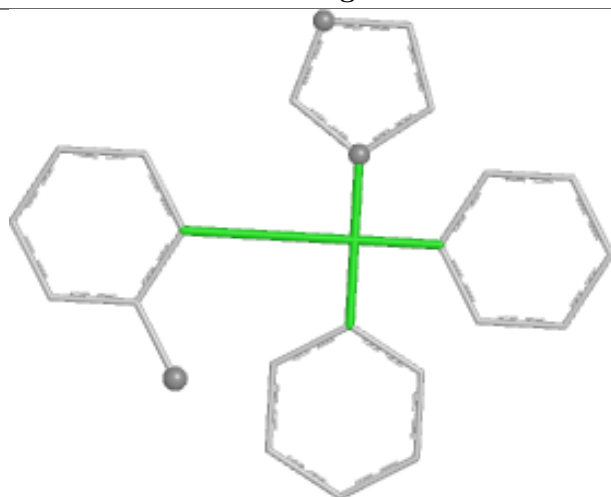
Ligand CL6 F 604



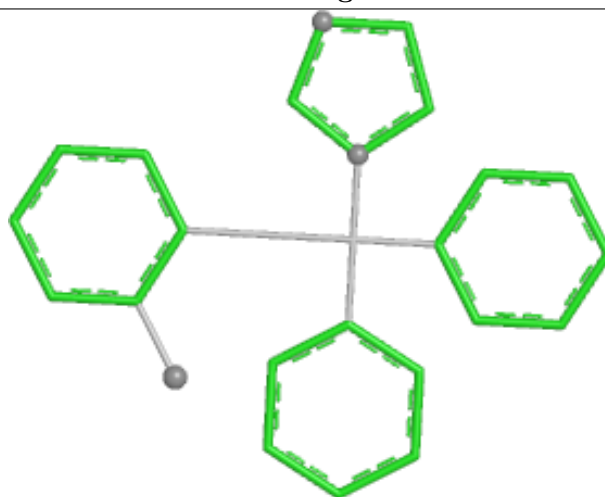
Bond lengths



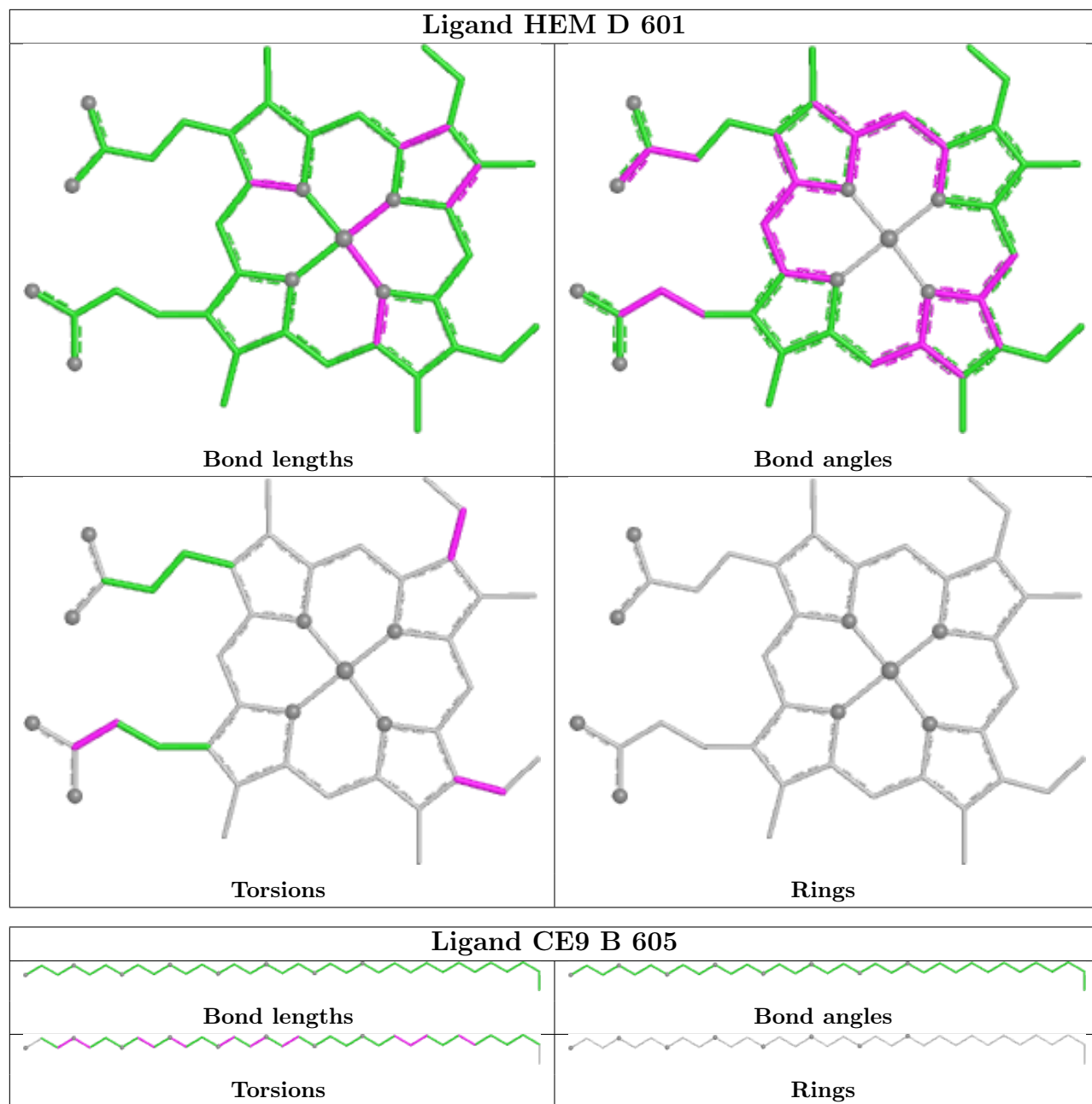
Bond angles



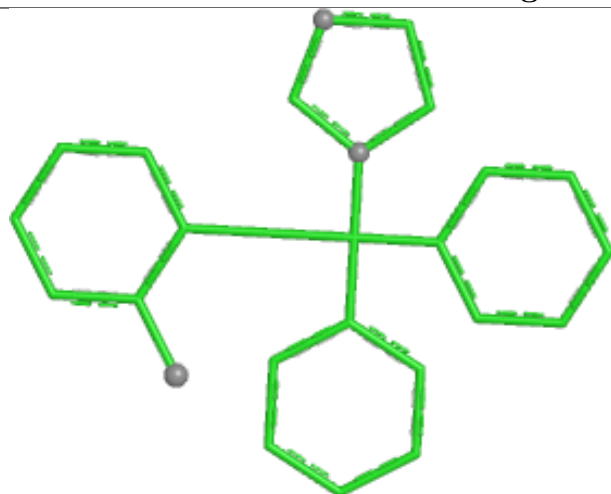
Torsions



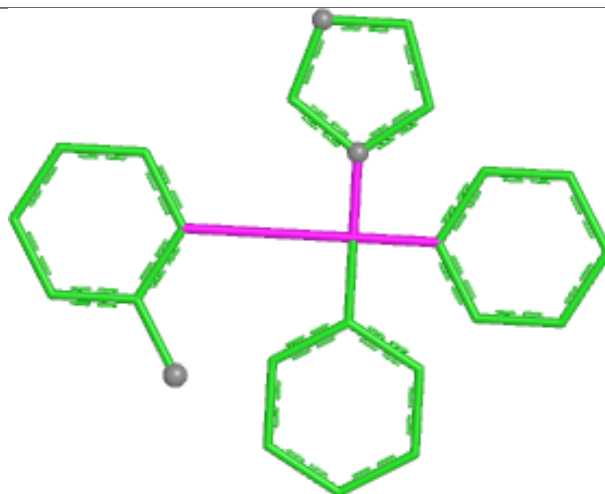
Rings



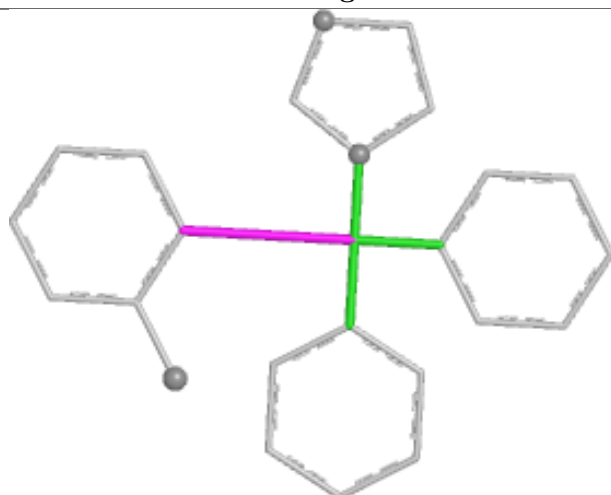
Ligand CL6 F 603



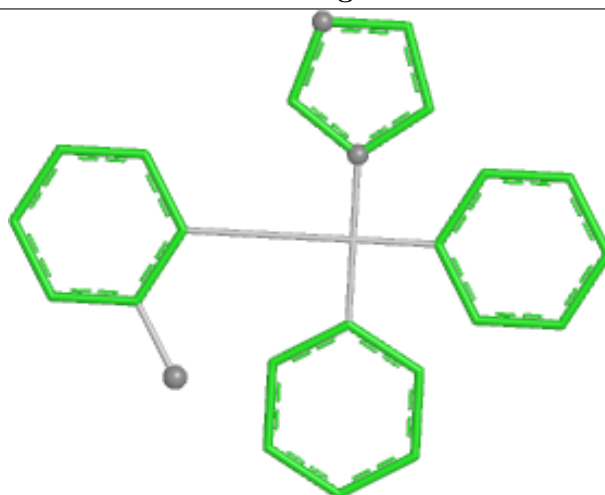
Bond lengths



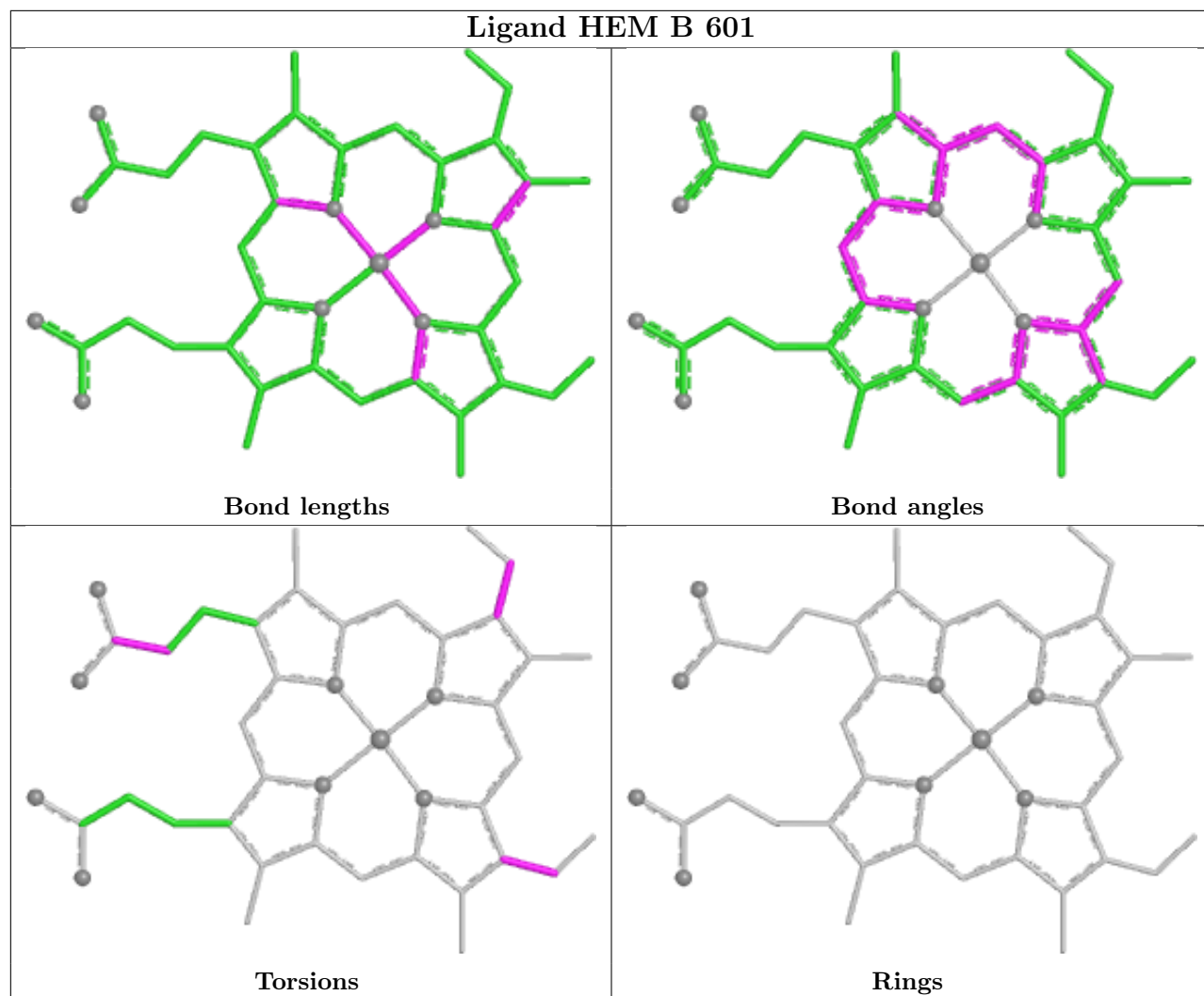
Bond angles



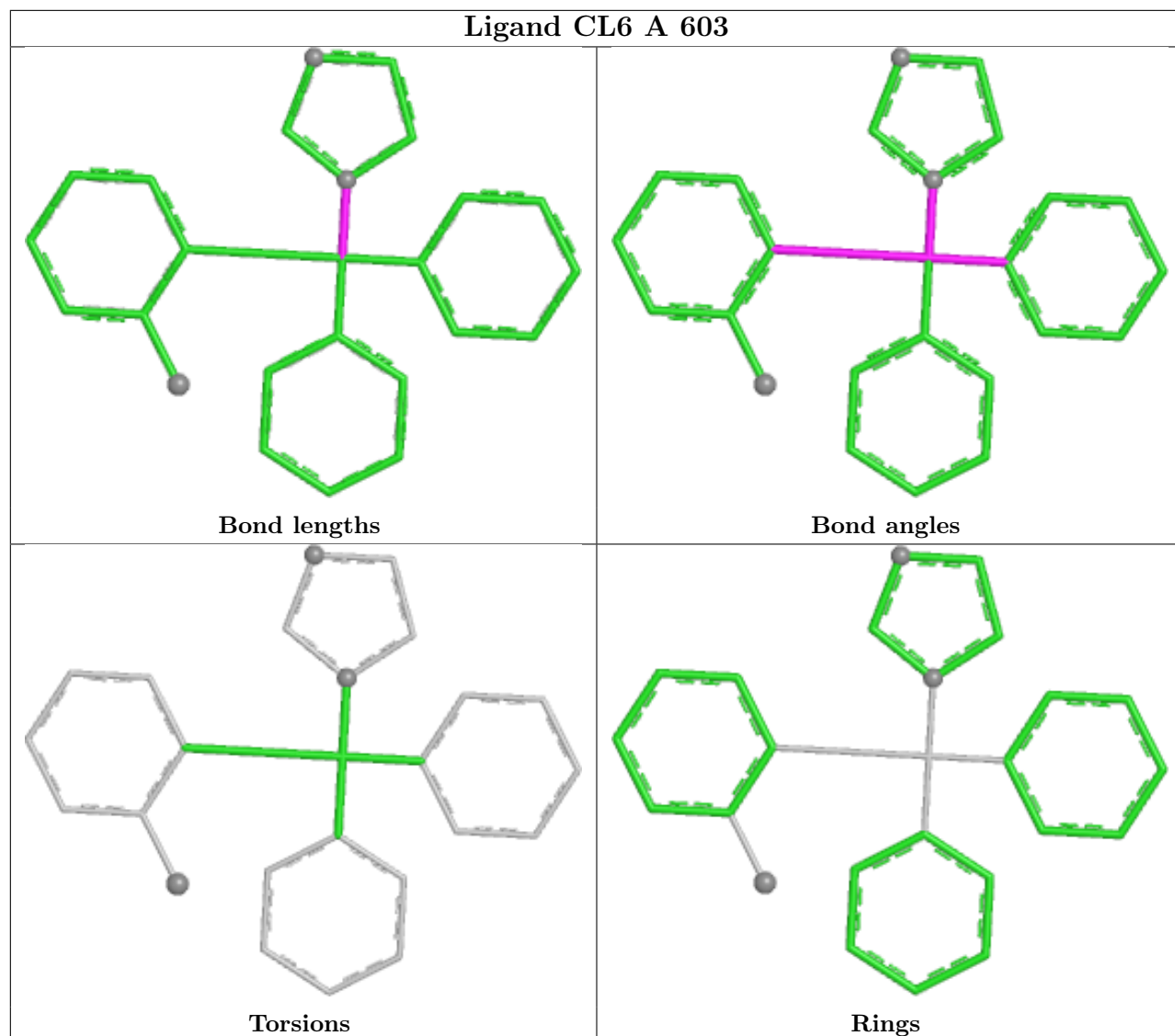
Torsions



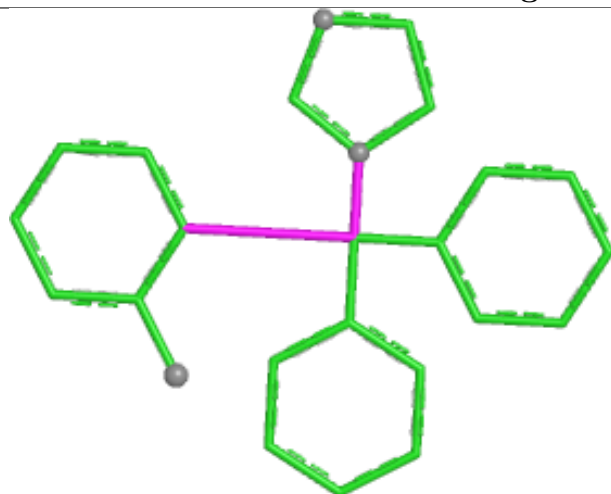
Rings



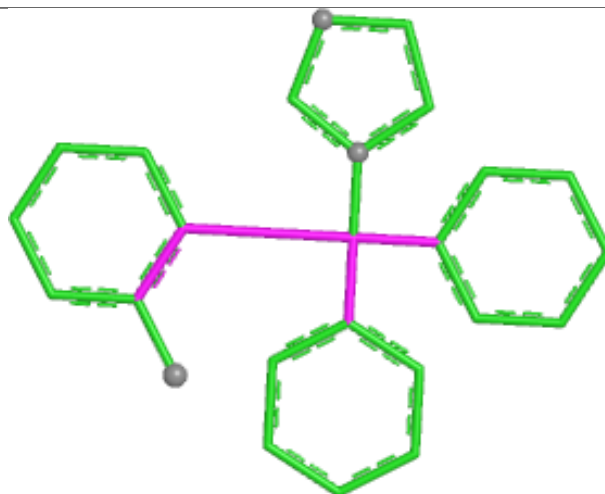
Ligand CL6 A 603



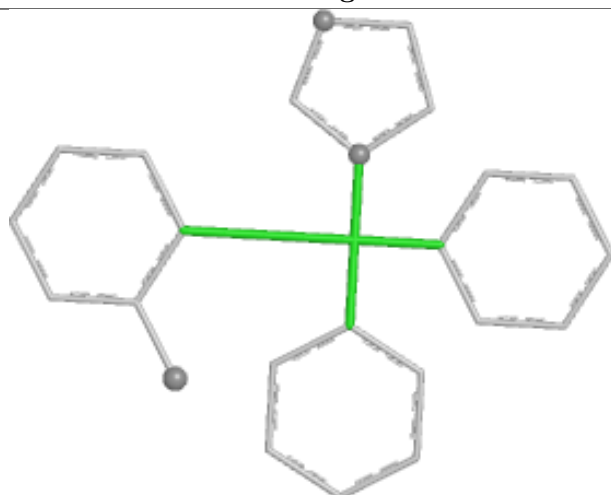
Ligand CL6 F 602



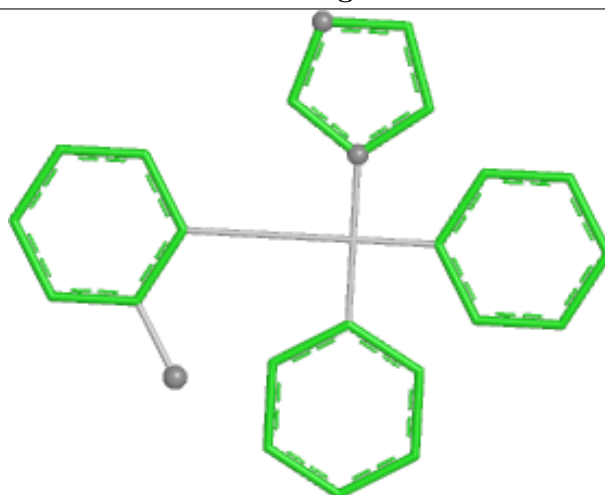
Bond lengths



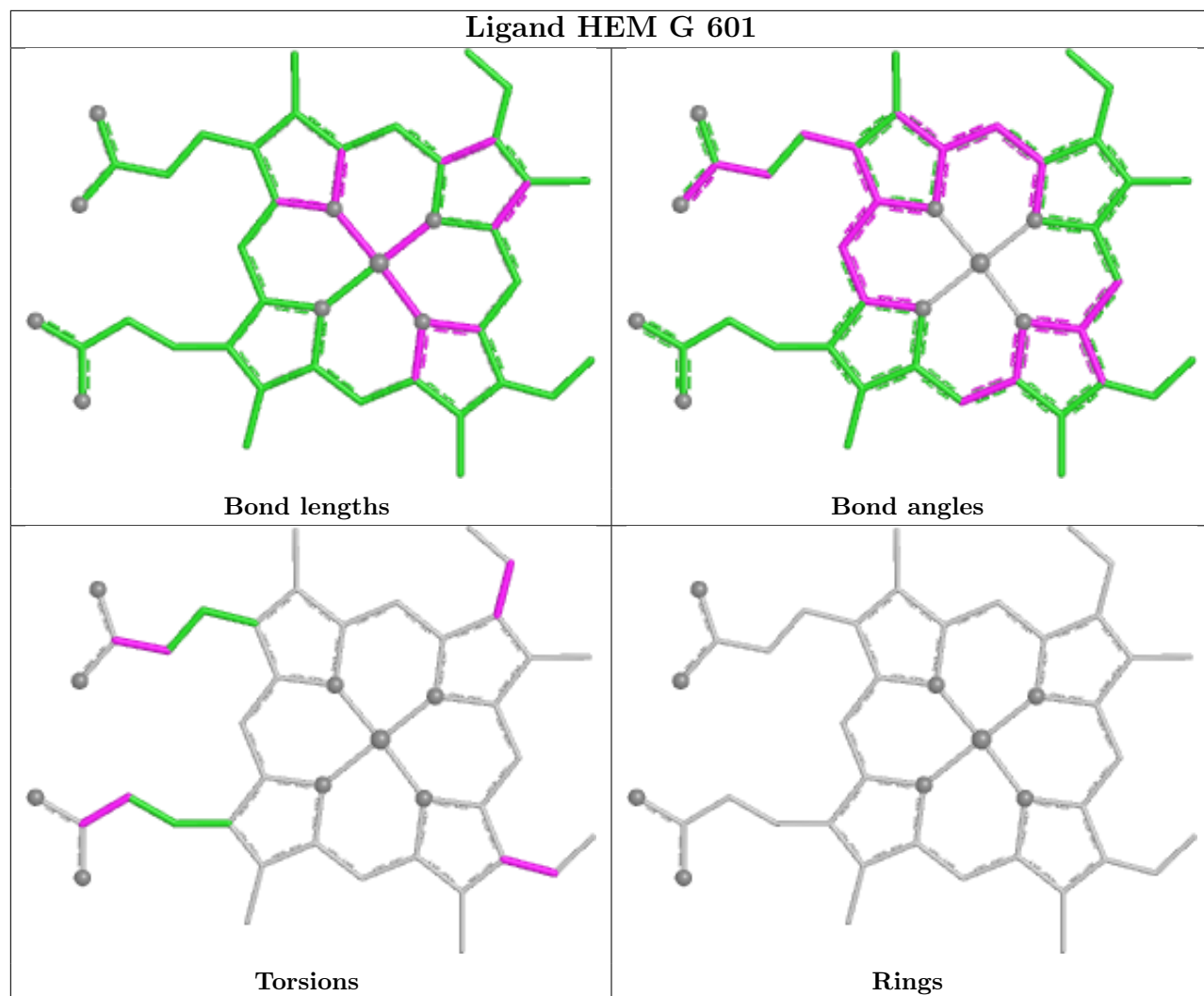
Bond angles



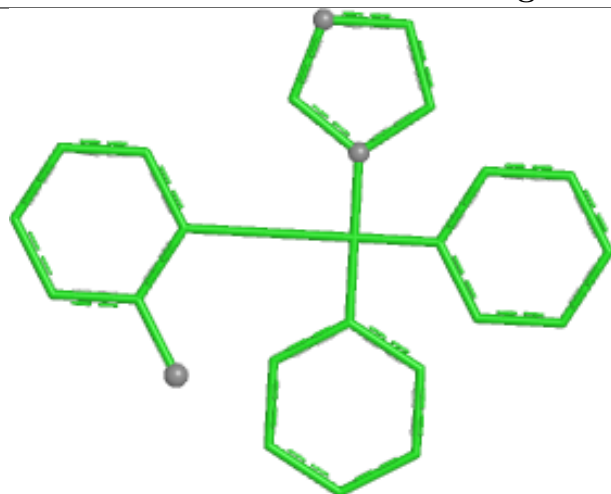
Torsions



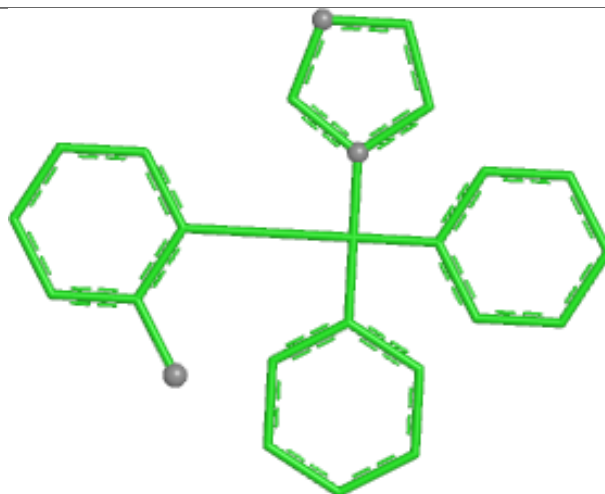
Rings



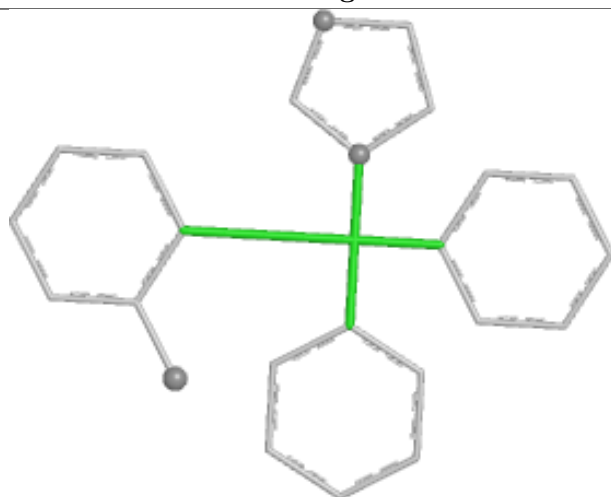
Ligand CL6 H 602



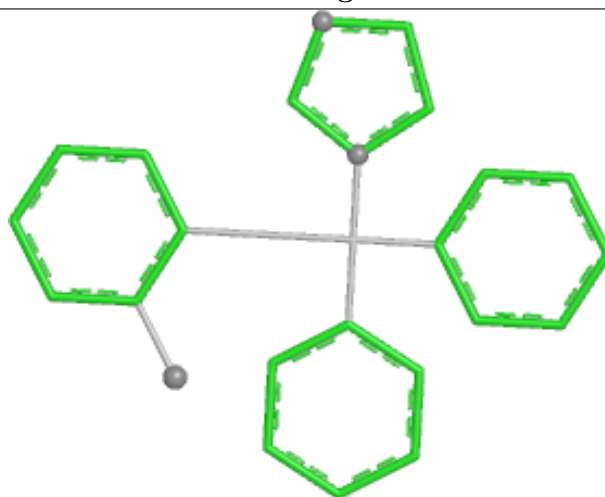
Bond lengths



Bond angles

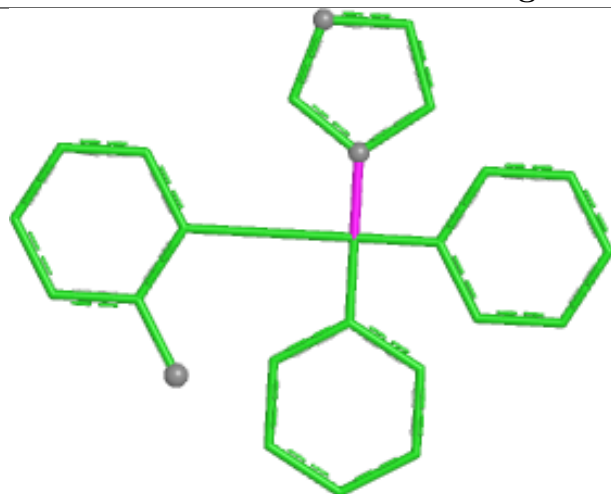


Torsions

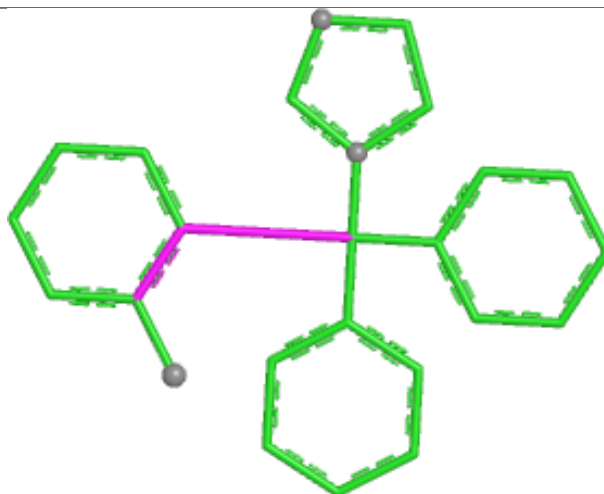


Rings

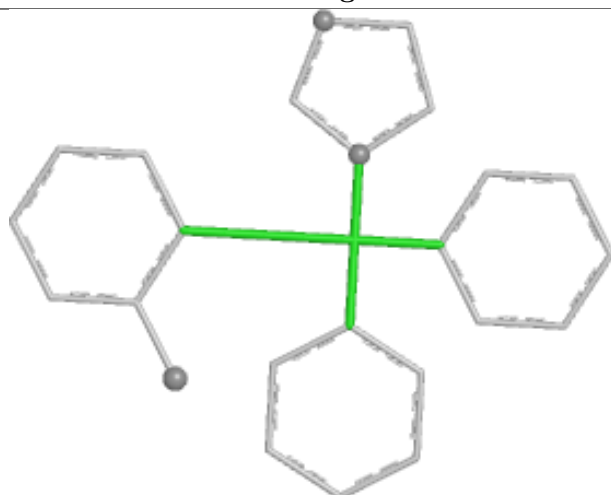
Ligand CL6 A 602



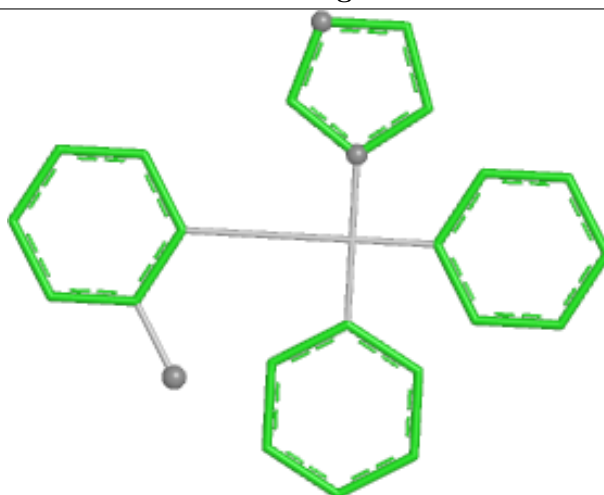
Bond lengths



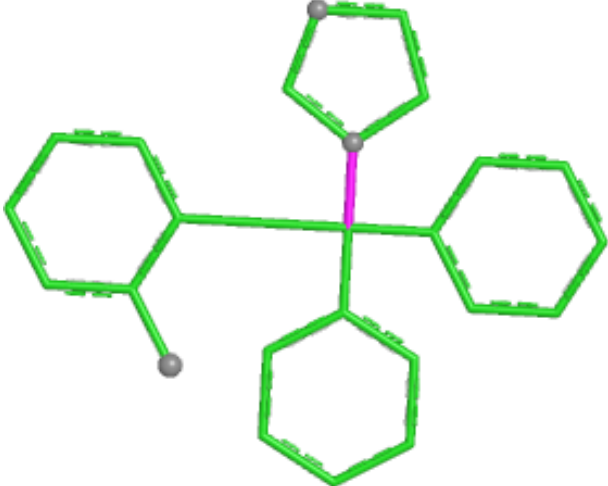
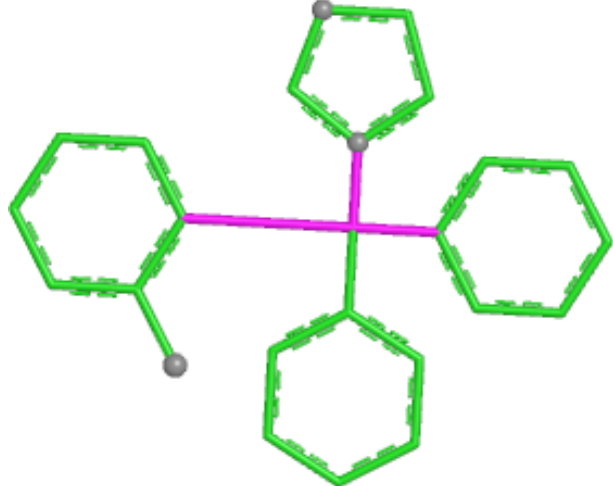
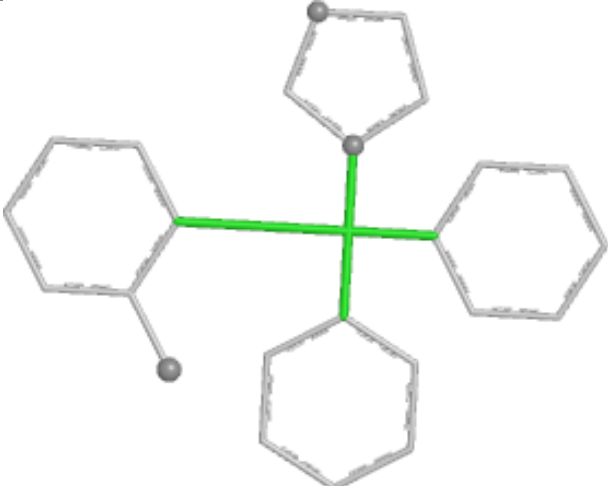
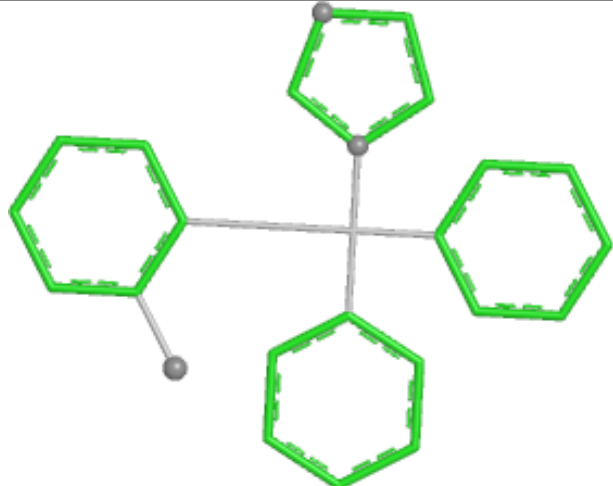
Bond angles



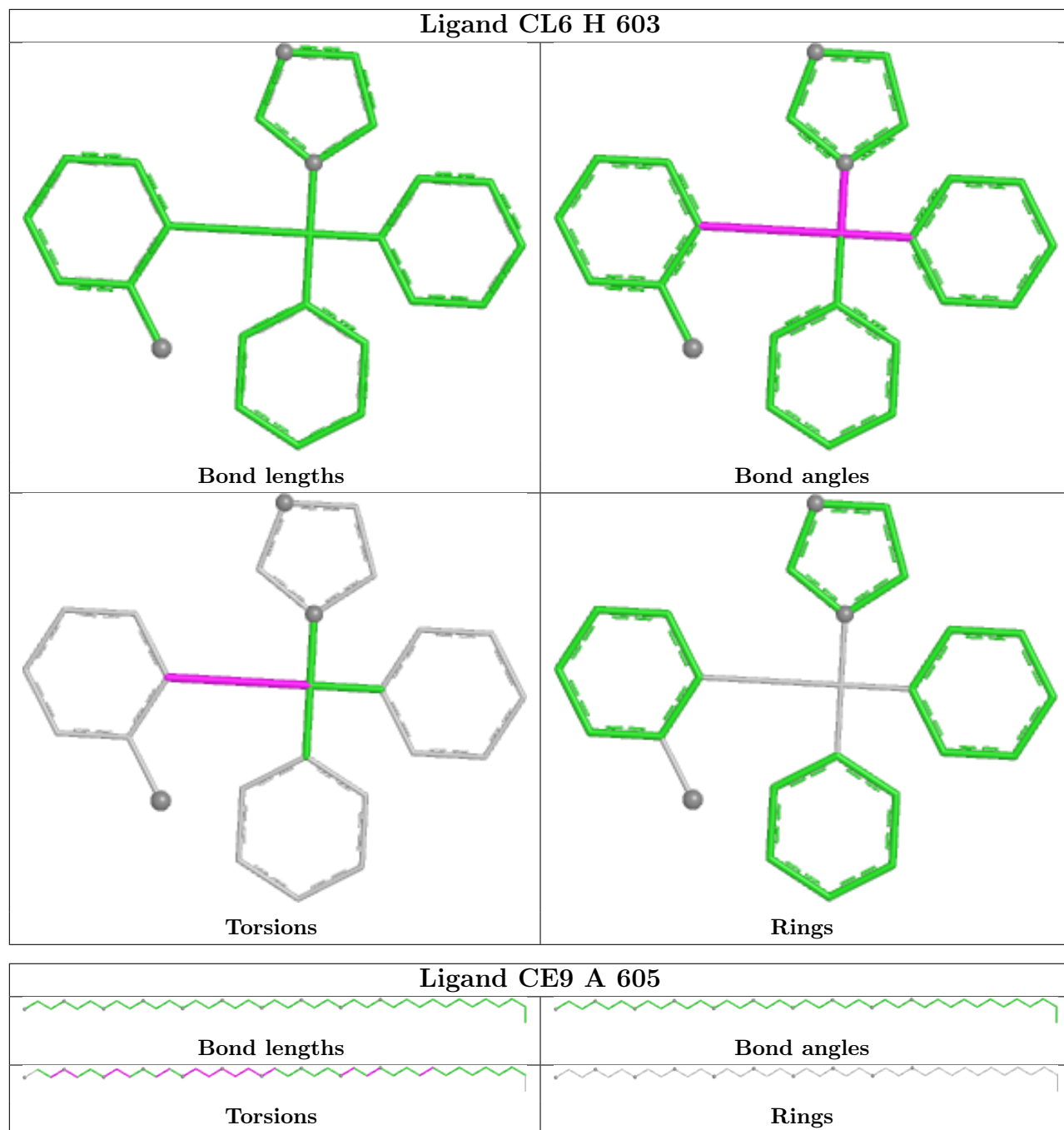
Torsions



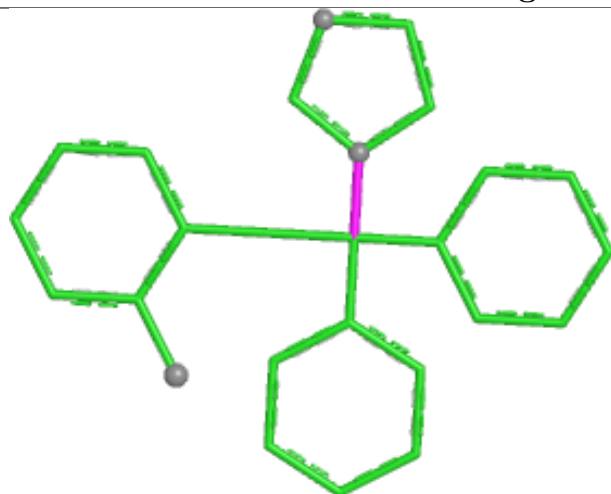
Rings

Ligand CL6 C 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

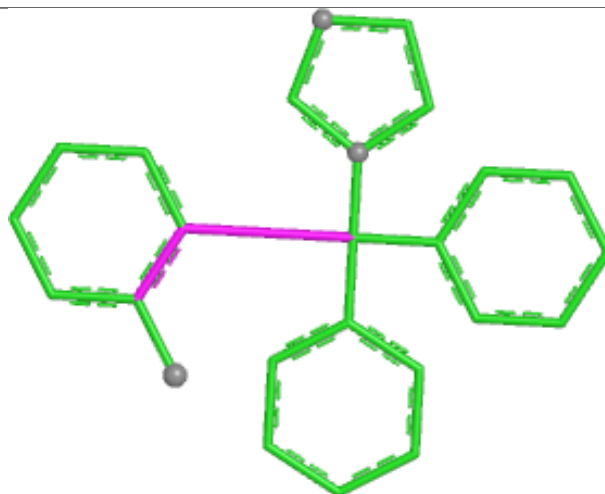
Ligand CE9 G 605	
	
Bond lengths	Bond angles
	
Torsions	Rings



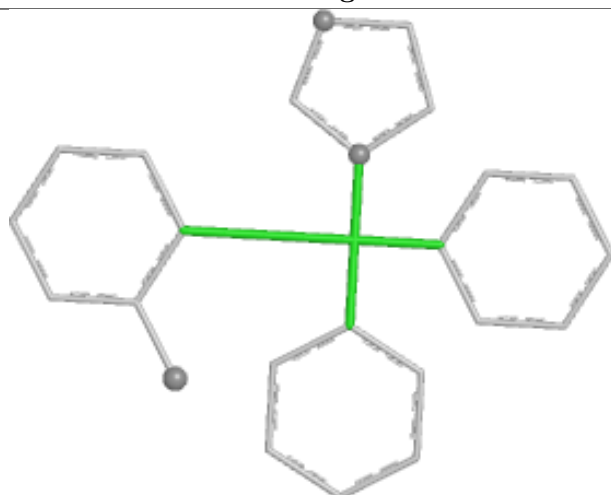
Ligand CL6 C 602



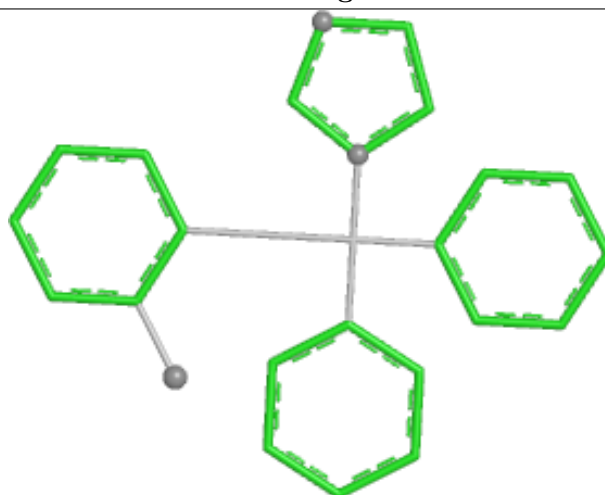
Bond lengths



Bond angles

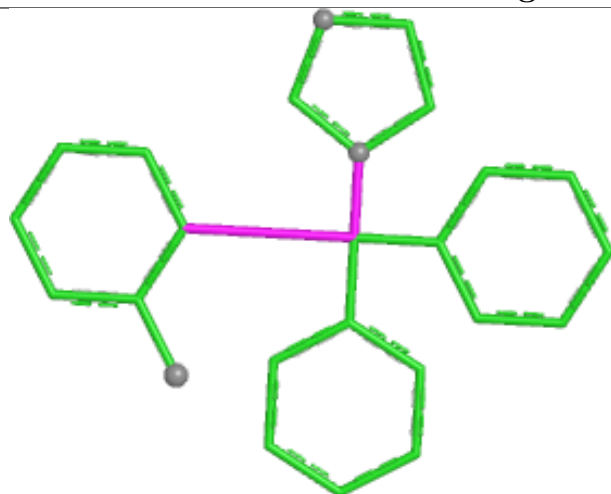


Torsions

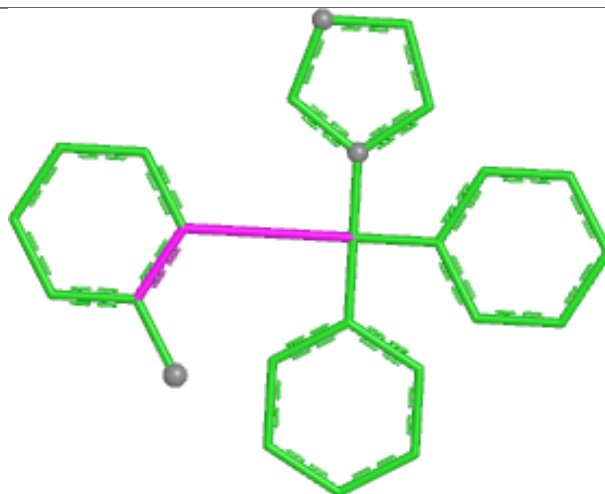


Rings

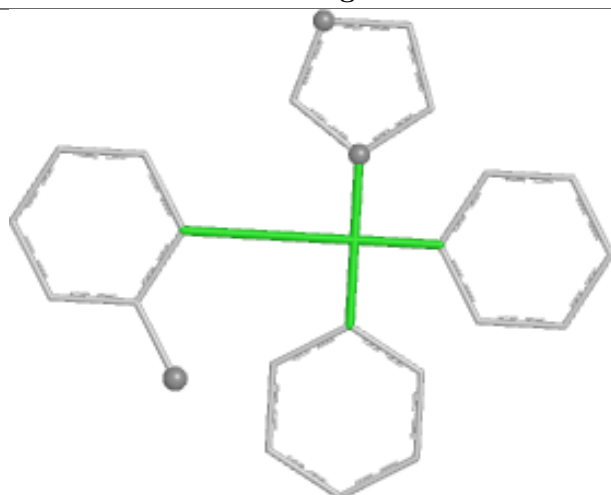
Ligand CL6 A 604



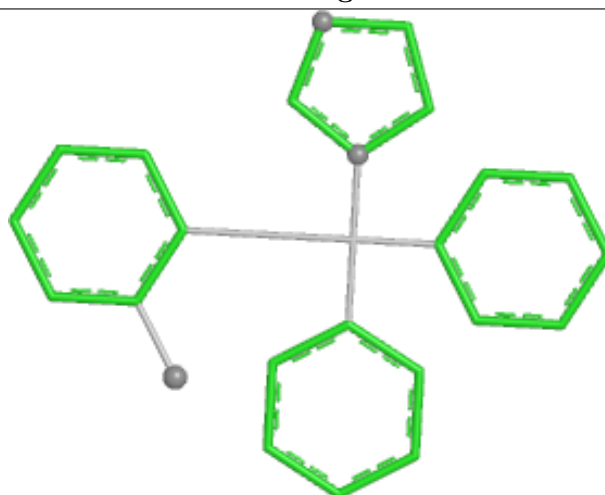
Bond lengths



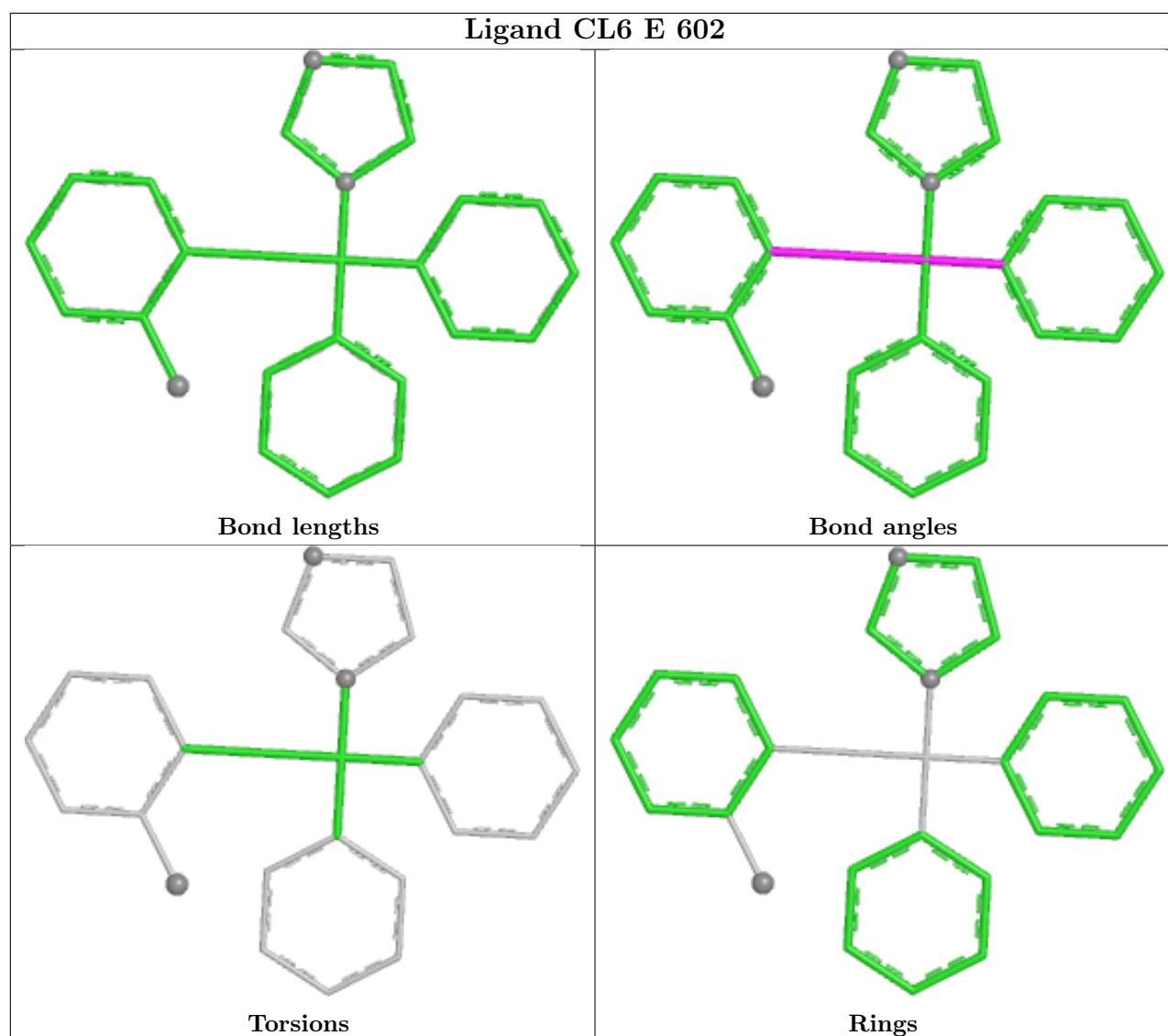
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	-0.20	5 (1%) 78 70	54, 78, 113, 181	0
1	B	456/480 (95%)	-0.24	4 (0%) 81 74	53, 80, 113, 151	0
1	C	451/480 (93%)	-0.16	7 (1%) 70 61	60, 80, 119, 199	0
1	D	453/480 (94%)	-0.13	4 (0%) 81 74	52, 77, 122, 183	0
1	E	452/480 (94%)	-0.12	4 (0%) 81 74	59, 83, 117, 170	0
1	F	452/480 (94%)	-0.07	6 (1%) 75 66	60, 87, 127, 180	0
1	G	449/480 (93%)	-0.02	7 (1%) 70 61	58, 87, 130, 163	0
1	H	446/480 (92%)	0.13	10 (2%) 62 52	56, 107, 155, 222	0
All	All	3615/3840 (94%)	-0.10	47 (1%) 75 66	52, 84, 130, 222	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	GLY	5.2
1	G	176	PHE	4.1
1	H	391	GLY	4.0
1	B	350	VAL	3.9
1	A	23	ALA	3.6
1	B	446	PHE	3.6
1	C	446	PHE	3.5
1	A	370	ALA	3.2
1	C	203	PHE	3.0
1	C	288	LYS	2.9
1	D	289	ALA	2.9
1	E	446	PHE	2.9
1	C	350	VAL	2.8
1	E	370	ALA	2.8
1	E	159	ASN	2.8
1	B	349	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	288	LYS	2.7
1	C	345	PRO	2.6
1	F	204	VAL	2.6
1	E	494	SER	2.6
1	F	193	ILE	2.6
1	H	383	ILE	2.6
1	G	160	LEU	2.5
1	H	288	LYS	2.5
1	H	360	VAL	2.5
1	F	203	PHE	2.5
1	H	446	PHE	2.5
1	C	370	ALA	2.5
1	C	193	ILE	2.4
1	G	153	GLY	2.4
1	H	189	PHE	2.4
1	H	356	LEU	2.3
1	A	27	THR	2.3
1	G	446	PHE	2.2
1	H	450	ASN	2.2
1	A	369	VAL	2.2
1	F	157	VAL	2.2
1	G	454	ALA	2.2
1	D	480	GLY	2.1
1	G	456	ILE	2.1
1	A	289	ALA	2.1
1	H	350	VAL	2.1
1	F	424	ASP	2.1
1	G	370	ALA	2.1
1	H	191	VAL	2.1
1	F	156	LEU	2.1
1	D	212	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.

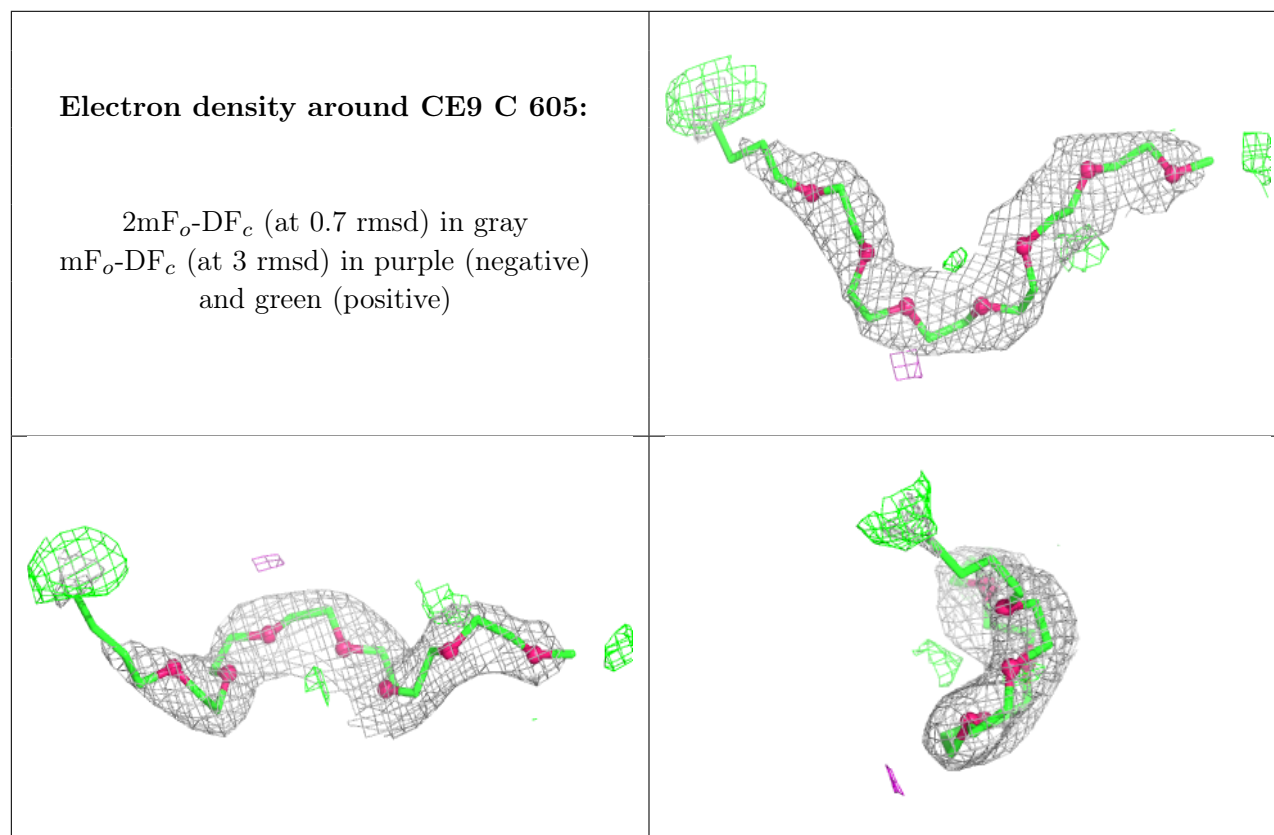
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CE9	C	605	24/40	0.78	0.17	73,79,99,105	0
4	CE9	D	605	24/40	0.87	0.14	60,76,81,83	0
4	CE9	B	605	34/40	0.88	0.13	63,70,95,101	0
4	CE9	F	605	29/40	0.88	0.14	65,76,90,103	0
4	CE9	G	605	30/40	0.88	0.13	60,70,94,94	0
4	CE9	A	605	40/40	0.89	0.13	60,73,106,107	0
3	CL6	D	604	25/25	0.89	0.12	72,75,79,98	0
3	CL6	H	604	25/25	0.90	0.10	75,80,84,106	0
3	CL6	B	604	25/25	0.91	0.10	57,65,68,93	0
4	CE9	E	605	22/40	0.92	0.12	50,65,71,73	0
3	CL6	F	604	25/25	0.92	0.11	70,77,80,104	0
3	CL6	C	604	25/25	0.92	0.10	61,70,74,93	0
3	CL6	A	604	25/25	0.93	0.10	59,65,68,84	0
3	CL6	B	603	25/25	0.93	0.09	59,64,67,80	0
3	CL6	E	604	25/25	0.93	0.10	62,67,74,88	0
3	CL6	F	603	25/25	0.93	0.10	70,72,75,89	0
3	CL6	A	603	25/25	0.93	0.10	57,61,64,72	0
3	CL6	H	603	25/25	0.93	0.09	68,73,80,80	0
3	CL6	C	603	25/25	0.93	0.09	62,65,69,80	0
3	CL6	E	602	25/25	0.94	0.10	61,68,70,73	0
3	CL6	D	603	25/25	0.94	0.10	66,70,73,84	0
3	CL6	G	604	25/25	0.94	0.09	65,70,75,94	0
3	CL6	G	603	25/25	0.95	0.09	65,69,74,76	0
3	CL6	F	602	25/25	0.95	0.09	64,68,72,74	0
3	CL6	H	602	25/25	0.95	0.09	78,82,87,87	0
2	HEM	H	601	43/43	0.96	0.10	85,91,95,97	0
3	CL6	E	603	25/25	0.96	0.08	62,68,72,79	0
3	CL6	B	602	25/25	0.96	0.08	56,61,63,65	0
3	CL6	G	602	25/25	0.96	0.09	65,68,71,71	0
3	CL6	A	602	25/25	0.97	0.07	52,56,58,61	0
2	HEM	A	601	43/43	0.97	0.09	58,62,65,69	0
3	CL6	D	602	25/25	0.97	0.07	59,63,67,68	0
3	CL6	C	602	25/25	0.97	0.07	58,63,66,68	0
2	HEM	D	601	43/43	0.98	0.07	51,62,67,69	0
2	HEM	E	601	43/43	0.98	0.07	66,71,75,76	0
2	HEM	F	601	43/43	0.98	0.06	62,69,74,75	0
2	HEM	G	601	43/43	0.98	0.09	68,73,83,87	0

Continued on next page...

Continued from previous page...

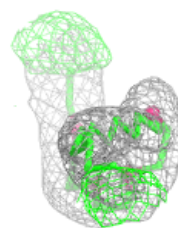
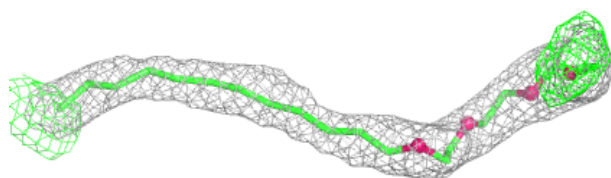
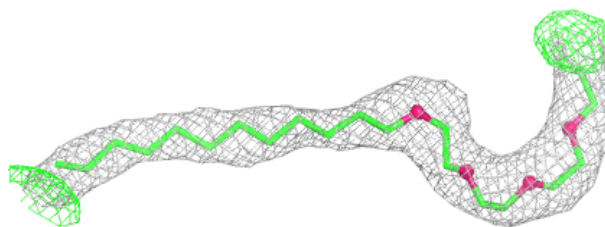
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	601	43/43	0.98	0.08	57,64,68,70	0
2	HEM	C	601	43/43	0.98	0.08	62,66,68,70	0

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.

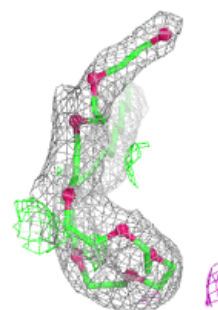
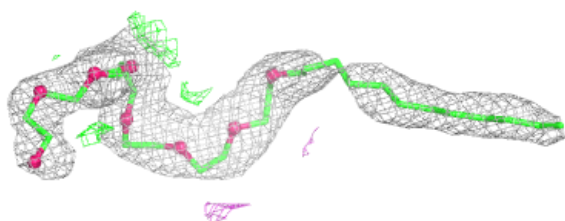
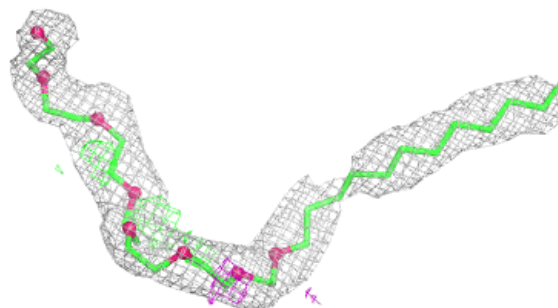


Electron density around CE9 D 605:

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

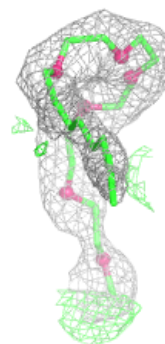
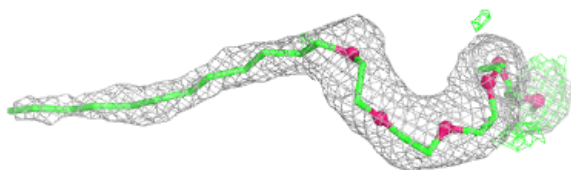
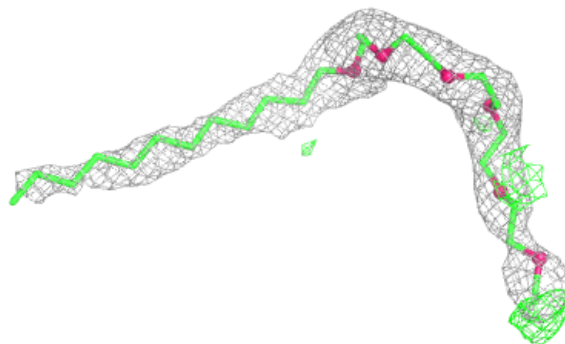
**Electron density around CE9 B 605:**

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

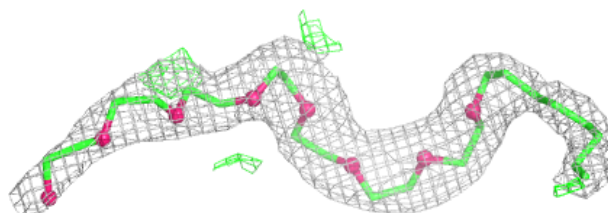
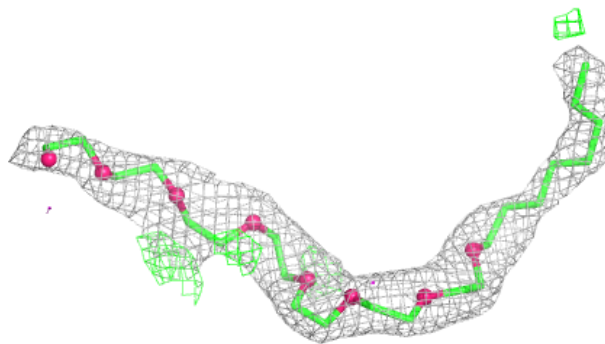


Electron density around CE9 F 605:

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

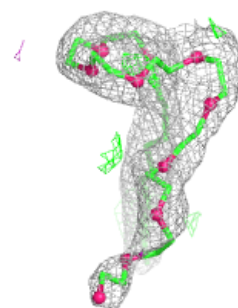
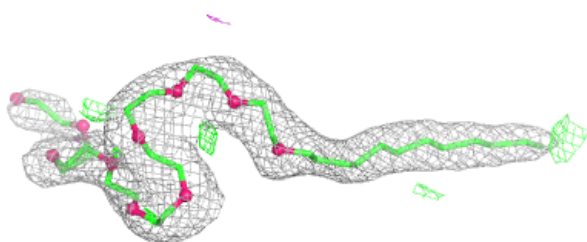
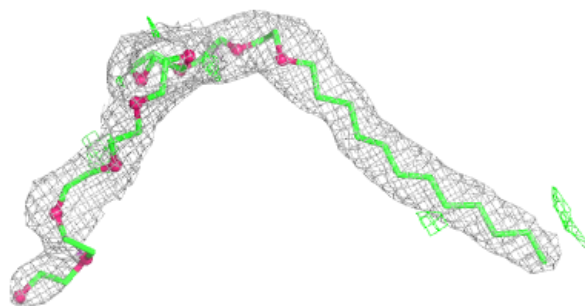
**Electron density around CE9 G 605:**

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



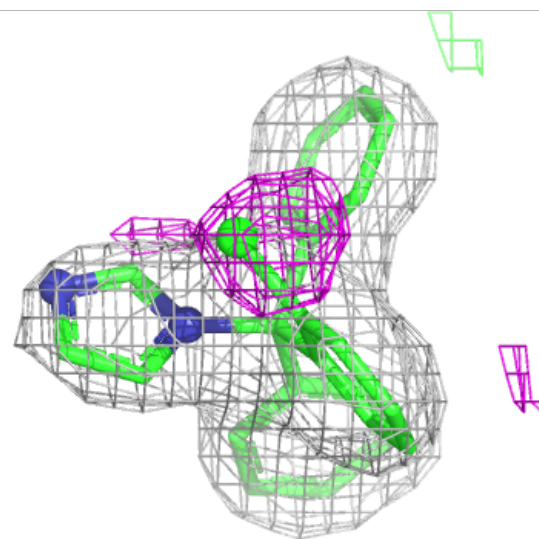
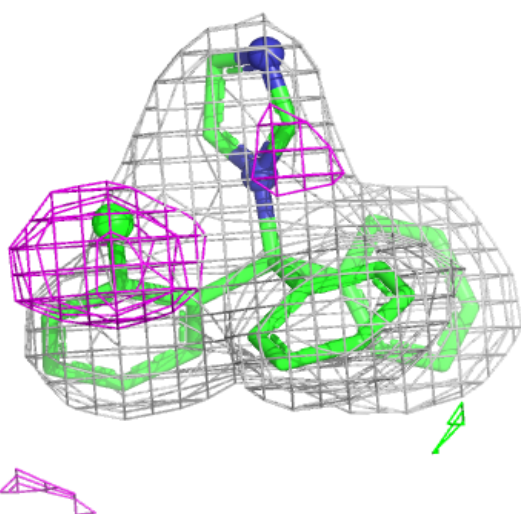
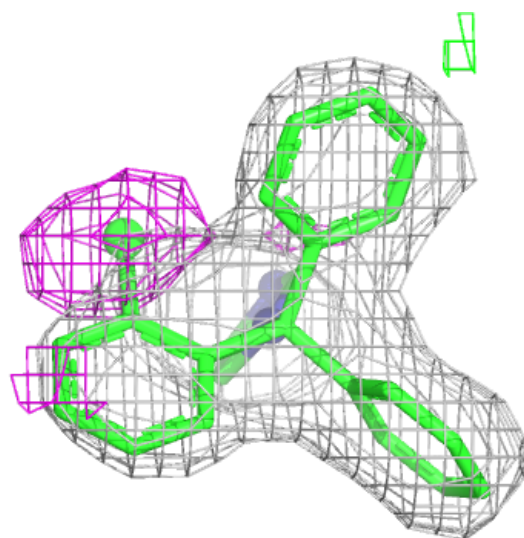
Electron density around CE9 A 605:

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



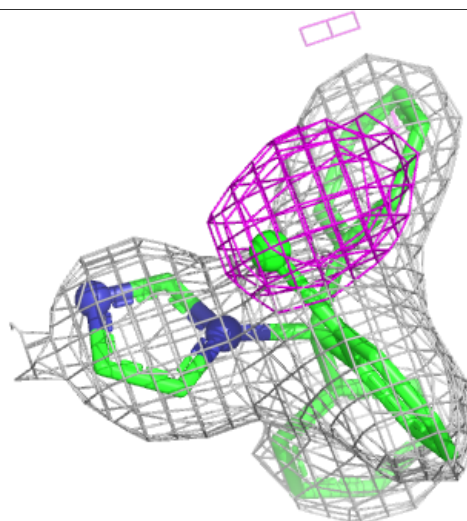
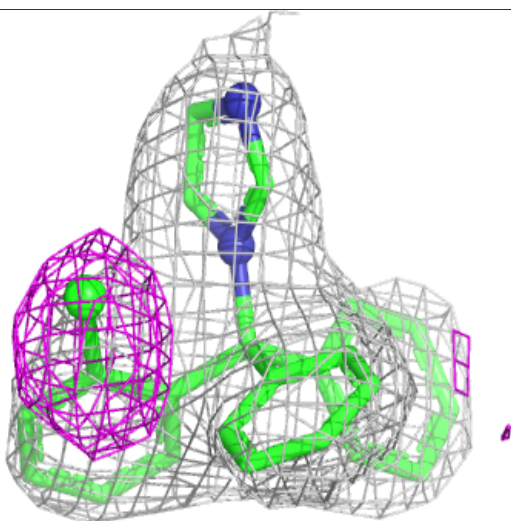
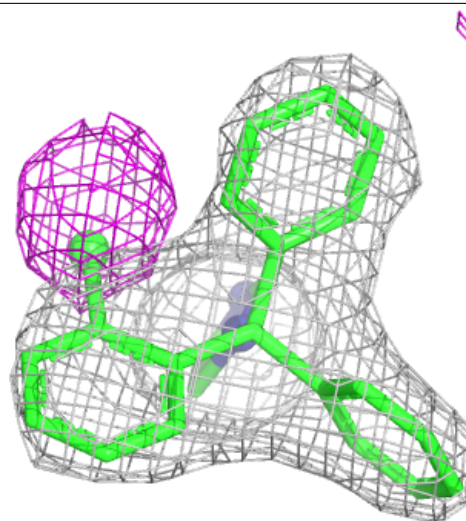
Electron density around CL6 D 604:

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



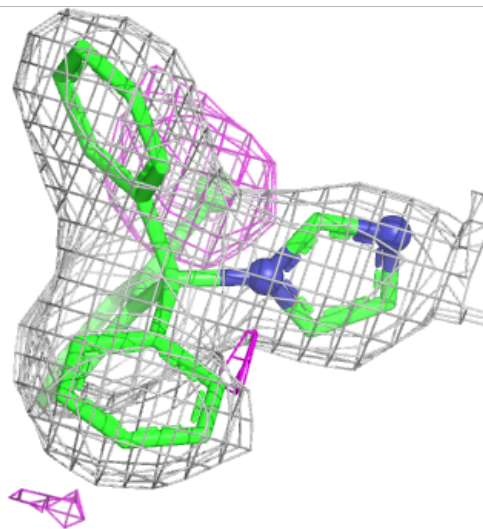
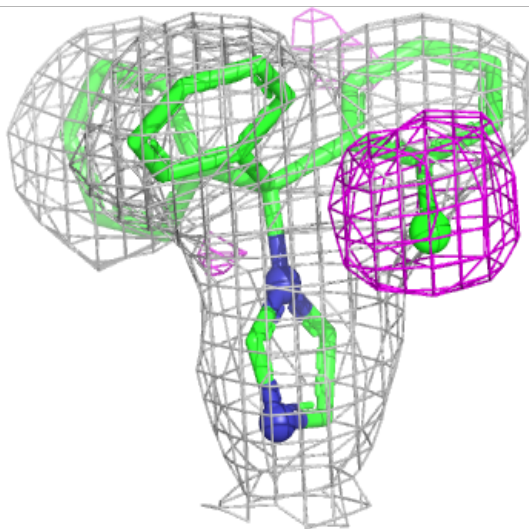
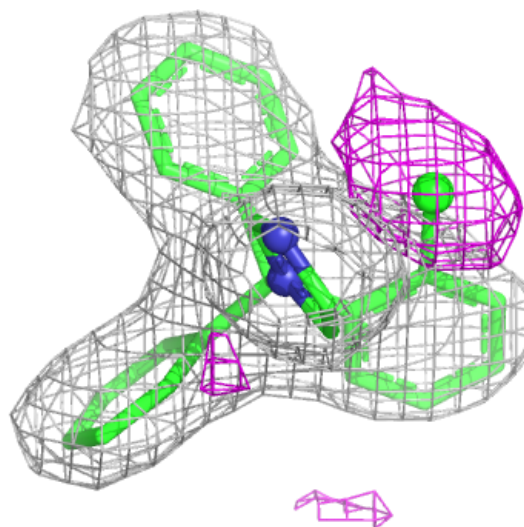
Electron density around CL6 H 604:

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



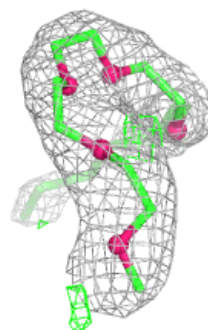
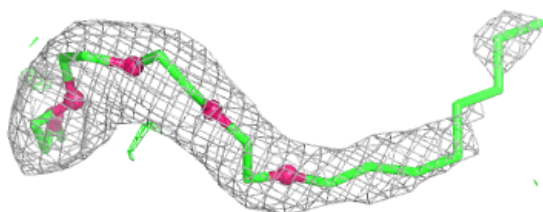
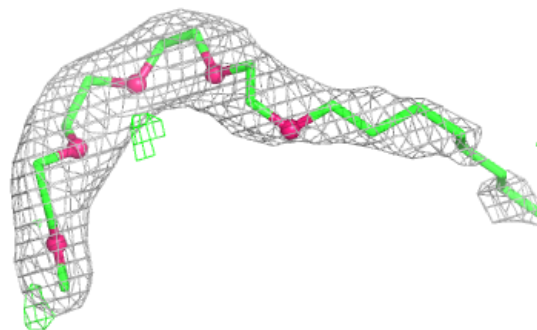
Electron density around CL6 B 604:

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



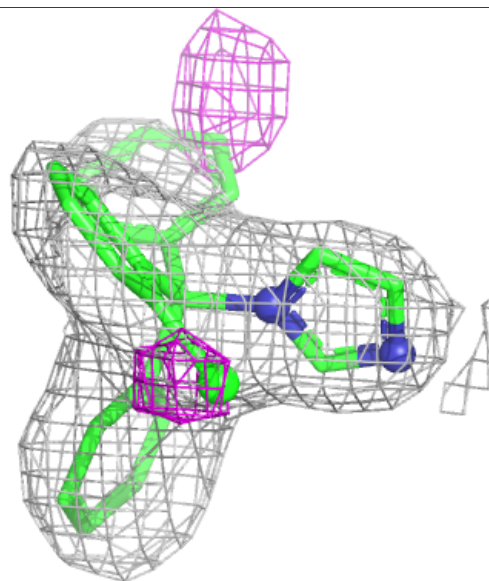
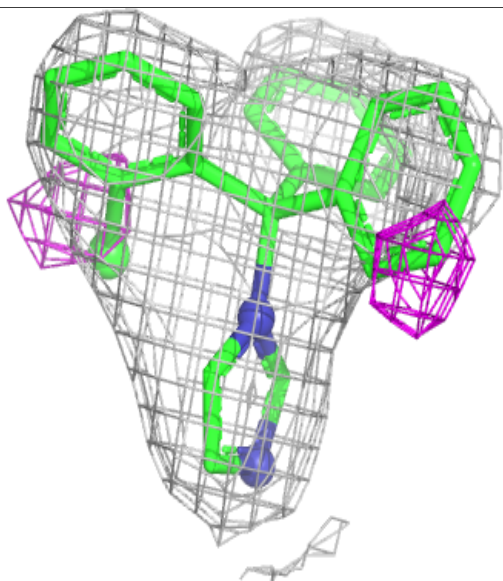
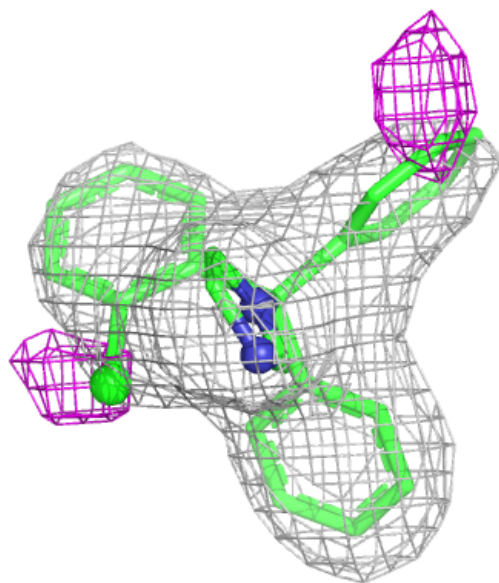
Electron density around CE9 E 605:

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



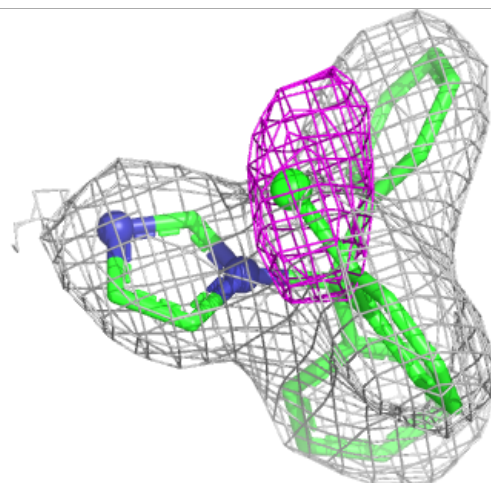
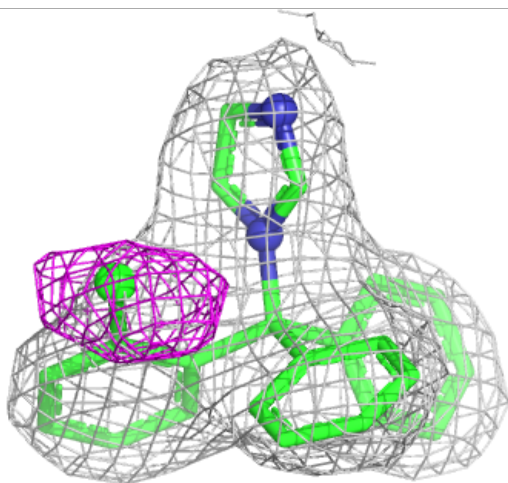
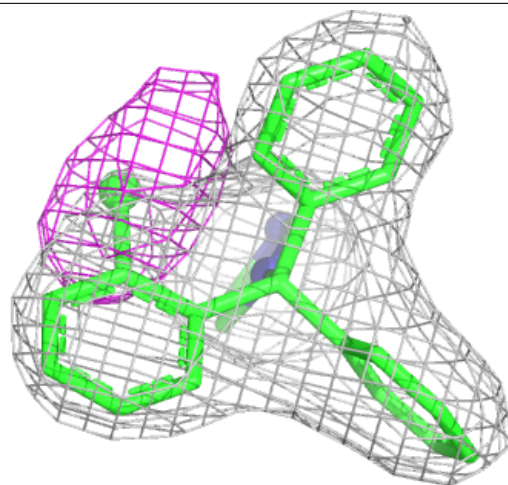
Electron density around CL6 F 604:

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



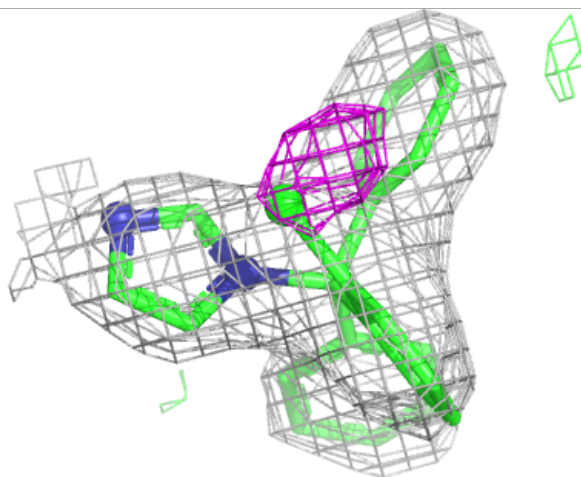
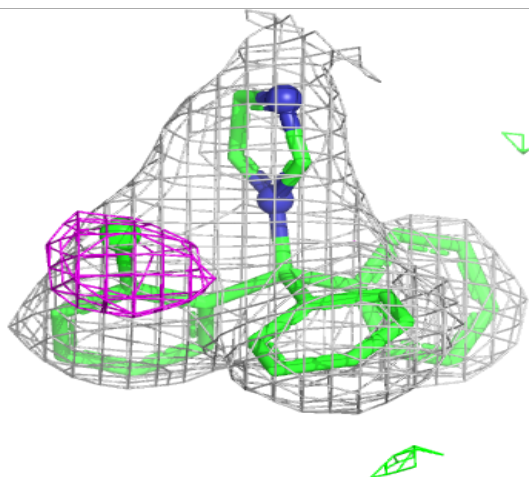
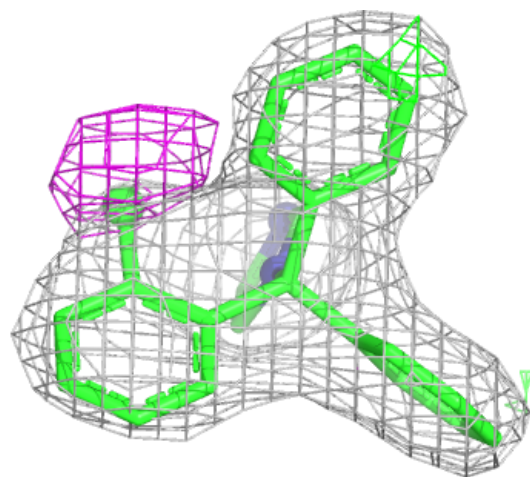
Electron density around CL6 C 604:

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



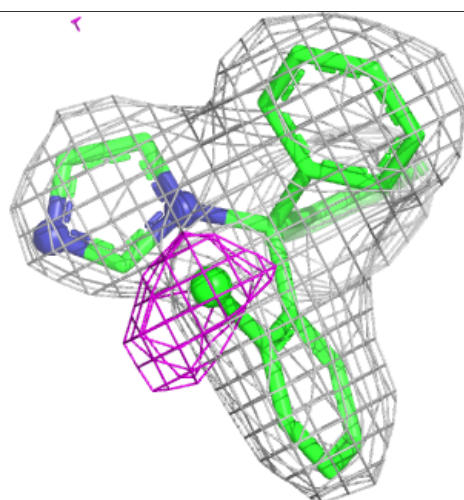
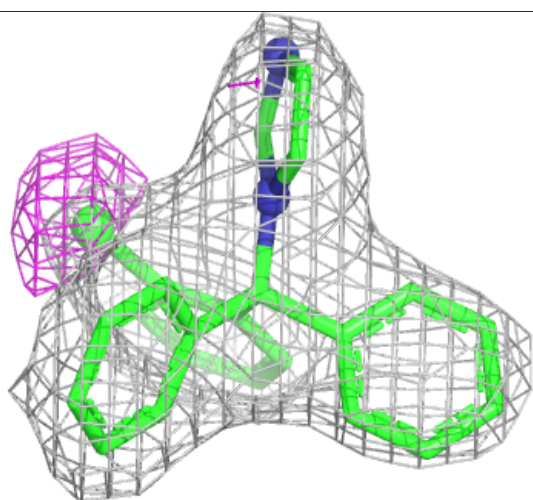
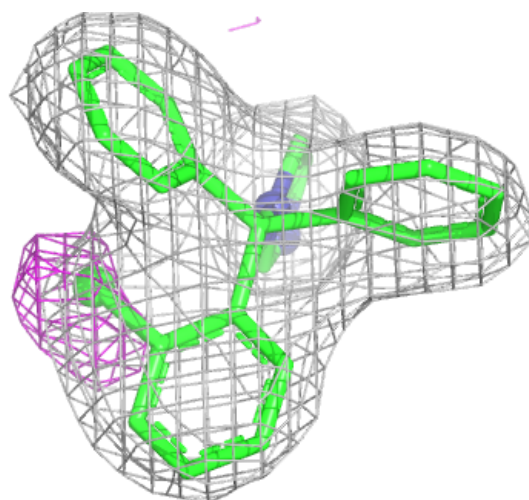
Electron density around CL6 A 604:

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



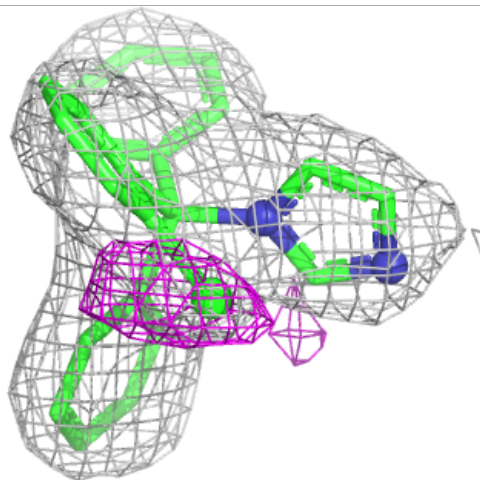
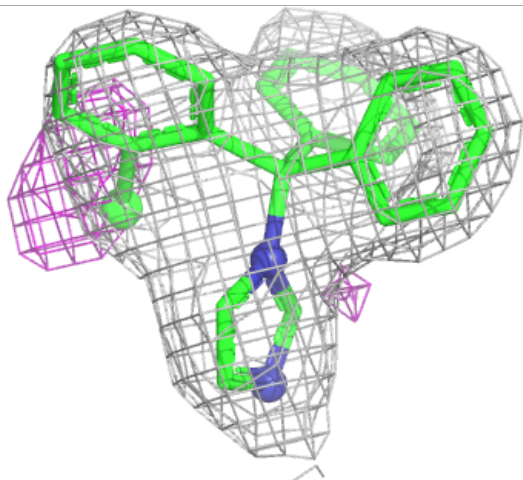
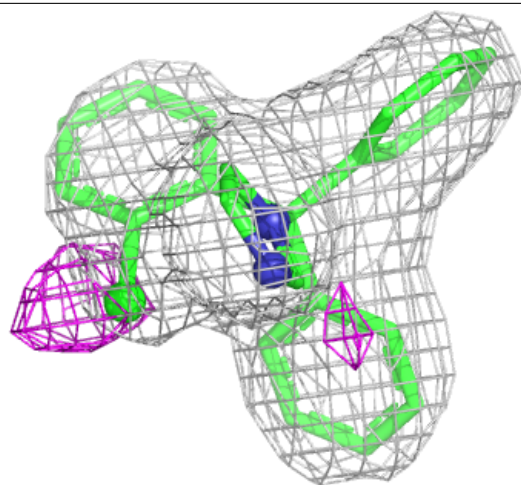
Electron density around CL6 B 603:

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



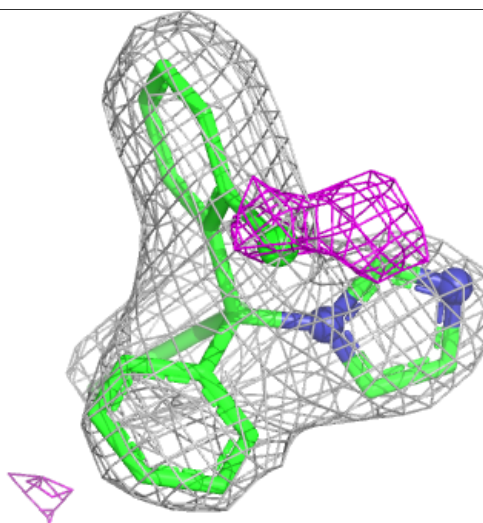
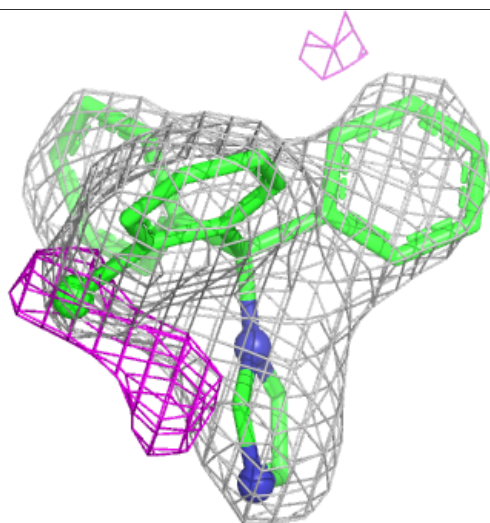
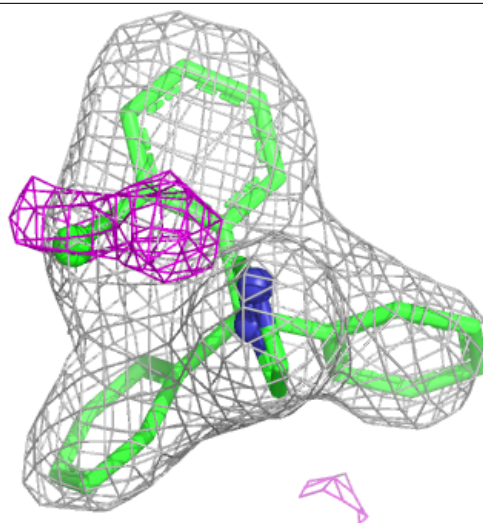
Electron density around CL6 E 604:

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



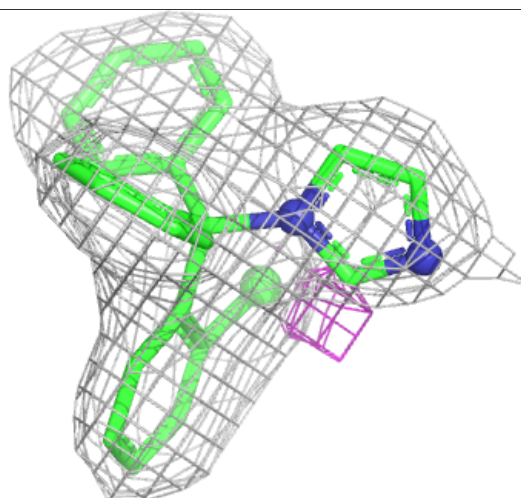
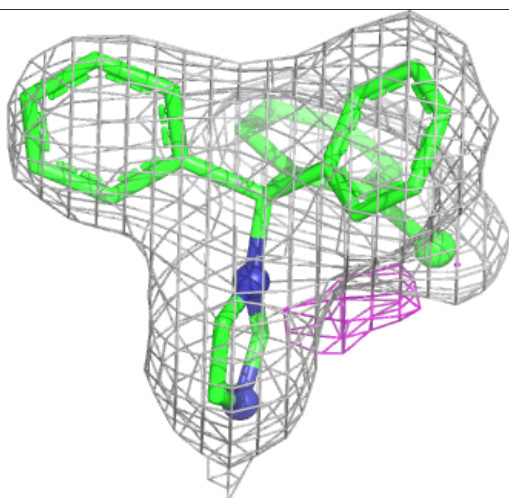
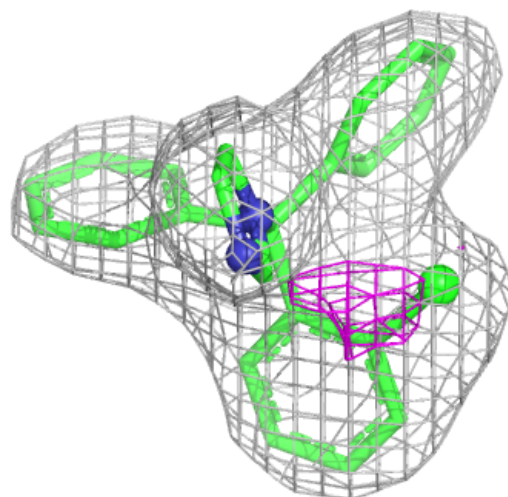
Electron density around CL6 F 603:

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



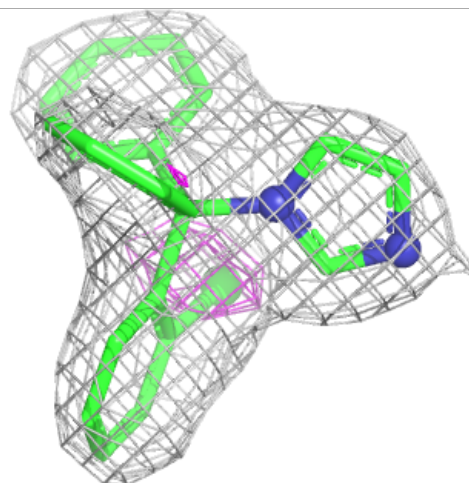
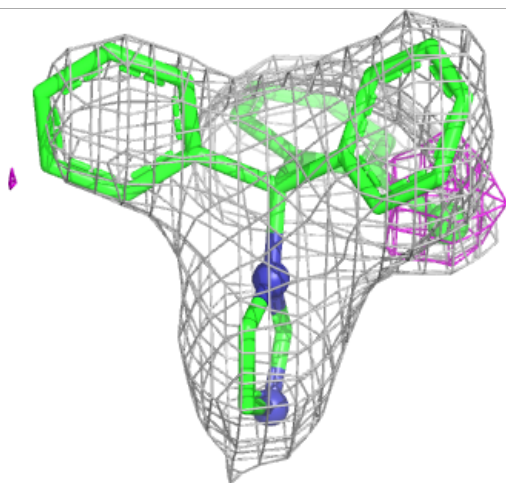
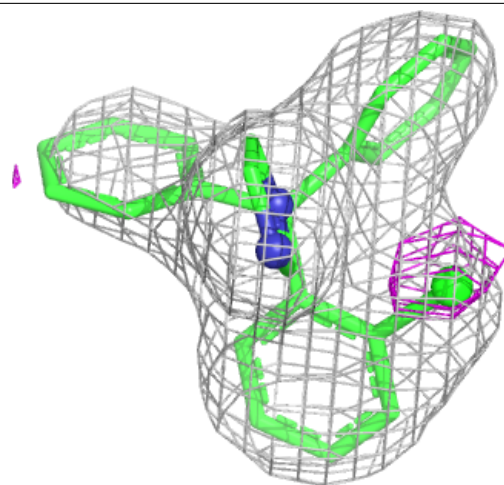
Electron density around CL6 A 603:

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



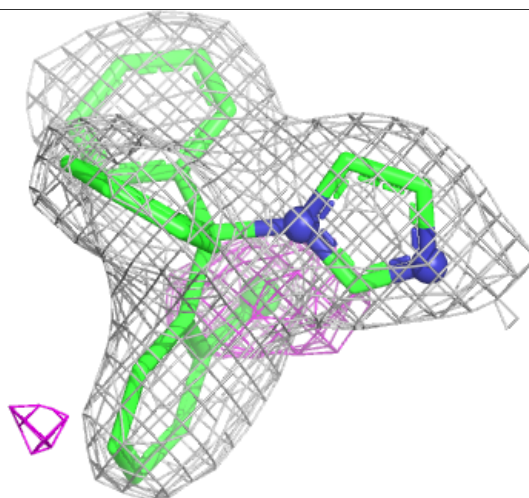
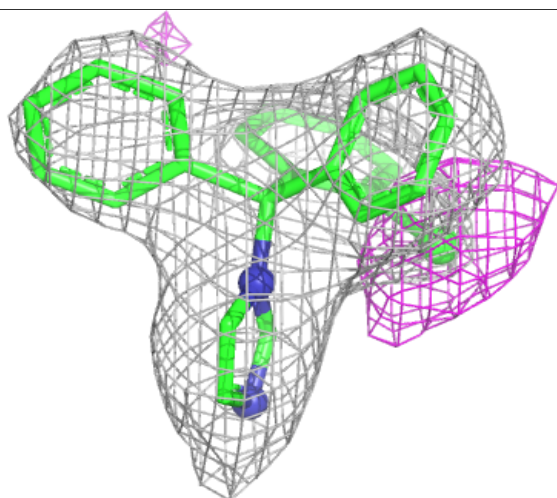
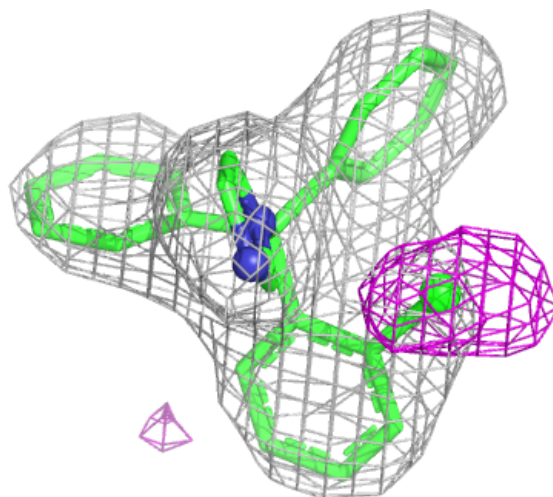
Electron density around CL6 H 603:

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



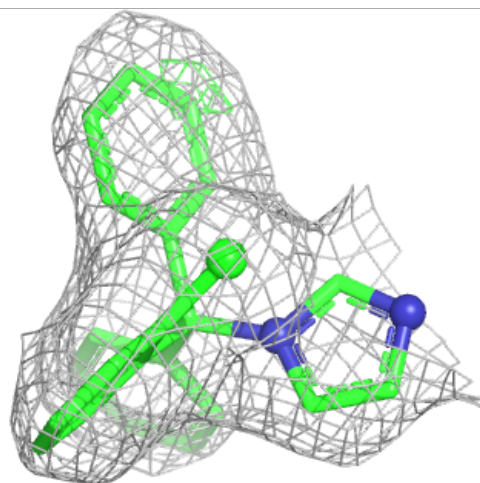
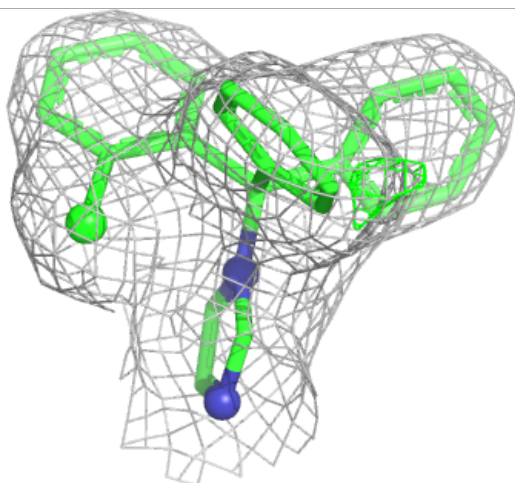
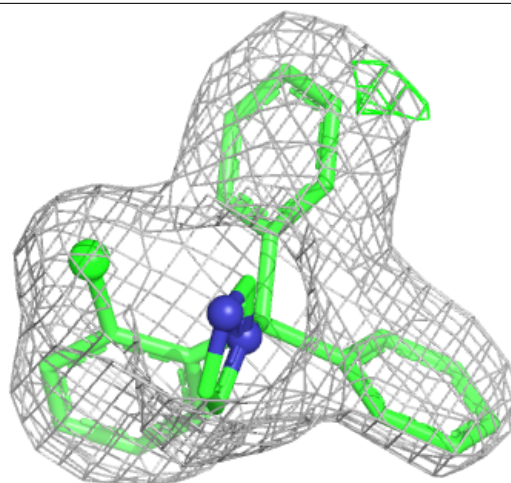
Electron density around CL6 C 603:

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



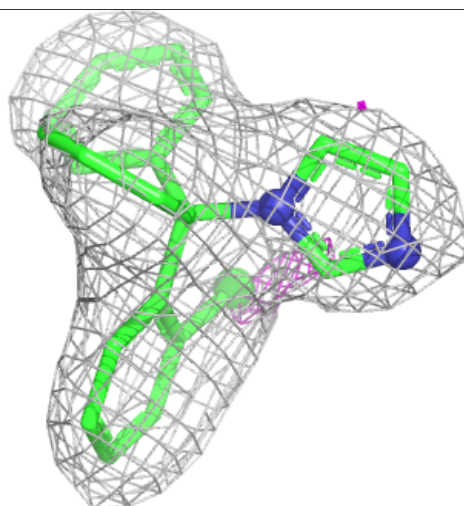
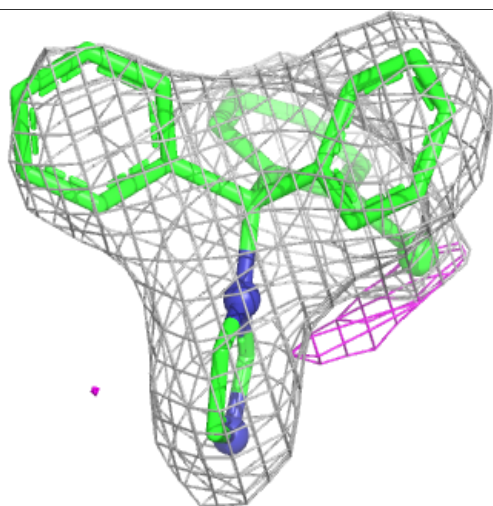
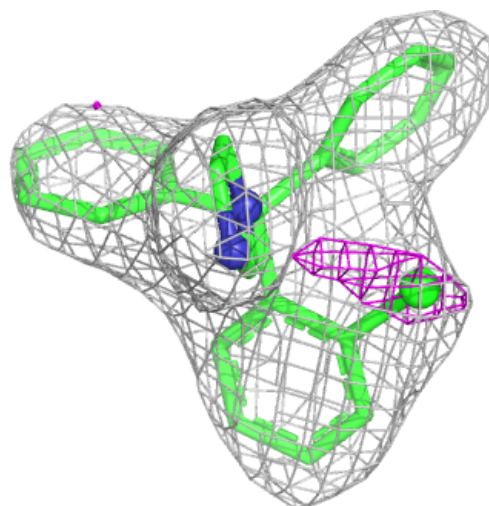
Electron density around CL6 E 602:

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



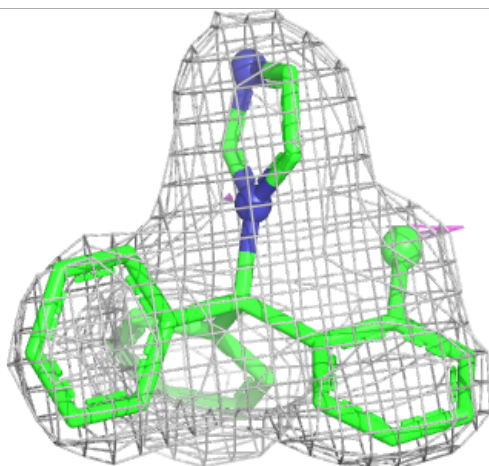
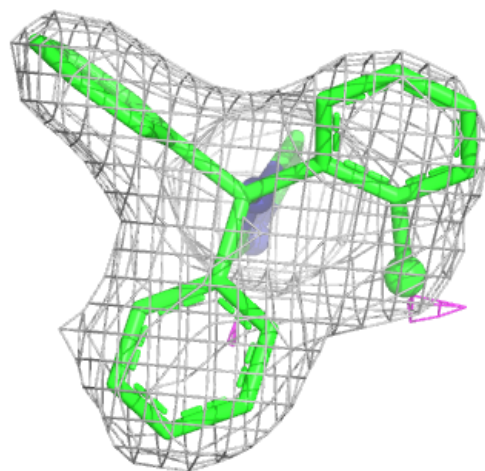
Electron density around CL6 D 603:

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



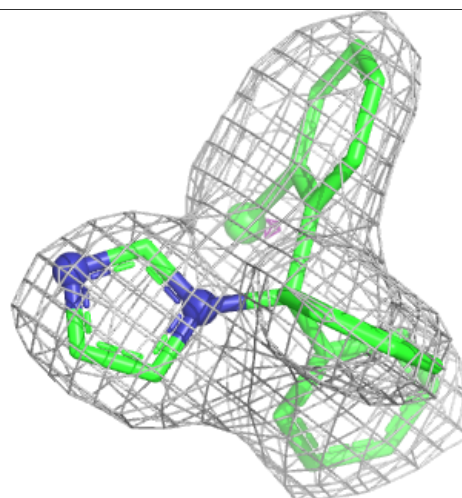
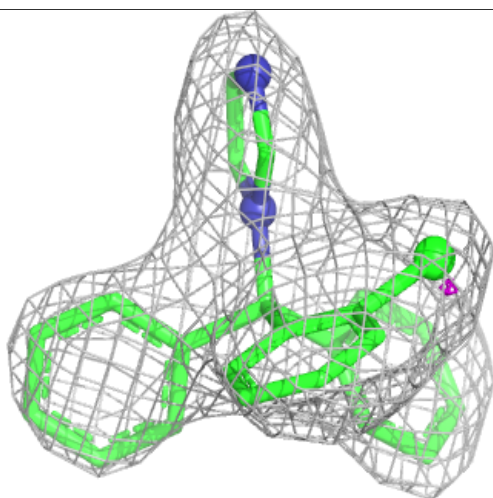
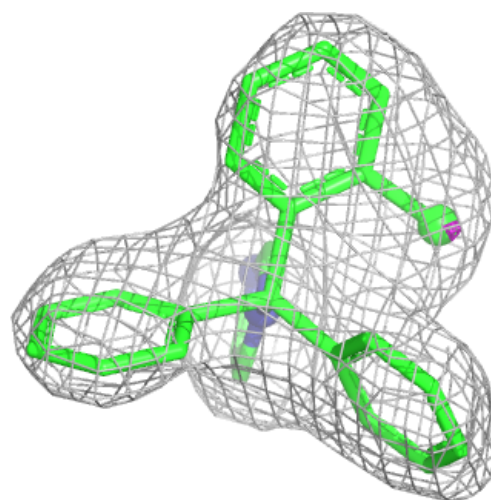
Electron density around CL6 G 604:

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



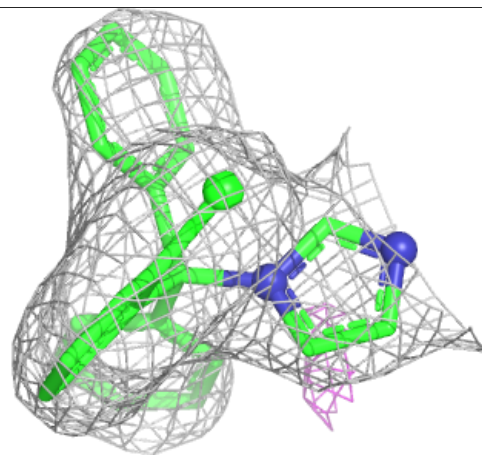
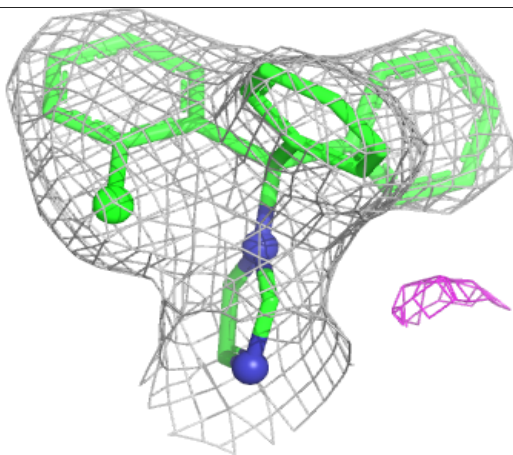
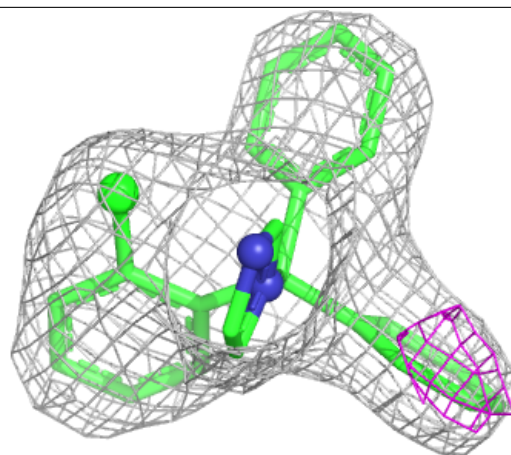
Electron density around CL6 G 603:

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



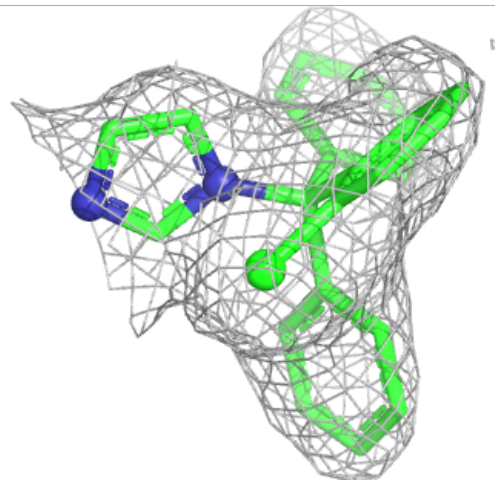
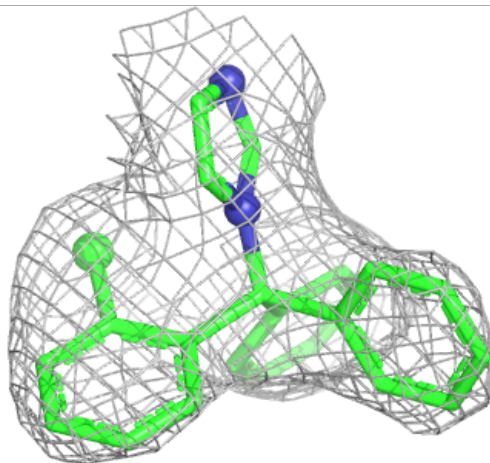
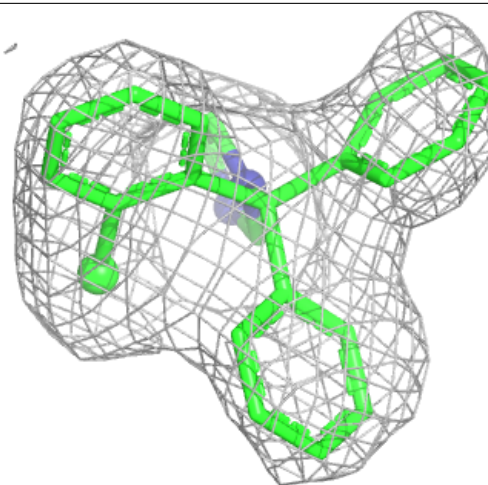
Electron density around CL6 F 602:

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



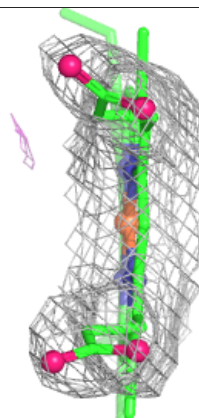
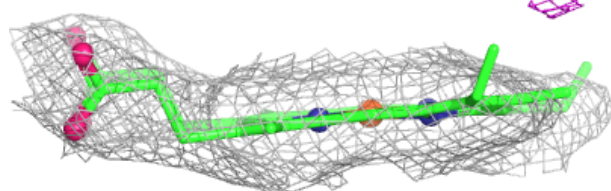
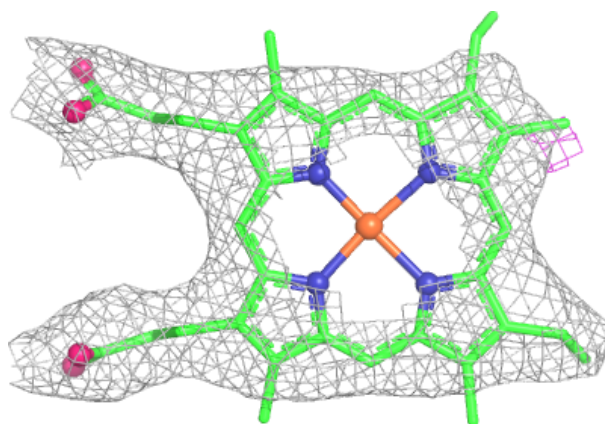
Electron density around CL6 H 602:

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



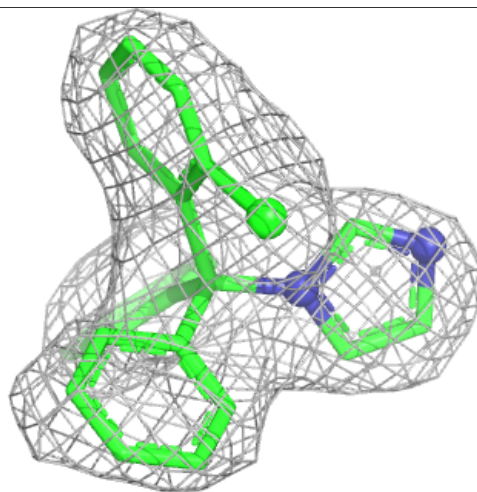
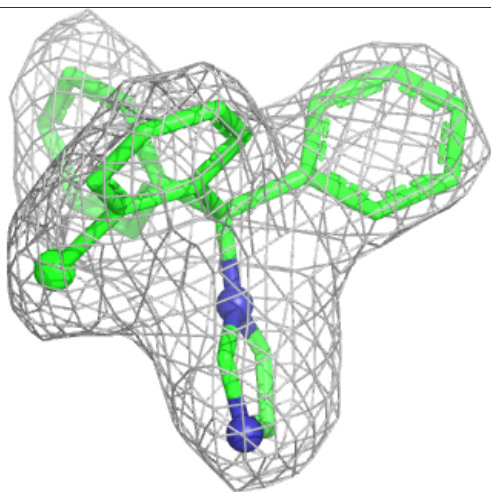
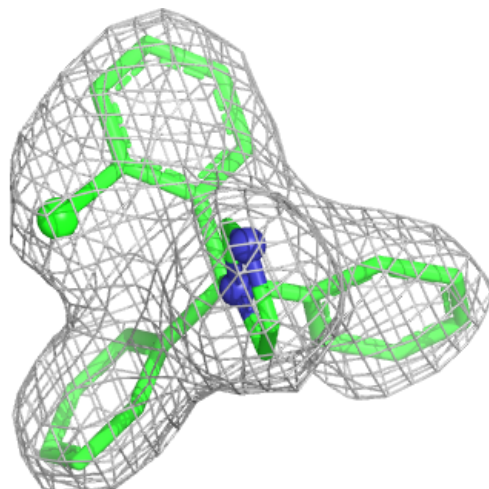
Electron density around HEM H 601:

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



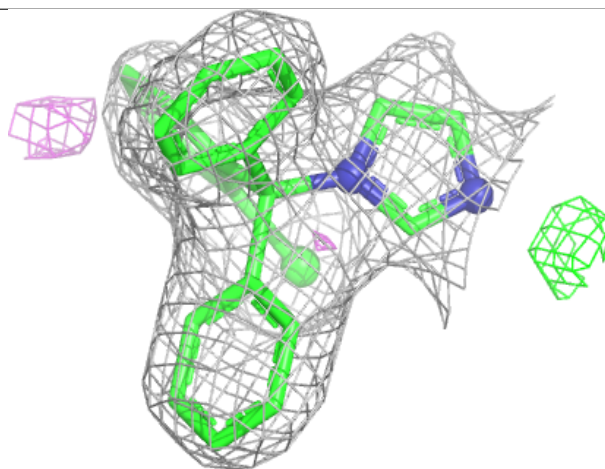
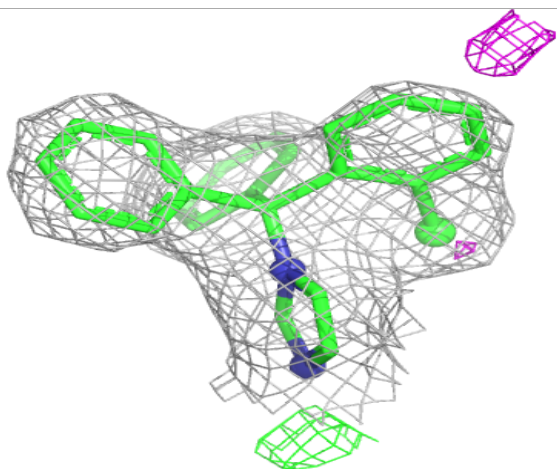
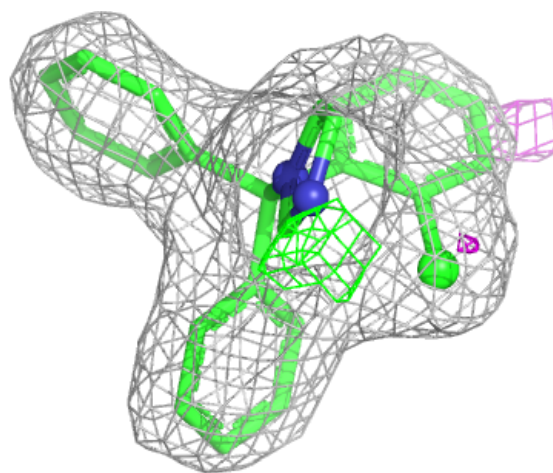
Electron density around CL6 E 603:

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



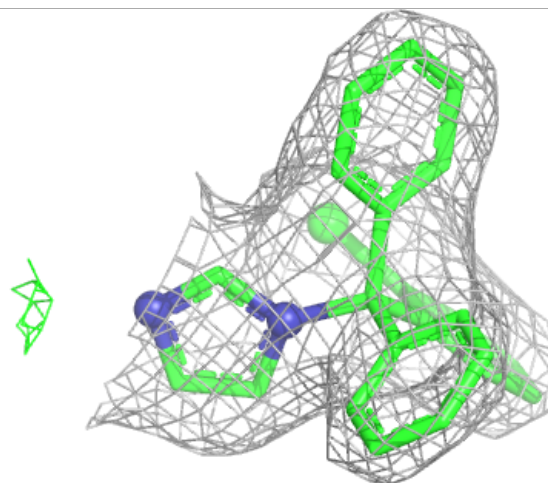
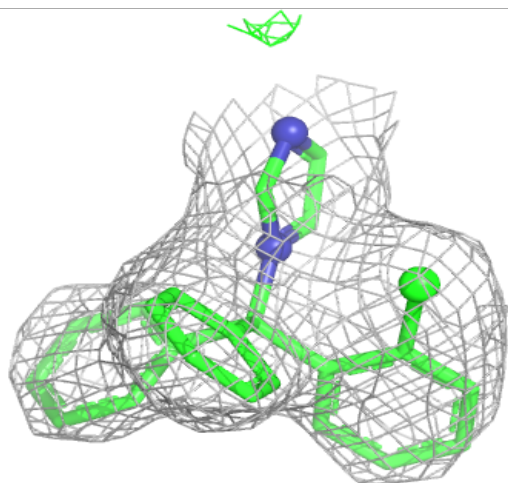
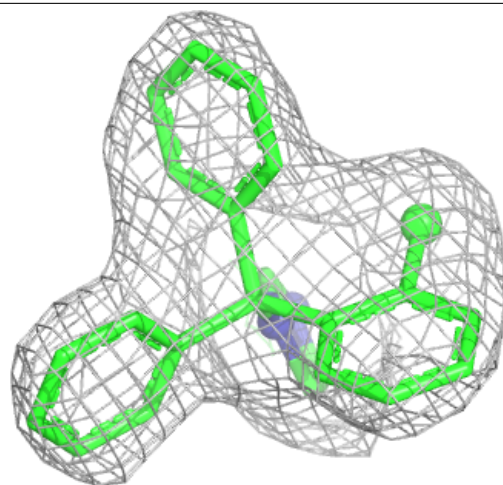
Electron density around CL6 B 602:

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



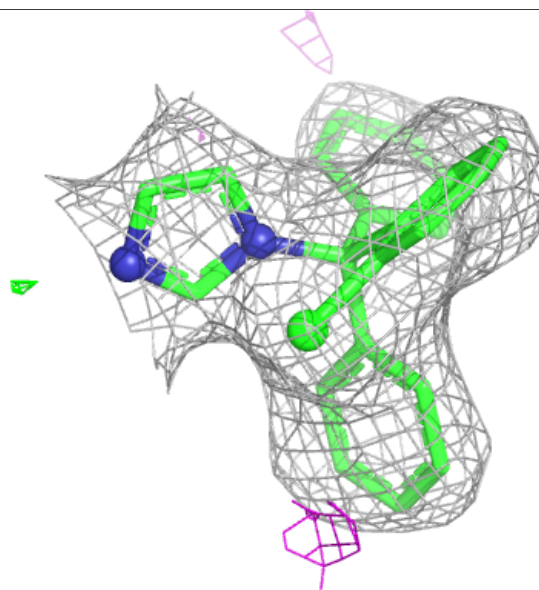
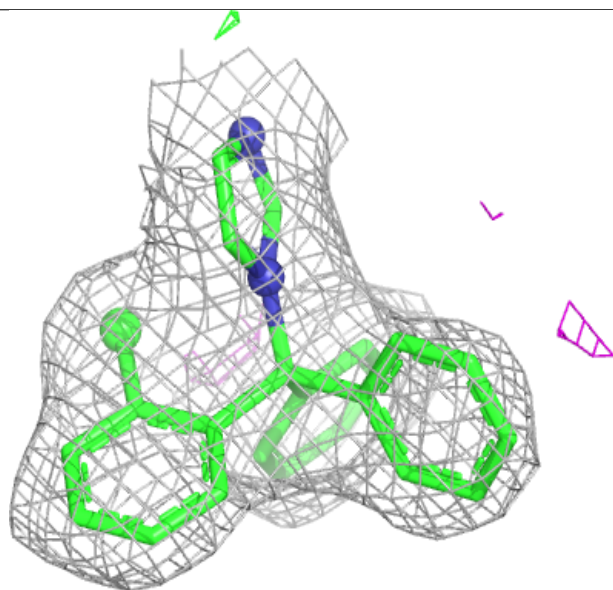
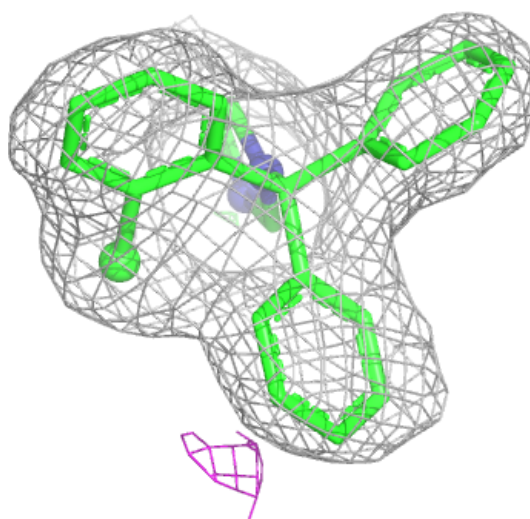
Electron density around CL6 G 602:

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



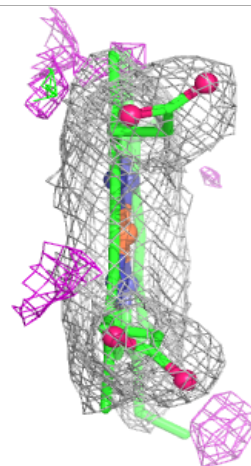
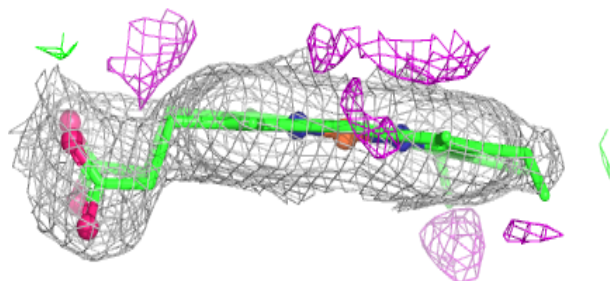
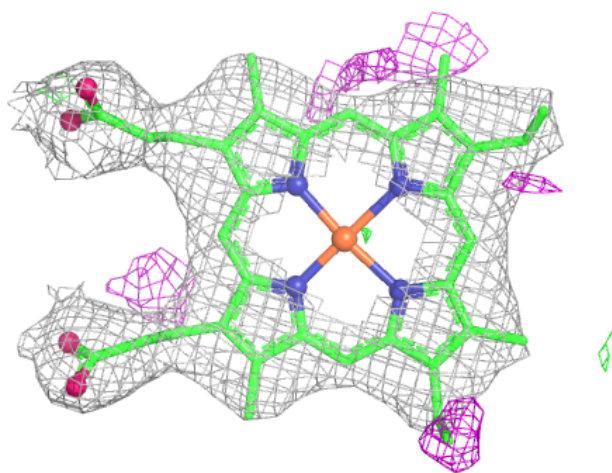
Electron density around CL6 A 602:

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



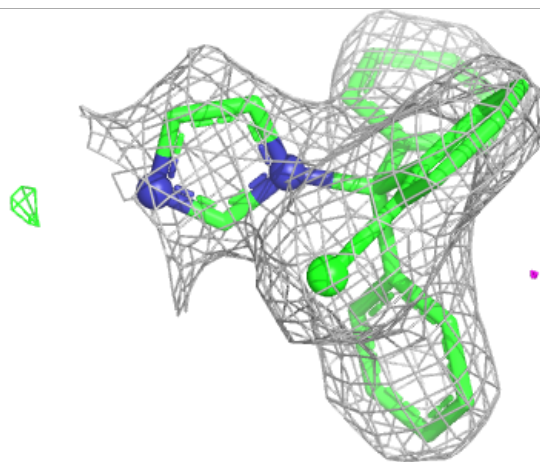
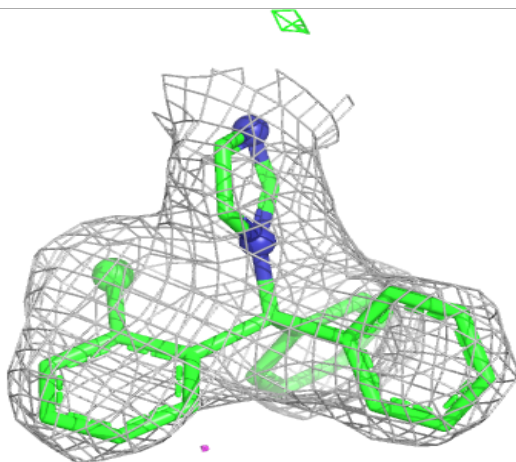
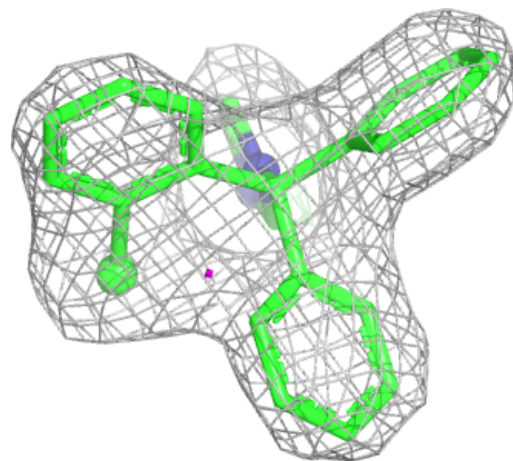
Electron density around HEM A 601:

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



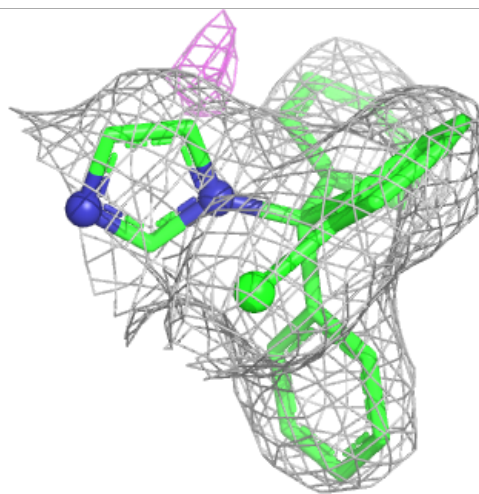
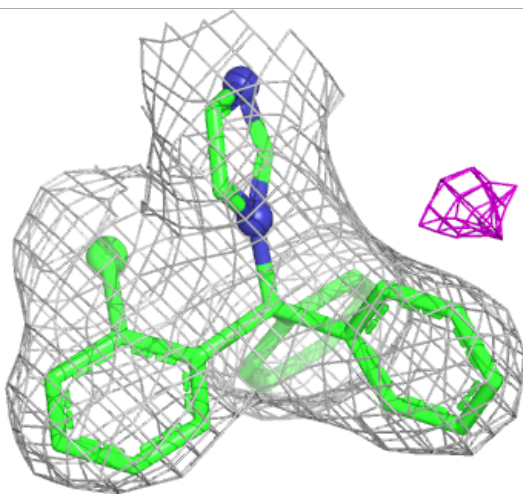
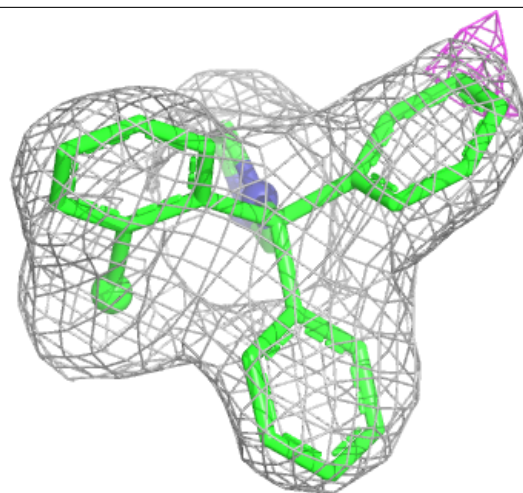
Electron density around CL6 D 602:

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



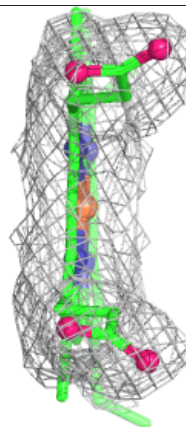
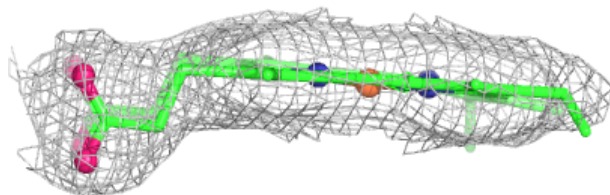
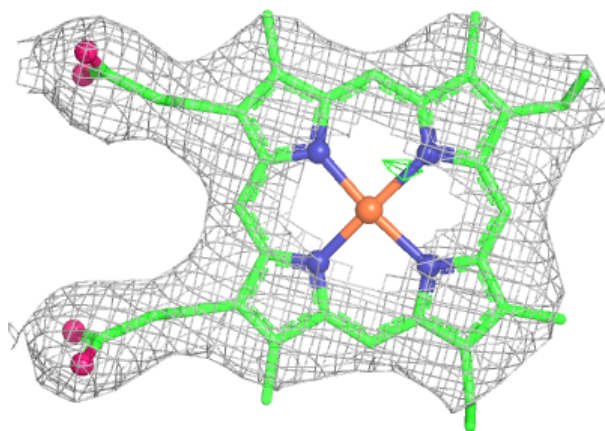
Electron density around CL6 C 602:

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



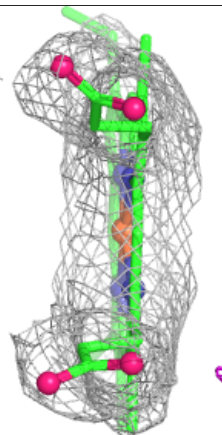
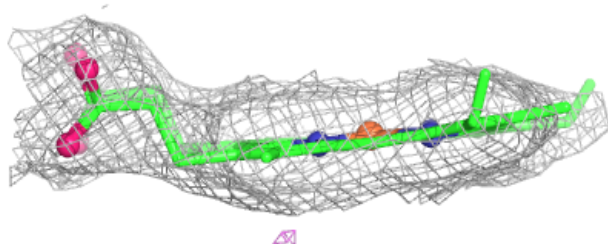
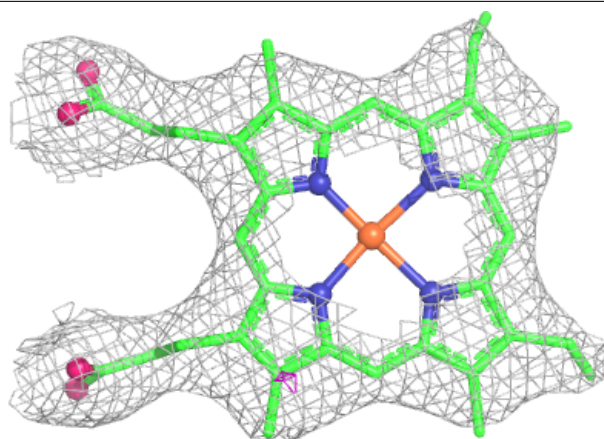
Electron density around HEM D 601:

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



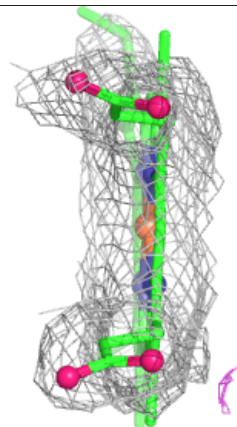
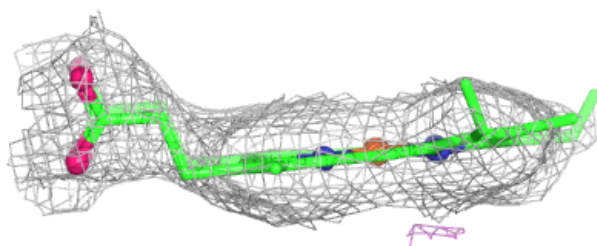
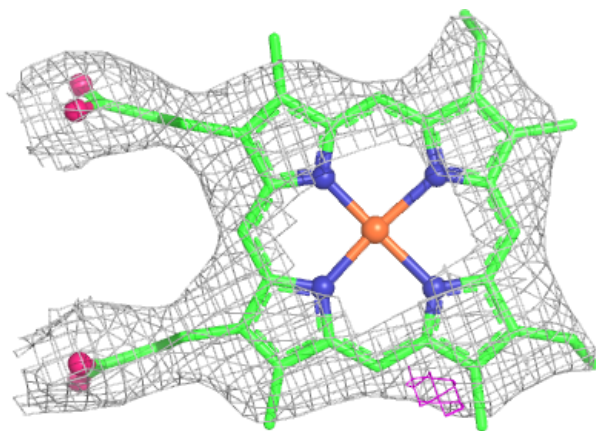
Electron density around HEM E 601:

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



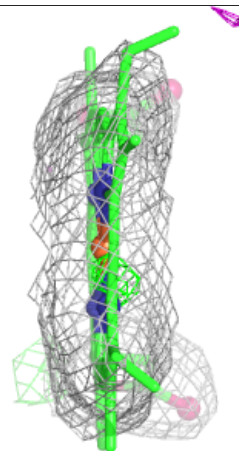
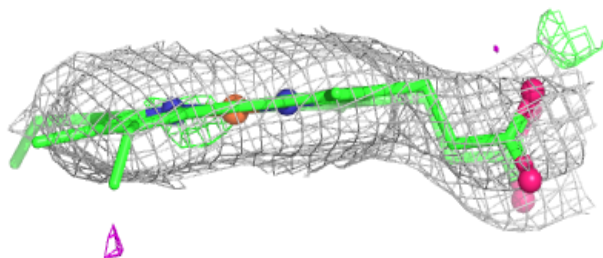
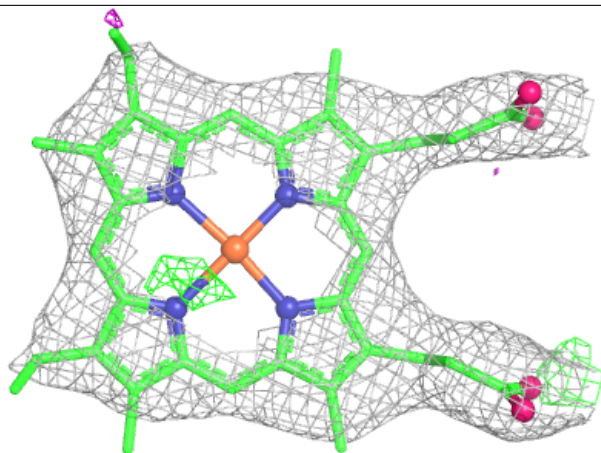
Electron density around HEM F 601:

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



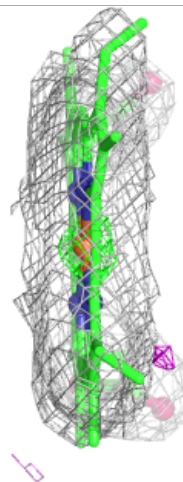
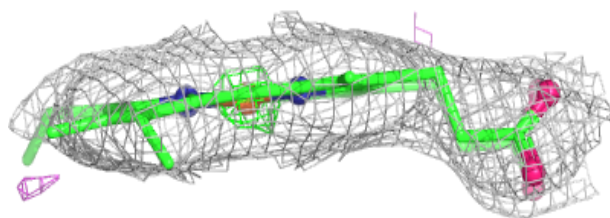
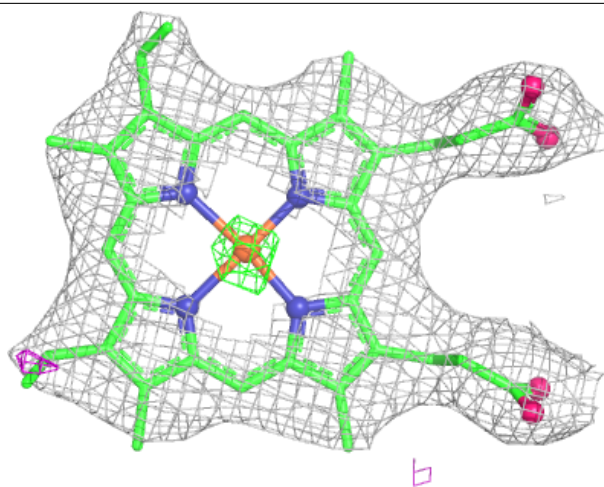
Electron density around HEM G 601:

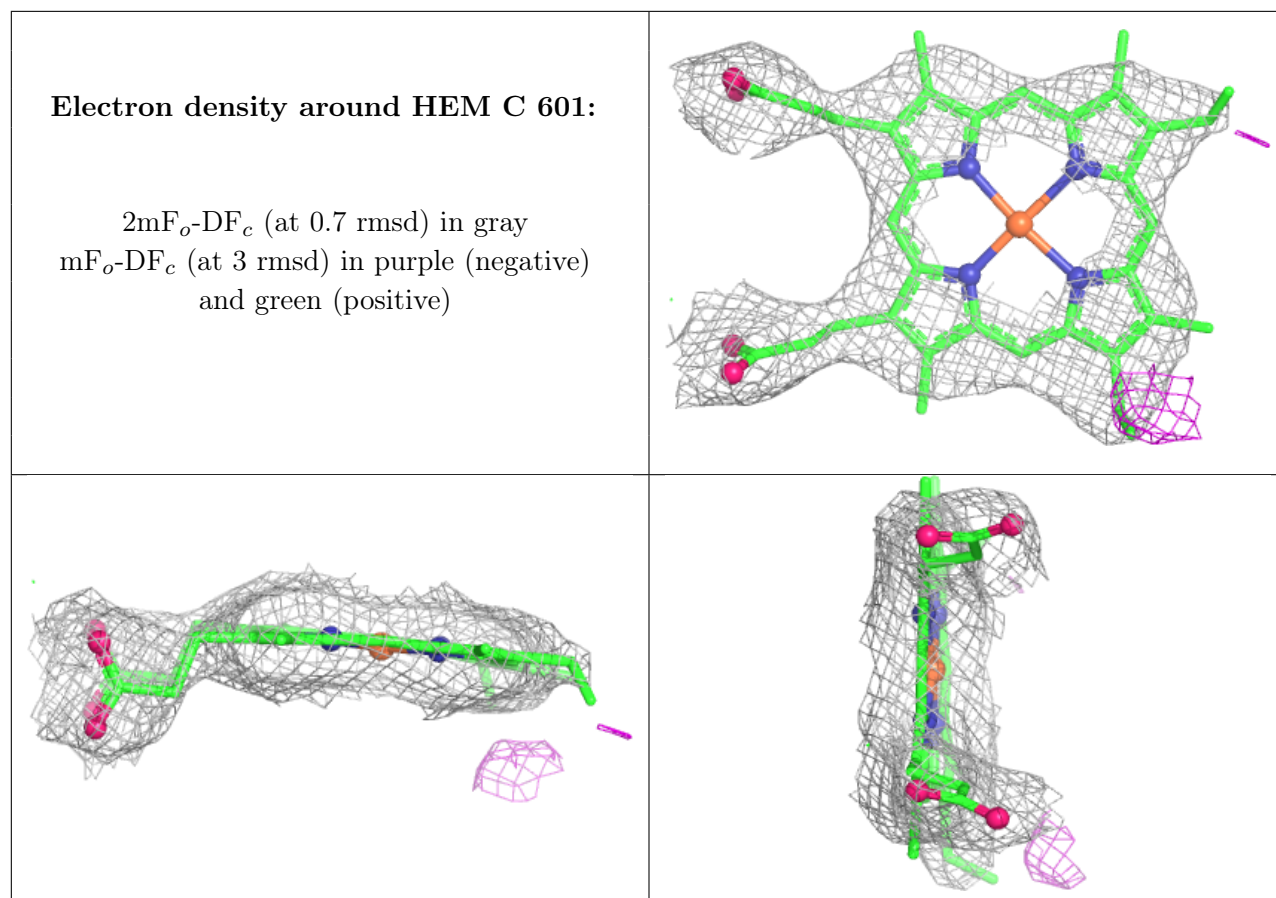
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.