



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 8, 2024 – 04:58 AM EDT

PDB ID : 4LMH  
Title : Crystal structure of the outer membrane decaheme cytochrome OmcA  
Authors : Edwards, M.J.; Baiden, N.; Clarke, T.A.  
Deposited on : 2013-07-10  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

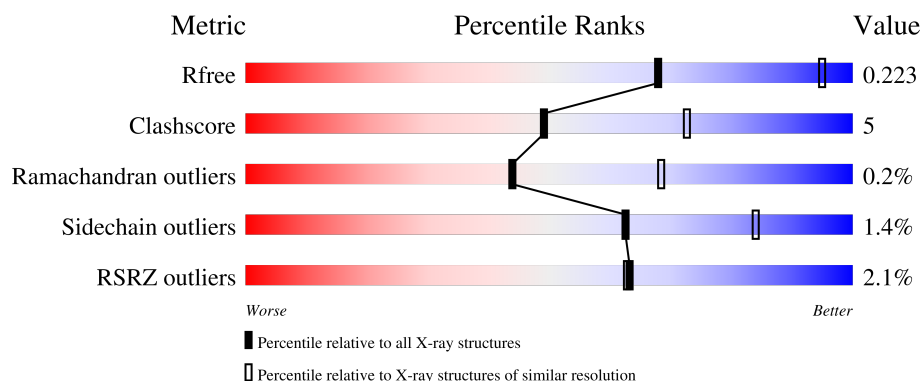
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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  $\geq 3$ , 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	760	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>9%</div> </div> </div>
1	B	760	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div> </div>
1	C	760	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	D	760	<div> <div>0%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	D	815	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24443 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 Extracellular iron oxide respiratory system surface decaheme cytochrome c component OmcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5222	3229	916	1047	30			
1	B	694	Total	C	N	O	S	0	0	0
			5231	3235	918	1048	30			
1	C	692	Total	C	N	O	S	0	0	0
			5215	3224	915	1046	30			
1	D	695	Total	C	N	O	S	0	0	0
			5235	3237	919	1049	30			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	initiating methionine	UNP Q8EG33
A	7	LYS	-	expression tag	UNP Q8EG33
A	8	PHE	-	expression tag	UNP Q8EG33
A	9	LYS	-	expression tag	UNP Q8EG33
A	10	LEU	-	expression tag	UNP Q8EG33
A	11	ASN	-	expression tag	UNP Q8EG33
A	12	LEU	-	expression tag	UNP Q8EG33
A	13	ILE	-	expression tag	UNP Q8EG33
A	14	THR	-	expression tag	UNP Q8EG33
A	15	LEU	-	expression tag	UNP Q8EG33
A	16	ALA	-	expression tag	UNP Q8EG33
A	17	LEU	-	expression tag	UNP Q8EG33
A	18	LEU	-	expression tag	UNP Q8EG33
A	19	ALA	-	expression tag	UNP Q8EG33
A	20	ASN	-	expression tag	UNP Q8EG33
A	21	THR	-	expression tag	UNP Q8EG33
A	22	GLY	-	expression tag	UNP Q8EG33
A	23	LEU	-	expression tag	UNP Q8EG33
A	24	ALA	-	expression tag	UNP Q8EG33
A	25	VAL	-	expression tag	UNP Q8EG33

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	-	expression tag	UNP Q8EG33
A	27	ALA	-	expression tag	UNP Q8EG33
A	736	LYS	-	expression tag	UNP Q8EG33
A	737	GLY	-	expression tag	UNP Q8EG33
A	738	GLU	-	expression tag	UNP Q8EG33
A	739	LEU	-	expression tag	UNP Q8EG33
A	740	LYS	-	expression tag	UNP Q8EG33
A	741	LEU	-	expression tag	UNP Q8EG33
A	742	GLU	-	expression tag	UNP Q8EG33
A	743	GLY	-	expression tag	UNP Q8EG33
A	744	LYS	-	expression tag	UNP Q8EG33
A	745	PRO	-	expression tag	UNP Q8EG33
A	746	ILE	-	expression tag	UNP Q8EG33
A	747	PRO	-	expression tag	UNP Q8EG33
A	748	ASN	-	expression tag	UNP Q8EG33
A	749	PRO	-	expression tag	UNP Q8EG33
A	750	LEU	-	expression tag	UNP Q8EG33
A	751	LEU	-	expression tag	UNP Q8EG33
A	752	GLY	-	expression tag	UNP Q8EG33
A	753	LEU	-	expression tag	UNP Q8EG33
A	754	ASP	-	expression tag	UNP Q8EG33
A	755	SER	-	expression tag	UNP Q8EG33
A	756	THR	-	expression tag	UNP Q8EG33
A	757	ARG	-	expression tag	UNP Q8EG33
A	758	THR	-	expression tag	UNP Q8EG33
A	759	GLY	-	expression tag	UNP Q8EG33
A	760	HIS	-	expression tag	UNP Q8EG33
A	761	HIS	-	expression tag	UNP Q8EG33
A	762	HIS	-	expression tag	UNP Q8EG33
A	763	HIS	-	expression tag	UNP Q8EG33
A	764	HIS	-	expression tag	UNP Q8EG33
A	765	HIS	-	expression tag	UNP Q8EG33
B	6	MET	-	initiating methionine	UNP Q8EG33
B	7	LYS	-	expression tag	UNP Q8EG33
B	8	PHE	-	expression tag	UNP Q8EG33
B	9	LYS	-	expression tag	UNP Q8EG33
B	10	LEU	-	expression tag	UNP Q8EG33
B	11	ASN	-	expression tag	UNP Q8EG33
B	12	LEU	-	expression tag	UNP Q8EG33
B	13	ILE	-	expression tag	UNP Q8EG33
B	14	THR	-	expression tag	UNP Q8EG33
B	15	LEU	-	expression tag	UNP Q8EG33

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	ALA	-	expression tag	UNP Q8EG33
B	17	LEU	-	expression tag	UNP Q8EG33
B	18	LEU	-	expression tag	UNP Q8EG33
B	19	ALA	-	expression tag	UNP Q8EG33
B	20	ASN	-	expression tag	UNP Q8EG33
B	21	THR	-	expression tag	UNP Q8EG33
B	22	GLY	-	expression tag	UNP Q8EG33
B	23	LEU	-	expression tag	UNP Q8EG33
B	24	ALA	-	expression tag	UNP Q8EG33
B	25	VAL	-	expression tag	UNP Q8EG33
B	26	ALA	-	expression tag	UNP Q8EG33
B	27	ALA	-	expression tag	UNP Q8EG33
B	736	LYS	-	expression tag	UNP Q8EG33
B	737	GLY	-	expression tag	UNP Q8EG33
B	738	GLU	-	expression tag	UNP Q8EG33
B	739	LEU	-	expression tag	UNP Q8EG33
B	740	LYS	-	expression tag	UNP Q8EG33
B	741	LEU	-	expression tag	UNP Q8EG33
B	742	GLU	-	expression tag	UNP Q8EG33
B	743	GLY	-	expression tag	UNP Q8EG33
B	744	LYS	-	expression tag	UNP Q8EG33
B	745	PRO	-	expression tag	UNP Q8EG33
B	746	ILE	-	expression tag	UNP Q8EG33
B	747	PRO	-	expression tag	UNP Q8EG33
B	748	ASN	-	expression tag	UNP Q8EG33
B	749	PRO	-	expression tag	UNP Q8EG33
B	750	LEU	-	expression tag	UNP Q8EG33
B	751	LEU	-	expression tag	UNP Q8EG33
B	752	GLY	-	expression tag	UNP Q8EG33
B	753	LEU	-	expression tag	UNP Q8EG33
B	754	ASP	-	expression tag	UNP Q8EG33
B	755	SER	-	expression tag	UNP Q8EG33
B	756	THR	-	expression tag	UNP Q8EG33
B	757	ARG	-	expression tag	UNP Q8EG33
B	758	THR	-	expression tag	UNP Q8EG33
B	759	GLY	-	expression tag	UNP Q8EG33
B	760	HIS	-	expression tag	UNP Q8EG33
B	761	HIS	-	expression tag	UNP Q8EG33
B	762	HIS	-	expression tag	UNP Q8EG33
B	763	HIS	-	expression tag	UNP Q8EG33
B	764	HIS	-	expression tag	UNP Q8EG33
B	765	HIS	-	expression tag	UNP Q8EG33

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	MET	-	initiating methionine	UNP Q8EG33
C	7	LYS	-	expression tag	UNP Q8EG33
C	8	PHE	-	expression tag	UNP Q8EG33
C	9	LYS	-	expression tag	UNP Q8EG33
C	10	LEU	-	expression tag	UNP Q8EG33
C	11	ASN	-	expression tag	UNP Q8EG33
C	12	LEU	-	expression tag	UNP Q8EG33
C	13	ILE	-	expression tag	UNP Q8EG33
C	14	THR	-	expression tag	UNP Q8EG33
C	15	LEU	-	expression tag	UNP Q8EG33
C	16	ALA	-	expression tag	UNP Q8EG33
C	17	LEU	-	expression tag	UNP Q8EG33
C	18	LEU	-	expression tag	UNP Q8EG33
C	19	ALA	-	expression tag	UNP Q8EG33
C	20	ASN	-	expression tag	UNP Q8EG33
C	21	THR	-	expression tag	UNP Q8EG33
C	22	GLY	-	expression tag	UNP Q8EG33
C	23	LEU	-	expression tag	UNP Q8EG33
C	24	ALA	-	expression tag	UNP Q8EG33
C	25	VAL	-	expression tag	UNP Q8EG33
C	26	ALA	-	expression tag	UNP Q8EG33
C	27	ALA	-	expression tag	UNP Q8EG33
C	736	LYS	-	expression tag	UNP Q8EG33
C	737	GLY	-	expression tag	UNP Q8EG33
C	738	GLU	-	expression tag	UNP Q8EG33
C	739	LEU	-	expression tag	UNP Q8EG33
C	740	LYS	-	expression tag	UNP Q8EG33
C	741	LEU	-	expression tag	UNP Q8EG33
C	742	GLU	-	expression tag	UNP Q8EG33
C	743	GLY	-	expression tag	UNP Q8EG33
C	744	LYS	-	expression tag	UNP Q8EG33
C	745	PRO	-	expression tag	UNP Q8EG33
C	746	ILE	-	expression tag	UNP Q8EG33
C	747	PRO	-	expression tag	UNP Q8EG33
C	748	ASN	-	expression tag	UNP Q8EG33
C	749	PRO	-	expression tag	UNP Q8EG33
C	750	LEU	-	expression tag	UNP Q8EG33
C	751	LEU	-	expression tag	UNP Q8EG33
C	752	GLY	-	expression tag	UNP Q8EG33
C	753	LEU	-	expression tag	UNP Q8EG33
C	754	ASP	-	expression tag	UNP Q8EG33
C	755	SER	-	expression tag	UNP Q8EG33

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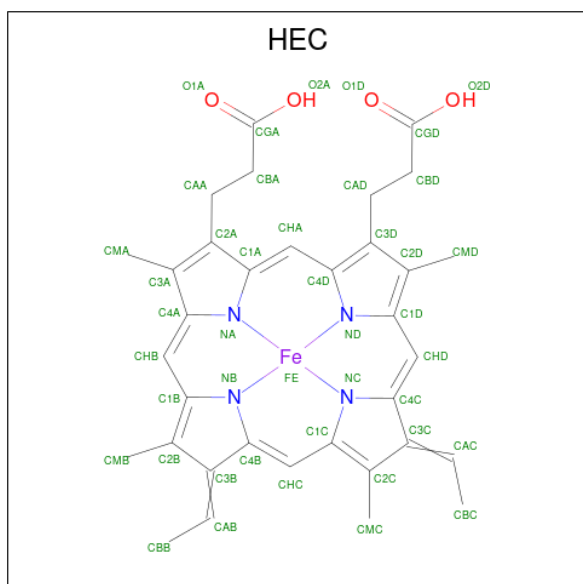
Chain	Residue	Modelled	Actual	Comment	Reference
C	756	THR	-	expression tag	UNP Q8EG33
C	757	ARG	-	expression tag	UNP Q8EG33
C	758	THR	-	expression tag	UNP Q8EG33
C	759	GLY	-	expression tag	UNP Q8EG33
C	760	HIS	-	expression tag	UNP Q8EG33
C	761	HIS	-	expression tag	UNP Q8EG33
C	762	HIS	-	expression tag	UNP Q8EG33
C	763	HIS	-	expression tag	UNP Q8EG33
C	764	HIS	-	expression tag	UNP Q8EG33
C	765	HIS	-	expression tag	UNP Q8EG33
D	6	MET	-	initiating methionine	UNP Q8EG33
D	7	LYS	-	expression tag	UNP Q8EG33
D	8	PHE	-	expression tag	UNP Q8EG33
D	9	LYS	-	expression tag	UNP Q8EG33
D	10	LEU	-	expression tag	UNP Q8EG33
D	11	ASN	-	expression tag	UNP Q8EG33
D	12	LEU	-	expression tag	UNP Q8EG33
D	13	ILE	-	expression tag	UNP Q8EG33
D	14	THR	-	expression tag	UNP Q8EG33
D	15	LEU	-	expression tag	UNP Q8EG33
D	16	ALA	-	expression tag	UNP Q8EG33
D	17	LEU	-	expression tag	UNP Q8EG33
D	18	LEU	-	expression tag	UNP Q8EG33
D	19	ALA	-	expression tag	UNP Q8EG33
D	20	ASN	-	expression tag	UNP Q8EG33
D	21	THR	-	expression tag	UNP Q8EG33
D	22	GLY	-	expression tag	UNP Q8EG33
D	23	LEU	-	expression tag	UNP Q8EG33
D	24	ALA	-	expression tag	UNP Q8EG33
D	25	VAL	-	expression tag	UNP Q8EG33
D	26	ALA	-	expression tag	UNP Q8EG33
D	27	ALA	-	expression tag	UNP Q8EG33
D	736	LYS	-	expression tag	UNP Q8EG33
D	737	GLY	-	expression tag	UNP Q8EG33
D	738	GLU	-	expression tag	UNP Q8EG33
D	739	LEU	-	expression tag	UNP Q8EG33
D	740	LYS	-	expression tag	UNP Q8EG33
D	741	LEU	-	expression tag	UNP Q8EG33
D	742	GLU	-	expression tag	UNP Q8EG33
D	743	GLY	-	expression tag	UNP Q8EG33
D	744	LYS	-	expression tag	UNP Q8EG33
D	745	PRO	-	expression tag	UNP Q8EG33

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Chain	Residue	Modelled	Actual	Comment	Reference
D	746	ILE	-	expression tag	UNP Q8EG33
D	747	PRO	-	expression tag	UNP Q8EG33
D	748	ASN	-	expression tag	UNP Q8EG33
D	749	PRO	-	expression tag	UNP Q8EG33
D	750	LEU	-	expression tag	UNP Q8EG33
D	751	LEU	-	expression tag	UNP Q8EG33
D	752	GLY	-	expression tag	UNP Q8EG33
D	753	LEU	-	expression tag	UNP Q8EG33
D	754	ASP	-	expression tag	UNP Q8EG33
D	755	SER	-	expression tag	UNP Q8EG33
D	756	THR	-	expression tag	UNP Q8EG33
D	757	ARG	-	expression tag	UNP Q8EG33
D	758	THR	-	expression tag	UNP Q8EG33
D	759	GLY	-	expression tag	UNP Q8EG33
D	760	HIS	-	expression tag	UNP Q8EG33
D	761	HIS	-	expression tag	UNP Q8EG33
D	762	HIS	-	expression tag	UNP Q8EG33
D	763	HIS	-	expression tag	UNP Q8EG33
D	764	HIS	-	expression tag	UNP Q8EG33
D	765	HIS	-	expression tag	UNP Q8EG33

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	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	C	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	C	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	C	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	D	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	D	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	D	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	D	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	D	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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

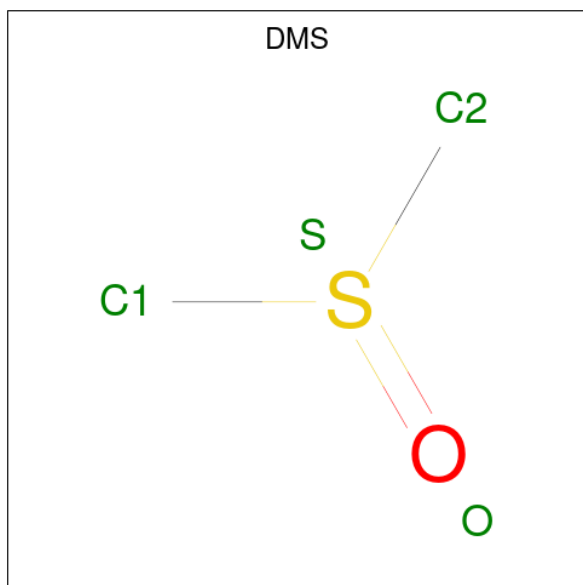
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0

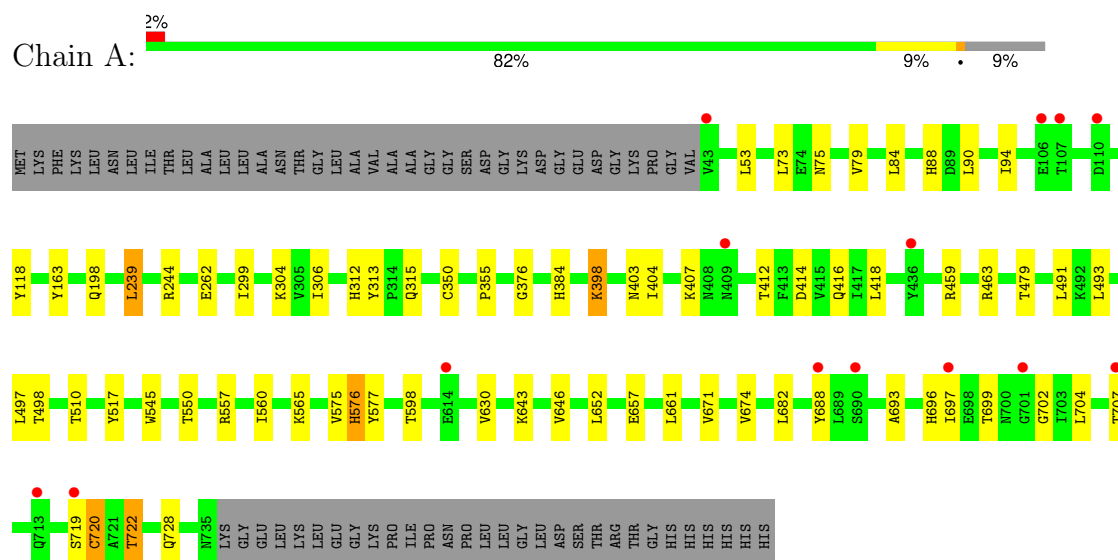
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	397	Total O 397 397	0	0
5	B	420	Total O 420 420	0	0
5	C	380	Total O 380 380	0	0
5	D	551	Total O 551 551	0	0

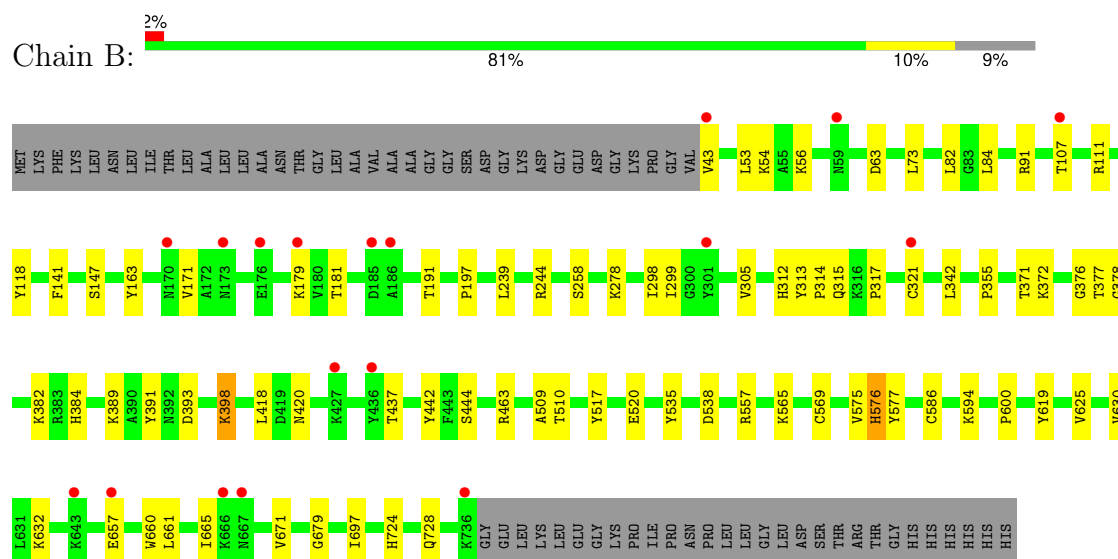
### 3 Residue-property plots [i](#)

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

- Molecule 1: Extracellular iron oxide respiratory system surface decaheme cytochrome c component OmcA



- Molecule 1: Extracellular iron oxide respiratory system surface decaheme cytochrome c component OmcA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.64Å 245.38Å 135.63Å 90.00° 97.89° 90.00°	Depositor
Resolution (Å)	50.97 – 2.70 50.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.97-2.70) 98.4 (50.97-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.193 , 0.230 0.186 , 0.223	Depositor DCC
$R_{free}$ test set	8083 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEC, DMS, CA

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	0.27	0/5337	0.44	0/7254
1	B	0.27	0/5346	0.44	0/7265
1	C	0.27	0/5330	0.43	0/7244
1	D	0.28	0/5350	0.44	0/7270
All	All	0.27	0/21363	0.44	0/29033

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	5222	0	4957	50	0
1	B	5231	0	4971	59	0
1	C	5215	0	4948	48	0
1	D	5235	0	4974	47	0
2	A	430	0	301	24	0
2	B	430	0	302	35	0
2	C	430	0	301	17	0
2	D	430	0	302	28	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	16	0	24	3	0
4	B	16	0	24	1	0
4	C	16	0	24	2	0
4	D	16	0	24	1	0
5	A	397	0	0	5	0
5	B	420	0	0	2	0
5	C	380	0	0	2	0
5	D	551	0	0	0	0
All	All	24443	0	21152	222	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 5.

The worst 5 of 222 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:D:253:CYS:SG	2:D:802:HEC:HAC	1.35	1.63
1:D:350:CYS:SG	2:D:804:HEC:HAC	1.53	1.47
1:C:350:CYS:SG	2:C:804:HEC:HAC	1.56	1.44
1:A:350:CYS:SG	2:A:804:HEC:HAC	1.64	1.34
1:B:586:CYS:SG	2:B:908:HEC:HAC	1.70	1.25

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	691/760 (91%)	656 (95%)	34 (5%)	1 (0%)	48 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	692/760 (91%)	669 (97%)	22 (3%)	1 (0%)	48	73
1	C	690/760 (91%)	664 (96%)	24 (4%)	2 (0%)	37	61
1	D	693/760 (91%)	670 (97%)	22 (3%)	1 (0%)	48	73
All	All	2766/3040 (91%)	2659 (96%)	102 (4%)	5 (0%)	44	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	575	VAL
1	A	575	VAL
1	C	676	SER
1	D	575	VAL
1	C	575	VAL

### 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	558/609 (92%)	547 (98%)	11 (2%)	50	78
1	B	559/609 (92%)	550 (98%)	9 (2%)	58	82
1	C	557/609 (92%)	552 (99%)	5 (1%)	75	90
1	D	559/609 (92%)	553 (99%)	6 (1%)	70	87
All	All	2233/2436 (92%)	2202 (99%)	31 (1%)	62	84

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	191	THR
1	D	288	THR
1	B	420	ASN
1	D	576	HIS
1	C	728	GLN

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

Mol	Chain	Res	Type
1	C	70	ASN
1	C	735	ASN
1	D	735	ASN
1	A	713	GLN
1	A	77	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 ⓘ

Of 64 ligands modelled in this entry, 8 are monoatomic - leaving 56 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	DMS	C	813	-	3,3,3	2.70	1 (33%)	3,3,3	0.46	0
2	HEC	B	906	1	32,50,50	2.04	3 (9%)	30,82,82	2.06	4 (13%)
2	HEC	D	801	1	32,50,50	2.07	3 (9%)	30,82,82	2.10	4 (13%)
2	HEC	C	807	1	32,50,50	2.01	3 (9%)	30,82,82	2.12	4 (13%)
2	HEC	D	808	1	32,50,50	2.02	4 (12%)	30,82,82	2.20	6 (20%)
4	DMS	B	901	-	3,3,3	2.71	1 (33%)	3,3,3	0.39	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	A	816	-	3,3,3	2.72	1 (33%)	3,3,3	0.37	0
2	HEC	A	808	1	32,50,50	2.08	3 (9%)	30,82,82	2.26	6 (20%)
4	DMS	D	816	-	3,3,3	2.74	1 (33%)	3,3,3	0.62	0
2	HEC	B	909	1	32,50,50	2.05	3 (9%)	30,82,82	2.23	5 (16%)
2	HEC	C	801	1	32,50,50	2.10	3 (9%)	30,82,82	2.11	6 (20%)
4	DMS	D	814	-	3,3,3	2.66	1 (33%)	3,3,3	0.43	0
2	HEC	C	805	1	32,50,50	2.02	3 (9%)	30,82,82	2.06	5 (16%)
2	HEC	B	904	1	32,50,50	1.92	4 (12%)	30,82,82	1.97	4 (13%)
4	DMS	D	815	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
2	HEC	A	802	3,1	32,50,50	2.02	3 (9%)	30,82,82	1.87	4 (13%)
2	HEC	D	806	1	32,50,50	2.05	3 (9%)	30,82,82	2.31	7 (23%)
2	HEC	D	804	1	32,50,50	2.08	3 (9%)	30,82,82	2.07	5 (16%)
2	HEC	C	809	1	32,50,50	2.05	3 (9%)	30,82,82	2.22	7 (23%)
2	HEC	A	809	1	32,50,50	2.06	3 (9%)	30,82,82	2.33	6 (20%)
4	DMS	A	814	-	3,3,3	2.71	1 (33%)	3,3,3	0.53	0
2	HEC	B	905	1	32,50,50	2.02	3 (9%)	30,82,82	2.04	6 (20%)
2	HEC	B	910	1	32,50,50	2.05	3 (9%)	30,82,82	2.30	6 (20%)
2	HEC	A	804	1	32,50,50	2.05	3 (9%)	30,82,82	2.08	7 (23%)
2	HEC	C	810	1	32,50,50	2.07	3 (9%)	30,82,82	2.25	4 (13%)
2	HEC	A	810	1	32,50,50	2.07	3 (9%)	30,82,82	2.30	4 (13%)
2	HEC	B	911	1	32,50,50	2.03	3 (9%)	30,82,82	2.06	4 (13%)
2	HEC	D	802	3,1	32,50,50	2.06	3 (9%)	30,82,82	1.89	5 (16%)
2	HEC	B	903	3,1	32,50,50	2.02	3 (9%)	30,82,82	1.96	6 (20%)
2	HEC	D	803	1	32,50,50	2.05	3 (9%)	30,82,82	2.24	5 (16%)
4	DMS	B	914	-	3,3,3	2.72	1 (33%)	3,3,3	0.42	0
2	HEC	B	908	1	32,50,50	1.96	3 (9%)	30,82,82	2.17	5 (16%)
2	HEC	D	805	1	32,50,50	2.05	3 (9%)	30,82,82	2.14	5 (16%)
4	DMS	B	916	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
2	HEC	A	807	1	32,50,50	2.02	3 (9%)	30,82,82	2.02	3 (10%)
2	HEC	D	807	1	32,50,50	1.94	3 (9%)	30,82,82	2.09	5 (16%)
4	DMS	A	813	-	3,3,3	2.69	1 (33%)	3,3,3	0.48	0
4	DMS	D	813	-	3,3,3	2.71	1 (33%)	3,3,3	0.42	0
2	HEC	B	902	1	32,50,50	2.05	3 (9%)	30,82,82	2.09	4 (13%)
2	HEC	C	802	3,1	32,50,50	2.00	3 (9%)	30,82,82	1.97	4 (13%)
2	HEC	C	803	1	32,50,50	2.06	3 (9%)	30,82,82	2.11	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEC	A	803	1	32,50,50	2.05	3 (9%)	30,82,82	2.20	6 (20%)
2	HEC	D	810	1	32,50,50	2.09	3 (9%)	30,82,82	2.21	4 (13%)
4	DMS	B	915	-	3,3,3	2.74	1 (33%)	3,3,3	0.57	0
2	HEC	A	805	1	32,50,50	2.03	3 (9%)	30,82,82	2.26	7 (23%)
2	HEC	A	801	1	32,50,50	2.08	3 (9%)	30,82,82	2.18	7 (23%)
2	HEC	D	809	1	32,50,50	2.06	3 (9%)	30,82,82	2.20	6 (20%)
4	DMS	C	816	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
4	DMS	C	814	-	3,3,3	2.68	1 (33%)	3,3,3	0.47	0
4	DMS	C	815	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0
2	HEC	B	907	1	32,50,50	2.10	3 (9%)	30,82,82	2.34	7 (23%)
2	HEC	C	808	1	32,50,50	2.04	3 (9%)	30,82,82	2.29	5 (16%)
2	HEC	C	804	1	32,50,50	2.04	3 (9%)	30,82,82	1.98	5 (16%)
4	DMS	A	815	-	3,3,3	2.73	1 (33%)	3,3,3	0.53	0
2	HEC	C	806	1	32,50,50	2.03	3 (9%)	30,82,82	2.27	7 (23%)
2	HEC	A	806	1	32,50,50	2.06	3 (9%)	30,82,82	2.33	7 (23%)

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
2	HEC	B	906	1	-	2/10/54/54	-
2	HEC	D	801	1	-	0/10/54/54	-
2	HEC	C	807	1	-	5/10/54/54	-
2	HEC	D	808	1	-	1/10/54/54	-
2	HEC	A	808	1	-	1/10/54/54	-
2	HEC	B	909	1	-	0/10/54/54	-
2	HEC	C	801	1	-	0/10/54/54	-
2	HEC	C	805	1	-	2/10/54/54	-
2	HEC	B	904	1	-	0/10/54/54	-
2	HEC	A	802	3,1	-	0/10/54/54	-
2	HEC	D	806	1	-	3/10/54/54	-
2	HEC	D	804	1	-	6/10/54/54	-
2	HEC	C	809	1	-	1/10/54/54	-
2	HEC	A	809	1	-	0/10/54/54	-
2	HEC	B	905	1	-	4/10/54/54	-
2	HEC	B	910	1	-	0/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	804	1	-	3/10/54/54	-
2	HEC	C	810	1	-	3/10/54/54	-
2	HEC	A	810	1	-	3/10/54/54	-
2	HEC	B	911	1	-	3/10/54/54	-
2	HEC	D	802	3,1	-	0/10/54/54	-
2	HEC	B	903	3,1	-	0/10/54/54	-
2	HEC	D	803	1	-	0/10/54/54	-
2	HEC	B	908	1	-	3/10/54/54	-
2	HEC	D	805	1	-	0/10/54/54	-
2	HEC	A	807	1	-	7/10/54/54	-
2	HEC	D	807	1	-	5/10/54/54	-
2	HEC	B	902	1	-	0/10/54/54	-
2	HEC	C	802	3,1	-	0/10/54/54	-
2	HEC	C	803	1	-	0/10/54/54	-
2	HEC	A	803	1	-	0/10/54/54	-
2	HEC	D	810	1	-	5/10/54/54	-
2	HEC	A	805	1	-	2/10/54/54	-
2	HEC	A	801	1	-	0/10/54/54	-
2	HEC	D	809	1	-	0/10/54/54	-
2	HEC	B	907	1	-	1/10/54/54	-
2	HEC	C	808	1	-	0/10/54/54	-
2	HEC	C	804	1	-	6/10/54/54	-
2	HEC	C	806	1	-	3/10/54/54	-
2	HEC	A	806	1	-	1/10/54/54	-

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	907	HEC	C2B-C3B	-5.96	1.34	1.40
2	A	805	HEC	C2B-C3B	-5.78	1.34	1.40
2	D	810	HEC	C2B-C3B	-5.77	1.34	1.40
2	B	902	HEC	C3C-C2C	-5.75	1.34	1.40
2	D	802	HEC	C2B-C3B	-5.73	1.34	1.40

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	907	HEC	CBB-CAB-C3B	-7.83	109.17	127.49
2	D	810	HEC	CBB-CAB-C3B	-7.64	109.61	127.49
2	A	810	HEC	CBC-CAC-C3C	-7.61	109.69	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	803	HEC	CBC-CAC-C3C	-7.54	109.84	127.49
2	C	810	HEC	CBC-CAC-C3C	-7.44	110.09	127.49

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	905	HEC	C3D-CAD-CBD-CGD
2	B	911	HEC	C2D-C3D-CAD-CBD
2	B	911	HEC	C4D-C3D-CAD-CBD
2	B	911	HEC	C3D-CAD-CBD-CGD
2	C	804	HEC	C3D-CAD-CBD-CGD

There are no ring outliers.

42 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	906	HEC	4	0
2	D	801	HEC	1	0
2	C	807	HEC	4	0
2	D	808	HEC	2	0
4	A	816	DMS	1	0
2	A	808	HEC	3	0
2	B	909	HEC	3	0
2	C	801	HEC	2	0
2	B	904	HEC	4	0
2	A	802	HEC	5	0
2	D	806	HEC	3	0
2	D	804	HEC	2	0
2	C	809	HEC	1	0
4	A	814	DMS	2	0
2	B	905	HEC	4	0
2	B	910	HEC	1	0
2	A	804	HEC	5	0
2	C	810	HEC	1	0
2	A	810	HEC	1	0
2	B	911	HEC	2	0
2	D	802	HEC	7	0
2	B	903	HEC	7	0
2	D	803	HEC	2	0
2	B	908	HEC	7	0

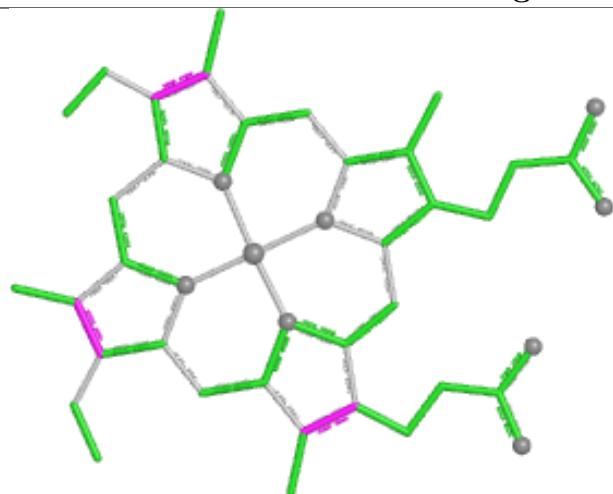
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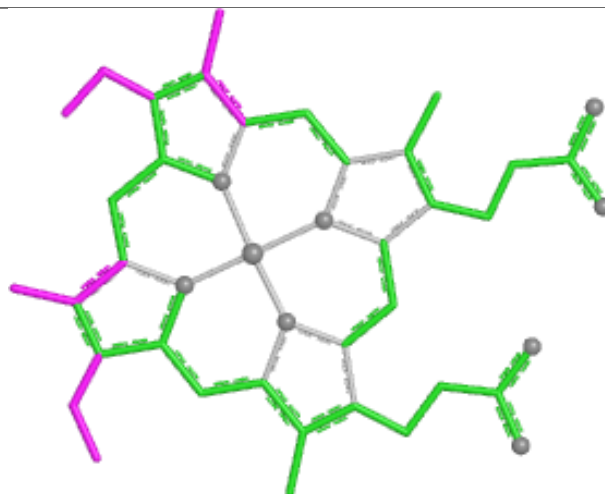
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	805	HEC	3	0
2	A	807	HEC	4	0
2	D	807	HEC	5	0
4	D	813	DMS	1	0
2	B	902	HEC	3	0
2	C	802	HEC	5	0
2	C	803	HEC	1	0
2	A	803	HEC	2	0
2	D	810	HEC	2	0
4	B	915	DMS	1	0
2	A	805	HEC	1	0
2	A	801	HEC	1	0
2	D	809	HEC	1	0
4	C	815	DMS	2	0
2	B	907	HEC	4	0
2	C	804	HEC	2	0
2	C	806	HEC	2	0
2	A	806	HEC	3	0

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

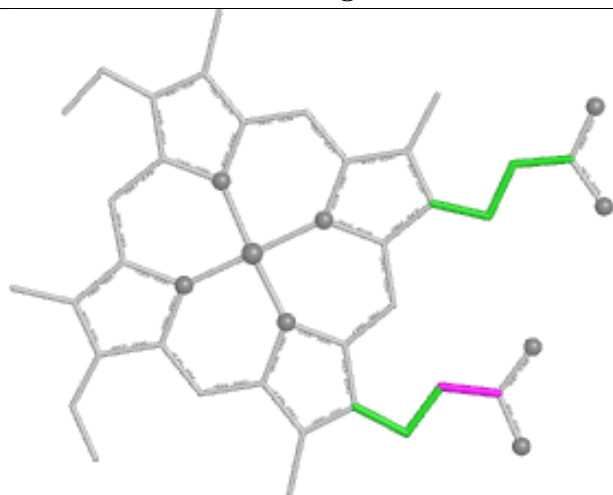
## Ligand HEC B 906



Bond lengths



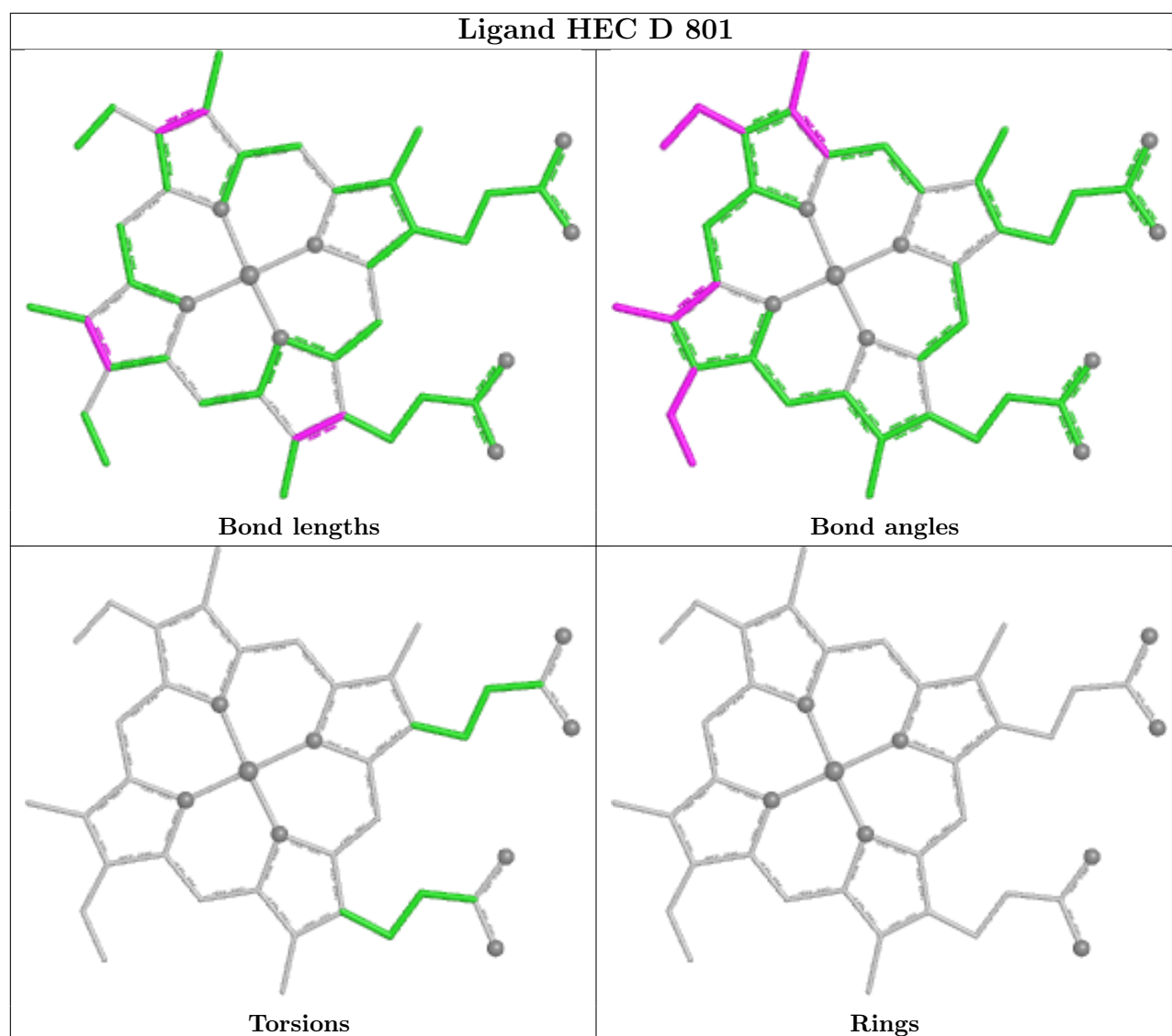
Bond angles



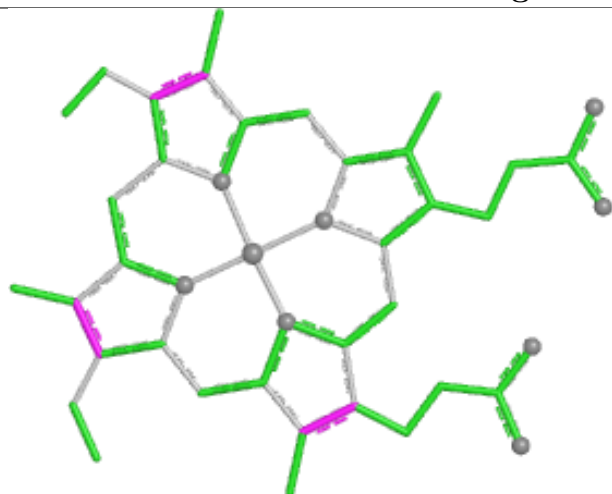
Torsions



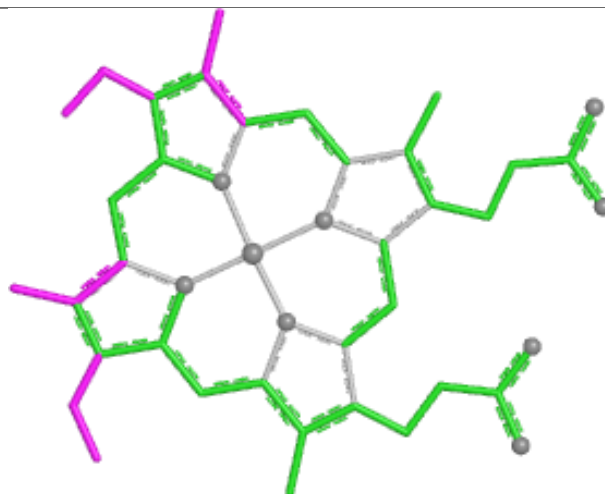
Rings



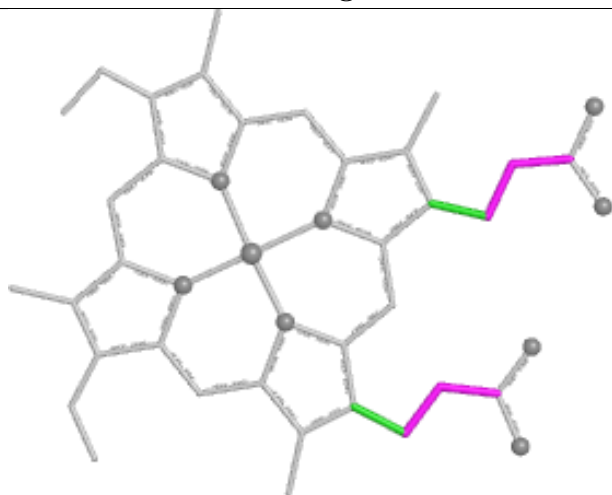
## Ligand HEC C 807



Bond lengths



Bond angles

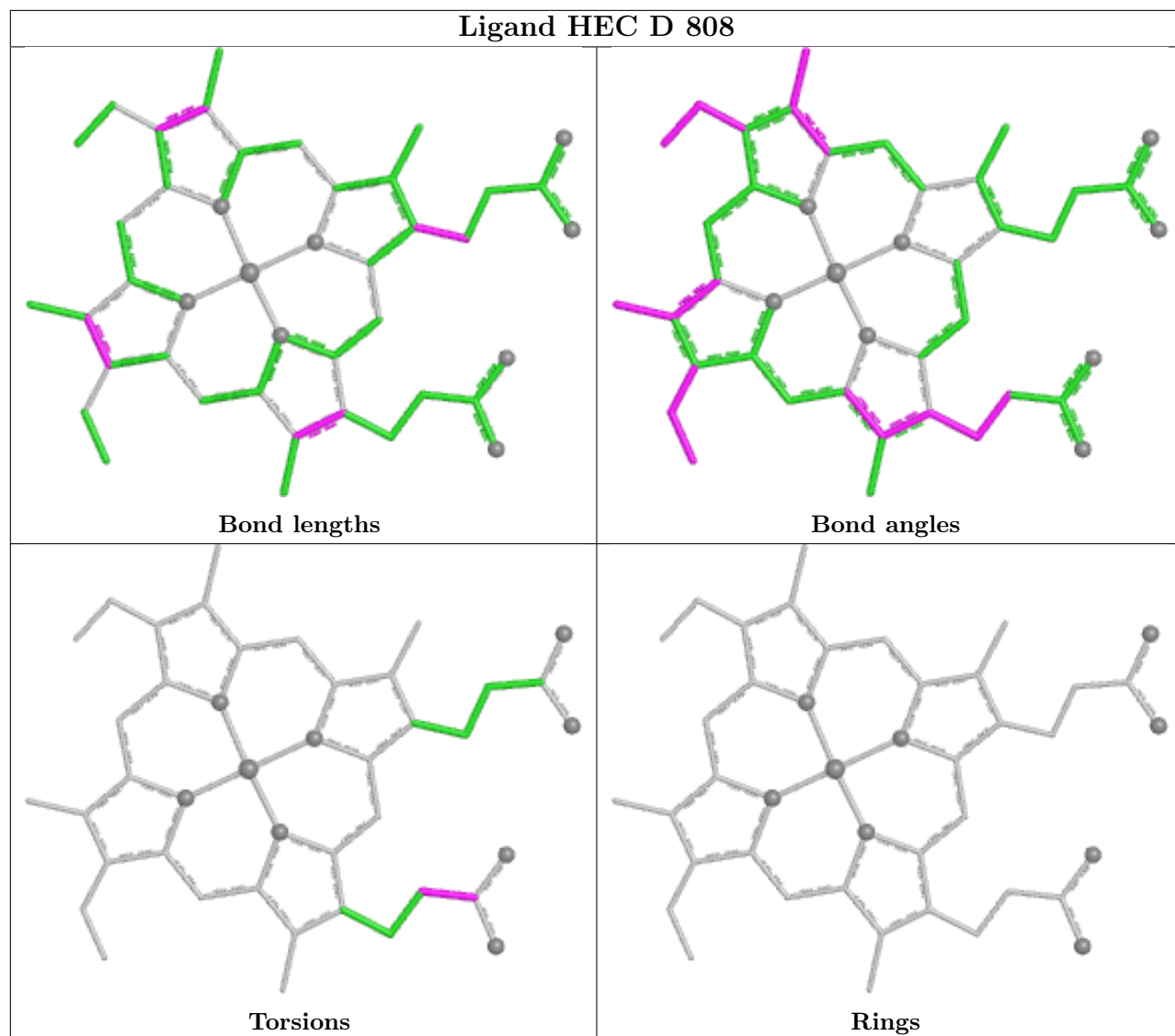


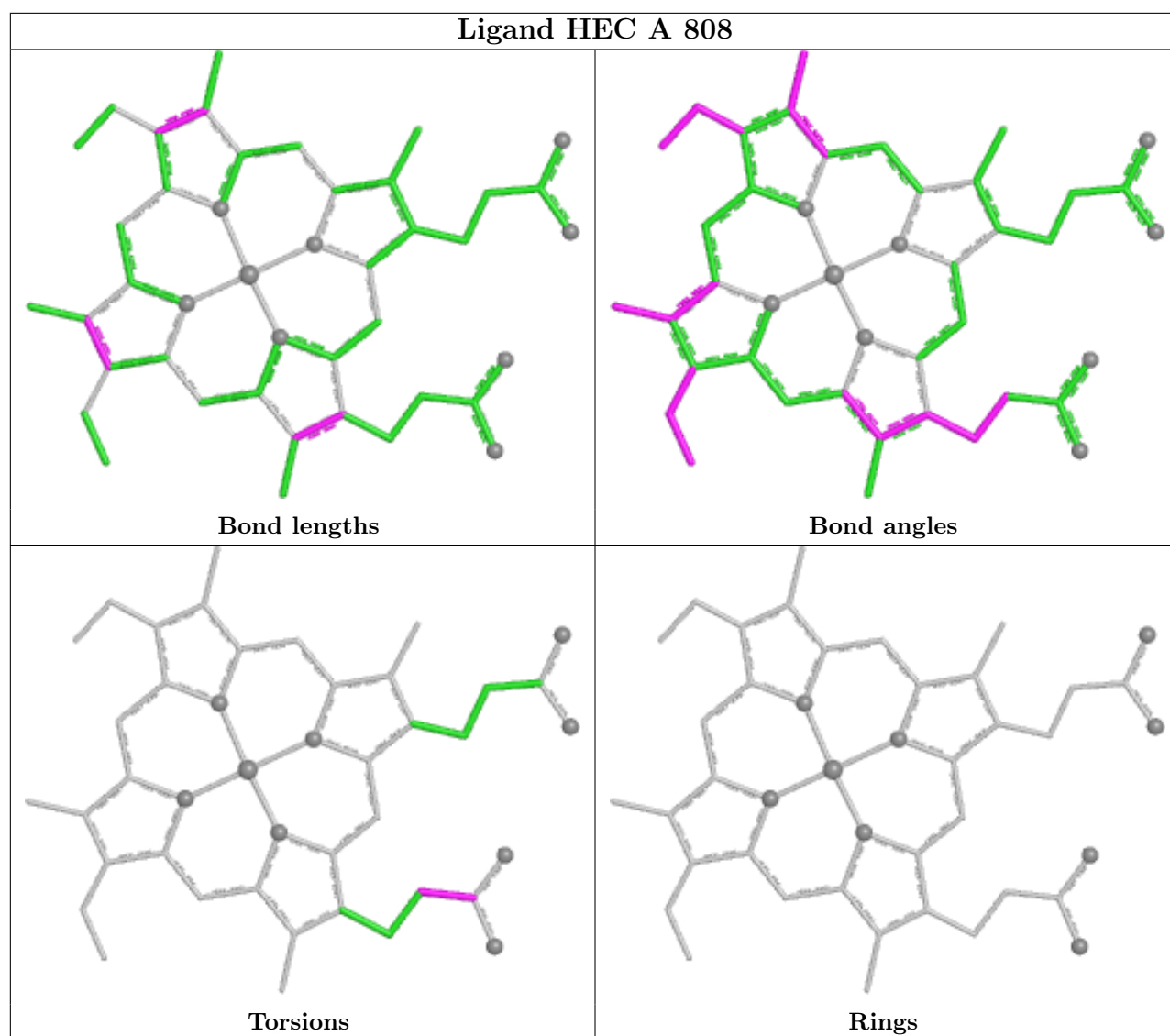
Torsions



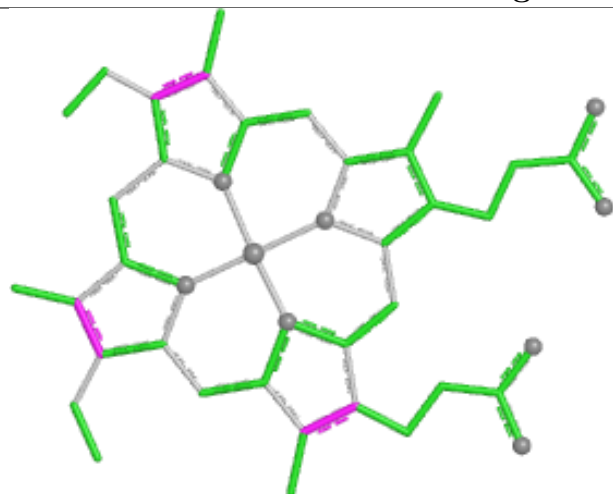
Rings



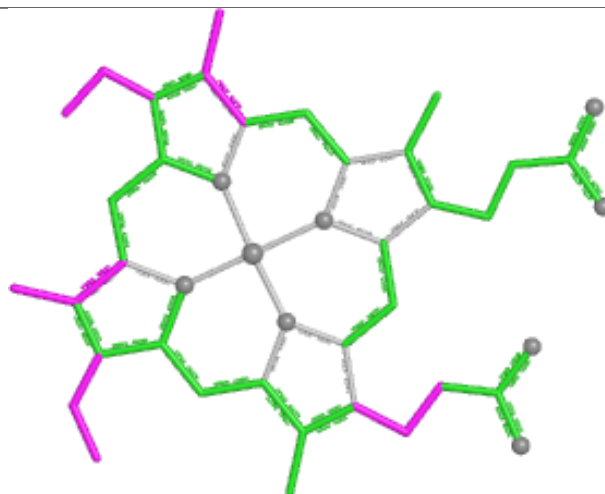




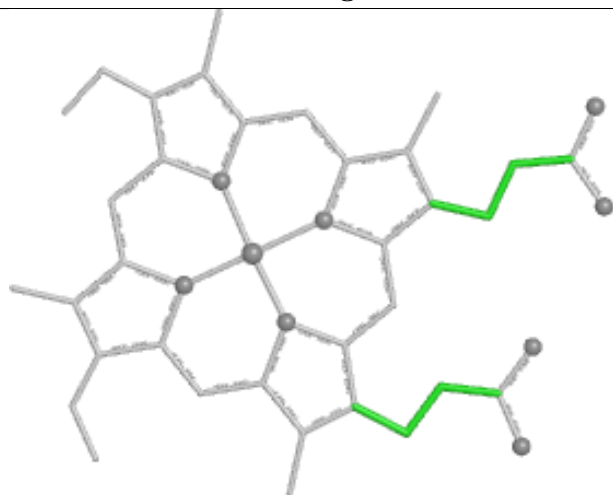
## Ligand HEC B 909



Bond lengths



Bond angles

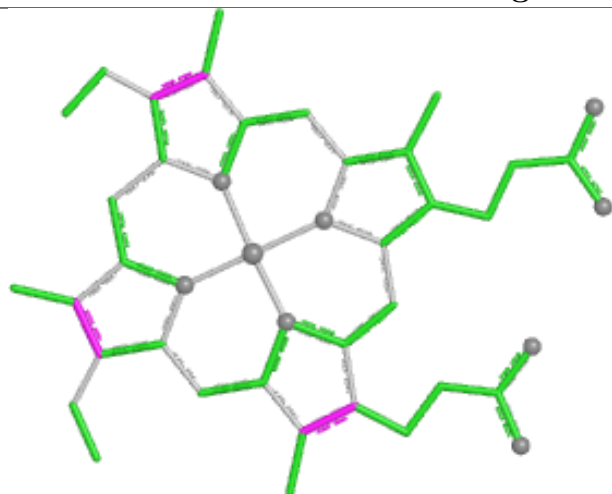


Torsions

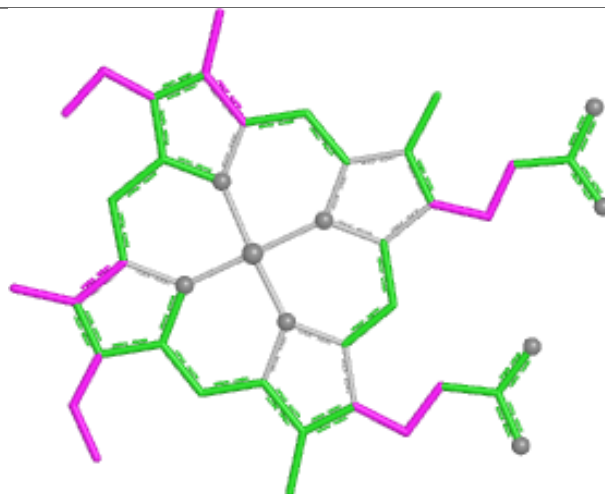


Rings

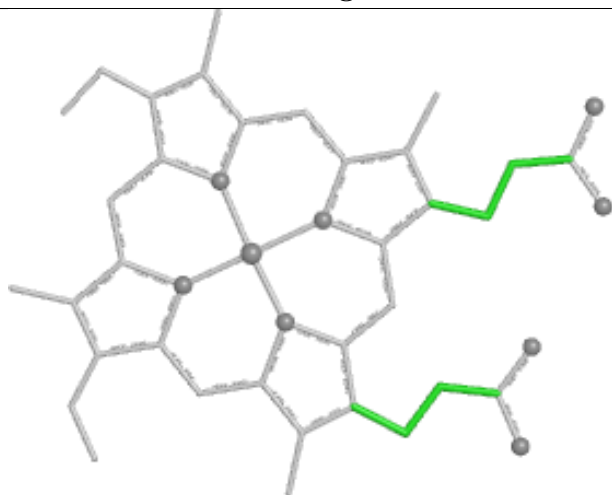
## Ligand HEC C 801



Bond lengths



Bond angles

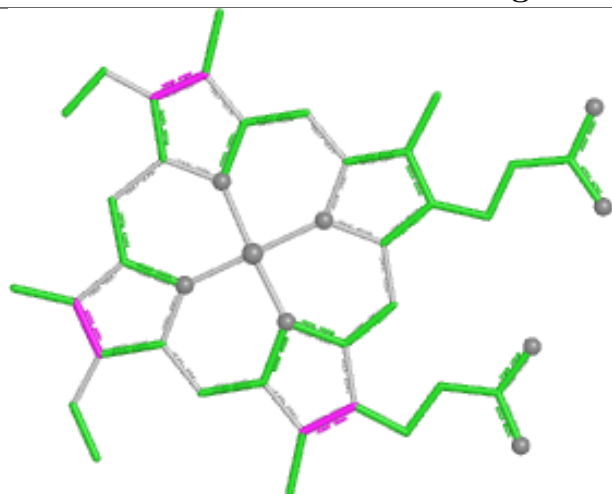


Torsions

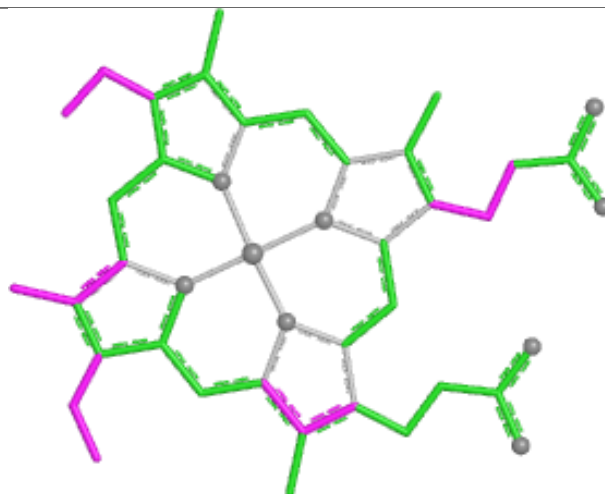


Rings

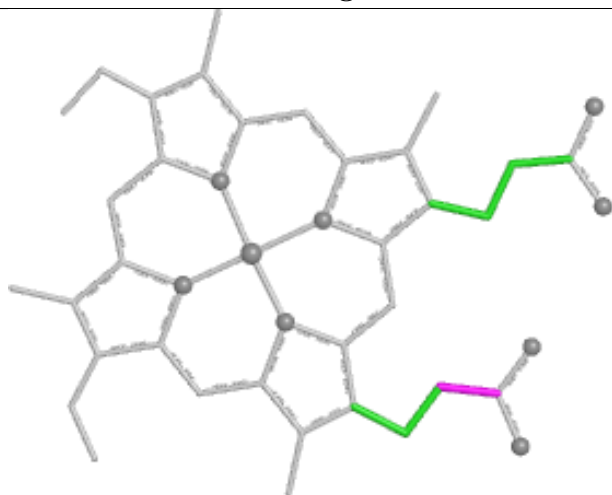
## Ligand HEC C 805



Bond lengths



Bond angles

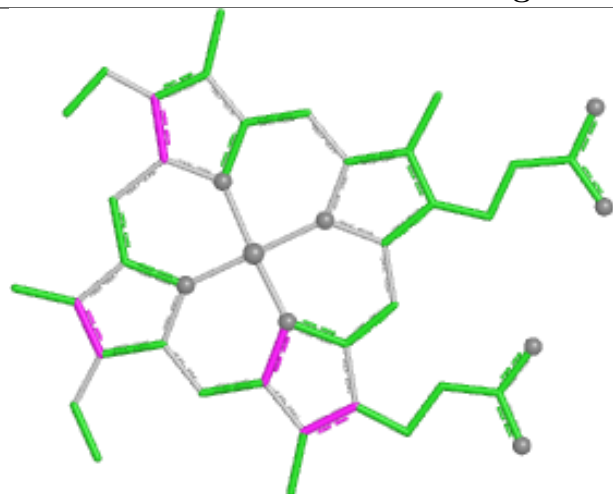


Torsions

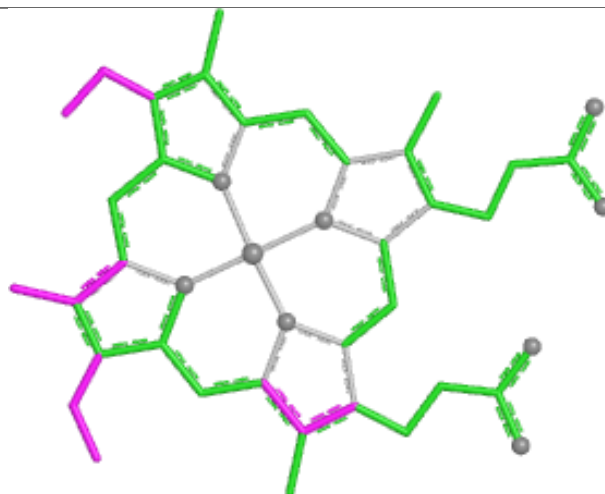


Rings

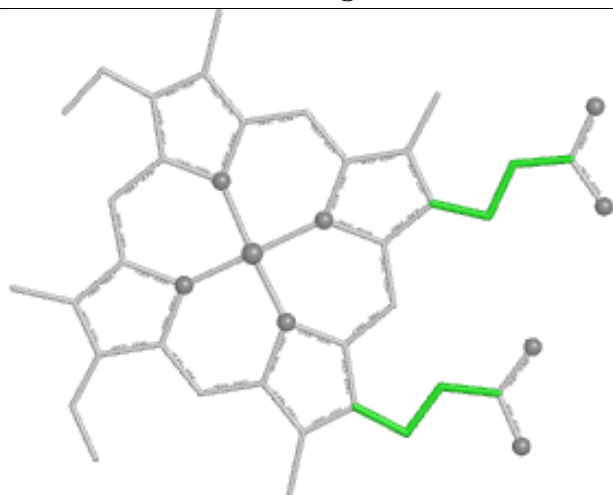
## Ligand HEC B 904



Bond lengths



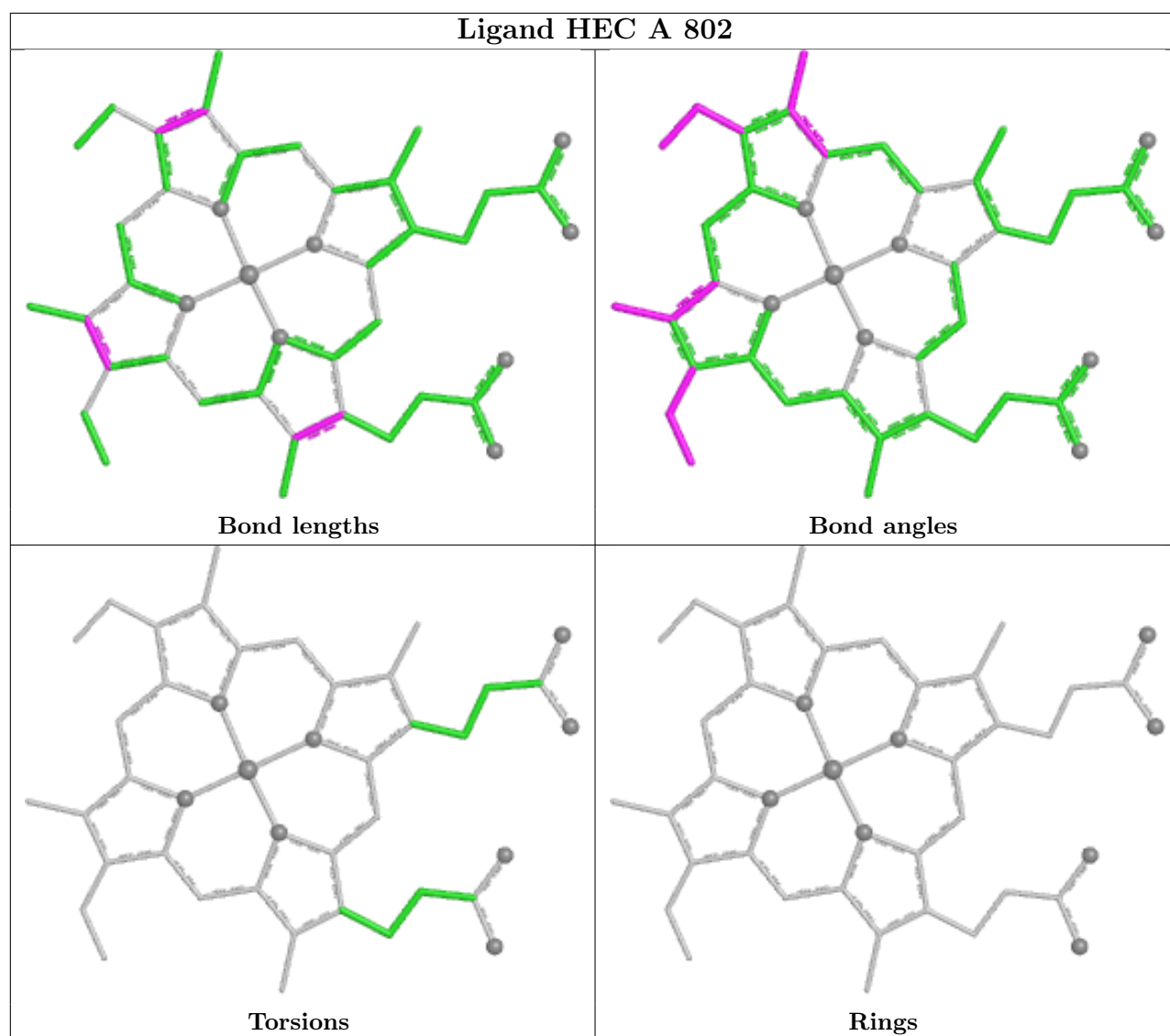
Bond angles

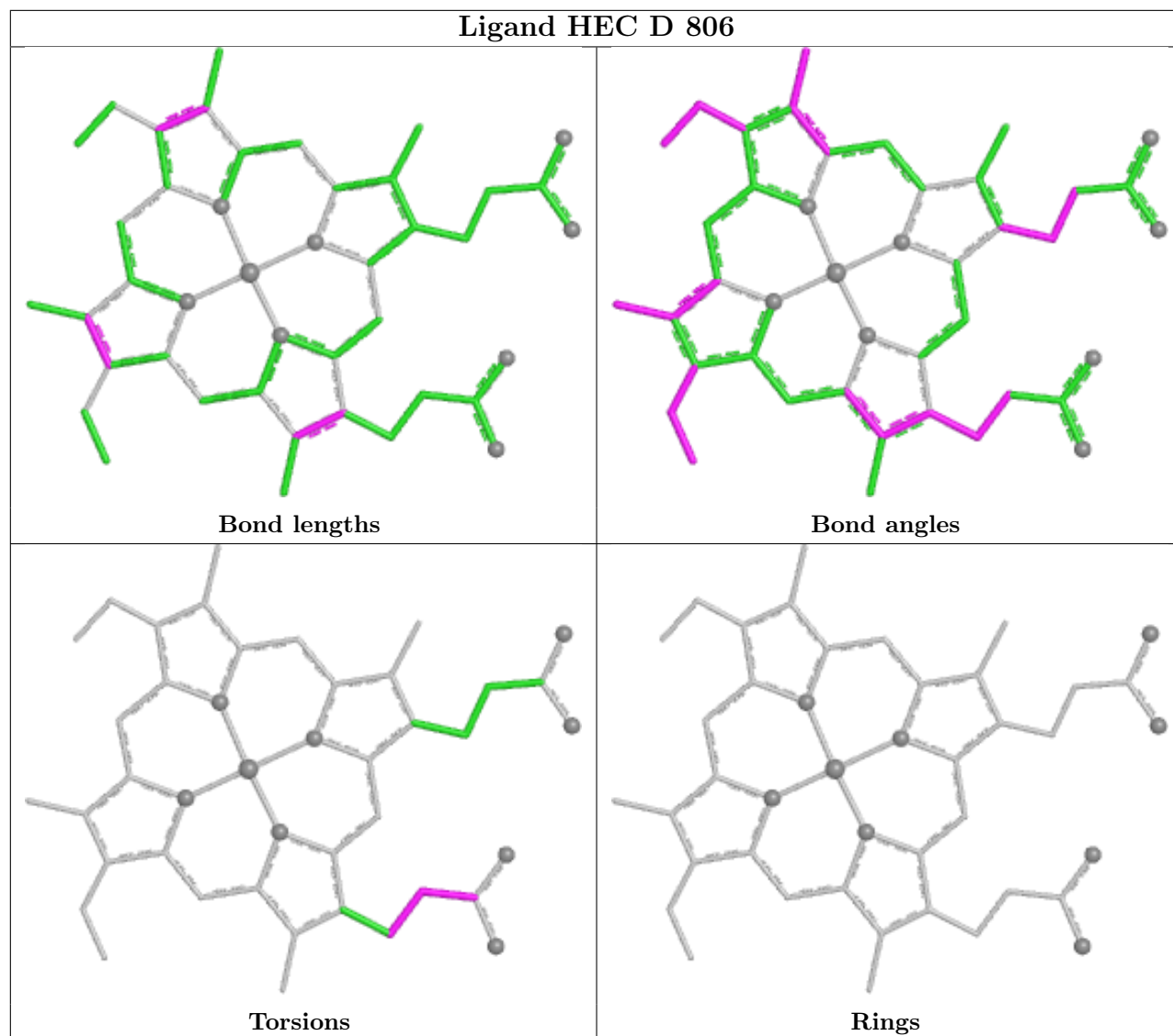


Torsions

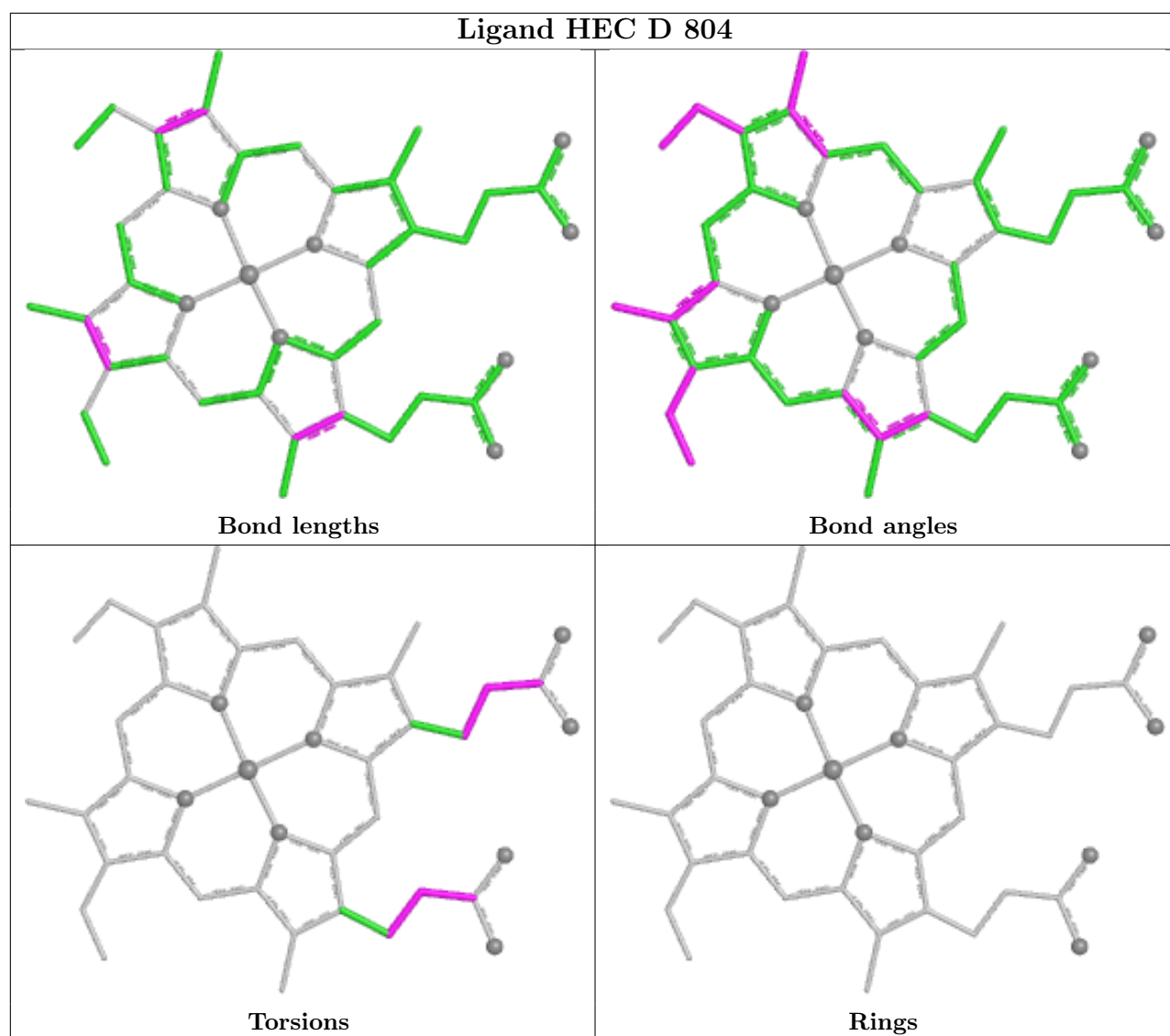


Rings

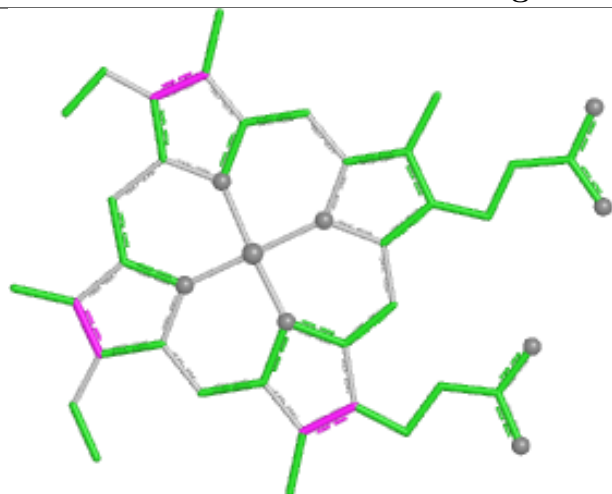




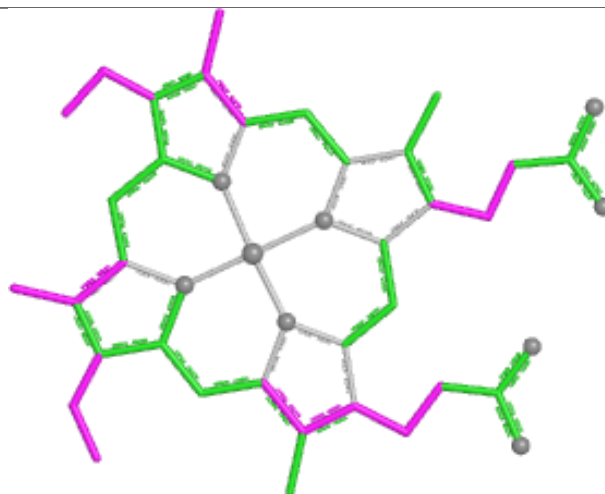




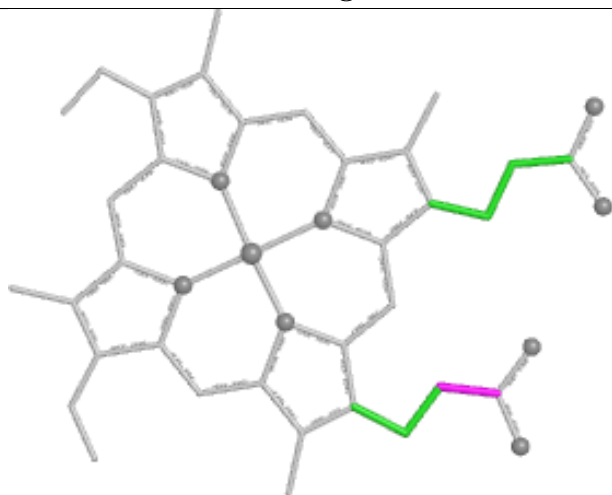
## Ligand HEC C 809



Bond lengths



Bond angles

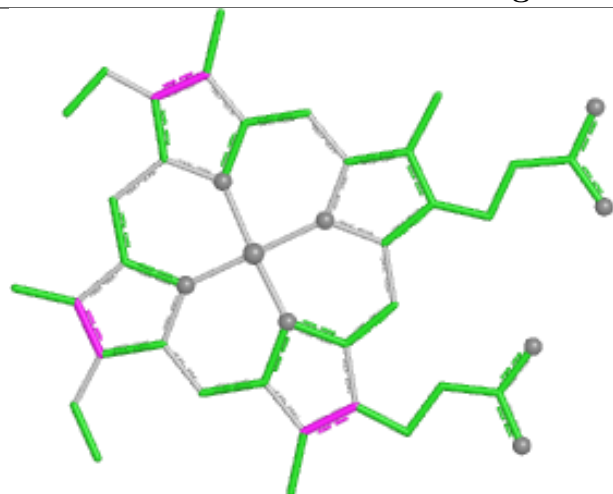


Torsions

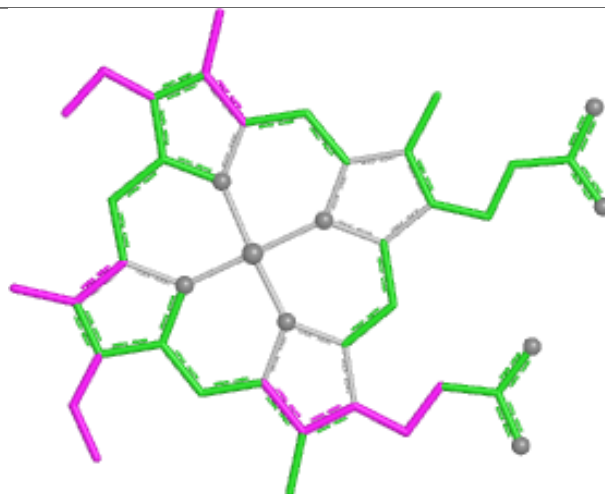


Rings

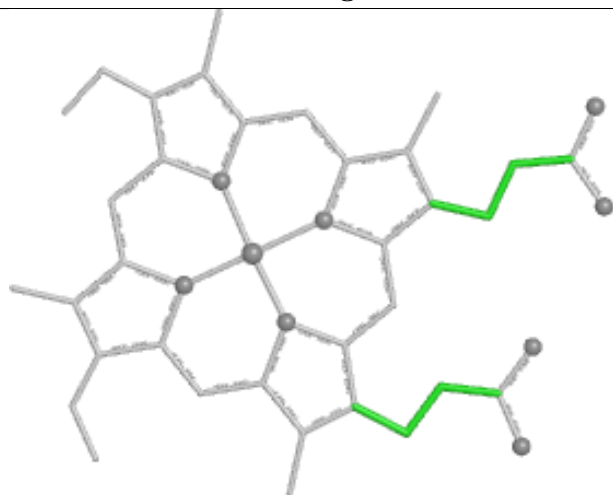
## Ligand HEC A 809



Bond lengths



Bond angles

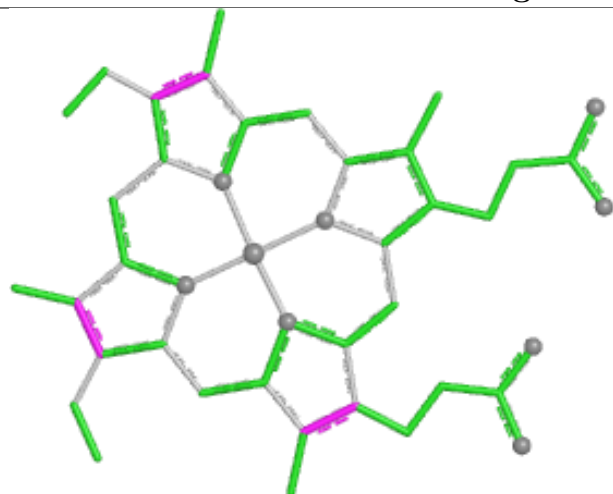


Torsions

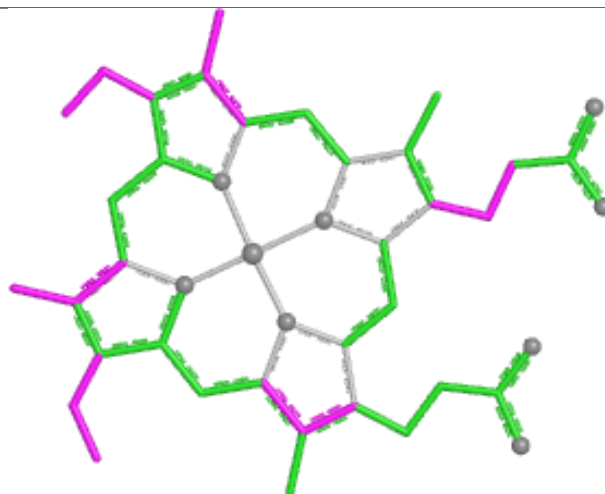


Rings

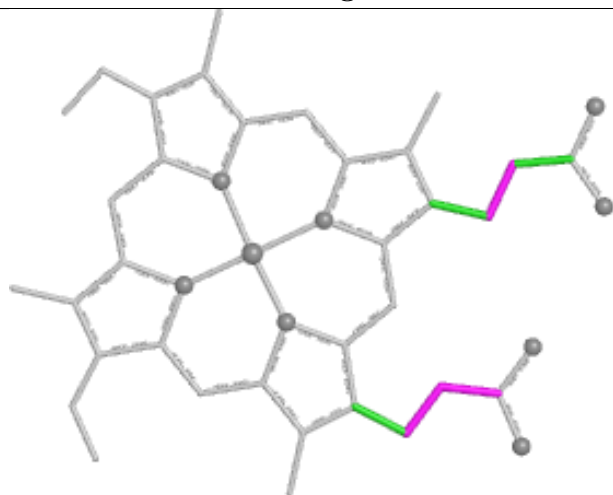
## Ligand HEC B 905



Bond lengths



Bond angles

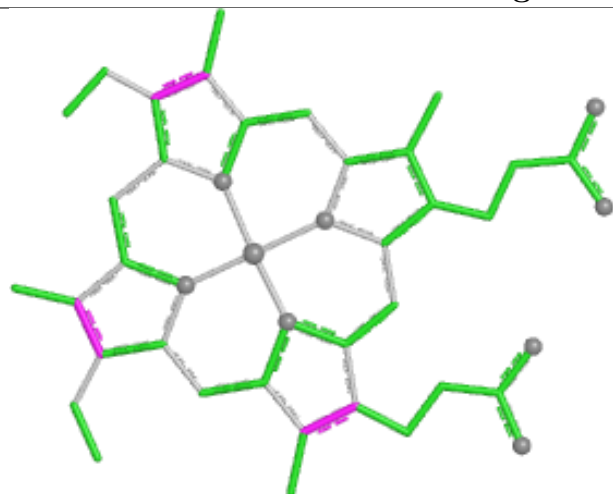


Torsions

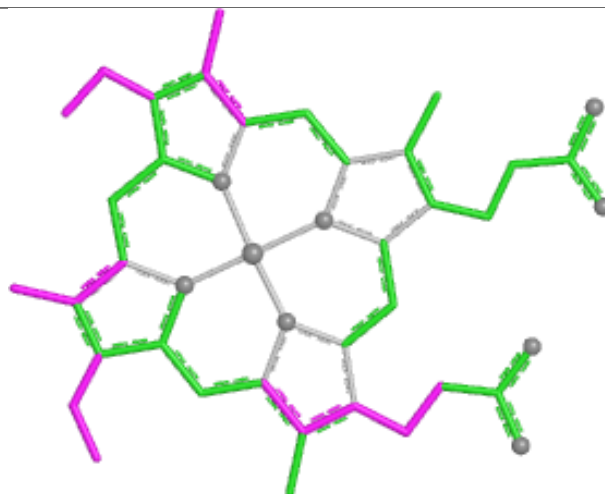


Rings

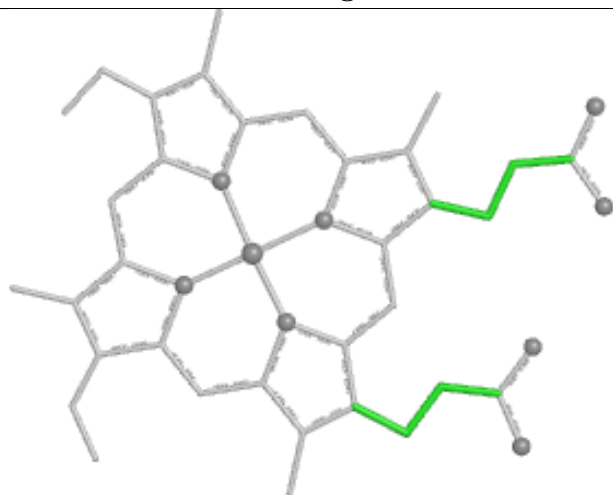
## Ligand HEC B 910



Bond lengths



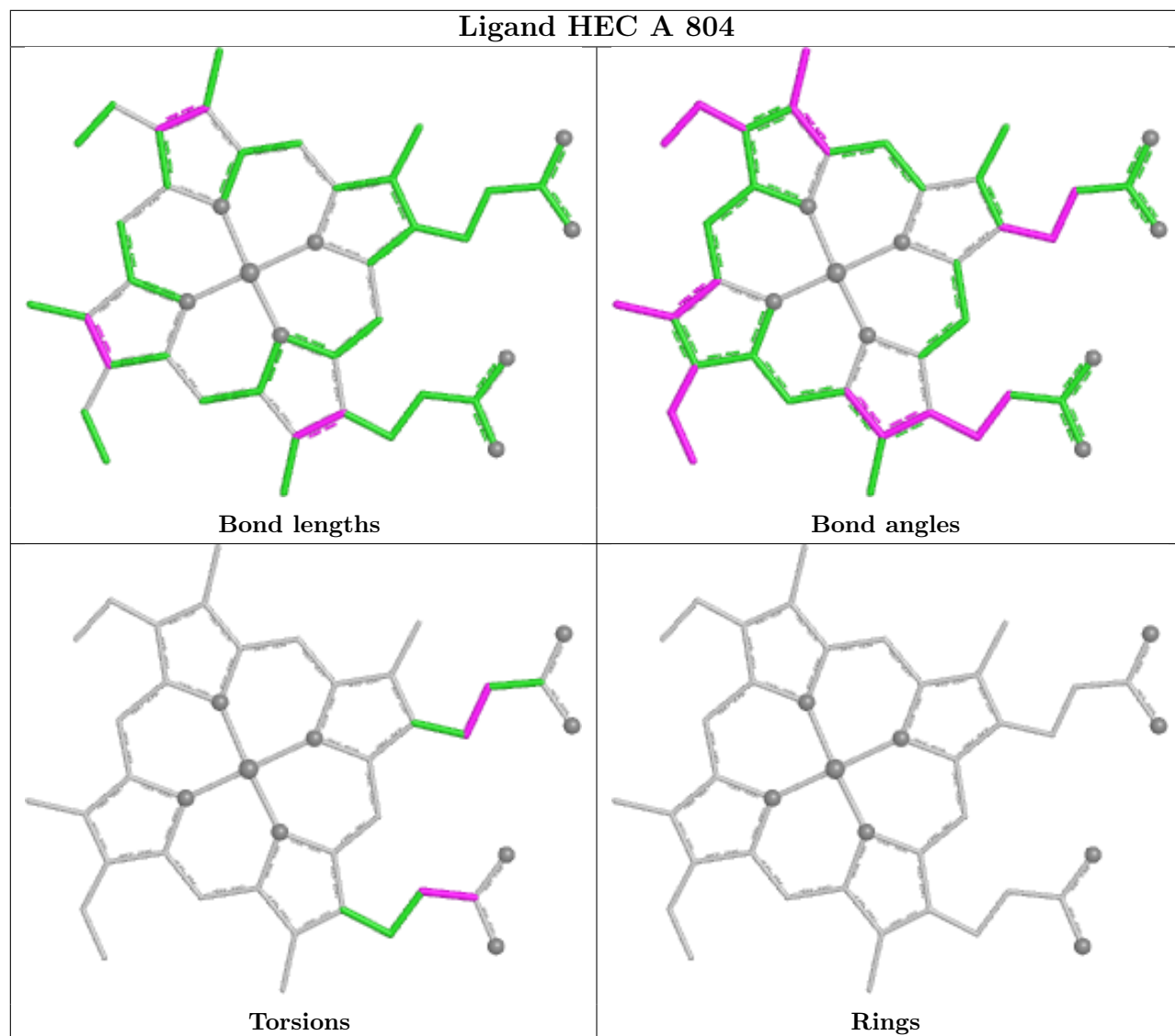
Bond angles



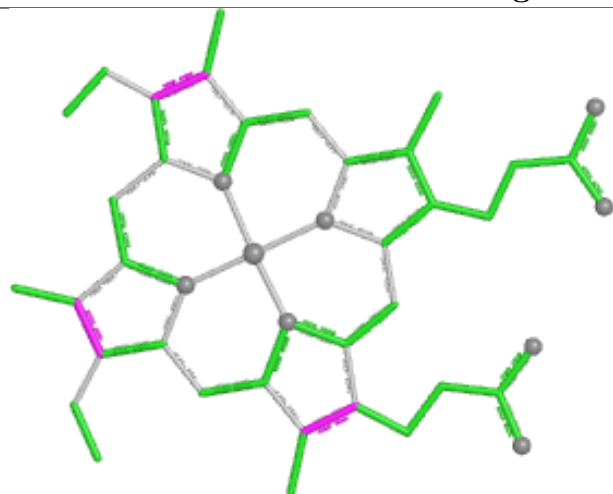
Torsions



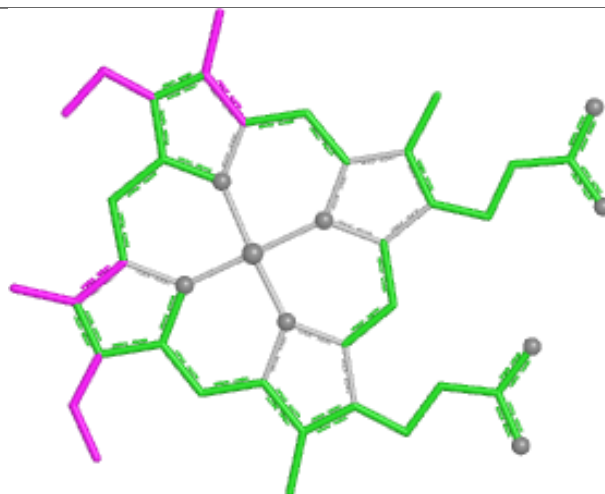
Rings



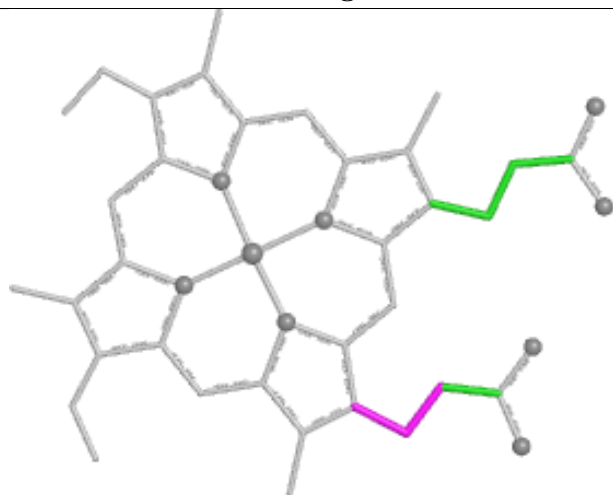
## Ligand HEC C 810



Bond lengths



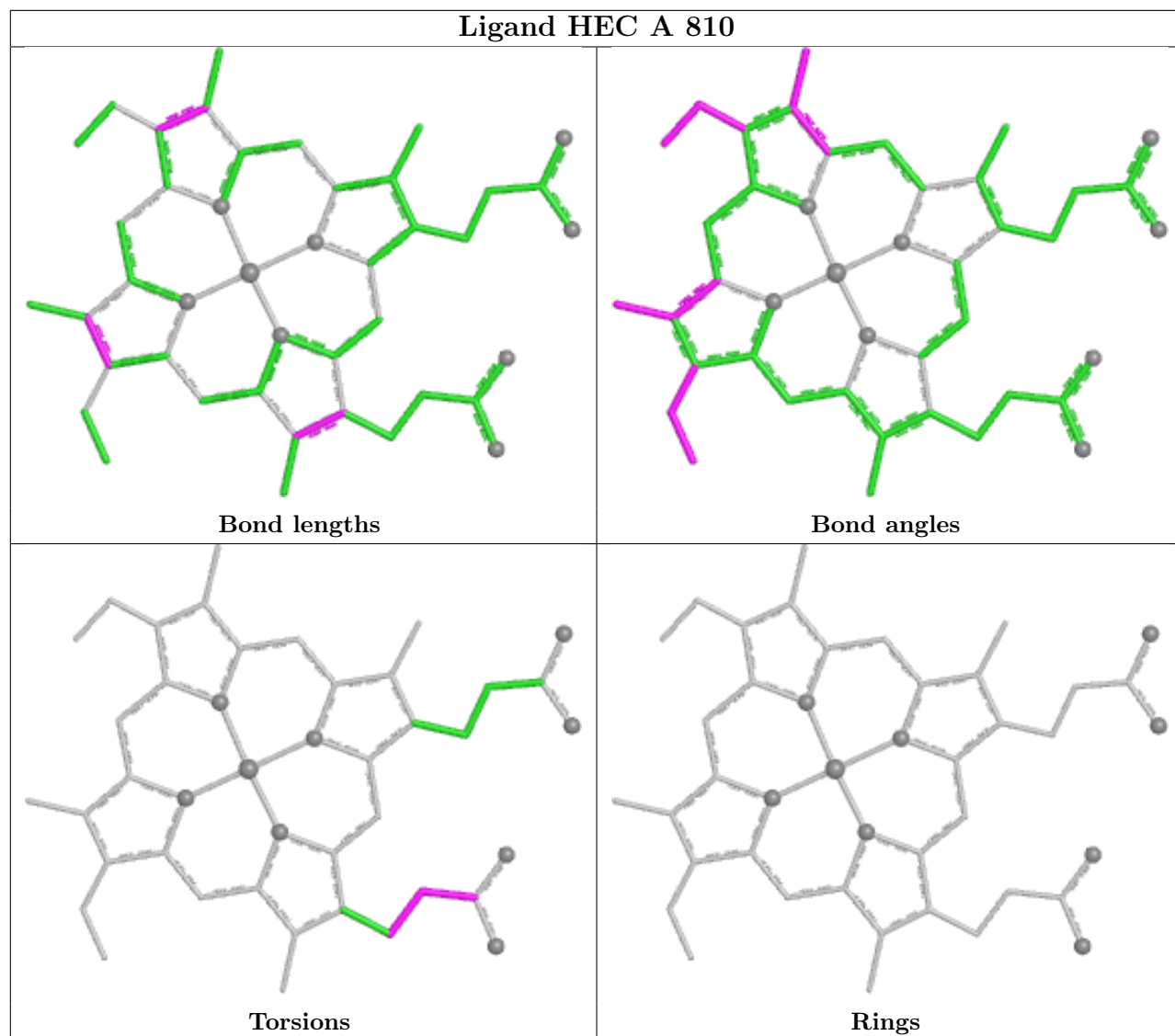
Bond angles



Torsions

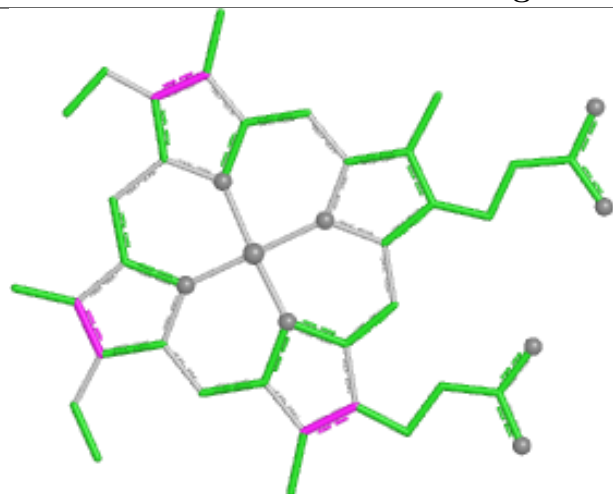


Rings

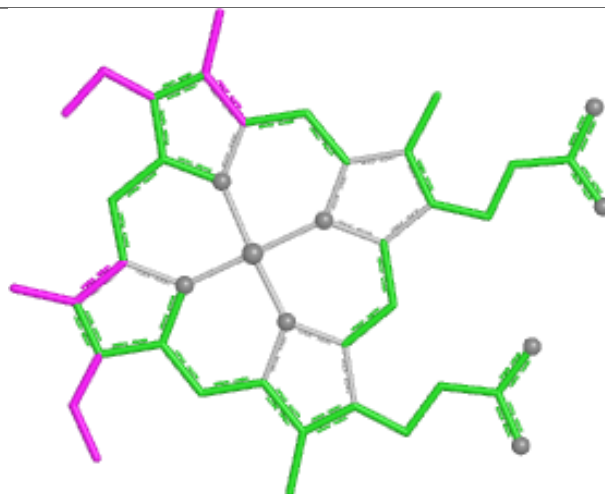




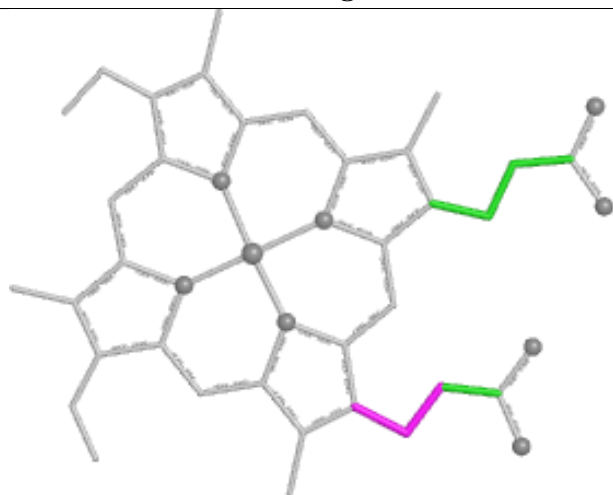
## Ligand HEC B 911



Bond lengths



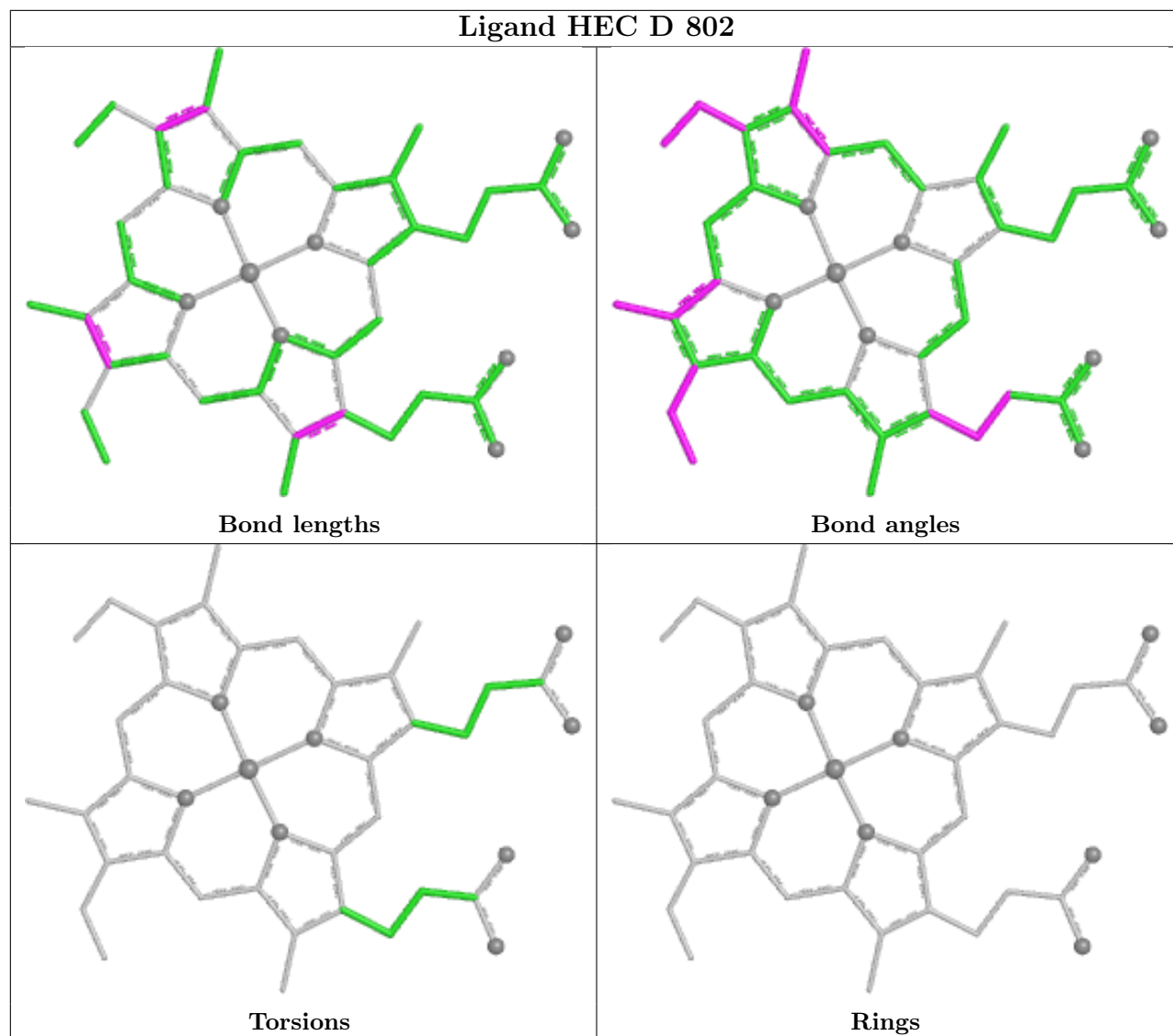
Bond angles



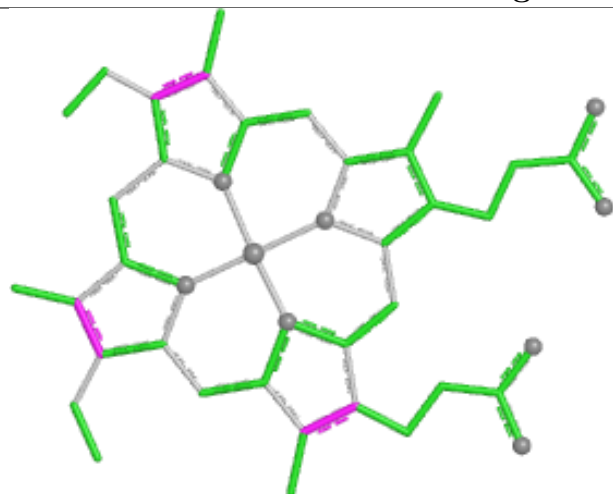
Torsions



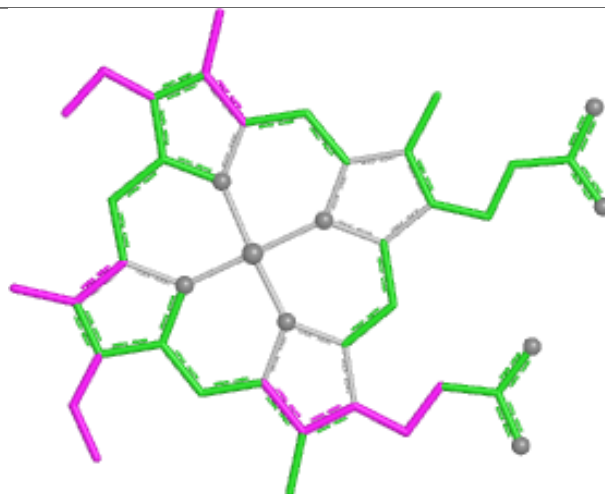
Rings



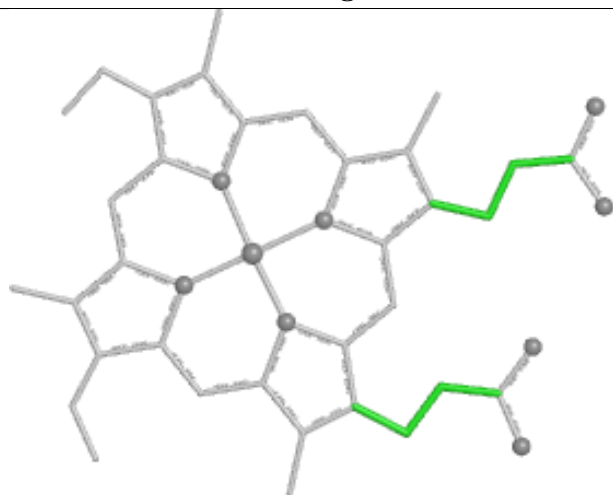
## Ligand HEC B 903



Bond lengths



Bond angles

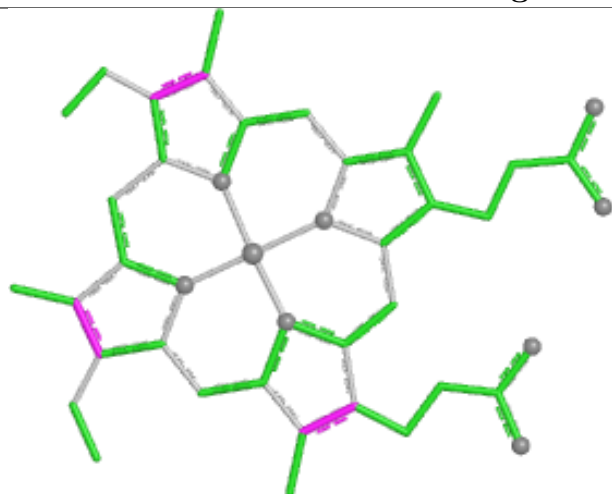


Torsions

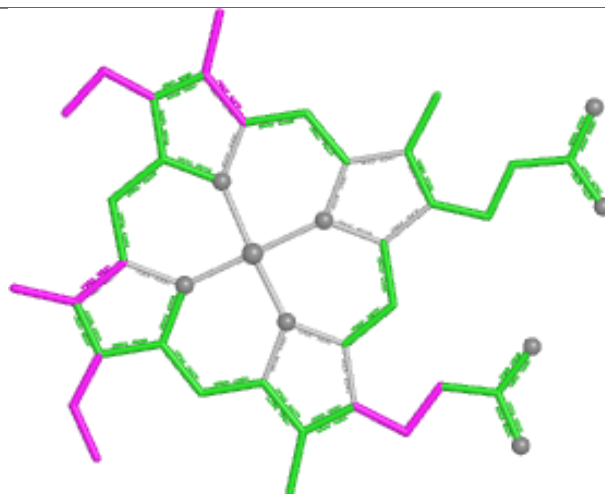


Rings

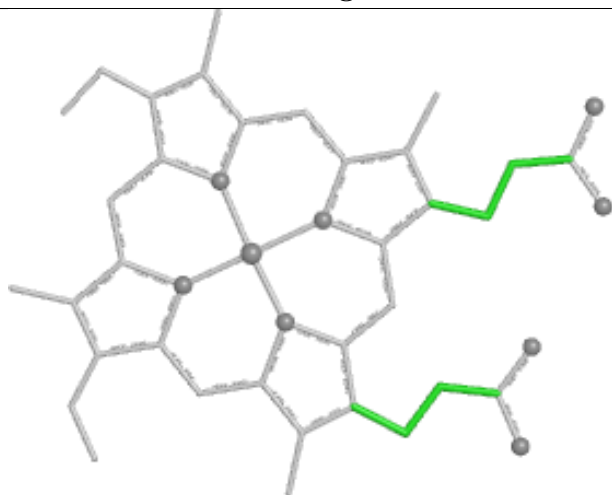
## Ligand HEC D 803



Bond lengths



Bond angles

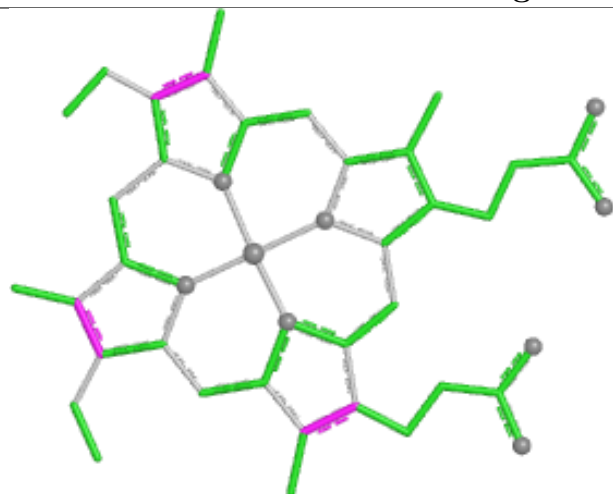


Torsions

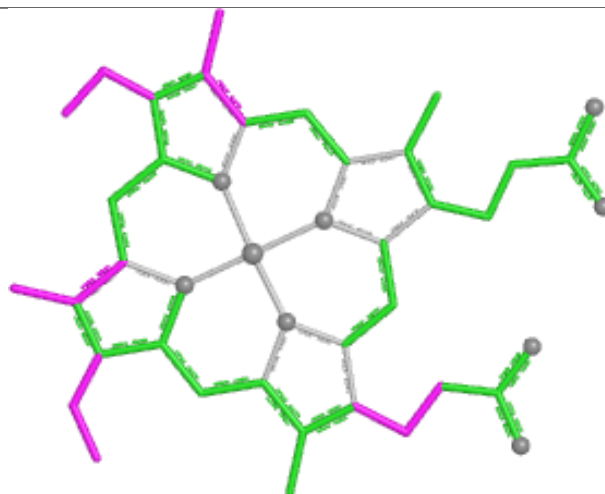


Rings

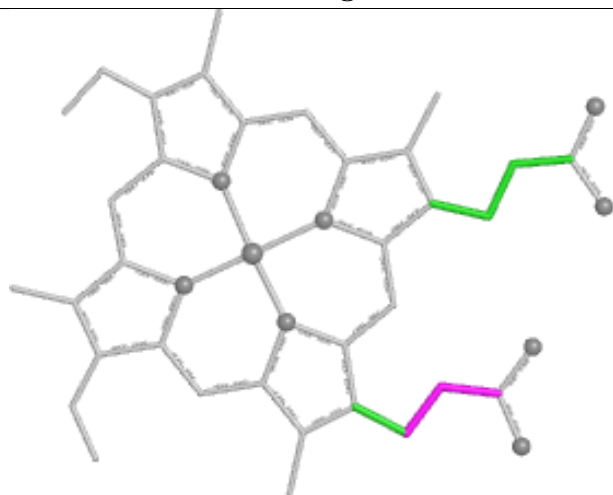
## Ligand HEC B 908



Bond lengths



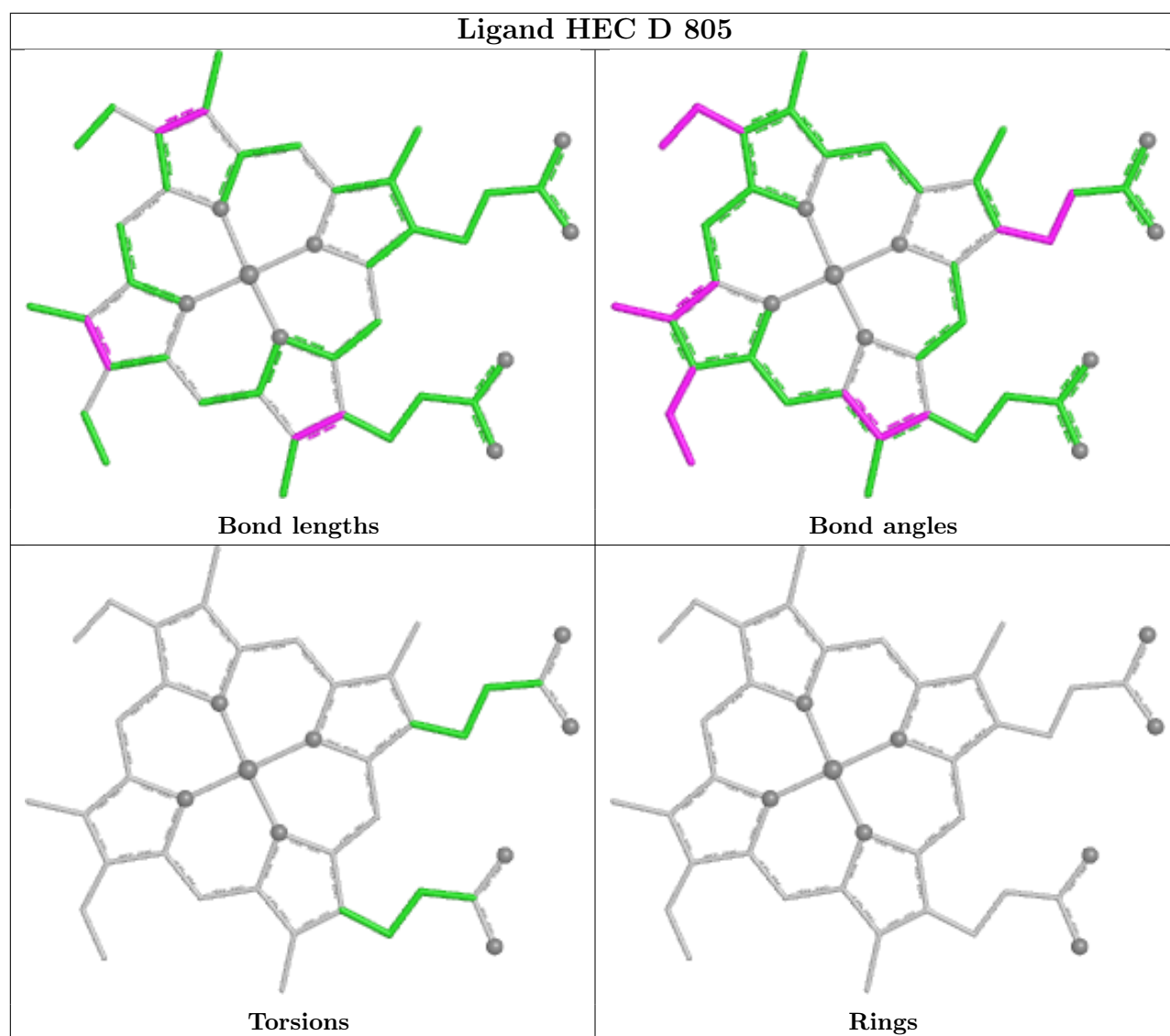
Bond angles



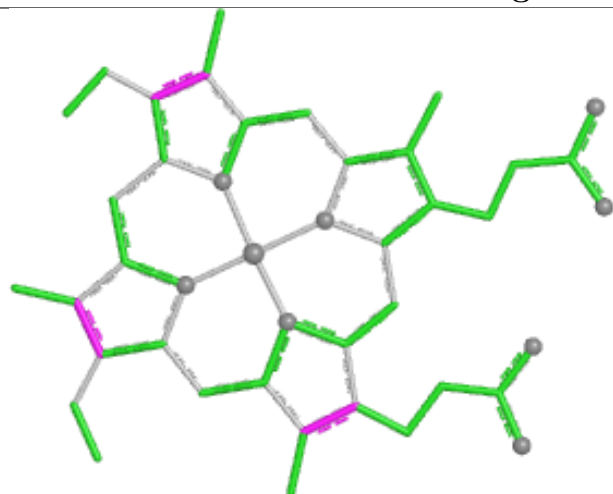
Torsions



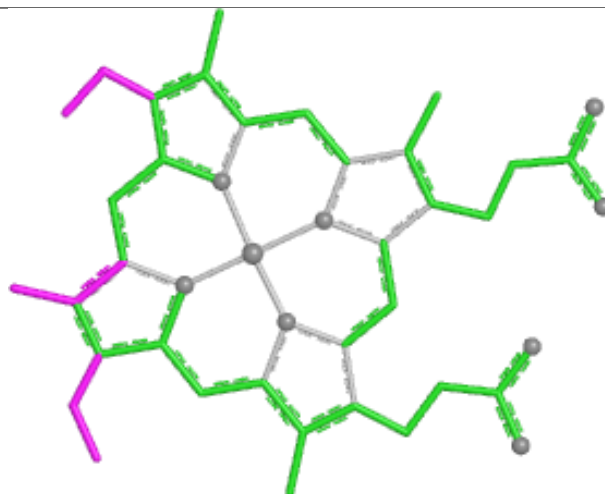
Rings



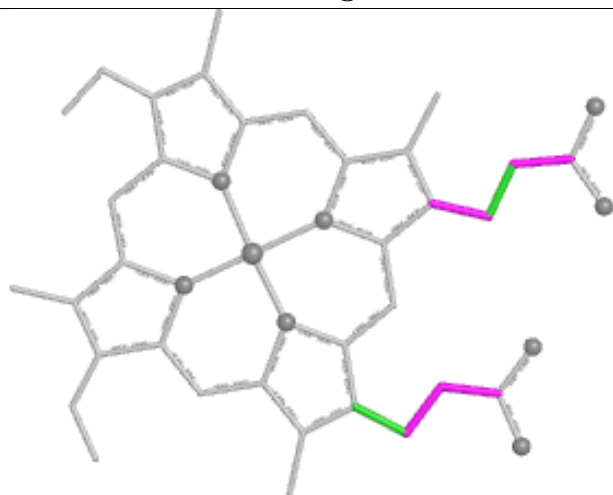
## Ligand HEC A 807



Bond lengths



Bond angles

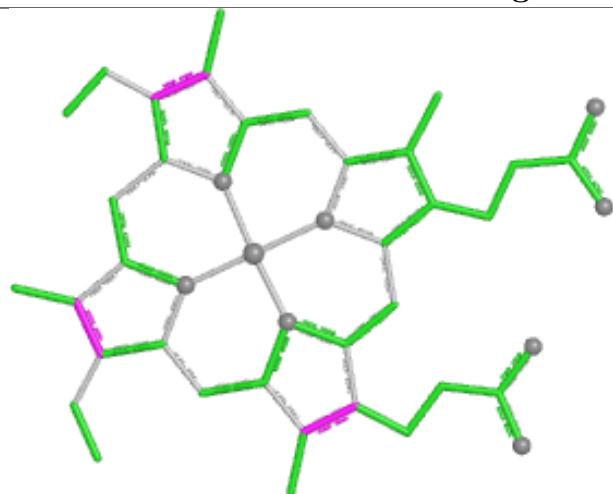


Torsions

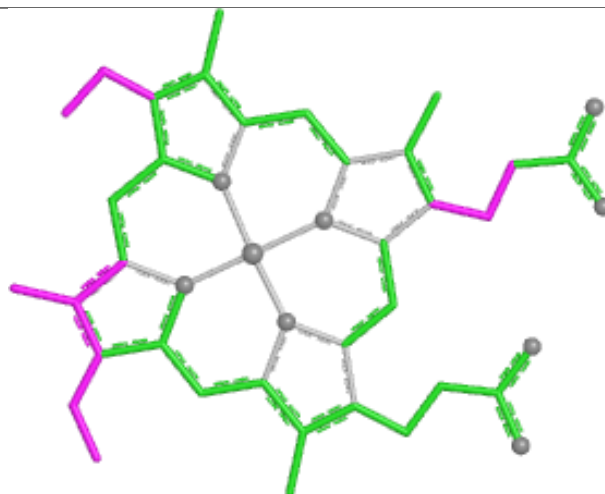


Rings

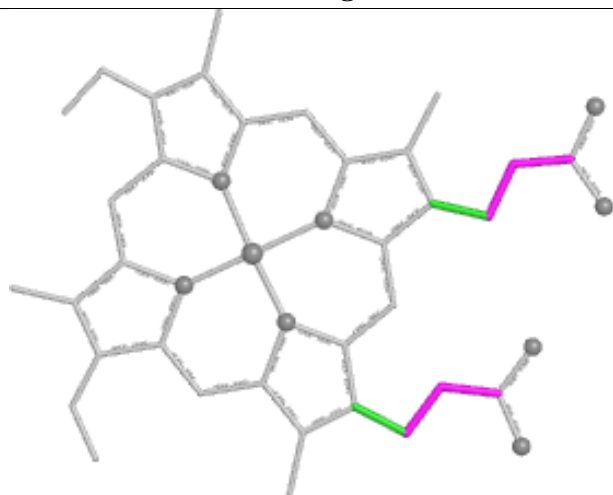
## Ligand HEC D 807



Bond lengths



Bond angles



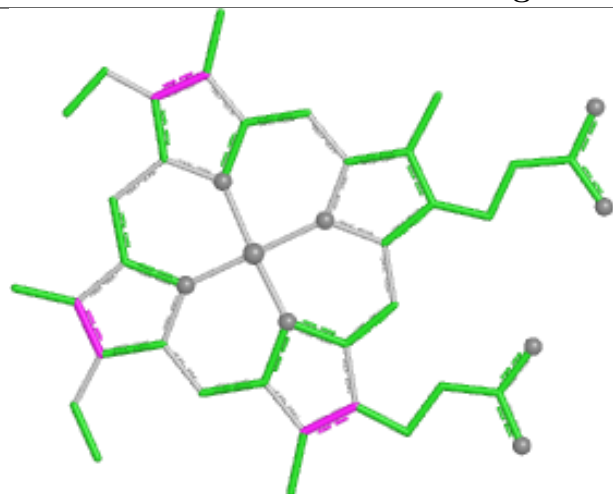
Torsions



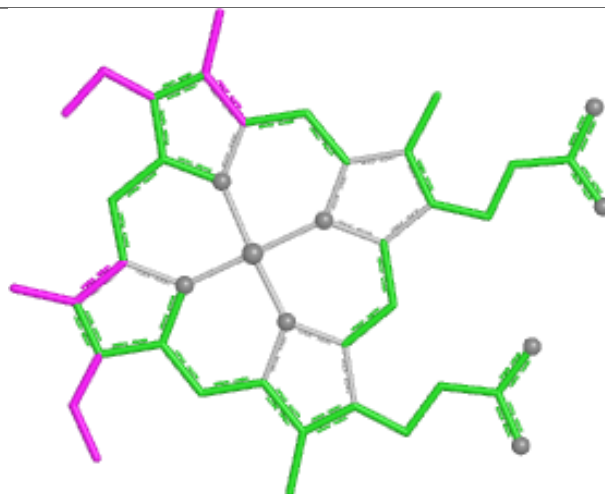
Rings



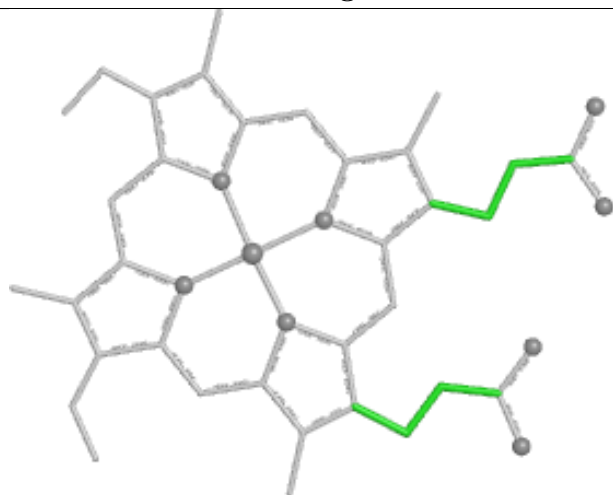
## Ligand HEC B 902



Bond lengths



Bond angles

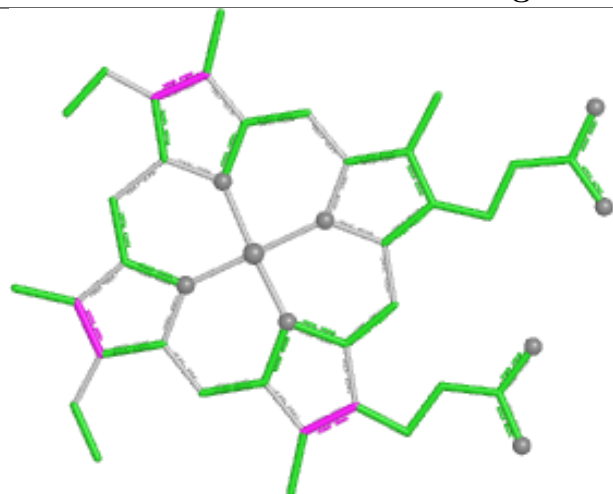


Torsions

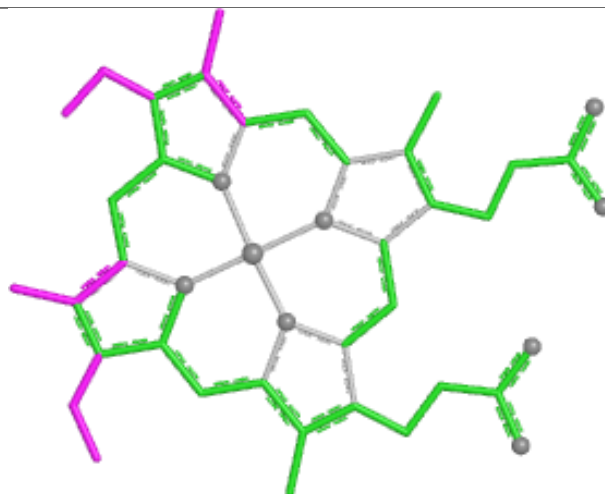


Rings

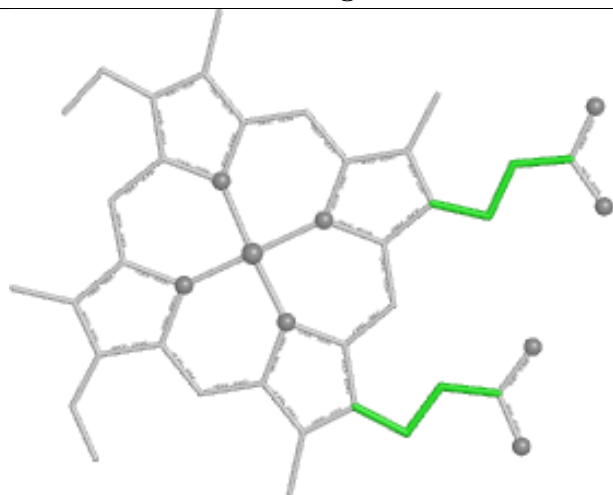
## Ligand HEC C 802



Bond lengths



Bond angles

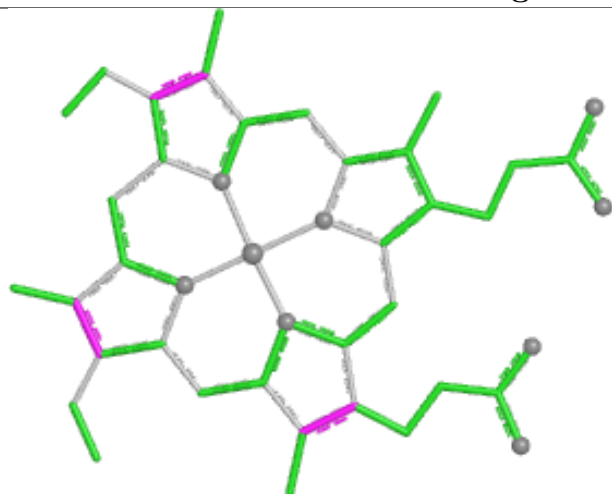


Torsions

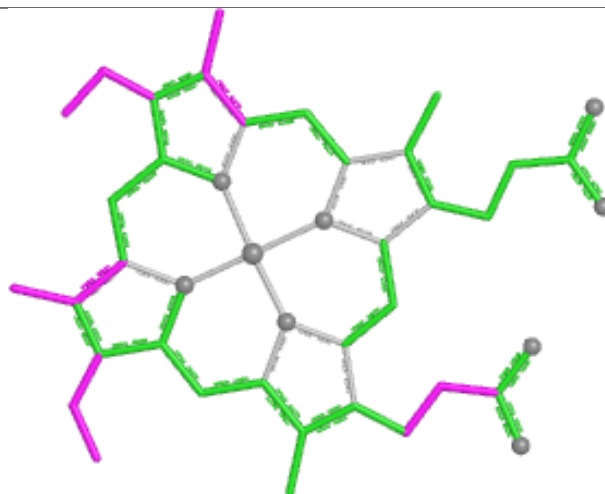


Rings

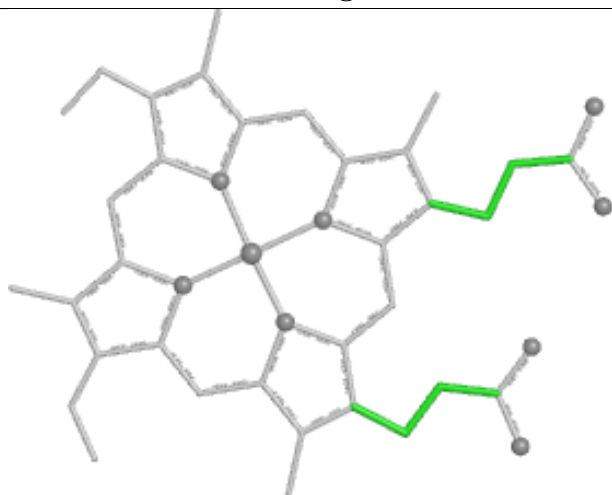
## Ligand HEC C 803



Bond lengths



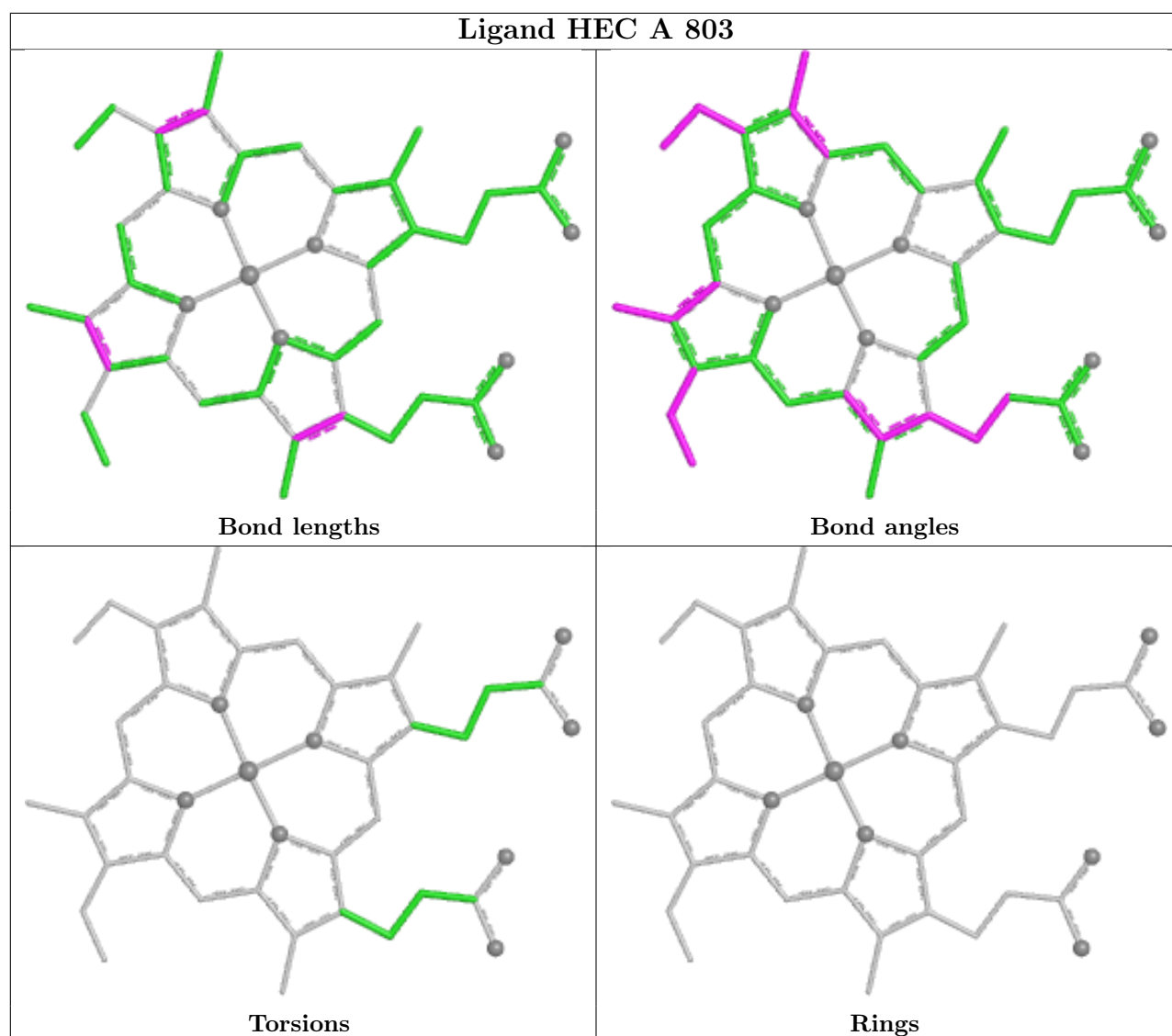
Bond angles

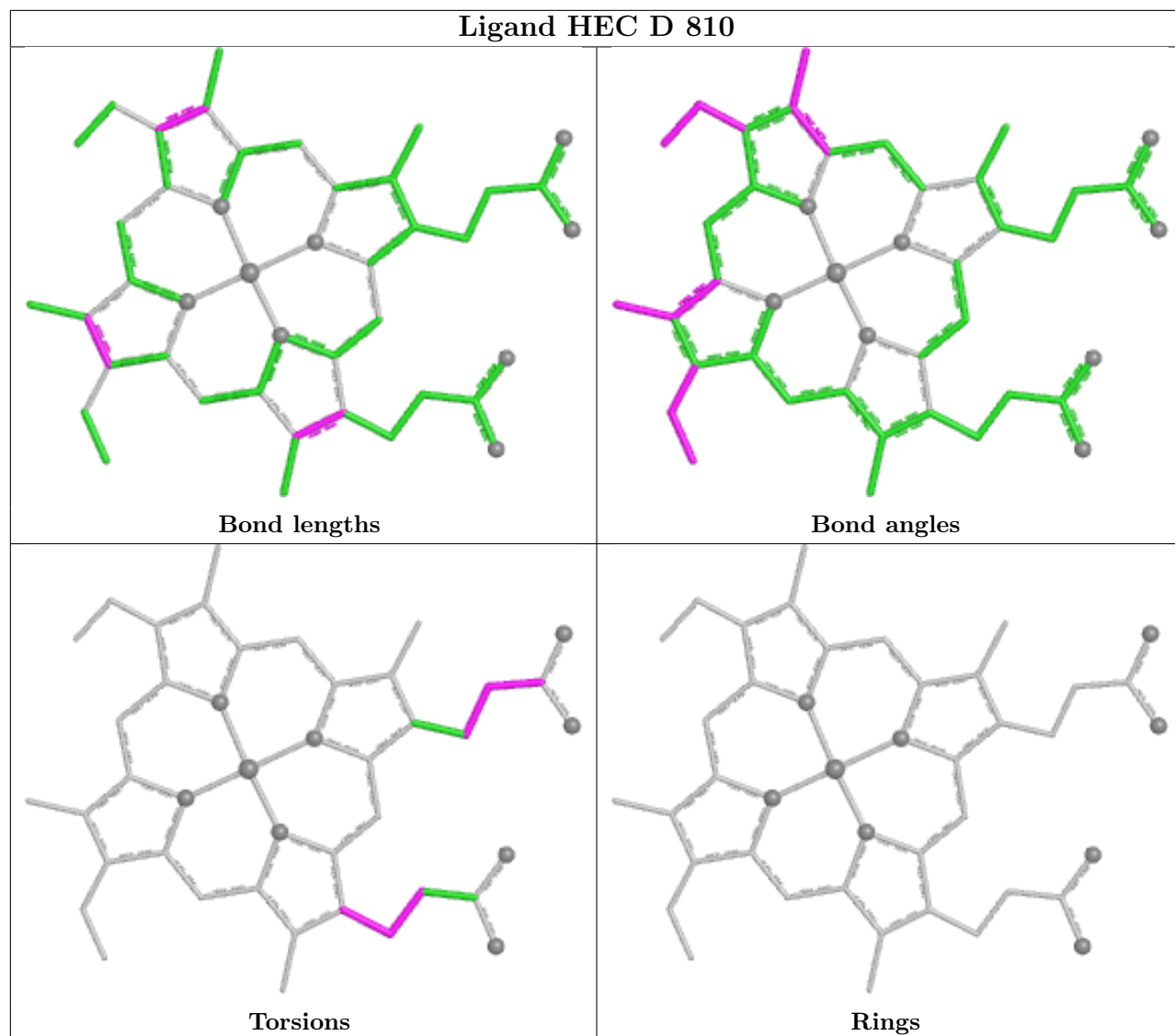


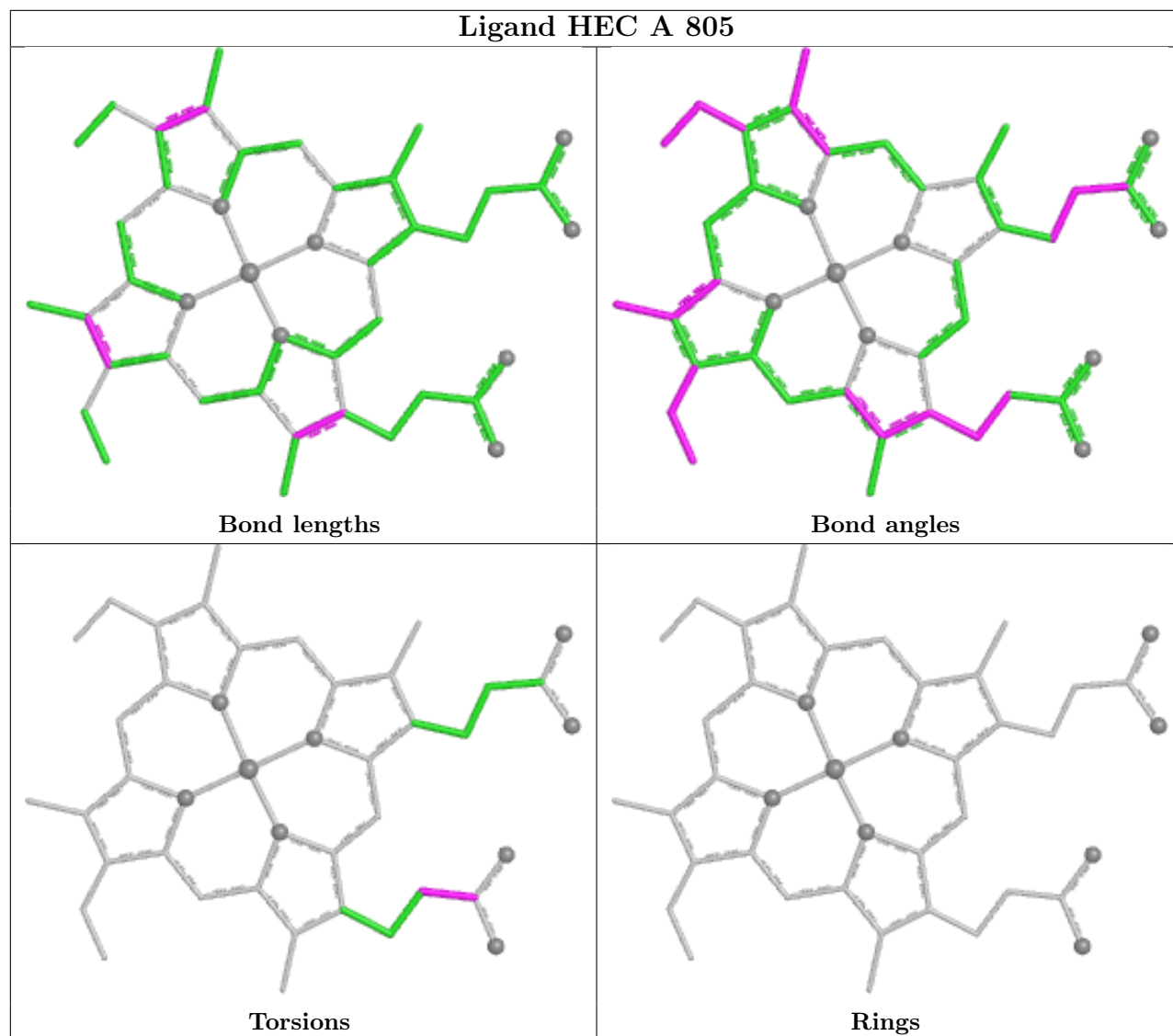
Torsions

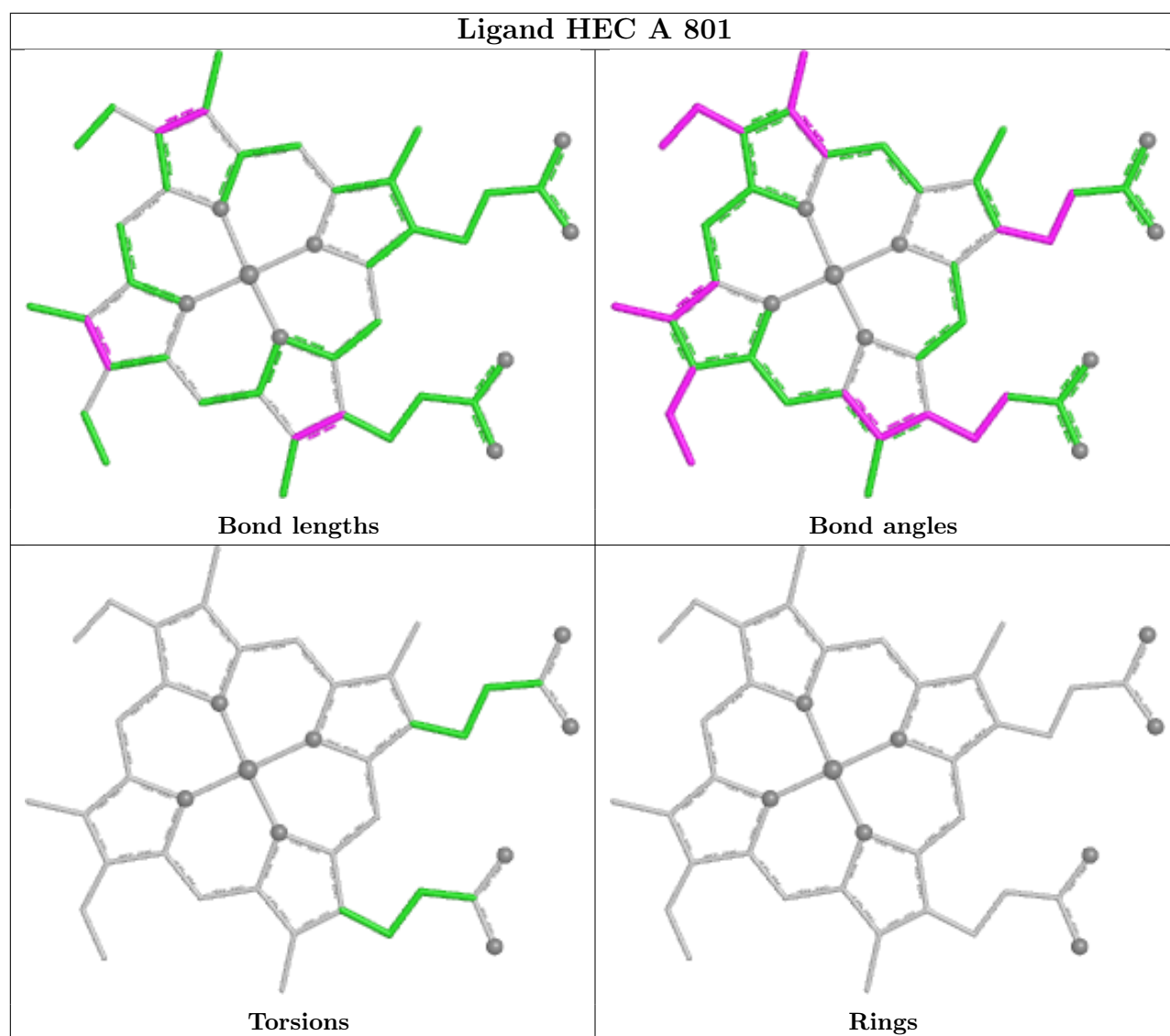


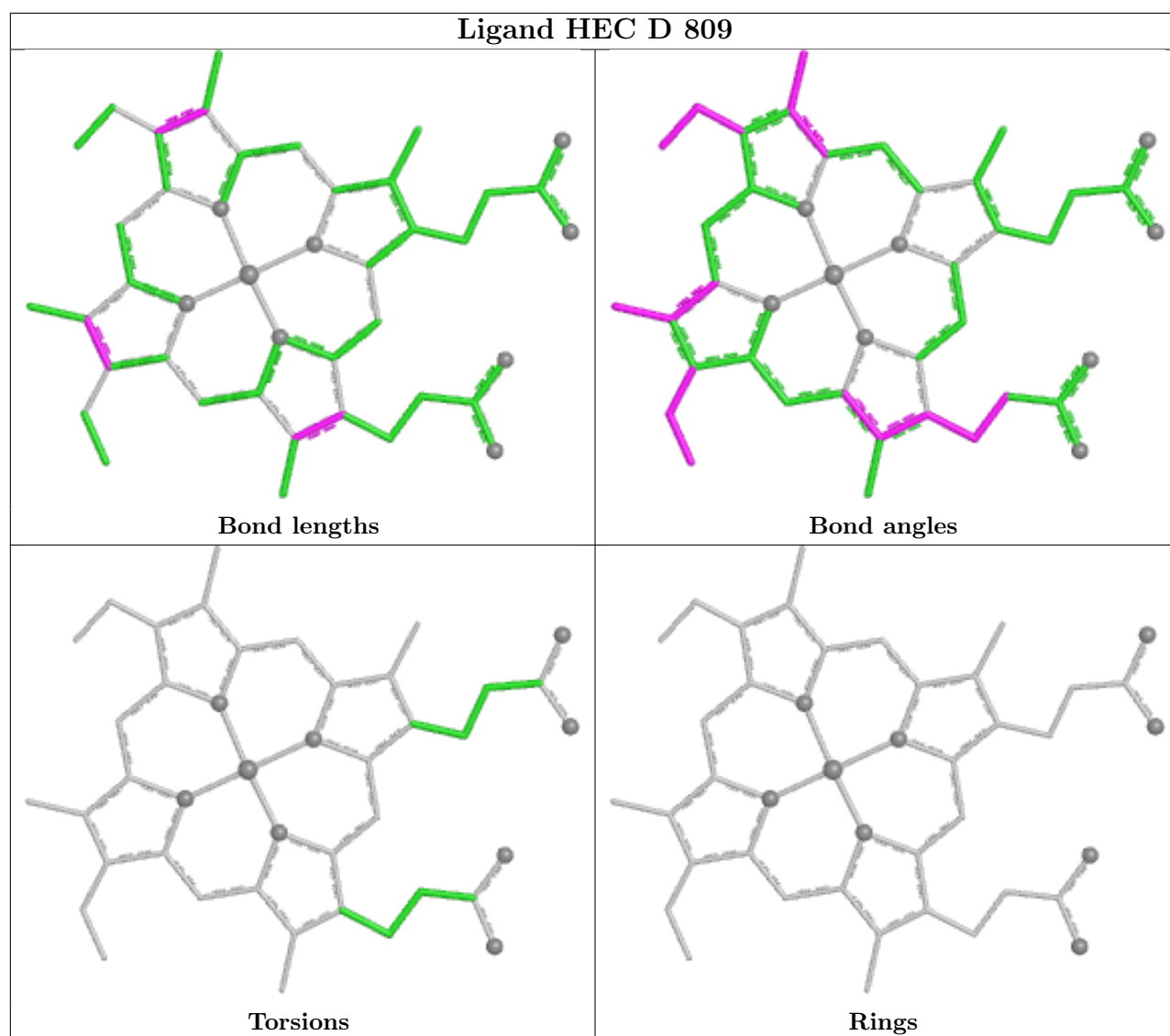
Rings





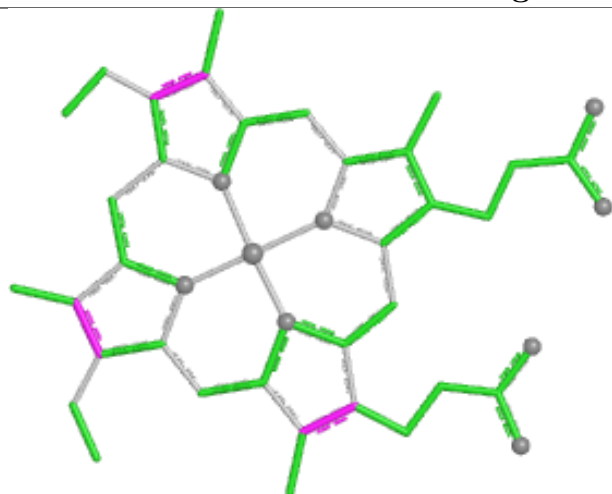




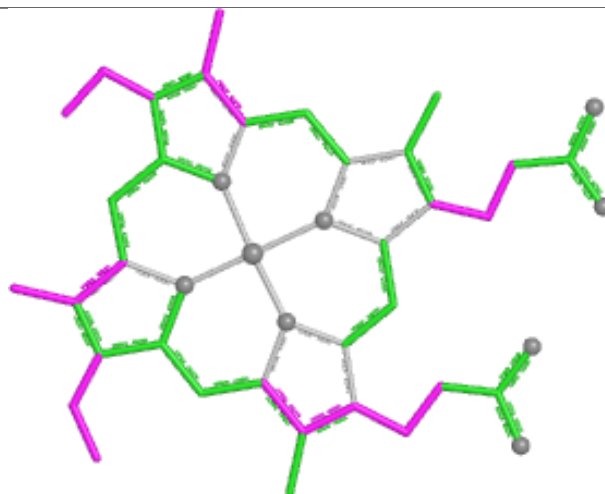




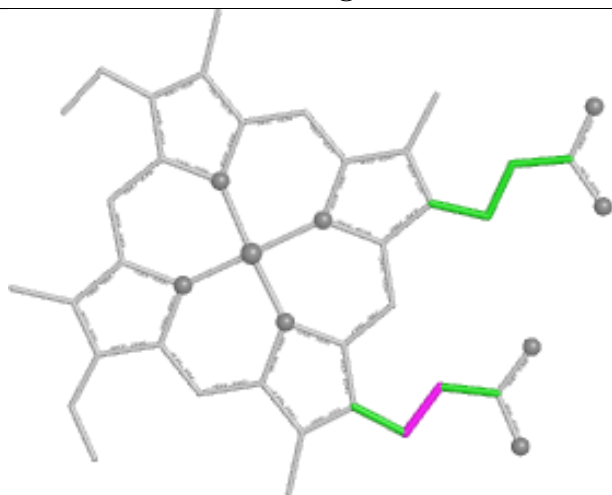
## Ligand HEC B 907



Bond lengths



Bond angles

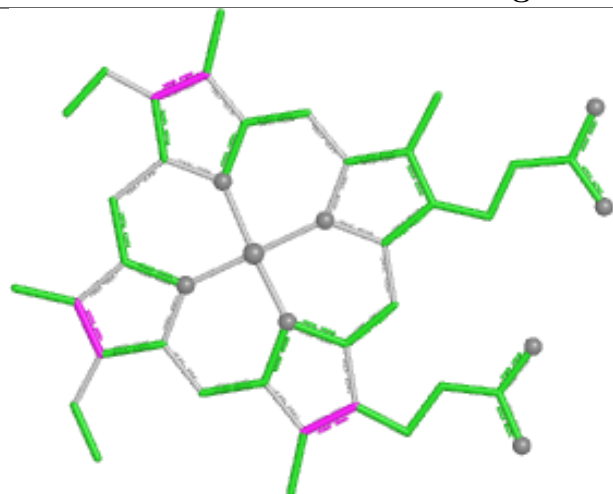


Torsions

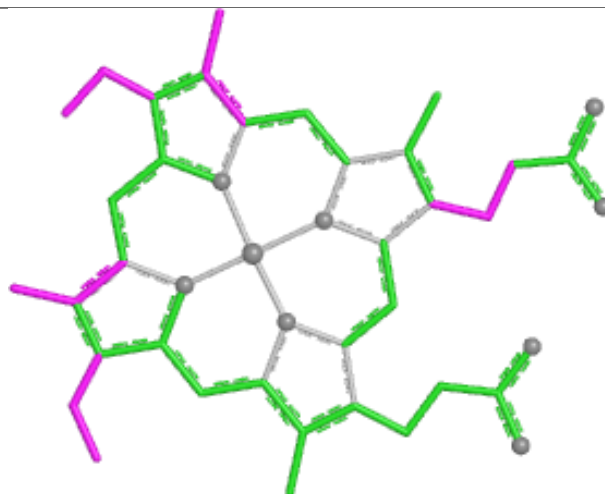


Rings

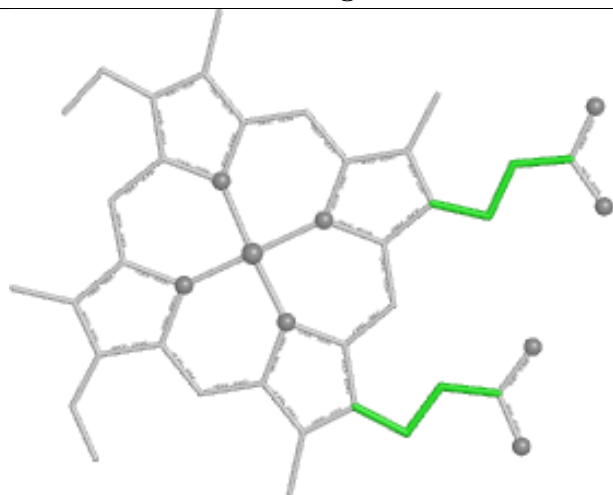
## Ligand HEC C 808



Bond lengths



Bond angles

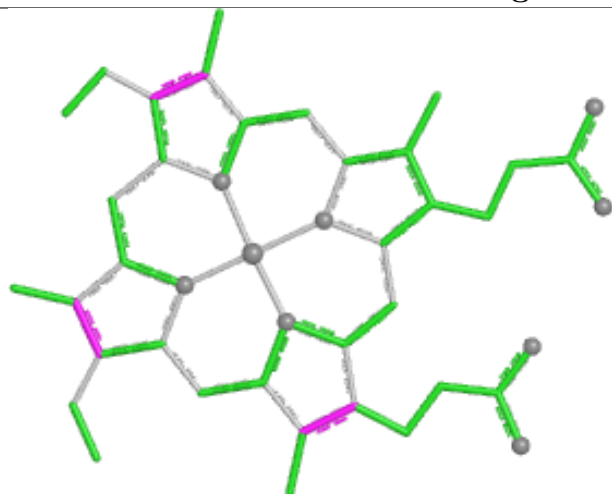


Torsions

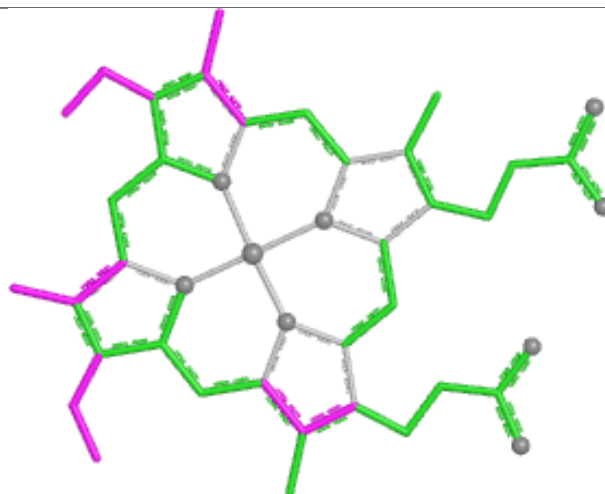


Rings

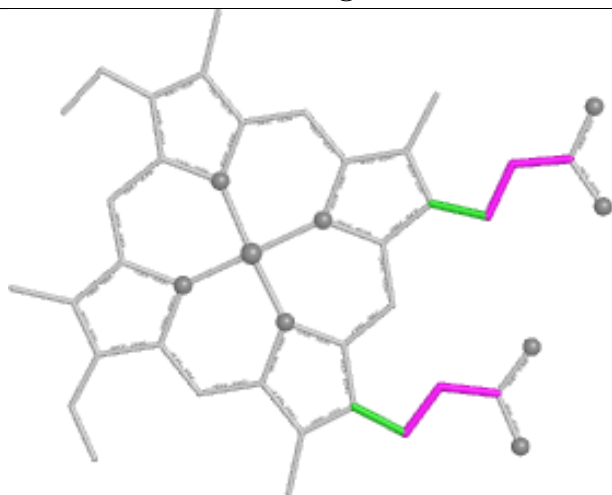
## Ligand HEC C 804



Bond lengths



Bond angles

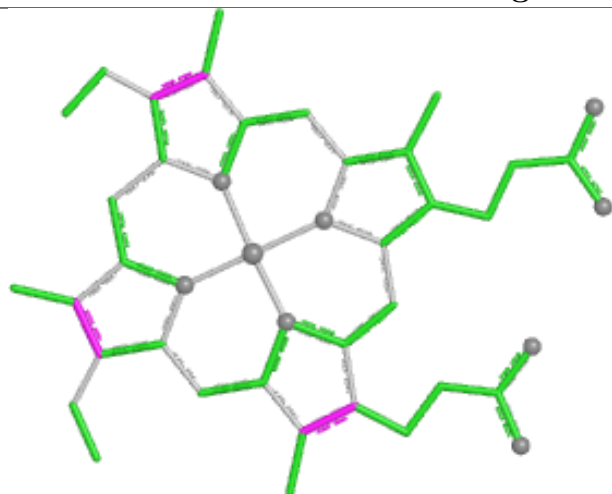


Torsions

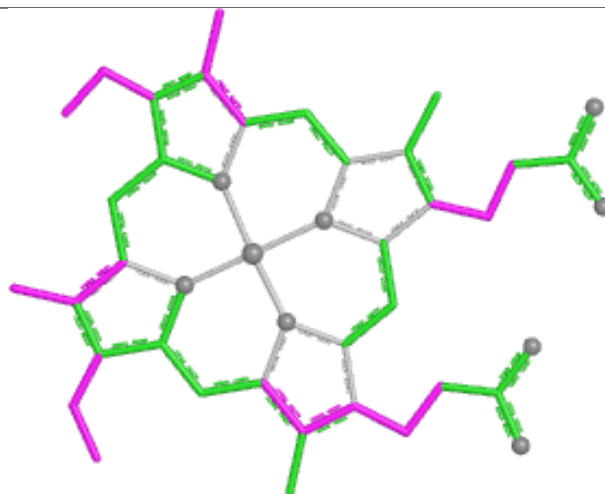


Rings

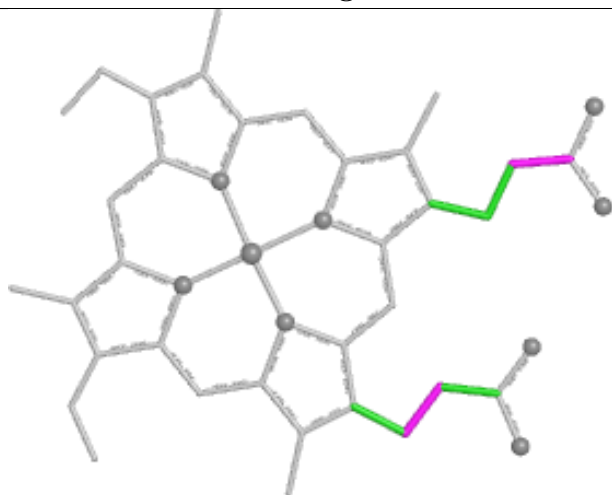
## Ligand HEC C 806



Bond lengths



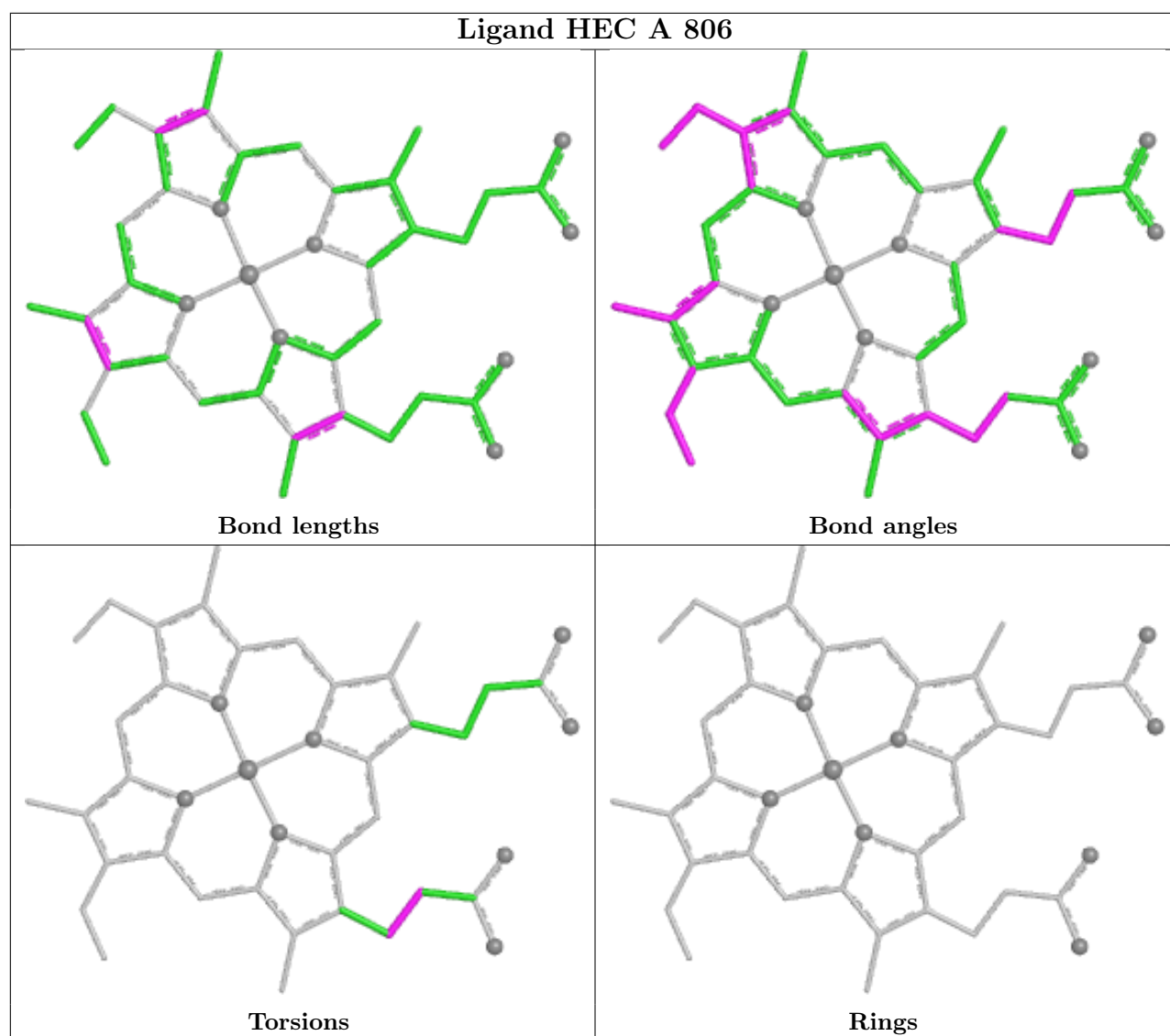
Bond angles



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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	693/760 (91%)	-0.30	14 (2%) 64 64	18, 36, 70, 148	0
1	B	694/760 (91%)	-0.26	18 (2%) 57 56	18, 35, 63, 113	0
1	C	692/760 (91%)	-0.27	16 (2%) 61 60	17, 37, 74, 110	0
1	D	695/760 (91%)	-0.46	11 (1%) 70 70	15, 31, 55, 111	0
All	All	2774/3040 (91%)	-0.32	59 (2%) 63 63	15, 34, 67, 148	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	688	TYR	8.2
1	D	43	VAL	6.1
1	D	737	GLY	6.1
1	A	43	VAL	5.6
1	B	736	LYS	4.6

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	DMS	B	915	4/4	0.73	0.35	92,92,92,92	0
4	DMS	D	815	4/4	0.73	0.41	115,115,115,115	0
3	CA	A	812	1/1	0.74	0.24	69,69,69,69	0
4	DMS	C	815	4/4	0.82	0.32	84,84,84,84	0
4	DMS	A	815	4/4	0.82	0.24	57,58,61,80	0
4	DMS	D	816	4/4	0.82	0.33	66,66,66,66	0
4	DMS	B	916	4/4	0.85	0.25	46,48,50,71	0
4	DMS	A	814	4/4	0.87	0.28	61,67,77,91	0
4	DMS	C	816	4/4	0.87	0.24	56,67,67,88	0
4	DMS	C	814	4/4	0.88	0.21	59,59,59,59	0
3	CA	D	812	1/1	0.92	0.09	60,60,60,60	0
3	CA	B	913	1/1	0.92	0.10	58,58,58,58	0
4	DMS	D	813	4/4	0.94	0.15	36,43,45,52	0
2	HEC	A	810	43/43	0.94	0.13	58,67,75,80	0
3	CA	C	812	1/1	0.94	0.09	57,57,57,57	0
2	HEC	C	810	43/43	0.95	0.12	62,71,76,83	0
4	DMS	B	914	4/4	0.95	0.16	46,49,57,59	0
2	HEC	B	911	43/43	0.97	0.10	26,32,52,58	0
3	CA	C	811	1/1	0.97	0.04	39,39,39,39	0
4	DMS	C	813	4/4	0.97	0.13	41,42,46,47	0
2	HEC	C	807	43/43	0.97	0.09	28,34,46,63	0
2	HEC	C	809	43/43	0.97	0.11	46,60,71,75	0
4	DMS	A	813	4/4	0.97	0.10	46,50,53,58	0
2	HEC	A	809	43/43	0.97	0.10	40,53,71,81	0
4	DMS	D	814	4/4	0.97	0.08	23,35,38,42	0
2	HEC	D	810	43/43	0.97	0.08	22,27,44,48	0
2	HEC	B	904	43/43	0.97	0.08	25,32,37,40	0
2	HEC	D	804	43/43	0.98	0.08	24,31,36,51	0
2	HEC	D	805	43/43	0.98	0.07	23,32,39,46	0
2	HEC	D	806	43/43	0.98	0.07	17,22,36,43	0
2	HEC	D	807	43/43	0.98	0.08	18,25,36,62	0
2	HEC	D	809	43/43	0.98	0.08	21,29,59,69	0
2	HEC	A	804	43/43	0.98	0.07	20,27,33,51	0
3	CA	A	811	1/1	0.98	0.04	30,30,30,30	0
2	HEC	B	903	43/43	0.98	0.08	24,31,43,46	0
3	CA	B	912	1/1	0.98	0.04	51,51,51,51	0
2	HEC	A	805	43/43	0.98	0.08	25,30,35,37	0
2	HEC	B	905	43/43	0.98	0.09	26,33,42,50	0
2	HEC	B	906	43/43	0.98	0.08	27,34,37,39	0
2	HEC	B	907	43/43	0.98	0.07	18,24,35,42	0
2	HEC	B	908	43/43	0.98	0.07	19,26,35,54	0
2	HEC	B	909	43/43	0.98	0.07	17,24,28,32	0
2	HEC	B	910	43/43	0.98	0.09	24,31,67,73	0

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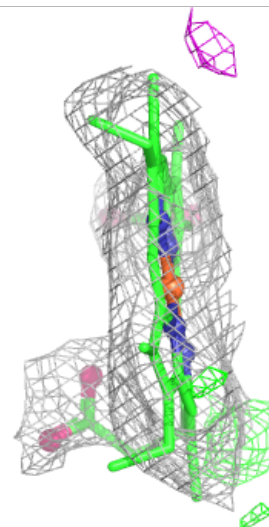
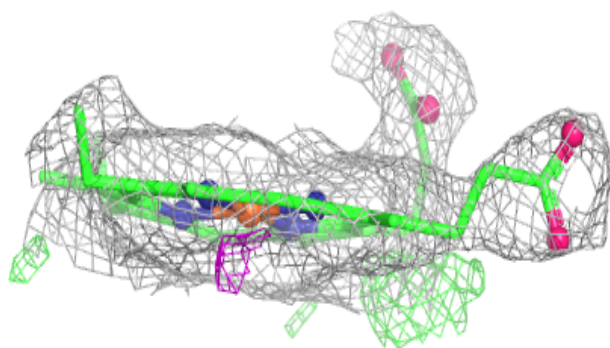
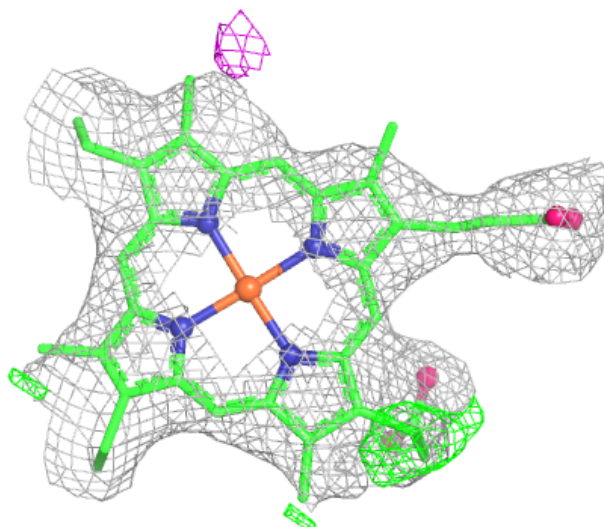
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	B	901	4/4	0.98	0.08	31,36,37,45	0
2	HEC	A	806	43/43	0.98	0.07	23,29,41,45	0
2	HEC	C	802	43/43	0.98	0.07	16,23,30,36	0
2	HEC	C	804	43/43	0.98	0.08	20,27,37,43	0
2	HEC	C	805	43/43	0.98	0.07	23,28,34,46	0
2	HEC	C	806	43/43	0.98	0.08	27,31,43,52	0
2	HEC	A	807	43/43	0.98	0.07	27,33,41,49	0
2	HEC	C	808	43/43	0.98	0.07	29,37,43,48	0
2	HEC	A	808	43/43	0.98	0.07	28,38,43,44	0
2	HEC	A	802	43/43	0.98	0.07	15,22,29,35	0
2	HEC	D	801	43/43	0.98	0.06	16,20,26,28	0
2	HEC	D	802	43/43	0.98	0.09	21,27,36,44	0
3	CA	D	811	1/1	0.99	0.03	38,38,38,38	0
2	HEC	D	803	43/43	0.99	0.06	19,26,30,33	0
2	HEC	C	803	43/43	0.99	0.06	18,23,27,32	0
2	HEC	A	801	43/43	0.99	0.06	18,22,29,34	0
2	HEC	B	902	43/43	0.99	0.06	19,24,27,30	0
4	DMS	A	816	4/4	0.99	0.06	28,31,36,41	0
2	HEC	C	801	43/43	0.99	0.06	20,23,28,30	0
2	HEC	D	808	43/43	0.99	0.05	16,23,27,30	0
2	HEC	A	803	43/43	0.99	0.05	16,20,24,32	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.



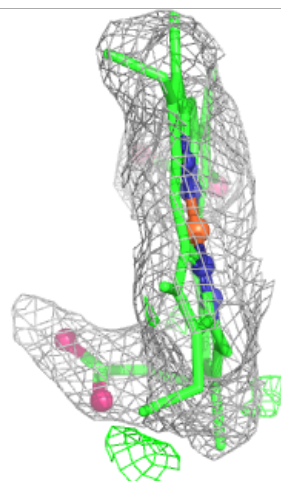
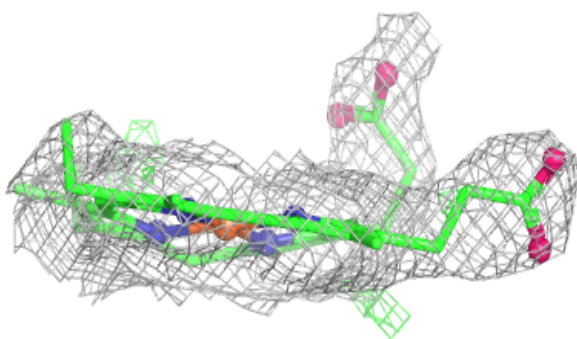
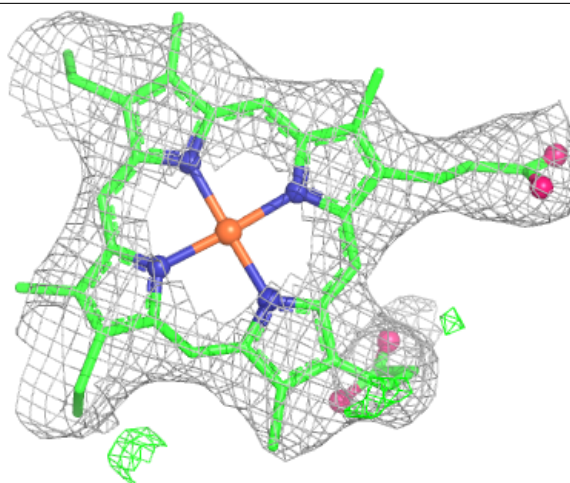
**Electron density around HEC A 810:**

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



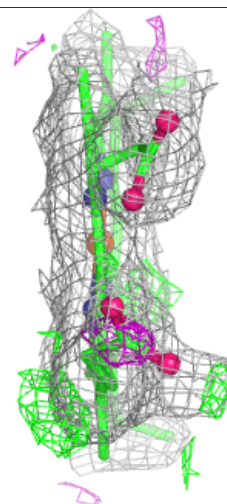
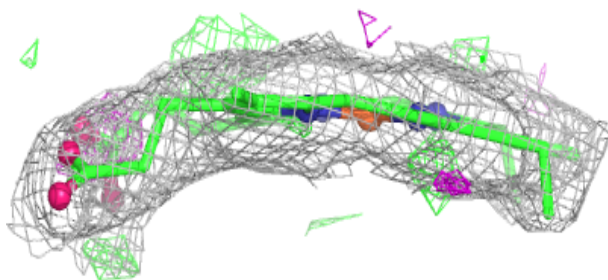
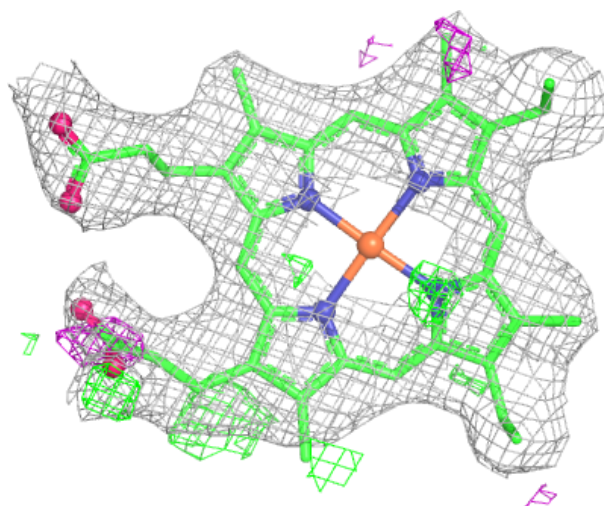
**Electron density around HEC C 810:**

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



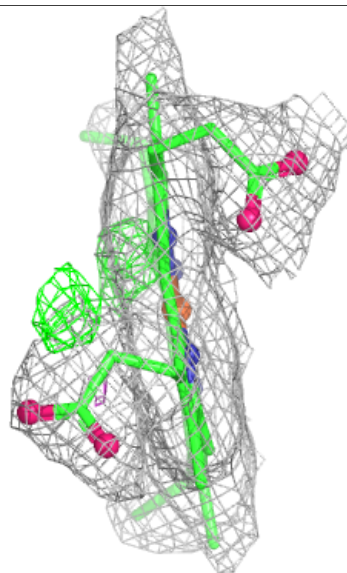
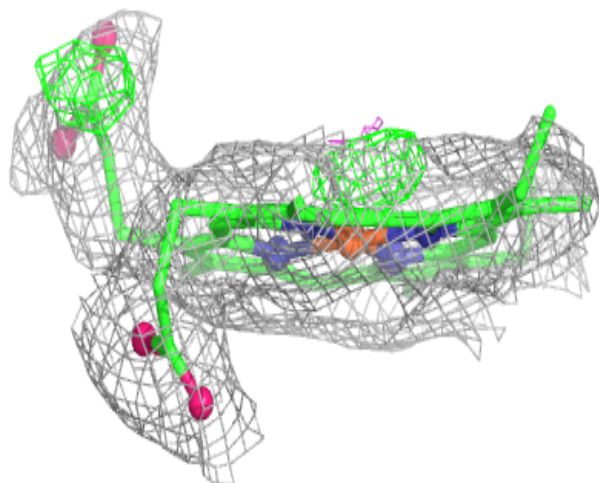
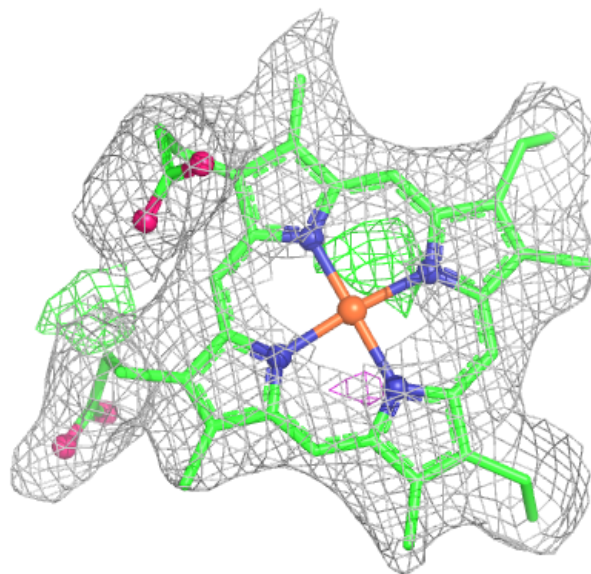
**Electron density around HEC B 911:**

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



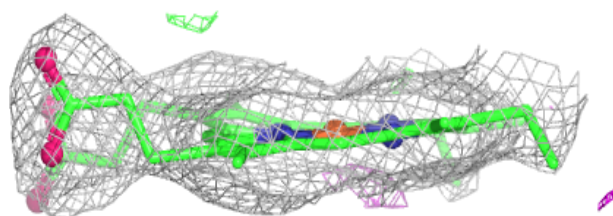
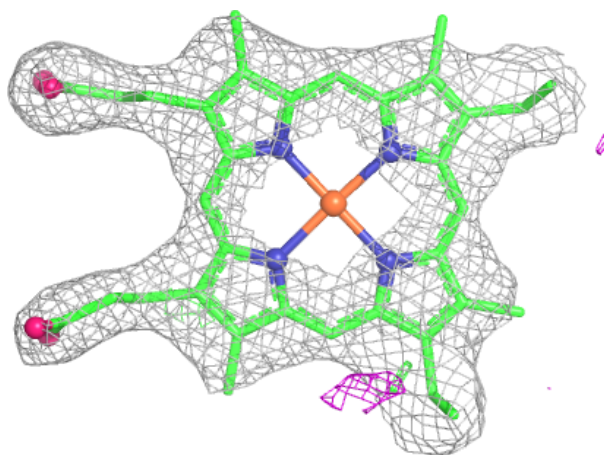
**Electron density around HEC C 807:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC C 809:**

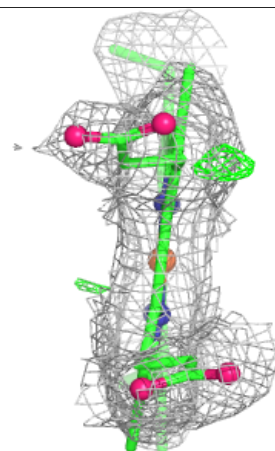
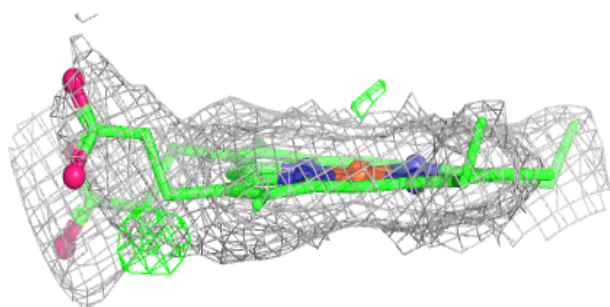
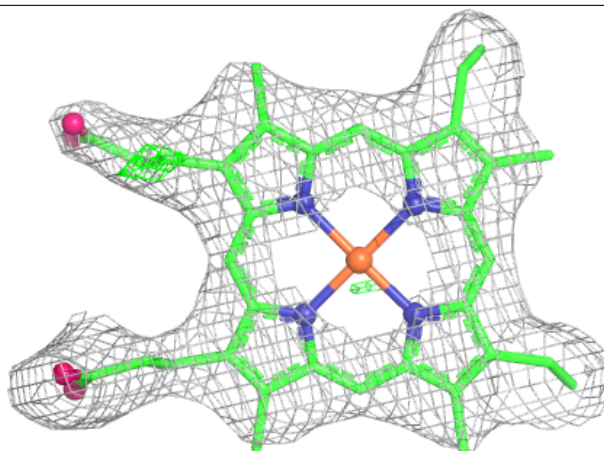
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





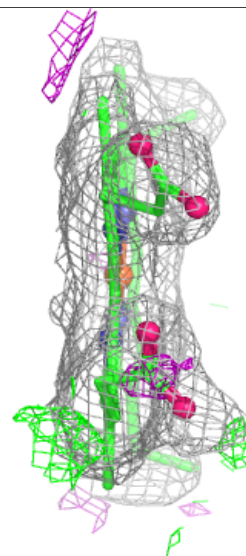
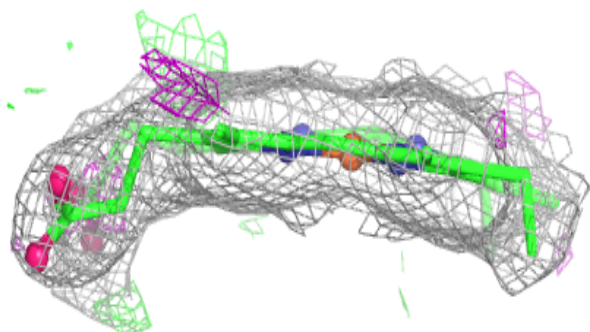
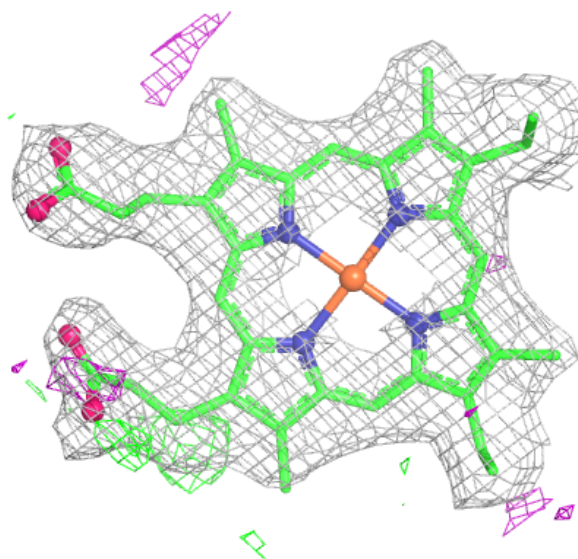
**Electron density around HEC A 809:**

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



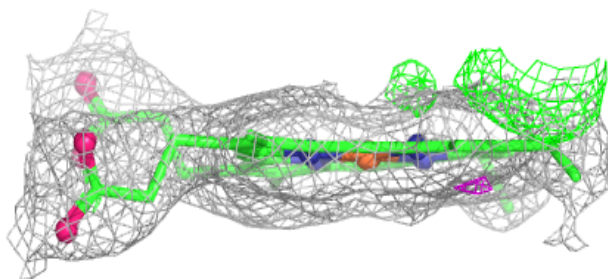
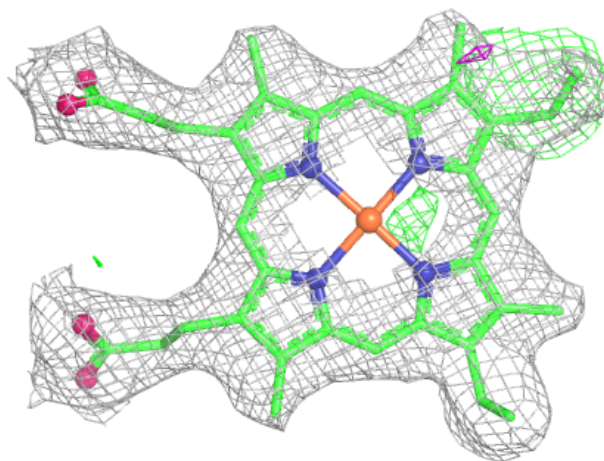
**Electron density around HEC D 810:**

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



**Electron density around HEC B 904:**

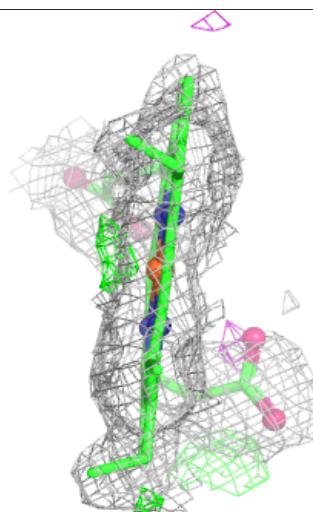
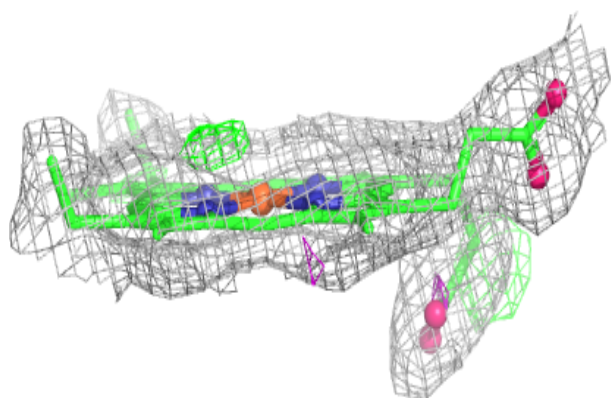
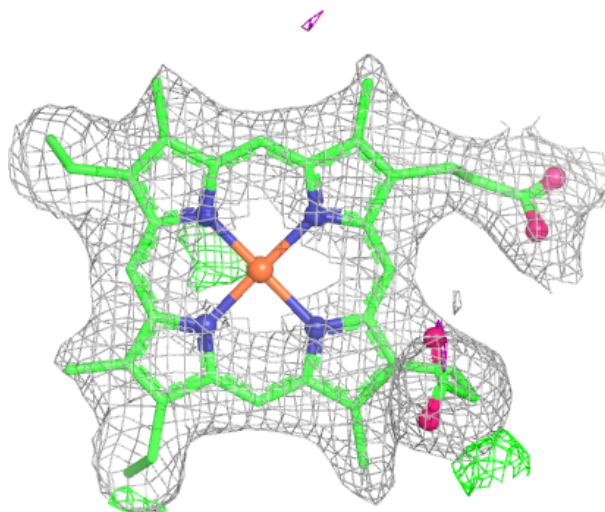
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





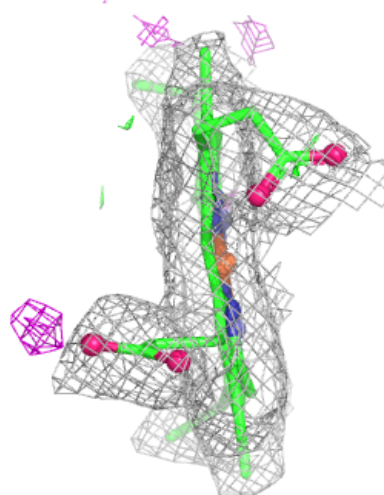
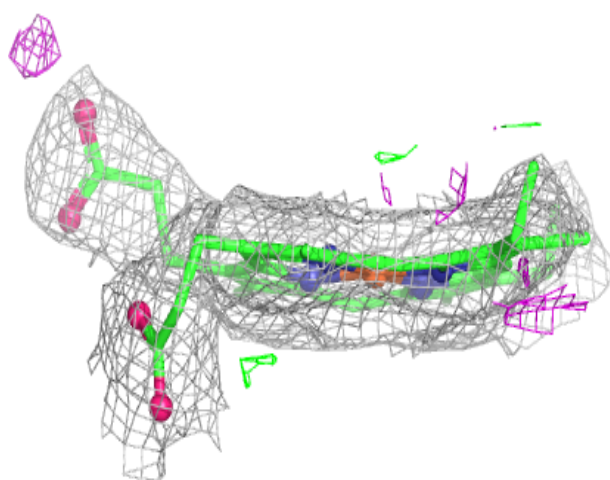
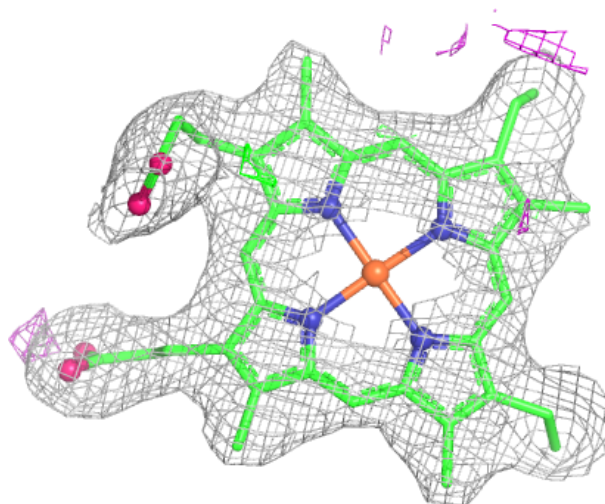
**Electron density around HEC D 804:**

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



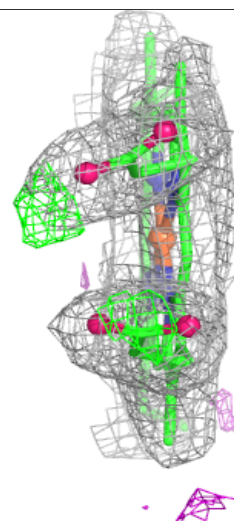
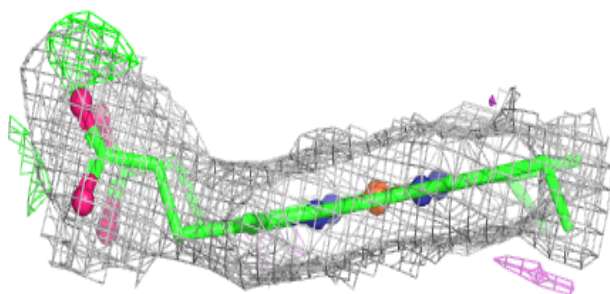
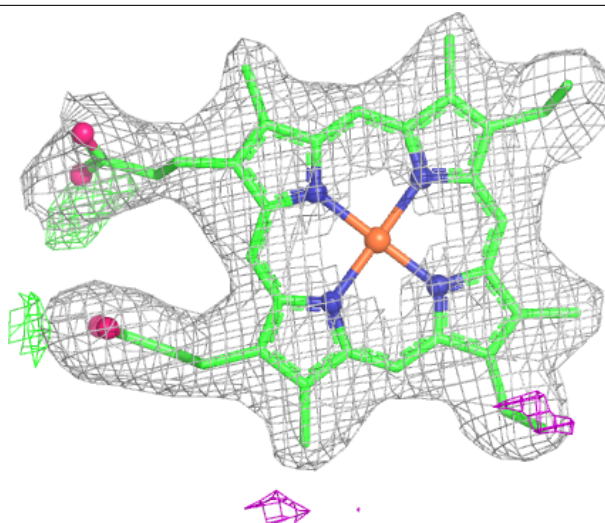
**Electron density around HEC D 805:**

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and green (positive)



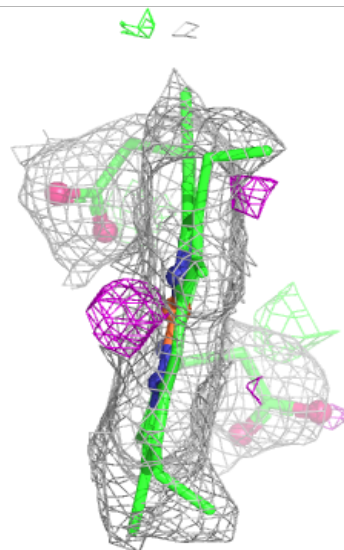
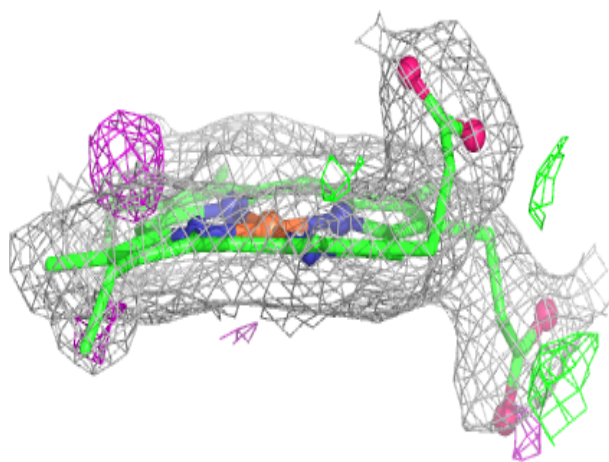
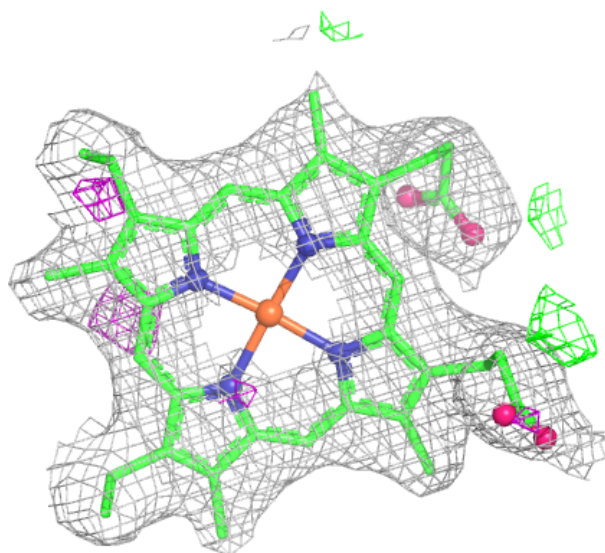
**Electron density around HEC D 806:**

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



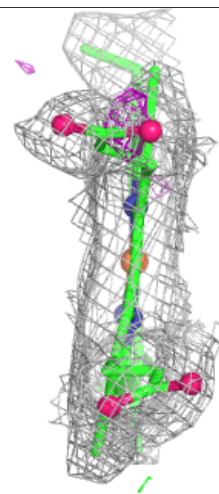
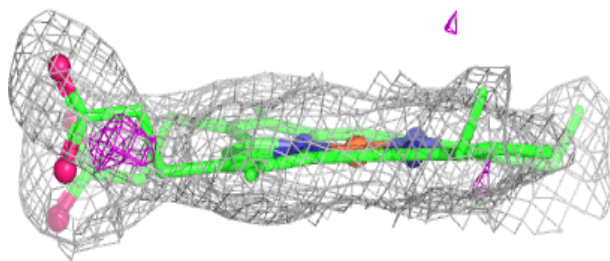
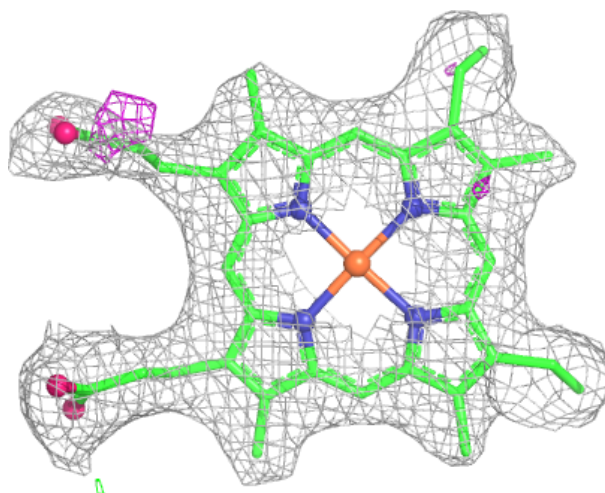
**Electron density around HEC D 807:**

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



**Electron density around HEC D 809:**

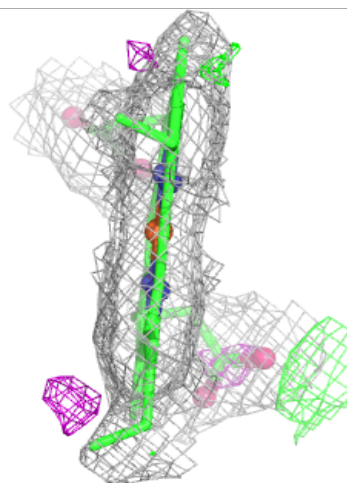
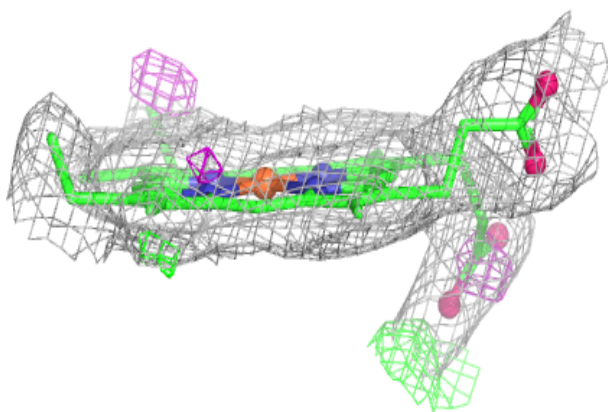
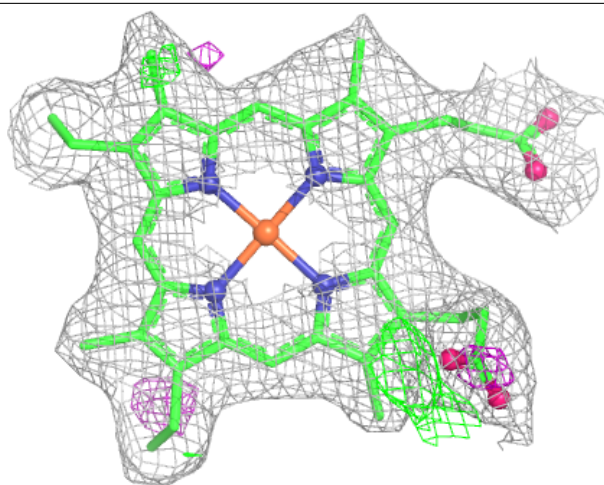
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)





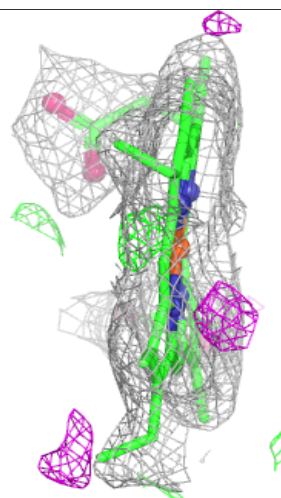
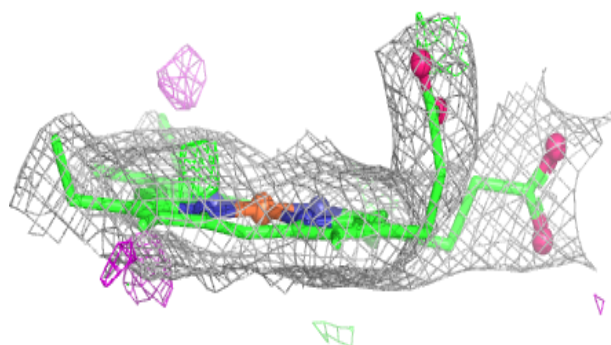
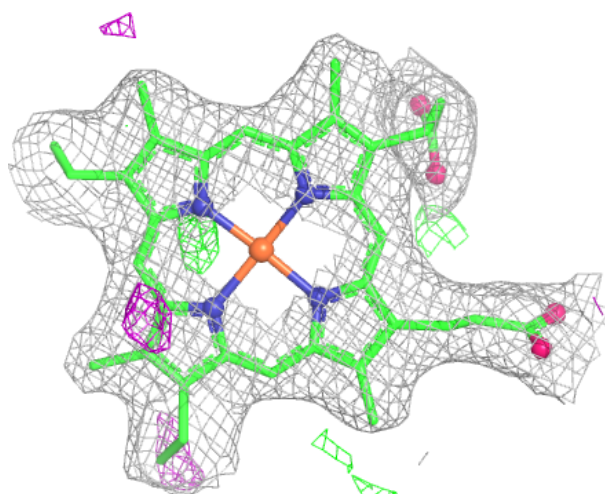
**Electron density around HEC A 804:**

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and green (positive)



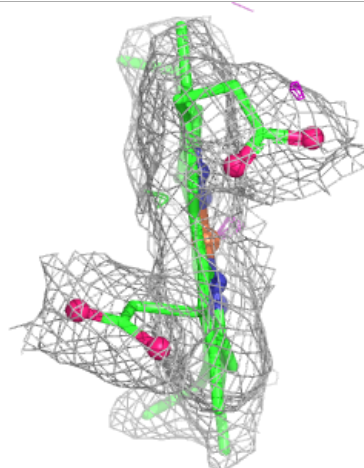
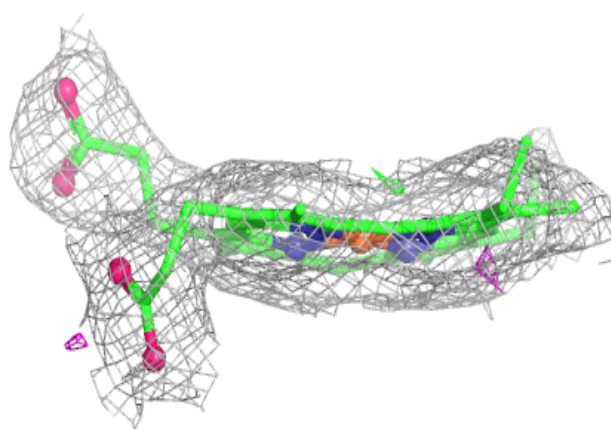
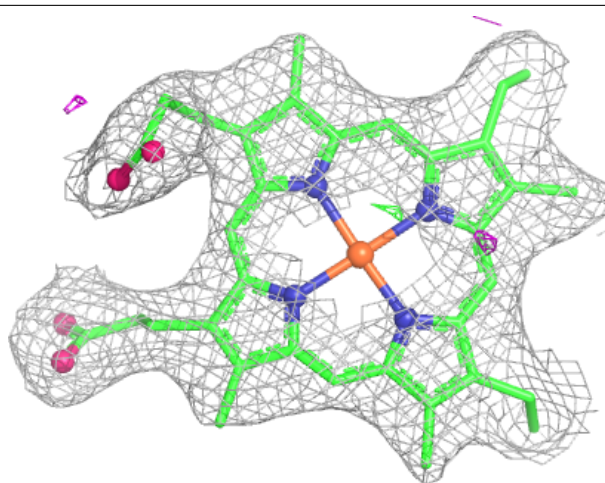
**Electron density around HEC B 903:**

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and green (positive)



**Electron density around HEC A 805:**

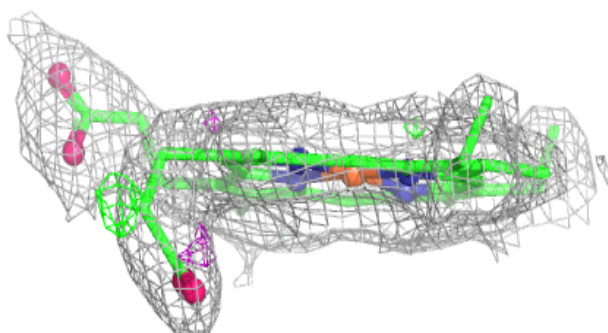
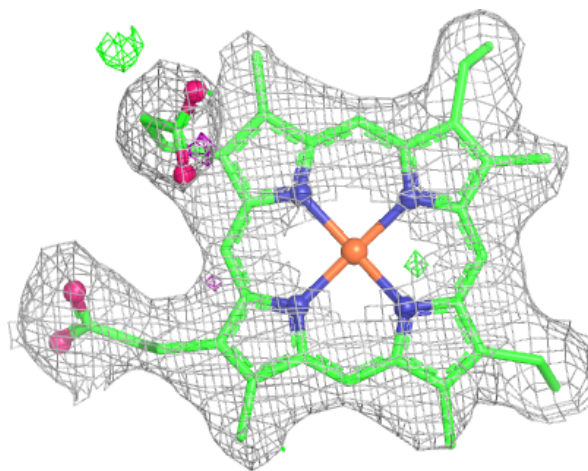
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





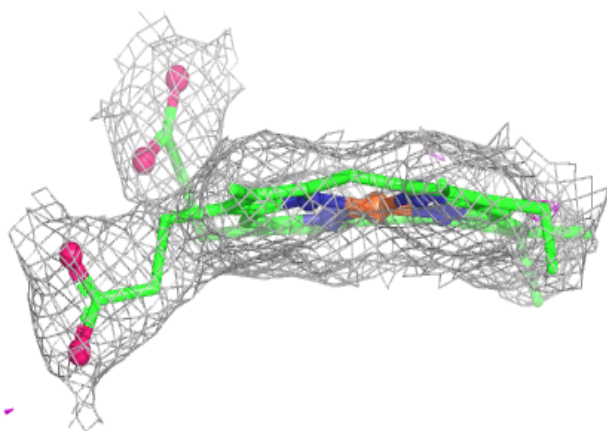
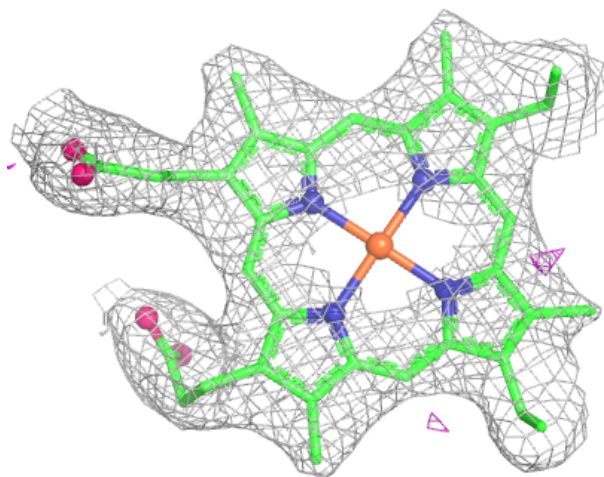
**Electron density around HEC B 905:**

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



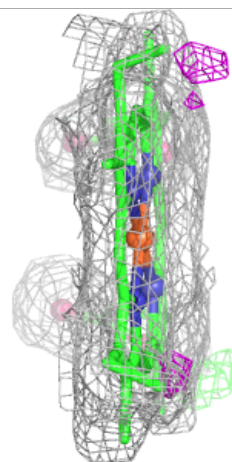
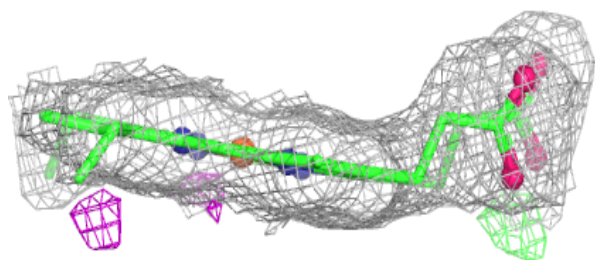
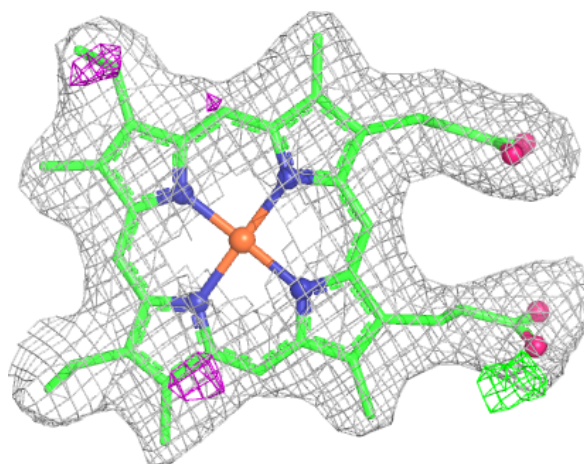
**Electron density around HEC B 906:**

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



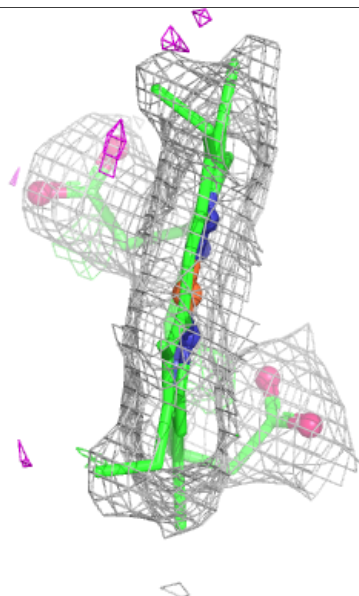
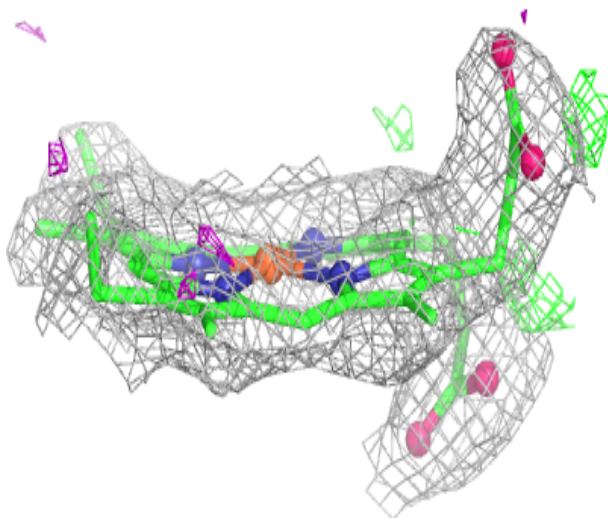
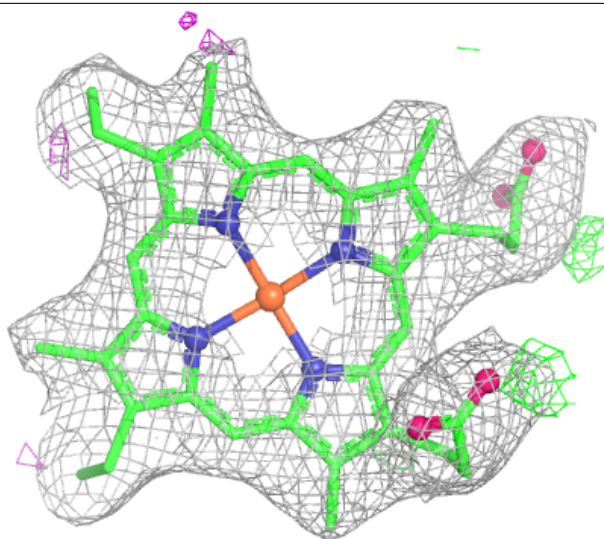
**Electron density around HEC B 907:**

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



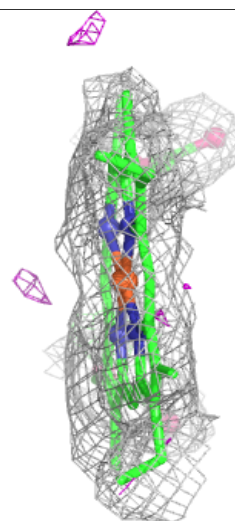
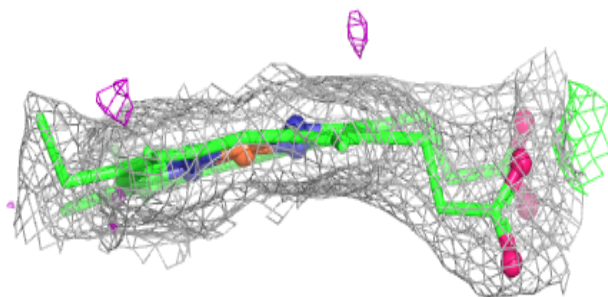
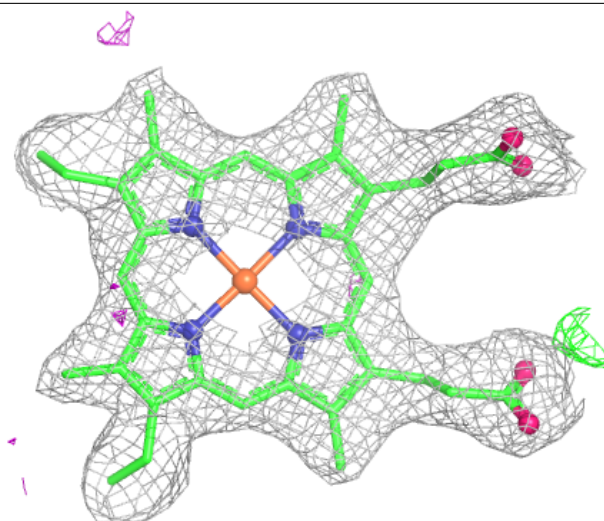
**Electron density around HEC B 908:**

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



**Electron density around HEC B 909:**

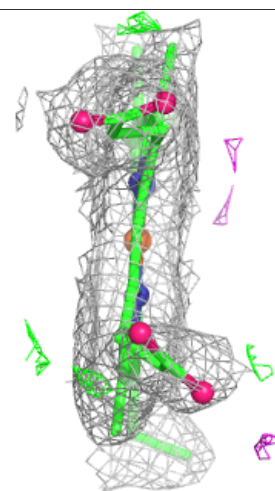
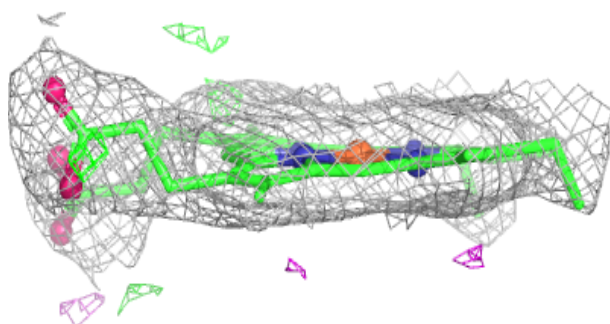
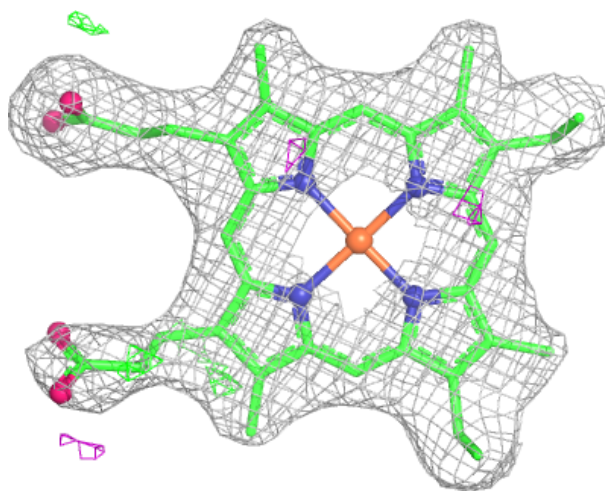
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





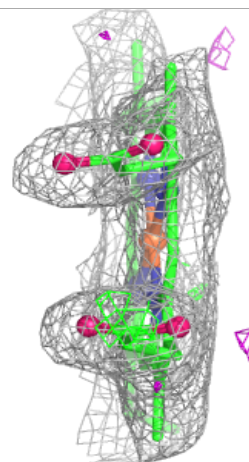
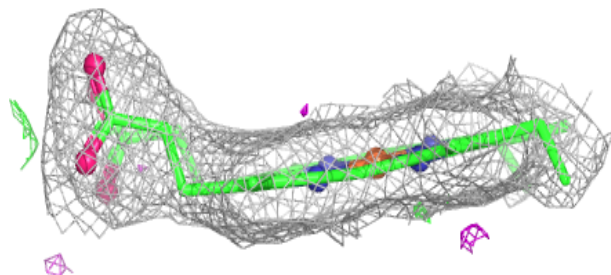
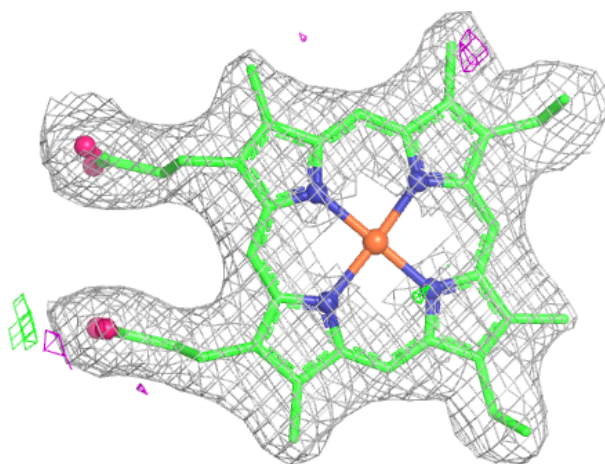
**Electron density around HEC B 910:**

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



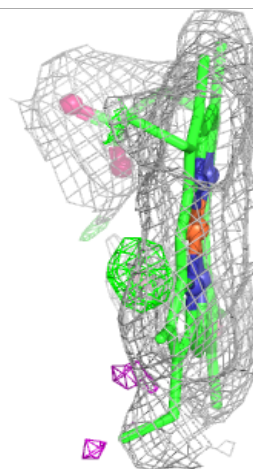
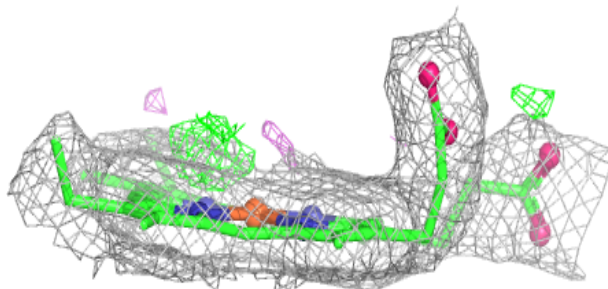
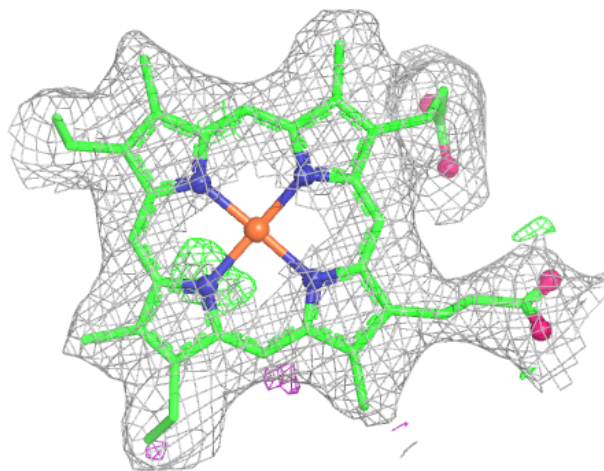
**Electron density around HEC A 806:**

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



**Electron density around HEC C 802:**

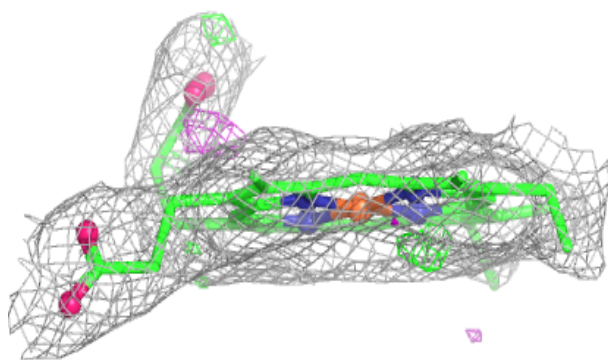
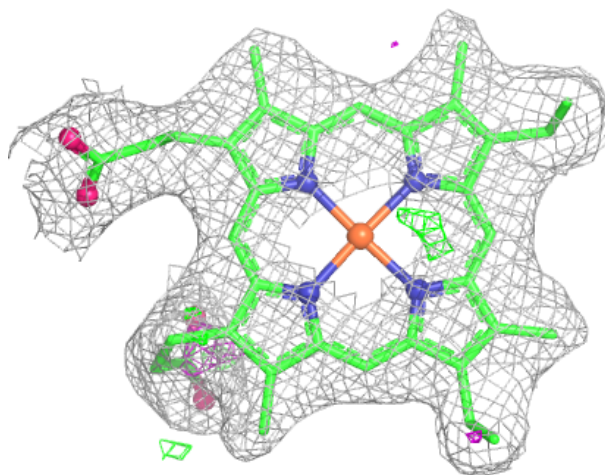
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





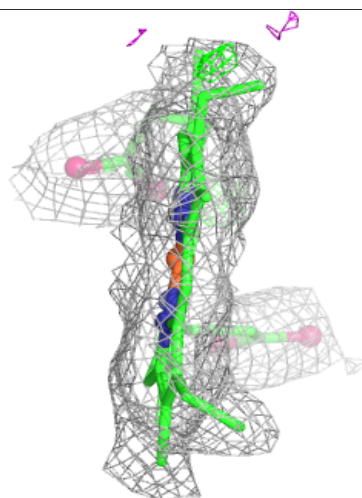
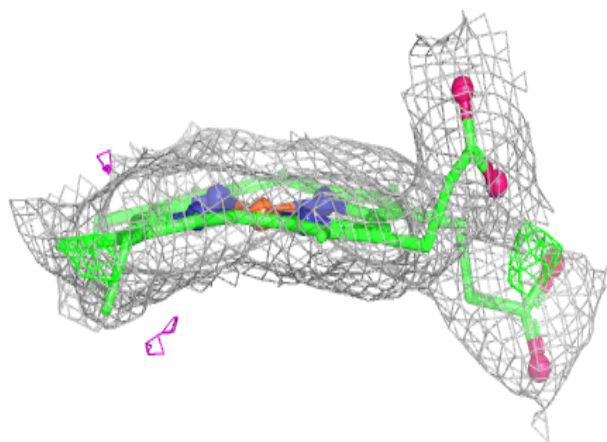
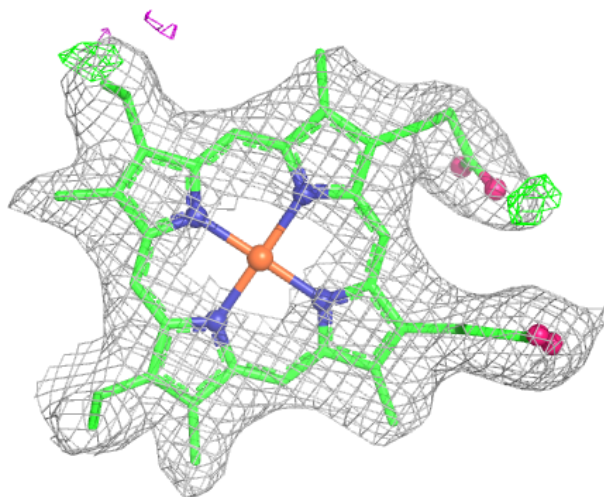
**Electron density around HEC C 804:**

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



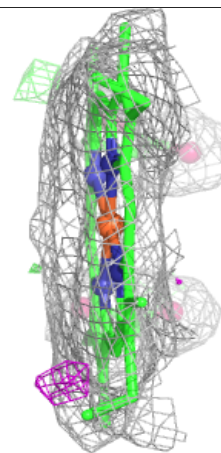
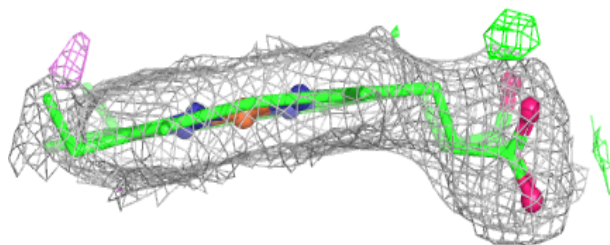
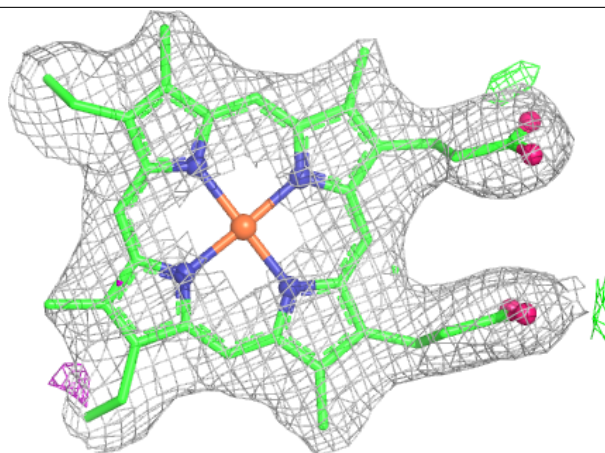
**Electron density around HEC C 805:**

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



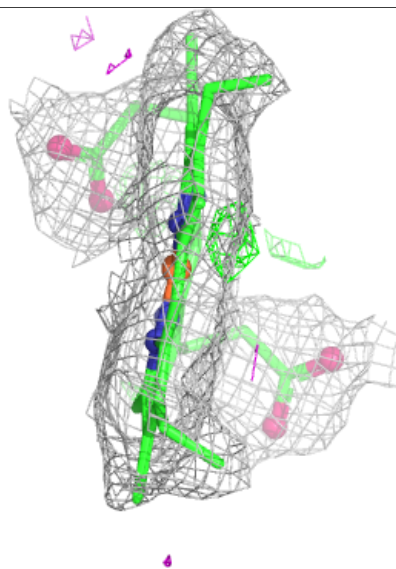
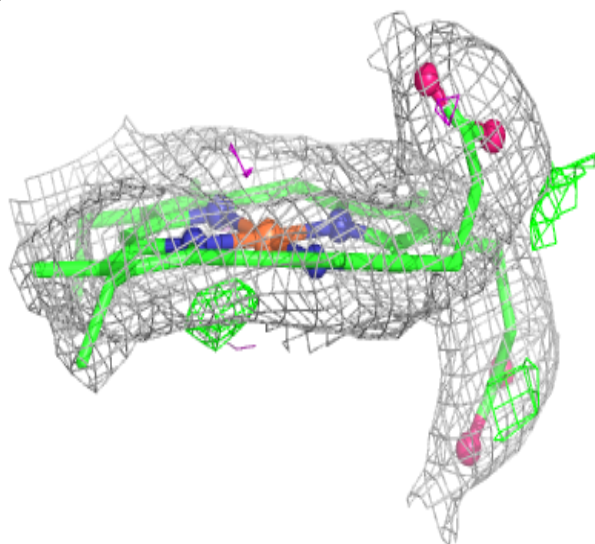
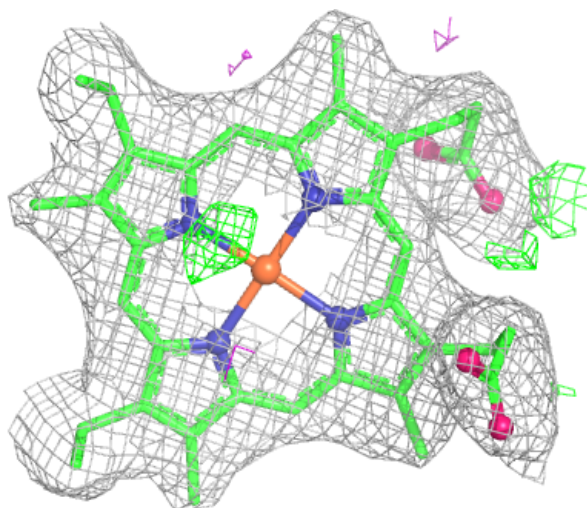
**Electron density around HEC C 806:**

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



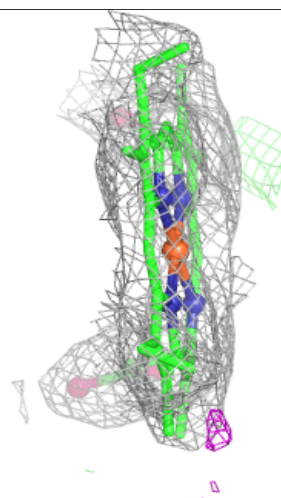
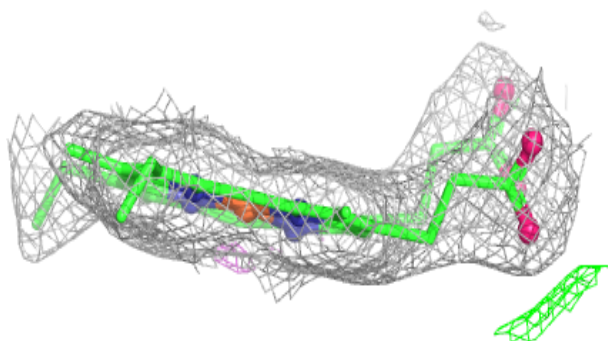
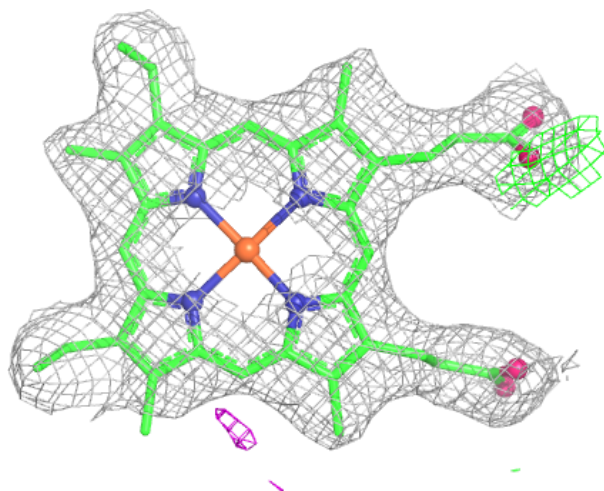
**Electron density around HEC A 807:**

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



**Electron density around HEC C 808:**

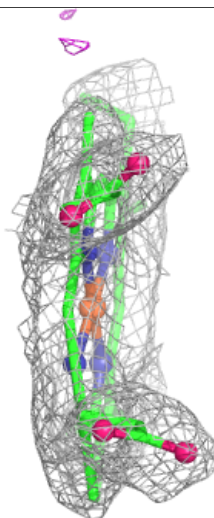
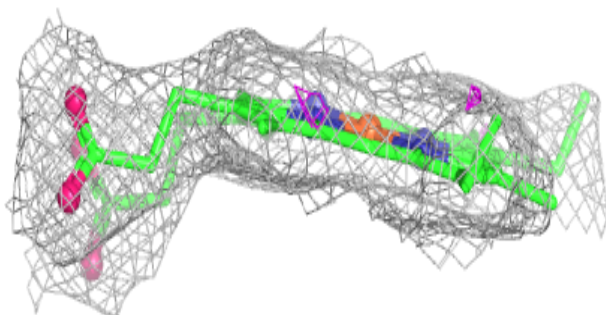
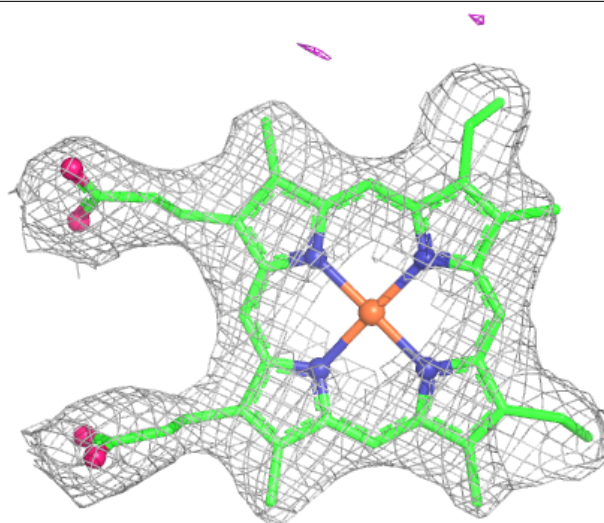
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





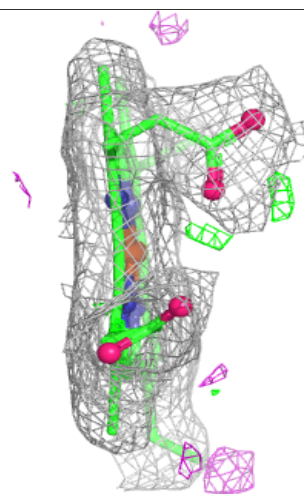
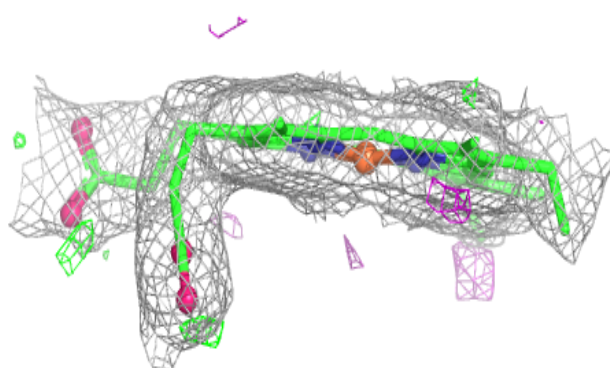
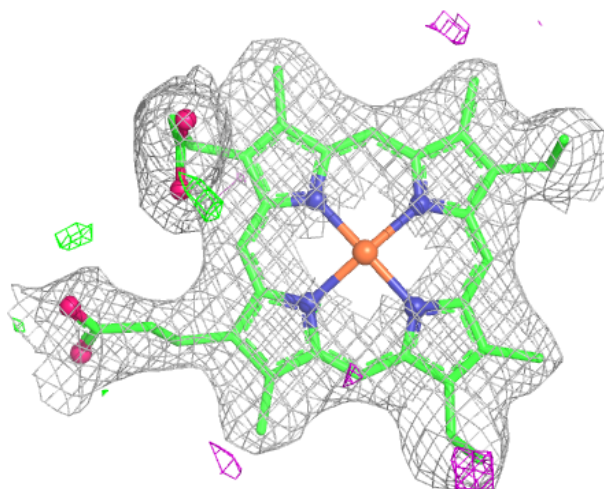
**Electron density around HEC A 808:**

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



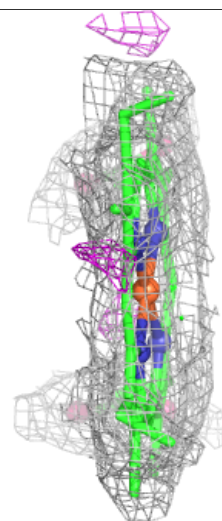
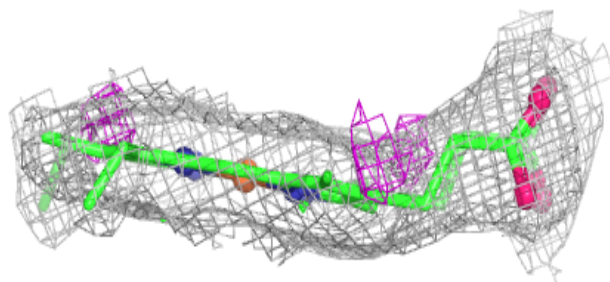
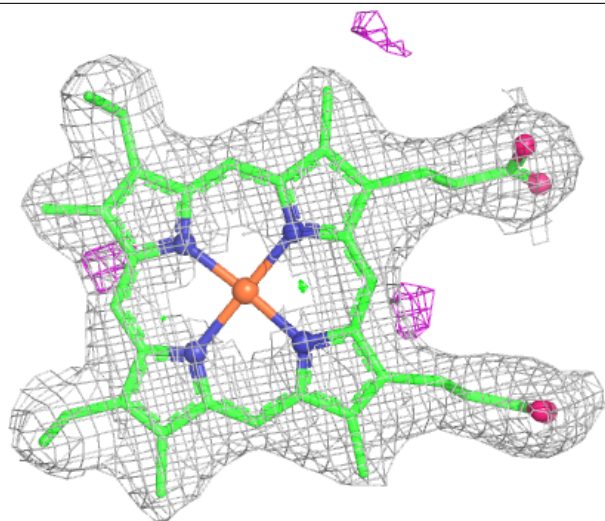
**Electron density around HEC A 802:**

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



**Electron density around HEC D 801:**

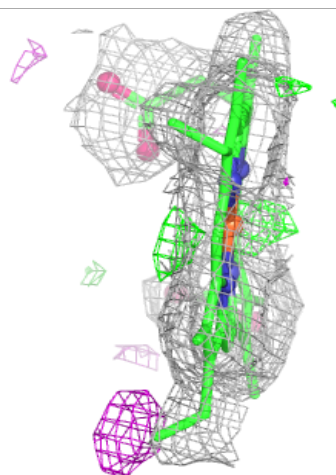
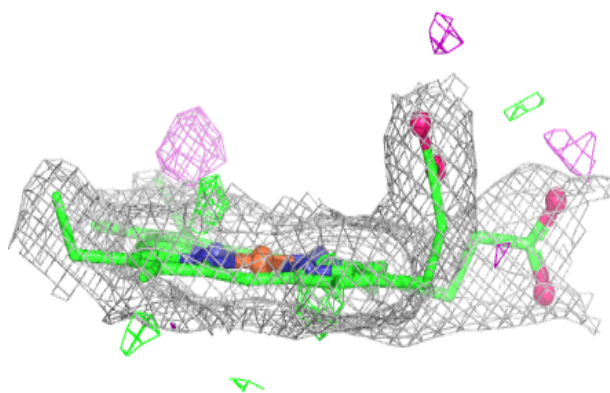
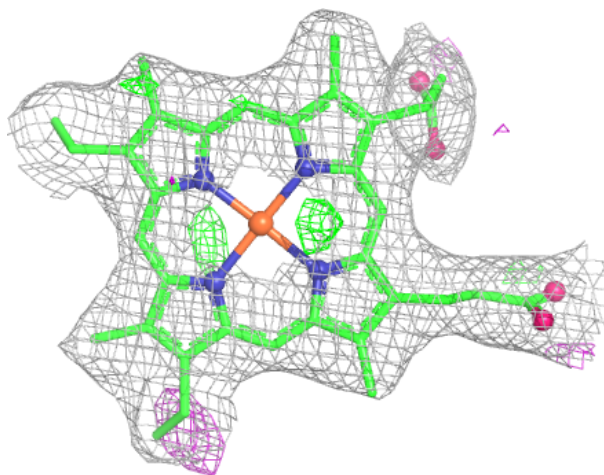
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





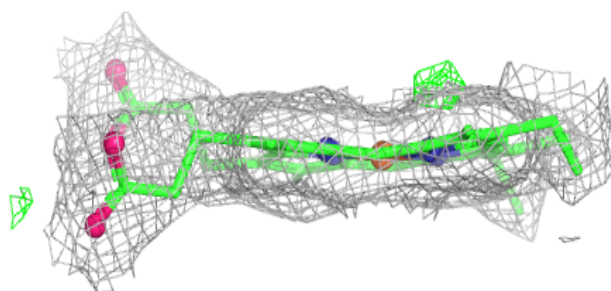
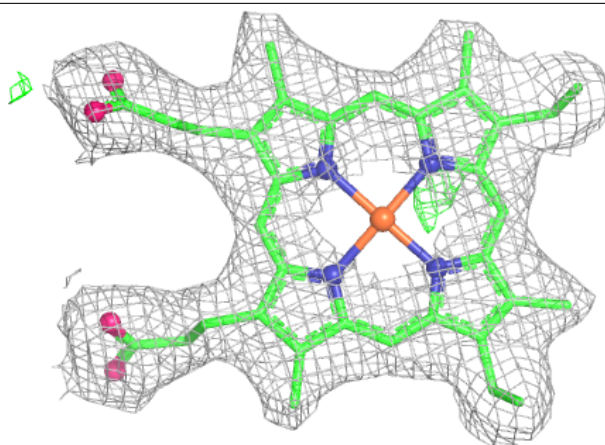
**Electron density around HEC D 802:**

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



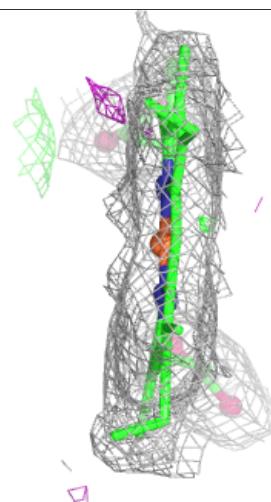
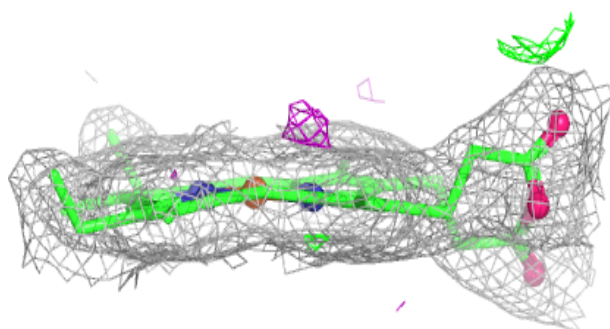
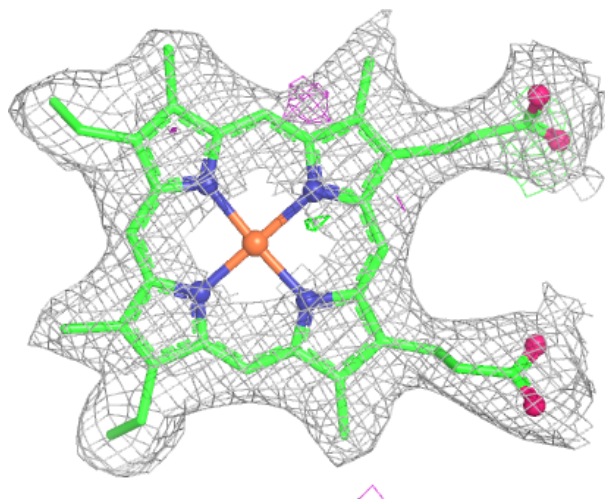
**Electron density around HEC D 803:**

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



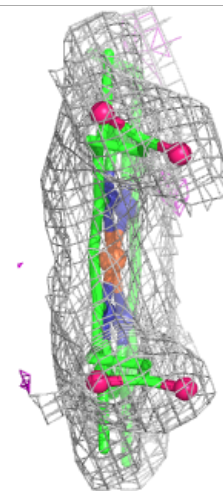
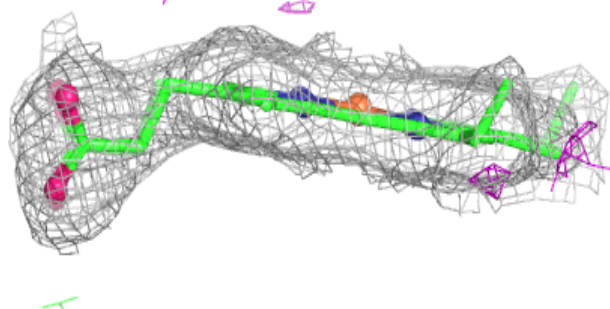
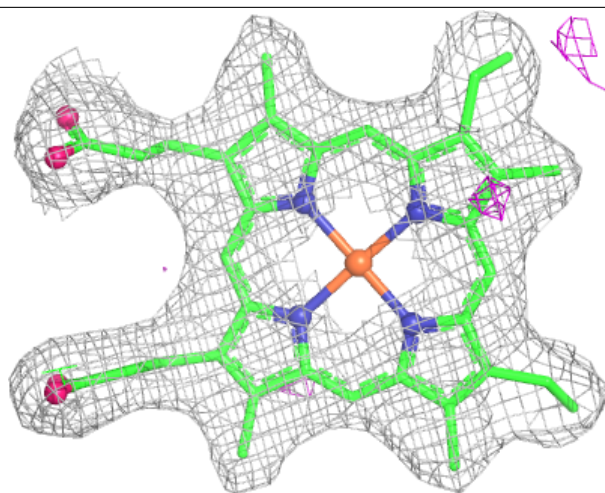
**Electron density around HEC C 803:**

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



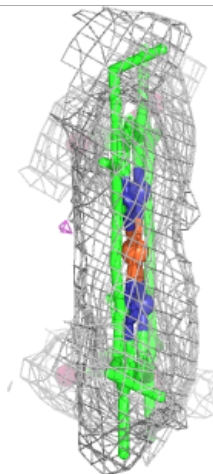
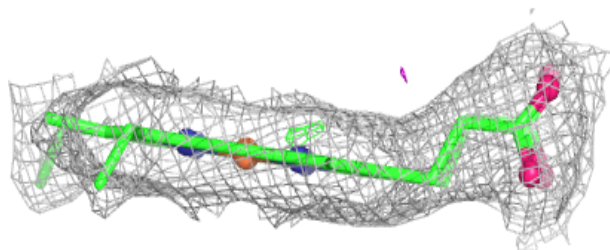
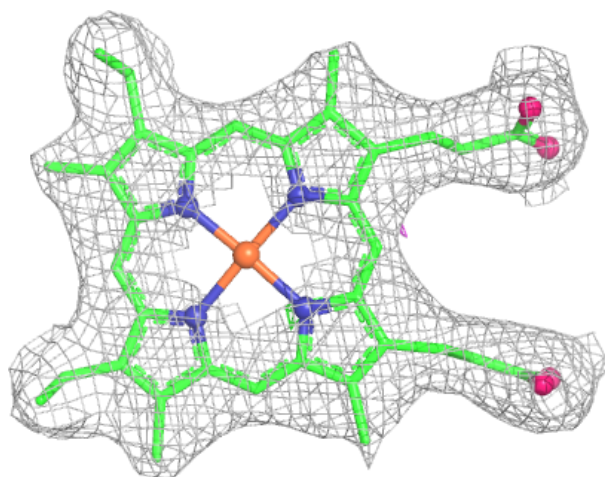
**Electron density around HEC A 801:**

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



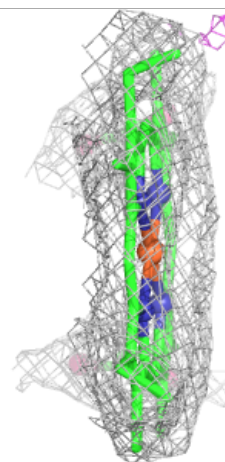
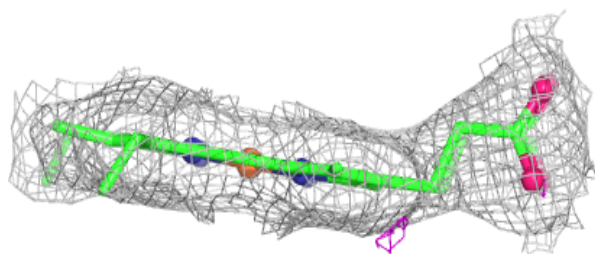
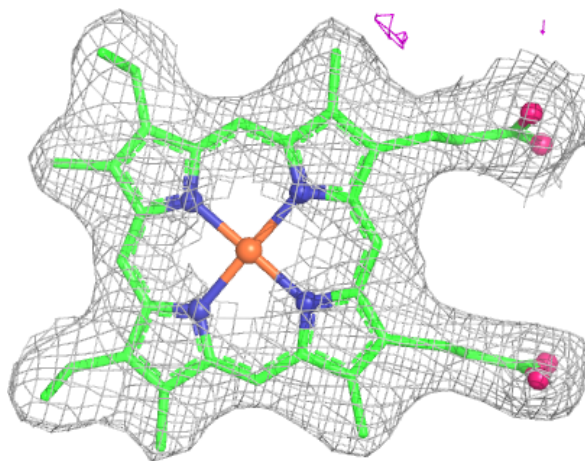
**Electron density around HEC B 902:**

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



**Electron density around HEC C 801:**

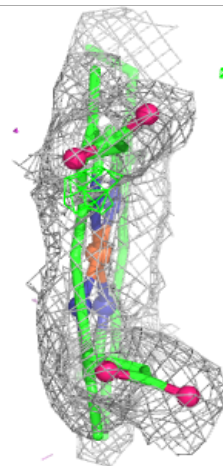
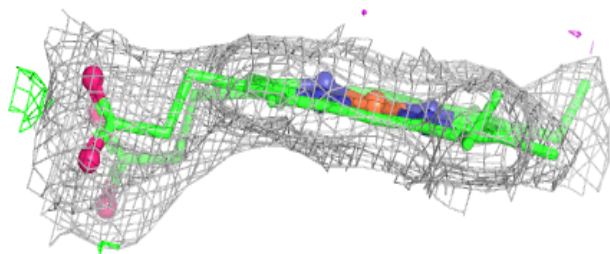
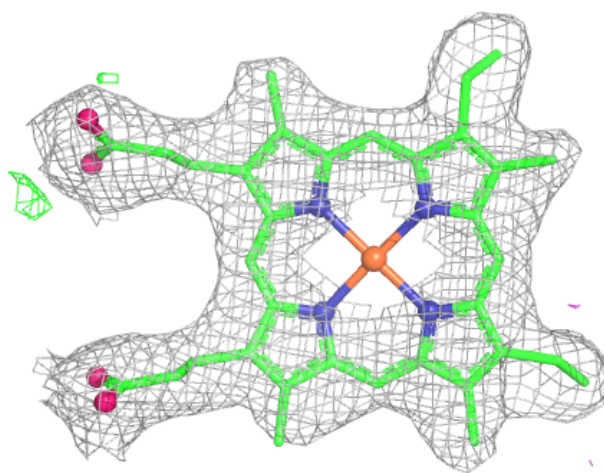
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

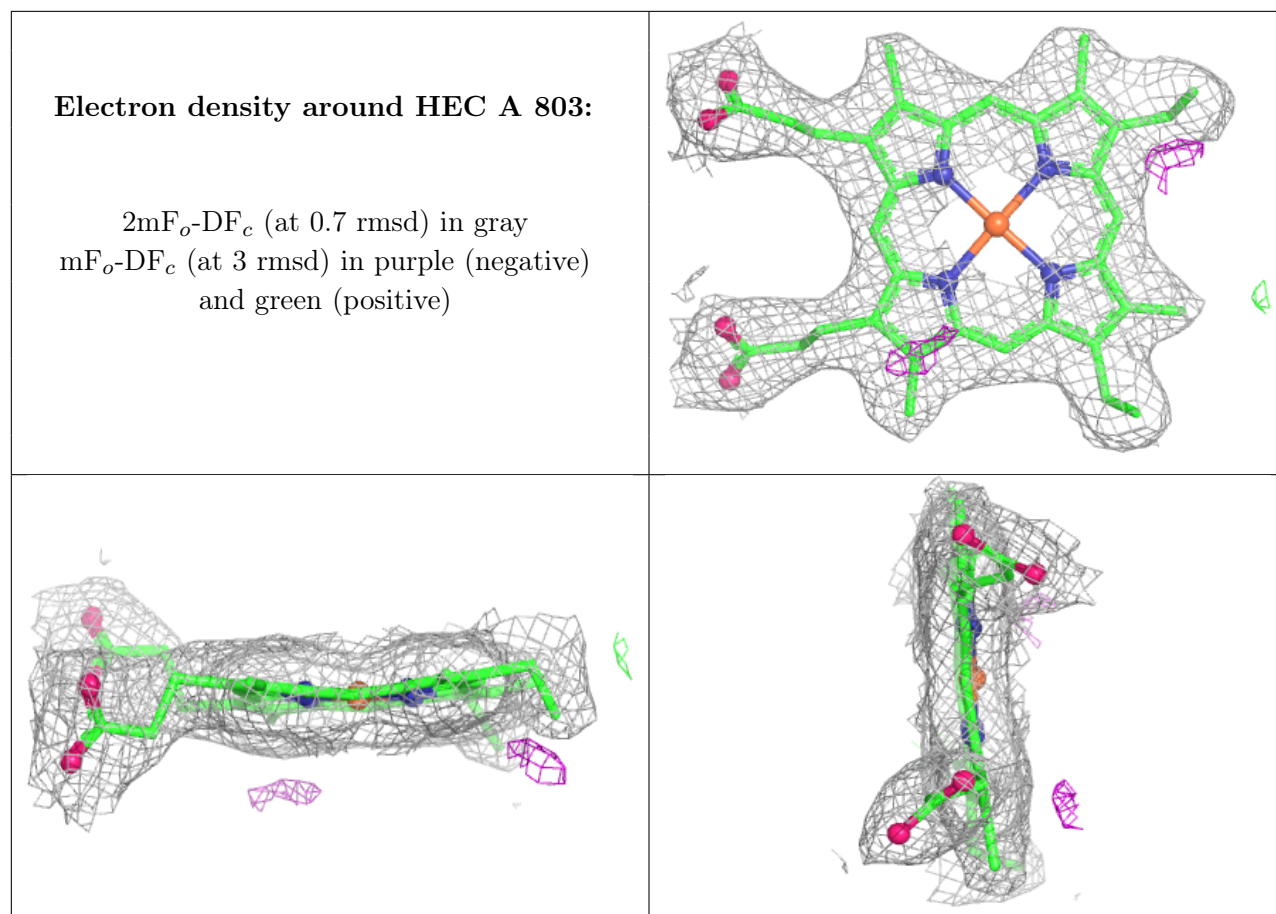




**Electron density around HEC D 808:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.