



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 03:34 am BST

PDB ID : 4BF4  
Title : PikC D50N mutant in complex with the engineered cycloalkane substrate mimic bearing a terminal N,N-dimethylamino group  
Authors : Podust, L.M.  
Deposited on : 2013-03-14  
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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

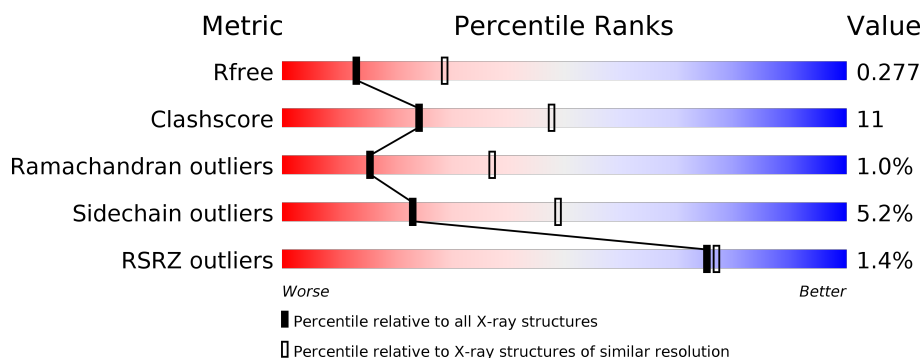
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 on 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	436	
1	B	436	
1	C	436	
1	D	436	
1	E	436	
1	F	436	

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Mol	Chain	Length	Quality of chain
1	G	436	
1	H	436	
1	I	436	
1	J	436	
1	K	436	
1	L	436	
1	M	436	
1	N	436	
1	O	436	
1	P	436	

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
3	SO4	A	1408	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 50342 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 HYDROXYLASE PIKC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3031	1912	545	561	13			
1	B	397	Total	C	N	O	S	0	2	0
			3069	1939	553	564	13			
1	C	396	Total	C	N	O	S	0	1	0
			3063	1937	549	564	13			
1	D	397	Total	C	N	O	S	0	2	0
			3076	1942	552	569	13			
1	E	397	Total	C	N	O	S	0	1	0
			3068	1938	550	567	13			
1	F	396	Total	C	N	O	S	0	4	0
			3075	1944	552	566	13			
1	G	396	Total	C	N	O	S	0	4	0
			3093	1952	557	571	13			
1	H	396	Total	C	N	O	S	0	1	0
			3057	1935	549	560	13			
1	I	396	Total	C	N	O	S	0	2	0
			3066	1939	550	564	13			
1	J	397	Total	C	N	O	S	0	1	0
			3060	1934	551	562	13			
1	K	397	Total	C	N	O	S	0	2	0
			3076	1944	551	568	13			
1	L	397	Total	C	N	O	S	0	2	0
			3065	1938	551	563	13			
1	M	397	Total	C	N	O	S	0	1	0
			3065	1936	551	565	13			
1	N	397	Total	C	N	O	S	0	1	0
			3064	1938	550	563	13			
1	O	397	Total	C	N	O	S	0	0	0
			3052	1931	548	560	13			
1	P	396	Total	C	N	O	S	0	1	0
			3058	1932	548	565	13			

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O87605
A	-18	GLY	-	expression tag	UNP O87605
A	-17	SER	-	expression tag	UNP O87605
A	-16	SER	-	expression tag	UNP O87605
A	-15	HIS	-	expression tag	UNP O87605
A	-14	HIS	-	expression tag	UNP O87605
A	-13	HIS	-	expression tag	UNP O87605
A	-12	HIS	-	expression tag	UNP O87605
A	-11	HIS	-	expression tag	UNP O87605
A	-10	HIS	-	expression tag	UNP O87605
A	-9	SER	-	expression tag	UNP O87605
A	-8	SER	-	expression tag	UNP O87605
A	-7	GLY	-	expression tag	UNP O87605
A	-6	LEU	-	expression tag	UNP O87605
A	-5	VAL	-	expression tag	UNP O87605
A	-4	PRO	-	expression tag	UNP O87605
A	-3	ARG	-	expression tag	UNP O87605
A	-2	GLY	-	expression tag	UNP O87605
A	-1	SER	-	expression tag	UNP O87605
A	0	HIS	-	expression tag	UNP O87605
A	50	ASN	ASP	engineered mutation	UNP O87605
B	-19	MET	-	expression tag	UNP O87605
B	-18	GLY	-	expression tag	UNP O87605
B	-17	SER	-	expression tag	UNP O87605
B	-16	SER	-	expression tag	UNP O87605
B	-15	HIS	-	expression tag	UNP O87605
B	-14	HIS	-	expression tag	UNP O87605
B	-13	HIS	-	expression tag	UNP O87605
B	-12	HIS	-	expression tag	UNP O87605
B	-11	HIS	-	expression tag	UNP O87605
B	-10	HIS	-	expression tag	UNP O87605
B	-9	SER	-	expression tag	UNP O87605
B	-8	SER	-	expression tag	UNP O87605
B	-7	GLY	-	expression tag	UNP O87605
B	-6	LEU	-	expression tag	UNP O87605
B	-5	VAL	-	expression tag	UNP O87605
B	-4	PRO	-	expression tag	UNP O87605
B	-3	ARG	-	expression tag	UNP O87605
B	-2	GLY	-	expression tag	UNP O87605
B	-1	SER	-	expression tag	UNP O87605
B	0	HIS	-	expression tag	UNP O87605
B	50	ASN	ASP	engineered mutation	UNP O87605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	expression tag	UNP 087605
C	-18	GLY	-	expression tag	UNP 087605
C	-17	SER	-	expression tag	UNP 087605
C	-16	SER	-	expression tag	UNP 087605
C	-15	HIS	-	expression tag	UNP 087605
C	-14	HIS	-	expression tag	UNP 087605
C	-13	HIS	-	expression tag	UNP 087605
C	-12	HIS	-	expression tag	UNP 087605
C	-11	HIS	-	expression tag	UNP 087605
C	-10	HIS	-	expression tag	UNP 087605
C	-9	SER	-	expression tag	UNP 087605
C	-8	SER	-	expression tag	UNP 087605
C	-7	GLY	-	expression tag	UNP 087605
C	-6	LEU	-	expression tag	UNP 087605
C	-5	VAL	-	expression tag	UNP 087605
C	-4	PRO	-	expression tag	UNP 087605
C	-3	ARG	-	expression tag	UNP 087605
C	-2	GLY	-	expression tag	UNP 087605
C	-1	SER	-	expression tag	UNP 087605
C	0	HIS	-	expression tag	UNP 087605
C	50	ASN	ASP	engineered mutation	UNP 087605
D	-19	MET	-	expression tag	UNP 087605
D	-18	GLY	-	expression tag	UNP 087605
D	-17	SER	-	expression tag	UNP 087605
D	-16	SER	-	expression tag	UNP 087605
D	-15	HIS	-	expression tag	UNP 087605
D	-14	HIS	-	expression tag	UNP 087605
D	-13	HIS	-	expression tag	UNP 087605
D	-12	HIS	-	expression tag	UNP 087605
D	-11	HIS	-	expression tag	UNP 087605
D	-10	HIS	-	expression tag	UNP 087605
D	-9	SER	-	expression tag	UNP 087605
D	-8	SER	-	expression tag	UNP 087605
D	-7	GLY	-	expression tag	UNP 087605
D	-6	LEU	-	expression tag	UNP 087605
D	-5	VAL	-	expression tag	UNP 087605
D	-4	PRO	-	expression tag	UNP 087605
D	-3	ARG	-	expression tag	UNP 087605
D	-2	GLY	-	expression tag	UNP 087605
D	-1	SER	-	expression tag	UNP 087605
D	0	HIS	-	expression tag	UNP 087605
D	50	ASN	ASP	engineered mutation	UNP 087605

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	expression tag	UNP 087605
E	-18	GLY	-	expression tag	UNP 087605
E	-17	SER	-	expression tag	UNP 087605
E	-16	SER	-	expression tag	UNP 087605
E	-15	HIS	-	expression tag	UNP 087605
E	-14	HIS	-	expression tag	UNP 087605
E	-13	HIS	-	expression tag	UNP 087605
E	-12	HIS	-	expression tag	UNP 087605
E	-11	HIS	-	expression tag	UNP 087605
E	-10	HIS	-	expression tag	UNP 087605
E	-9	SER	-	expression tag	UNP 087605
E	-8	SER	-	expression tag	UNP 087605
E	-7	GLY	-	expression tag	UNP 087605
E	-6	LEU	-	expression tag	UNP 087605
E	-5	VAL	-	expression tag	UNP 087605
E	-4	PRO	-	expression tag	UNP 087605
E	-3	ARG	-	expression tag	UNP 087605
E	-2	GLY	-	expression tag	UNP 087605
E	-1	SER	-	expression tag	UNP 087605
E	0	HIS	-	expression tag	UNP 087605
E	50	ASN	ASP	engineered mutation	UNP 087605
F	-19	MET	-	expression tag	UNP 087605
F	-18	GLY	-	expression tag	UNP 087605
F	-17	SER	-	expression tag	UNP 087605
F	-16	SER	-	expression tag	UNP 087605
F	-15	HIS	-	expression tag	UNP 087605
F	-14	HIS	-	expression tag	UNP 087605
F	-13	HIS	-	expression tag	UNP 087605
F	-12	HIS	-	expression tag	UNP 087605
F	-11	HIS	-	expression tag	UNP 087605
F	-10	HIS	-	expression tag	UNP 087605
F	-9	SER	-	expression tag	UNP 087605
F	-8	SER	-	expression tag	UNP 087605
F	-7	GLY	-	expression tag	UNP 087605
F	-6	LEU	-	expression tag	UNP 087605
F	-5	VAL	-	expression tag	UNP 087605
F	-4	PRO	-	expression tag	UNP 087605
F	-3	ARG	-	expression tag	UNP 087605
F	-2	GLY	-	expression tag	UNP 087605
F	-1	SER	-	expression tag	UNP 087605
F	0	HIS	-	expression tag	UNP 087605
F	50	ASN	ASP	engineered mutation	UNP 087605

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	MET	-	expression tag	UNP 087605
G	-18	GLY	-	expression tag	UNP 087605
G	-17	SER	-	expression tag	UNP 087605
G	-16	SER	-	expression tag	UNP 087605
G	-15	HIS	-	expression tag	UNP 087605
G	-14	HIS	-	expression tag	UNP 087605
G	-13	HIS	-	expression tag	UNP 087605
G	-12	HIS	-	expression tag	UNP 087605
G	-11	HIS	-	expression tag	UNP 087605
G	-10	HIS	-	expression tag	UNP 087605
G	-9	SER	-	expression tag	UNP 087605
G	-8	SER	-	expression tag	UNP 087605
G	-7	GLY	-	expression tag	UNP 087605
G	-6	LEU	-	expression tag	UNP 087605
G	-5	VAL	-	expression tag	UNP 087605
G	-4	PRO	-	expression tag	UNP 087605
G	-3	ARG	-	expression tag	UNP 087605
G	-2	GLY	-	expression tag	UNP 087605
G	-1	SER	-	expression tag	UNP 087605
G	0	HIS	-	expression tag	UNP 087605
G	50	ASN	ASP	engineered mutation	UNP 087605
H	-19	MET	-	expression tag	UNP 087605
H	-18	GLY	-	expression tag	UNP 087605
H	-17	SER	-	expression tag	UNP 087605
H	-16	SER	-	expression tag	UNP 087605
H	-15	HIS	-	expression tag	UNP 087605
H	-14	HIS	-	expression tag	UNP 087605
H	-13	HIS	-	expression tag	UNP 087605
H	-12	HIS	-	expression tag	UNP 087605
H	-11	HIS	-	expression tag	UNP 087605
H	-10	HIS	-	expression tag	UNP 087605
H	-9	SER	-	expression tag	UNP 087605
H	-8	SER	-	expression tag	UNP 087605
H	-7	GLY	-	expression tag	UNP 087605
H	-6	LEU	-	expression tag	UNP 087605
H	-5	VAL	-	expression tag	UNP 087605
H	-4	PRO	-	expression tag	UNP 087605
H	-3	ARG	-	expression tag	UNP 087605
H	-2	GLY	-	expression tag	UNP 087605
H	-1	SER	-	expression tag	UNP 087605
H	0	HIS	-	expression tag	UNP 087605
H	50	ASN	ASP	engineered mutation	UNP 087605

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-19	MET	-	expression tag	UNP 087605
I	-18	GLY	-	expression tag	UNP 087605
I	-17	SER	-	expression tag	UNP 087605
I	-16	SER	-	expression tag	UNP 087605
I	-15	HIS	-	expression tag	UNP 087605
I	-14	HIS	-	expression tag	UNP 087605
I	-13	HIS	-	expression tag	UNP 087605
I	-12	HIS	-	expression tag	UNP 087605
I	-11	HIS	-	expression tag	UNP 087605
I	-10	HIS	-	expression tag	UNP 087605
I	-9	SER	-	expression tag	UNP 087605
I	-8	SER	-	expression tag	UNP 087605
I	-7	GLY	-	expression tag	UNP 087605
I	-6	LEU	-	expression tag	UNP 087605
I	-5	VAL	-	expression tag	UNP 087605
I	-4	PRO	-	expression tag	UNP 087605
I	-3	ARG	-	expression tag	UNP 087605
I	-2	GLY	-	expression tag	UNP 087605
I	-1	SER	-	expression tag	UNP 087605
I	0	HIS	-	expression tag	UNP 087605
I	50	ASN	ASP	engineered mutation	UNP 087605
J	-19	MET	-	expression tag	UNP 087605
J	-18	GLY	-	expression tag	UNP 087605
J	-17	SER	-	expression tag	UNP 087605
J	-16	SER	-	expression tag	UNP 087605
J	-15	HIS	-	expression tag	UNP 087605
J	-14	HIS	-	expression tag	UNP 087605
J	-13	HIS	-	expression tag	UNP 087605
J	-12	HIS	-	expression tag	UNP 087605
J	-11	HIS	-	expression tag	UNP 087605
J	-10	HIS	-	expression tag	UNP 087605
J	-9	SER	-	expression tag	UNP 087605
J	-8	SER	-	expression tag	UNP 087605
J	-7	GLY	-	expression tag	UNP 087605
J	-6	LEU	-	expression tag	UNP 087605
J	-5	VAL	-	expression tag	UNP 087605
J	-4	PRO	-	expression tag	UNP 087605
J	-3	ARG	-	expression tag	UNP 087605
J	-2	GLY	-	expression tag	UNP 087605
J	-1	SER	-	expression tag	UNP 087605
J	0	HIS	-	expression tag	UNP 087605
J	50	ASN	ASP	engineered mutation	UNP 087605

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-19	MET	-	expression tag	UNP 087605
K	-18	GLY	-	expression tag	UNP 087605
K	-17	SER	-	expression tag	UNP 087605
K	-16	SER	-	expression tag	UNP 087605
K	-15	HIS	-	expression tag	UNP 087605
K	-14	HIS	-	expression tag	UNP 087605
K	-13	HIS	-	expression tag	UNP 087605
K	-12	HIS	-	expression tag	UNP 087605
K	-11	HIS	-	expression tag	UNP 087605
K	-10	HIS	-	expression tag	UNP 087605
K	-9	SER	-	expression tag	UNP 087605
K	-8	SER	-	expression tag	UNP 087605
K	-7	GLY	-	expression tag	UNP 087605
K	-6	LEU	-	expression tag	UNP 087605
K	-5	VAL	-	expression tag	UNP 087605
K	-4	PRO	-	expression tag	UNP 087605
K	-3	ARG	-	expression tag	UNP 087605
K	-2	GLY	-	expression tag	UNP 087605
K	-1	SER	-	expression tag	UNP 087605
K	0	HIS	-	expression tag	UNP 087605
K	50	ASN	ASP	engineered mutation	UNP 087605
L	-19	MET	-	expression tag	UNP 087605
L	-18	GLY	-	expression tag	UNP 087605
L	-17	SER	-	expression tag	UNP 087605
L	-16	SER	-	expression tag	UNP 087605
L	-15	HIS	-	expression tag	UNP 087605
L	-14	HIS	-	expression tag	UNP 087605
L	-13	HIS	-	expression tag	UNP 087605
L	-12	HIS	-	expression tag	UNP 087605
L	-11	HIS	-	expression tag	UNP 087605
L	-10	HIS	-	expression tag	UNP 087605
L	-9	SER	-	expression tag	UNP 087605
L	-8	SER	-	expression tag	UNP 087605
L	-7	GLY	-	expression tag	UNP 087605
L	-6	LEU	-	expression tag	UNP 087605
L	-5	VAL	-	expression tag	UNP 087605
L	-4	PRO	-	expression tag	UNP 087605
L	-3	ARG	-	expression tag	UNP 087605
L	-2	GLY	-	expression tag	UNP 087605
L	-1	SER	-	expression tag	UNP 087605
L	0	HIS	-	expression tag	UNP 087605
L	50	ASN	ASP	engineered mutation	UNP 087605

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	expression tag	UNP 087605
M	-18	GLY	-	expression tag	UNP 087605
M	-17	SER	-	expression tag	UNP 087605
M	-16	SER	-	expression tag	UNP 087605
M	-15	HIS	-	expression tag	UNP 087605
M	-14	HIS	-	expression tag	UNP 087605
M	-13	HIS	-	expression tag	UNP 087605
M	-12	HIS	-	expression tag	UNP 087605
M	-11	HIS	-	expression tag	UNP 087605
M	-10	HIS	-	expression tag	UNP 087605
M	-9	SER	-	expression tag	UNP 087605
M	-8	SER	-	expression tag	UNP 087605
M	-7	GLY	-	expression tag	UNP 087605
M	-6	LEU	-	expression tag	UNP 087605
M	-5	VAL	-	expression tag	UNP 087605
M	-4	PRO	-	expression tag	UNP 087605
M	-3	ARG	-	expression tag	UNP 087605
M	-2	GLY	-	expression tag	UNP 087605
M	-1	SER	-	expression tag	UNP 087605
M	0	HIS	-	expression tag	UNP 087605
M	50	ASN	ASP	engineered mutation	UNP 087605
N	-19	MET	-	expression tag	UNP 087605
N	-18	GLY	-	expression tag	UNP 087605
N	-17	SER	-	expression tag	UNP 087605
N	-16	SER	-	expression tag	UNP 087605
N	-15	HIS	-	expression tag	UNP 087605
N	-14	HIS	-	expression tag	UNP 087605
N	-13	HIS	-	expression tag	UNP 087605
N	-12	HIS	-	expression tag	UNP 087605
N	-11	HIS	-	expression tag	UNP 087605
N	-10	HIS	-	expression tag	UNP 087605
N	-9	SER	-	expression tag	UNP 087605
N	-8	SER	-	expression tag	UNP 087605
N	-7	GLY	-	expression tag	UNP 087605
N	-6	LEU	-	expression tag	UNP 087605
N	-5	VAL	-	expression tag	UNP 087605
N	-4	PRO	-	expression tag	UNP 087605
N	-3	ARG	-	expression tag	UNP 087605
N	-2	GLY	-	expression tag	UNP 087605
N	-1	SER	-	expression tag	UNP 087605
N	0	HIS	-	expression tag	UNP 087605
N	50	ASN	ASP	engineered mutation	UNP 087605

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-19	MET	-	expression tag	UNP O87605
O	-18	GLY	-	expression tag	UNP O87605
O	-17	SER	-	expression tag	UNP O87605
O	-16	SER	-	expression tag	UNP O87605
O	-15	HIS	-	expression tag	UNP O87605
O	-14	HIS	-	expression tag	UNP O87605
O	-13	HIS	-	expression tag	UNP O87605
O	-12	HIS	-	expression tag	UNP O87605
O	-11	HIS	-	expression tag	UNP O87605
O	-10	HIS	-	expression tag	UNP O87605
O	-9	SER	-	expression tag	UNP O87605
O	-8	SER	-	expression tag	UNP O87605
O	-7	GLY	-	expression tag	UNP O87605
O	-6	LEU	-	expression tag	UNP O87605
O	-5	VAL	-	expression tag	UNP O87605
O	-4	PRO	-	expression tag	UNP O87605
O	-3	ARG	-	expression tag	UNP O87605
O	-2	GLY	-	expression tag	UNP O87605
O	-1	SER	-	expression tag	UNP O87605
O	0	HIS	-	expression tag	UNP O87605
O	50	ASN	ASP	engineered mutation	UNP O87605
P	-19	MET	-	expression tag	UNP O87605
P	-18	GLY	-	expression tag	UNP O87605
P	-17	SER	-	expression tag	UNP O87605
P	-16	SER	-	expression tag	UNP O87605
P	-15	HIS	-	expression tag	UNP O87605
P	-14	HIS	-	expression tag	UNP O87605
P	-13	HIS	-	expression tag	UNP O87605
P	-12	HIS	-	expression tag	UNP O87605
P	-11	HIS	-	expression tag	UNP O87605
P	-10	HIS	-	expression tag	UNP O87605
P	-9	SER	-	expression tag	UNP O87605
P	-8	SER	-	expression tag	UNP O87605
P	-7	GLY	-	expression tag	UNP O87605
P	-6	LEU	-	expression tag	UNP O87605
P	-5	VAL	-	expression tag	UNP O87605
P	-4	PRO	-	expression tag	UNP O87605
P	-3	ARG	-	expression tag	UNP O87605
P	-2	GLY	-	expression tag	UNP O87605
P	-1	SER	-	expression tag	UNP O87605
P	0	HIS	-	expression tag	UNP O87605
P	50	ASN	ASP	engineered mutation	UNP O87605

- # HEM

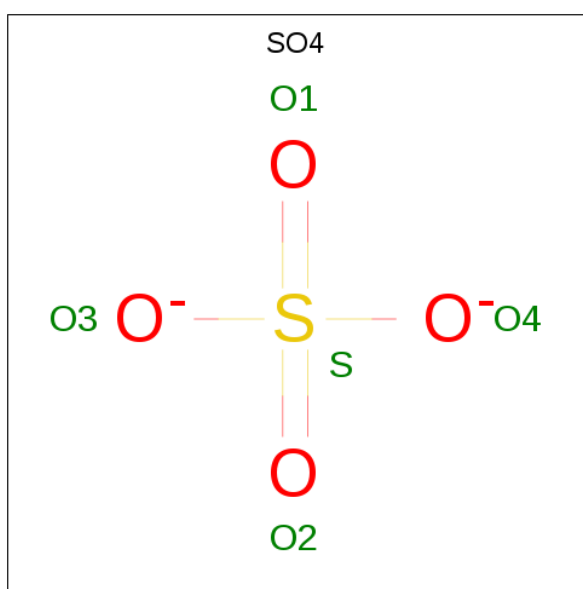
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



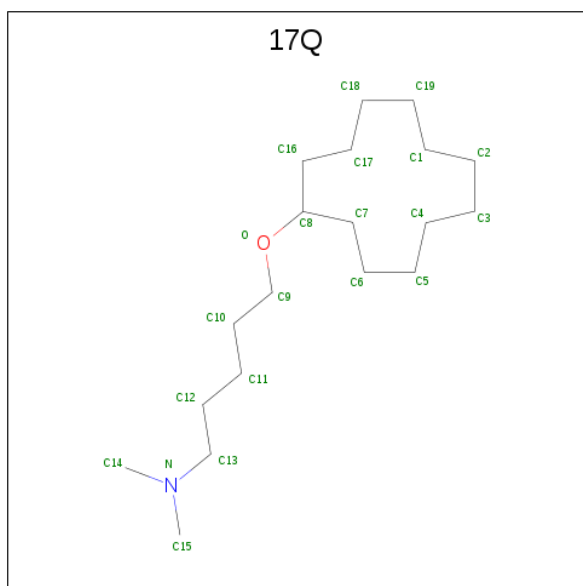
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1.7.6 5-cyclododecyloxy-N,N-dimethyl-pentan-1-amine (three-letter code: 17Q) (formula: C<sub>19</sub>H<sub>39</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			21	19	1	1		
4	G	1	Total	C	N	O	0	0
			21	19	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		

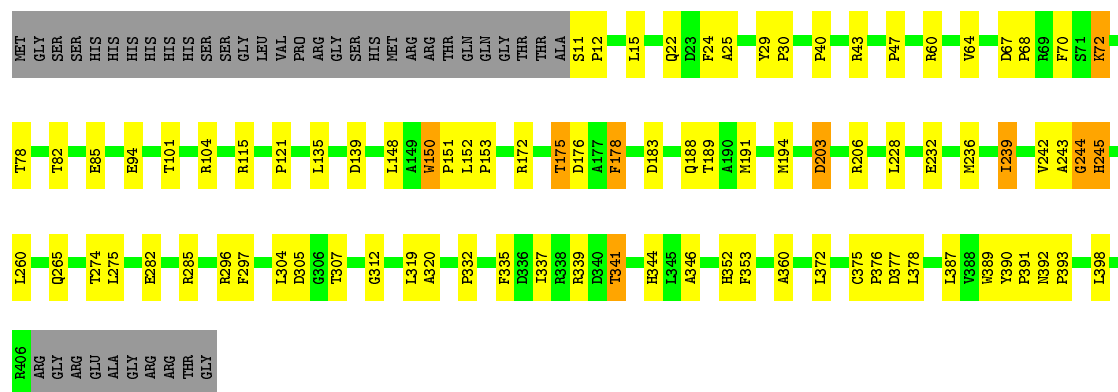
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	43	Total 43	O 43	0	0
5	D	46	Total 46	O 46	0	0
5	E	37	Total 37	O 37	0	0
5	F	39	Total 39	O 39	0	0
5	G	57	Total 57	O 57	0	0
5	H	35	Total 35	O 35	0	0
5	I	39	Total 39	O 39	0	0
5	J	34	Total 34	O 34	0	0
5	K	28	Total 28	O 28	0	0
5	L	21	Total 21	O 21	0	0
5	M	16	Total 16	O 16	0	0
5	N	15	Total 15	O 15	0	0
5	O	20	Total 20	O 20	0	0
5	P	17	Total 17	O 17	0	0

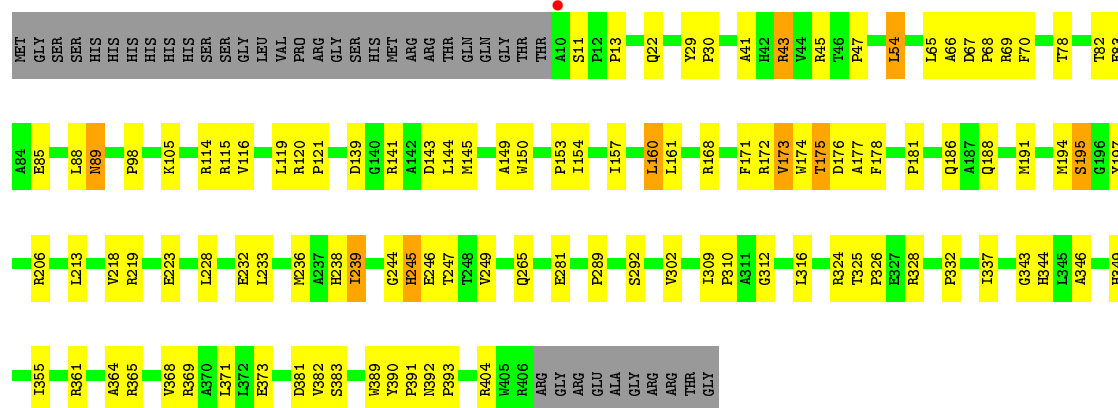






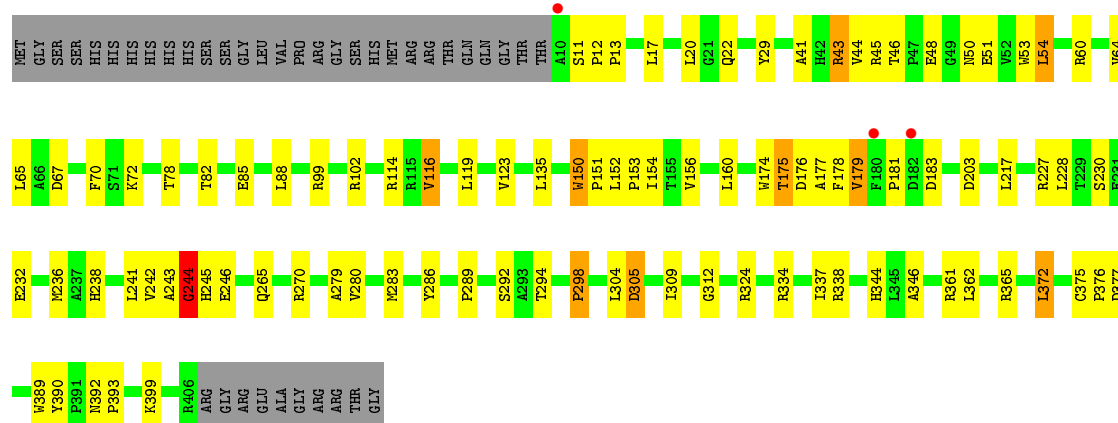
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain D: 66% 23% 9%



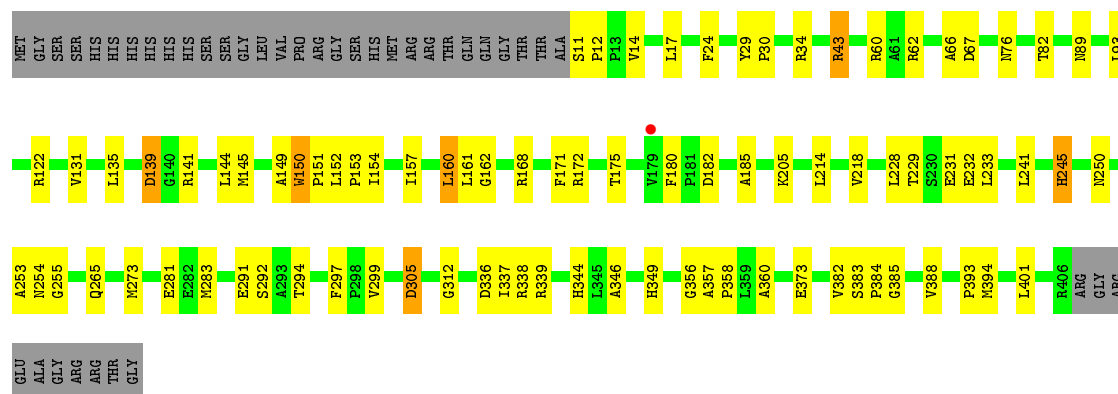
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain E: 69% 19% 9%



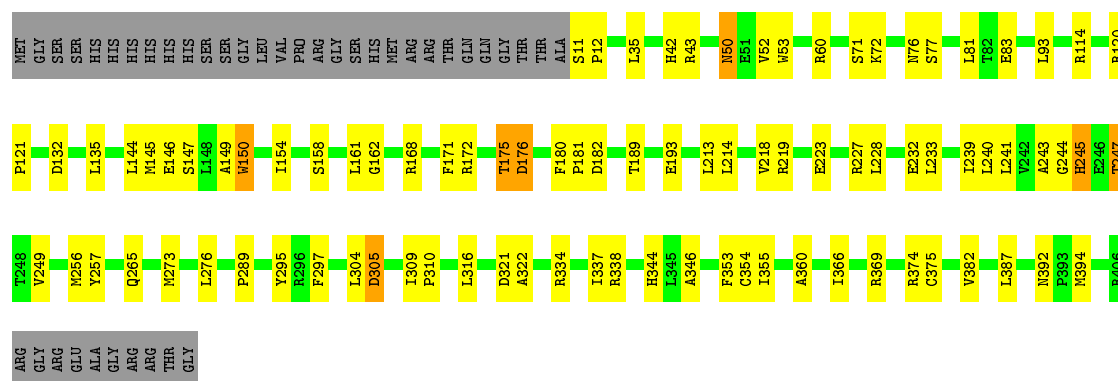
● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain F: 71% 18% 9%



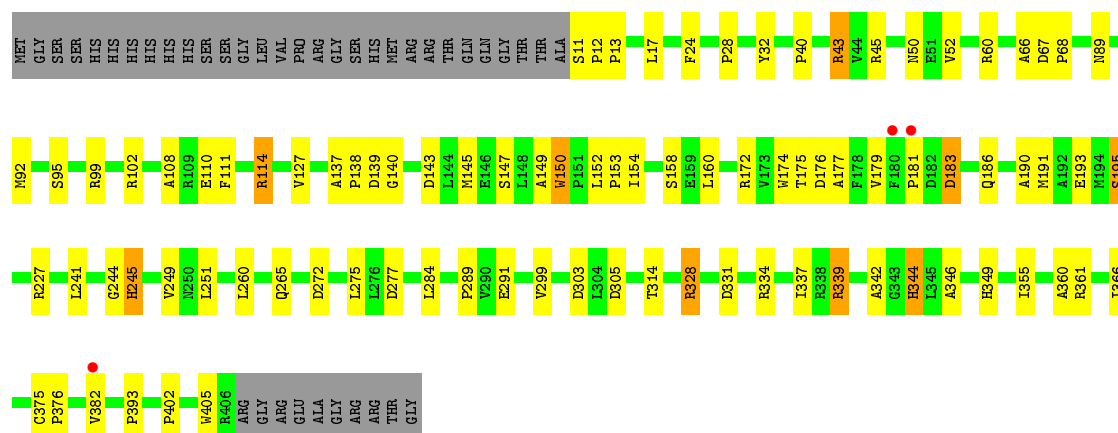
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain G: 70% 19% 9%



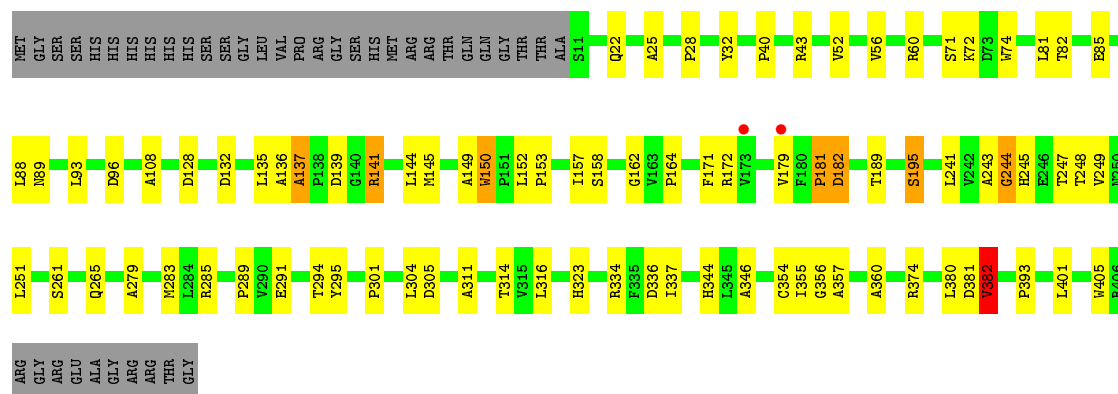
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain H: 70% 19% 9%

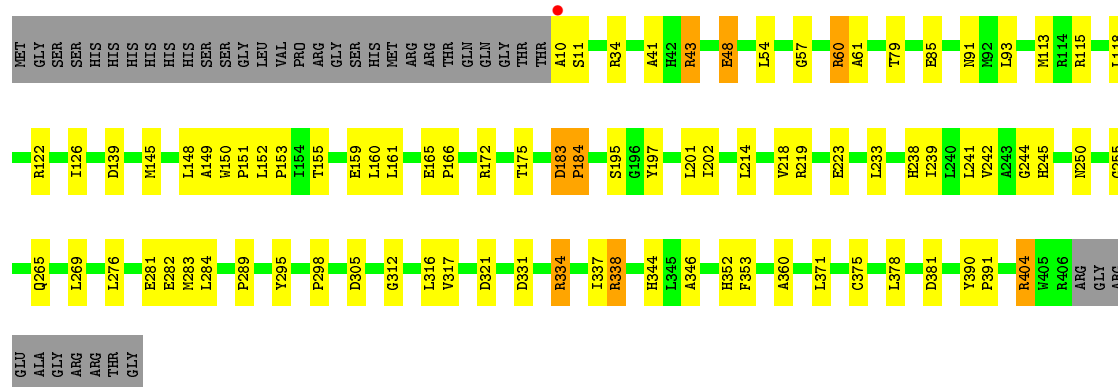


• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

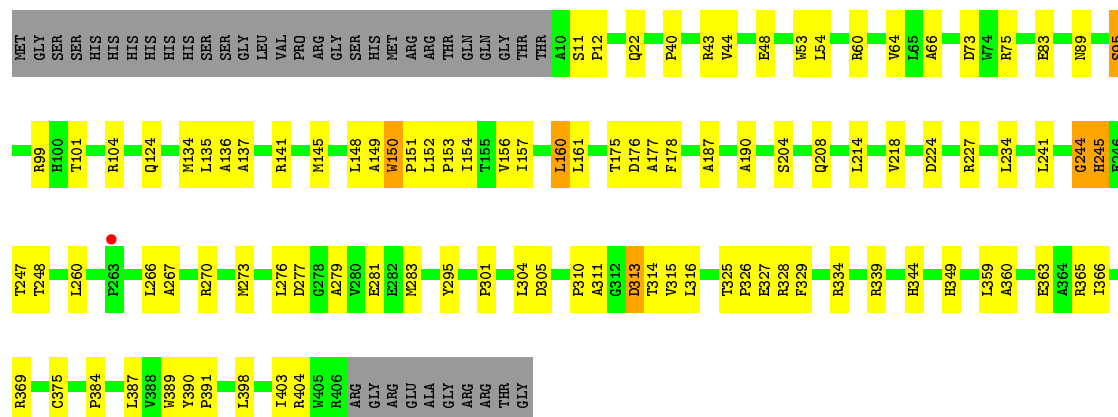
Chain I: 71% 18% 9%



- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

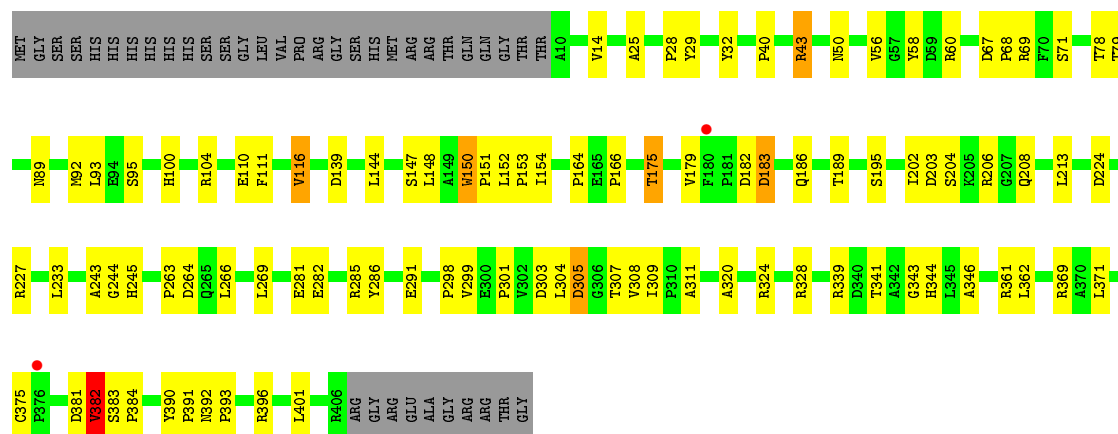


● Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

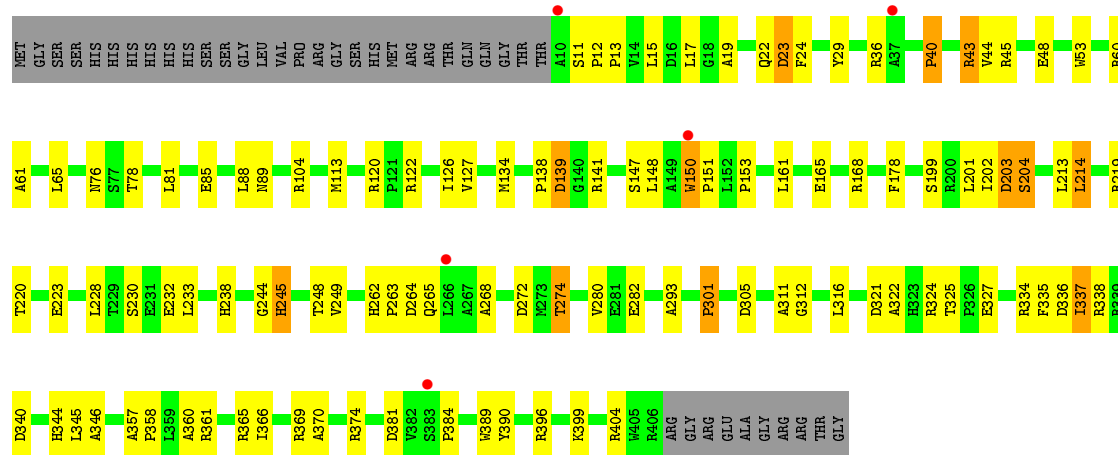


- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

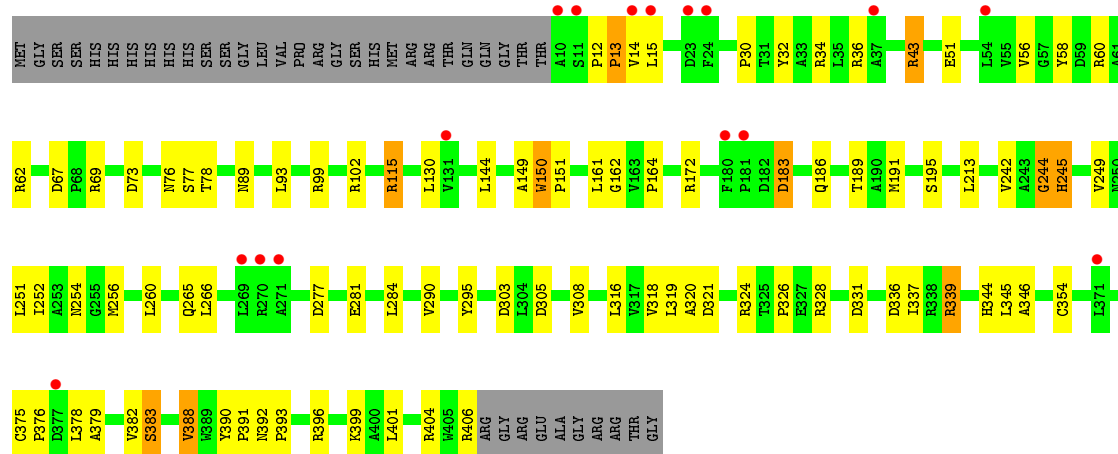




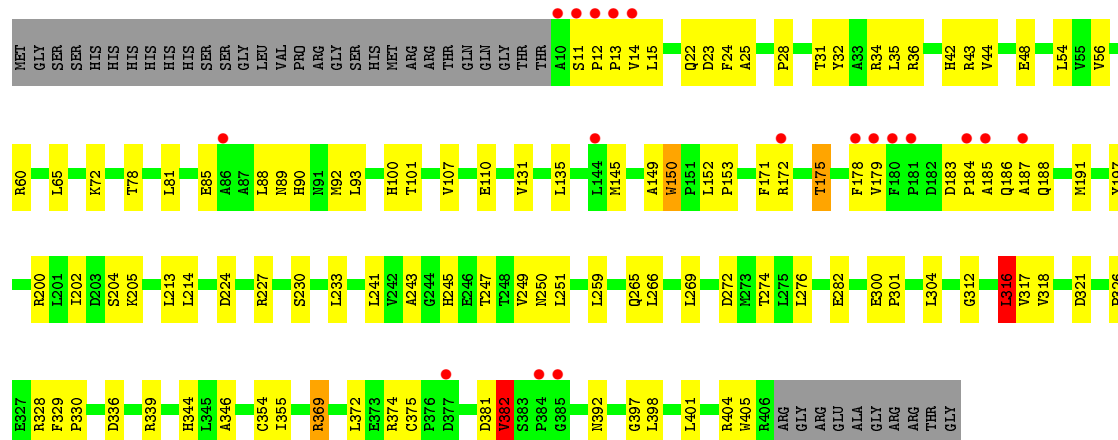
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



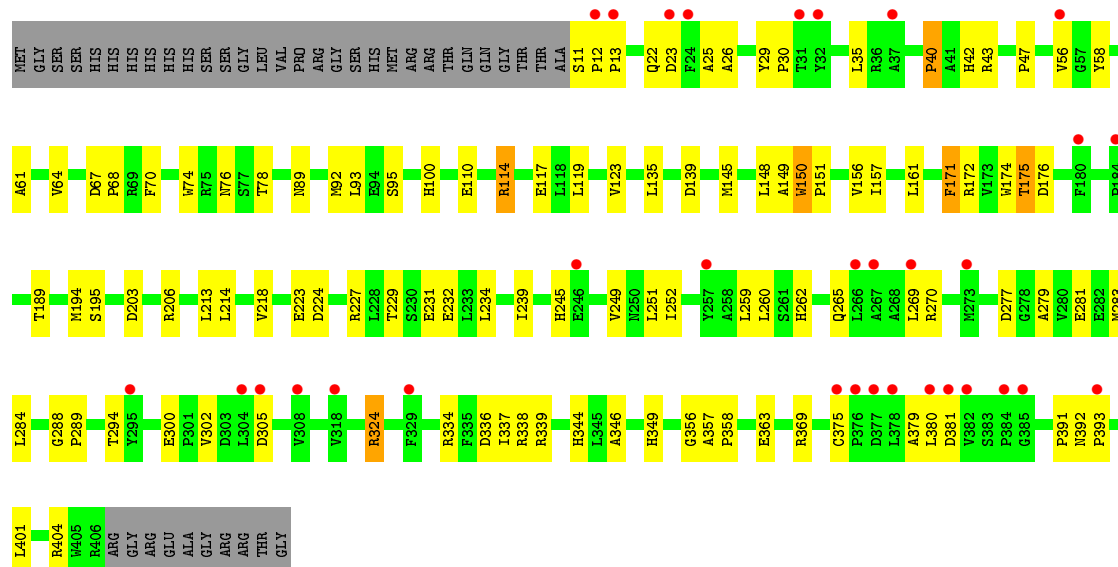
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.27Å 130.11Å 134.90Å 66.48° 70.25° 72.23°	Depositor
Resolution (Å)	119.84 – 2.70 91.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (119.84-2.70) 97.3 (91.88-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.196 , 0.279 0.199 , 0.277	Depositor DCC
$R_{free}$ test set	8479 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.030 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8815e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: HEM, SO4, 17Q

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	0.61	0/3100	0.75	0/4234
1	B	0.60	0/3142	0.72	0/4292
1	C	0.62	0/3136	0.75	1/4283 (0.0%)
1	D	0.63	0/3149	0.75	1/4301 (0.0%)
1	E	0.66	0/3141	0.77	1/4290 (0.0%)
1	F	0.59	0/3149	0.71	0/4303
1	G	0.61	0/3166	0.71	0/4324
1	H	0.62	0/3130	0.74	0/4275
1	I	0.57	0/3139	0.72	0/4288
1	J	0.58	0/3133	0.69	0/4280
1	K	0.55	0/3149	0.70	0/4301
1	L	0.54	0/3138	0.70	0/4287
1	M	0.54	0/3138	0.68	0/4286
1	N	0.48	0/3137	0.63	0/4285
1	O	0.51	0/3125	0.67	1/4269 (0.0%)
1	P	0.47	0/3131	0.64	0/4276
All	All	0.58	0/50203	0.71	4/68574 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	E	54	LEU	CA-CB-CG	5.09	127.00	115.30
1	D	65	LEU	CA-CB-CG	5.05	126.92	115.30
1	O	316	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	244	GLY	Peptide
1	I	179	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3031	0	2990	67	0
1	B	3069	0	3026	93	0
1	C	3063	0	3024	71	0
1	D	3076	0	3027	78	0
1	E	3068	0	3022	63	0
1	F	3075	0	3019	70	0
1	G	3093	0	3049	78	0
1	H	3057	0	3020	57	0
1	I	3066	0	3020	65	0
1	J	3060	0	3016	61	0
1	K	3076	0	3032	60	0
1	L	3065	0	3014	61	0
1	M	3065	0	3014	68	0
1	N	3064	0	3025	63	0
1	O	3052	0	3008	70	0
1	P	3058	0	3006	60	0
2	A	43	0	30	1	0
2	B	43	0	30	6	0
2	C	43	0	30	6	0
2	D	43	0	30	8	0
2	E	43	0	30	5	0
2	F	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	43	0	30	6	0
2	H	43	0	30	7	0
2	I	43	0	30	5	0
2	J	43	0	30	4	0
2	K	43	0	30	3	0
2	L	43	0	30	4	0
2	M	43	0	30	5	0
2	N	43	0	30	7	0
2	O	43	0	30	4	0
2	P	43	0	30	5	0
3	A	5	0	0	2	0
3	B	10	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	1	0
3	H	10	0	0	1	0
3	I	10	0	0	0	0
3	J	5	0	0	0	0
3	O	10	0	0	1	0
4	C	21	0	39	6	0
4	G	21	0	39	5	0
5	A	35	0	0	0	0
5	B	32	0	0	0	0
5	C	43	0	0	3	0
5	D	46	0	0	3	0
5	E	37	0	0	1	0
5	F	39	0	0	2	0
5	G	57	0	0	2	0
5	H	35	0	0	4	0
5	I	39	0	0	0	0
5	J	34	0	0	1	0
5	K	28	0	0	1	0
5	L	21	0	0	0	0
5	M	16	0	0	0	0
5	N	15	0	0	0	0
5	O	20	0	0	0	0
5	P	17	0	0	1	0
All	All	50342	0	48870	1084	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 11.

The worst 5 of 1084 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:O:227:ARG:NH1	1:O:227:ARG:HB3	1.69	1.07
1:I:128:ASP:HA	1:I:374:ARG:HH12	1.21	1.06
1:G:171:PHE:O	1:G:175:THR:HG22	1.56	1.05
1:N:390:TYR:HE1	1:N:399:LYS:HG3	1.20	1.04
1:F:171:PHE:O	1:F:175:THR:HG22	1.59	1.02

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	394/436 (90%)	370 (94%)	20 (5%)	4 (1%)	15	37
1	B	397/436 (91%)	367 (92%)	29 (7%)	1 (0%)	41	66
1	C	395/436 (91%)	370 (94%)	23 (6%)	2 (0%)	29	54
1	D	397/436 (91%)	366 (92%)	28 (7%)	3 (1%)	19	43
1	E	396/436 (91%)	367 (93%)	26 (7%)	3 (1%)	19	43
1	F	398/436 (91%)	362 (91%)	30 (8%)	6 (2%)	10	26
1	G	398/436 (91%)	373 (94%)	22 (6%)	3 (1%)	19	43
1	H	395/436 (91%)	368 (93%)	26 (7%)	1 (0%)	41	66
1	I	396/436 (91%)	363 (92%)	29 (7%)	4 (1%)	15	37
1	J	396/436 (91%)	370 (93%)	24 (6%)	2 (0%)	29	54
1	K	397/436 (91%)	362 (91%)	30 (8%)	5 (1%)	12	30
1	L	397/436 (91%)	357 (90%)	33 (8%)	7 (2%)	8	21
1	M	396/436 (91%)	367 (93%)	22 (6%)	7 (2%)	8	21
1	N	396/436 (91%)	355 (90%)	37 (9%)	4 (1%)	15	37
1	O	395/436 (91%)	343 (87%)	47 (12%)	5 (1%)	12	30
1	P	395/436 (91%)	356 (90%)	35 (9%)	4 (1%)	15	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6338/6976 (91%)	5816 (92%)	461 (7%)	61 (1%)	15 37

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL
1	E	179	VAL
1	E	305	ASP
1	F	245[A]	HIS
1	F	245[B]	HIS

### 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	312/355 (88%)	293 (94%)	19 (6%)	18 41
1	B	316/355 (89%)	298 (94%)	18 (6%)	20 44
1	C	317/355 (89%)	300 (95%)	17 (5%)	22 47
1	D	318/355 (90%)	300 (94%)	18 (6%)	20 44
1	E	317/355 (89%)	304 (96%)	13 (4%)	30 59
1	F	317/355 (89%)	307 (97%)	10 (3%)	39 68
1	G	321/355 (90%)	307 (96%)	14 (4%)	28 56
1	H	315/355 (89%)	298 (95%)	17 (5%)	22 47
1	I	316/355 (89%)	302 (96%)	14 (4%)	28 56
1	J	315/355 (89%)	301 (96%)	14 (4%)	28 56
1	K	318/355 (90%)	302 (95%)	16 (5%)	24 51
1	L	314/355 (88%)	289 (92%)	25 (8%)	12 27
1	M	315/355 (89%)	295 (94%)	20 (6%)	18 40
1	N	316/355 (89%)	304 (96%)	12 (4%)	33 62
1	O	313/355 (88%)	295 (94%)	18 (6%)	20 43
1	P	315/355 (89%)	296 (94%)	19 (6%)	19 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5055/5680 (89%)	4791 (95%)	264 (5%)	23 49

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	241	LEU
1	J	139	ASP
1	O	382	VAL
1	H	303	ASP
1	I	189	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	245	HIS
1	I	238	HIS
1	O	265	GLN
1	G	265	GLN
1	H	245	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

30 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
2	HEM	H	1407	1	27,50,50	2.20	8 (29%)	17,82,82	1.52	2 (11%)
2	HEM	J	1407	1	27,50,50	2.19	6 (22%)	17,82,82	1.49	3 (17%)
3	SO4	B	1408	-	4,4,4	0.27	0	6,6,6	0.33	0
2	HEM	B	1407	1	27,50,50	2.05	5 (18%)	17,82,82	2.09	5 (29%)
4	17Q	G	1410	-	21,21,21	0.47	0	21,23,23	0.68	0
2	HEM	D	1407	1	27,50,50	2.05	6 (22%)	17,82,82	1.69	3 (17%)
4	17Q	C	1410	-	21,21,21	0.30	0	21,23,23	0.97	2 (9%)
3	SO4	H	1409	-	4,4,4	0.29	0	6,6,6	0.31	0
2	HEM	P	1407	1	27,50,50	2.17	6 (22%)	17,82,82	1.54	4 (23%)
2	HEM	K	1407	1	27,50,50	2.13	5 (18%)	17,82,82	1.56	4 (23%)
2	HEM	N	1407	1	27,50,50	2.17	6 (22%)	17,82,82	1.40	2 (11%)
2	HEM	C	1407	1	27,50,50	2.28	7 (25%)	17,82,82	2.32	5 (29%)
2	HEM	F	1407	1	27,50,50	2.21	8 (29%)	17,82,82	1.94	4 (23%)
2	HEM	E	1407	1	27,50,50	2.02	7 (25%)	17,82,82	2.22	5 (29%)
3	SO4	O	1409	-	4,4,4	0.48	0	6,6,6	0.88	0
3	SO4	I	1409	-	4,4,4	0.23	0	6,6,6	0.38	0
3	SO4	H	1408	-	4,4,4	0.48	0	6,6,6	0.52	0
2	HEM	M	1407	1	27,50,50	2.29	7 (25%)	17,82,82	1.54	4 (23%)
3	SO4	O	1408	-	4,4,4	0.55	0	6,6,6	0.60	0
3	SO4	A	1408	-	4,4,4	0.27	0	6,6,6	0.53	0
2	HEM	O	1407	1	27,50,50	2.15	6 (22%)	17,82,82	1.83	4 (23%)
3	SO4	J	1408	-	4,4,4	0.60	0	6,6,6	0.47	0
2	HEM	G	1407	1	27,50,50	2.20	6 (22%)	17,82,82	1.74	2 (11%)
2	HEM	I	1407	1	27,50,50	2.12	7 (25%)	17,82,82	2.13	4 (23%)
2	HEM	L	1407	1	27,50,50	2.06	5 (18%)	17,82,82	1.78	4 (23%)
3	SO4	D	1408	-	4,4,4	0.67	0	6,6,6	0.79	0
3	SO4	F	1408	-	4,4,4	0.51	0	6,6,6	0.52	0
3	SO4	I	1408	-	4,4,4	0.68	0	6,6,6	0.77	0
2	HEM	A	1407	1	27,50,50	2.09	5 (18%)	17,82,82	1.68	5 (29%)
3	SO4	B	1409	-	4,4,4	0.26	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	H	1407	1	-	0/6/54/54	-
2	HEM	G	1407	1	-	0/6/54/54	-
2	HEM	J	1407	1	-	0/6/54/54	-
2	HEM	I	1407	1	-	0/6/54/54	-
2	HEM	L	1407	1	-	0/6/54/54	-
2	HEM	K	1407	1	-	0/6/54/54	-
2	HEM	N	1407	1	-	0/6/54/54	-
2	HEM	M	1407	1	-	0/6/54/54	-
2	HEM	B	1407	1	-	0/6/54/54	-
2	HEM	A	1407	1	-	0/6/54/54	-
2	HEM	D	1407	1	-	0/6/54/54	-
2	HEM	C	1407	1	-	0/6/54/54	-
4	17Q	C	1410	-	-	14/23/23/23	1/1/1/1
2	HEM	E	1407	1	-	0/6/54/54	-
4	17Q	G	1410	-	-	14/23/23/23	1/1/1/1
2	HEM	F	1407	1	-	0/6/54/54	-
2	HEM	P	1407	1	-	0/6/54/54	-
2	HEM	O	1407	1	-	0/6/54/54	-

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1407	HEM	C3D-C2D	5.63	1.54	1.37
2	M	1407	HEM	C3D-C2D	5.57	1.54	1.37
2	C	1407	HEM	C3C-C2C	-5.46	1.32	1.40
2	P	1407	HEM	C3B-C2B	-5.42	1.32	1.40
2	P	1407	HEM	C3D-C2D	5.34	1.53	1.37

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1407	HEM	C1D-C2D-C3D	-5.57	103.12	107.00
2	E	1407	HEM	C1D-C2D-C3D	-4.97	103.54	107.00
2	F	1407	HEM	CBD-CAD-C3D	-4.95	103.36	112.48
2	I	1407	HEM	CBD-CAD-C3D	-4.88	103.48	112.48
2	C	1407	HEM	CBD-CAD-C3D	-4.84	103.55	112.48

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1410	17Q	C7-C8-O-C9
4	C	1410	17Q	C7-C8-O-C9
4	C	1410	17Q	C6-C7-C8-O
4	C	1410	17Q	C2-C1-C19-C18
4	C	1410	17Q	C1-C2-C3-C4

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1410	17Q	C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8
4	G	1410	17Q	C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8

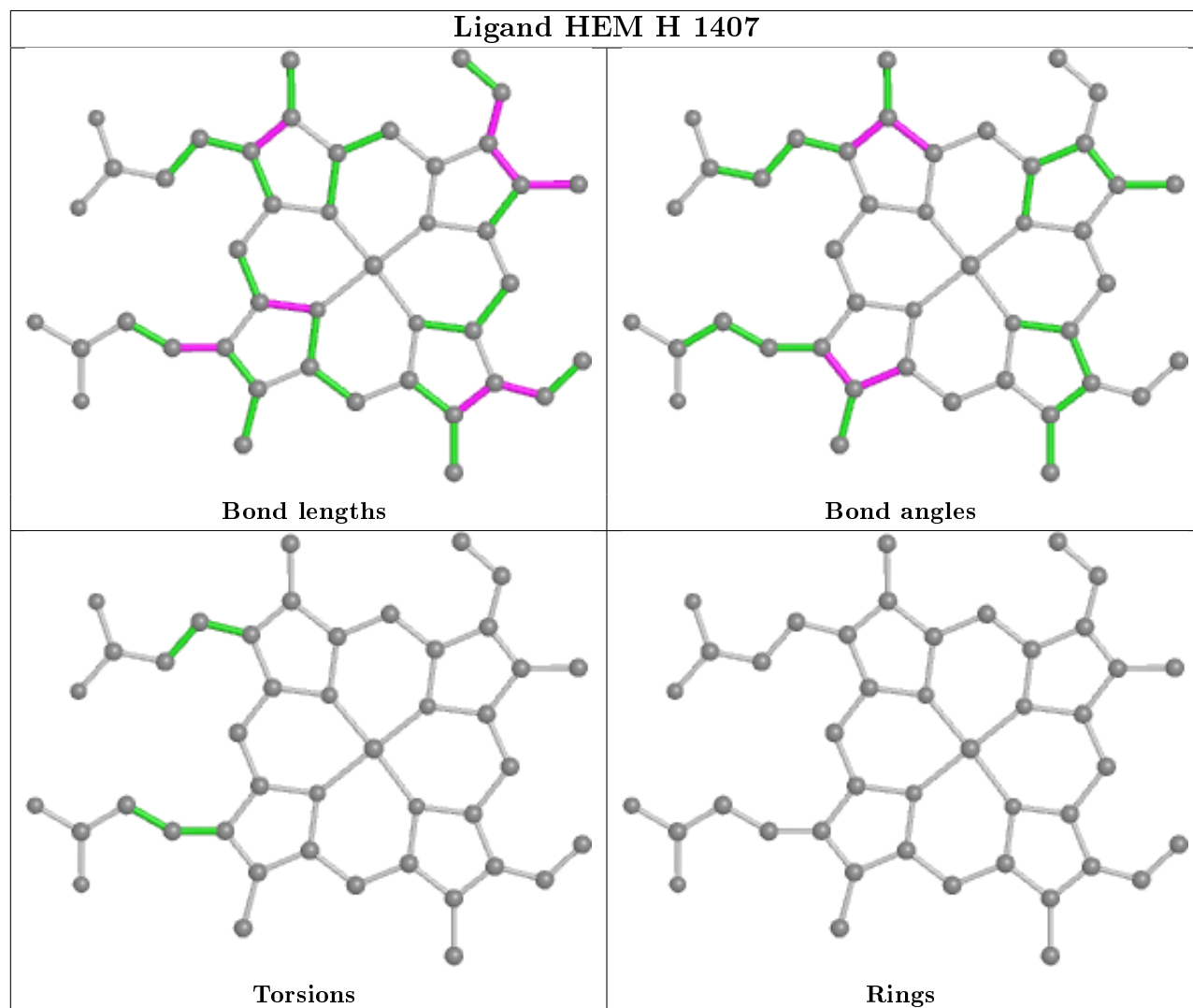
22 monomers are involved in 94 short contacts:

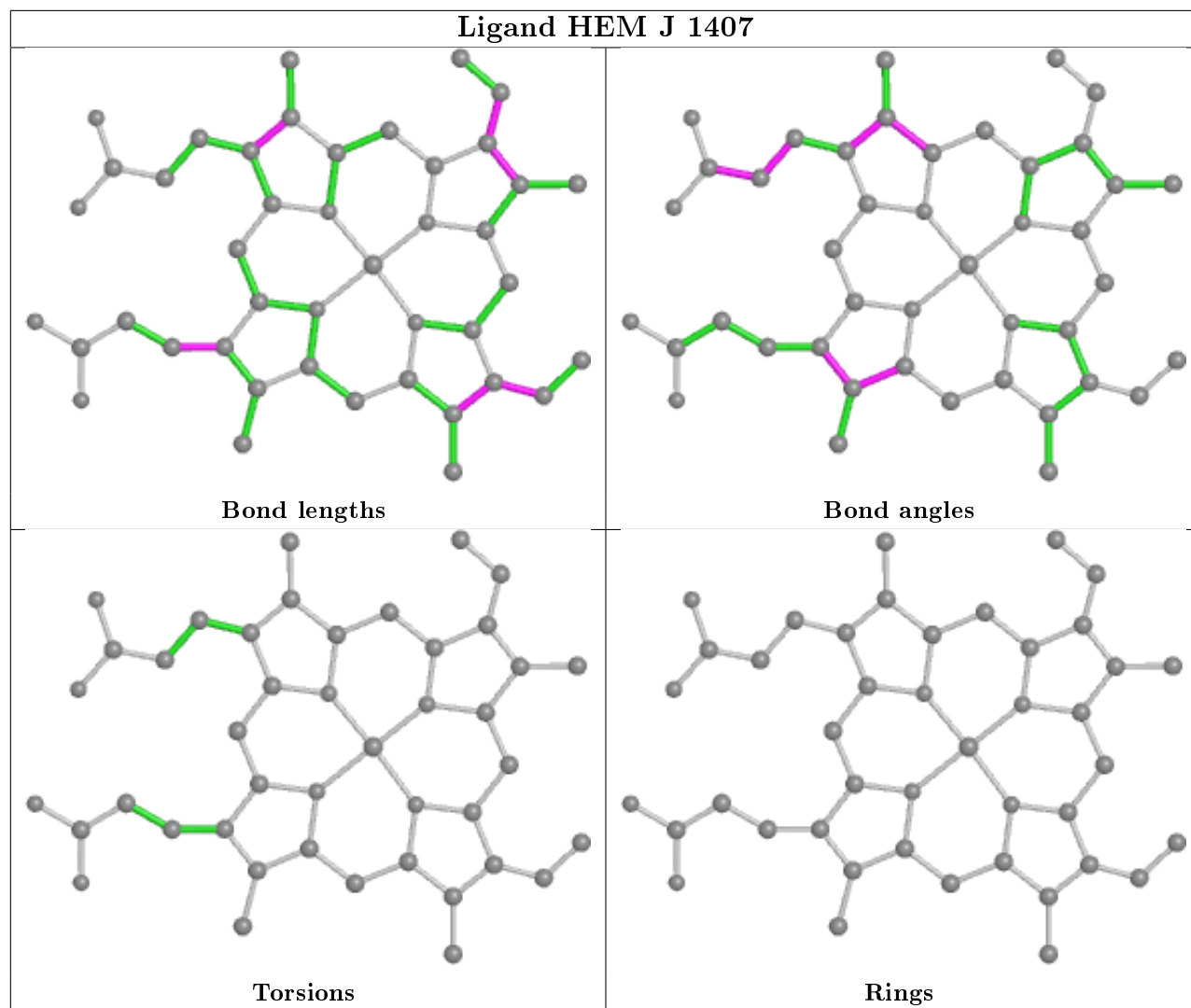
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1407	HEM	7	0
2	J	1407	HEM	4	0
2	B	1407	HEM	6	0
4	G	1410	17Q	5	0
2	D	1407	HEM	8	0
4	C	1410	17Q	6	0
3	H	1409	SO4	1	0
2	P	1407	HEM	5	0
2	K	1407	HEM	3	0
2	N	1407	HEM	7	0
2	C	1407	HEM	6	0
2	F	1407	HEM	3	0
2	E	1407	HEM	5	0
3	O	1409	SO4	1	0
2	M	1407	HEM	5	0
3	A	1408	SO4	2	0
2	O	1407	HEM	4	0
2	G	1407	HEM	6	0
2	I	1407	HEM	5	0
2	L	1407	HEM	4	0
3	F	1408	SO4	1	0
2	A	1407	HEM	1	0

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

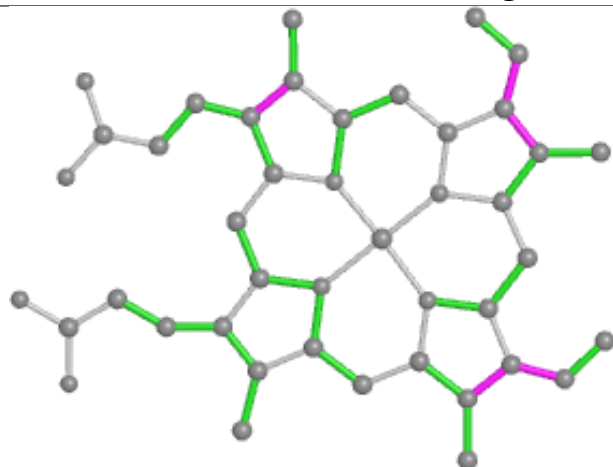


Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

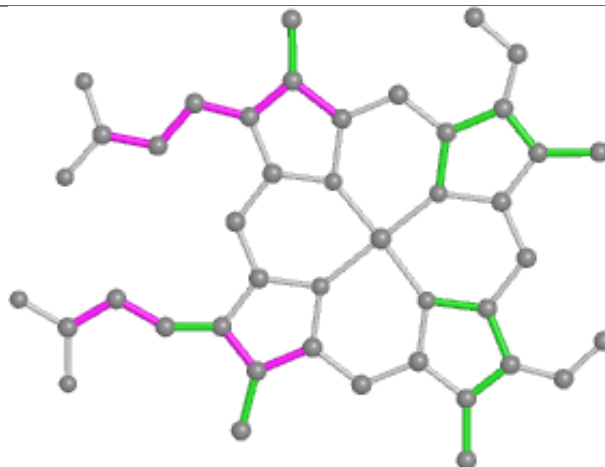




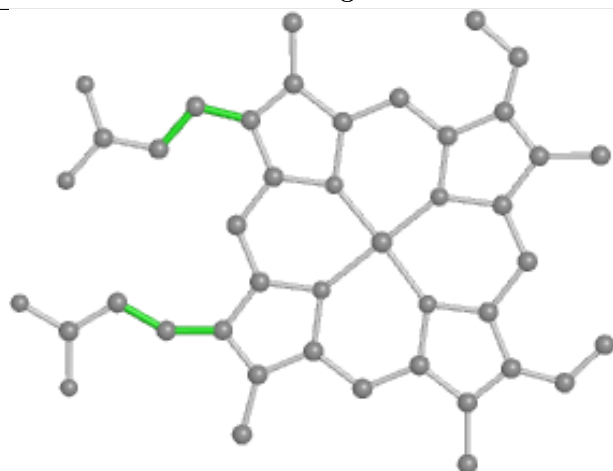
## Ligand HEM B 1407



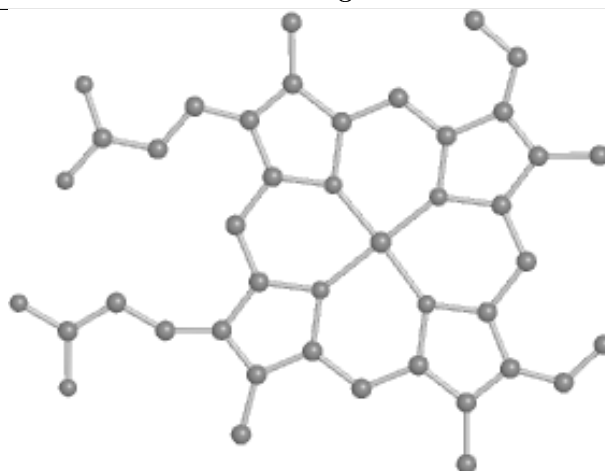
Bond lengths



Bond angles

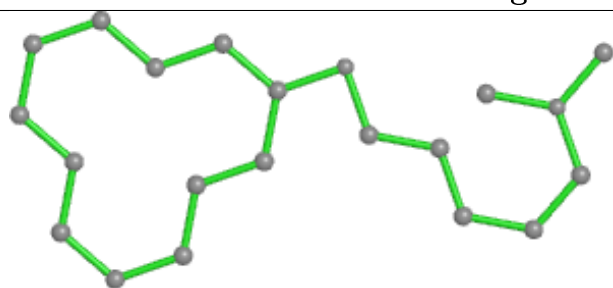


Torsions

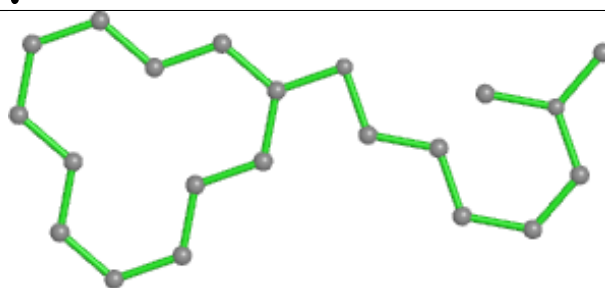


Rings

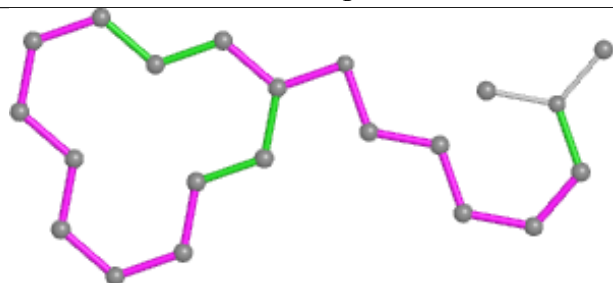
## Ligand 17Q G 1410



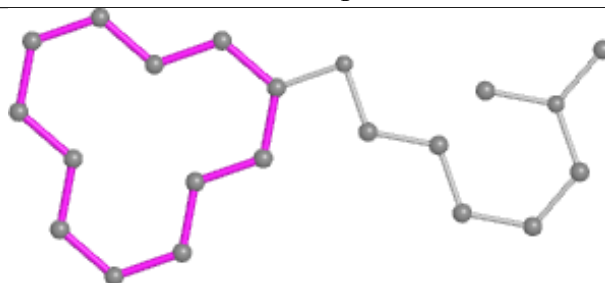
Bond lengths



Bond angles

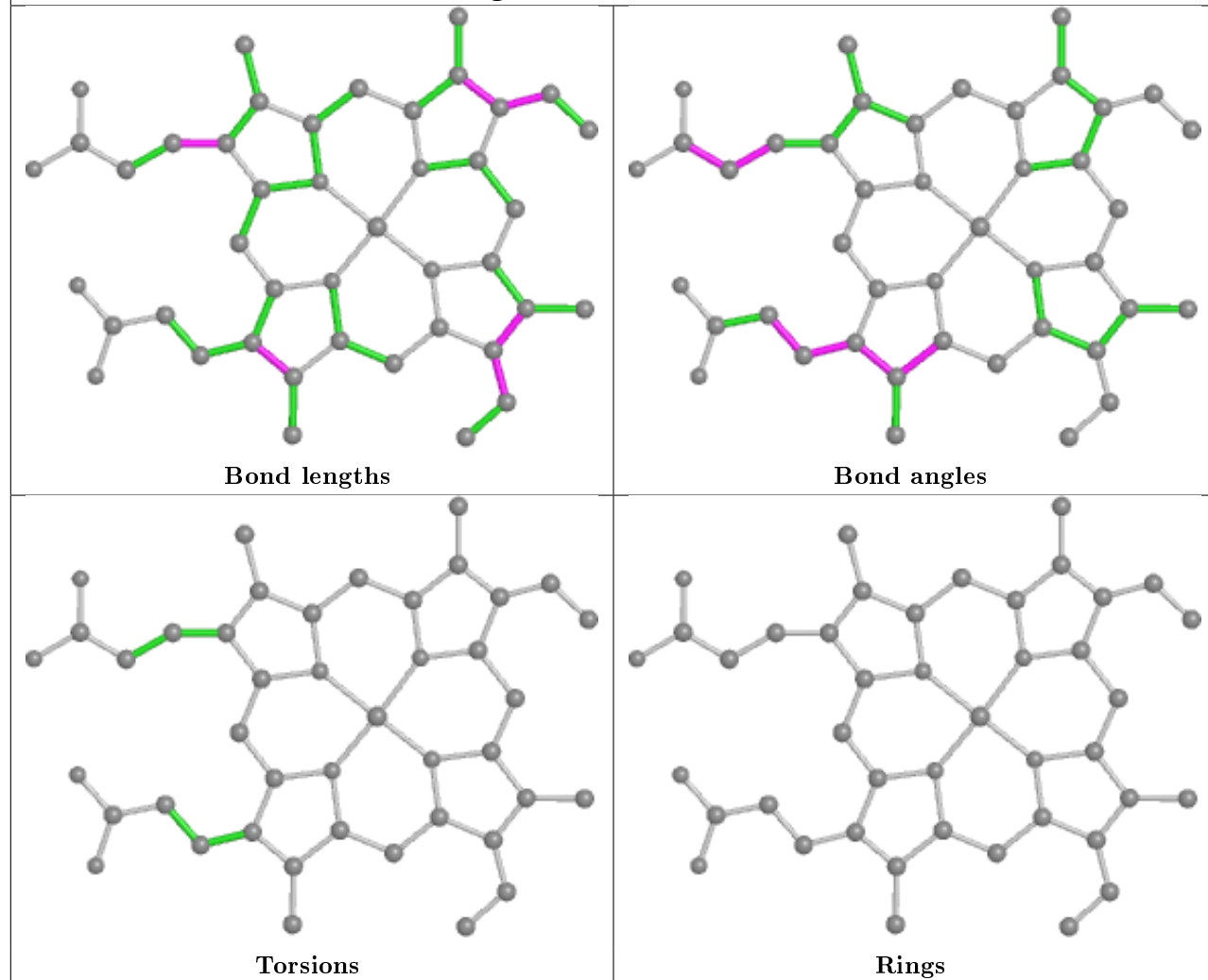


Torsions

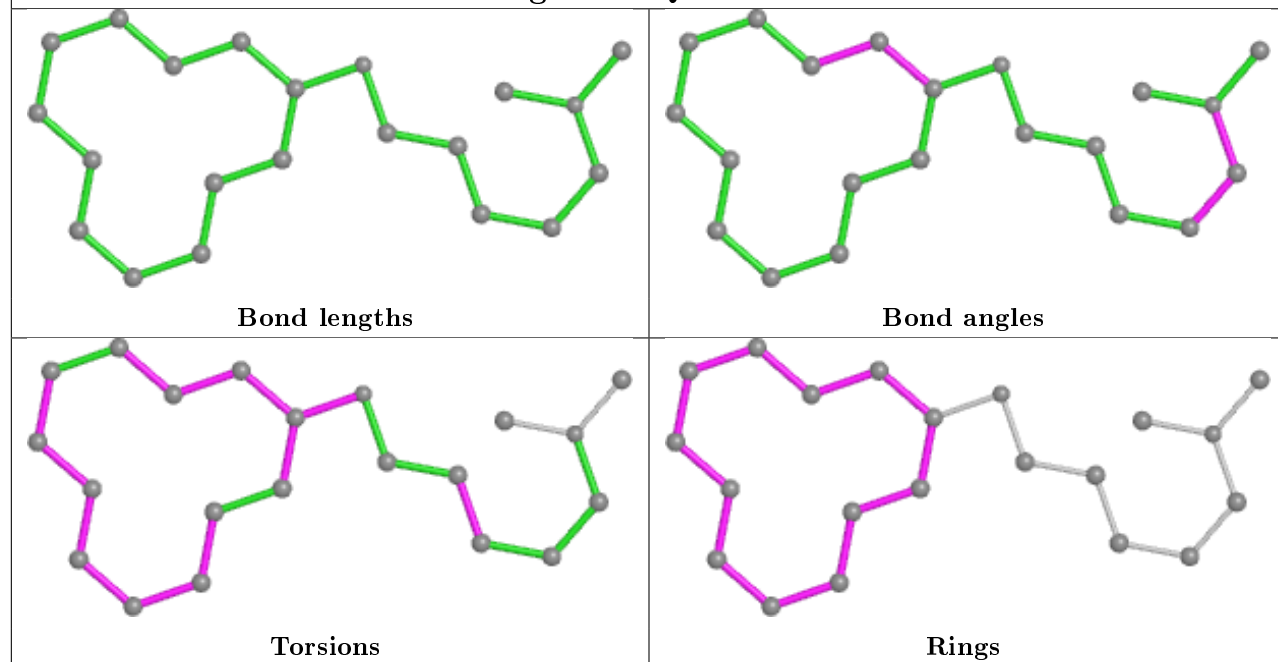


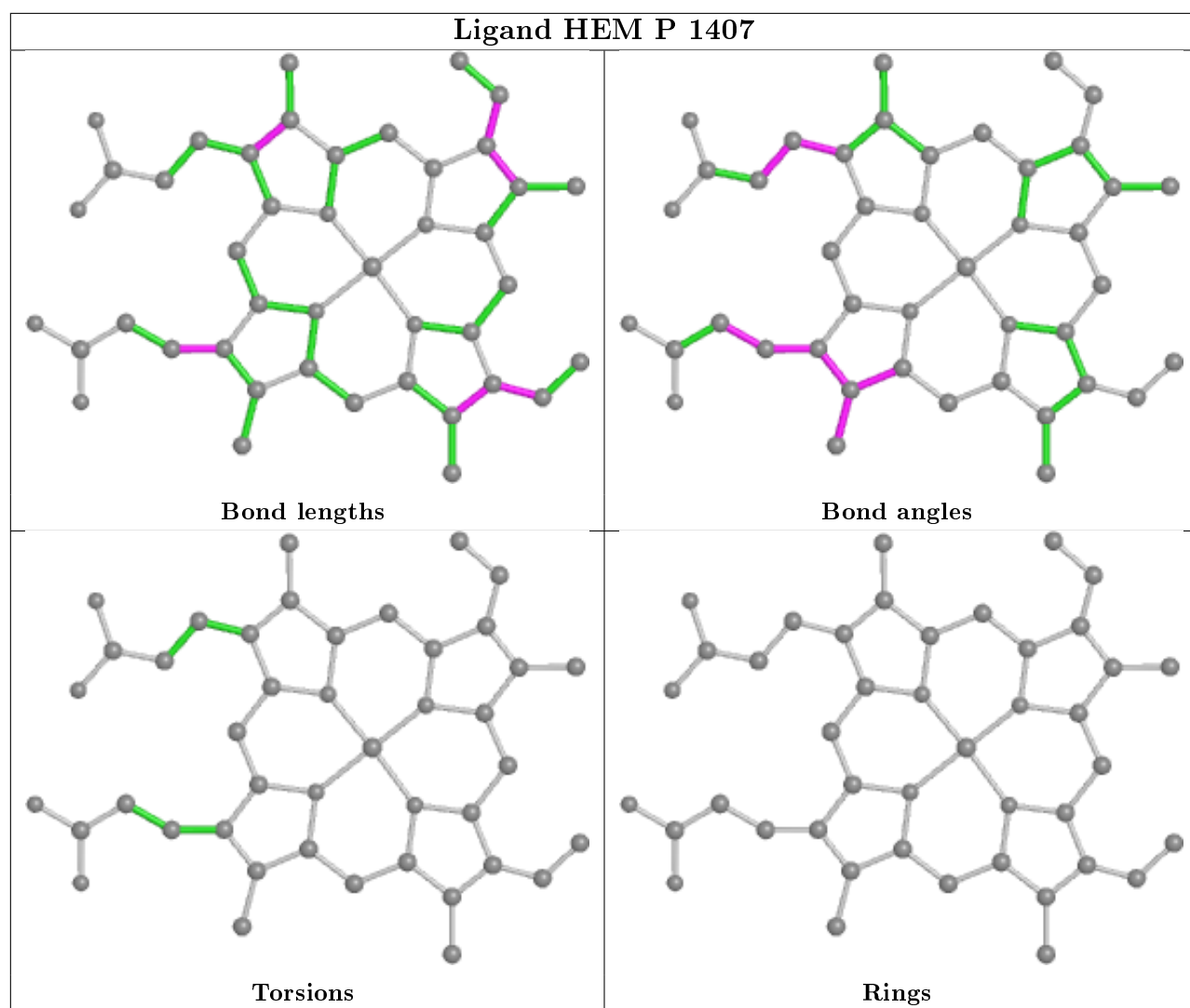
Rings

## Ligand HEM D 1407

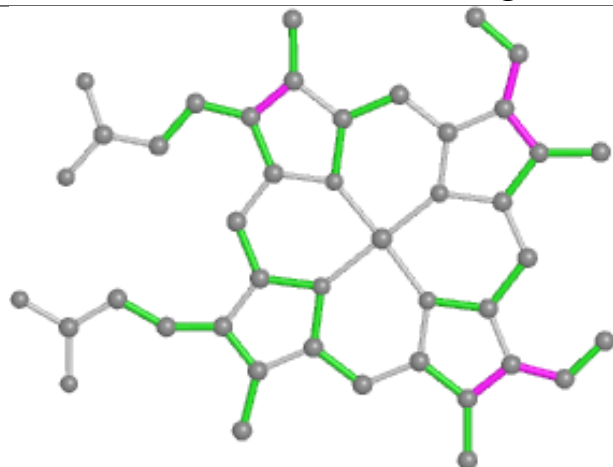


## Ligand 17Q C 1410

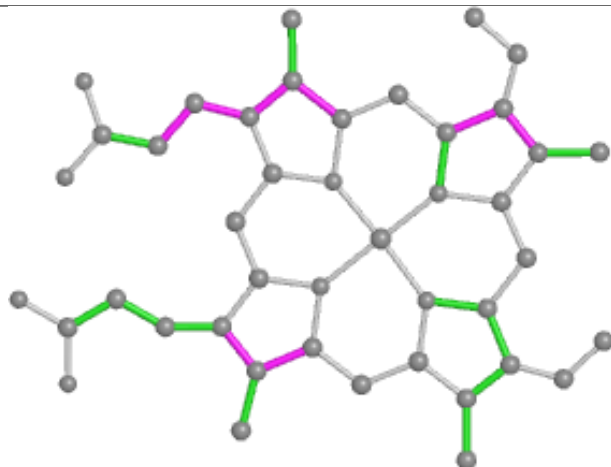




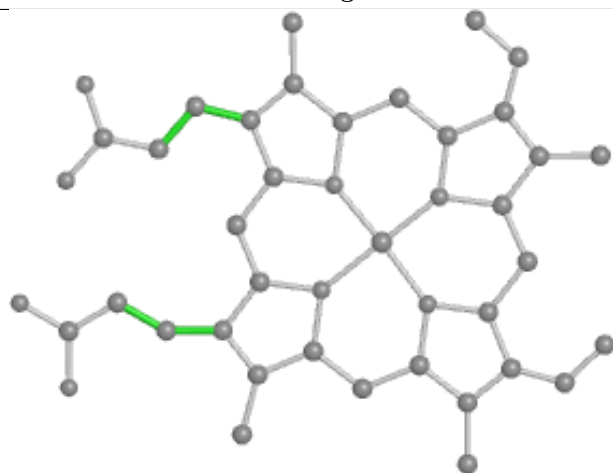
## Ligand HEM K 1407



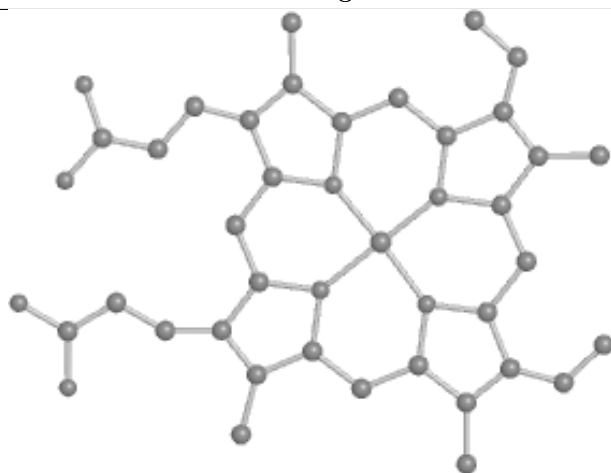
Bond lengths



Bond angles

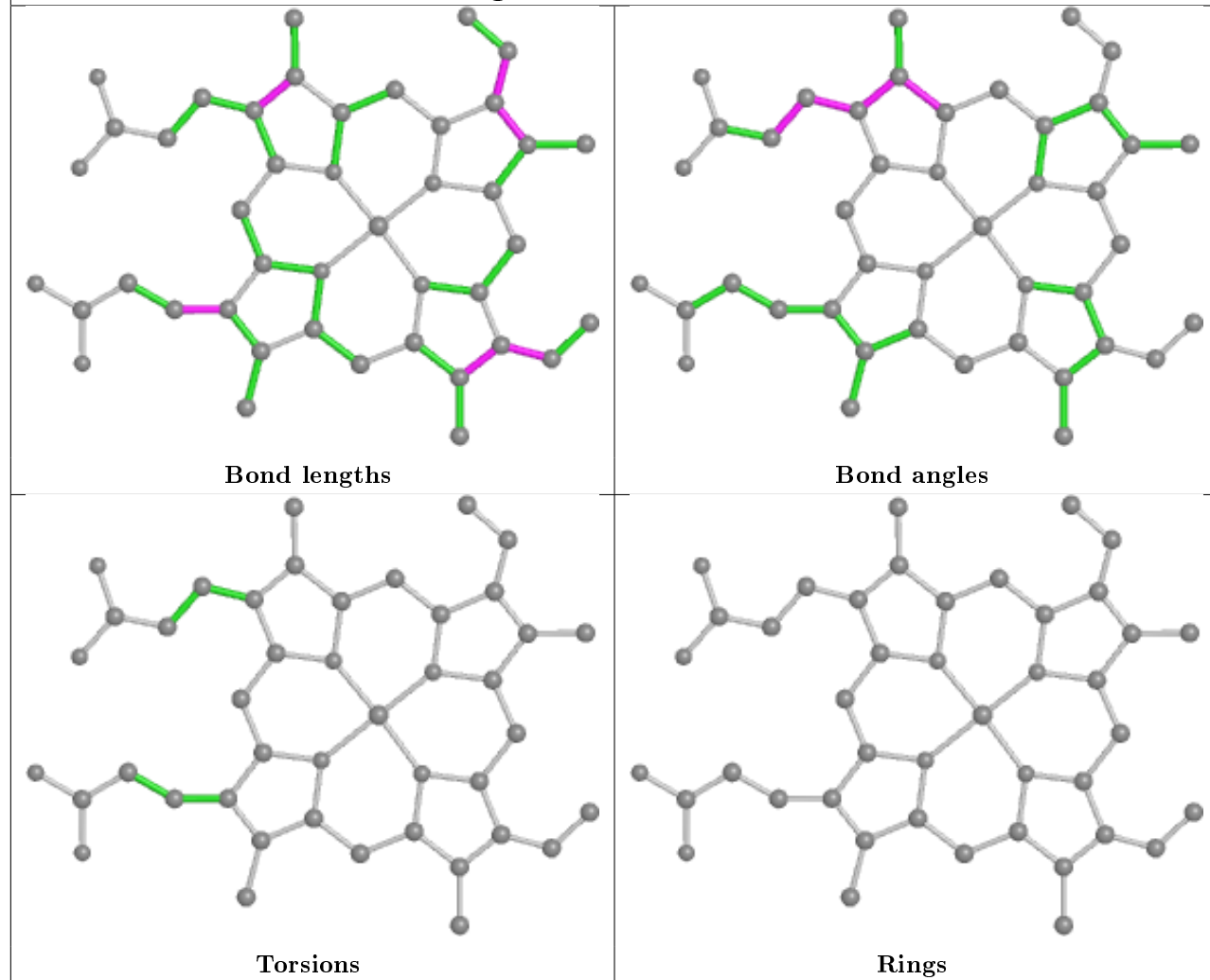


Torsions

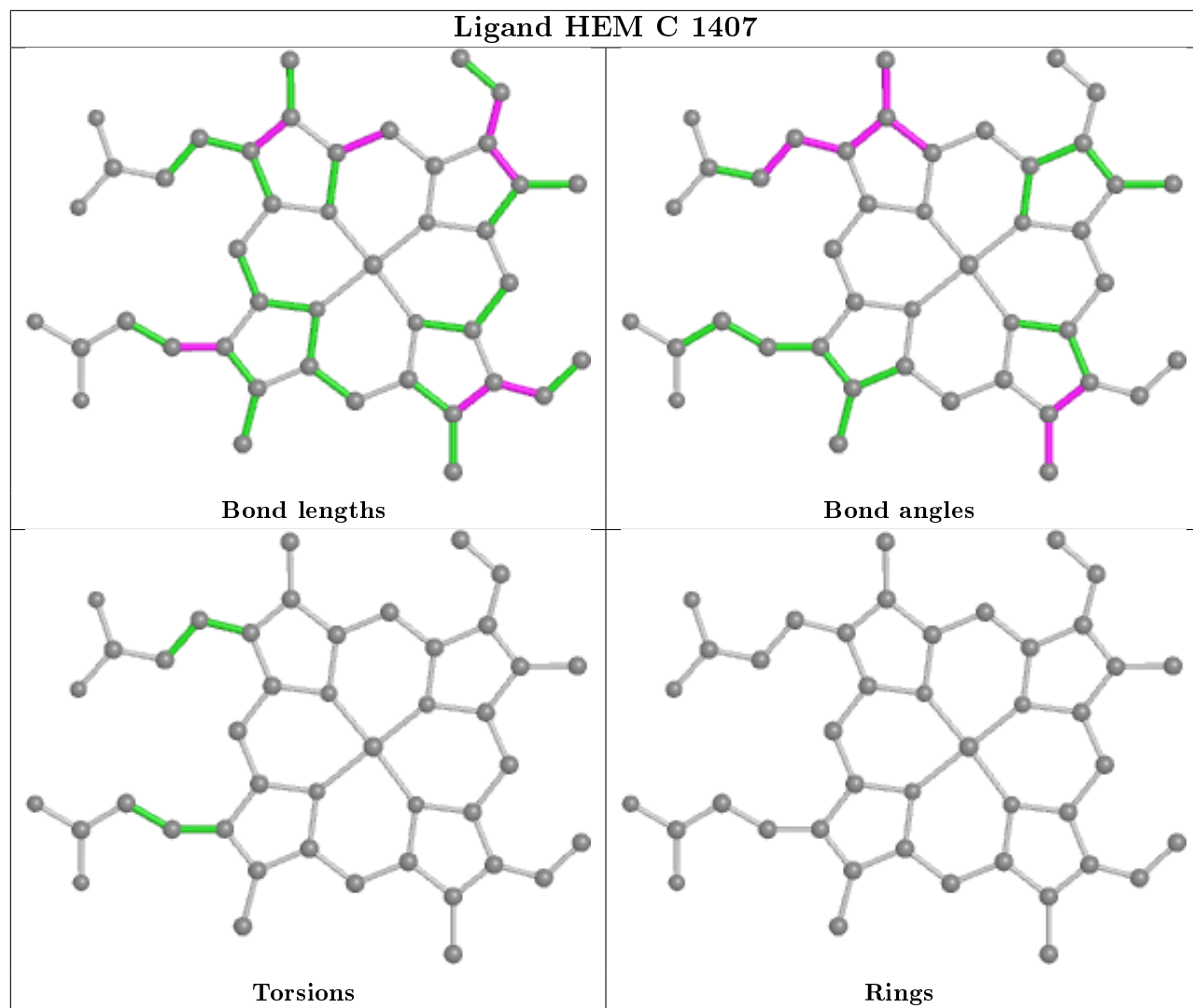


Rings

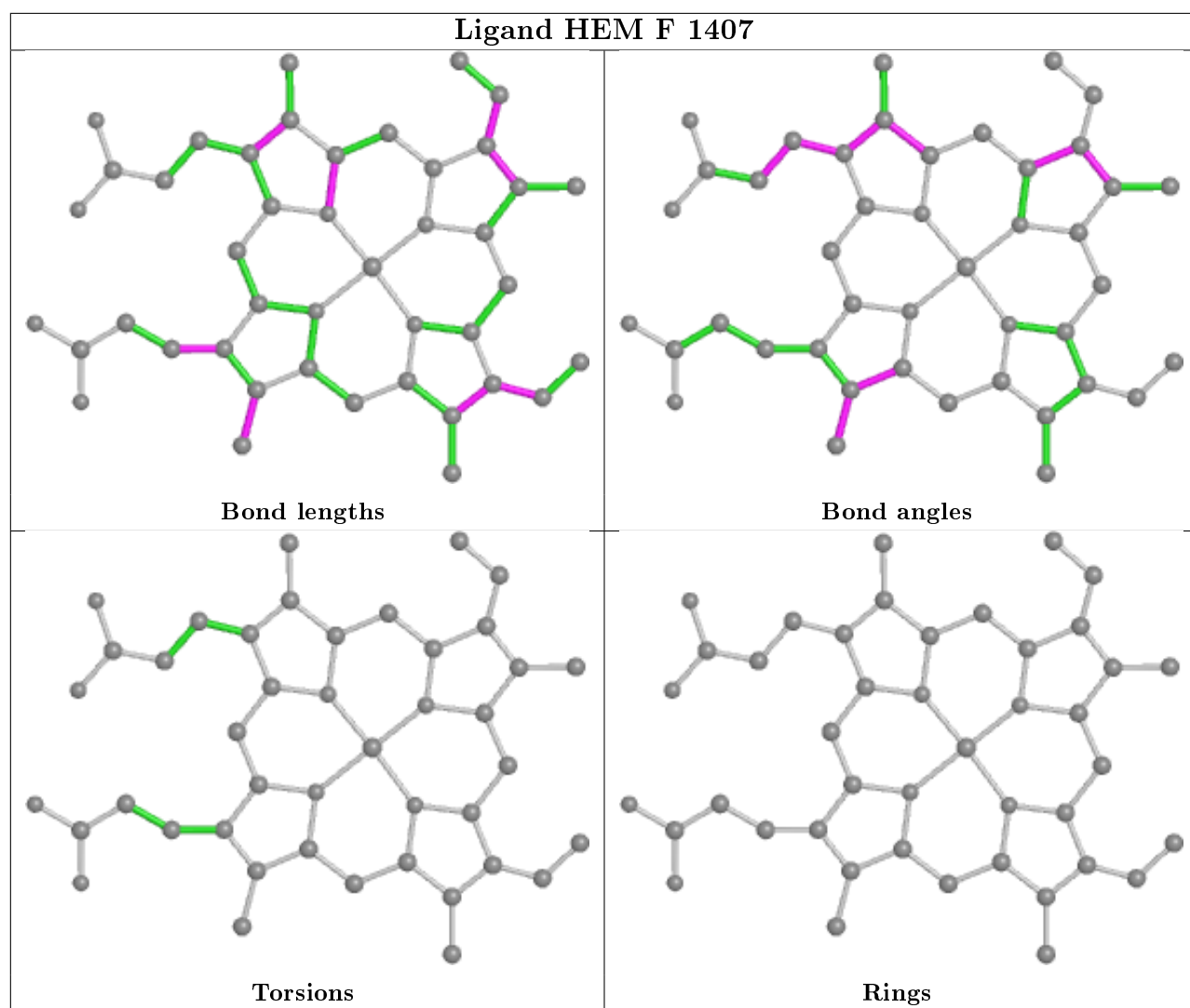
## Ligand HEM N 1407

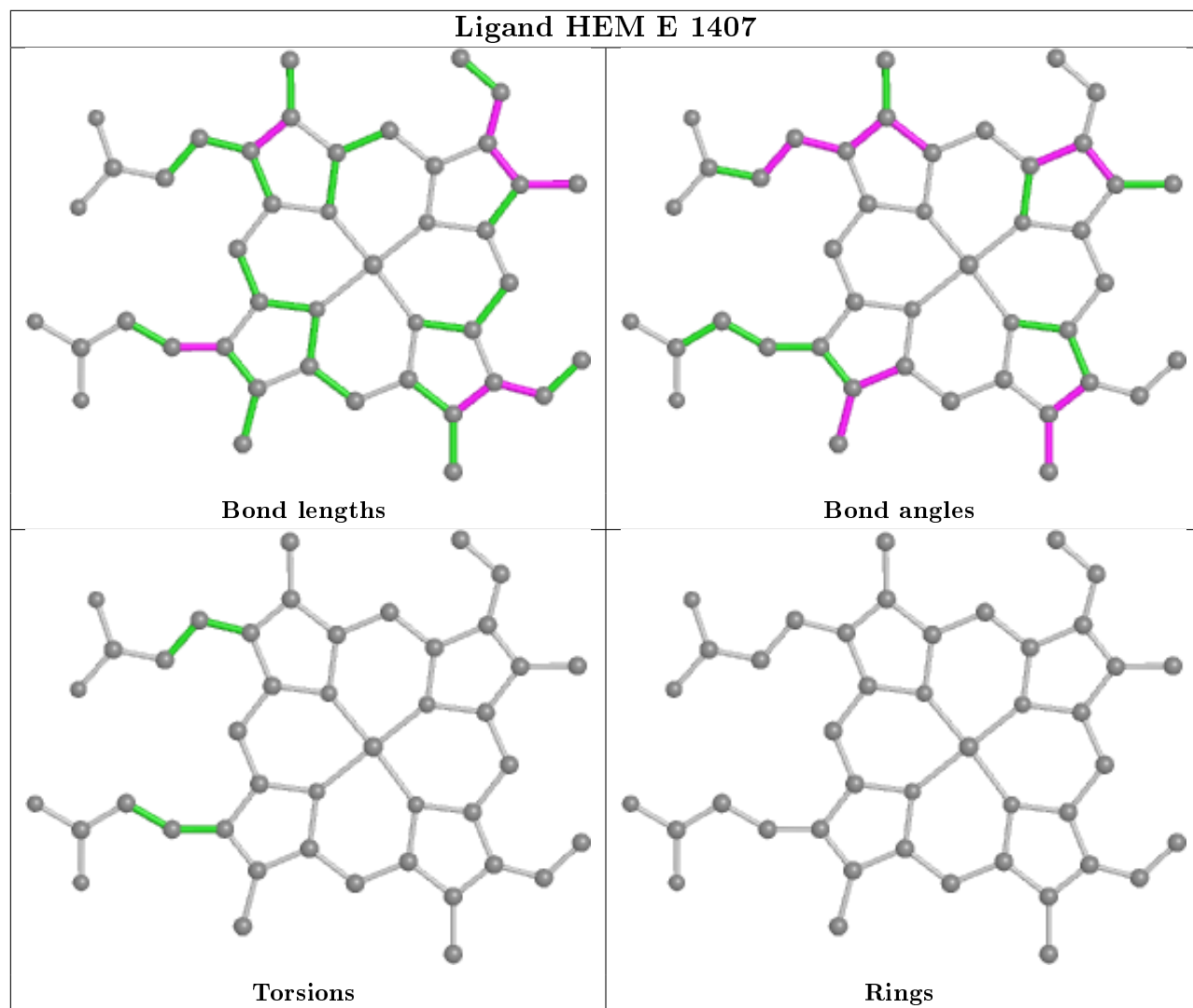


## Ligand HEM C 1407

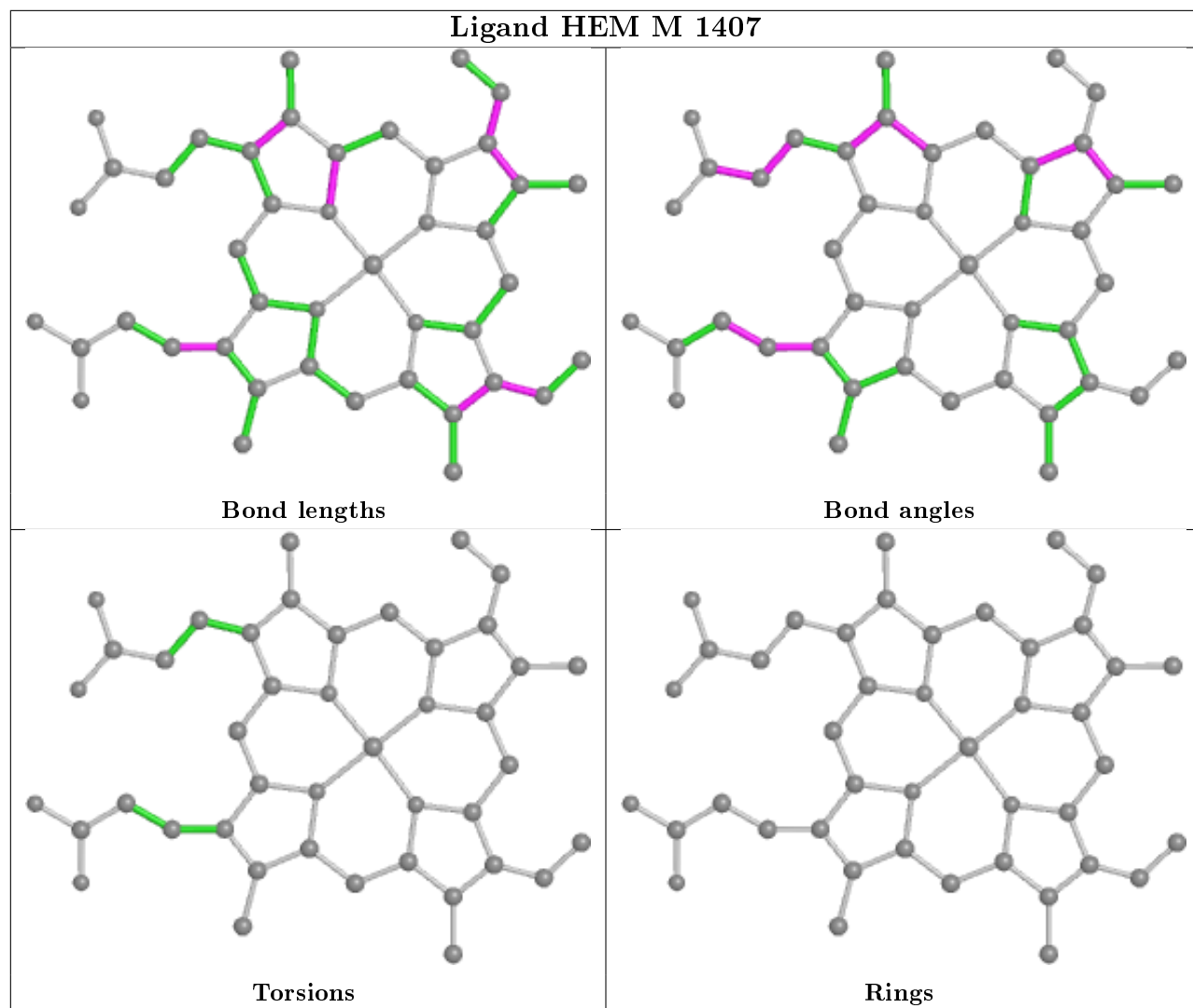




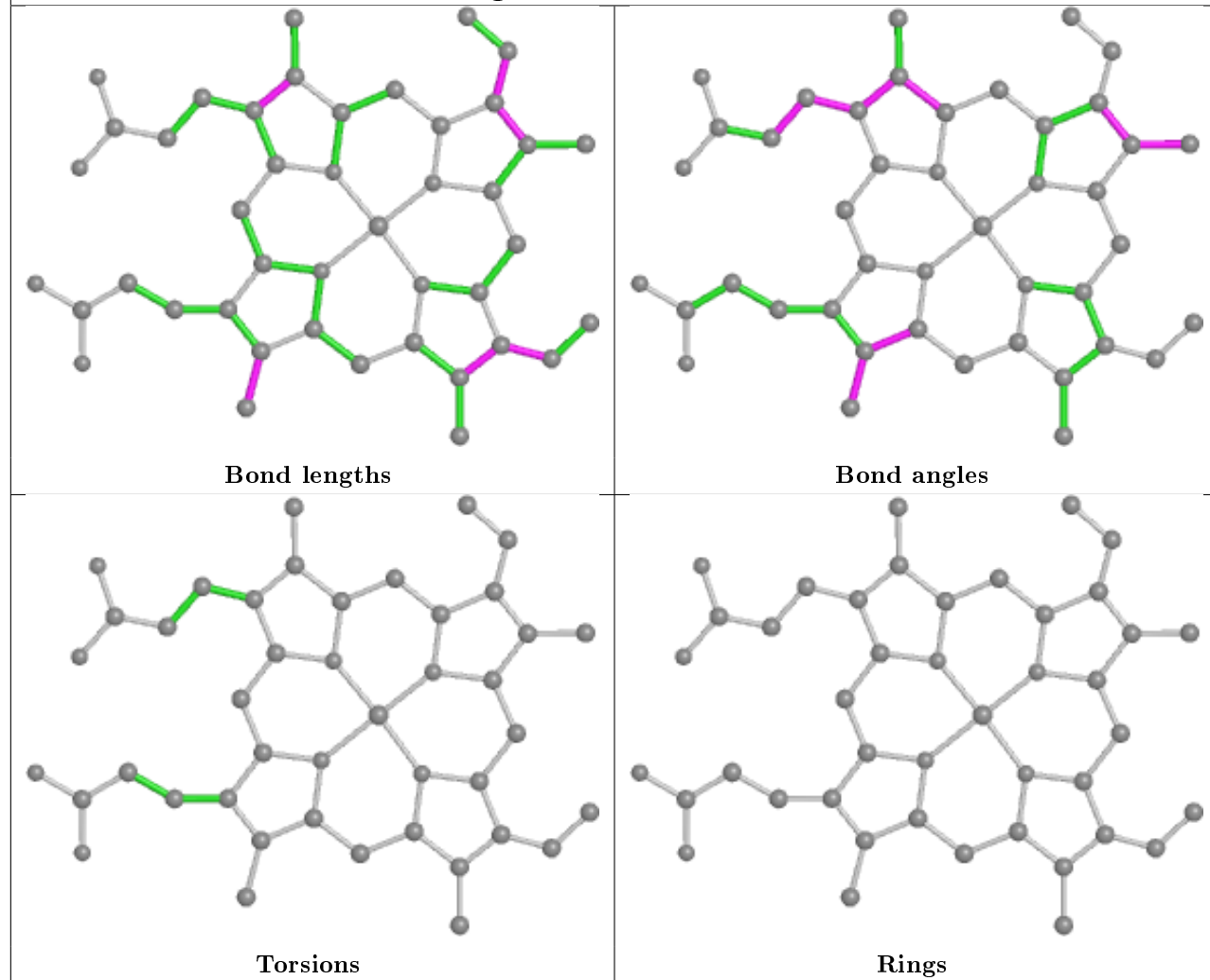




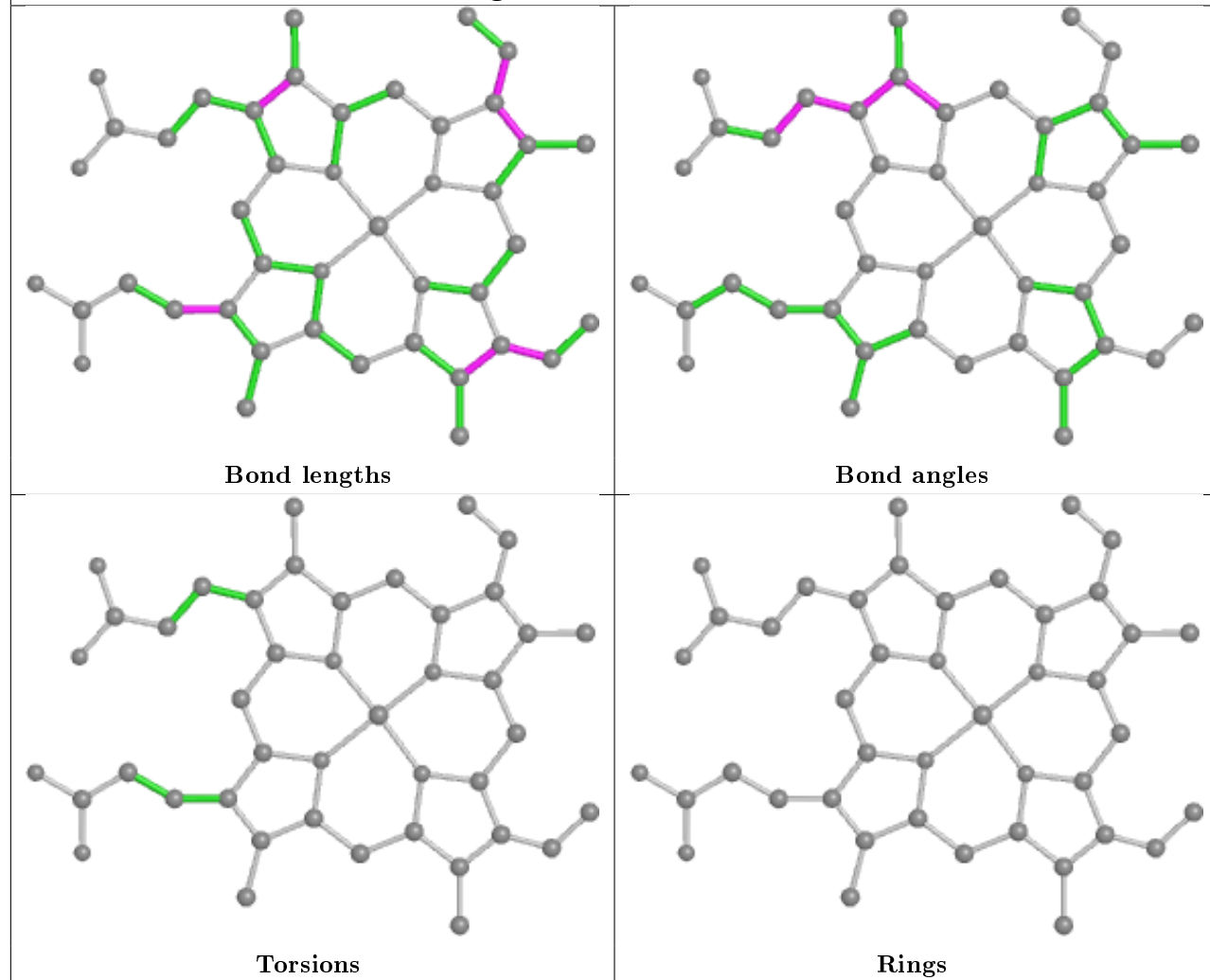
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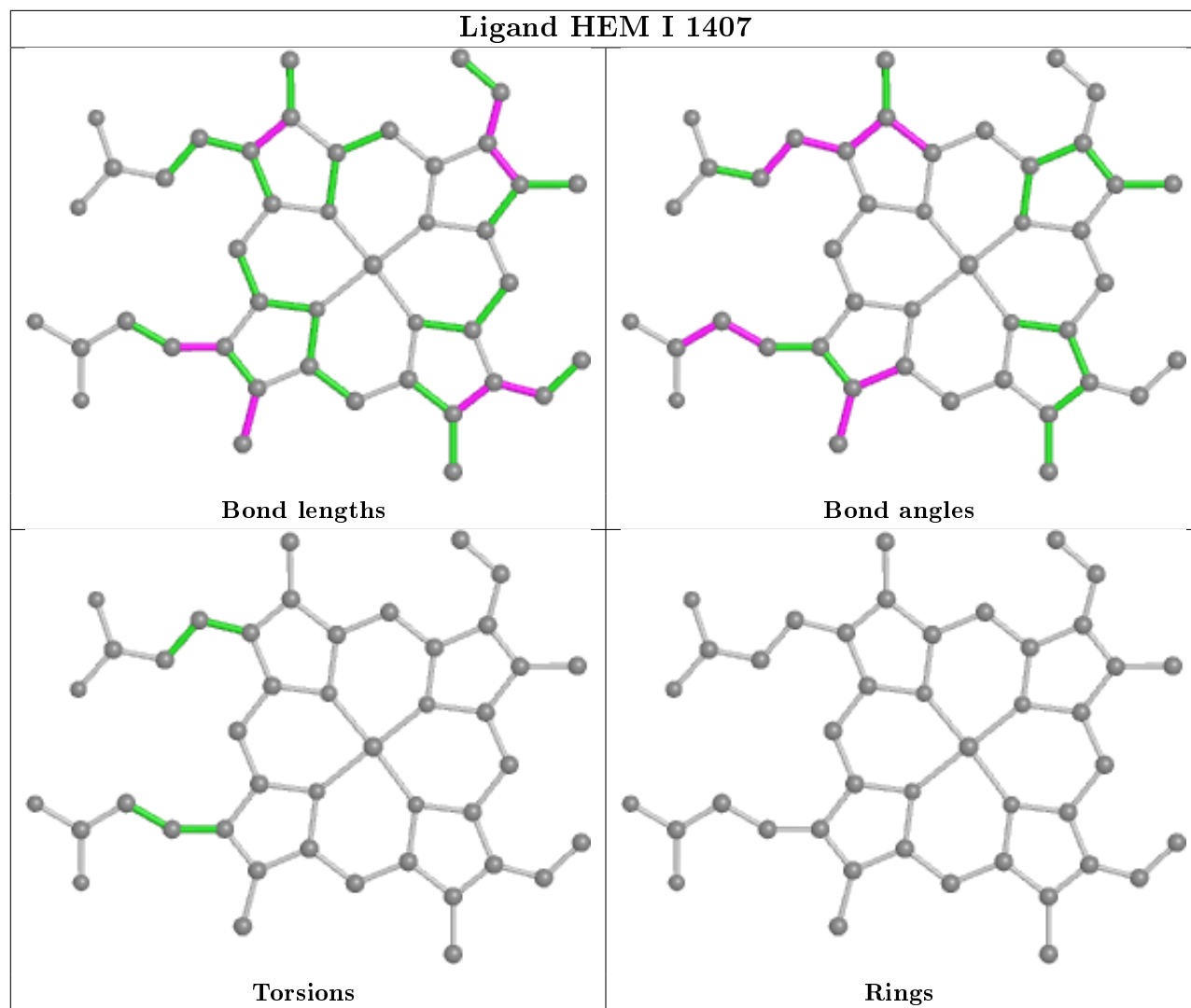


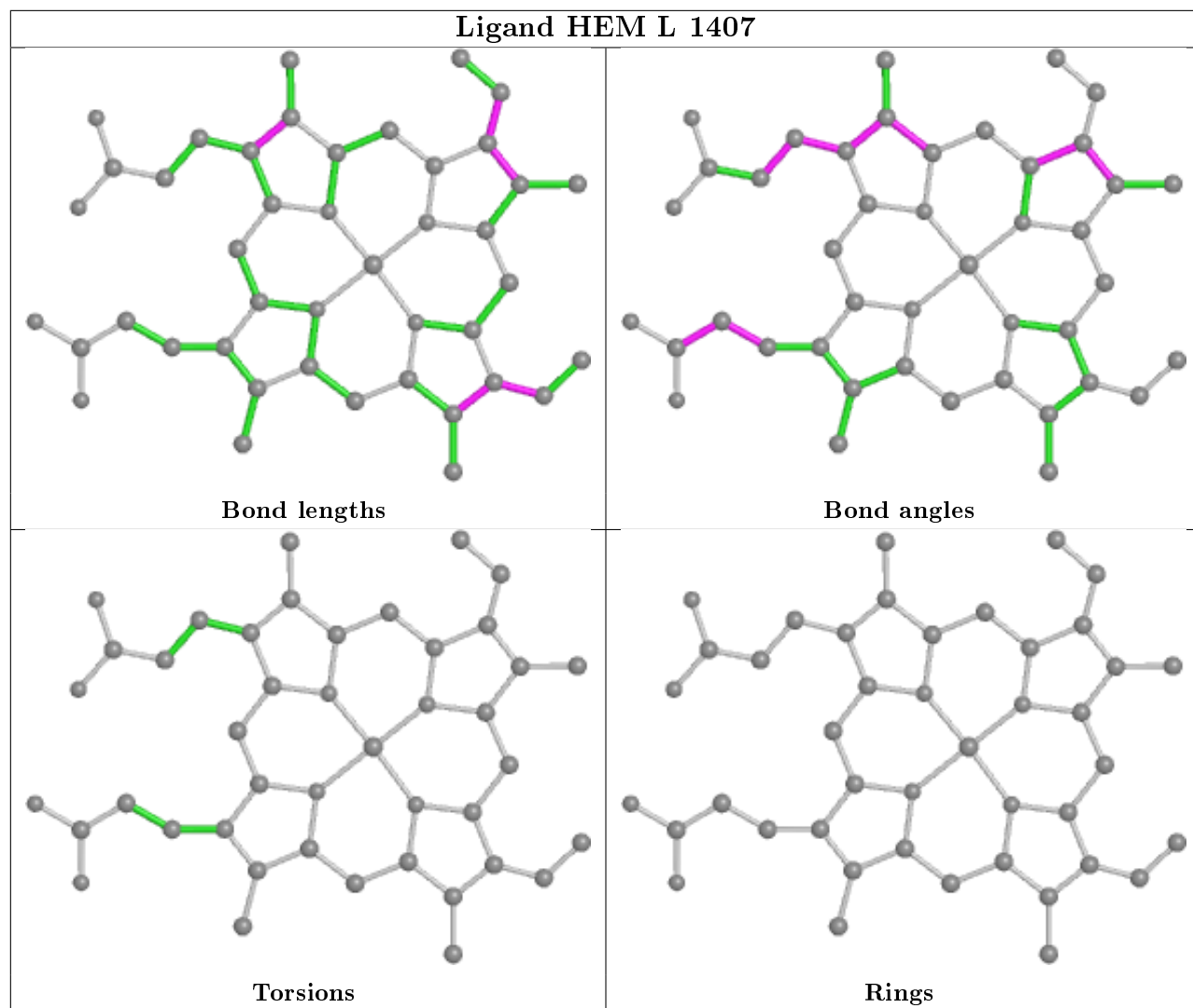
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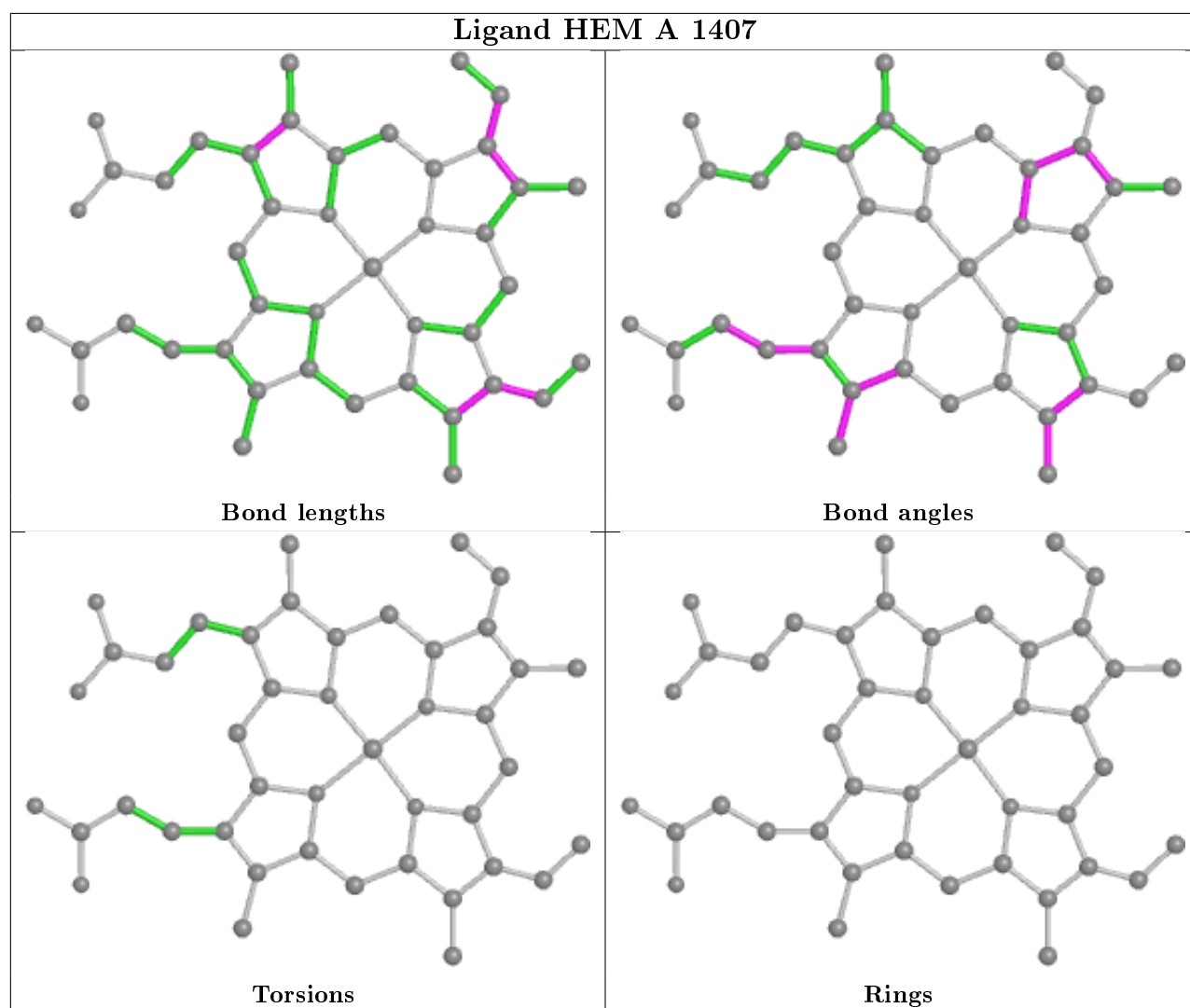


## Ligand HEM G 1407









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	396/436 (90%)	-0.56	0 100 100	17, 33, 55, 71	0
1	B	397/436 (91%)	-0.48	2 (0%) 91 92	20, 35, 57, 76	0
1	C	396/436 (90%)	-0.54	0 100 100	16, 33, 55, 73	0
1	D	397/436 (91%)	-0.49	1 (0%) 94 95	18, 32, 55, 81	0
1	E	397/436 (91%)	-0.47	3 (0%) 86 87	16, 33, 55, 73	0
1	F	396/436 (90%)	-0.47	1 (0%) 94 95	16, 39, 66, 84	0
1	G	396/436 (90%)	-0.54	0 100 100	19, 35, 52, 61	0
1	H	396/436 (90%)	-0.46	3 (0%) 86 87	18, 35, 61, 87	0
1	I	396/436 (90%)	-0.45	2 (0%) 91 92	20, 39, 66, 79	0
1	J	397/436 (91%)	-0.42	1 (0%) 94 95	21, 42, 68, 91	0
1	K	397/436 (91%)	-0.34	1 (0%) 94 95	25, 46, 72, 90	0
1	L	397/436 (91%)	-0.26	2 (0%) 91 92	21, 50, 86, 99	0
1	M	397/436 (91%)	-0.17	5 (1%) 77 78	30, 53, 85, 91	0
1	N	397/436 (91%)	0.09	16 (4%) 38 37	34, 72, 116, 158	0
1	O	397/436 (91%)	0.04	18 (4%) 33 31	28, 57, 105, 133	0
1	P	396/436 (90%)	0.30	32 (8%) 12 10	29, 78, 129, 155	0
All	All	6345/6976 (90%)	-0.33	87 (1%) 75 77	16, 41, 91, 158	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	184	PRO	8.3
1	O	179	VAL	6.6
1	O	180	PHE	6.3
1	O	10	ALA	5.5
1	N	10	ALA	4.8

## 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 carbohydrates 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.

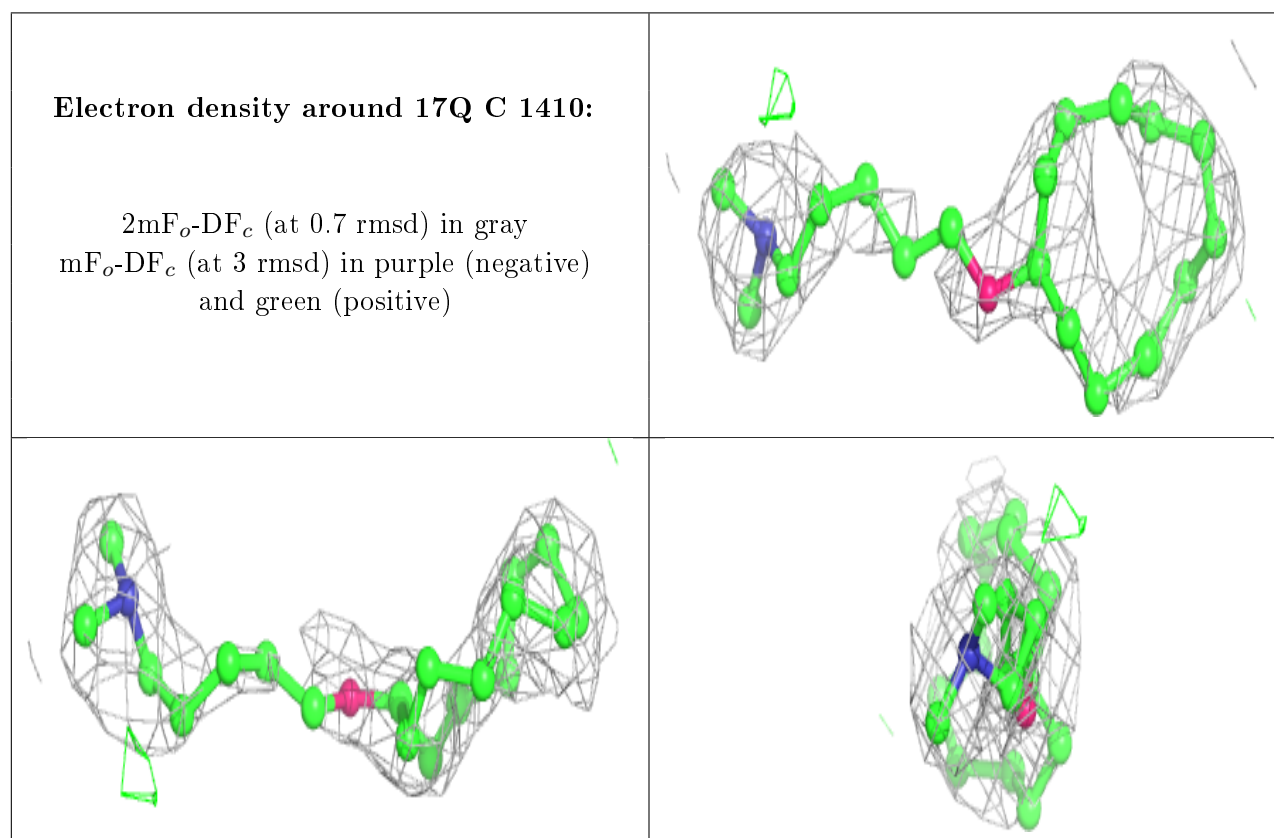
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	17Q	C	1410	21/21	0.86	0.29	53,57,60,60	0
4	17Q	G	1410	21/21	0.90	0.27	39,49,55,55	0
3	SO4	D	1408	5/5	0.91	0.16	37,37,39,40	0
3	SO4	O	1409	5/5	0.95	0.19	39,39,40,40	0
3	SO4	H	1408	5/5	0.95	0.18	42,42,44,45	0
3	SO4	A	1408	5/5	0.95	0.10	41,42,43,43	0
3	SO4	J	1408	5/5	0.95	0.20	41,42,42,43	0
3	SO4	B	1408	5/5	0.95	0.16	61,62,63,63	0
3	SO4	I	1408	5/5	0.95	0.24	39,41,42,43	0
3	SO4	H	1409	5/5	0.96	0.13	38,39,40,40	0
3	SO4	F	1408	5/5	0.96	0.15	38,39,40,41	0
2	HEM	P	1407	43/43	0.96	0.16	36,46,51,54	0
2	HEM	I	1407	43/43	0.97	0.14	23,25,29,31	0
2	HEM	E	1407	43/43	0.97	0.13	13,18,21,23	0
2	HEM	O	1407	43/43	0.97	0.14	29,33,38,41	0
3	SO4	O	1408	5/5	0.97	0.18	41,41,42,42	0
2	HEM	J	1407	43/43	0.98	0.15	26,28,31,32	0
2	HEM	K	1407	43/43	0.98	0.13	21,25,27,29	0
2	HEM	N	1407	43/43	0.98	0.13	29,33,44,49	0
2	HEM	F	1407	43/43	0.98	0.14	17,22,24,26	0
2	HEM	G	1407	43/43	0.98	0.13	17,23,24,28	0
2	HEM	D	1407	43/43	0.98	0.12	13,18,22,23	0
2	HEM	L	1407	43/43	0.98	0.13	19,24,27,31	0
2	HEM	H	1407	43/43	0.98	0.14	15,19,21,22	0
2	HEM	B	1407	43/43	0.98	0.12	19,25,27,29	0
2	HEM	M	1407	43/43	0.98	0.12	18,23,26,31	0
3	SO4	B	1409	5/5	0.98	0.12	49,49,51,51	0

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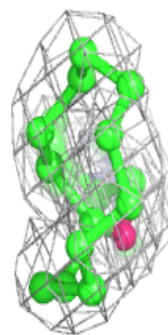
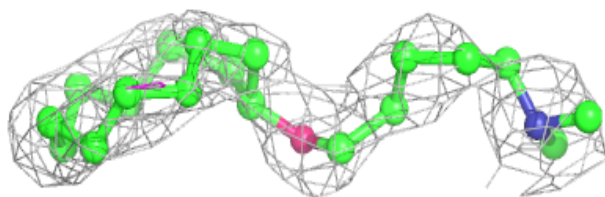
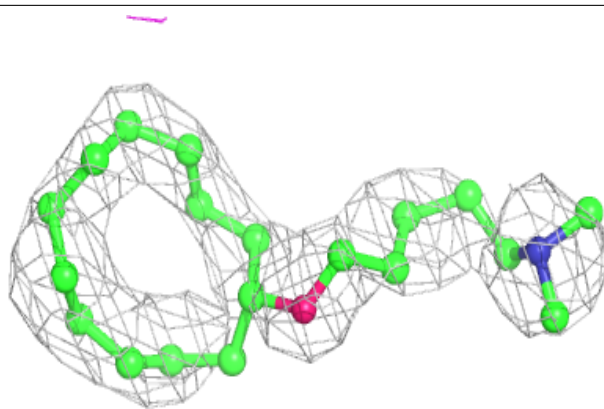
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	I	1409	5/5	0.99	0.05	53,54,55,55	0
2	HEM	A	1407	43/43	0.99	0.12	14,20,24,28	0
2	HEM	C	1407	43/43	0.99	0.14	12,14,19,24	0

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.



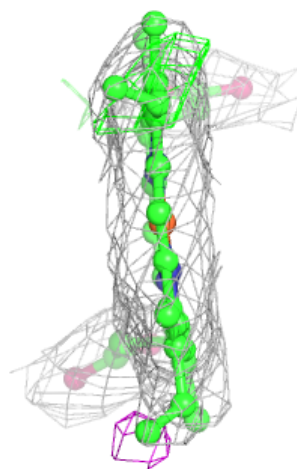
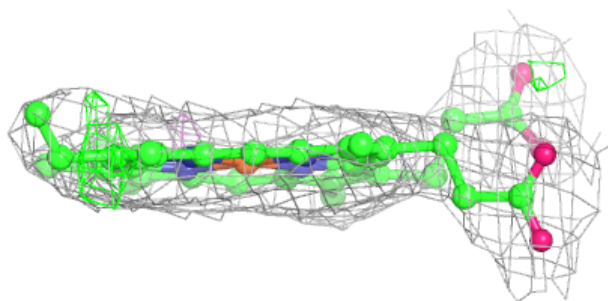
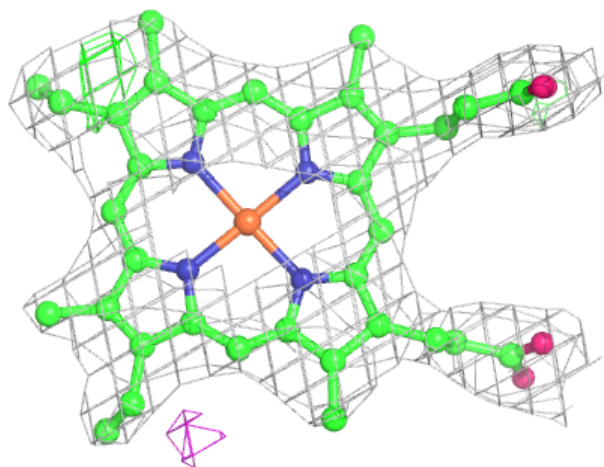
**Electron density around 17Q G 1410:**

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



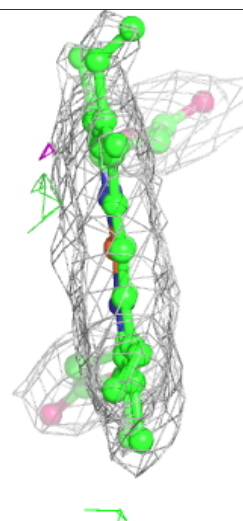
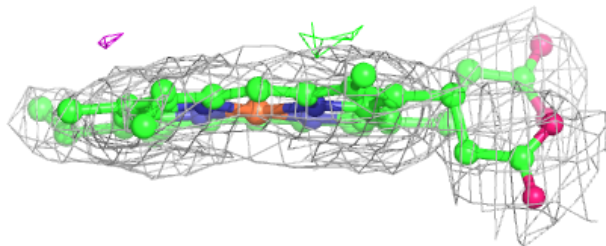
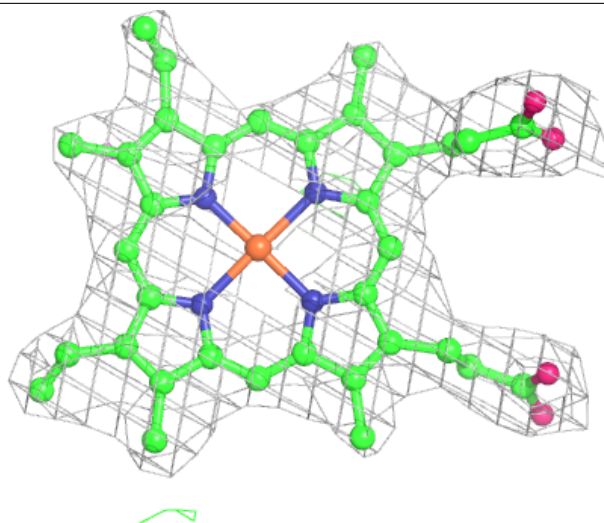
**Electron density around HEM P 1407:**

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



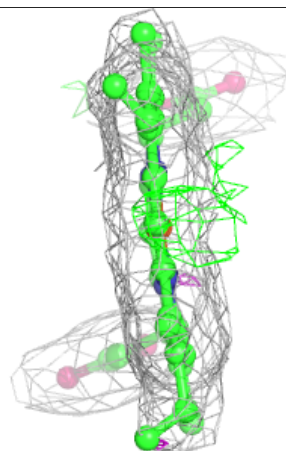
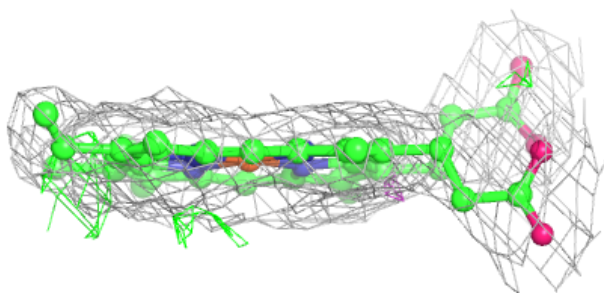
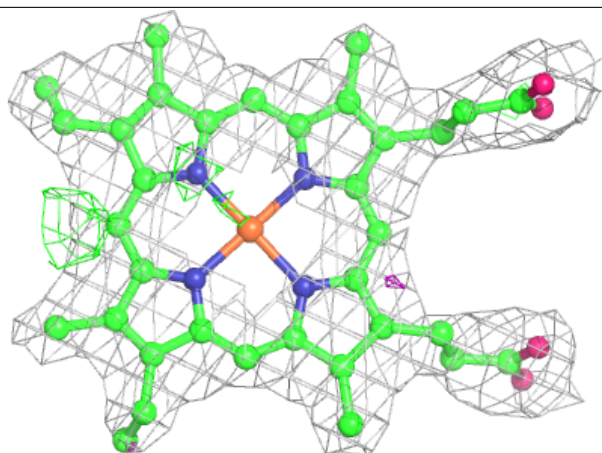
**Electron density around HEM I 1407:**

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



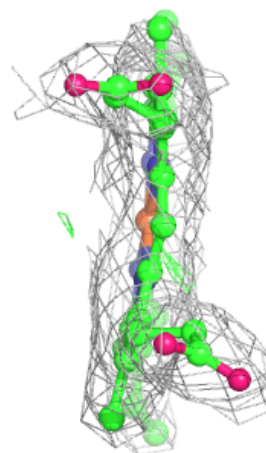
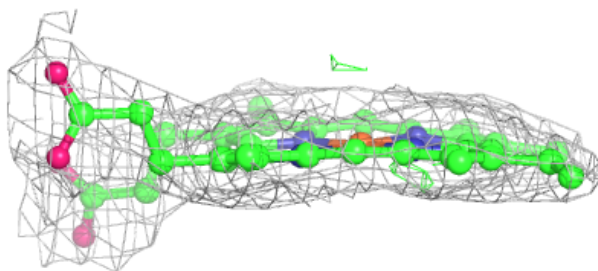
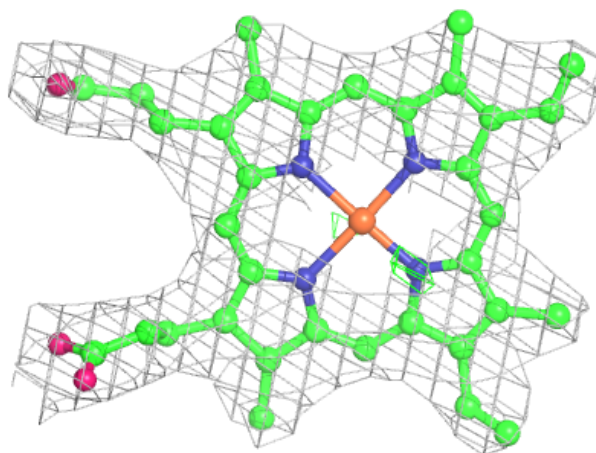
**Electron density around HEM E 1407:**

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



**Electron density around HEM O 1407:**

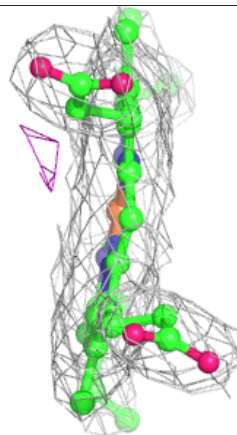
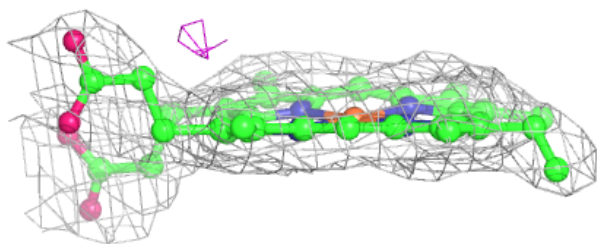
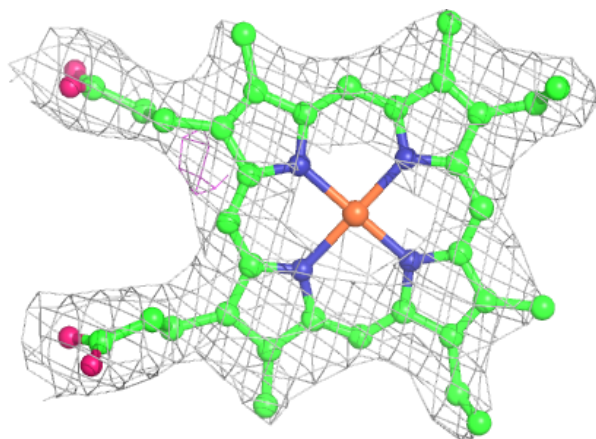
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





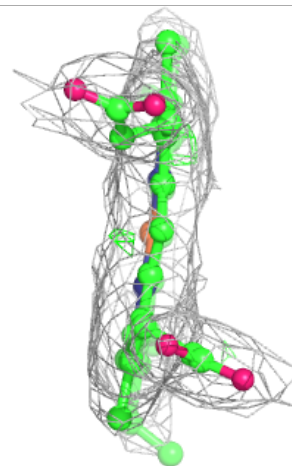
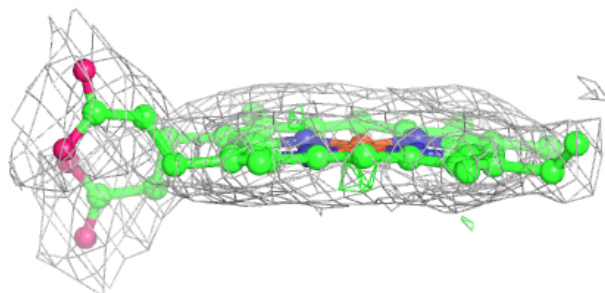
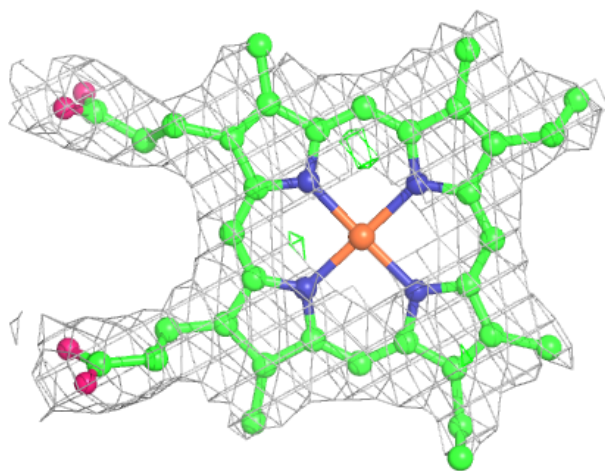
**Electron density around HEM J 1407:**

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



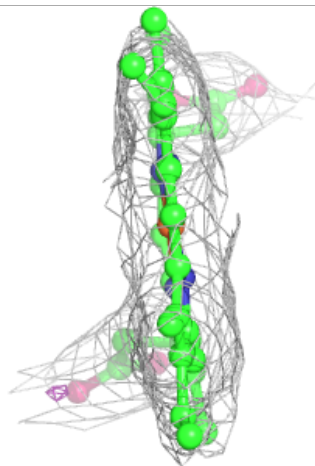
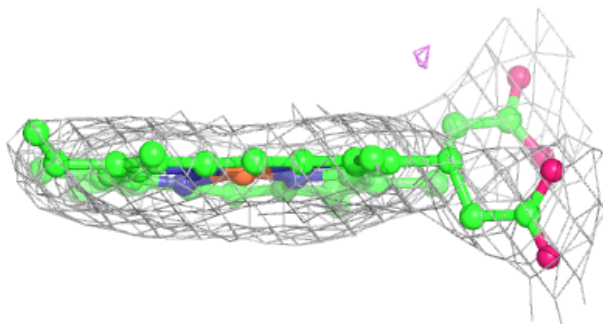
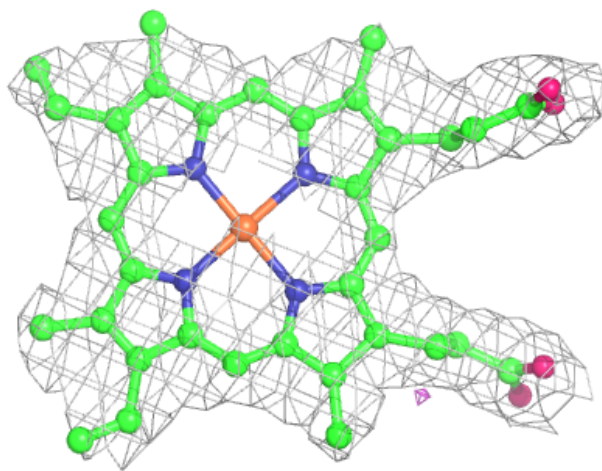
**Electron density around HEM K 1407:**

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



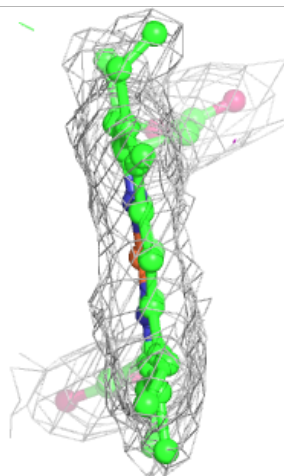
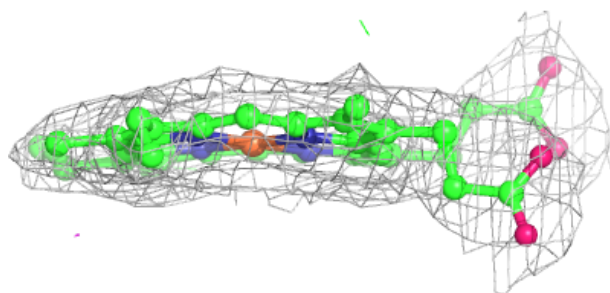
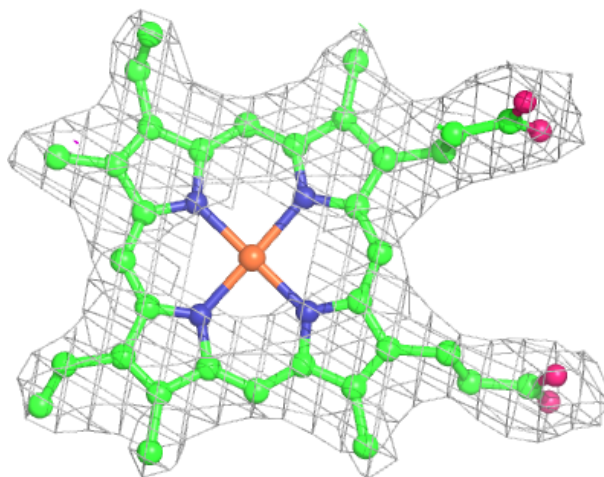
**Electron density around HEM N 1407:**

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



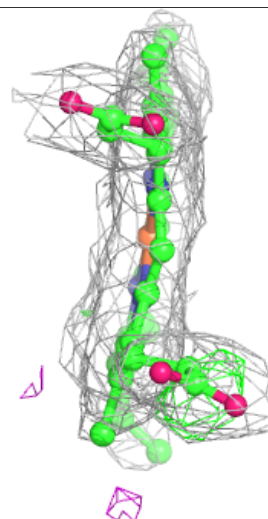
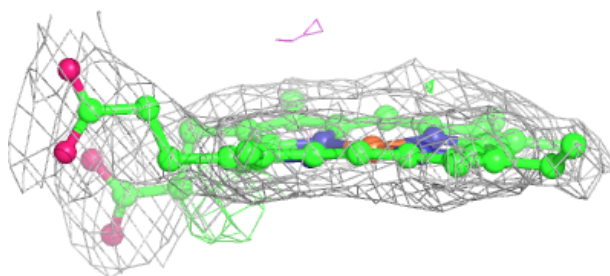
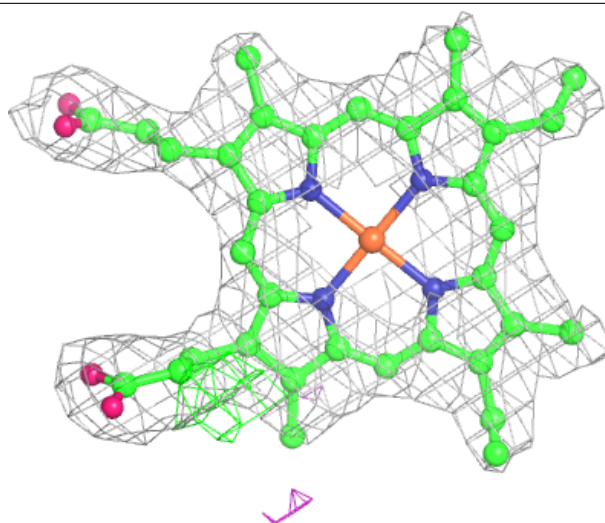
**Electron density around HEM F 1407:**

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



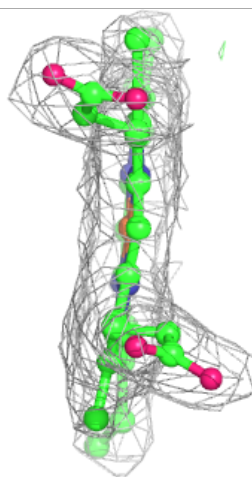
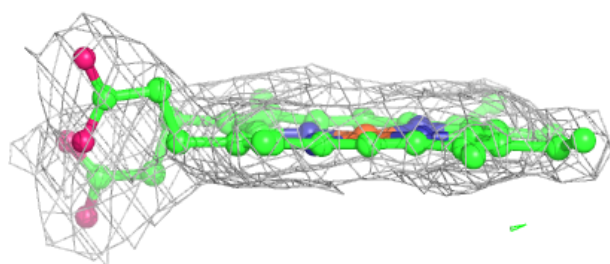
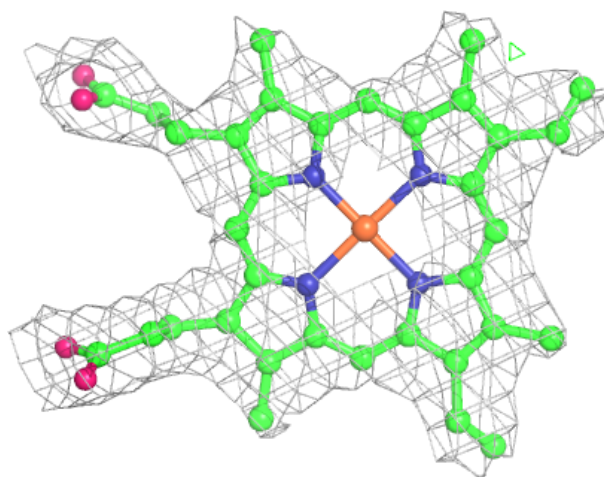
**Electron density around HEM G 1407:**

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



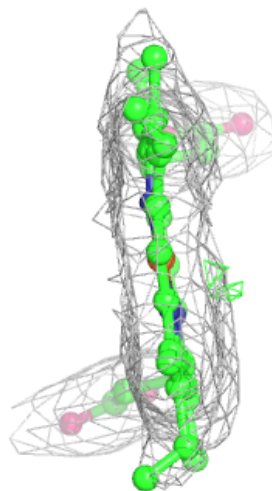
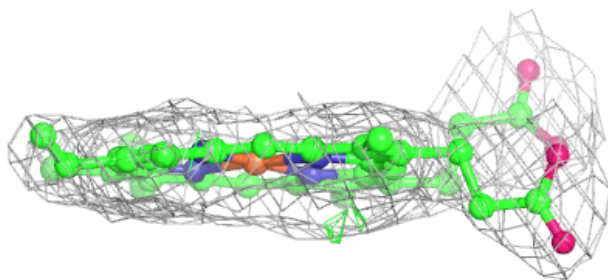
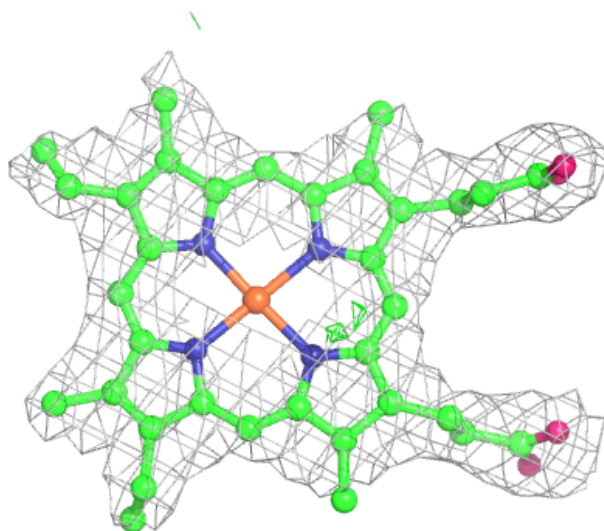
**Electron density around HEM D 1407:**

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



**Electron density around HEM L 1407:**

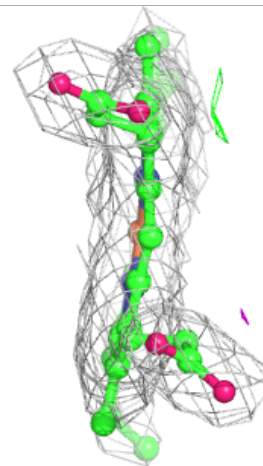
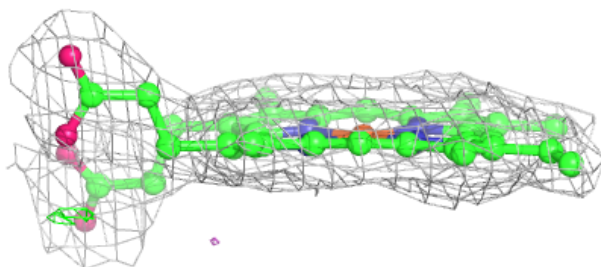
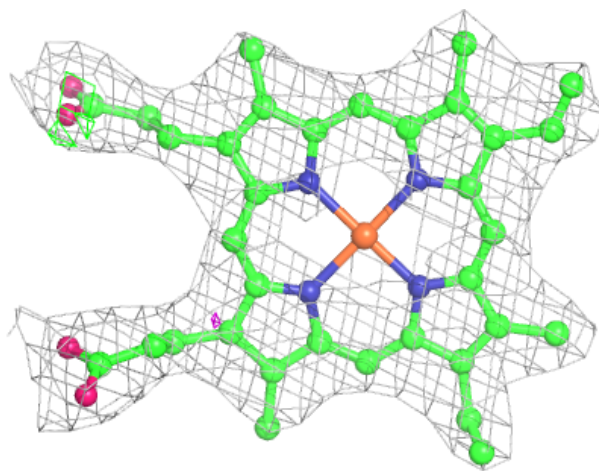
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM H 1407:**

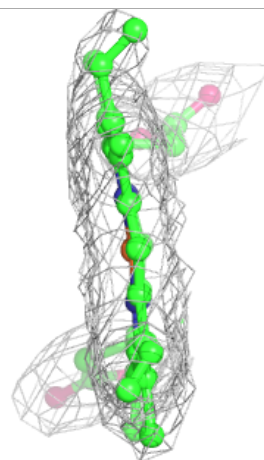
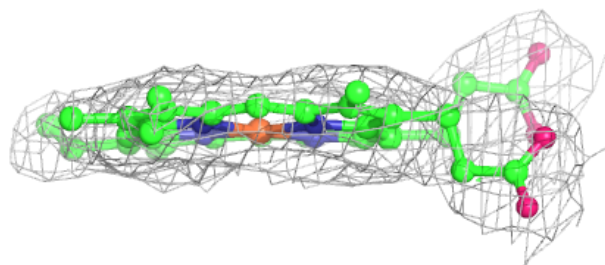
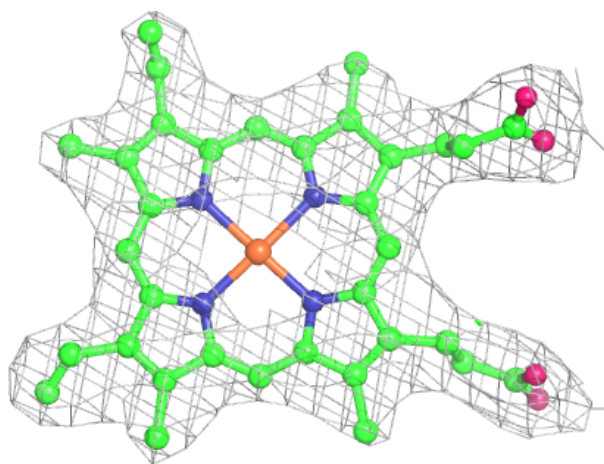
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





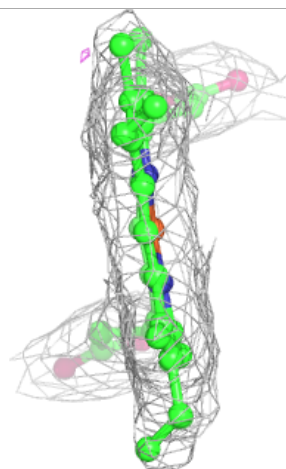
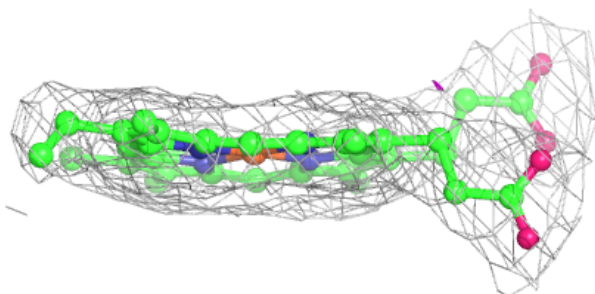
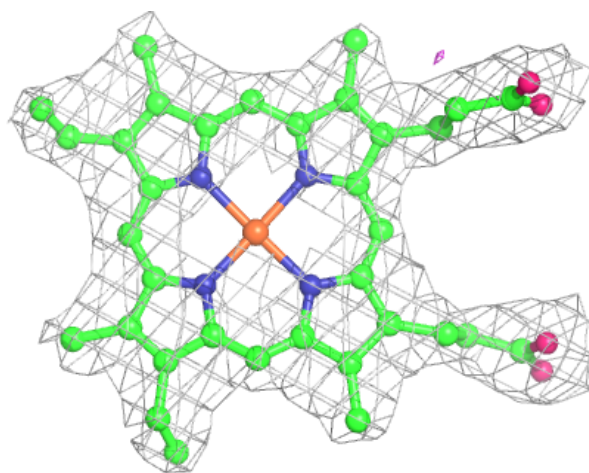
**Electron density around HEM B 1407:**

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



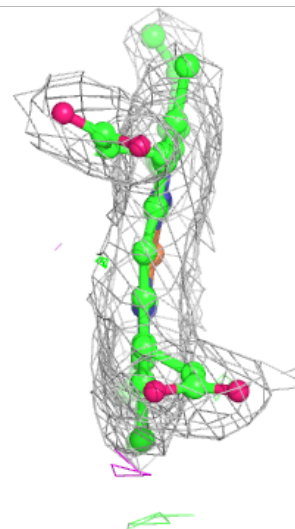
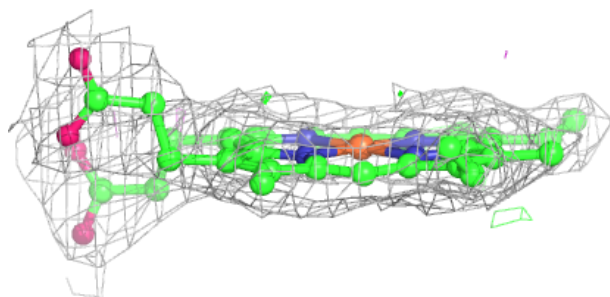
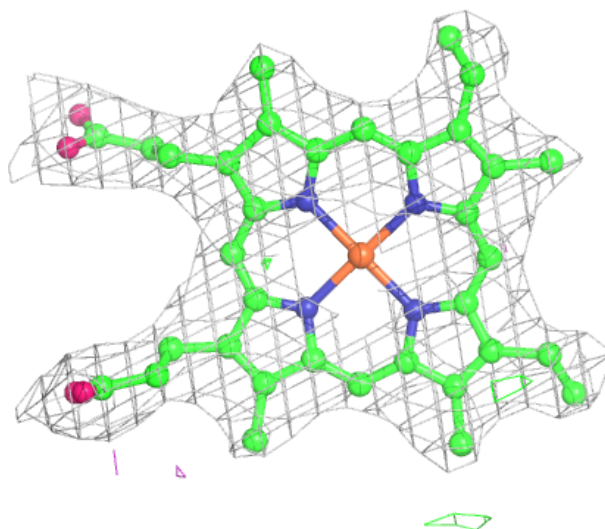
**Electron density around HEM M 1407:**

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



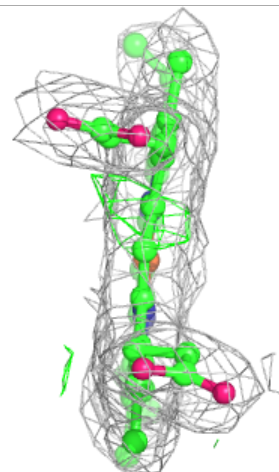
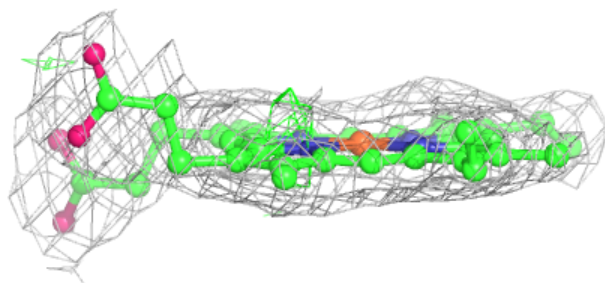
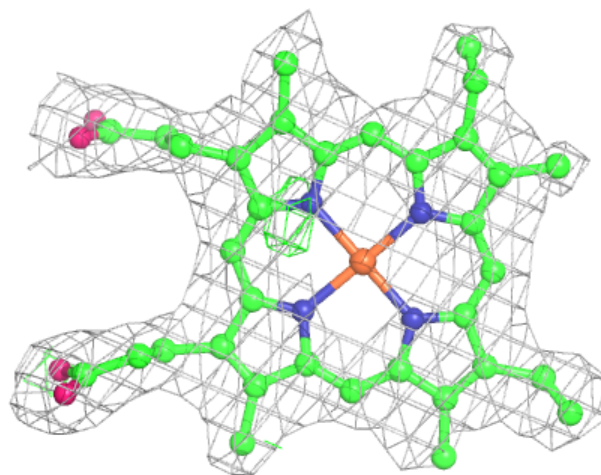
**Electron density around HEM A 1407:**

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



**Electron density around HEM C 1407:**

$2mF_o-DF_c$  (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.