



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:12 AM UTC

PDB ID : 4BF4 / pdb_00004bf4
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

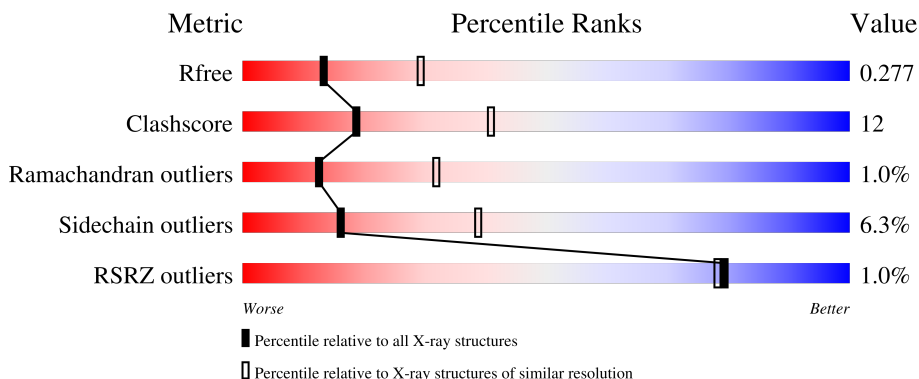
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	436	 66% 24% 9%
1	G	436	 68% 20% 9%
1	H	436	 68% 22% 9%
1	I	436	 70% 18% 9%
1	J	436	 67% 22% 9%
1	K	436	 65% 24% 9%
1	L	436	 1% 66% 23% 9%
1	M	436	 61% 27% 9%
1	N	436	 2% 67% 20% 9%
1	O	436	 3% 65% 24% 9%
1	P	436	 4% 64% 25% 9%

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

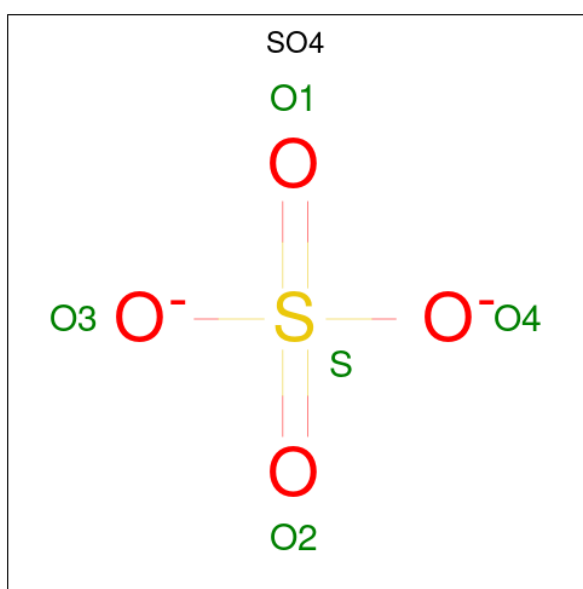
Continued from previous page...

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

Continued from previous page...

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 (CCD ID: SO4) (formula: O₄S).



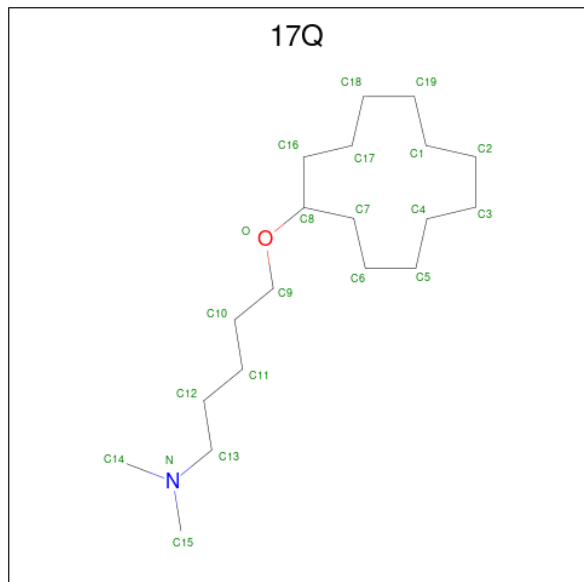
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	D	1	Total	O S	0	0
			5	4 1		
3	F	1	Total	O S	0	0
			5	4 1		
3	H	1	Total	O S	0	0
			5	4 1		
3	H	1	Total	O S	0	0
			5	4 1		

Continued on next page...

Continued from previous page...

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 (CCD ID: 17Q) (formula: C₁₉H₃₉NO).



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		

Continued on next page...

Continued from previous page...

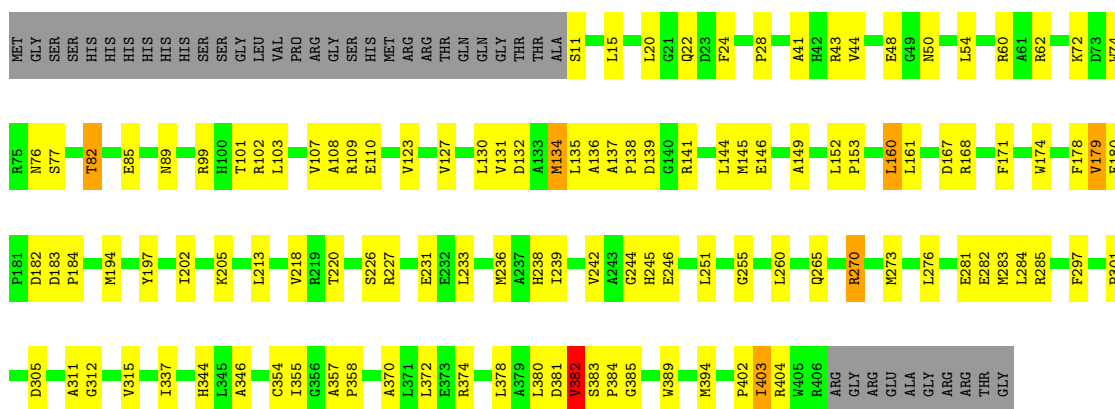
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	43	Total 43	O 43	0	0
5	D	46	Total 46	O 46	0	0
5	E	37	Total 37	O 37	0	0
5	F	39	Total 39	O 39	0	0
5	G	57	Total 57	O 57	0	0
5	H	35	Total 35	O 35	0	0
5	I	39	Total 39	O 39	0	0
5	J	34	Total 34	O 34	0	0
5	K	28	Total 28	O 28	0	0
5	L	21	Total 21	O 21	0	0
5	M	16	Total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

3 Residue-property plots

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

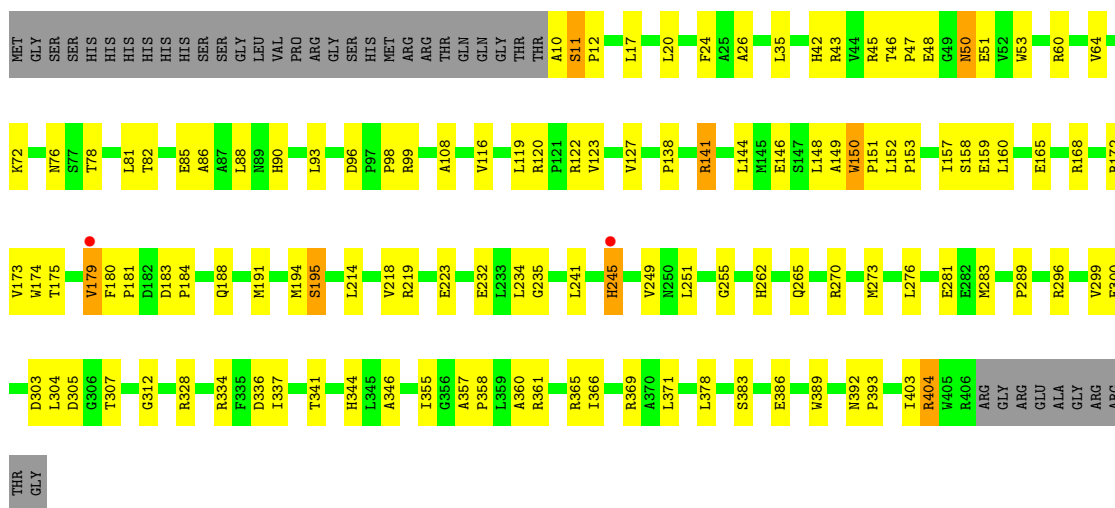
- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain A: 



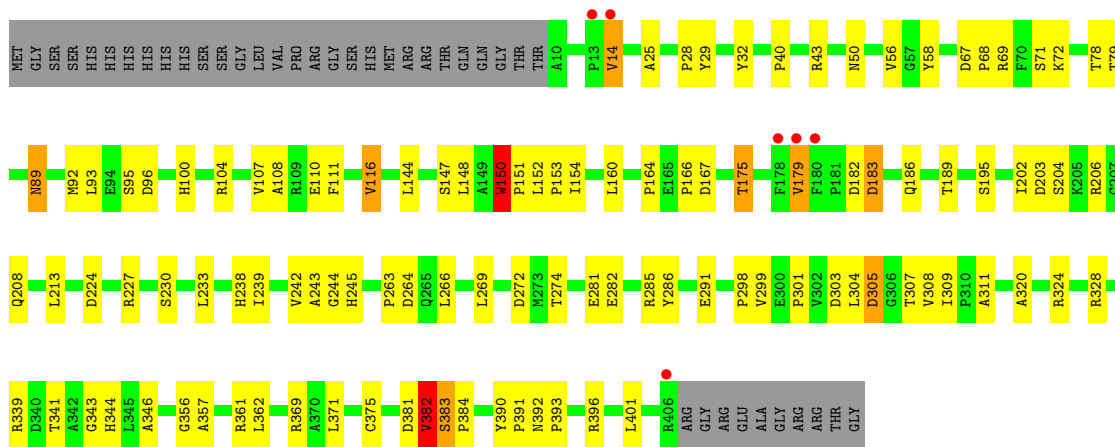
- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain B: 

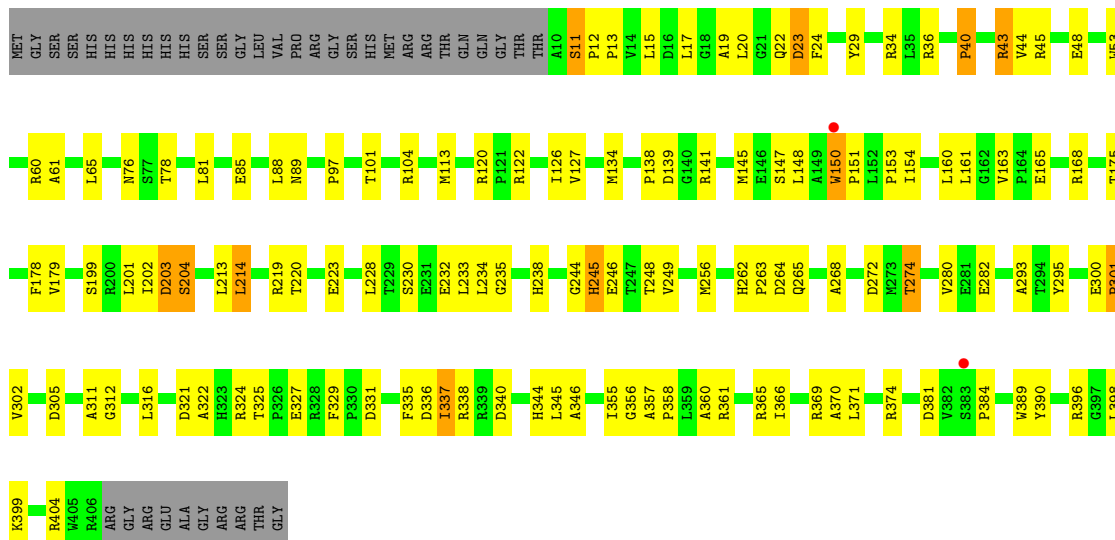


- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

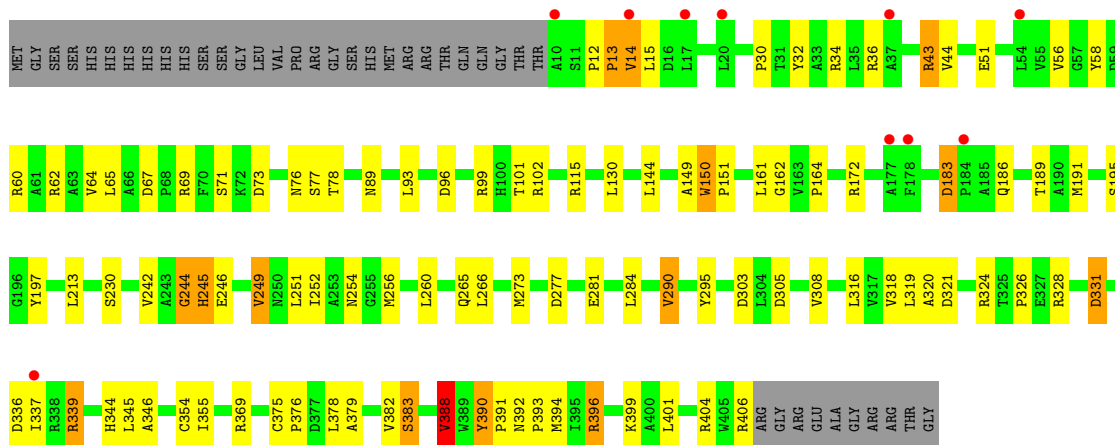
Chain C: 



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.27Å 130.11Å 134.90Å 66.48° 70.25° 72.23°	Depositor
Resolution (Å)	119.84 – 2.70 119.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (119.84-2.70) 97.3 (119.84-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.69Å)	Xtrriage
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 ²)	44.7	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.030 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50342	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, HEM, 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	0.80	0/3100	1.07	6/4234 (0.1%)
1	B	0.79	0/3142	1.02	5/4292 (0.1%)
1	C	0.80	0/3136	1.06	9/4283 (0.2%)
1	D	0.83	1/3149 (0.0%)	1.07	10/4301 (0.2%)
1	E	0.82	0/3141	1.12	11/4290 (0.3%)
1	F	0.78	0/3149	1.00	3/4303 (0.1%)
1	G	0.79	0/3166	1.03	4/4324 (0.1%)
1	H	0.82	0/3130	1.04	0/4275
1	I	0.75	0/3139	1.01	2/4288 (0.0%)
1	J	0.75	0/3133	1.00	2/4280 (0.0%)
1	K	0.73	1/3149 (0.0%)	1.02	8/4301 (0.2%)
1	L	0.72	0/3138	1.01	7/4287 (0.2%)
1	M	0.70	1/3138 (0.0%)	1.00	11/4286 (0.3%)
1	N	0.63	0/3137	0.98	8/4285 (0.2%)
1	O	0.68	0/3125	0.99	4/4269 (0.1%)
1	P	0.63	0/3131	0.96	4/4276 (0.1%)
All	All	0.75	3/50203 (0.0%)	1.02	94/68574 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	154	ILE	CA-CB	8.53	1.64	1.54
1	M	154	ILE	CA-CB	5.54	1.61	1.54
1	K	154	ILE	CA-CB	5.36	1.60	1.54

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	39	GLY	CA-C-N	8.36	128.33	119.05
1	K	39	GLY	C-N-CA	8.36	128.33	119.05
1	D	390	TYR	CA-C-N	8.09	128.18	119.28
1	D	390	TYR	C-N-CA	8.09	128.18	119.28
1	N	246	GLU	N-CA-C	7.96	119.64	110.97

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 [\(i\)](#)

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	3031	0	2990	70	0
1	B	3069	0	3026	99	0
1	C	3063	0	3024	75	0
1	D	3076	0	3027	87	0
1	E	3068	0	3022	68	0
1	F	3075	0	3019	79	0
1	G	3093	0	3049	87	0
1	H	3057	0	3020	63	0
1	I	3066	0	3020	67	0
1	J	3060	0	3016	68	0
1	K	3076	0	3032	68	0
1	L	3065	0	3014	67	0
1	M	3065	0	3014	75	0
1	N	3064	0	3025	68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3052	0	3008	74	0
1	P	3058	0	3006	65	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
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	5	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	20	0	0	0	0
5	P	17	0	0	1	0
All	All	50342	0	48870	1177	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 12.

The worst 5 of 1177 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:C:85:GLU:HG3	1:C:191:MET:HE1	1.17	1.11
1:G:273:MET:HE2	1:G:369:ARG:HG3	1.33	1.10
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

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%)	12 32
1	B	397/436 (91%)	367 (92%)	29 (7%)	1 (0%)	36 60
1	C	395/436 (91%)	370 (94%)	23 (6%)	2 (0%)	24 48
1	D	397/436 (91%)	366 (92%)	28 (7%)	3 (1%)	16 37
1	E	396/436 (91%)	367 (93%)	26 (7%)	3 (1%)	16 37
1	F	398/436 (91%)	362 (91%)	30 (8%)	6 (2%)	8 22
1	G	398/436 (91%)	373 (94%)	22 (6%)	3 (1%)	16 37
1	H	395/436 (91%)	368 (93%)	26 (7%)	1 (0%)	36 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	396/436 (91%)	363 (92%)	29 (7%)	4 (1%)	12	32
1	J	396/436 (91%)	370 (93%)	24 (6%)	2 (0%)	24	48
1	K	397/436 (91%)	362 (91%)	30 (8%)	5 (1%)	9	25
1	L	397/436 (91%)	357 (90%)	33 (8%)	7 (2%)	6	18
1	M	396/436 (91%)	367 (93%)	22 (6%)	7 (2%)	6	18
1	N	396/436 (91%)	355 (90%)	37 (9%)	4 (1%)	12	32
1	O	395/436 (91%)	343 (87%)	47 (12%)	5 (1%)	9	25
1	P	395/436 (91%)	356 (90%)	35 (9%)	4 (1%)	12	32
All	All	6338/6976 (91%)	5816 (92%)	461 (7%)	61 (1%)	12	32

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/355 (88%)	288 (92%)	24 (8%)	12	30
1	B	316/355 (89%)	296 (94%)	20 (6%)	16	39
1	C	317/355 (89%)	298 (94%)	19 (6%)	17	41
1	D	318/355 (90%)	297 (93%)	21 (7%)	15	36
1	E	317/355 (89%)	300 (95%)	17 (5%)	20	45
1	F	317/355 (89%)	300 (95%)	17 (5%)	20	45
1	G	321/355 (90%)	303 (94%)	18 (6%)	19	44
1	H	315/355 (89%)	295 (94%)	20 (6%)	16	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	316/355 (89%)	297 (94%)	19 (6%)	17	41
1	J	315/355 (89%)	298 (95%)	17 (5%)	20	45
1	K	318/355 (90%)	300 (94%)	18 (6%)	18	43
1	L	314/355 (88%)	286 (91%)	28 (9%)	9	23
1	M	315/355 (89%)	291 (92%)	24 (8%)	12	30
1	N	316/355 (89%)	299 (95%)	17 (5%)	20	45
1	O	313/355 (88%)	294 (94%)	19 (6%)	17	40
1	P	315/355 (89%)	294 (93%)	21 (7%)	15	36
All	All	5055/5680 (89%)	4736 (94%)	319 (6%)	16	39

5 of 319 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	304	LEU
1	O	160	LEU
1	M	11	SER
1	M	369	ARG
1	P	78	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	245	HIS
1	L	344	HIS
1	J	265	GLN
1	K	245	HIS
1	M	344	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	SO4	F	1408	-	4,4,4	0.60	0	6,6,6	0.54	0
2	HEM	D	1407	1	50,50,50	1.85	9 (18%)	67,82,82	1.24	8 (11%)
2	HEM	F	1407	1	50,50,50	1.83	11 (22%)	67,82,82	1.30	6 (8%)
2	HEM	L	1407	1	50,50,50	1.68	7 (14%)	67,82,82	1.36	10 (14%)
3	SO4	A	1408	-	4,4,4	0.38	0	6,6,6	0.54	0
3	SO4	I	1409	-	4,4,4	0.34	0	6,6,6	0.37	0
3	SO4	O	1409	-	4,4,4	0.55	0	6,6,6	0.80	0
2	HEM	I	1407	1	50,50,50	1.90	8 (16%)	67,82,82	1.48	8 (11%)
3	SO4	J	1408	-	4,4,4	0.68	0	6,6,6	0.49	0
2	HEM	M	1407	1	50,50,50	1.88	10 (20%)	67,82,82	1.34	6 (8%)
2	HEM	G	1407	1	50,50,50	1.88	8 (16%)	67,82,82	1.38	8 (11%)
3	SO4	B	1409	-	4,4,4	0.37	0	6,6,6	0.22	0
2	HEM	O	1407	1	50,50,50	1.90	9 (18%)	67,82,82	1.23	6 (8%)
3	SO4	H	1409	-	4,4,4	0.39	0	6,6,6	0.31	0
4	17Q	C	1410	-	21,21,21	0.30	0	23,23,23	1.02	2 (8%)
2	HEM	J	1407	1	50,50,50	1.78	9 (18%)	67,82,82	1.16	4 (5%)
2	HEM	A	1407	1	50,50,50	1.78	7 (14%)	67,82,82	1.27	6 (8%)
3	SO4	D	1408	-	4,4,4	0.73	0	6,6,6	0.77	0
2	HEM	P	1407	1	50,50,50	1.87	9 (18%)	67,82,82	1.30	8 (11%)
2	HEM	K	1407	1	50,50,50	1.75	11 (22%)	67,82,82	1.33	11 (16%)
3	SO4	B	1408	-	4,4,4	0.38	0	6,6,6	0.28	0
4	17Q	G	1410	-	21,21,21	0.48	0	23,23,23	0.75	0
3	SO4	H	1408	-	4,4,4	0.56	0	6,6,6	0.49	0
2	HEM	E	1407	1	50,50,50	1.71	7 (14%)	67,82,82	1.45	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	1407	1	50,50,50	1.85	8 (16%)	67,82,82	1.47	11 (16%)
3	SO4	I	1408	-	4,4,4	0.75	0	6,6,6	0.77	0
2	HEM	N	1407	1	50,50,50	1.74	6 (12%)	67,82,82	1.21	8 (11%)
2	HEM	B	1407	1	50,50,50	1.85	7 (14%)	67,82,82	1.51	13 (19%)
3	SO4	O	1408	-	4,4,4	0.64	0	6,6,6	0.49	0
2	HEM	H	1407	1	50,50,50	1.79	7 (14%)	67,82,82	1.06	3 (4%)

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	D	1407	1	-	2/14/54/54	-
2	HEM	C	1407	1	-	3/14/54/54	-
2	HEM	I	1407	1	-	4/14/54/54	-
2	HEM	L	1407	1	-	4/14/54/54	-
2	HEM	P	1407	1	-	4/14/54/54	-
2	HEM	K	1407	1	-	6/14/54/54	-
2	HEM	M	1407	1	-	6/14/54/54	-
4	17Q	G	1410	-	-	14/23/23/23	1/1/1/1
2	HEM	F	1407	1	-	2/14/54/54	-
2	HEM	E	1407	1	-	4/14/54/54	-
2	HEM	G	1407	1	-	4/14/54/54	-
2	HEM	J	1407	1	-	4/14/54/54	-
2	HEM	N	1407	1	-	0/14/54/54	-
2	HEM	B	1407	1	-	4/14/54/54	-
2	HEM	O	1407	1	-	1/14/54/54	-
4	17Q	C	1410	-	-	14/23/23/23	1/1/1/1
2	HEM	H	1407	1	-	4/14/54/54	-
2	HEM	A	1407	1	-	3/14/54/54	-

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1407	HEM	C3D-C2D	8.15	1.54	1.36
2	M	1407	HEM	C3D-C2D	8.07	1.54	1.36
2	P	1407	HEM	C3D-C2D	7.76	1.53	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1407	HEM	C3D-C2D	7.73	1.53	1.36
2	O	1407	HEM	C3D-C2D	7.61	1.53	1.36

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1407	HEM	C4D-ND-C1D	5.14	111.29	105.21
2	P	1407	HEM	C4D-ND-C1D	5.07	111.21	105.21
2	A	1407	HEM	C4D-ND-C1D	4.80	110.89	105.21
2	O	1407	HEM	C4D-ND-C1D	4.80	110.89	105.21
2	F	1407	HEM	C4D-ND-C1D	4.54	110.58	105.21

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1407	HEM	C2C-C3C-CAC-CBC
2	B	1407	HEM	C4C-C3C-CAC-CBC
2	C	1407	HEM	C2C-C3C-CAC-CBC
2	C	1407	HEM	C4C-C3C-CAC-CBC
2	E	1407	HEM	C2C-C3C-CAC-CBC

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 92 short contacts:

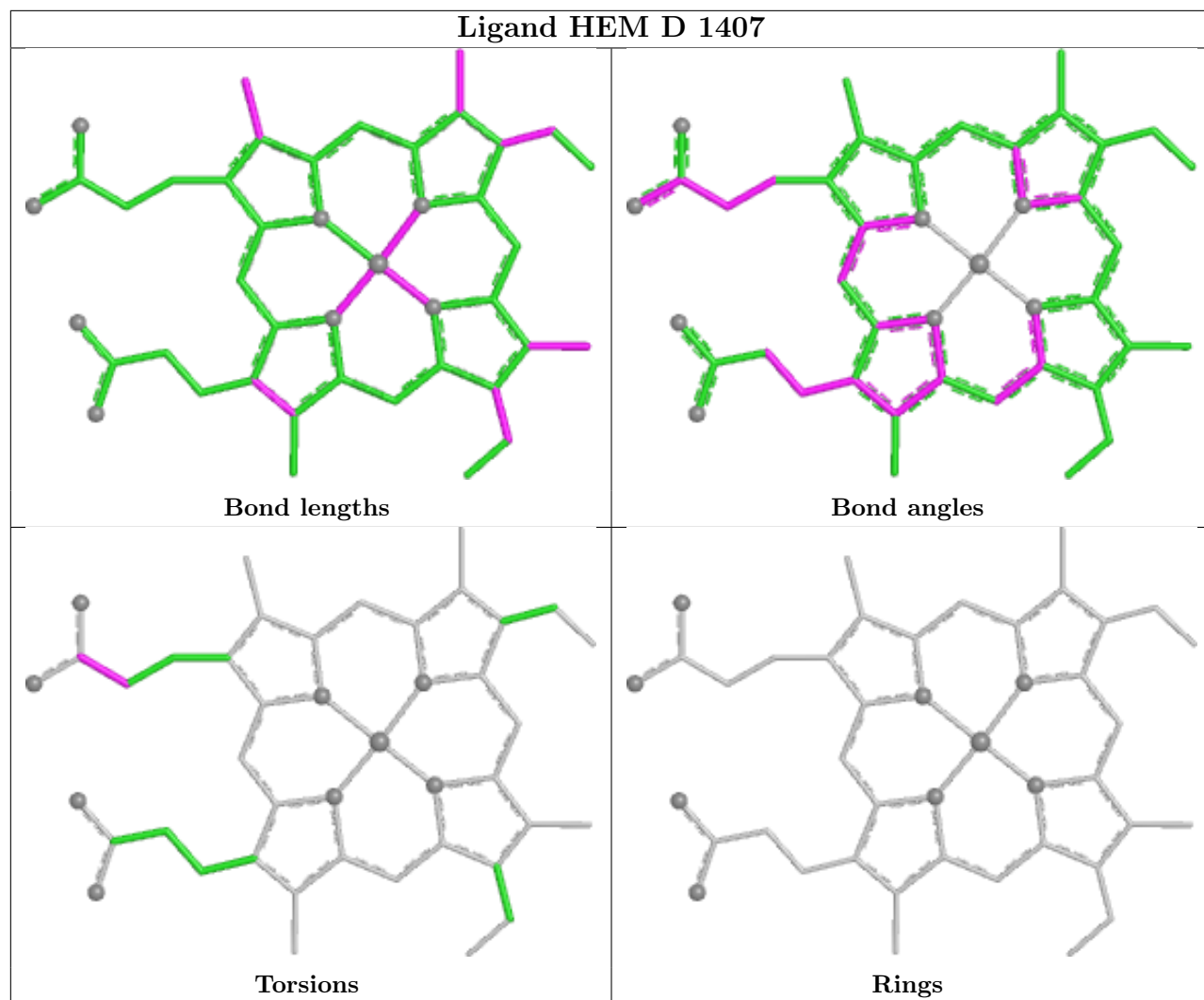
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1408	SO4	1	0
2	D	1407	HEM	8	0
2	F	1407	HEM	3	0
2	L	1407	HEM	4	0
3	A	1408	SO4	2	0
3	O	1409	SO4	1	0
2	I	1407	HEM	5	0
2	M	1407	HEM	5	0
2	G	1407	HEM	6	0
2	O	1407	HEM	4	0

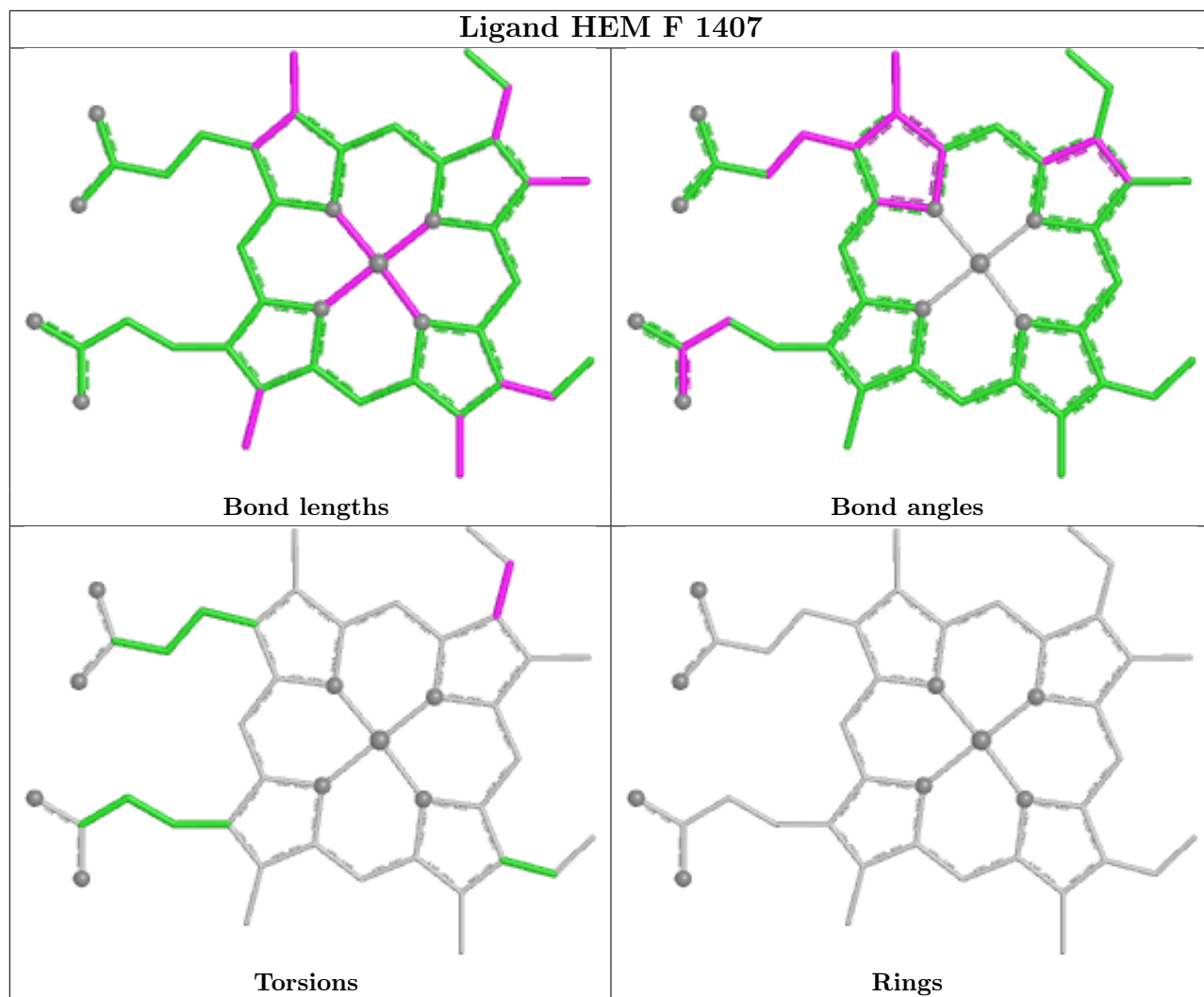
Continued on next page...

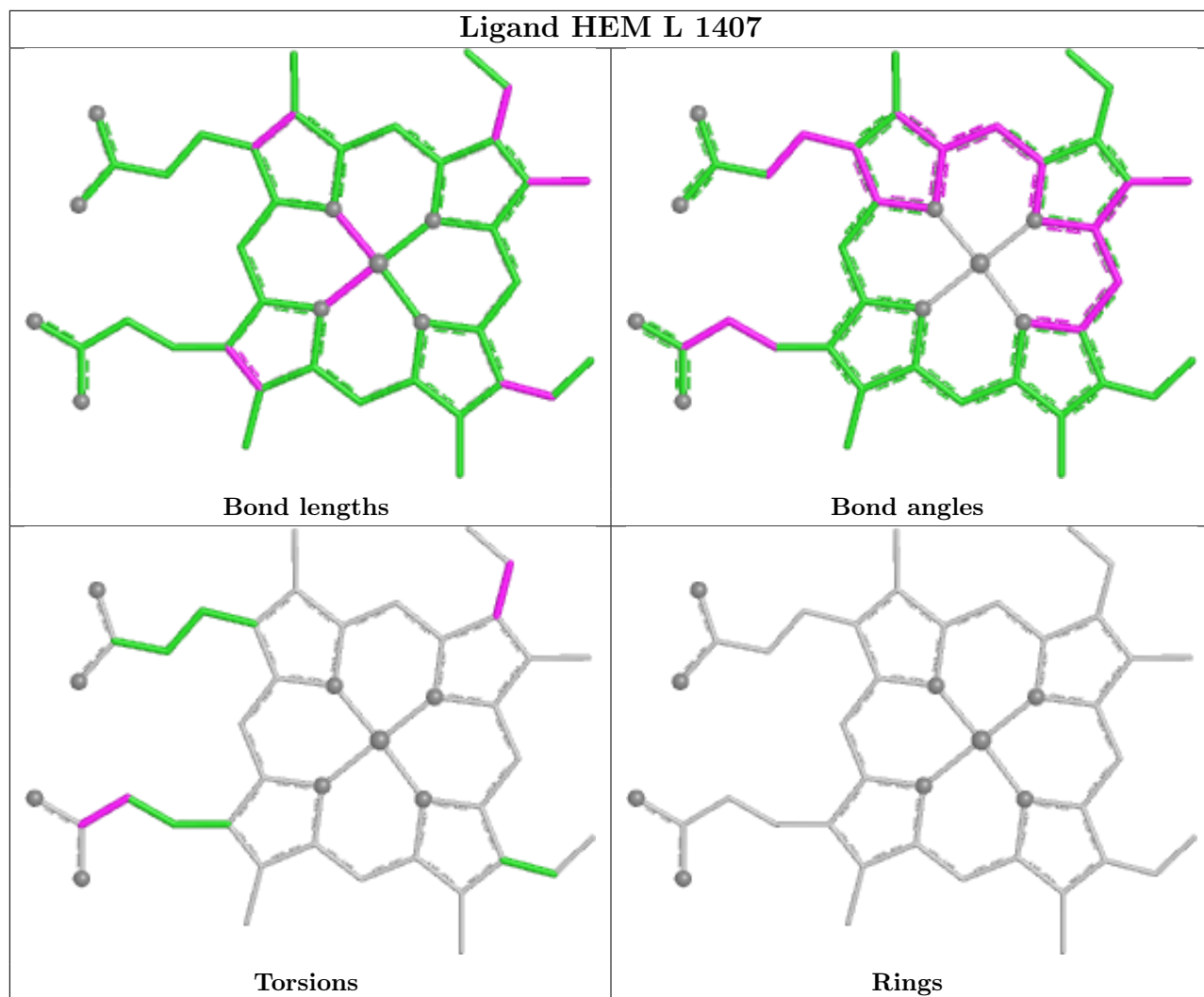
Continued from previous page...

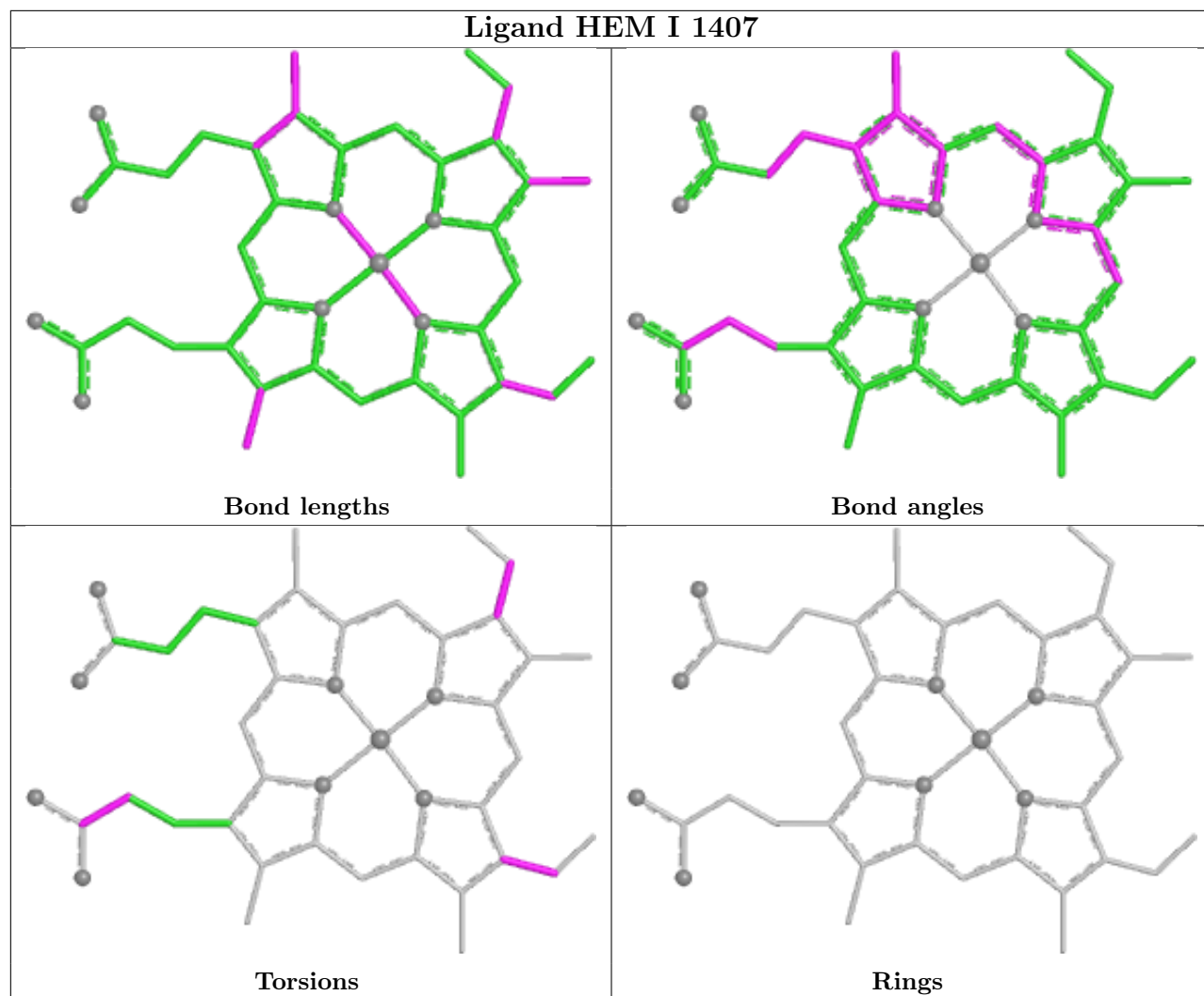
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1409	SO4	1	0
4	C	1410	17Q	6	0
2	J	1407	HEM	4	0
2	A	1407	HEM	1	0
2	P	1407	HEM	5	0
2	K	1407	HEM	3	0
4	G	1410	17Q	5	0
2	E	1407	HEM	5	0
2	C	1407	HEM	6	0
2	N	1407	HEM	5	0
2	B	1407	HEM	6	0
2	H	1407	HEM	7	0

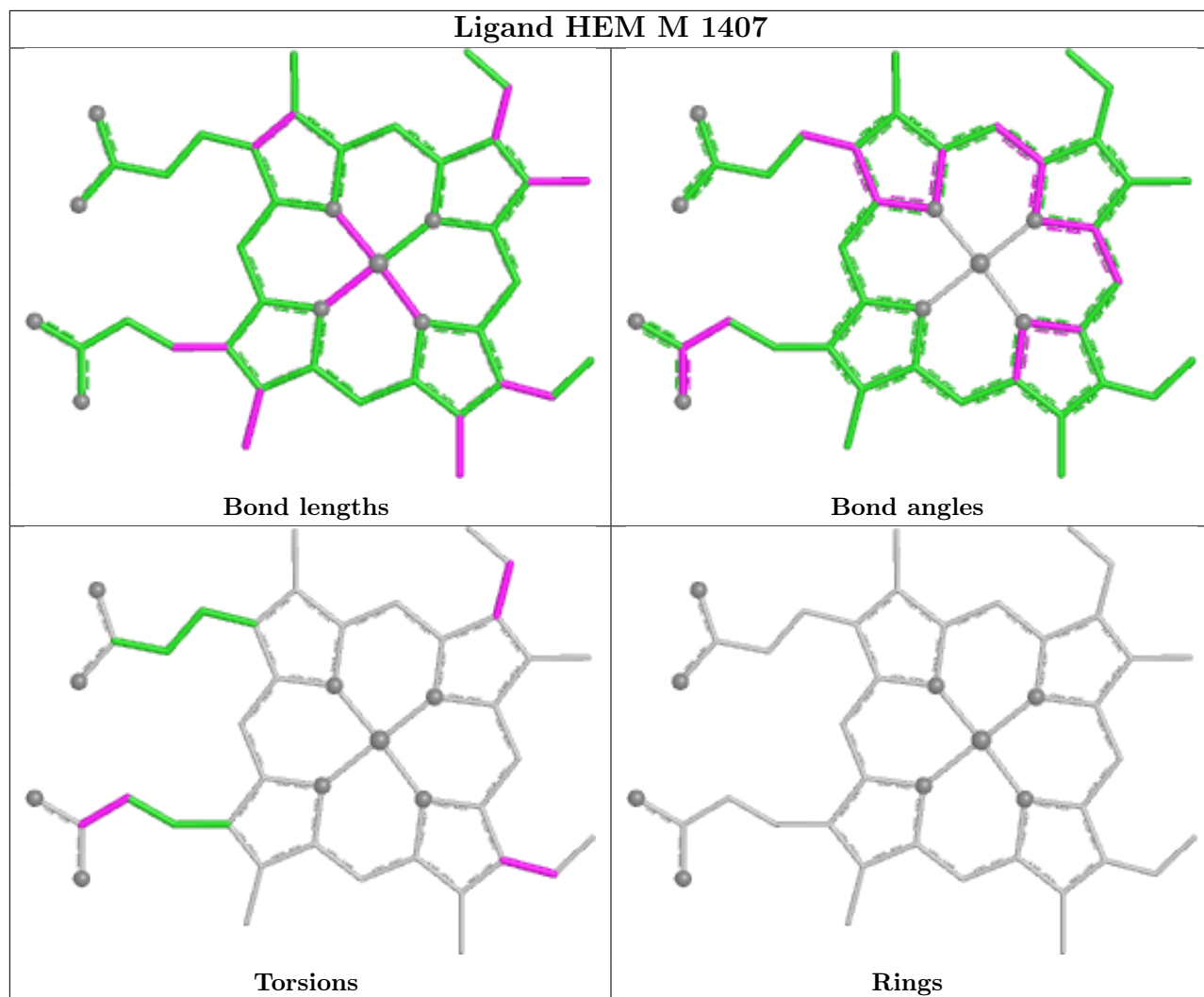
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

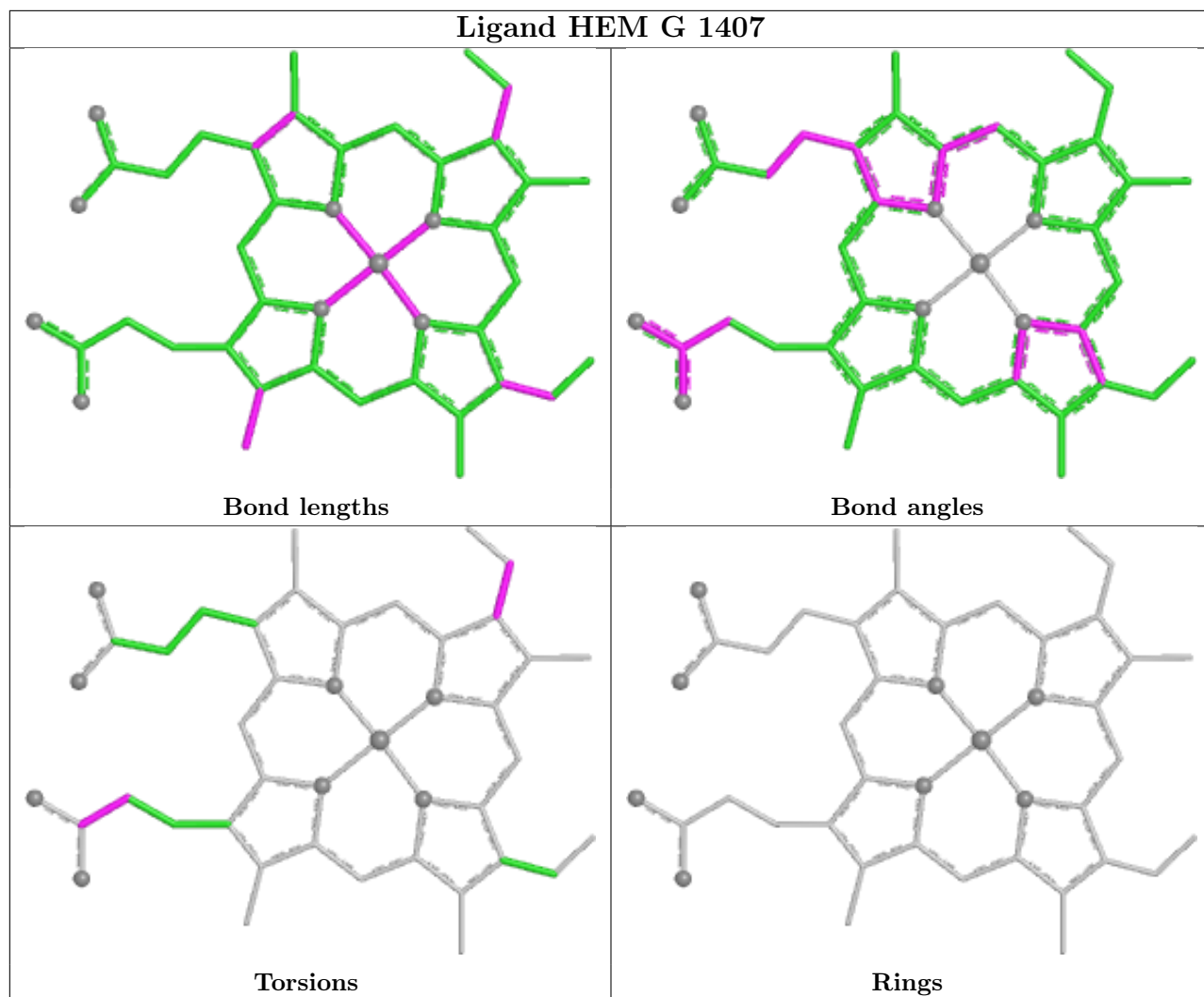


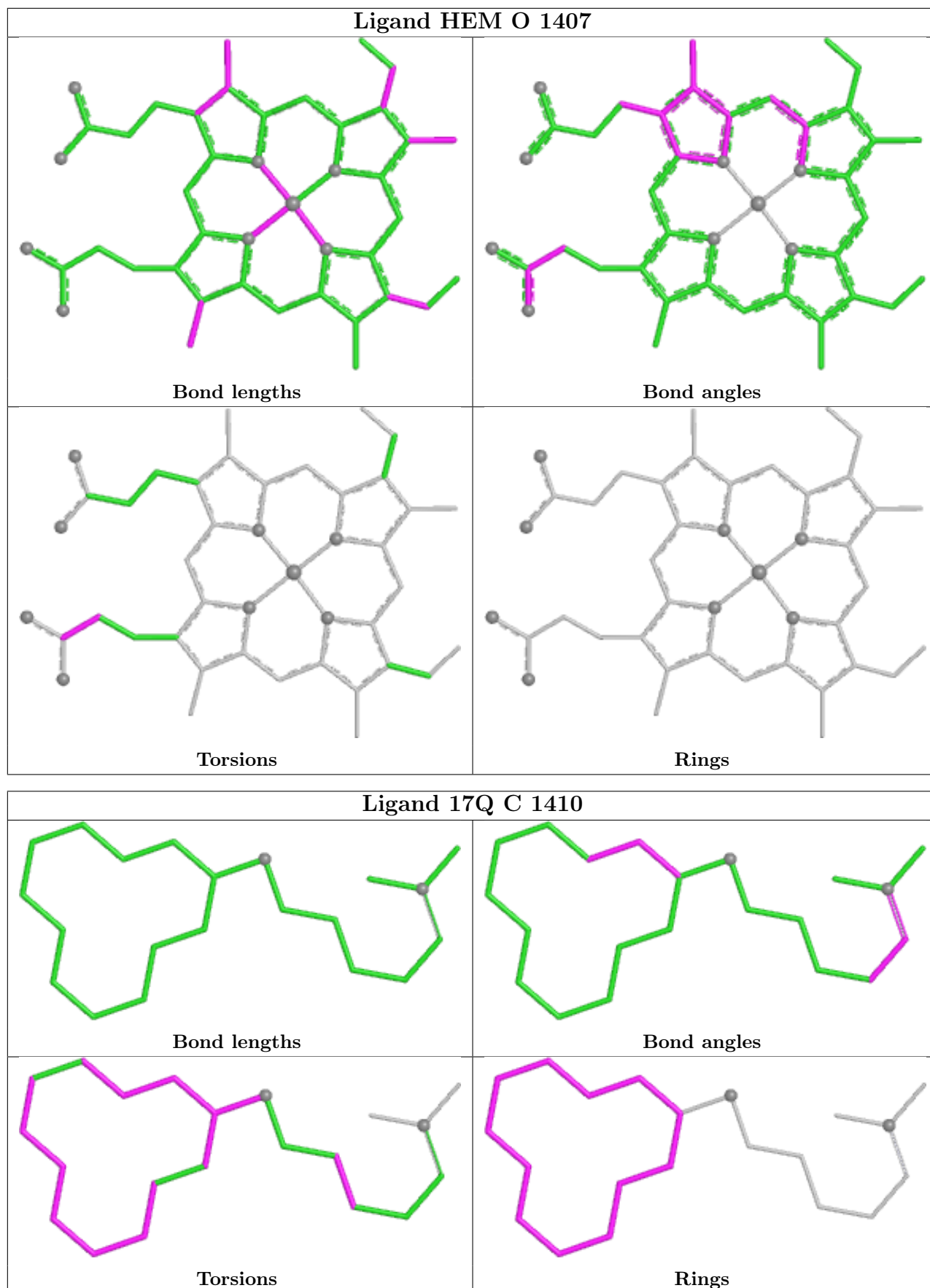


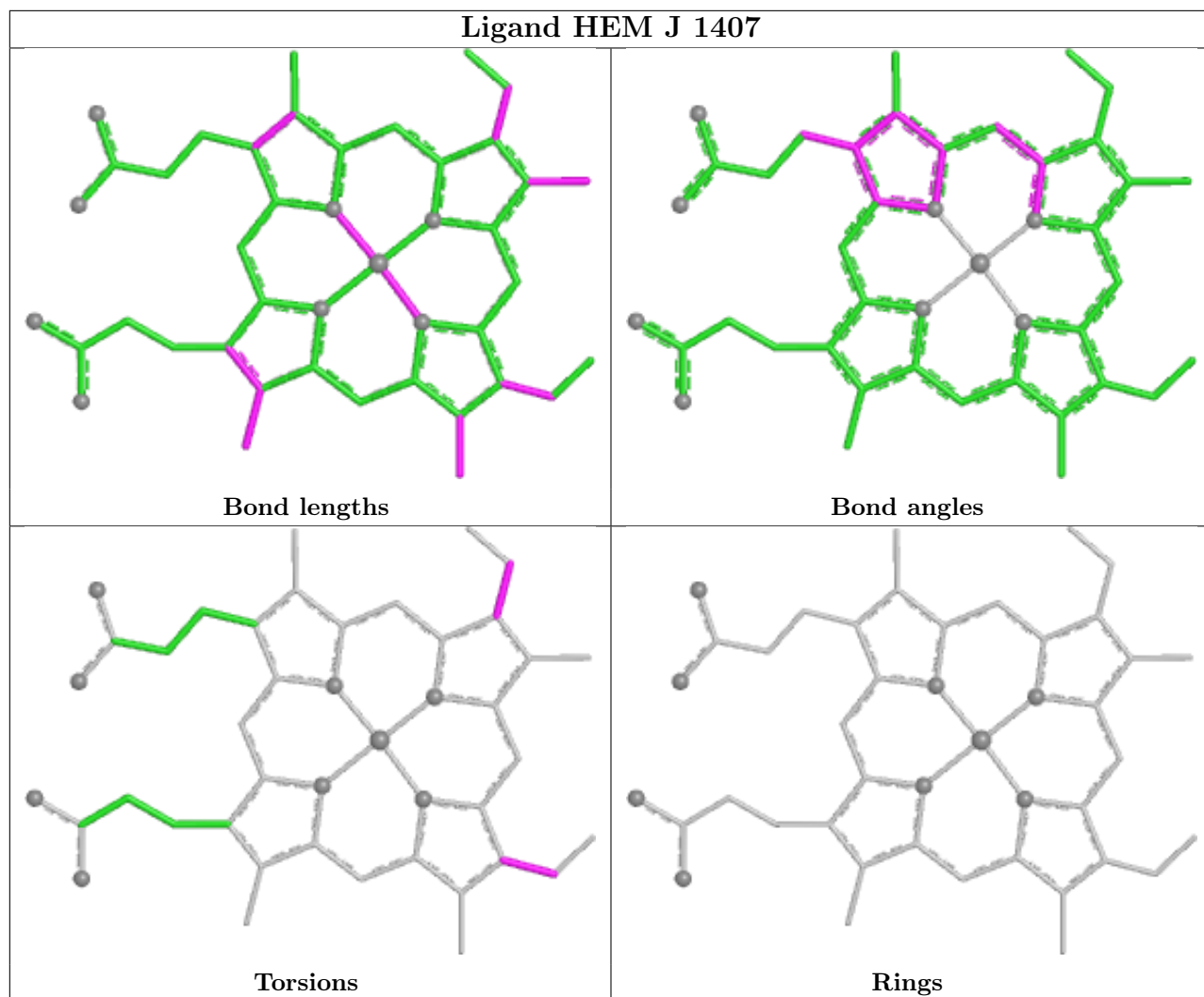


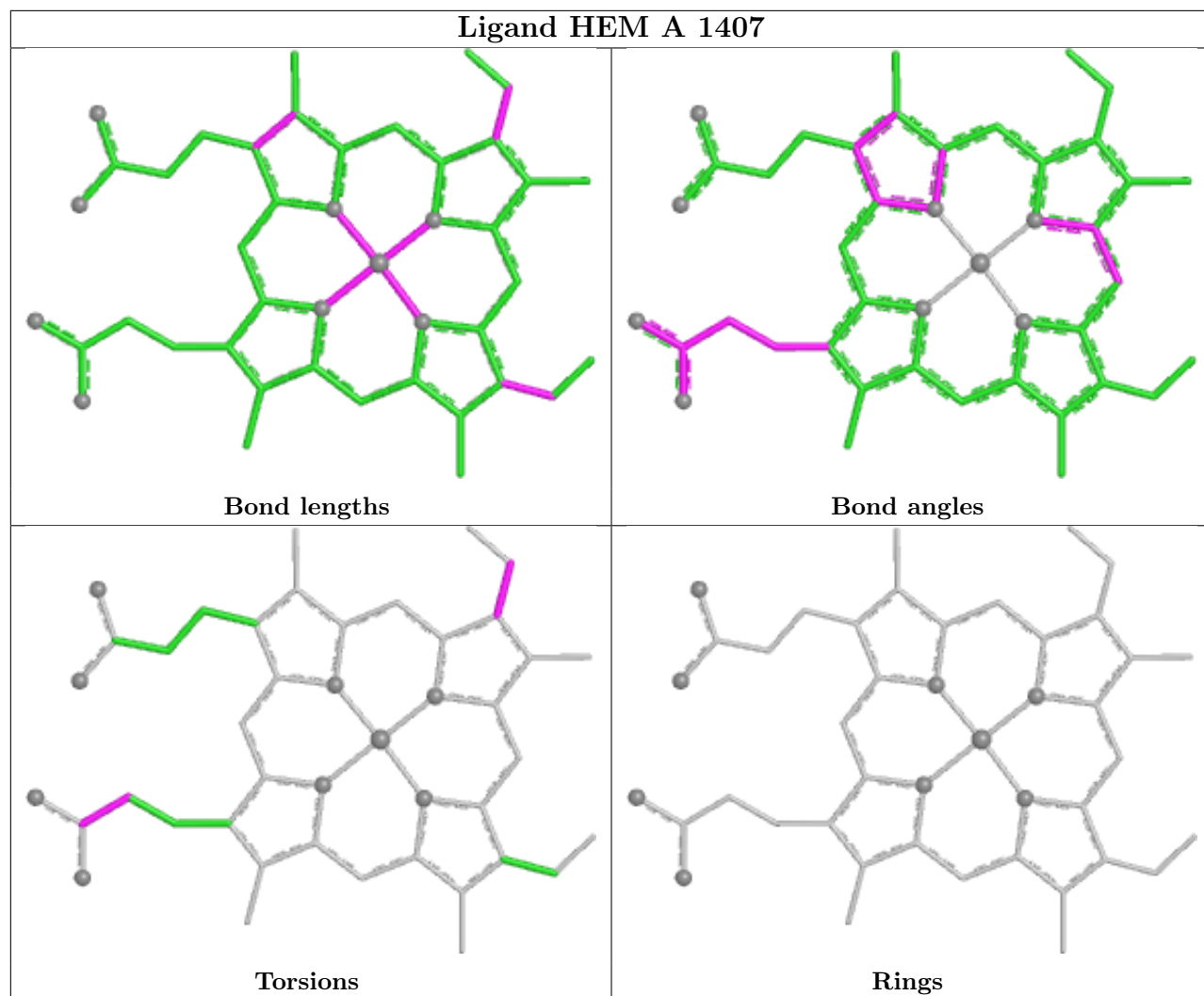


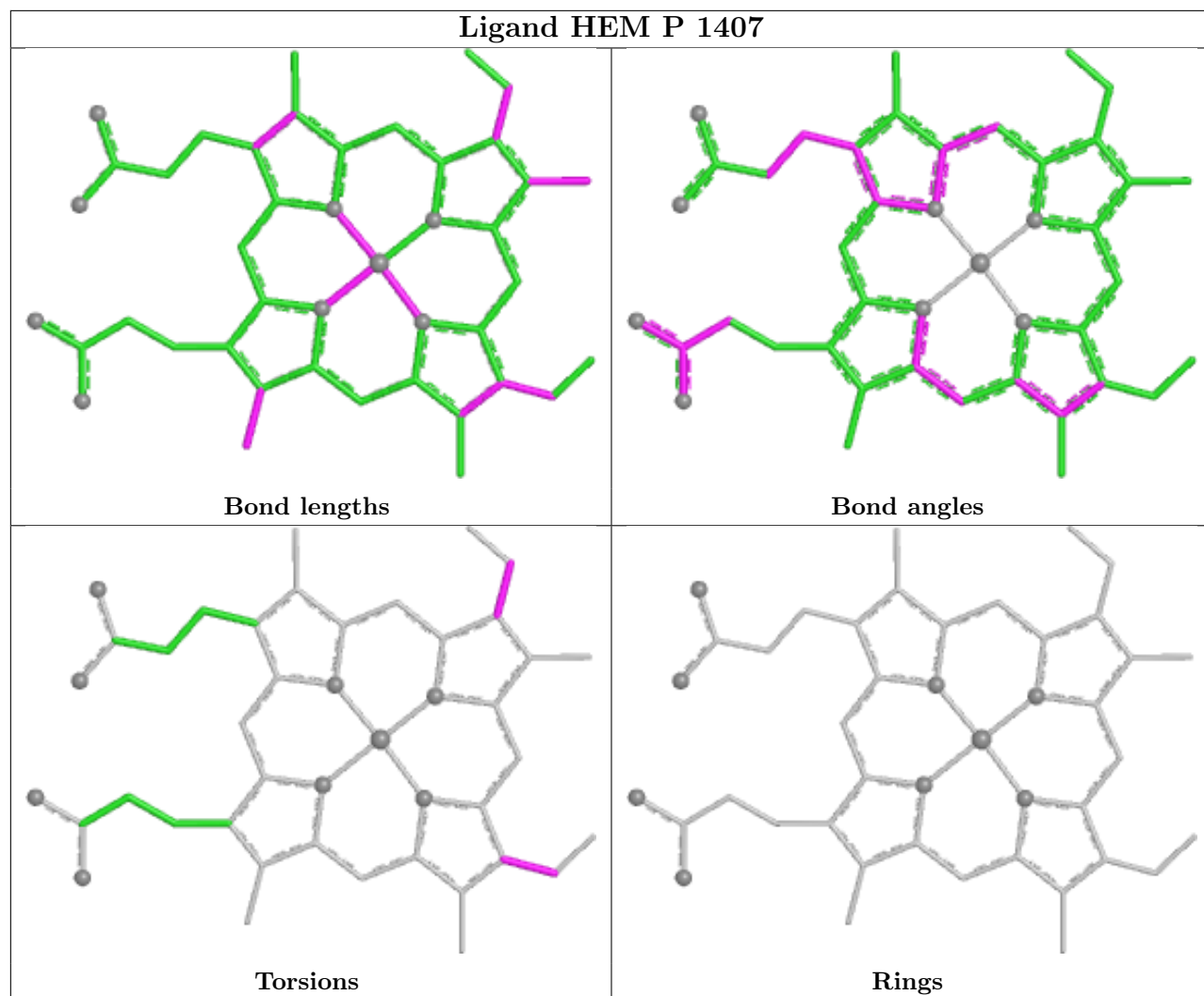


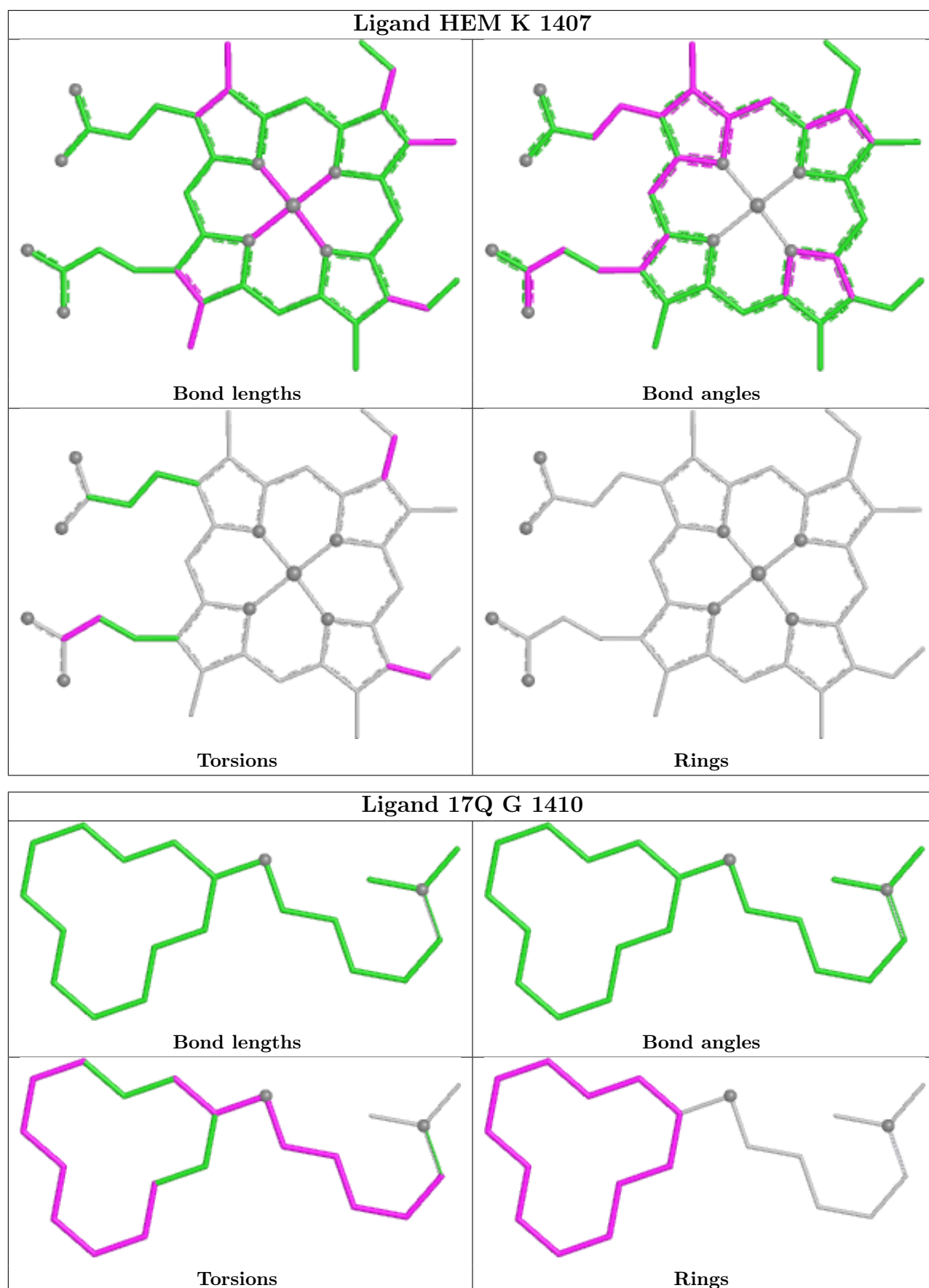


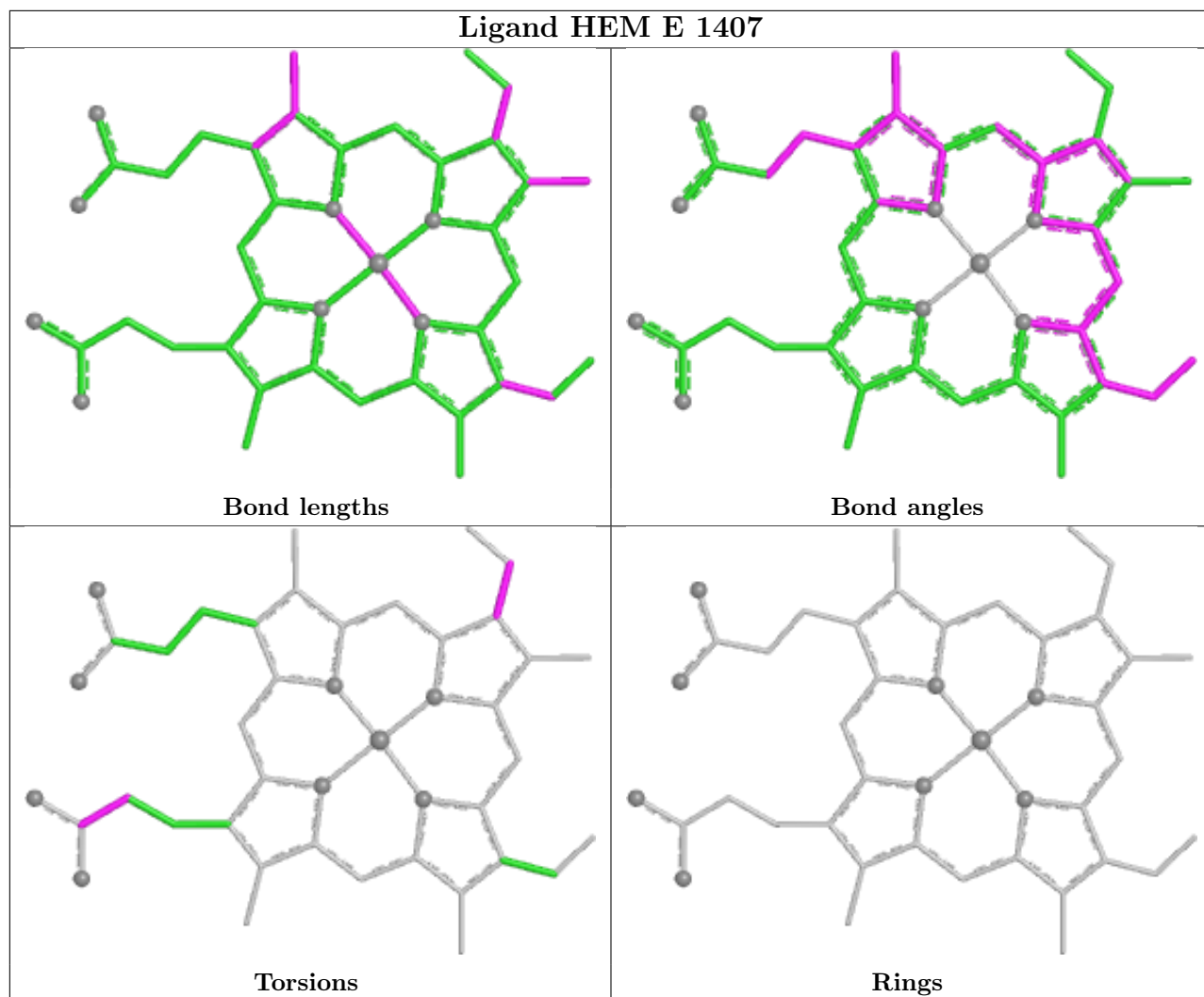


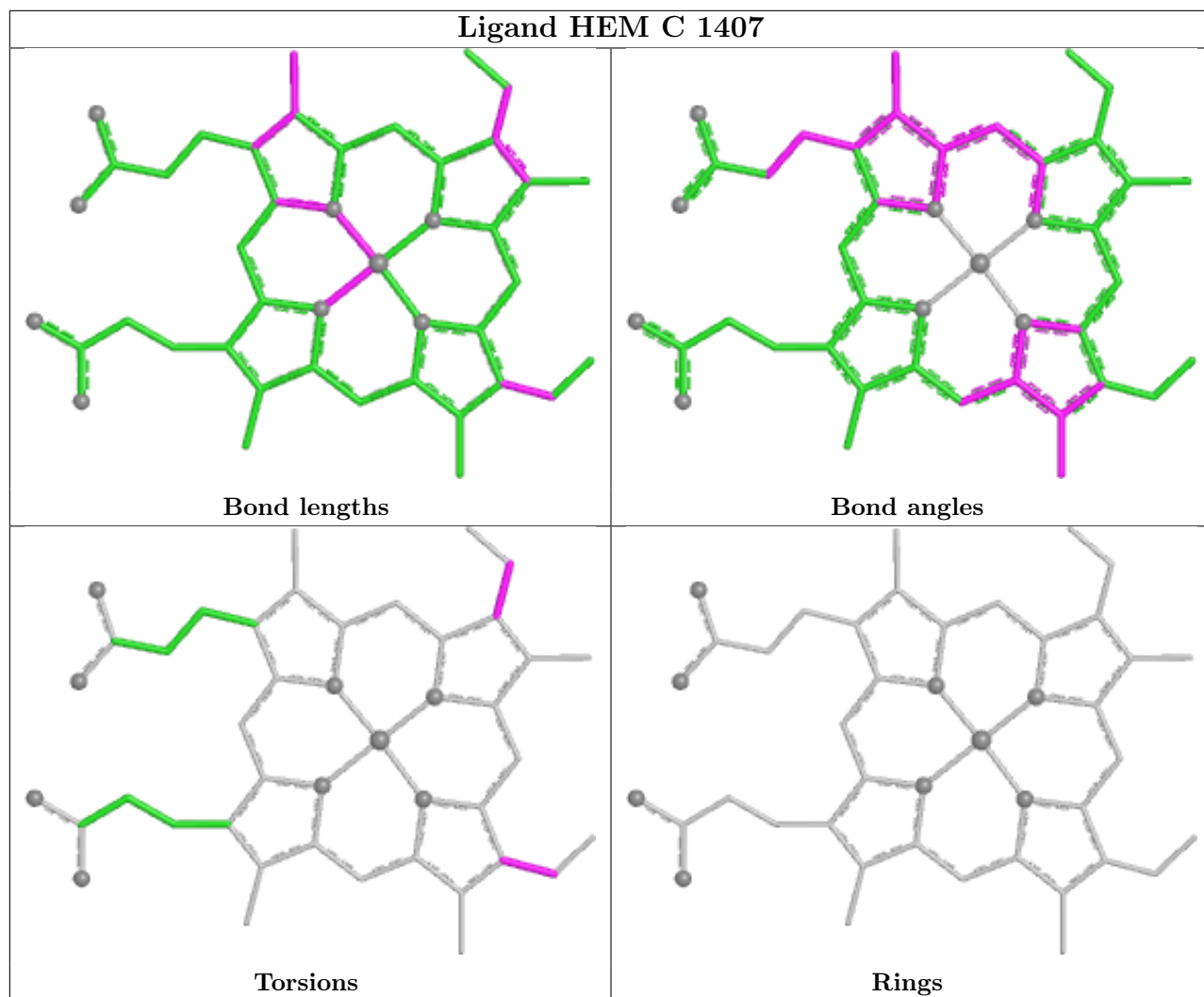


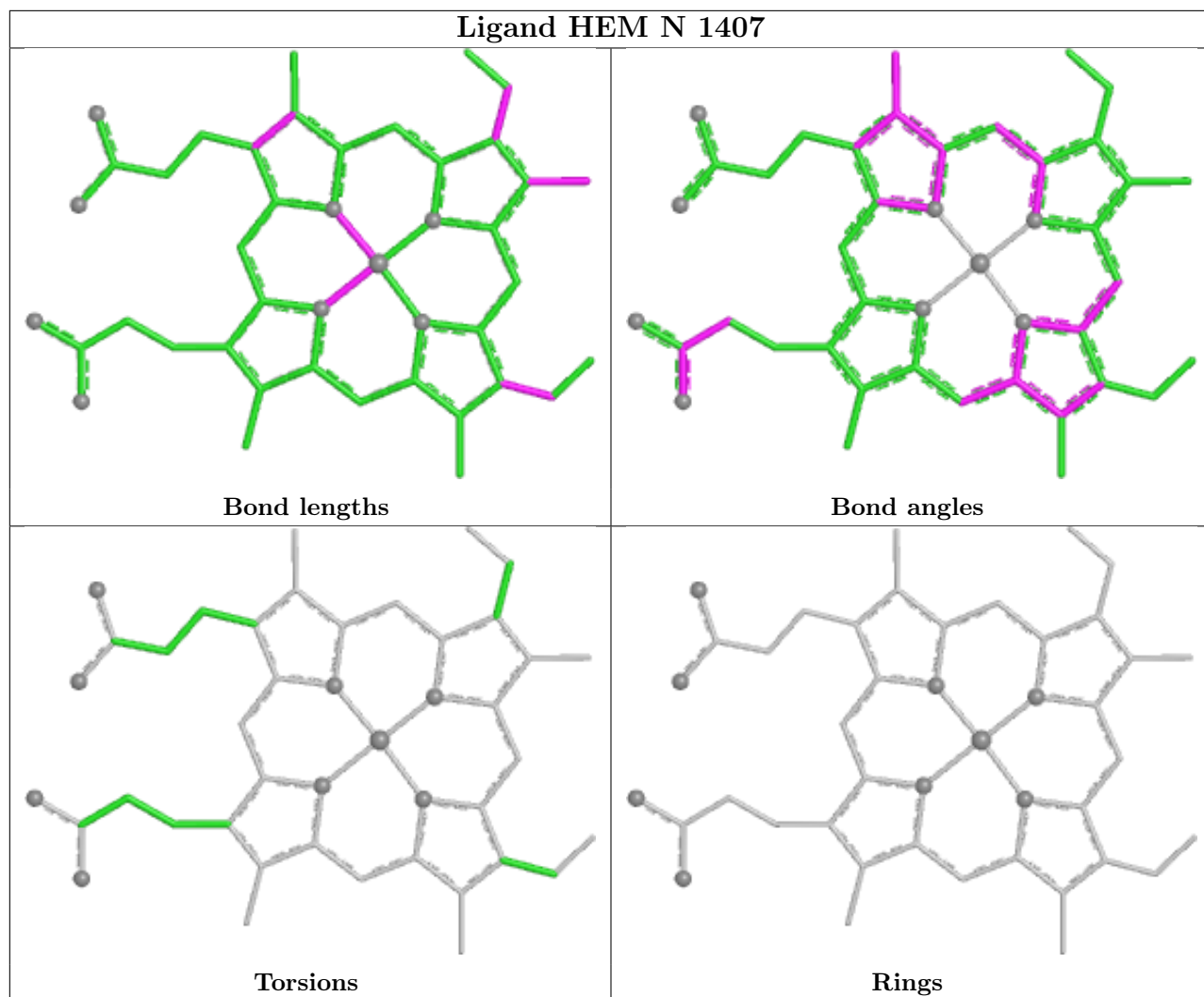


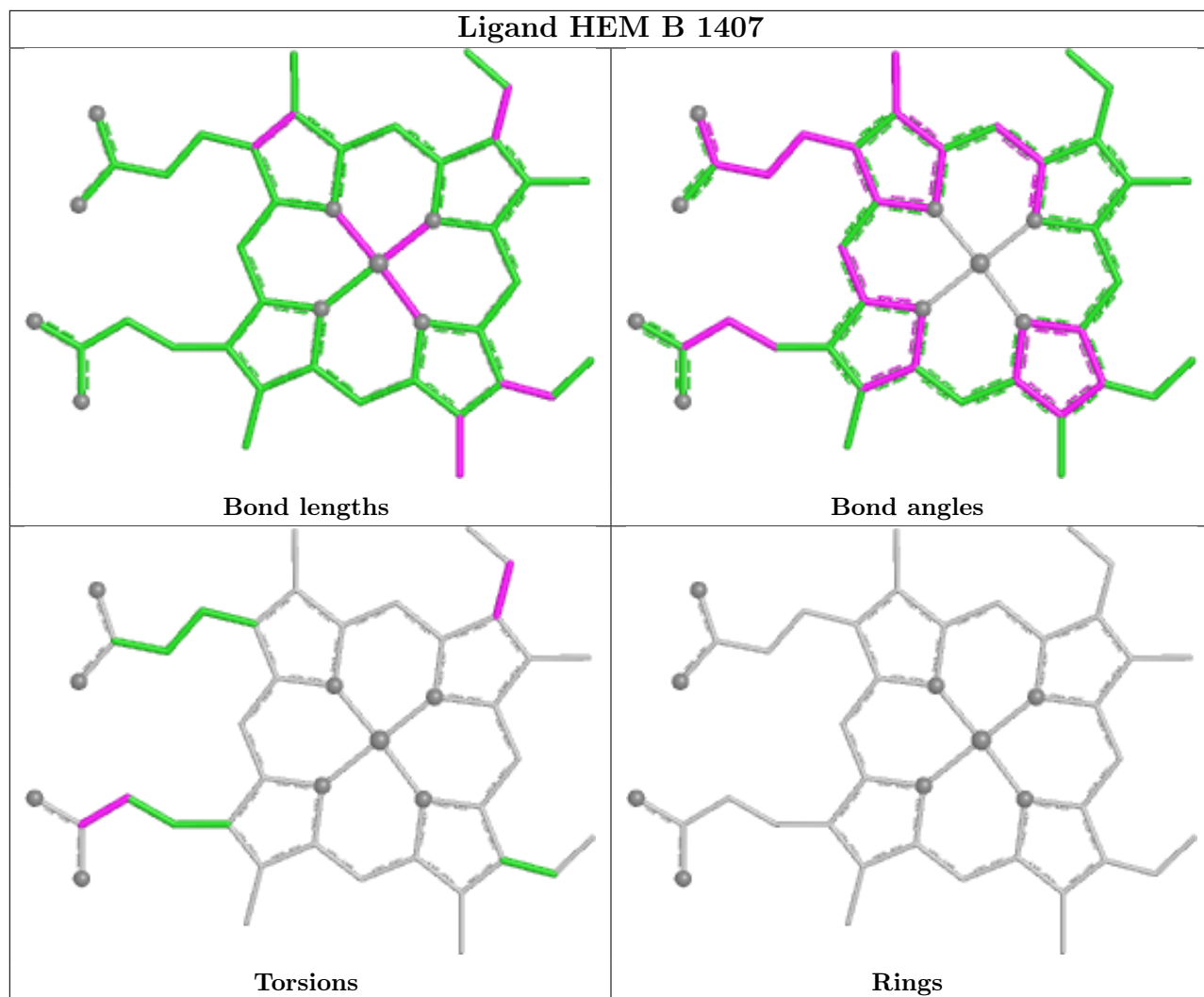


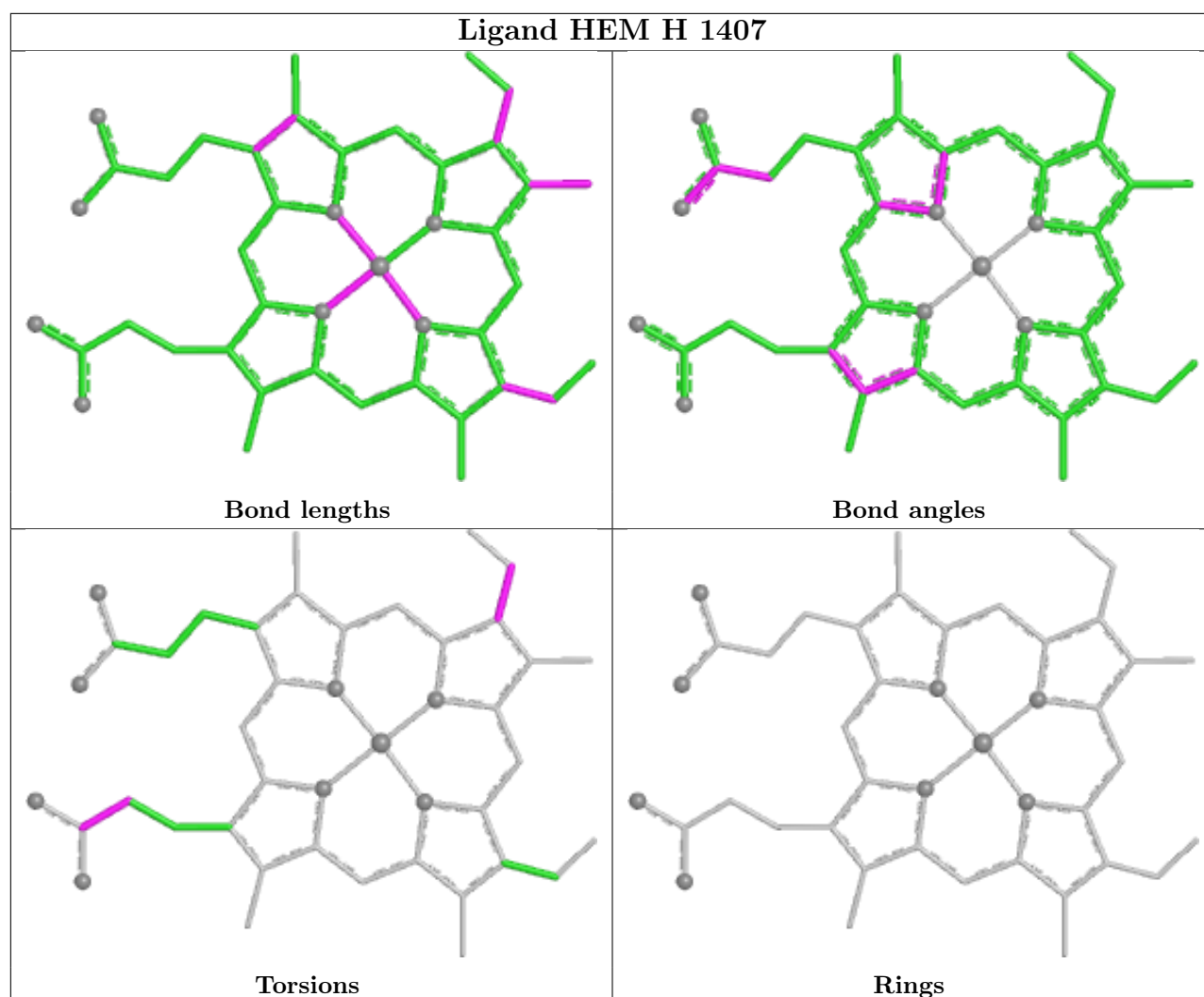












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/436 (90%)	-0.54	0 100 100	17, 33, 55, 71	0
1	B	397/436 (91%)	-0.43	2 (0%) 87 86	15, 35, 57, 76	2 (0%)
1	C	396/436 (90%)	-0.51	1 (0%) 90 89	13, 33, 55, 73	1 (0%)
1	D	397/436 (91%)	-0.49	2 (0%) 87 86	18, 32, 55, 81	2 (0%)
1	E	397/436 (91%)	-0.44	1 (0%) 90 89	16, 33, 55, 73	1 (0%)
1	F	396/436 (90%)	-0.36	1 (0%) 90 89	14, 39, 66, 84	4 (1%)
1	G	396/436 (90%)	-0.47	1 (0%) 90 89	12, 35, 52, 61	4 (1%)
1	H	396/436 (90%)	-0.42	2 (0%) 87 86	12, 35, 61, 87	1 (0%)
1	I	396/436 (90%)	-0.41	1 (0%) 90 89	12, 38, 66, 79	2 (0%)
1	J	397/436 (91%)	-0.30	1 (0%) 90 89	21, 42, 68, 91	1 (0%)
1	K	397/436 (91%)	-0.20	2 (0%) 87 86	17, 46, 72, 90	2 (0%)
1	L	397/436 (91%)	-0.09	6 (1%) 72 70	18, 50, 86, 99	2 (0%)
1	M	397/436 (91%)	-0.02	2 (0%) 87 86	30, 53, 85, 91	1 (0%)
1	N	397/436 (91%)	0.30	10 (2%) 58 55	34, 72, 116, 158	1 (0%)
1	O	397/436 (91%)	0.14	13 (3%) 49 45	28, 57, 105, 133	0
1	P	396/436 (90%)	0.47	19 (4%) 35 32	20, 78, 129, 155	1 (0%)
All	All	6345/6976 (90%)	-0.24	64 (1%) 79 78	12, 41, 91, 158	25 (0%)

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	VAL	4.8
1	N	10	ALA	3.8
1	M	150	TRP	3.3
1	O	13	PRO	3.2
1	O	184	PRO	3.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

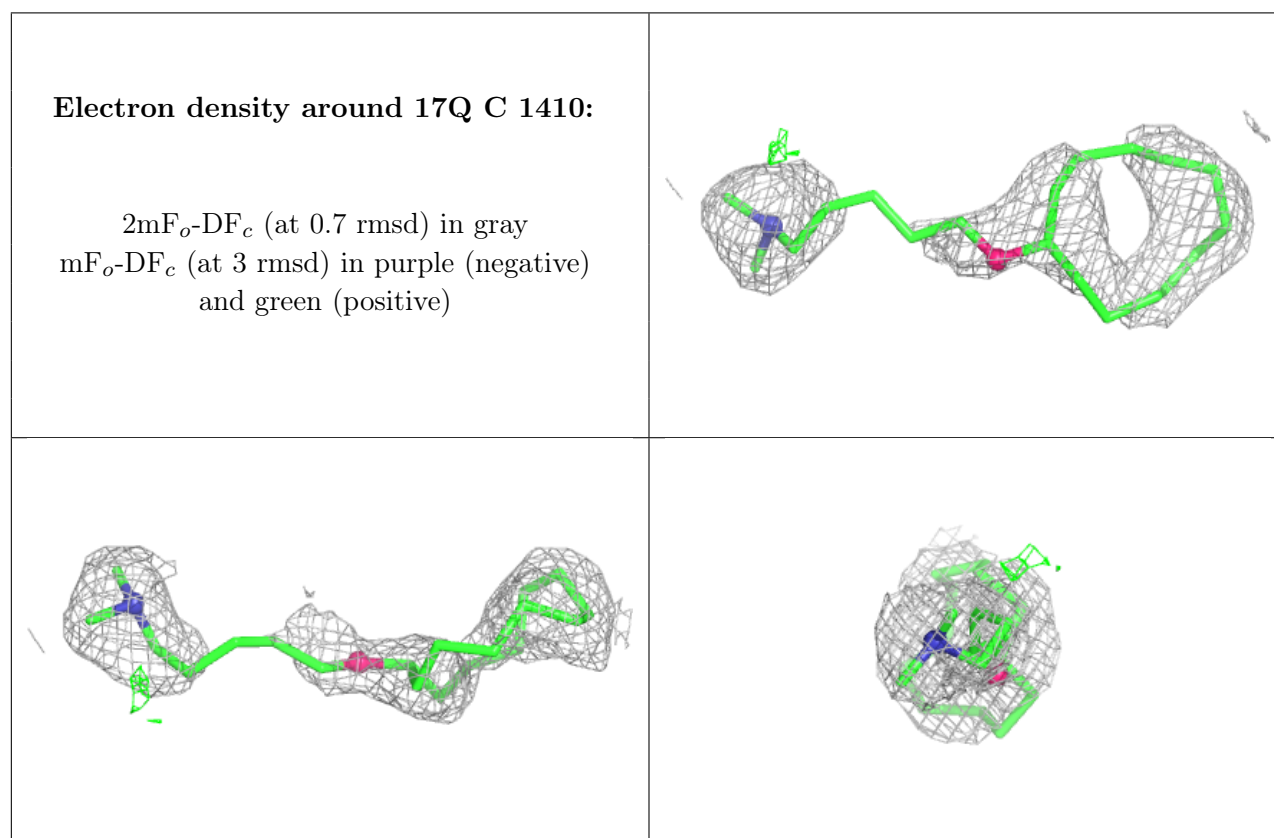
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	D	1408	5/5	0.89	0.18	37,37,39,40	0
3	SO4	O	1409	5/5	0.90	0.19	39,39,40,40	0
4	17Q	C	1410	21/21	0.90	0.14	53,57,60,60	0
3	SO4	O	1408	5/5	0.91	0.20	41,41,42,42	0
3	SO4	B	1408	5/5	0.91	0.12	61,62,63,63	0
3	SO4	J	1408	5/5	0.91	0.17	41,42,42,43	0
4	17Q	G	1410	21/21	0.91	0.13	39,49,55,55	0
3	SO4	I	1408	5/5	0.93	0.20	39,41,42,43	0
3	SO4	B	1409	5/5	0.93	0.12	49,49,51,51	0
3	SO4	H	1408	5/5	0.94	0.15	42,42,44,45	0
3	SO4	A	1408	5/5	0.95	0.09	41,42,43,43	0
3	SO4	I	1409	5/5	0.96	0.07	53,54,55,55	0
2	HEM	P	1407	43/43	0.96	0.08	36,46,51,54	0
3	SO4	F	1408	5/5	0.96	0.15	38,39,40,41	0
2	HEM	E	1407	43/43	0.97	0.06	13,18,21,23	0
3	SO4	H	1409	5/5	0.97	0.10	38,39,40,40	0
2	HEM	O	1407	43/43	0.97	0.07	29,33,38,41	0
2	HEM	G	1407	43/43	0.98	0.06	17,23,24,28	0
2	HEM	H	1407	43/43	0.98	0.06	15,19,21,22	0
2	HEM	I	1407	43/43	0.98	0.07	23,25,29,31	0
2	HEM	J	1407	43/43	0.98	0.06	26,28,31,32	0
2	HEM	K	1407	43/43	0.98	0.06	21,25,27,29	0
2	HEM	L	1407	43/43	0.98	0.06	19,24,27,31	0
2	HEM	M	1407	43/43	0.98	0.06	18,23,26,31	0
2	HEM	N	1407	43/43	0.98	0.07	29,33,44,49	0
2	HEM	B	1407	43/43	0.98	0.06	19,25,27,29	0
2	HEM	C	1407	43/43	0.98	0.06	12,14,19,24	0

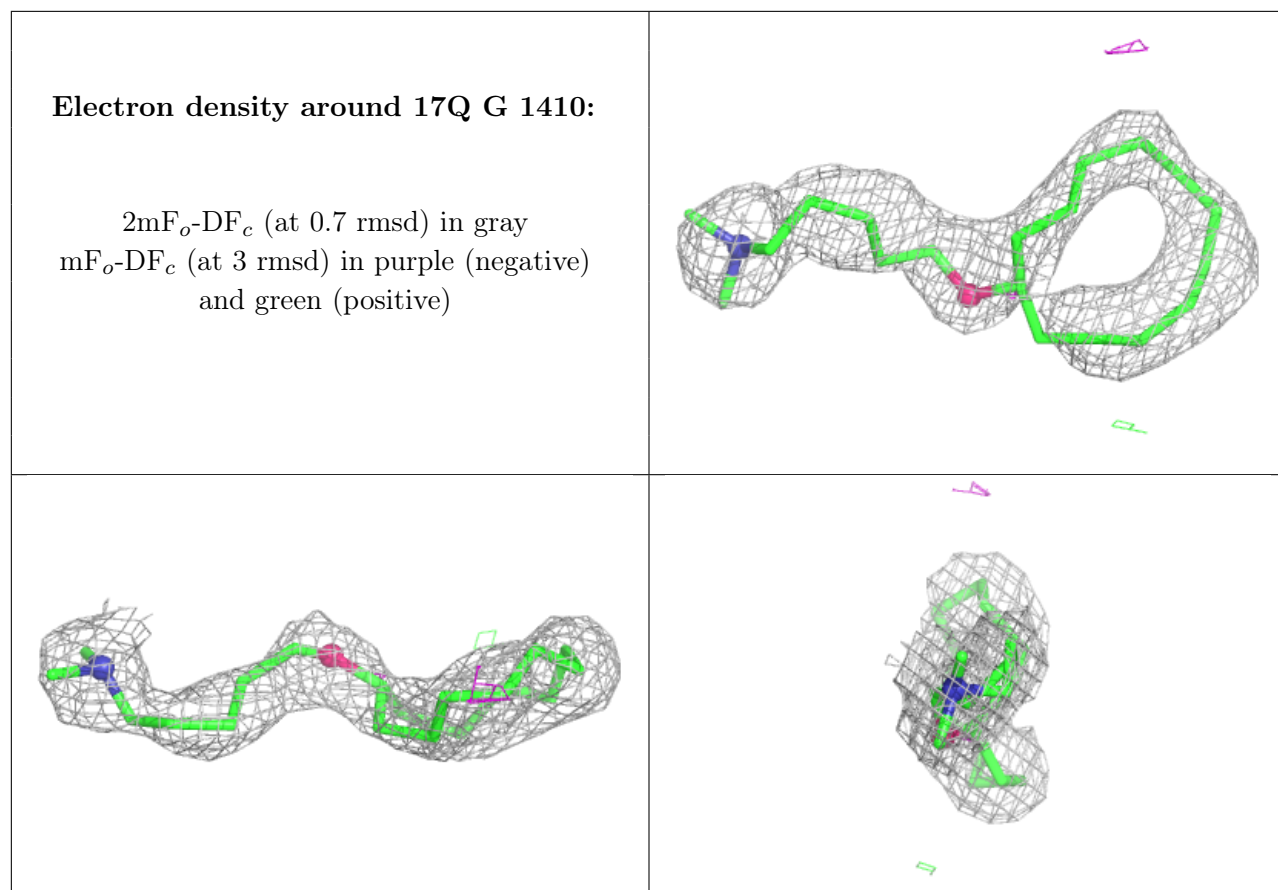
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	1407	43/43	0.98	0.05	14,20,24,28	0
2	HEM	F	1407	43/43	0.98	0.06	17,22,24,26	0
2	HEM	D	1407	43/43	0.99	0.05	13,18,22,23	0

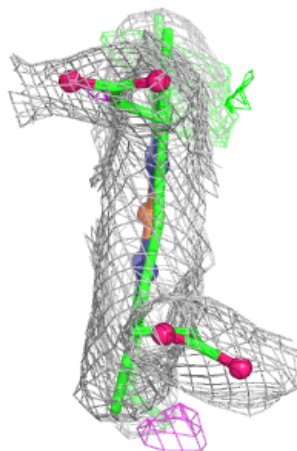
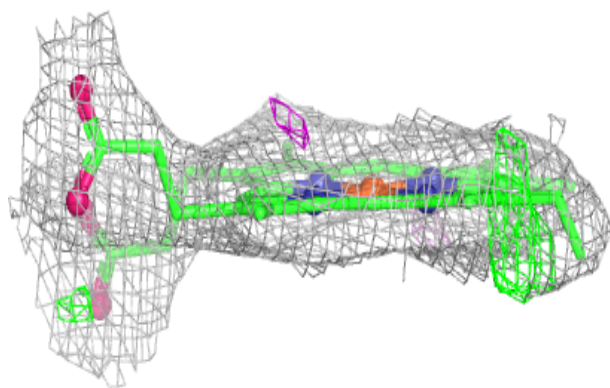
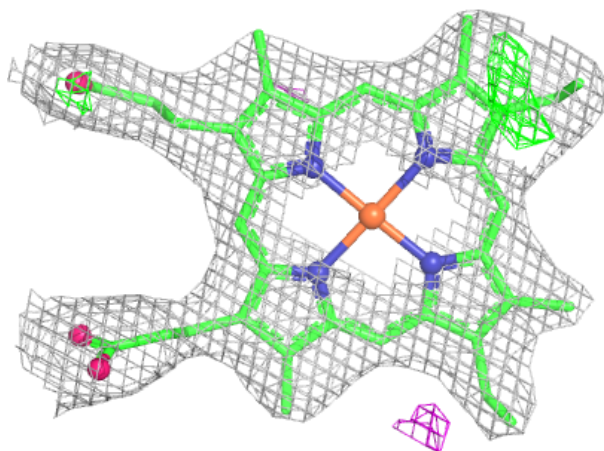
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





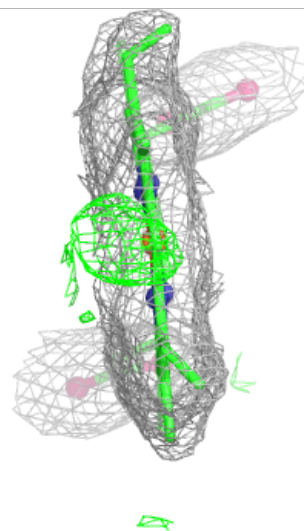
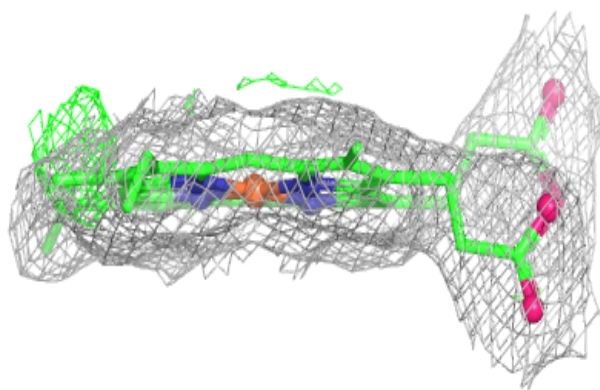
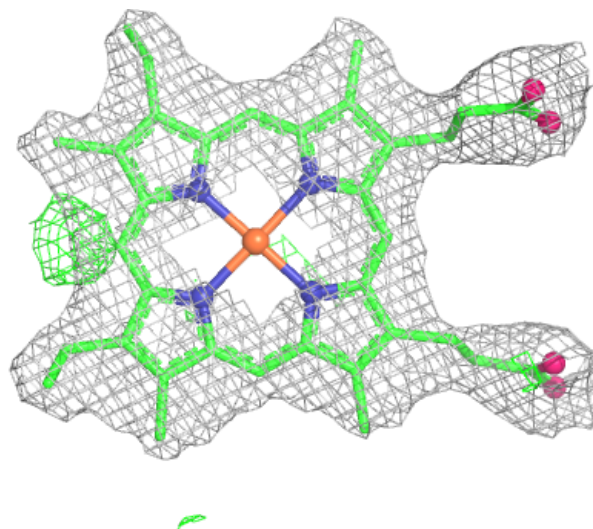
Electron density around HEM P 1407:

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



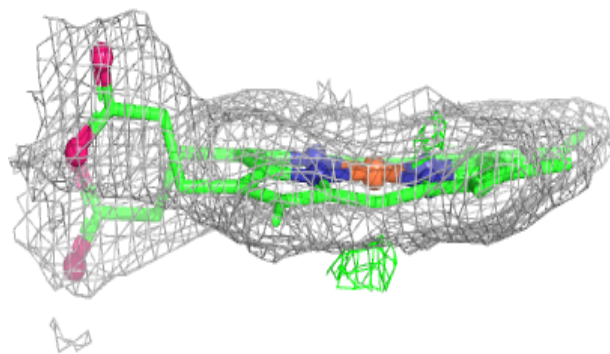
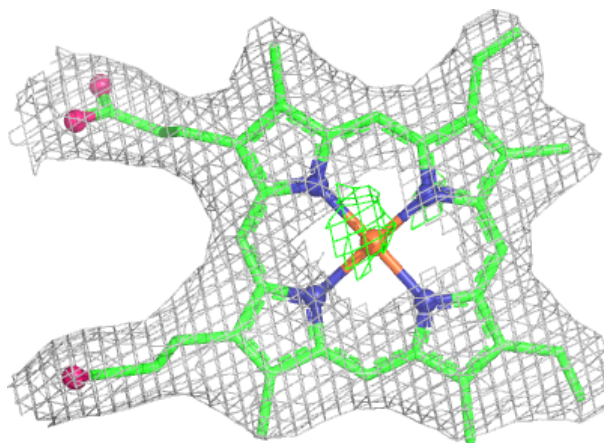
Electron density around HEM E 1407:

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



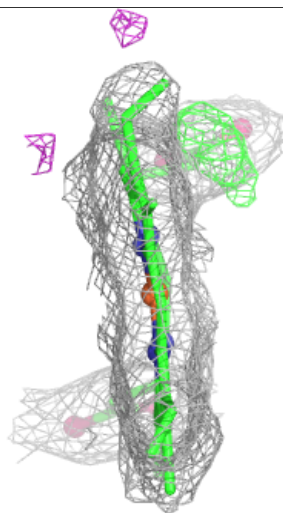
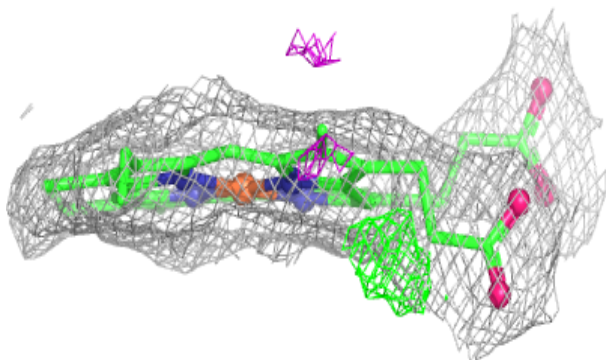
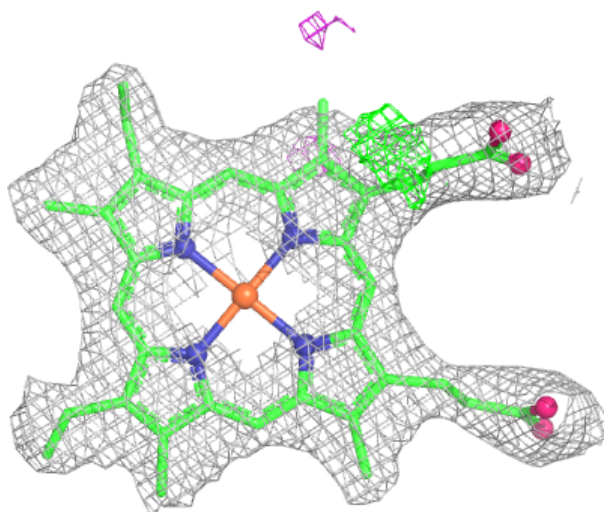
Electron density around HEM O 1407:

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



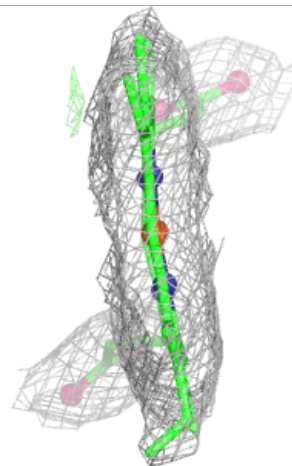
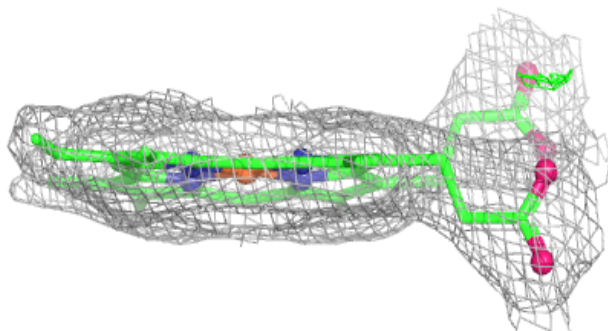
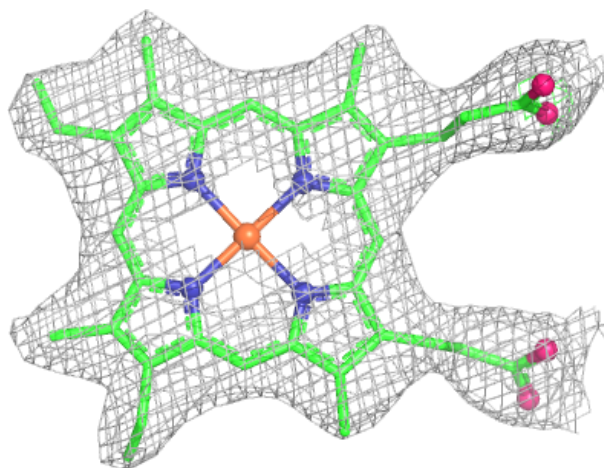
Electron density around HEM G 1407:

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



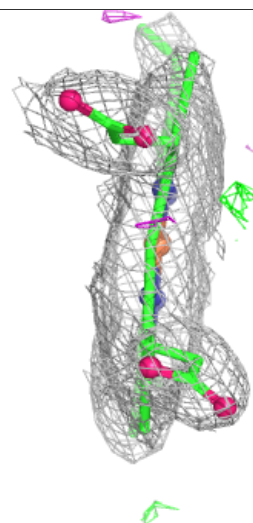
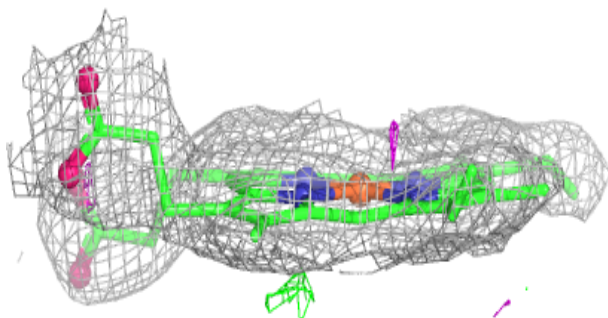
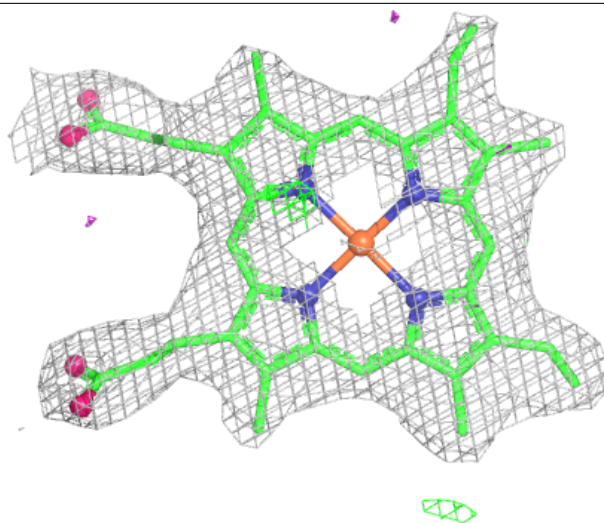
Electron density around HEM H 1407:

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



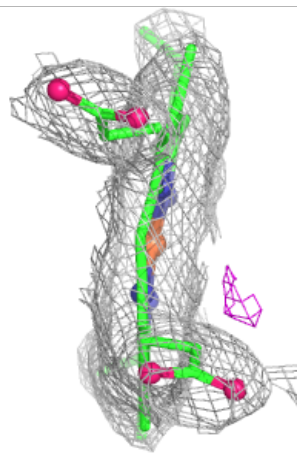
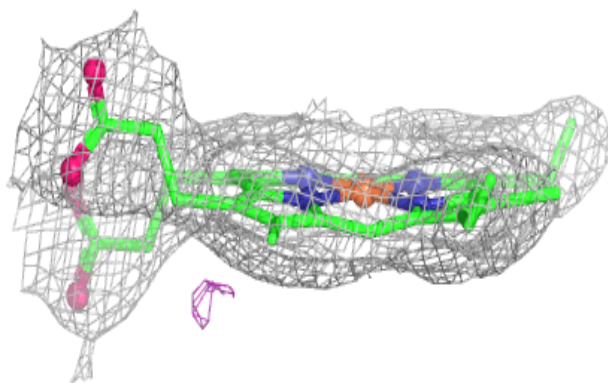
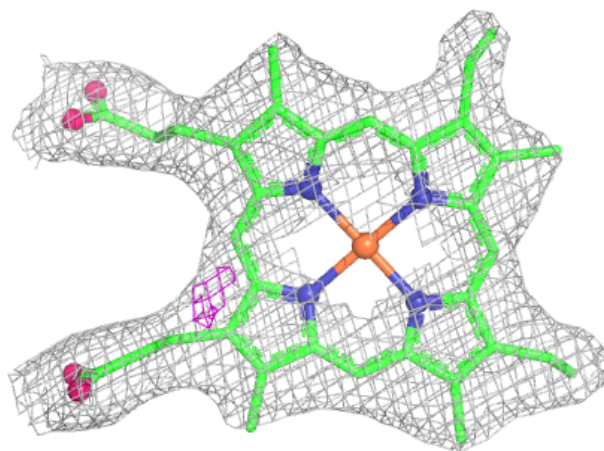
Electron density around HEM I 1407:

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



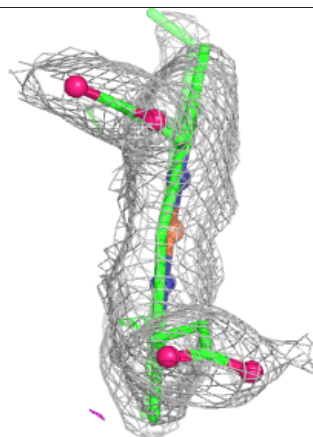
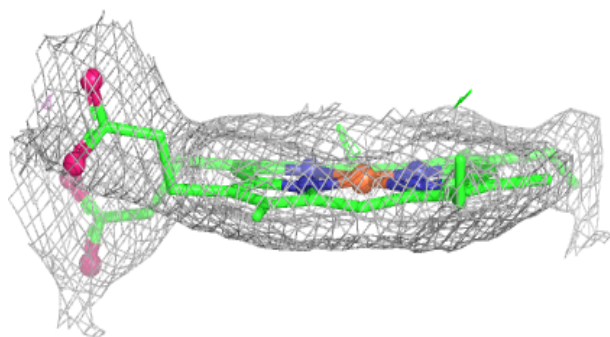
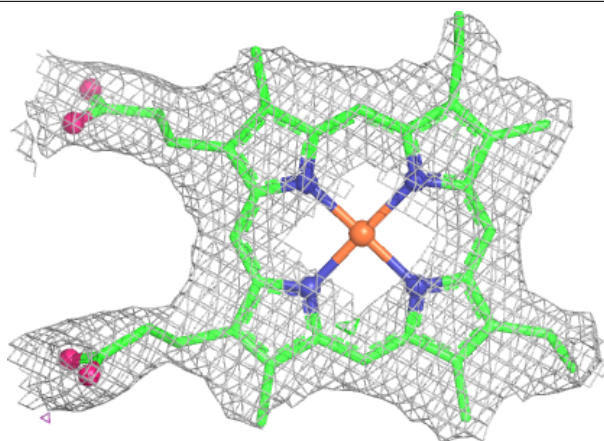
Electron density around HEM J 1407:

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



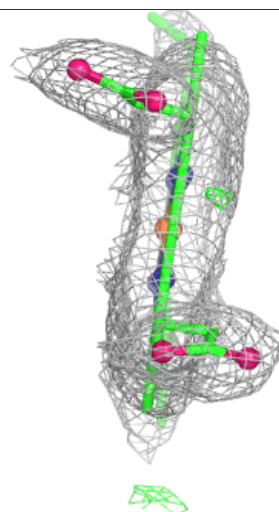
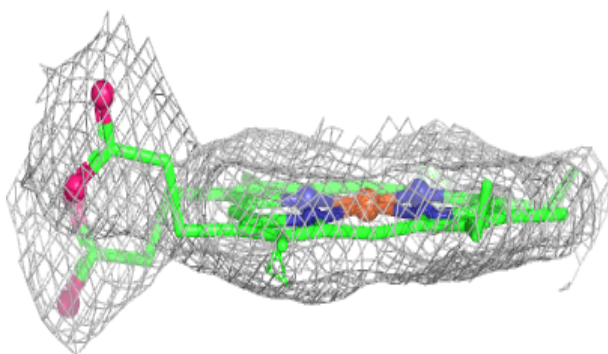
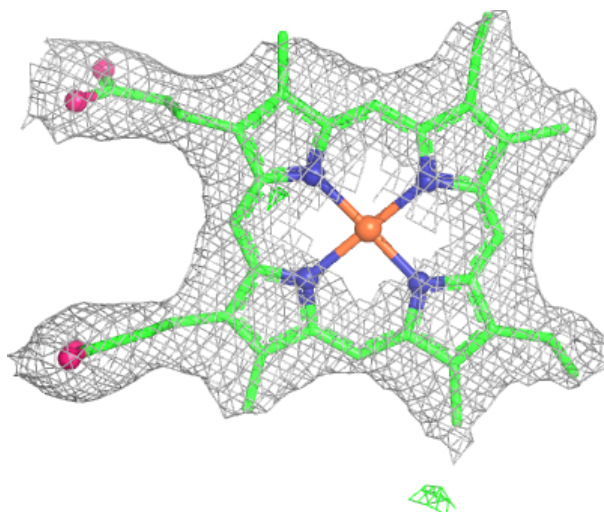
Electron density around HEM K 1407:

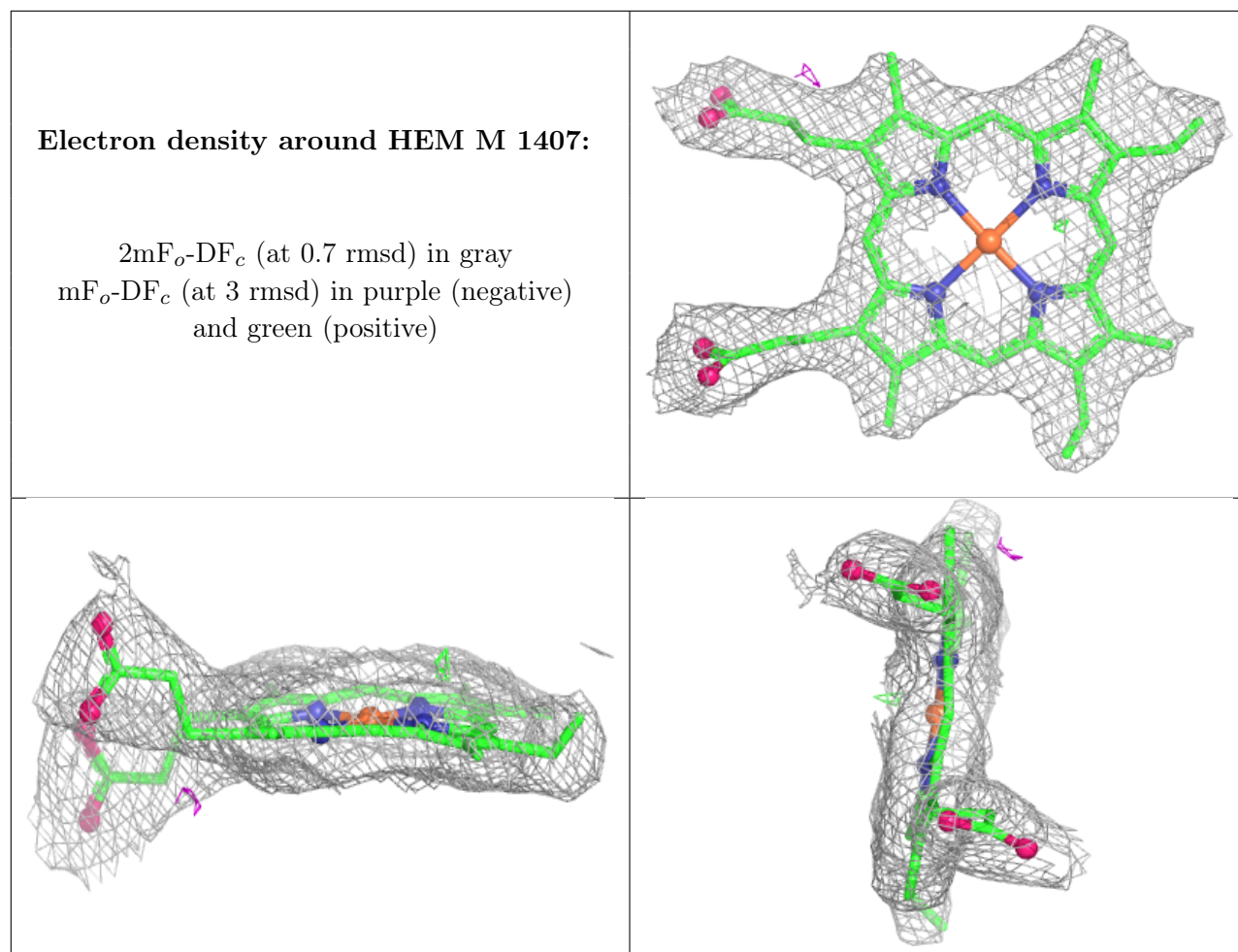
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM L 1407:

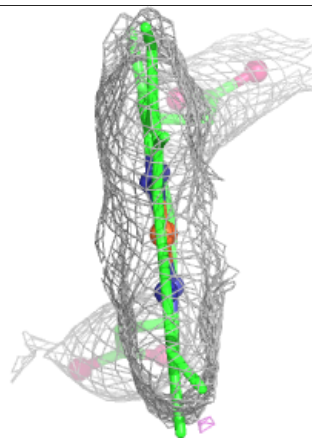
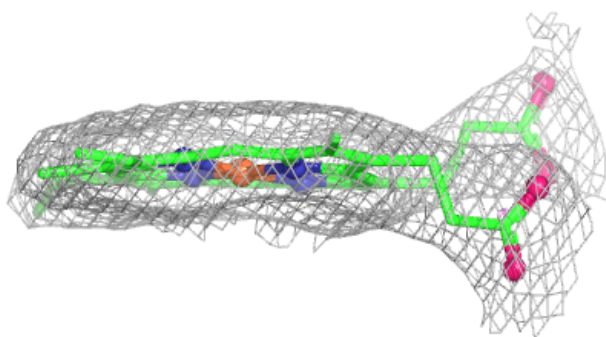
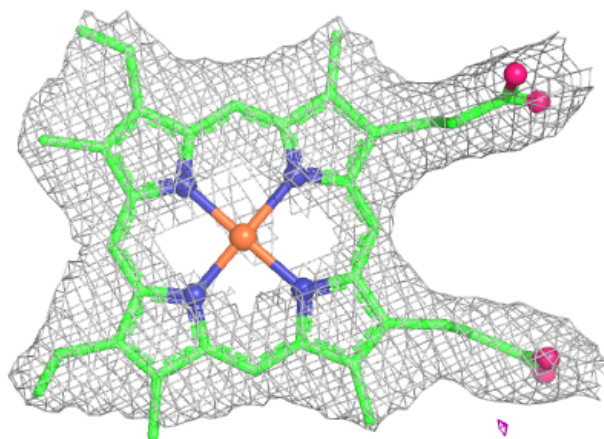
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





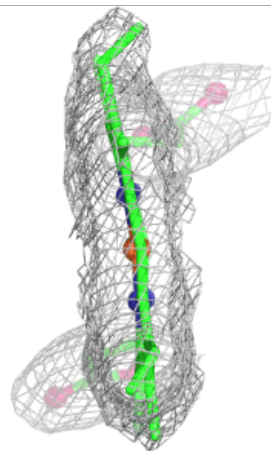
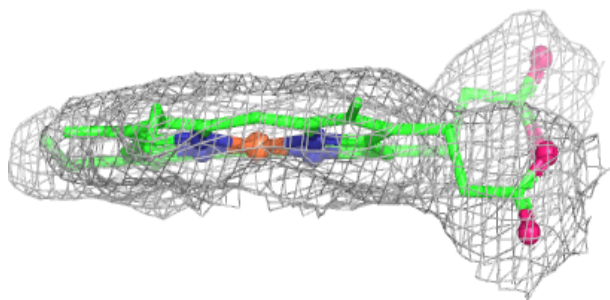
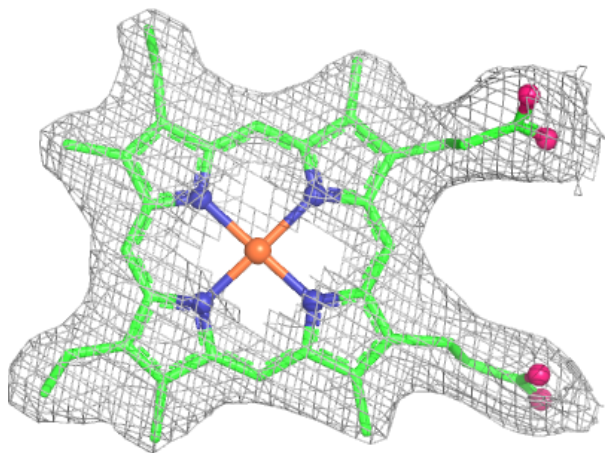
Electron density around HEM N 1407:

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



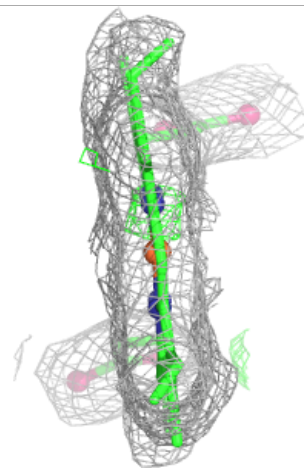
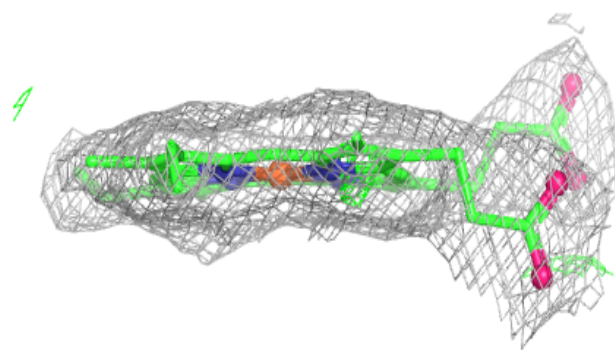
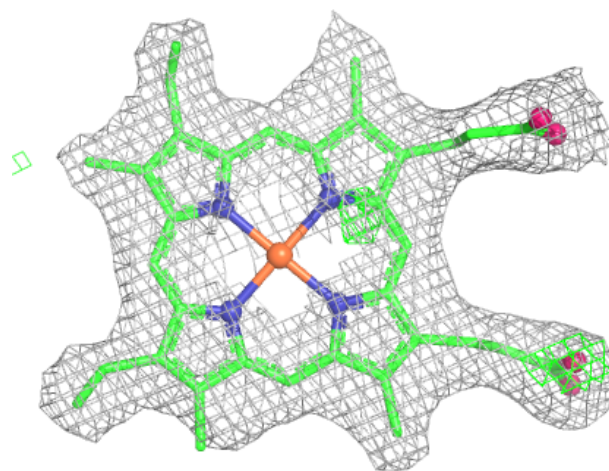
Electron density around HEM B 1407:

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



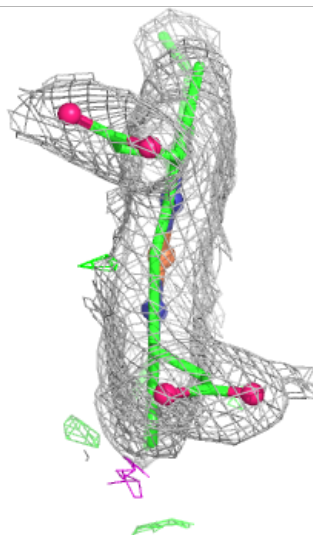
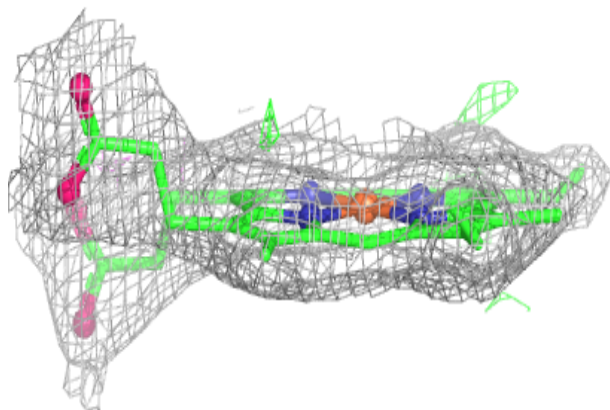
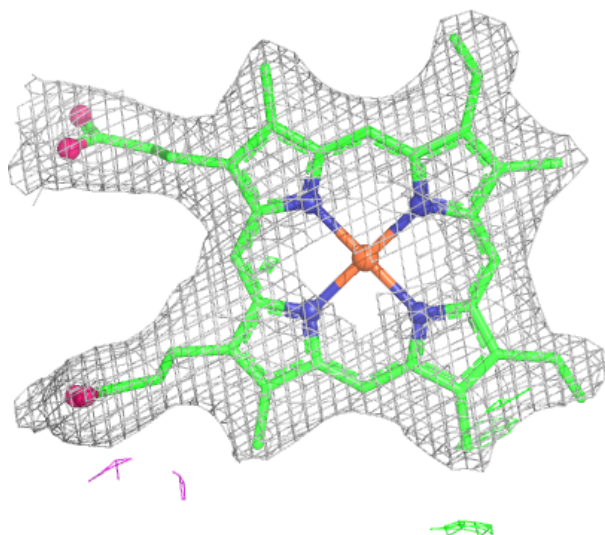
Electron density around HEM C 1407:

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



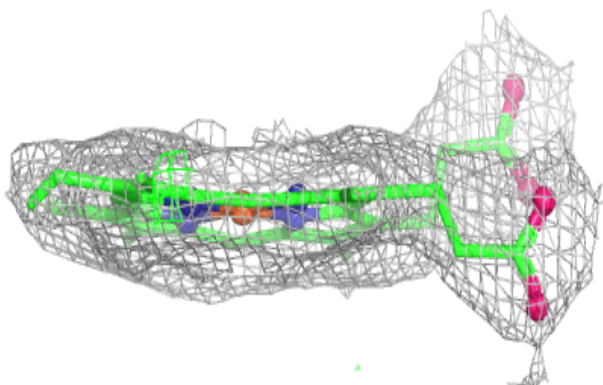
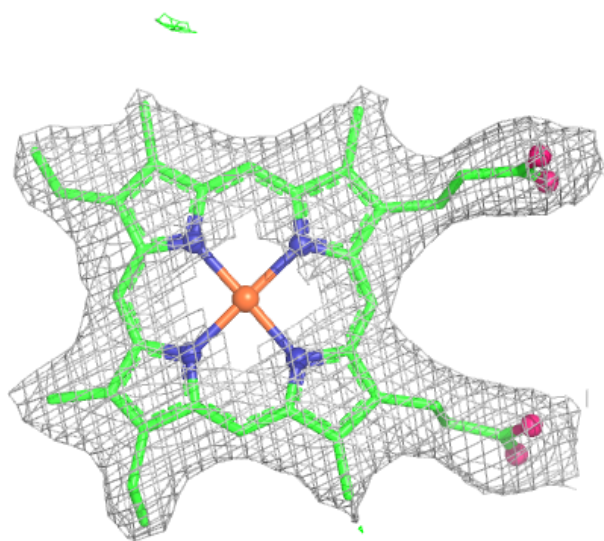
Electron density around HEM A 1407:

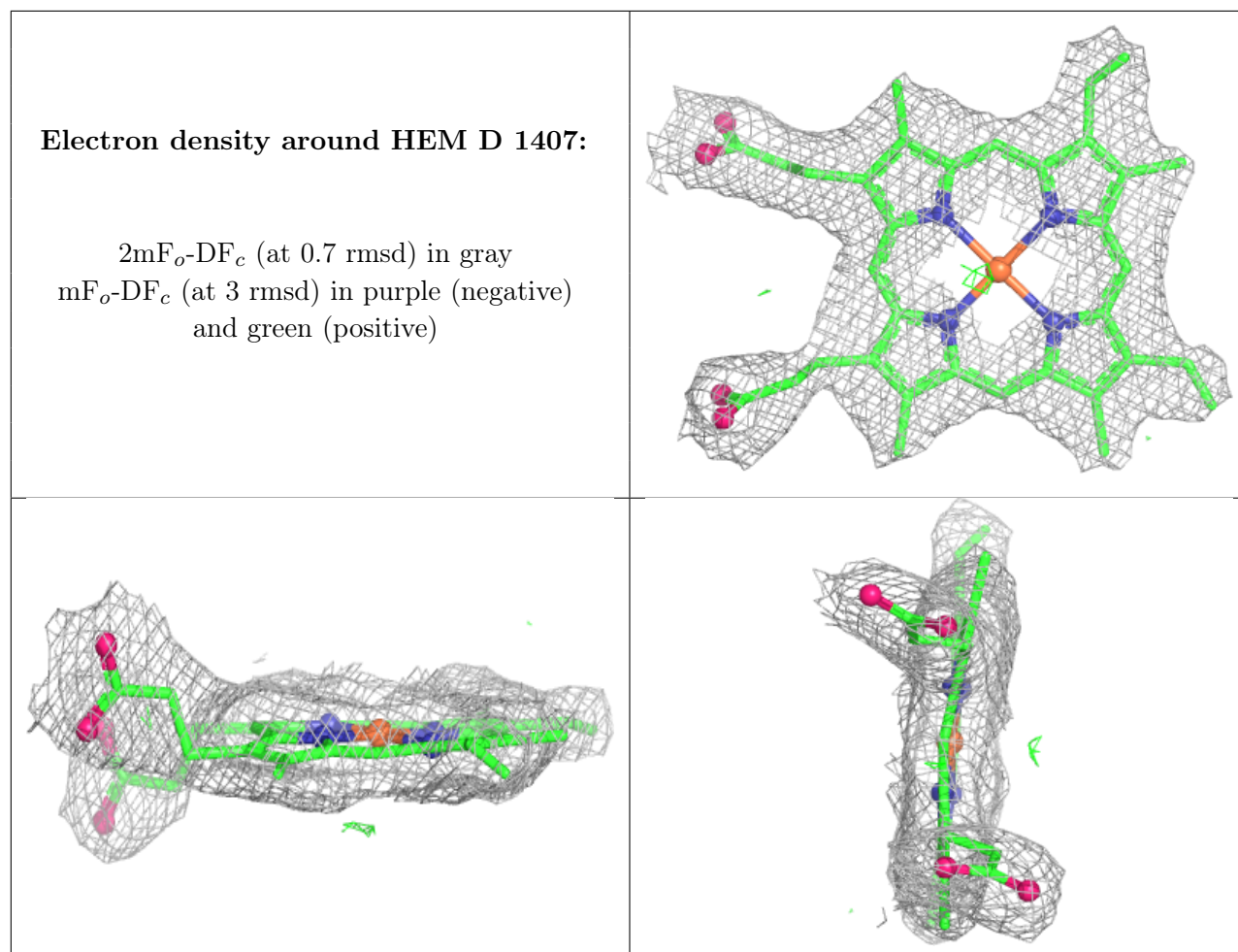
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.