



wwPDB X-ray Structure Validation Summary Report i

Dec 17, 2023 – 06:06 pm GMT

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
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

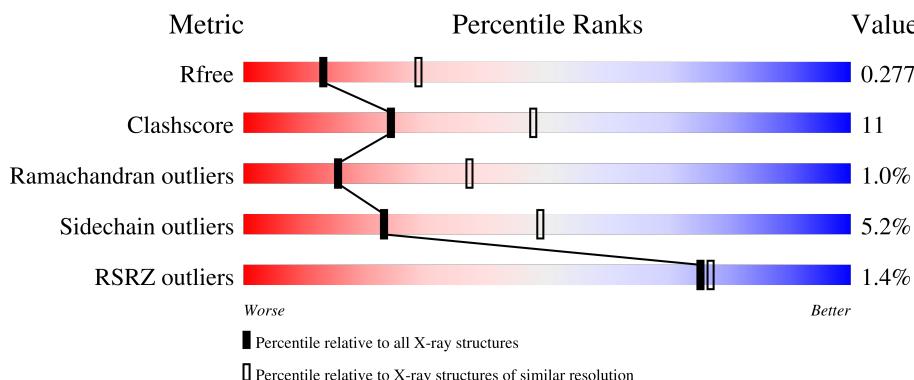
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

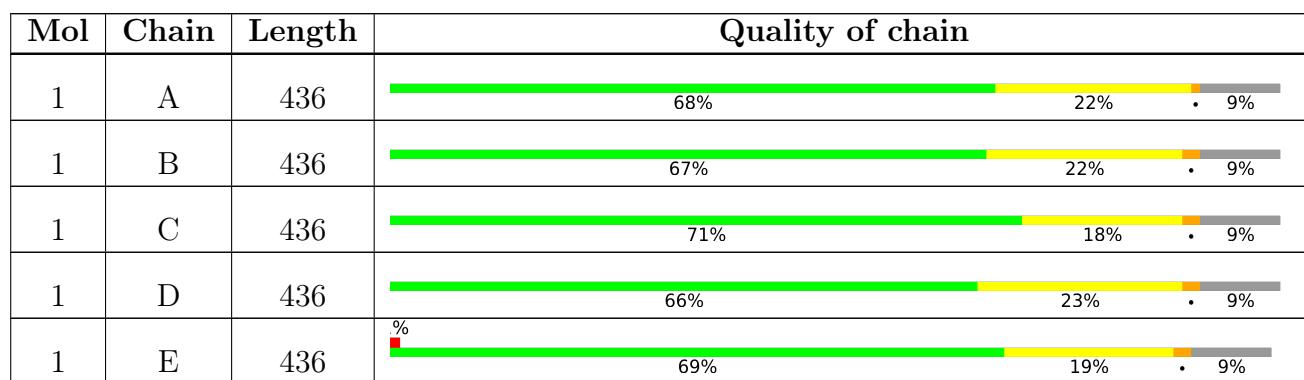
The reported resolution of this entry is 2.70 Å.

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.



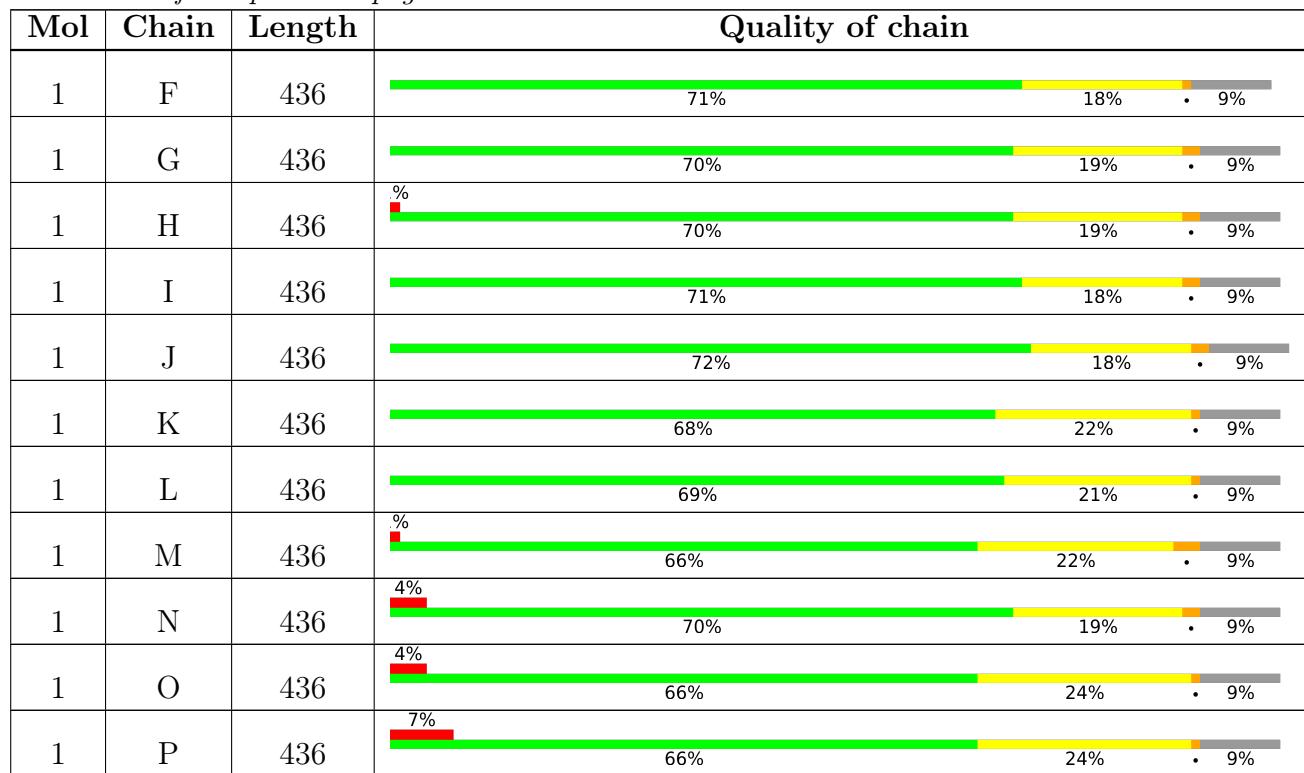
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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.



Continued on next page...

Continued from previous page...



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 [\(i\)](#)

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 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...

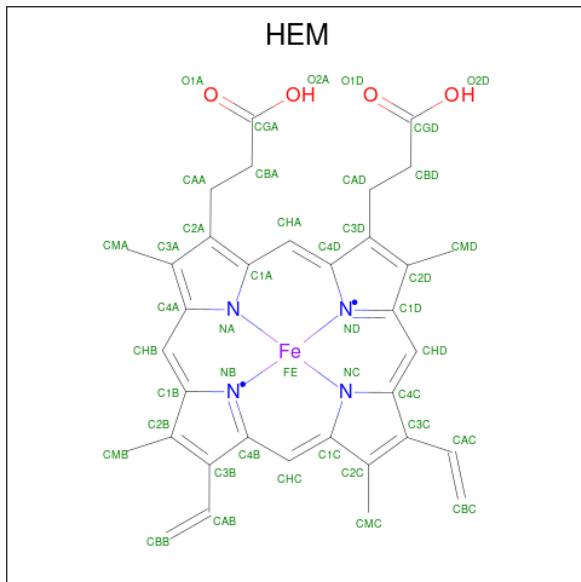
Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	expression tag	UNP O87605
M	-18	GLY	-	expression tag	UNP O87605
M	-17	SER	-	expression tag	UNP O87605
M	-16	SER	-	expression tag	UNP O87605
M	-15	HIS	-	expression tag	UNP O87605
M	-14	HIS	-	expression tag	UNP O87605
M	-13	HIS	-	expression tag	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

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



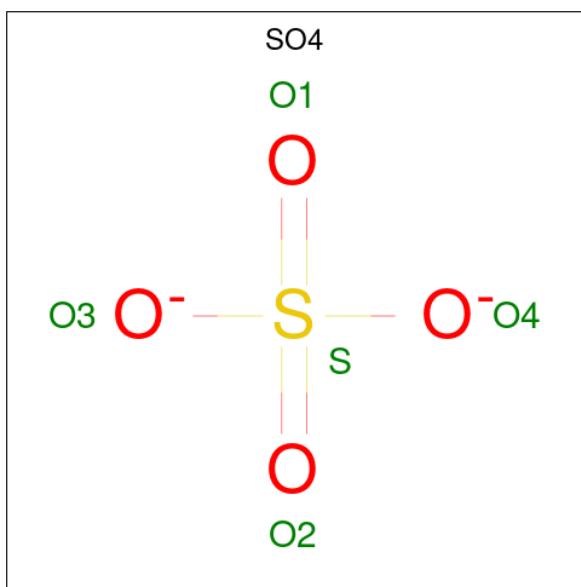
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G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

Continued on next page...

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 (three-letter code: SO4) (formula: O₄S).



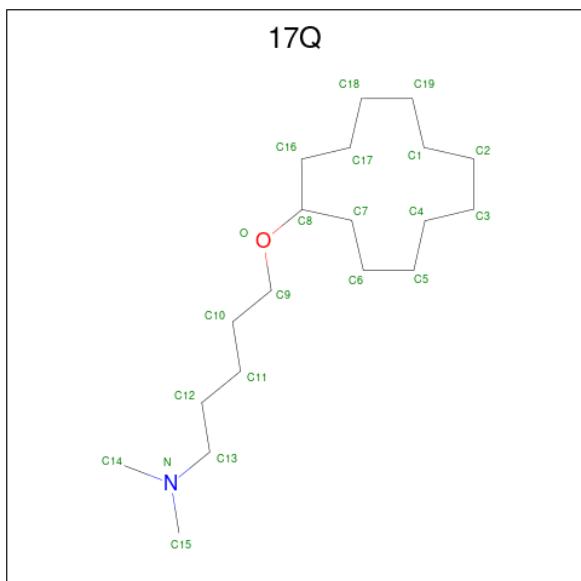
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is 1.7.6 5-cyclododecyloxy-N,N-dimethyl-pentan-1-amine (three-letter code: 17Q) (formula: C₁₉H₃₉NO).



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

- Molecule 5 is water.

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

Continued on next page...

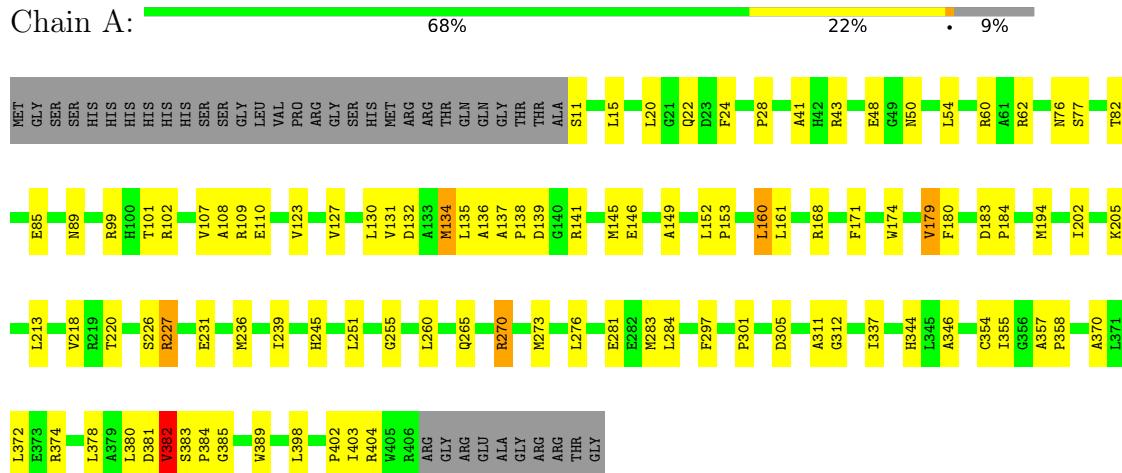
Continued from previous page...

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

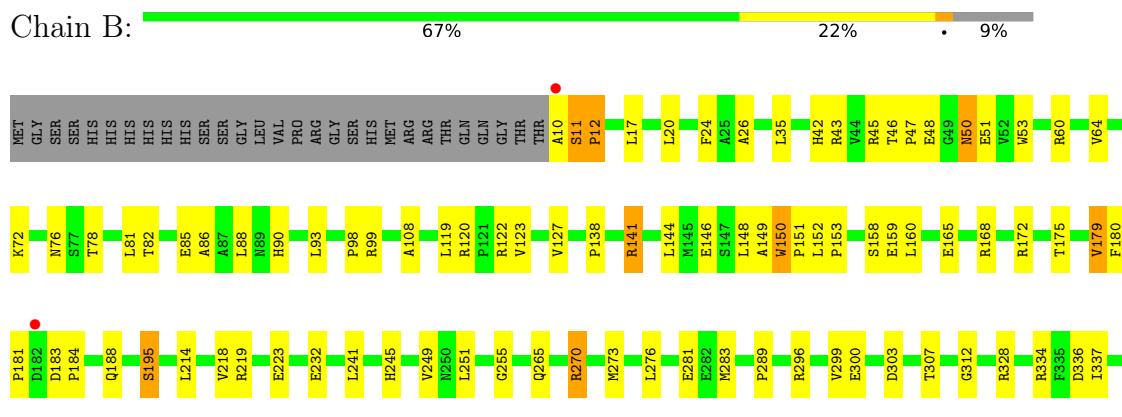
3 Residue-property plots

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

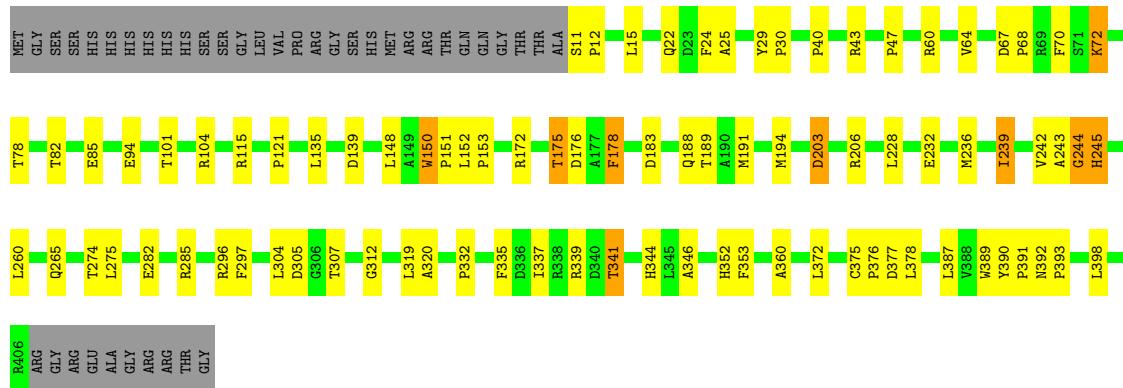


- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

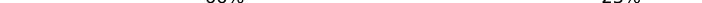


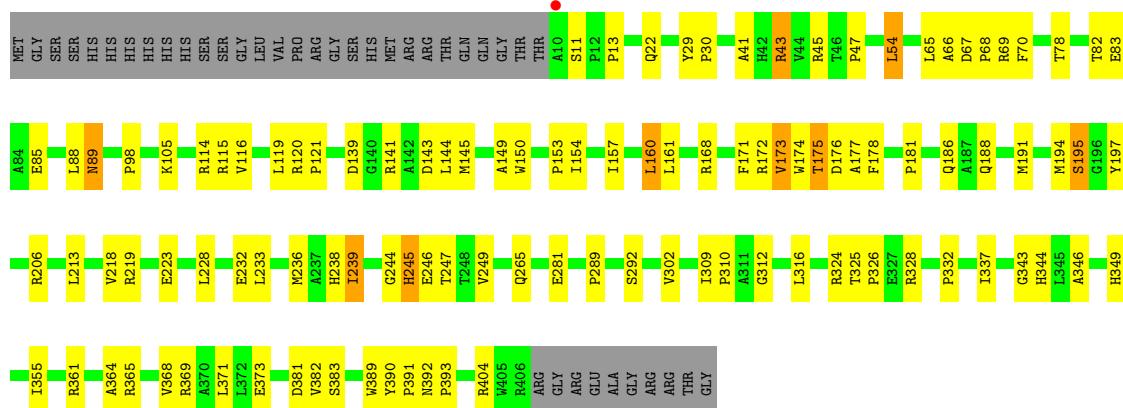
- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC





- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

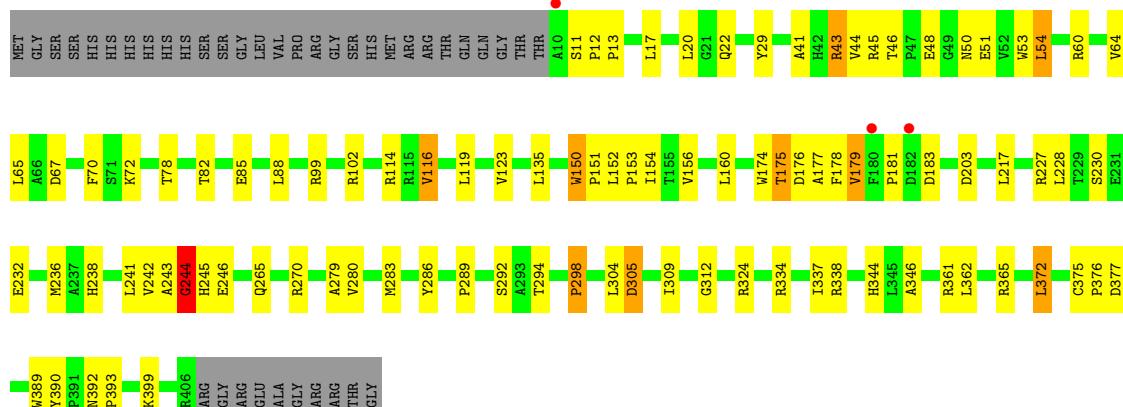
Chain D:  66% 23% • 9%



- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

A horizontal bar chart titled "Chain E:" at the top left. The x-axis represents percentages from 0% to 100%, with major tick marks at 0%, 69%, 19%, and 9%. The y-axis has a single tick mark at the top labeled "%". A single green bar spans from 0% to approximately 85%. To the right of the bar, there is a small yellow segment representing 9%.

Category	Percentage
Chain E	85%
Other	9%



• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain F: 71% 18% : 9%



- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain G:



- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain H:



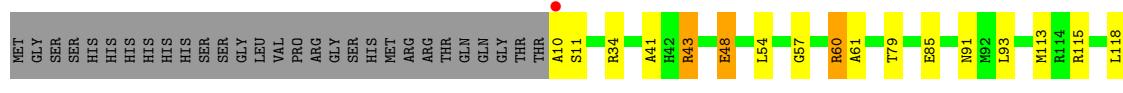
- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

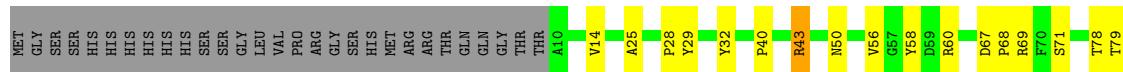
Chain I:



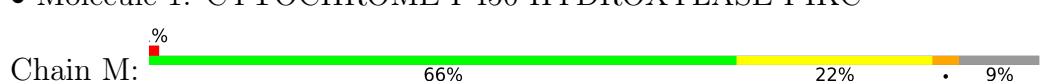
• Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC

Chain J:

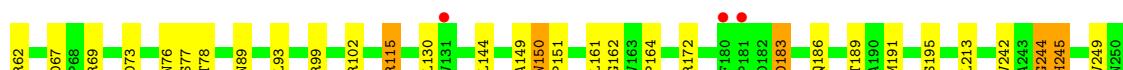




- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



<img alt="Diagram showing the distribution of mutations across the SARS-CoV-2 genome. The genome is represented as a horizontal bar divided into segments by vertical lines. Colored boxes indicate mutation types: red for R60, yellow for L65, K72, T78, L81, E85, A86, H90, M92, L93, L241, H100, T101, V107, E110, V131, L135, L144, M145, A149, W150, P151, L152, P153, F171, R172, T176, V178, V179, P181, D182, P184, A185, Q186, A187, Q188, M191, and Y197. Green boxes indicate mutations R200, F228, F229, P301, D336, R339, C354, I355, R369, L571, E373, R374, C375, P376, D377, D381, V382, S383, P384, G385, N392, L398, L401, R404, W405, R406, A407, G408, A409, G410, R411, T412, L413, V414, P415, D416, V417, P418, D419, V419, P420, D421, V422, P423, D424, V425, P426, D427, V428, P429, D429, V430, P431, D432, V433, P434, D435, V436, P437, D438, V439, P439, D440, V441, P442, D443, V444, P445, D446, V447, P448, D449, V449, P450, D451, V452, P453, D454, V455, P456, D457, V458, P459, D460, V461, P462, D463, V464, P465, D466, V467, P468, D469, V468, P470, D471, V472, P473, D474, V475, P476, D477, V478, P479, D479, V480, P481, D482, V483, P484, D485, V486, P487, D488, V489, P490, D491, V492, P493, D494, V495, P496, D497, V498, P499, D499, V500, P501, D502, V503, P504, D505, V506, P507, D508, V509, P510, D511, V512, P513, D514, V515, P516, D517, V518, P519, D520, V521, P522, D523, V524, P525, D526, V527, P528, D529, V528, P529, D529, V529, P530, D531, V531, P532, D533, V534, P535, D536, V537, P538, D539, V539, P540, D541, V542, P543, D544, V545, P546, D547, V548, P549, D550, V551, P552, D553, V554, P555, D556, V557, P558, D559, V558, P559, D559, V559, P560, D561, V560, P562, D563, V564, P565, D566, V567, P568, D569, V568, P569, D569, V569, P570, D571, V570, P571, D572, V571, P573, D574, V572, P575, D576, V577, P578, D579, V578, P579, D579, V579, P580, D581, V580, P582, D583, V584, P585, D586, V587, P588, D589, V589, P590, D591, V592, P593, D594, V595, P596, D597, V598, P599, D599, V599, P600, D601, V600, P601, D602, V603, P604, D605, V606, P607, D608, V609, P610, D611, V612, P613, D614, V615, P616, D617, V618, P619, D620, V621, P622, D623, V624, P625, D626, V627, P628, D629, V628, P629, D629, V629, P630, D631, V632, P633, D634, V635, P636, D637, V638, P639, D640, V641, P642, D643, V644, P645, D646, V647, P648, D649, V648, P649, D649, V649, P650, D651, V652, P653, D654, V655, P656, D657, V658, P659, D660, V661, P662, D663, V664, P665, D666, V667, P668, D669, V668, P669, D669, V669, P670, D671, V672, P673, D674, V675, P676, D677, V678, P679, D680, V681, P682, D683, V684, P685, D686, V687, P688, D689, V689, P690, D691, V692, P693, D694, V695, P696, D697, V698, P699, D699, V699, P700, D701, V702, P703, D704, V705, P706, D707, V708, P709, D7010, V7011, P7012, D7013, V7014, P7015, D7016, V7017, P7018, D7019, V7019, P7020, D7021, V7022, P7023, D7024, V7025, P7026, D7027, V7028, P7029, D7029, V7029, P7030, D7031, V7032, P7033, D7034, V7035, P7036, D7037, V7038, P7039, D7038, V7039, P7040, D7041, V7042, P7043, D7044, V7045, P7046, D7047, V7048, P7049, D7050, V7051, P7052, D7053, V7054, P7055, D7056, V7057, P7058, D7059, V7058, P7059, D7059, V7059, P7060, D7061, V7062, P7063, D7064, V7065, P7066, D7067, V7068, P7068, D7069, V7069, P7070, D7071, V7072, P7073, D7074, V7075, P7076, D7077, V7078, P7079, D7080, V7081, P7082, D7083, V7084, P7085, D7086, V7087, P7088, D7089, V7089, P7090, D7091, V7092, P7093, D7094, V7095, P7096, D7097, V7098, P7099, D7099, V7099, P7100, D7101, V7102, P7103, D7104, V7105, P7106, D7107, V7108, P7109, D7110, V7109, P7111, D7112, V7113, P7114, D7115, V7116, P7117, D7118, V7119, P7120, D7121, V7122, P7123, D7124, V7125, P7126, D7127, V7128, P7129, D7130, V7131, P7132, D7133, V7134, P7135, D7136, V7137, P7138, D7139, V7138, P7140, D7141, V7142, P7143, D7144, V7145, P7146, D7147, V7148, P7149, D7150, V7151, P7152, D7153, V7154, P7155, D7156, V7157, P7158, D7159, V7158, P7159, D7159, V7159, P7160, D7161, V7162, P7163, D7164, V7165, P7166, D7167, V7168, P7169, D7170, V7171, P7172, D7173, V7174, P7175, D7176, V7177, P7178, D7179, V7178, P7180, D7181, V7182, P7183, D7184, V7185, P7186, D7187, V7188, P7189, D7190, V7191, P7192, D7193, V7194, P7195, D7196, V7197, P7198, D7199, V7198, P7199, D7199, V7199, P7200, D7201, V7202, P7203, D7204, V7205, P7206, D7207, V7208, P7209, D7210, V7209, P7211, D7212, V7213, P7214, D7215, V7216, P7217, D7218, V7219, P7220, D7221, V7222, P7223, D7224, V7225, P7226, D7227, V7228, P7229, D7230, V7229, P7231, D7232, V7233, P7234, D7235, V7236, P7237, D7238, V7239, P7239, D7239, V7239, P7240, D7241, V7242, P7243, D7244, V7245, P7246, D7247, V7248, P7248, D7248, V7249, P7249, D7249, V7249, P7250, D7251, V7251, P7252, D7253, V7253, P7254, D7255, V7255, P7256, D7257, V7257, P7258, D7259, V7259, P7259, D7259, V7259, P7260, D7261, V7261, P7262, D7263, V7263, P7264, D7265, V7265, P7266, D7266, V7266, P7267, D7268, V7268, P7269, D7269, V7269, P7270, D7271, V7271, P7272, D7272, V7272, P7273, D7274, V7274, P7275, D7275, V7276, P7276, D7277, V7277, P7278, D7278, V7278, P7279, D7279, V7279, P7280, D7281, V7280, P7281, D7282, V7281, P7283, D7284, V7282, P7285, D7286, V7283, P7287, D7288, V7284, P7289, D7289, V7285, P7290, D7291, V7290, P7291, D7292, V7291, P7293, D7294, V7292, P7295, D7296, V7293, P7297, D7298, V7294, P7298, D7299, V7295, P7299, D7299, V7295, P7300, D7301, V7300, P7302, D7303, V7301, P7304, D7305, V7302, P7306, D7307, V7303, P7308, D7309, V7304, P7309, D7310, V7305, P7311, D7312, V7306, P7313, D7314, V7307, P7315, D7316, V7308, P7317, D7318, V7309, P7318, D7319, V7310, P7319, D7320, V7311, P7321, D7322, V7312, P7323, D7324, V7313, P7325, D7326, V7314, P7327, D7328, V7315, P7329, D7330, V7316, P7331, D7332, V7317, P7333, D7334, V7318, P7334, D7335, V7319, P7335, D7336, V7320, P7336, D7337, V7321, P7337, D7338, V7322, P7338, D7339, V7323, P7339, D7340, V7324, P7341, D7342, V7325, P7343, D7344, V7326, P7345, D7346, V7327, P7347, D7348, V7328, P7349, D7350, V7329, P7351, D7352, V7330, P7353, D7354, V7331, P7355, D7356, V7332, P7357, D7358, V7333, P7359, D7360, V7334, P7361, D7362, V7335, P7363, D7364, V7336, P7365, D7366, V7337, P7367, D7368, V7338, P7368, D7369, V7339, P7369, D7370, V7340, P7371, D7372, V7341, P7373, D7374, V7342, P7375, D7376, V7343, P7377, D7378, V7344, P7379, D7380, V7345, P7381, D7382, V7346, P7383, D7384, V7347, P7385, D7386, V7348, P7387, D7388, V7349, P7389, D7390, V7350, P7391, D7392, V7351, P7393, D7394, V7352, P7395, D7396, V7353, P7397, D7398, V7354, P7399, D73100, V7355, P73101, D73102, V7356, P73103, D73104, V7357, P73105, D73106, V7358, P73107, D73108, V7359, P73109, D73110, V7360, P73111, D73112, V7361, P73113, D73114, V7362, P73115, D73116, V7363, P73117, D73118, V7364, P73119, D73120, V7365, P73121, D73122, V7366, P73123, D73124, V7367, P73125, D73126, V7368, P73127, D73128, V7369, P73129, D73130, V7370, P73131, D73132, V7371, P73133, D73134, V7372, P73135, D73136, V7373, P73137, D73138, V7374, P73139, D73140, V7375, P73141, D73142, V7376, P73143, D73144, V7377, P73145, D73146, V7378, P73147, D73148, V7379, P73149, D73150, V7380, P73151, D73152, V7381, P73153, D73154, V7382, P73155, D73156, V7383, P73157, D73158, V7384, P73159, D73160, V7385, P73161, D73162, V7386, P73163, D73164, V7387, P73165, D73166, V7388, P73167, D73168, V7389, P73169, D73170, V7390, P73171, D73172, V7391, P73173, D73174, V7392, P73175, D73176, V7393, P73177, D73178, V7394, P73179, D73180, V7395, P73181, D73182, V7396, P73183, D73184, V7397, P73185, D73186, V7398, P73187, D73188, V7399, P73189, D73190, V73100, P73191, D73192, V73101, P73193, D73194, V73102, P73195, D73196, V73103, P73197, D73198, V73104, P73199, D73100, V73105, P73101, D73102, V73106, P73102, D73103, V73107, P73103, D73104, V73108, P73104, D73105, V73109, P73105, D73106, V73110, P73106, D73107, V73111, P73107, D73108, V73112, P73108, D73109, V73113, P73109, D73110, V73114, P73110, D73111, V73115, P73111, D73112, V73116, P73112, D73113, V73117, P73113, D73114, V73118, P73114, D73115, V73119, P73115, D73116, V73120, P73116, D73117, V73121, P73117, D73118, V73122, P73118, D73119, V73123, P73119, D73120, V73124, P73120, D73121, V73125, P73121, D73122, V73126, P73122, D73123, V73127, P73123, D73124, V73128, P73124, D73125, V73129, P73125, D73126, V73130, P73126, D73127, V73131, P73127, D73128, V73132, P73128, D73129, V73133, P73129, D73130, V73134, P73130, D73131, V73135, P73131, D73132, V73136, P73132, D73133, V73137, P73133, D73134, V73138, P73134, D73135, V73139, P73135, D73136, V73140, P73136, D73137, V73141, P73137, D73138, V73142, P73138, D73139, V73143, P73139, D73140, V73144, P73140, D73141, V73145, P73141, D73142, V73146, P73142, D73143, V73147, P73143, D73144, V73148, P73144, D73145, V73149, P73145, D73146, V73150, P73146, D73147, V73151, P73147, D73148, V73152, P73148, D73149, V73153, P73149, D73150, V73154, P73150, D73151, V73155, P73151, D73152, V73156, P73152, D73153, V73157, P73153, D73154, V73158, P73154, D73155, V73159, P73155, D73156, V73160, P73156, D73157, V73161, P73157, D73158, V73162, P73158, D73159, V73163, P73159, D73160, V73164, P73160, D73161, V73165, P73161, D73162, V73166, P73162, D73163, V73167, P73163, D73164, V73168, P73164, D73165, V73169, P73165, D73166, V73170, P73166, D73167, V73171, P73167, D73168, V73172, P73168, D73169, V73173, P73169, D73170, V73174, P73170, D73171, V73175, P73171, D73172, V73176, P73172, D73173, V73177, P73173, D73174, V73178, P73174, D73175, V73179, P73175, D73176, V73180, P73176, D73177, V73181, P73177, D73178, V73182, P73178, D73179, V73183, P73179, D73180, V73184, P73180, D73181, V73185, P73181, D73182, V73186, P73182, D73183, V73187, P73183, D73184, V73188, P73184, D73185, V73189, P73185, D73186, V73190, P73186, D73187, V73191, P73187, D73188, V73192, P73188, D73189, V73193, P73189, D73190, V73194, P73190, D73191, V73195, P73191, D73192, V73196, P73192, D73193, V73197, P73193, D73194, V73198, P73194, D73195, V73199, P73195, D73196, V73200, P73196, D73197, V73201, P73197, D73198, V73202, P73198, D73199, V73203, P73199, D73200, V73204, P73201, D73202, V73205, P73202, D73203, V73206, P73203, D73204, V73207, P73204, D73205, V73208, P73205, D73206, V73209, P73206, D73207, V73210, P73207, D73208, V73211, P73208, D73209, V73212, P73209, D73210, V73213, P73210, D73211, V73214, P73211, D73212, V73215, P73212, D73213, V73216, P73213, D73214, V73217, P73214, D73215, V73218, P73215, D73216, V73219, P73216, D73217, V73220, P73217, D73218, V73221, P73218, D73219, V73222, P73219, D73220, V73223, P73220, D73221, V73224, P73221, D73222, V73225, P73222, D73223, V73226, P73223, D73224, V73227, P73224, D73225, V73228, P73225, D73226, V73229, P73226, D73227, V73230, P73227, D73228, V73231, P73228, D73229, V73232, P73229, D73230, V73233, P73230, D73231, V73234, P73231, D73232, V73235, P73232, D73233, V73236, P73233, D73234, V73237, P73234, D73235, V73238, P73235, D73236, V73239, P73236, D73237, V73240, P73237, D73238, V73241, P73238, D73239, V73242, P73239, D73240, V73243, P73240, D73241, V73244, P73241, D73242, V73245, P73242, D73243, V73246, P73243, D73244, V73247, P73244, D73245, V73248, P73245, D73246, V73249, P73246, D73247, V73250, P73247, D73248, V73251, P73248, D73249, V73252, P73249, D73250, V73253, P73250, D73251, V73254, P73251, D73252, V73255, P73252, D73253, V73256, P73253, D73254, V73257, P73254, D73255, V73258, P73255, D73256, V73259, P73256, D73257, V73260, P73257, D73258, V73261, P73258, D73259, V73262, P73259, D73260, V73263, P73260, D73261, V73264, P73261, D73262, V73265, P73262, D73263, V73266, P73263, D73264, V73267, P73264, D73265, V73268, P73265, D73266, V73269, P73266, D73267, V73270, P73267, D73268, V73271, P73268, D73269, V73272, P73269, D73270, V73273, P73270, D73271, V73274, P73271, D73272, V73275, P73272, D73273, V73276, P73273, D73274, V73277, P73274, D73275, V73278, P73275, D73276, V73279, P73276, D73277, V73280, P73277, D73278, V73281, P73278, D73279, V73282, P73279, D73280, V73283, P73280, D73281, V73284, P73281, D73282, V73285, P73282, D73283, V73286, P73283, D73284, V73287, P73284, D73285, V73288, P73285, D73286, V73289, P73286, D73287, V73290, P73287, D73288, V73291, P73288, D73289, V73292, P73289, D73290, V73293, P73290, D73291, V73294, P73291, D73292, V73295, P73292, D73293, V73296, P73293, D73294, V73297, P73294, D73295, V73298, P73295, D73296, V73299, P73296, D73297, V73200, P73297, D73298, V73201, P73298, D73299, V73202, P73299, D73200, V73203, P73200, D73201, V73204, P73201, D73202, V73205, P73202, D73203, V73206, P73203, D73204, V73207, P73204, D73205, V73208, P73205, D73206, V73209, P73206, D73207, V73210, P73207, D73208, V73211, P73208, D73209, V73212, P73209, D73210, V73213, P73210, D73211, V73214, P73211, D73212, V73215, P73212, D73213, V73216, P73213, D73214, V73217, P73214, D73215, V73218, P73215, D73216, V73219, P73216, D73217, V73220, P73217, D73218, V73221, P73218, D73219, V73222, P73219, D73220, V73223, P73220, D73221, V73224, P73221, D73222, V73225, P73222, D73223, V73226, P73223, D73224, V73227, P73224, D73225, V73228, P73225, D73226, V73229, P73226, D73227, V73230, P73227, D73228, V73231, P73228, D73229, V73232, P73229, D73230, V73233, P73230, D73231, V73234, P73231, D73232, V73235, P73232, D73233, V73236, P73233, D73234, V73237, P73234, D73235, V73238, P73235, D73236, V73239, P73236, D73237, V73240, P73237, D73238, V73241, P73238, D73239, V73242, P73239, D73240, V73243, P73240, D73241, V73244, P73241, D73242, V73245, P73242, D73243, V73246, P73243, D73244, V73247, P73244, D73245, V73248, P73245, D73246, V73249, P73246, D73247, V73250, P73247, D73248, V73251, P73248, D73249, V73252, P73249, D73250, V73253, P73250, D73251, V73254, P73251, D73252, V73255, P73252, D73253, V73256, P73253, D73254, V73257, P73254, D73255, V73258, P73255, D73256, V73259, P73256, D73257, V73260, P73257, D73258, V73261, P73258, D73259, V73262, P73259, D73260, V73263, P73260, D73261, V73264, P73261, D73262, V73265, P73262, D73263, V73266, P73263, D73264, V73267, P73264, D73265, V73268, P73265, D73266, V73269, P73266, D73267, V73270, P73267, D73268, V73271, P73268, D73269, V73272, P73269, D73270, V73273, P73270, D73271, V73274, P73271, D73272, V73275, P73272, D73273, V73276, P73273, D73274, V73277, P73274, D73275, V73278, P73275, D73276, V73279, P73276, D73277, V73280, P73277, D73278, V73281, P73278, D73279, V73282, P73279, D73280, V73283, P73280, D73281, V73284, P73281, D73282, V73285, P73282, D73283, V73286, P73283, D73284, V73287, P73284, D73285, V73288, P73285, D73286, V73289, P73286, D73287, V73290, P7

- Molecule 1: CYTOCHROME P450 HYDROXYLASE PIKC



The phylogenetic tree illustrates the evolutionary relationships and specific mutations across three main clades. The tree is rooted at the bottom and branches upwards. Nodes are labeled with sequence identifiers and amino acid positions. Colored bars indicate specific mutations or features along the branches. Red dots mark specific sites of interest.

- Clade 1 (Top Branch):**
 - Root: A61 (M194)
 - Sub-branch 1: V64 (S195)
 - Sub-branch 2: D67 (D203)
 - Sub-branch 3: P68 (R206)
 - Sub-branch 4: R69 (P401)
 - Sub-branch 5: F70 (V302)
 - Sub-branch 6: L74 (L213)
 - Sub-branch 7: T78 (L214)
 - Sub-branch 8: N76 (L223)
 - Sub-branch 9: S77 (D224)
 - Sub-branch 10: M89 (E223)
 - Sub-branch 11: H100 (D224)
 - Sub-branch 12: M92 (R227)
 - Sub-branch 13: L93 (L228)
 - Sub-branch 14: E94 (T229)
 - Sub-branch 15: S95 (S230)
 - Sub-branch 16: I10 (E231)
 - Sub-branch 17: E110 (E232)
 - Sub-branch 18: R114 (L233)
 - Sub-branch 19: R114 (L234)
 - Sub-branch 20: E117 (T239)
 - Sub-branch 21: L118 (R334)
 - Sub-branch 22: L119 (F246)
 - Sub-branch 23: V123 (P249)
 - Sub-branch 24: L135 (W250)
 - Sub-branch 25: D139 (L251)
 - Sub-branch 26: M145 (I252)
 - Sub-branch 27: Q226 (H245)
 - Sub-branch 28: D223 (F24)
 - Sub-branch 29: P30 (Y229)
 - Sub-branch 30: T31 (Y32)
 - Sub-branch 31: L35 (D223)
 - Sub-branch 32: R36 (F24)
 - Sub-branch 33: A37 (Y229)
 - Sub-branch 34: L161 (Y32)
 - Sub-branch 35: F40 (R172)
 - Sub-branch 36: A441 (R43)
 - Sub-branch 37: H42 (P47)
 - Sub-branch 38: R43 (V56)
 - Sub-branch 39: P47 (G57)
 - Sub-branch 40: V56 (Y58)
 - Sub-branch 41: P180 (P194)
 - Sub-branch 42: P180 (P194)
- Clade 2 (Middle Branch):**
 - Root: T189 (L284)
 - Sub-branch 1: G288 (P289)
 - Sub-branch 2: W405 (R406)
 - Sub-branch 3: R404 (R406)
 - Sub-branch 4: Y295 (T294)
 - Sub-branch 5: D324 (D303)
 - Sub-branch 6: L304 (L305)
 - Sub-branch 7: P299 (P336)
 - Sub-branch 8: D336 (I337)
 - Sub-branch 9: I337 (R338)
 - Sub-branch 10: R338 (R339)
 - Sub-branch 11: V308 (V318)
 - Sub-branch 12: R324 (R324)
 - Sub-branch 13: F299 (F336)
 - Sub-branch 14: L336 (L337)
 - Sub-branch 15: L337 (R338)
 - Sub-branch 16: R338 (R339)
 - Sub-branch 17: H344 (H344)
 - Sub-branch 18: L345 (A346)
 - Sub-branch 19: A346 (H349)
 - Sub-branch 20: H349 (G356)
 - Sub-branch 21: A357 (P358)
 - Sub-branch 22: P358 (E363)
 - Sub-branch 23: E363 (R369)
 - Sub-branch 24: R369 (Q225)
 - Sub-branch 25: D277 (P376)
 - Sub-branch 26: P376 (D377)
 - Sub-branch 27: D377 (L378)
 - Sub-branch 28: L378 (A379)
 - Sub-branch 29: A379 (L380)
 - Sub-branch 30: L380 (D381)
 - Sub-branch 31: D381 (V382)
 - Sub-branch 32: V382 (S383)
 - Sub-branch 33: S383 (P384)
 - Sub-branch 34: P384 (G385)
 - Sub-branch 35: G385 (P391)
 - Sub-branch 36: P391 (M392)
 - Sub-branch 37: M392 (P393)
 - Sub-branch 38: P393 (M283)
- Clade 3 (Bottom Branch):**
 - Root: L401 (L401)
 - Sub-branch 1: R404 (R404)
 - Sub-branch 2: W405 (W405)
 - Sub-branch 3: R406 (R406)
 - Sub-branch 4: Y295 (Y295)
 - Sub-branch 5: D324 (D324)
 - Sub-branch 6: L304 (L304)
 - Sub-branch 7: P299 (P299)
 - Sub-branch 8: D336 (D336)
 - Sub-branch 9: I337 (I337)
 - Sub-branch 10: R338 (R338)
 - Sub-branch 11: R339 (R339)
 - Sub-branch 12: V308 (V308)
 - Sub-branch 13: R324 (R324)
 - Sub-branch 14: F299 (F299)
 - Sub-branch 15: L336 (L336)
 - Sub-branch 16: I337 (I337)
 - Sub-branch 17: R338 (R338)
 - Sub-branch 18: R339 (R339)
 - Sub-branch 19: H344 (H344)
 - Sub-branch 20: L345 (A346)
 - Sub-branch 21: A346 (H349)
 - Sub-branch 22: H349 (G356)
 - Sub-branch 23: A357 (P358)
 - Sub-branch 24: P358 (E363)
 - Sub-branch 25: E363 (R369)
 - Sub-branch 26: R369 (Q225)
 - Sub-branch 27: D277 (P376)
 - Sub-branch 28: P376 (D377)
 - Sub-branch 29: D377 (L378)
 - Sub-branch 30: L378 (A379)
 - Sub-branch 31: A379 (L380)
 - Sub-branch 32: L380 (D381)
 - Sub-branch 33: D381 (V382)
 - Sub-branch 34: V382 (S383)
 - Sub-branch 35: S383 (P384)
 - Sub-branch 36: P384 (G385)
 - Sub-branch 37: G385 (P391)
 - Sub-branch 38: P391 (M392)
 - Sub-branch 39: M392 (P393)
 - Sub-branch 40: P393 (M283)

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.27 Å 130.11 Å 134.90 Å 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
$< I/\sigma(I) >$ ¹	1.73 (at 2.69 Å)	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 ²)	44.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$< L > = 0.46$, $< L^2 > = 0.28$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [\(i\)](#)

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 [\(i\)](#)

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	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 [\(i\)](#)

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%)	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

Continued on next page...

Continued from previous page...

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	O	48	GLU
1	O	241	LEU
1	P	324	ARG
1	G	50[B]	ASN
1	F	388	VAL

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

Mol	Chain	Res	Type
1	L	344	HIS
1	P	188	GLN
1	M	188	GLN
1	N	265	GLN
1	E	265	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

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	H	1408	-	4,4,4	0.48	0	6,6,6	0.52	0
4	17Q	G	1410	-	21,21,21	0.47	0	21,23,23	0.68	0
3	SO4	A	1408	-	4,4,4	0.27	0	6,6,6	0.53	0
2	HEM	K	1407	1	41,50,50	1.86	5 (12%)	45,82,82	1.61	11 (24%)
3	SO4	B	1408	-	4,4,4	0.27	0	6,6,6	0.33	0
2	HEM	B	1407	1	41,50,50	1.89	6 (14%)	45,82,82	1.89	12 (26%)
3	SO4	O	1408	-	4,4,4	0.55	0	6,6,6	0.60	0
2	HEM	H	1407	1	41,50,50	1.96	8 (19%)	45,82,82	1.50	6 (13%)
2	HEM	A	1407	1	41,50,50	1.91	5 (12%)	45,82,82	1.69	11 (24%)
3	SO4	J	1408	-	4,4,4	0.60	0	6,6,6	0.47	0
4	17Q	C	1410	-	21,21,21	0.30	0	21,23,23	0.97	2 (9%)
2	HEM	M	1407	1	41,50,50	2.06	7 (17%)	45,82,82	1.67	8 (17%)
2	HEM	L	1407	1	41,50,50	1.85	4 (9%)	45,82,82	1.59	10 (22%)
2	HEM	I	1407	1	41,50,50	1.95	9 (21%)	45,82,82	1.70	10 (22%)
2	HEM	F	1407	1	41,50,50	1.98	9 (21%)	45,82,82	1.75	9 (20%)
3	SO4	I	1409	-	4,4,4	0.23	0	6,6,6	0.38	0
2	HEM	G	1407	1	41,50,50	1.97	5 (12%)	45,82,82	1.75	7 (15%)
3	SO4	I	1408	-	4,4,4	0.68	0	6,6,6	0.77	0
2	HEM	N	1407	1	41,50,50	1.91	6 (14%)	45,82,82	1.48	9 (20%)
2	HEM	C	1407	1	41,50,50	2.07	7 (17%)	45,82,82	1.79	11 (24%)
3	SO4	F	1408	-	4,4,4	0.51	0	6,6,6	0.52	0
3	SO4	B	1409	-	4,4,4	0.26	0	6,6,6	0.23	0
2	HEM	J	1407	1	41,50,50	1.93	6 (14%)	45,82,82	1.43	6 (13%)
2	HEM	O	1407	1	41,50,50	1.96	7 (17%)	45,82,82	1.67	9 (20%)
3	SO4	O	1409	-	4,4,4	0.48	0	6,6,6	0.88	0
2	HEM	P	1407	1	41,50,50	1.95	8 (19%)	45,82,82	1.77	13 (28%)
2	HEM	D	1407	1	41,50,50	1.92	9 (21%)	45,82,82	1.45	7 (15%)
3	SO4	D	1408	-	4,4,4	0.67	0	6,6,6	0.79	0
2	HEM	E	1407	1	41,50,50	1.88	7 (17%)	45,82,82	1.71	10 (22%)
3	SO4	H	1409	-	4,4,4	0.29	0	6,6,6	0.31	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
4	17Q	C	1410	-	-	14/23/23/23	1/1/1/1
4	17Q	G	1410	-	-	14/23/23/23	1/1/1/1
2	HEM	I	1407	1	-	1/12/54/54	-
2	HEM	M	1407	1	-	4/12/54/54	-
2	HEM	F	1407	1	-	0/12/54/54	-
2	HEM	H	1407	1	-	2/12/54/54	-
2	HEM	A	1407	1	-	2/12/54/54	-
2	HEM	G	1407	1	-	2/12/54/54	-
2	HEM	J	1407	1	-	2/12/54/54	-
2	HEM	K	1407	1	-	4/12/54/54	-
2	HEM	B	1407	1	-	2/12/54/54	-
2	HEM	N	1407	1	-	0/12/54/54	-
2	HEM	O	1407	1	-	1/12/54/54	-
2	HEM	P	1407	1	-	2/12/54/54	-
2	HEM	D	1407	1	-	2/12/54/54	-
2	HEM	E	1407	1	-	2/12/54/54	-
2	HEM	C	1407	1	-	2/12/54/54	-
2	HEM	L	1407	1	-	2/12/54/54	-

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1407	HEM	C3D-C2D	8.28	1.54	1.36
2	M	1407	HEM	C3D-C2D	8.20	1.54	1.36
2	P	1407	HEM	C3D-C2D	7.88	1.53	1.36
2	C	1407	HEM	C3D-C2D	7.85	1.53	1.36
2	O	1407	HEM	C3D-C2D	7.73	1.53	1.36

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1407	HEM	C4D-ND-C1D	6.02	111.29	105.07
2	P	1407	HEM	C4D-ND-C1D	5.95	111.21	105.07
2	A	1407	HEM	C4D-ND-C1D	5.64	110.89	105.07
2	O	1407	HEM	C4D-ND-C1D	5.63	110.89	105.07
2	F	1407	HEM	C4D-ND-C1D	5.33	110.58	105.07

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	1407	HEM	C2B-C3B-CAB-CBB
2	J	1407	HEM	C4B-C3B-CAB-CBB
2	P	1407	HEM	C2B-C3B-CAB-CBB
2	P	1407	HEM	C4B-C3B-CAB-CBB
4	C	1410	17Q	C7-C8-O-C9

All (2) ring outliers are listed below:

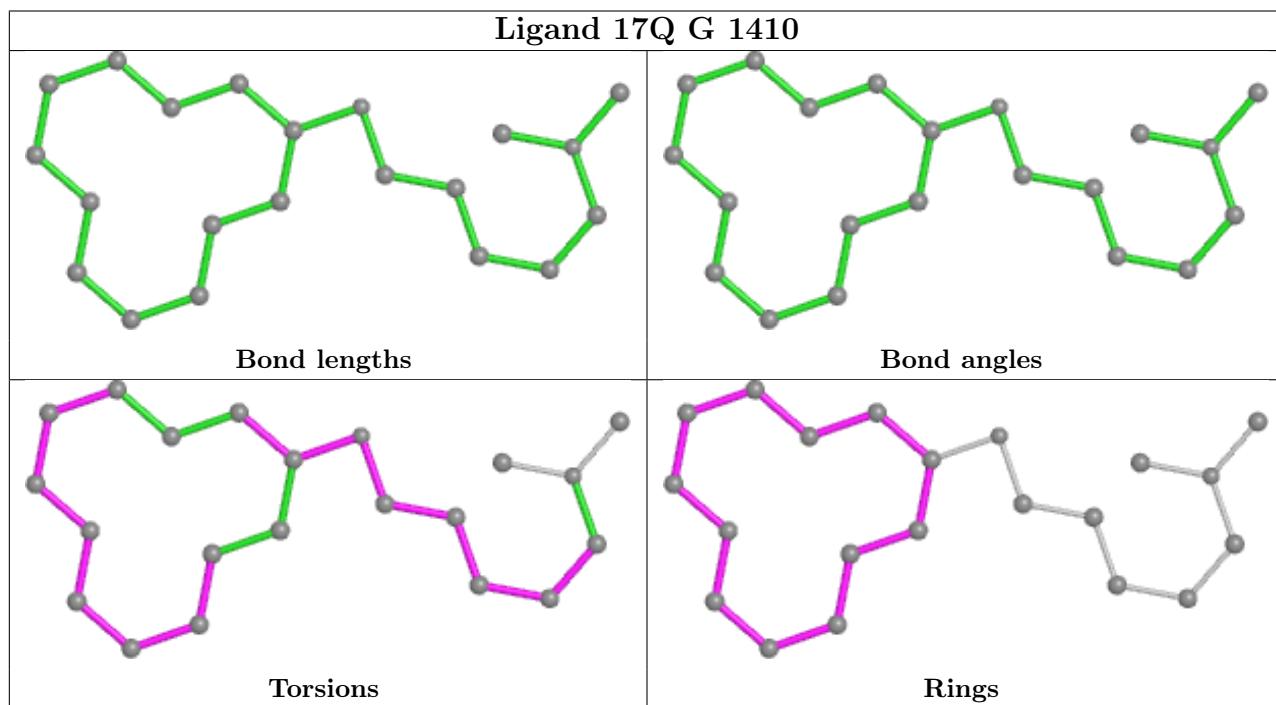
Mol	Chain	Res	Type	Atoms
4	C	1410	17Q	C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8
4	G	1410	17Q	C1-C16-C17-C18-C19-C2-C3-C4-C5-C6-C7-C8

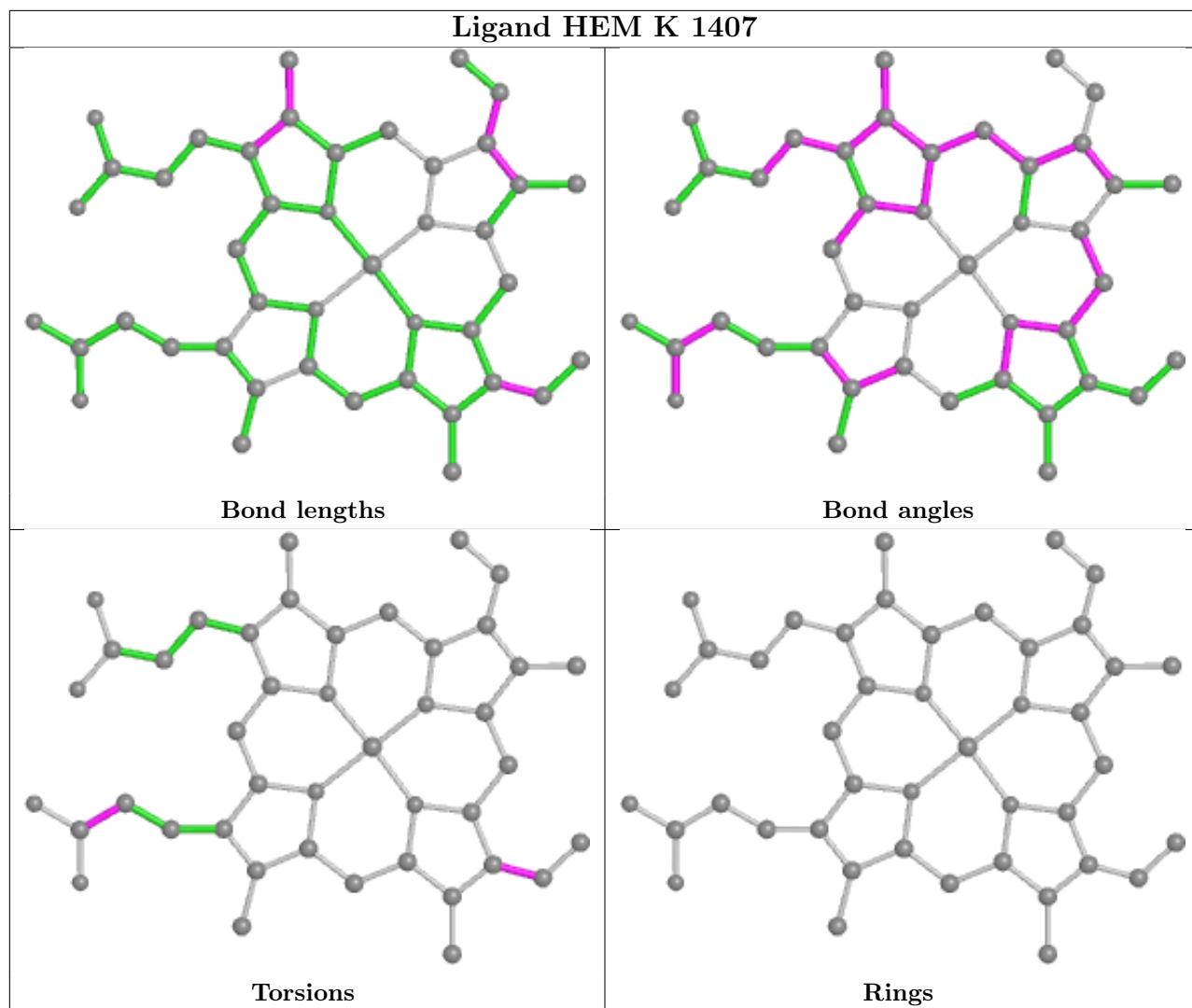
22 monomers are involved in 94 short contacts:

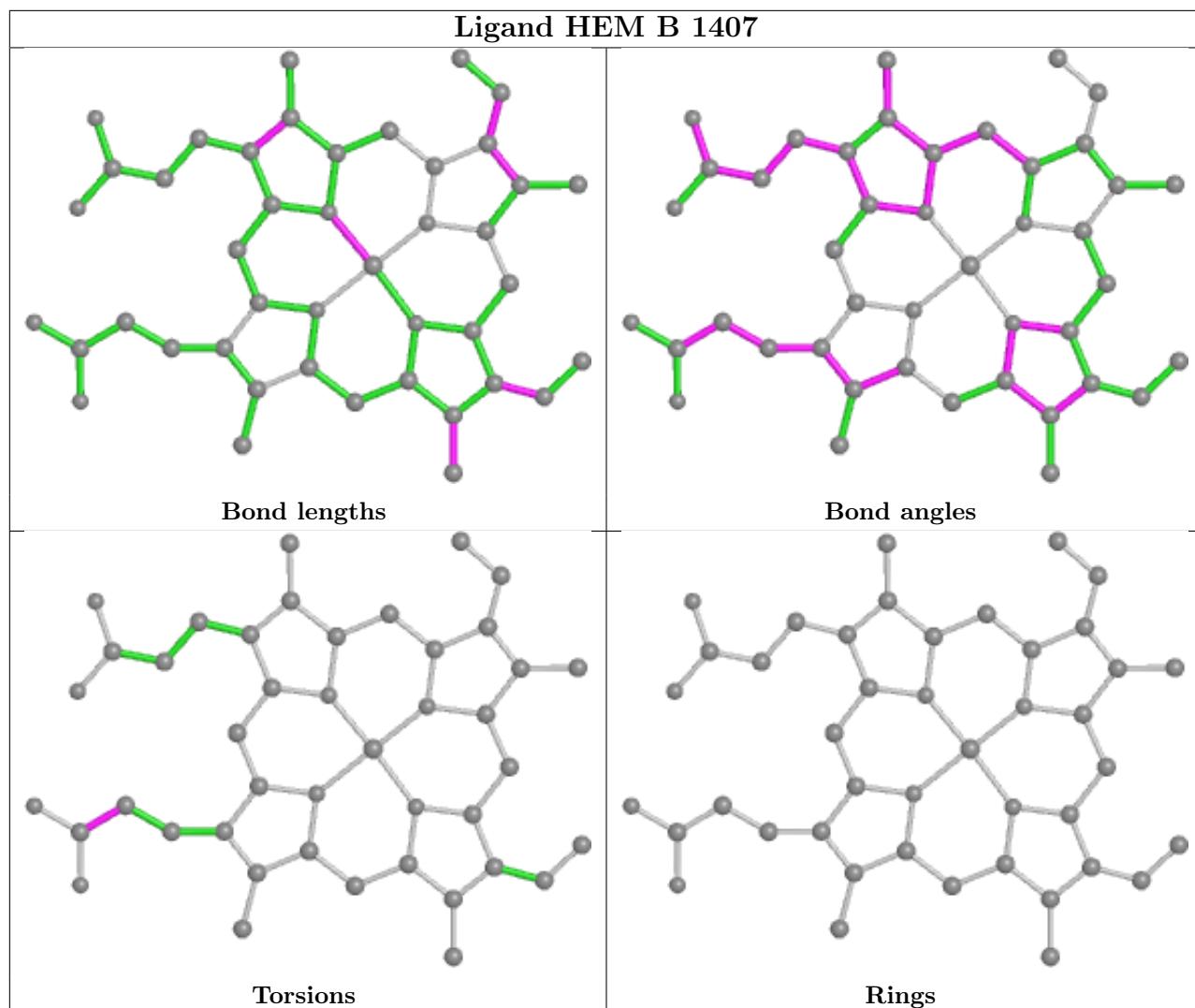
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1410	17Q	5	0
3	A	1408	SO4	2	0
2	K	1407	HEM	3	0
2	B	1407	HEM	6	0
2	H	1407	HEM	7	0
2	A	1407	HEM	1	0
4	C	1410	17Q	6	0
2	M	1407	HEM	5	0
2	L	1407	HEM	4	0
2	I	1407	HEM	5	0
2	F	1407	HEM	3	0
2	G	1407	HEM	6	0
2	N	1407	HEM	7	0
2	C	1407	HEM	6	0
3	F	1408	SO4	1	0
2	J	1407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

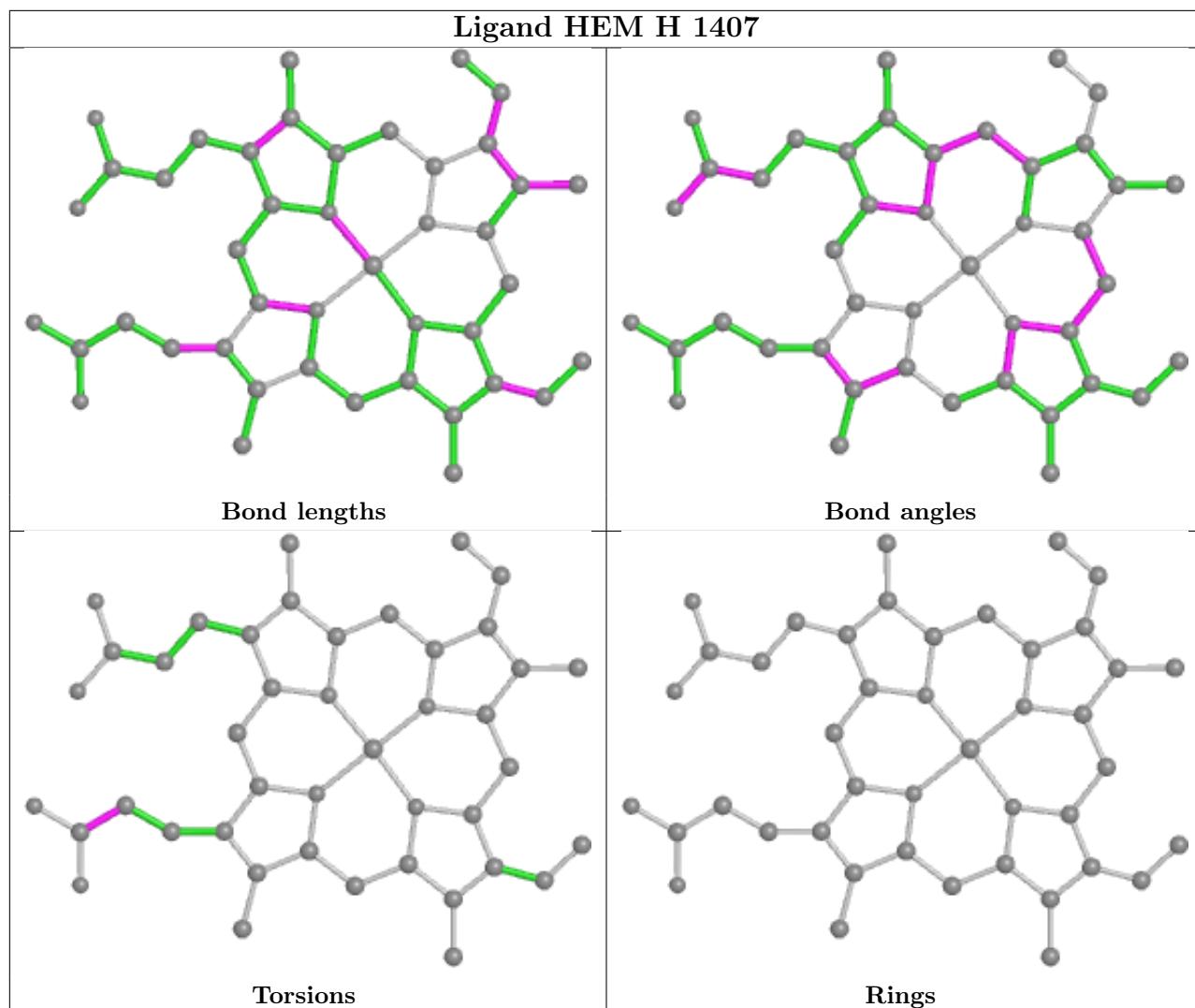
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

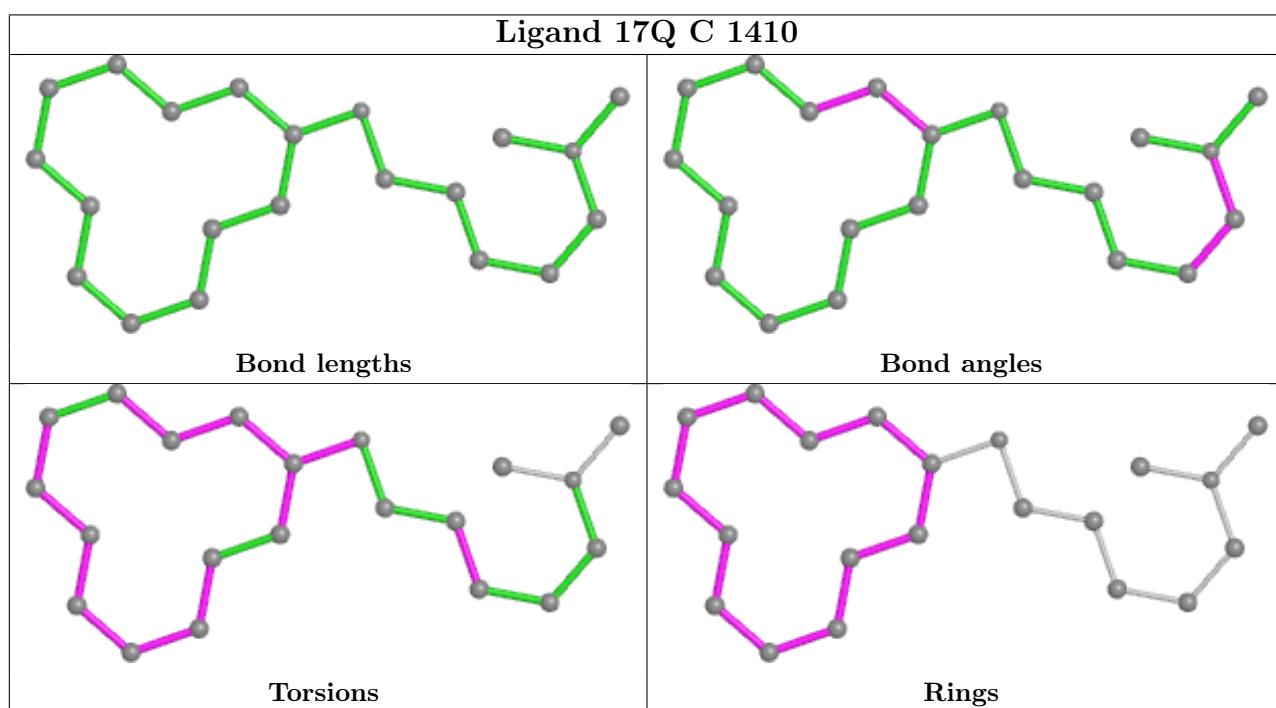
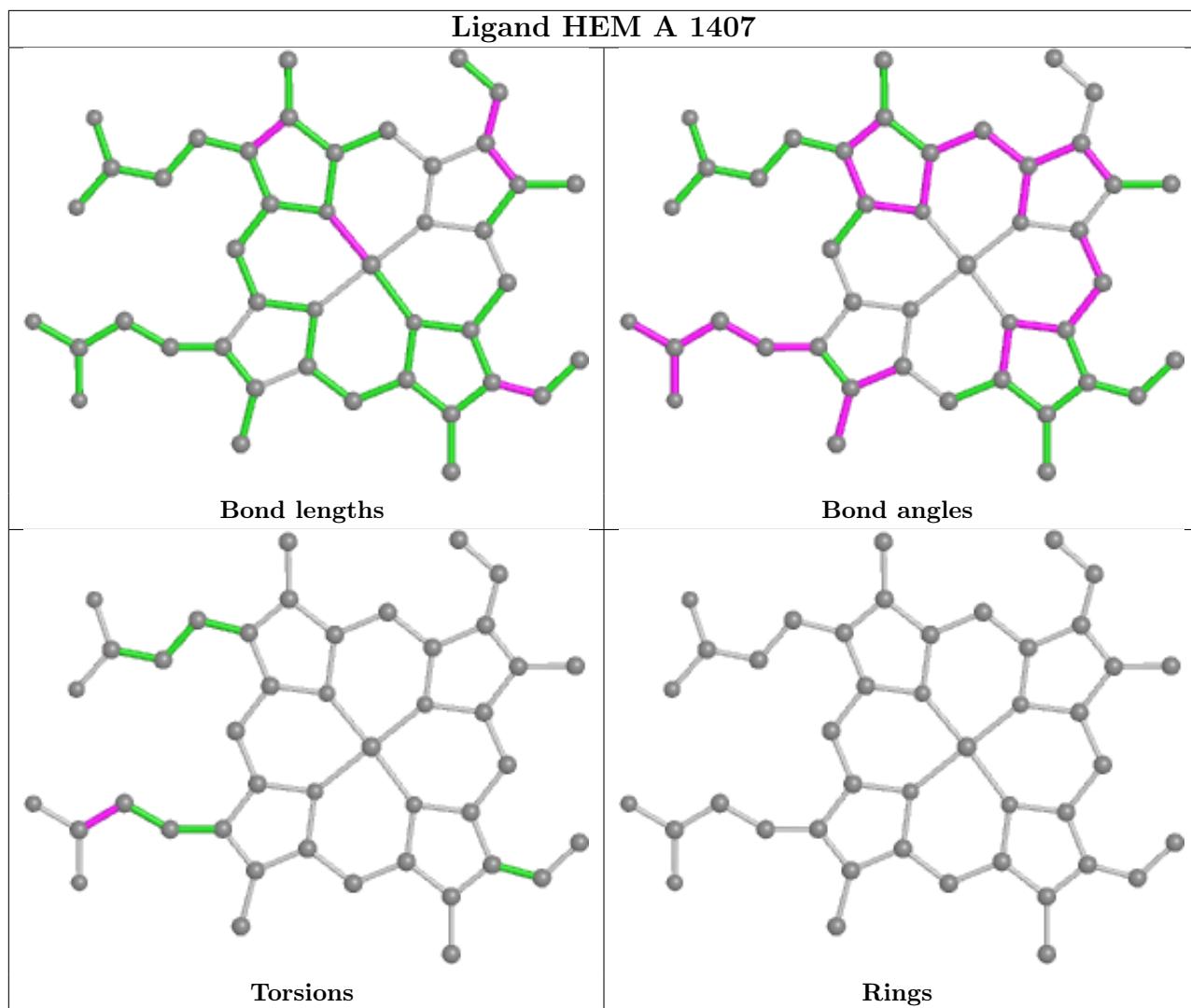
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

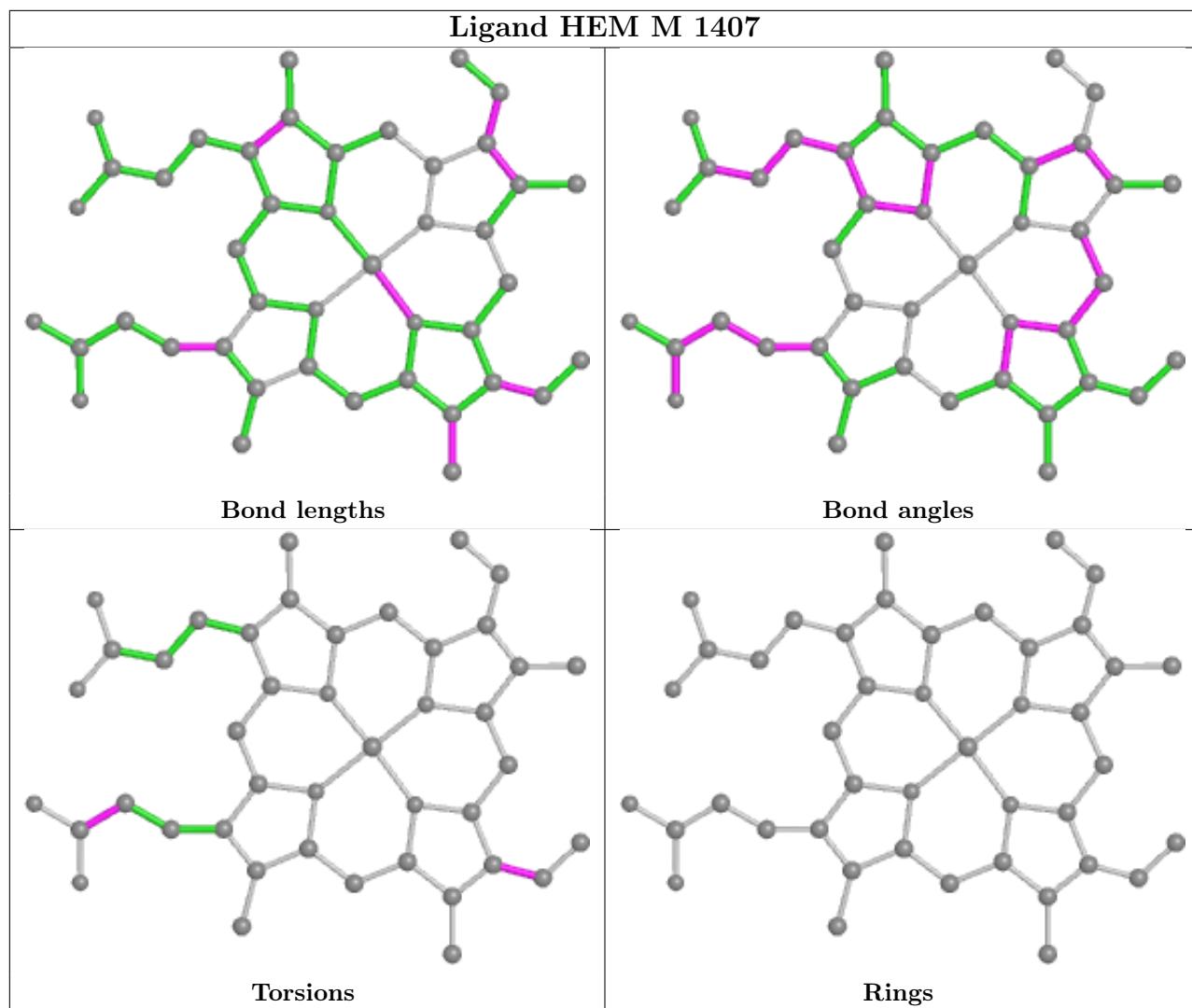


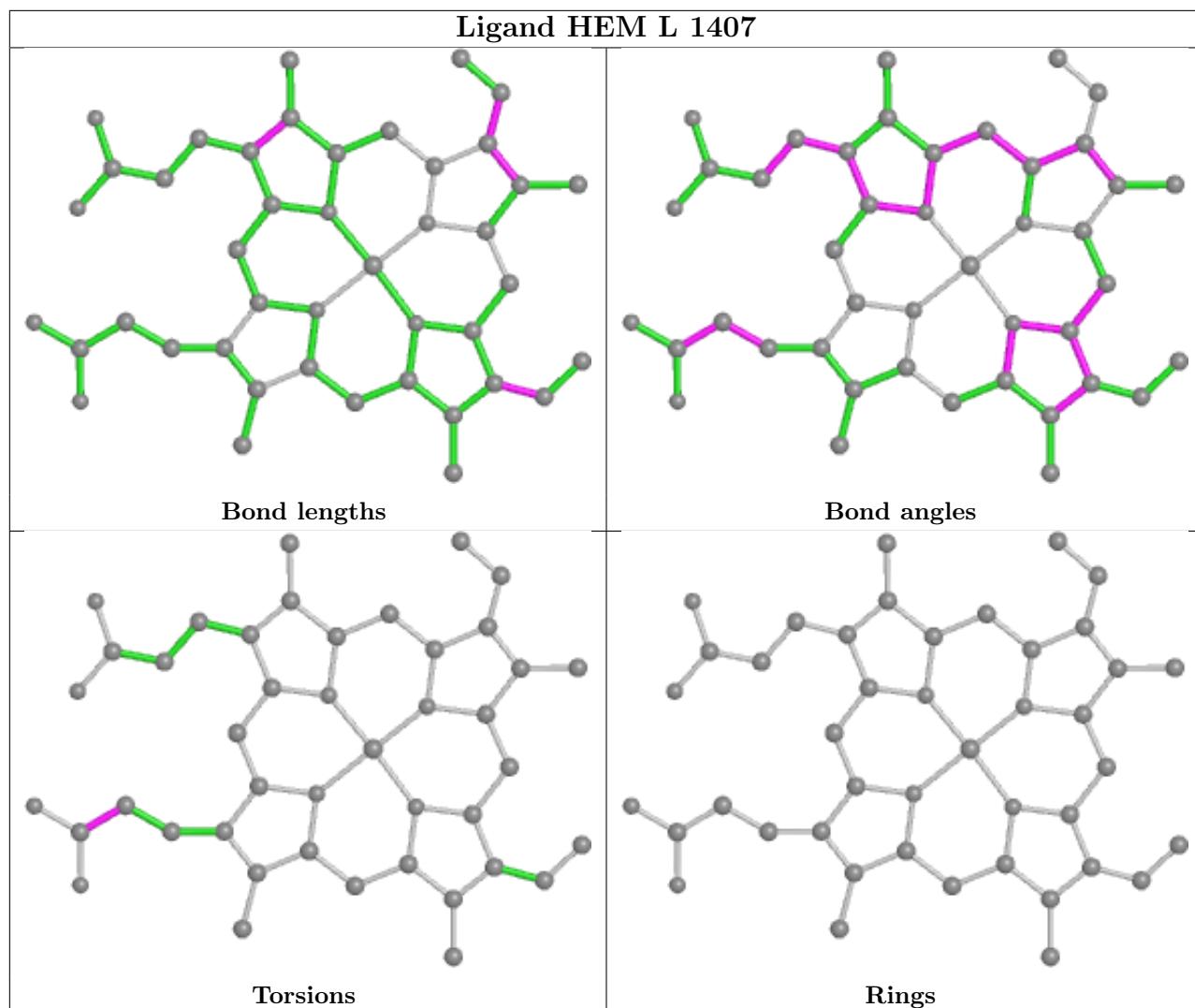


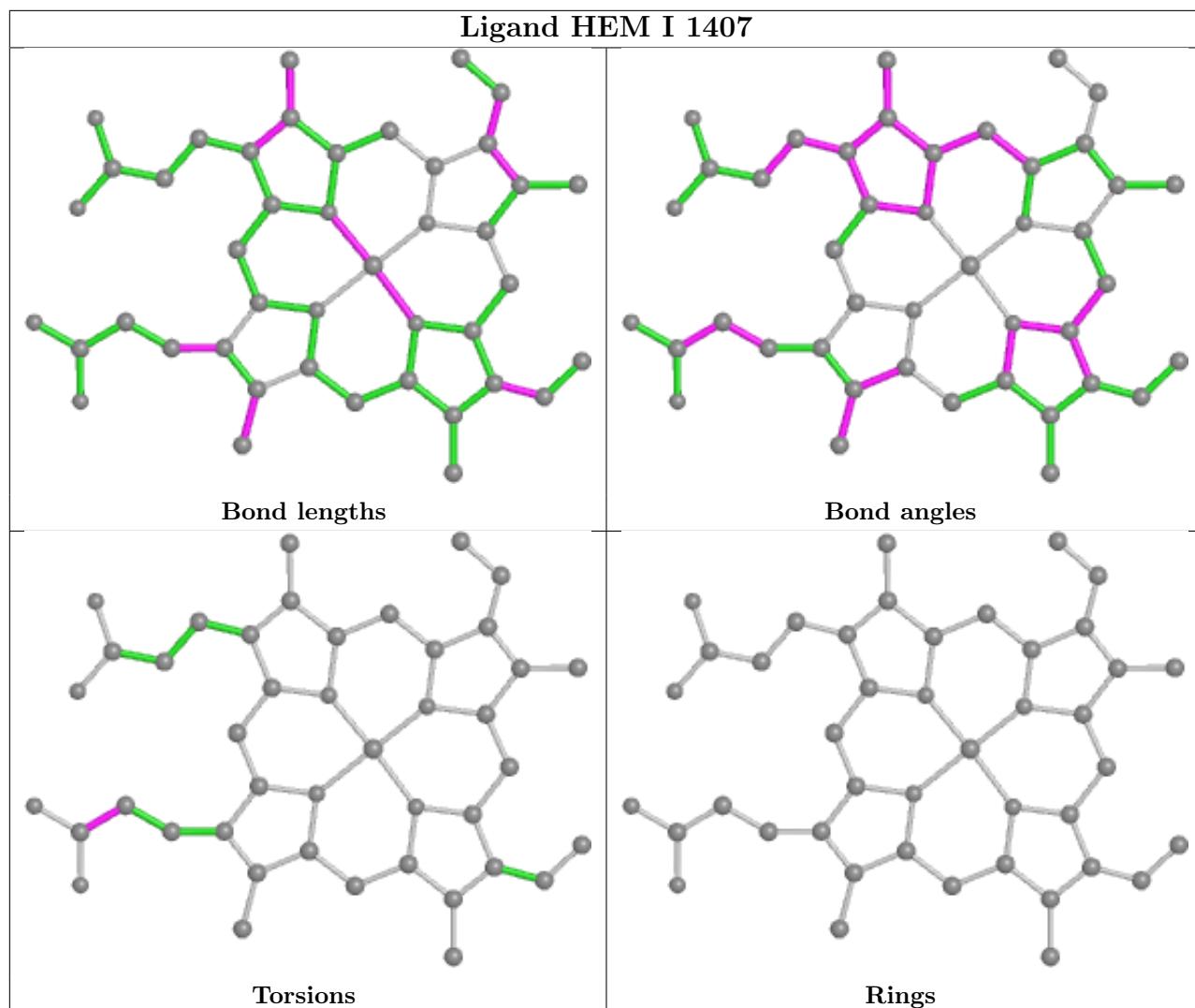


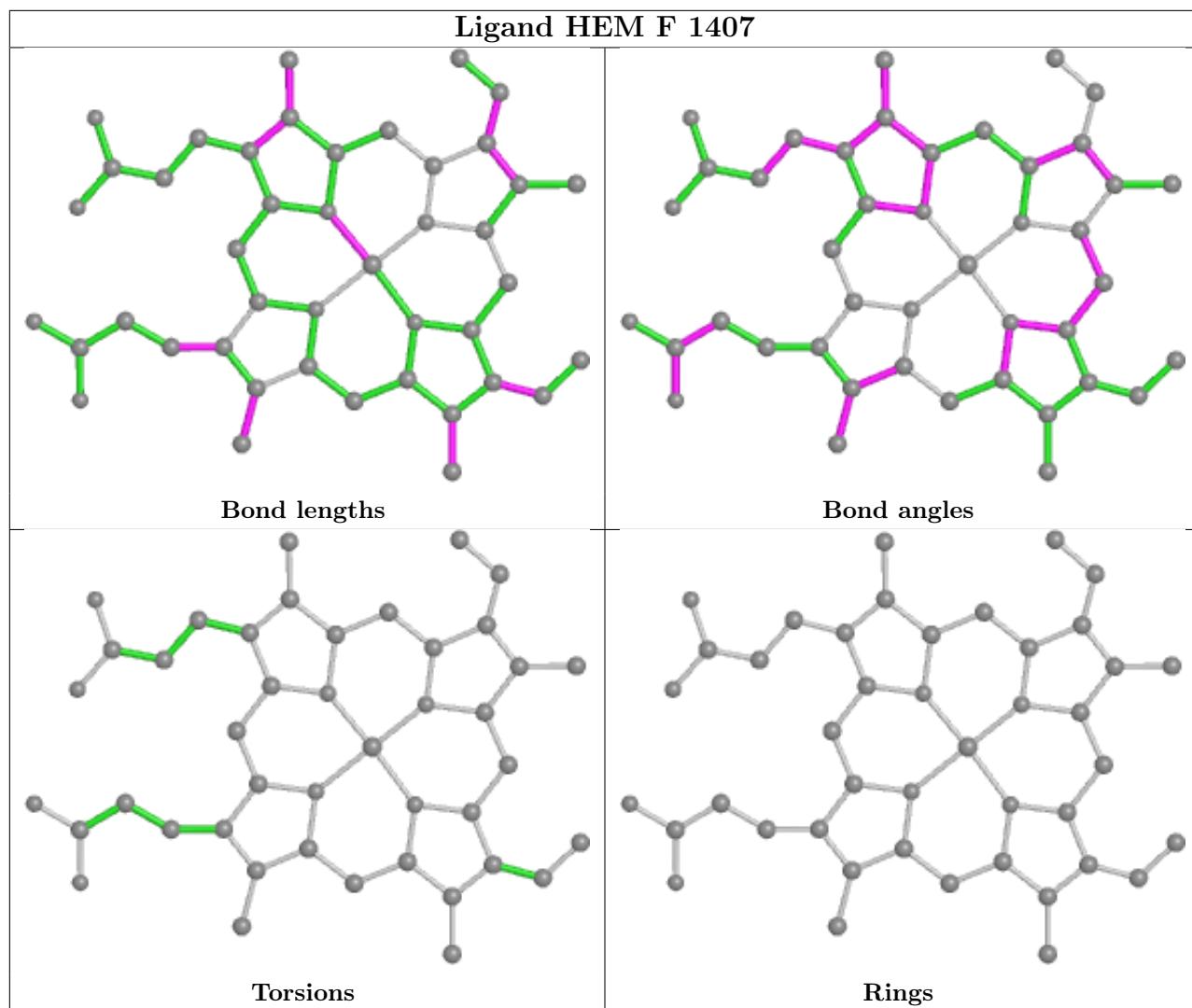


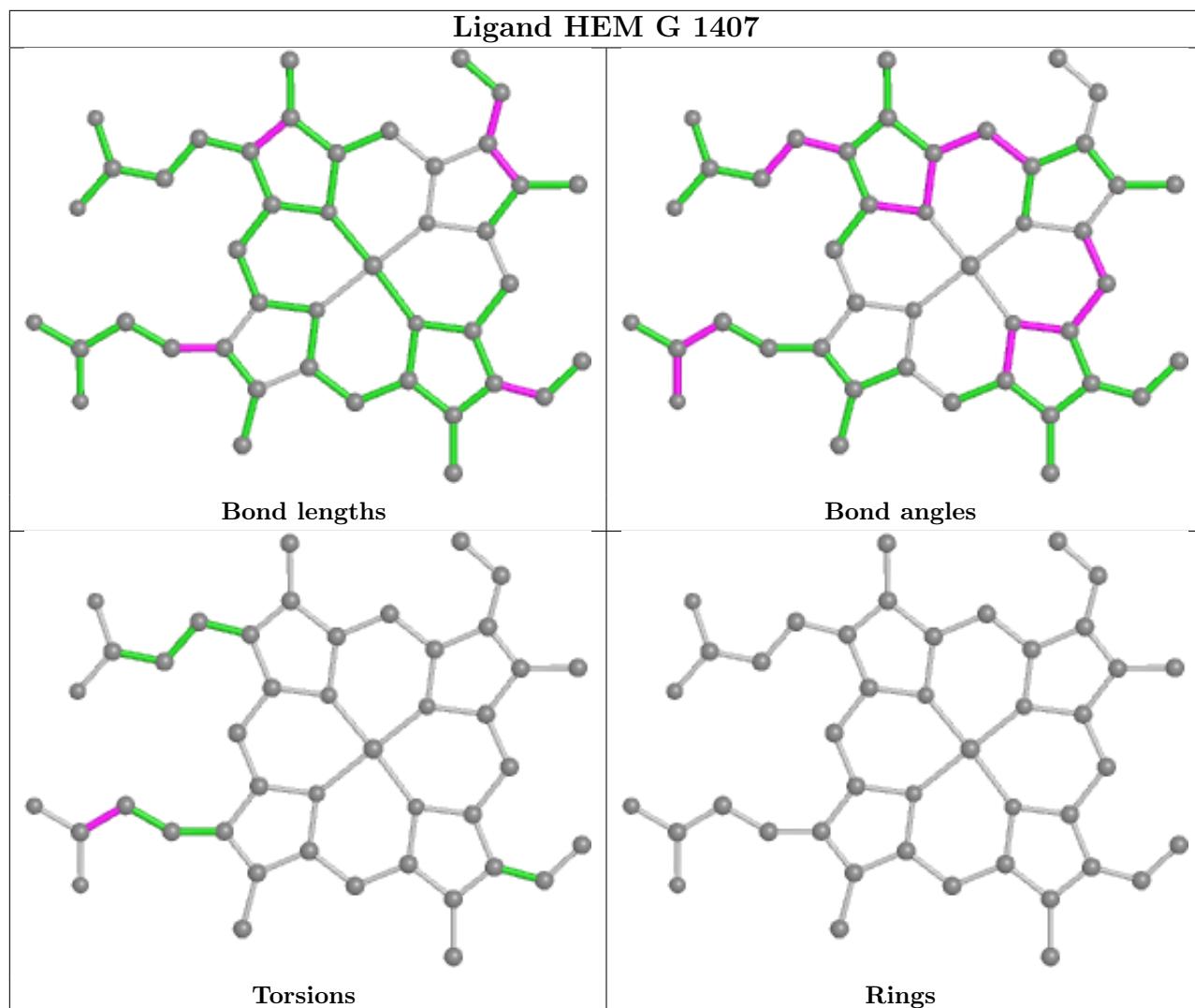


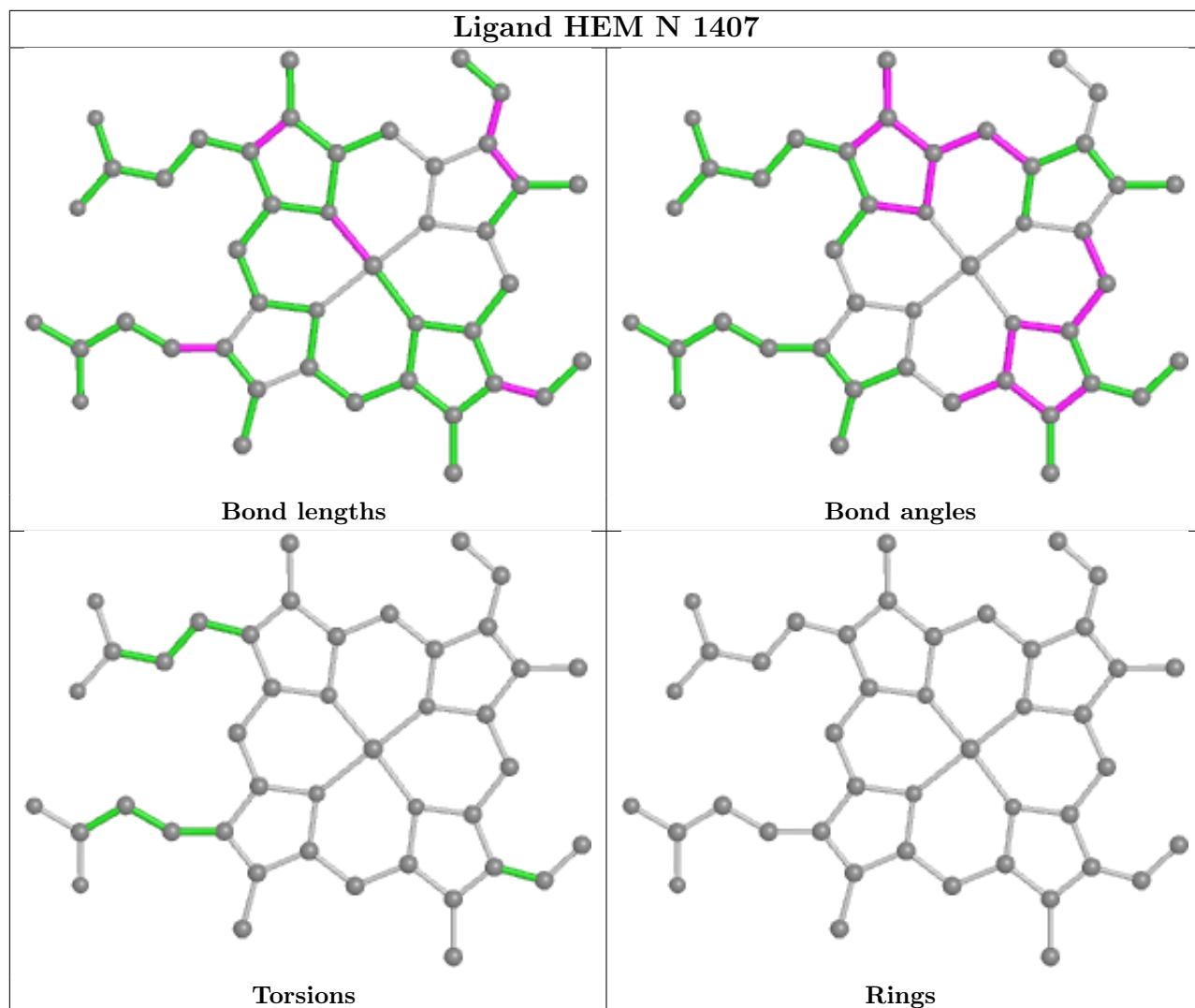


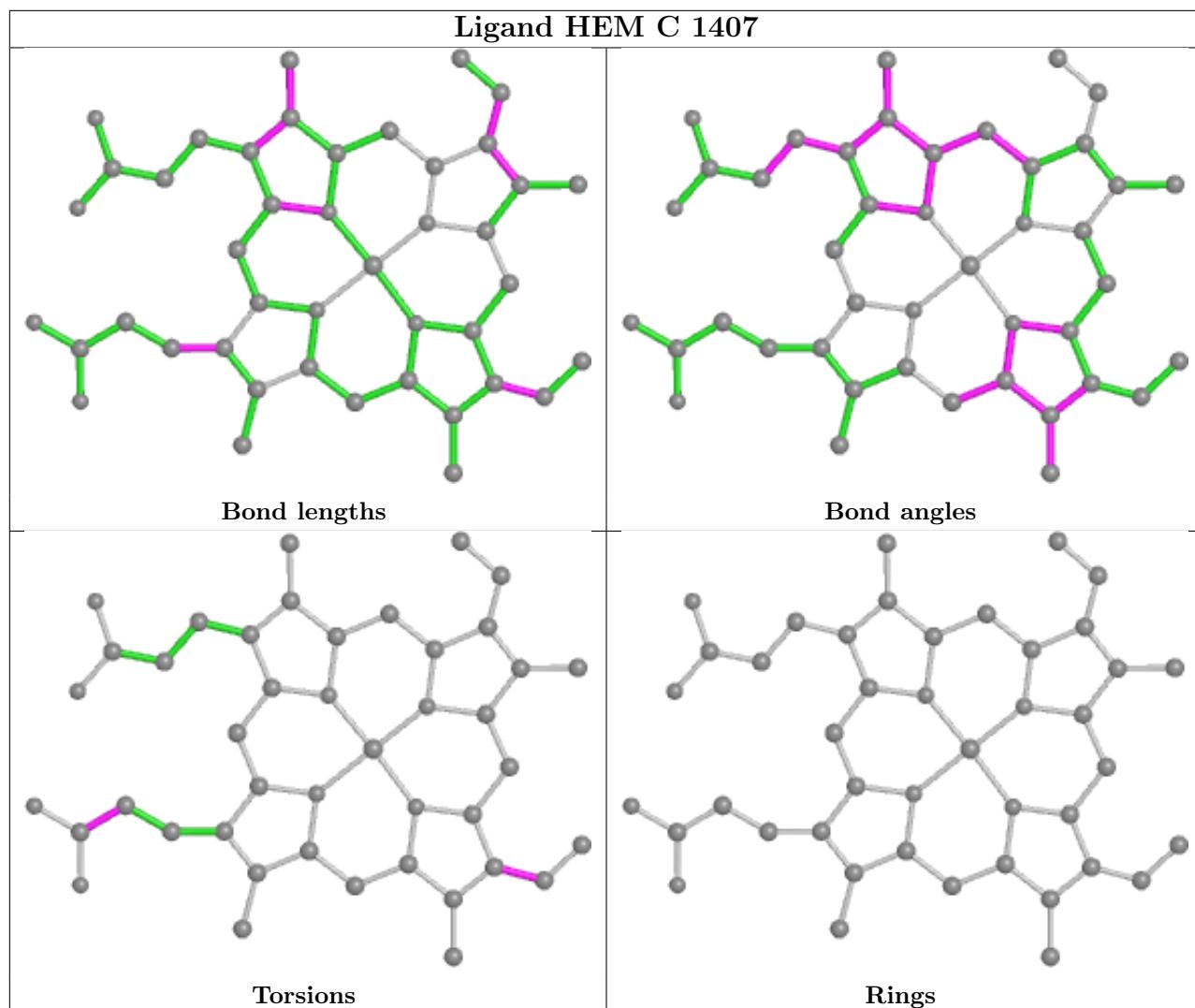


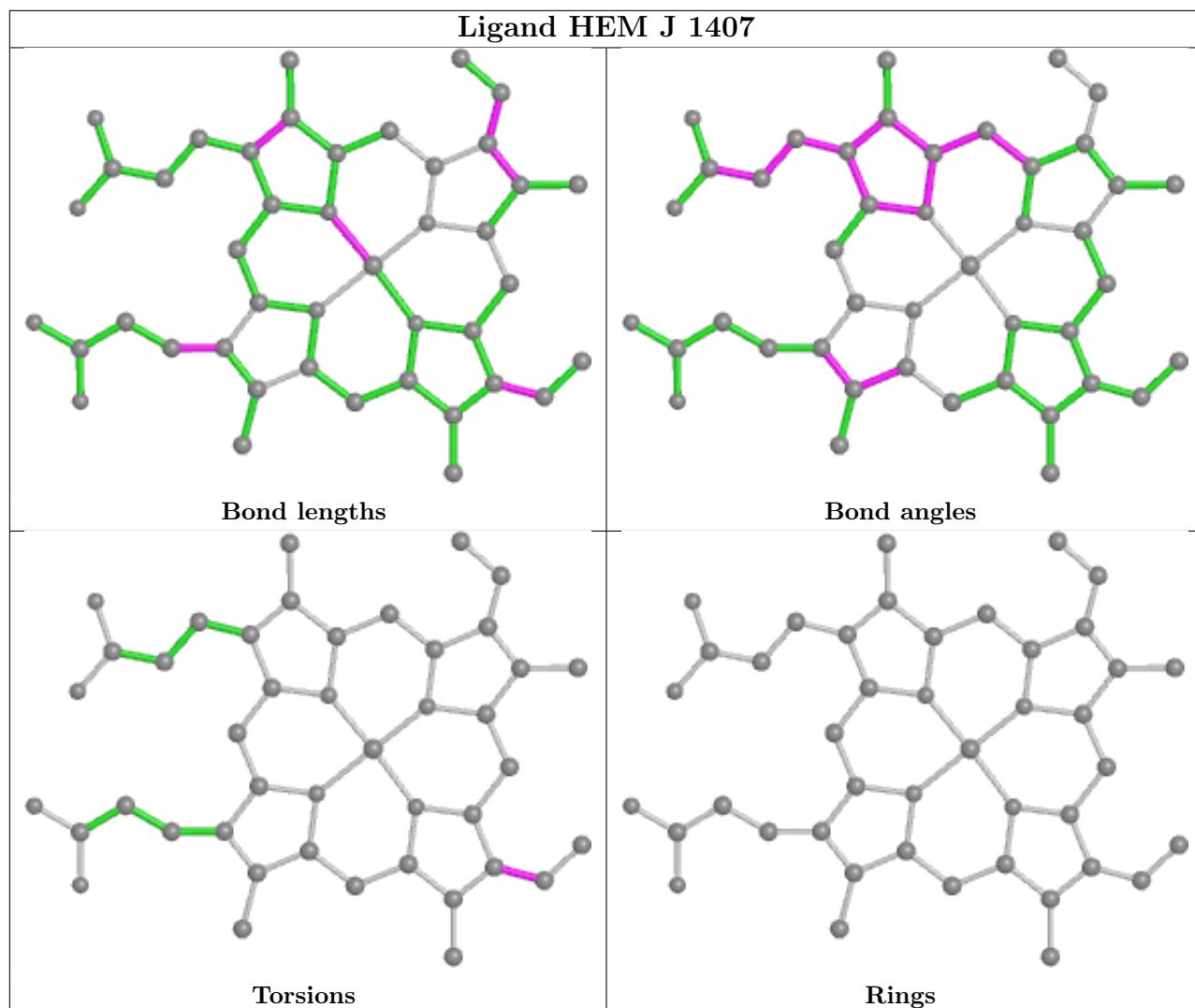


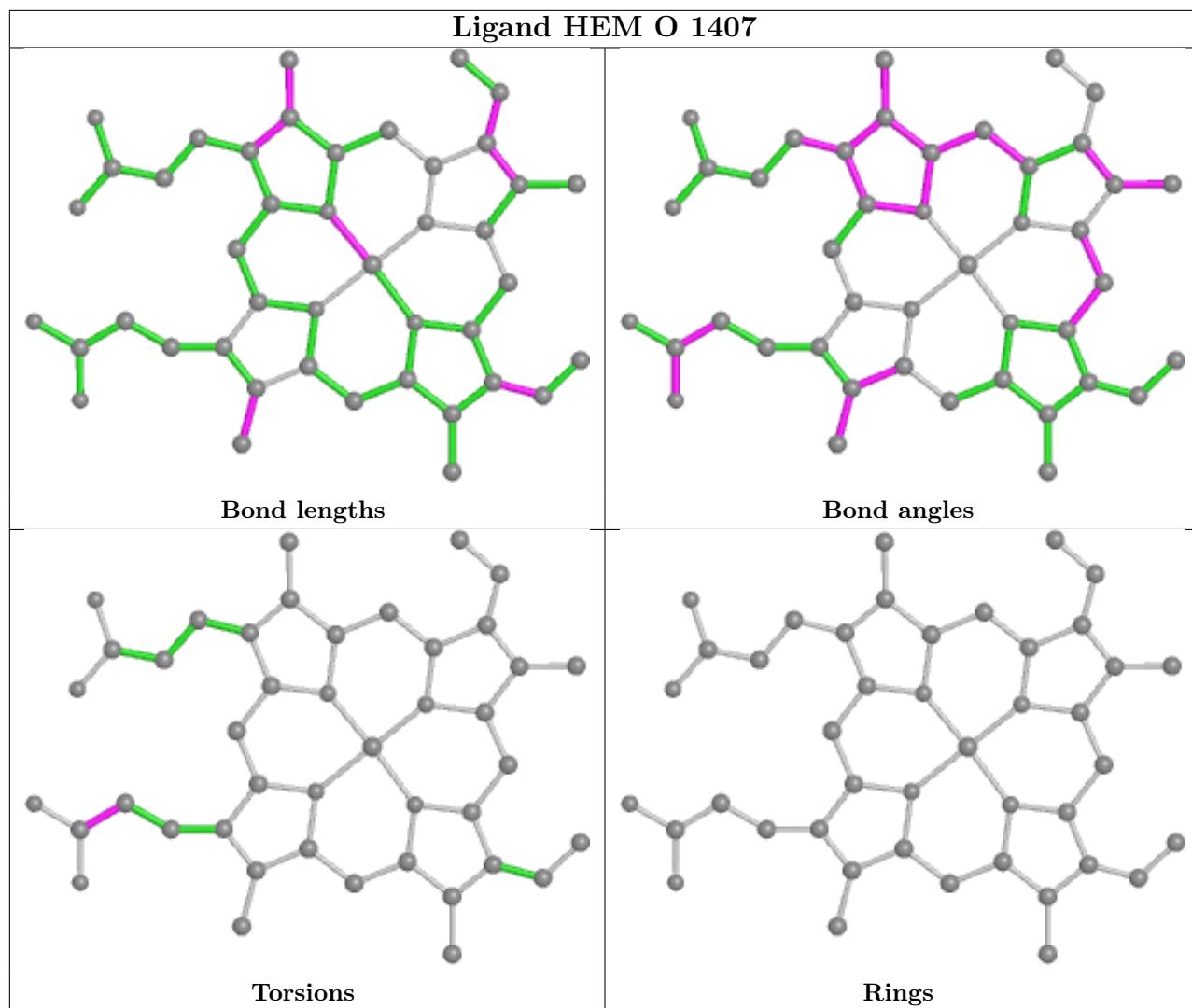


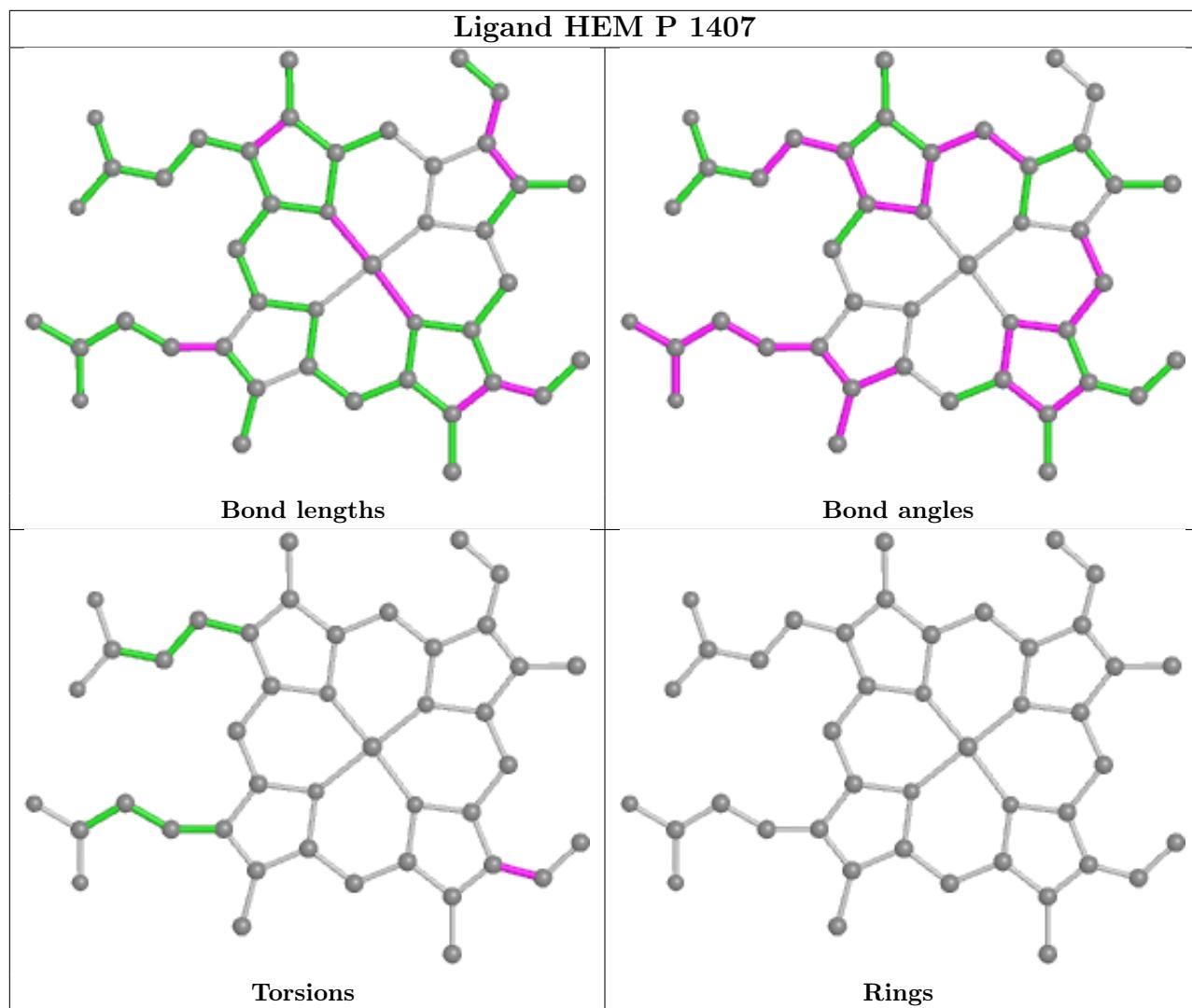


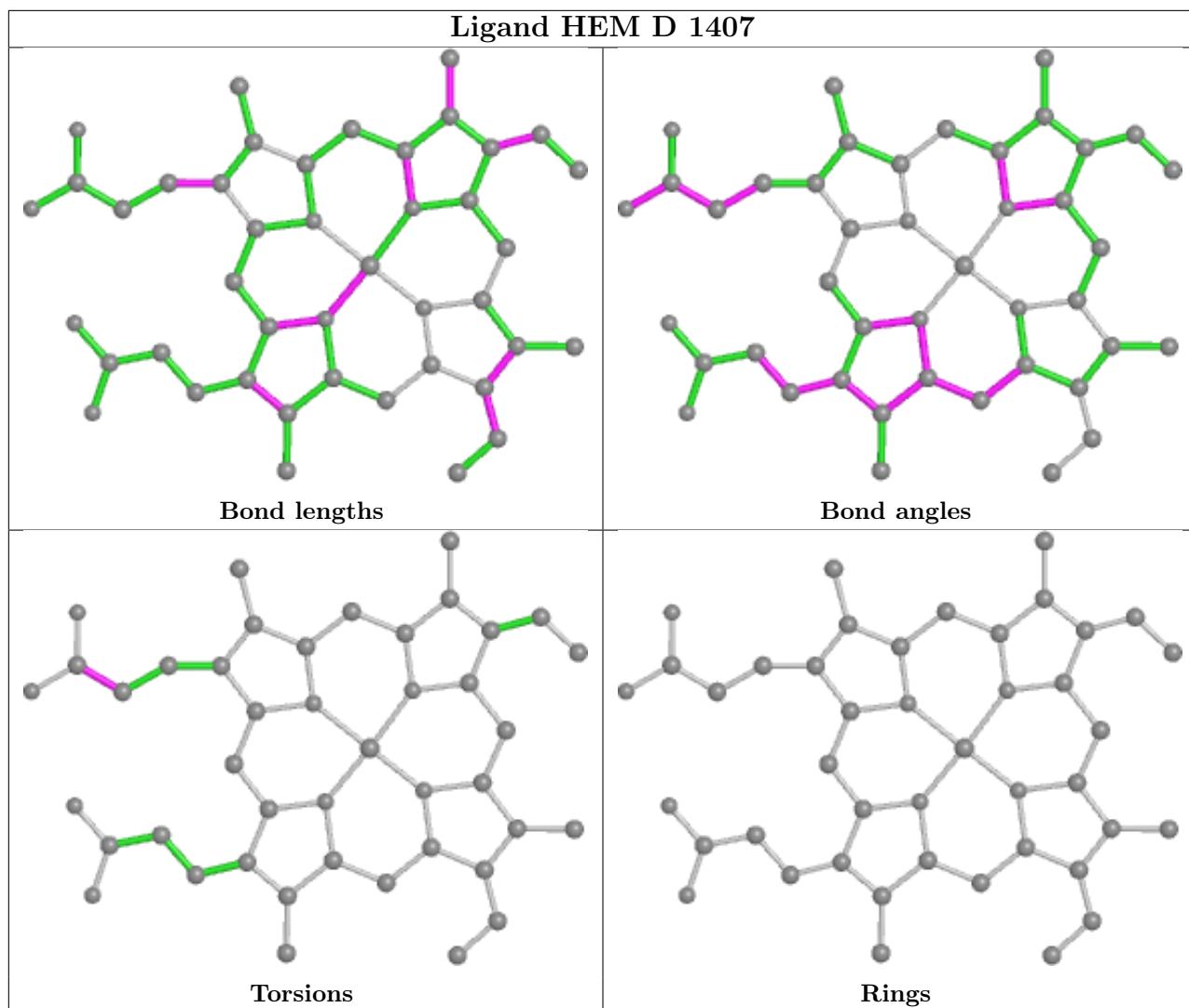


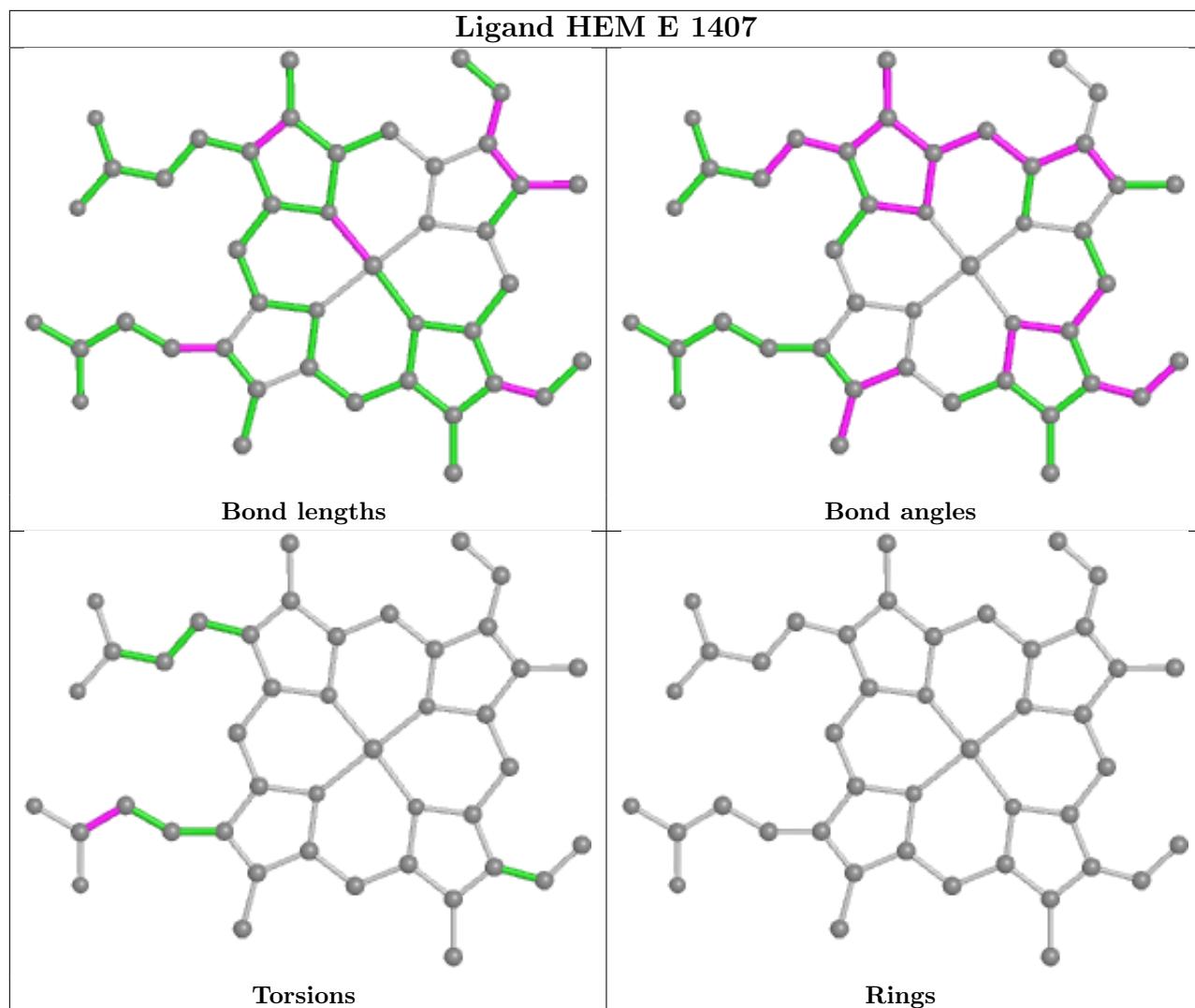












5.7 Other polymers [\(i\)](#)

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%)	-0.56	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, 38, 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 monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

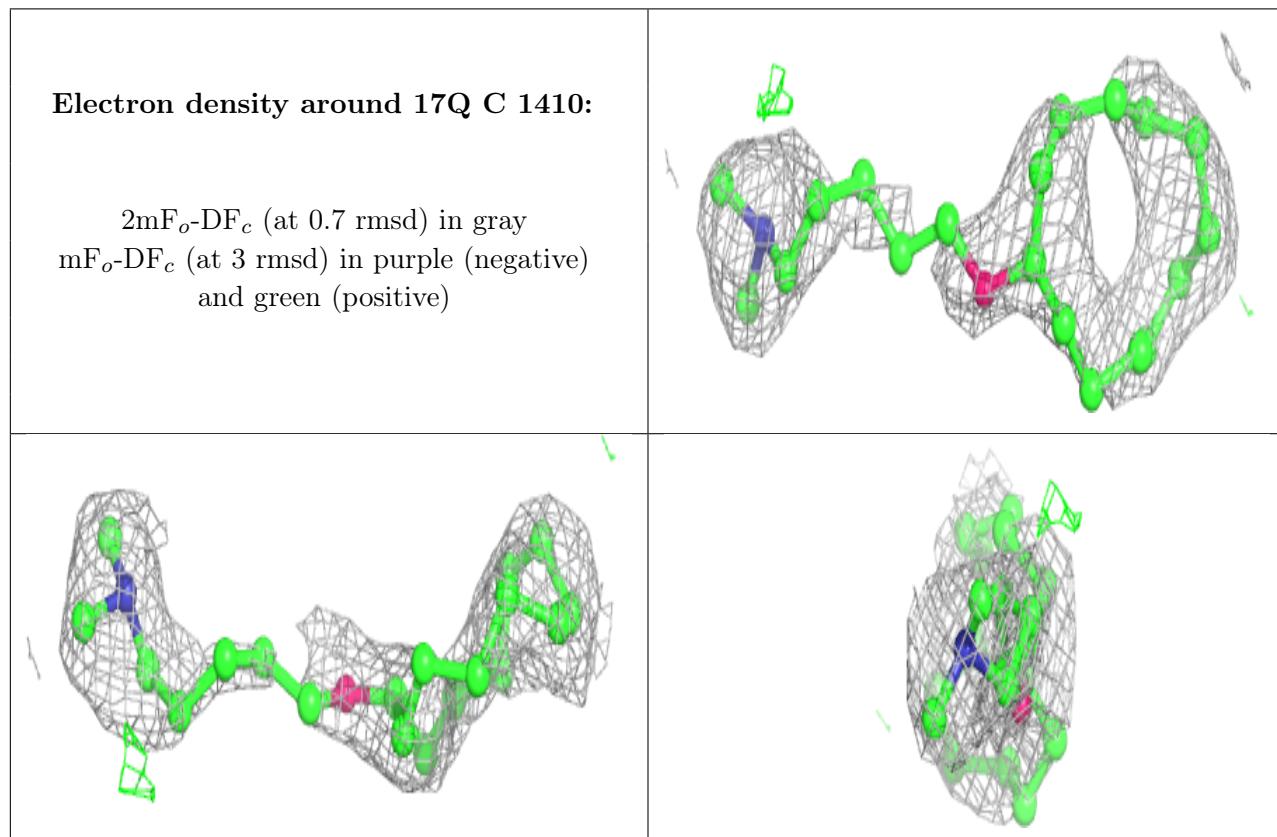
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	17Q	C	1410	21/21	0.86	0.29	53,57,60,60	0
4	17Q	G	1410	21/21	0.90	0.27	39,49,55,55	0
3	SO4	D	1408	5/5	0.91	0.16	37,37,39,40	0
3	SO4	H	1408	5/5	0.95	0.18	42,42,44,45	0
3	SO4	I	1408	5/5	0.95	0.24	39,41,42,43	0
3	SO4	J	1408	5/5	0.95	0.20	41,42,42,43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

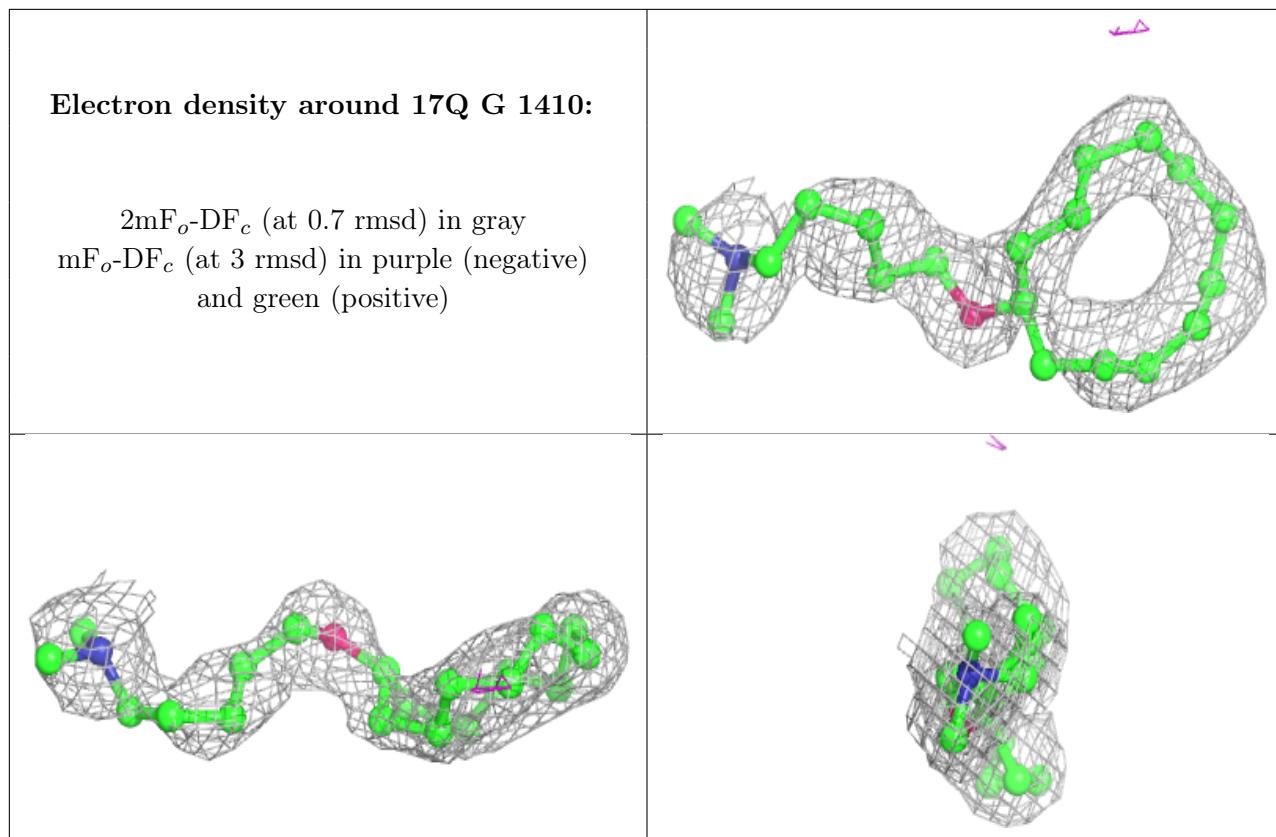
Continued on next page...

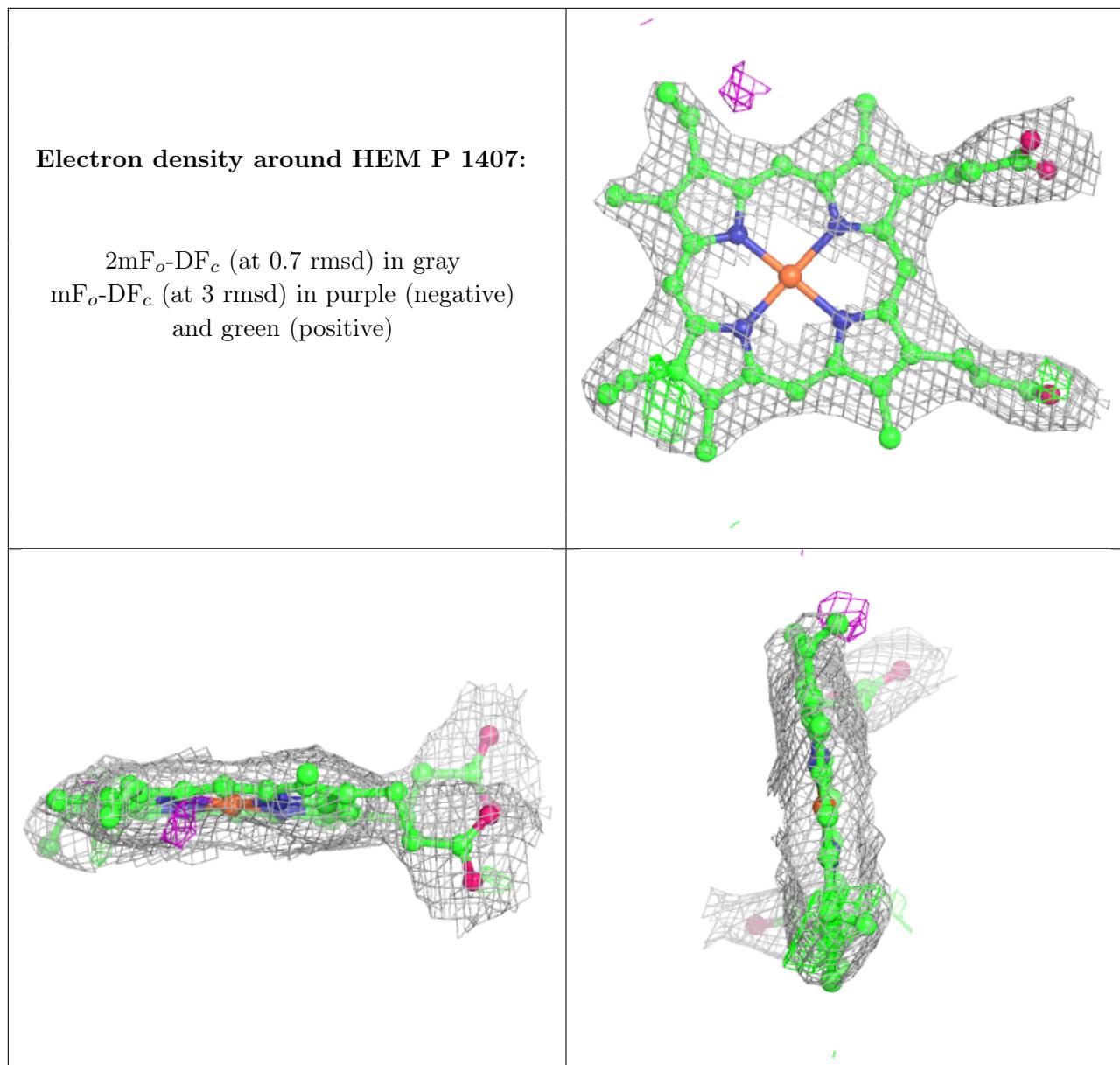
Continued from previous page...

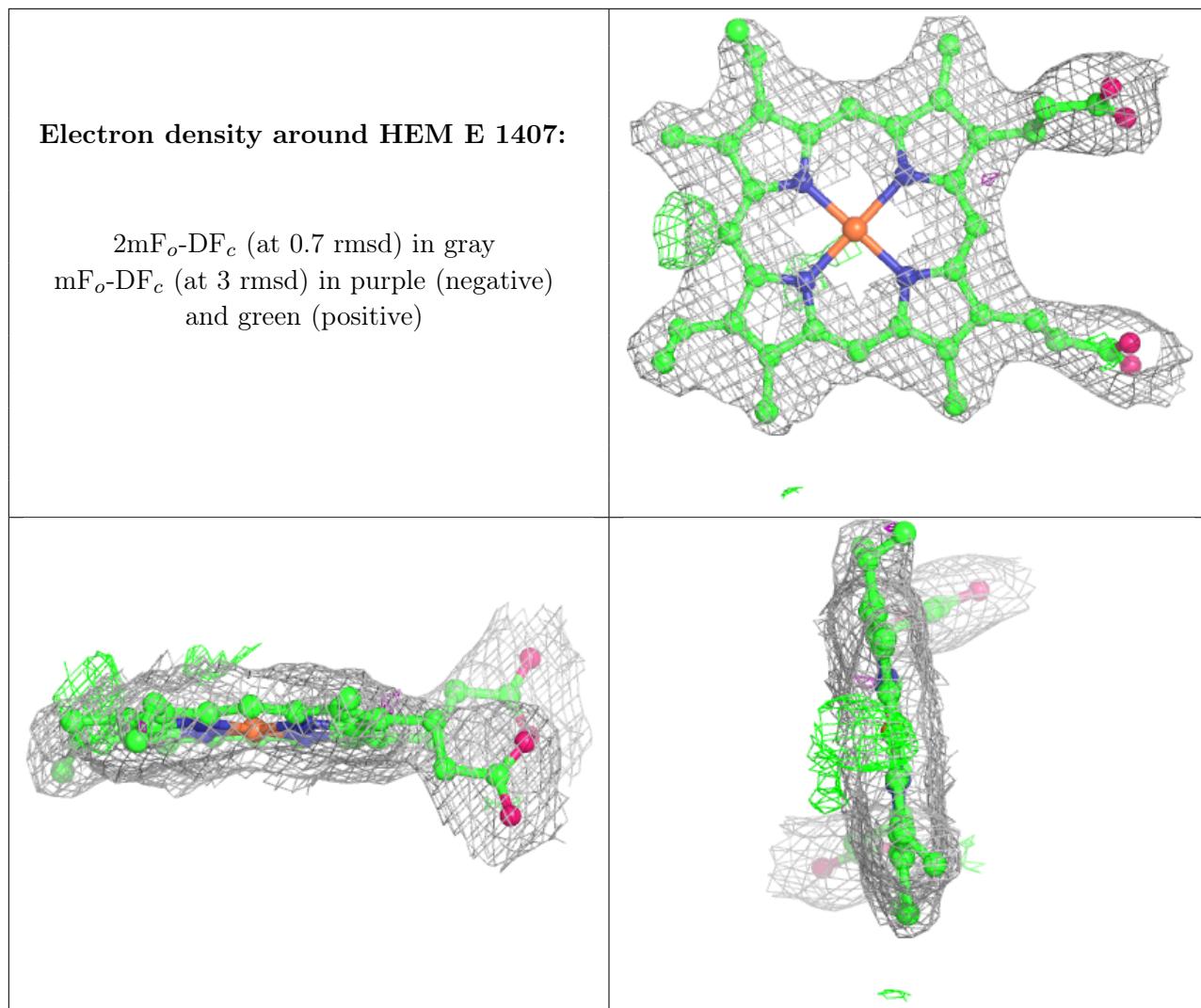
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	I	1409	5/5	0.99	0.05	53,54,55,55	0
2	HEM	C	1407	43/43	0.99	0.14	12,14,19,24	0
2	HEM	A	1407	43/43	0.99	0.12	14,20,24,28	0

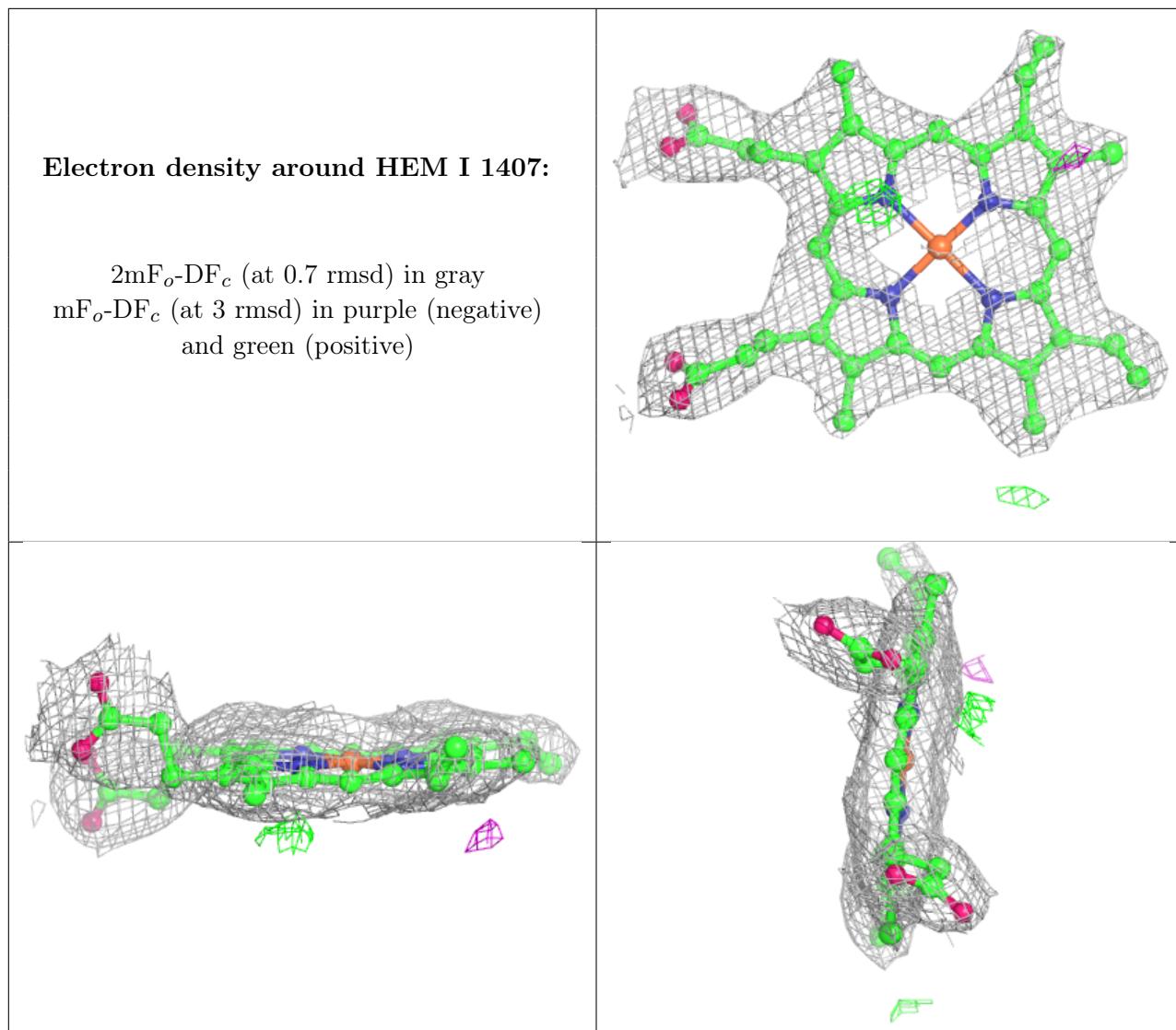
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

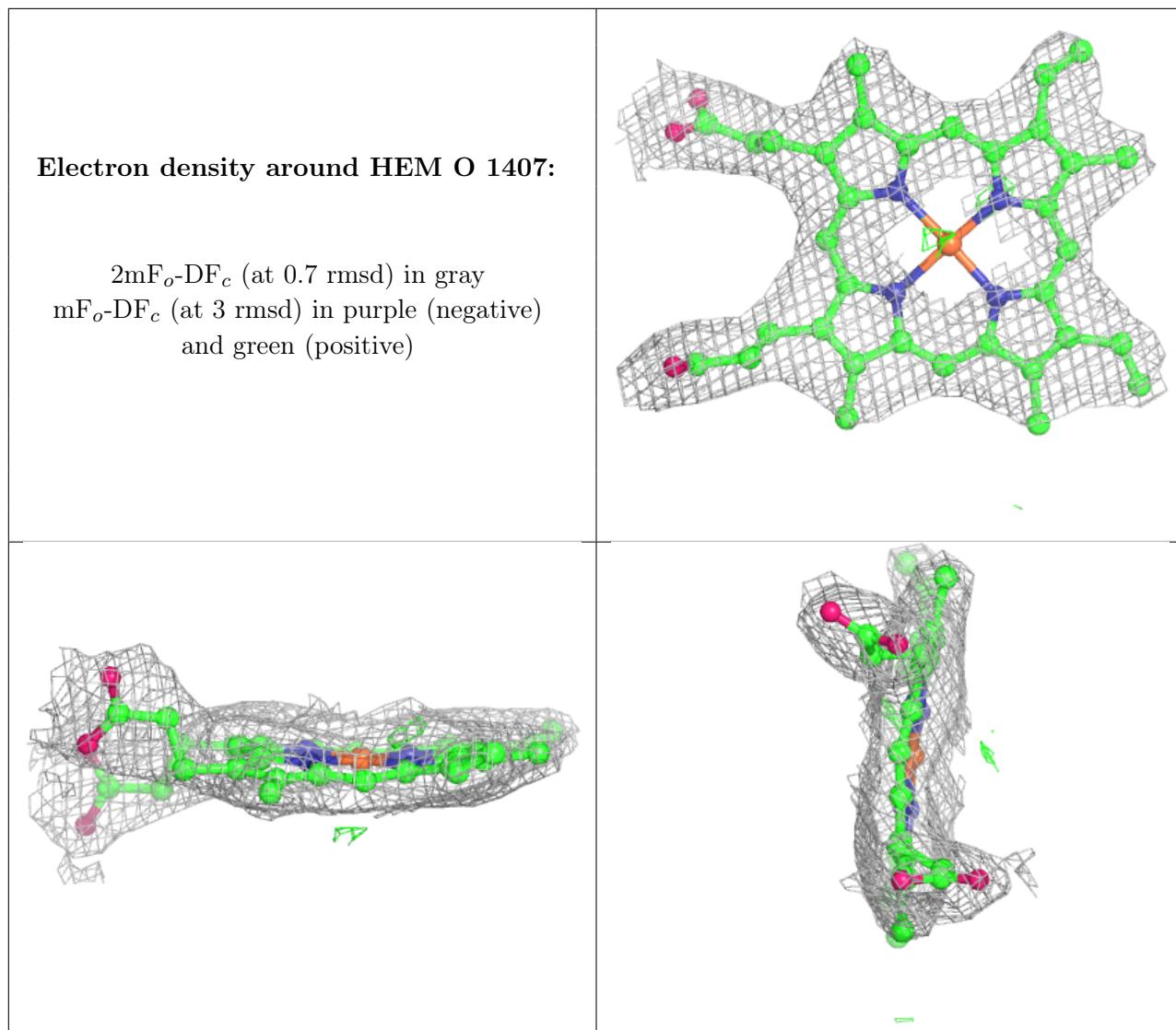


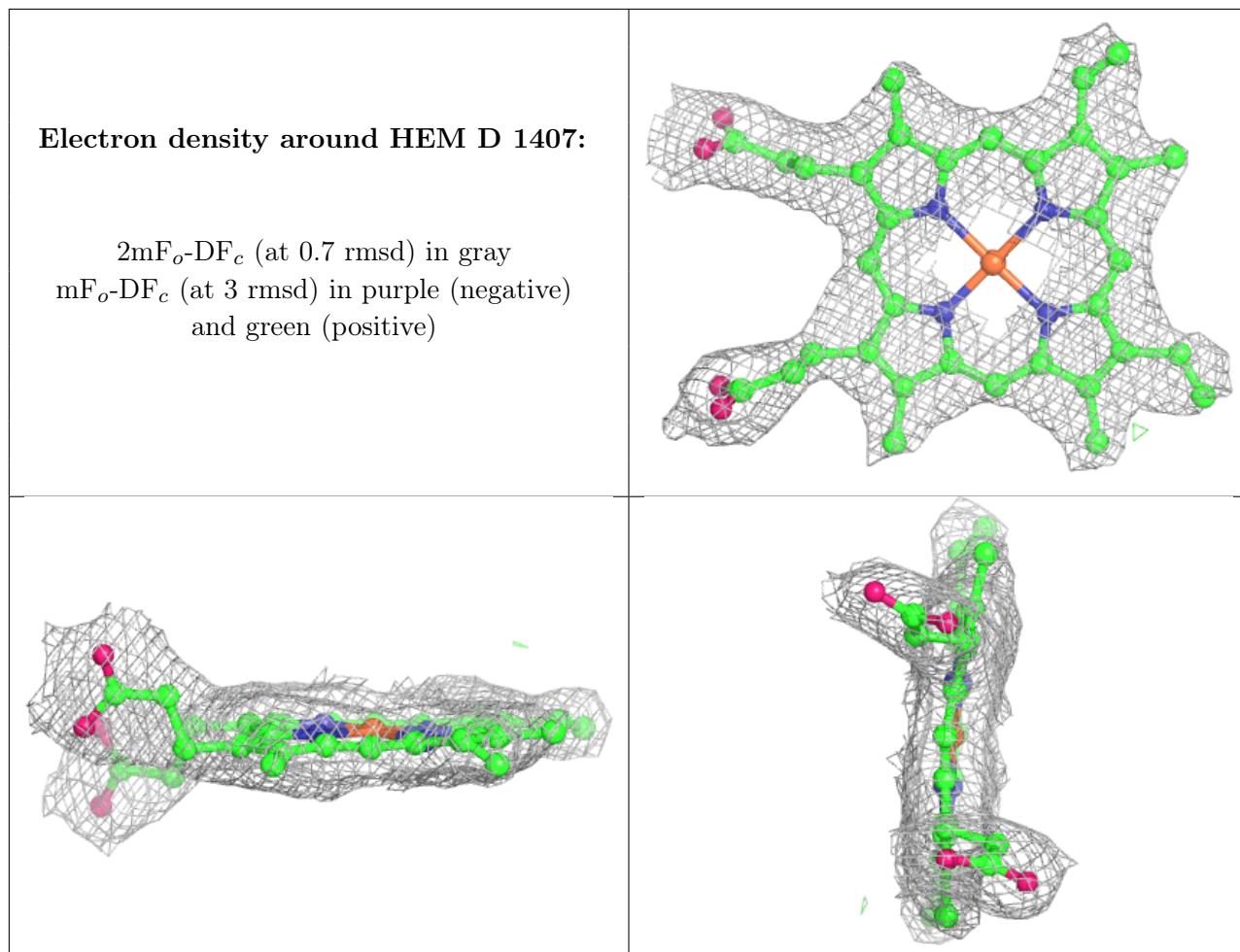


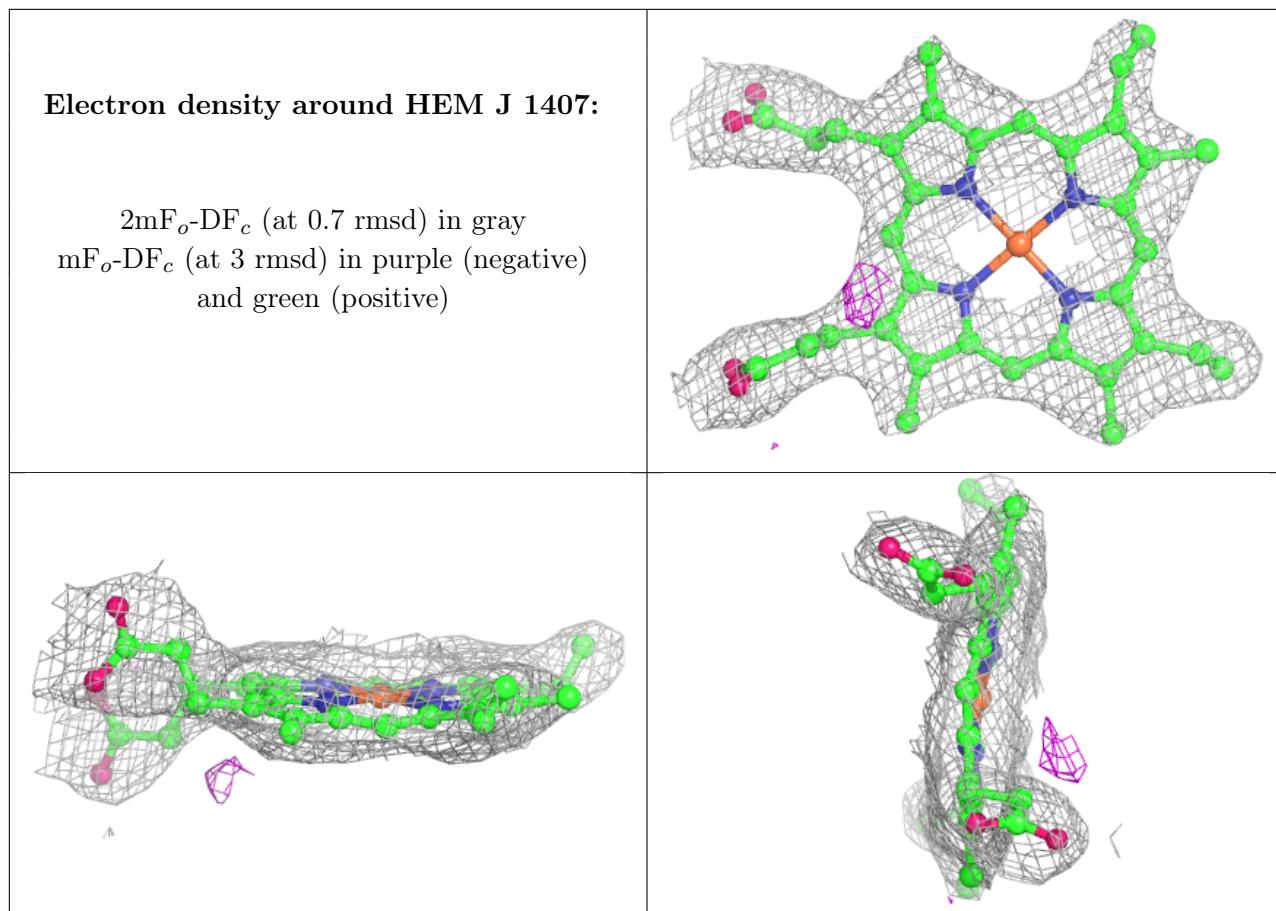


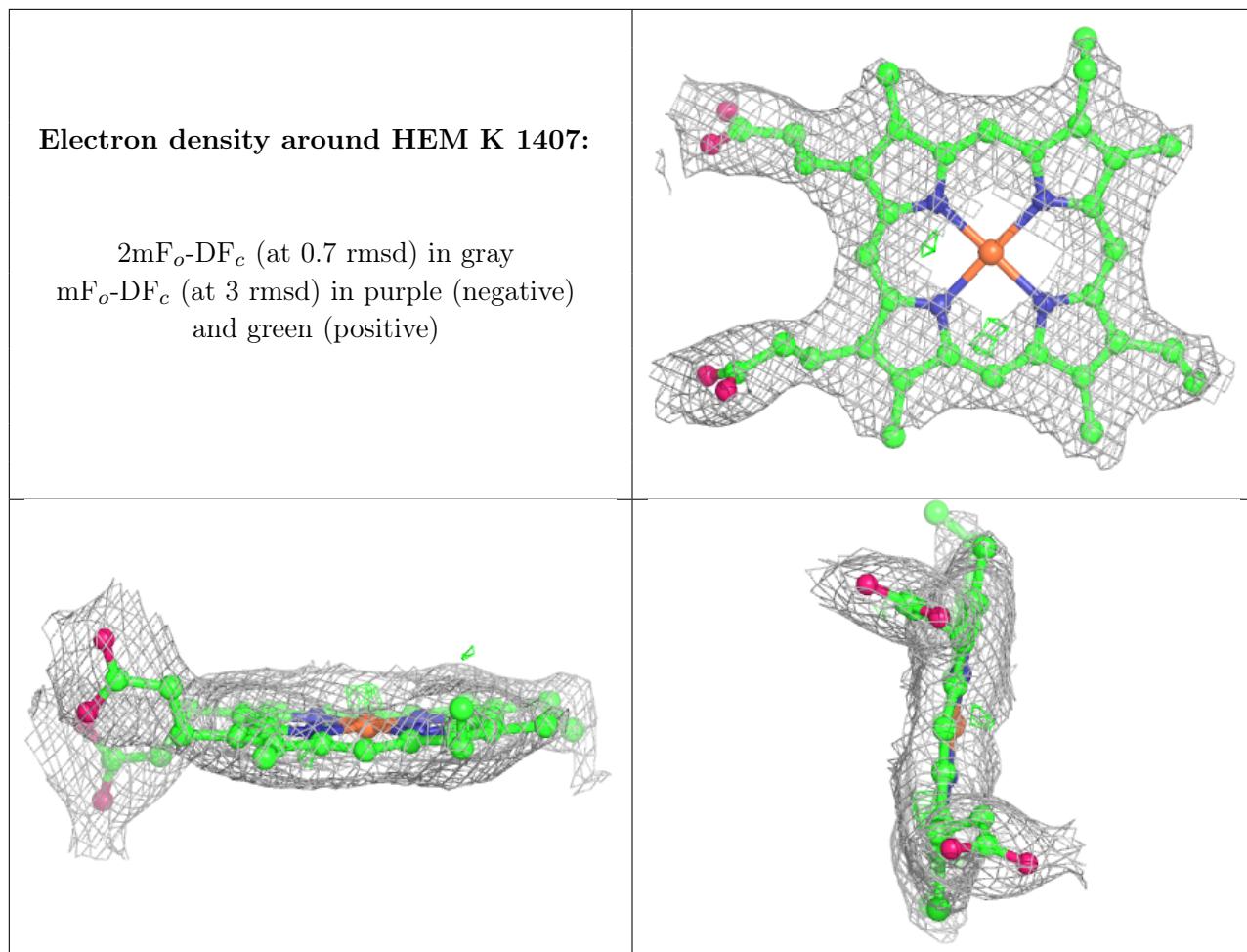


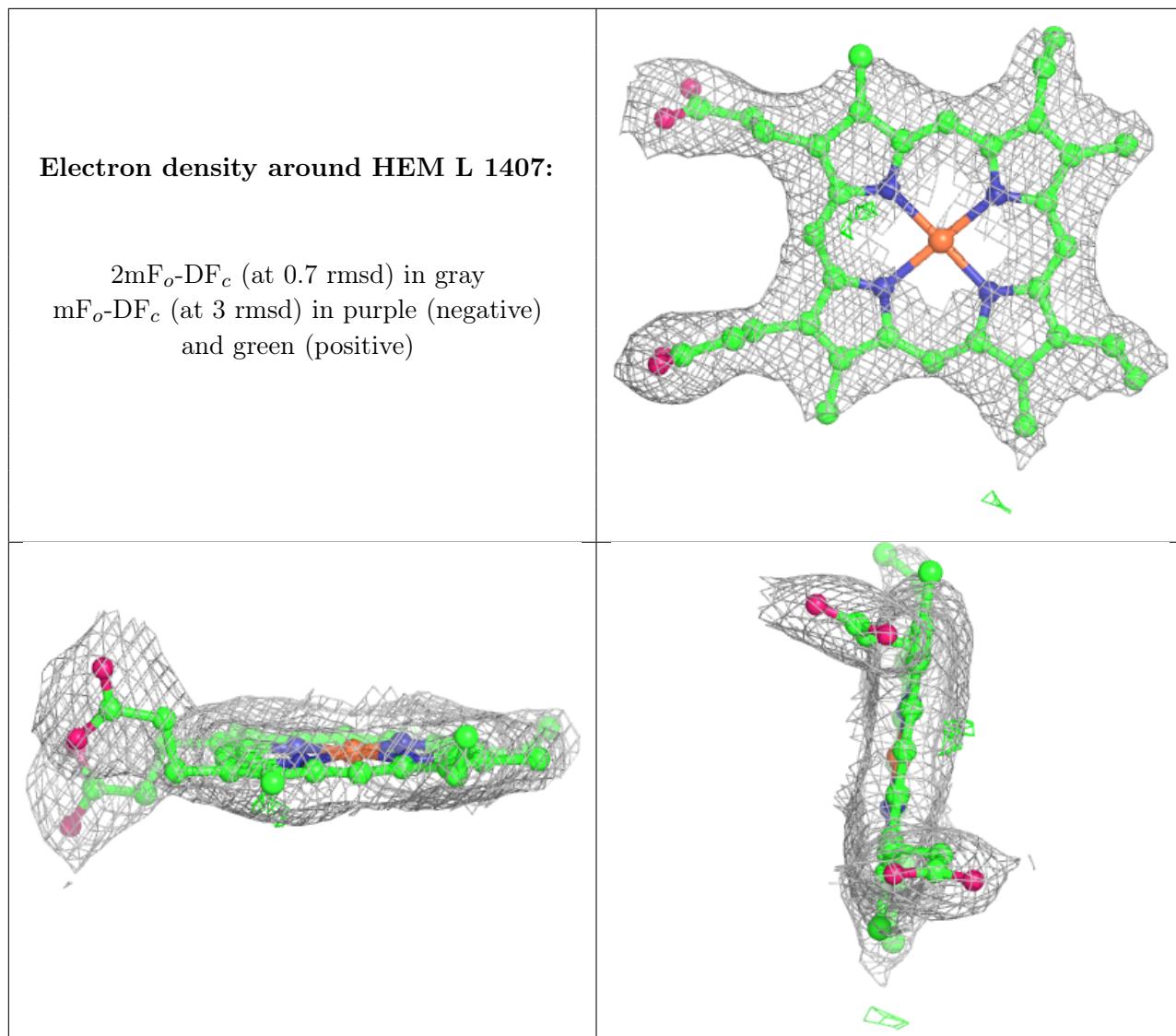


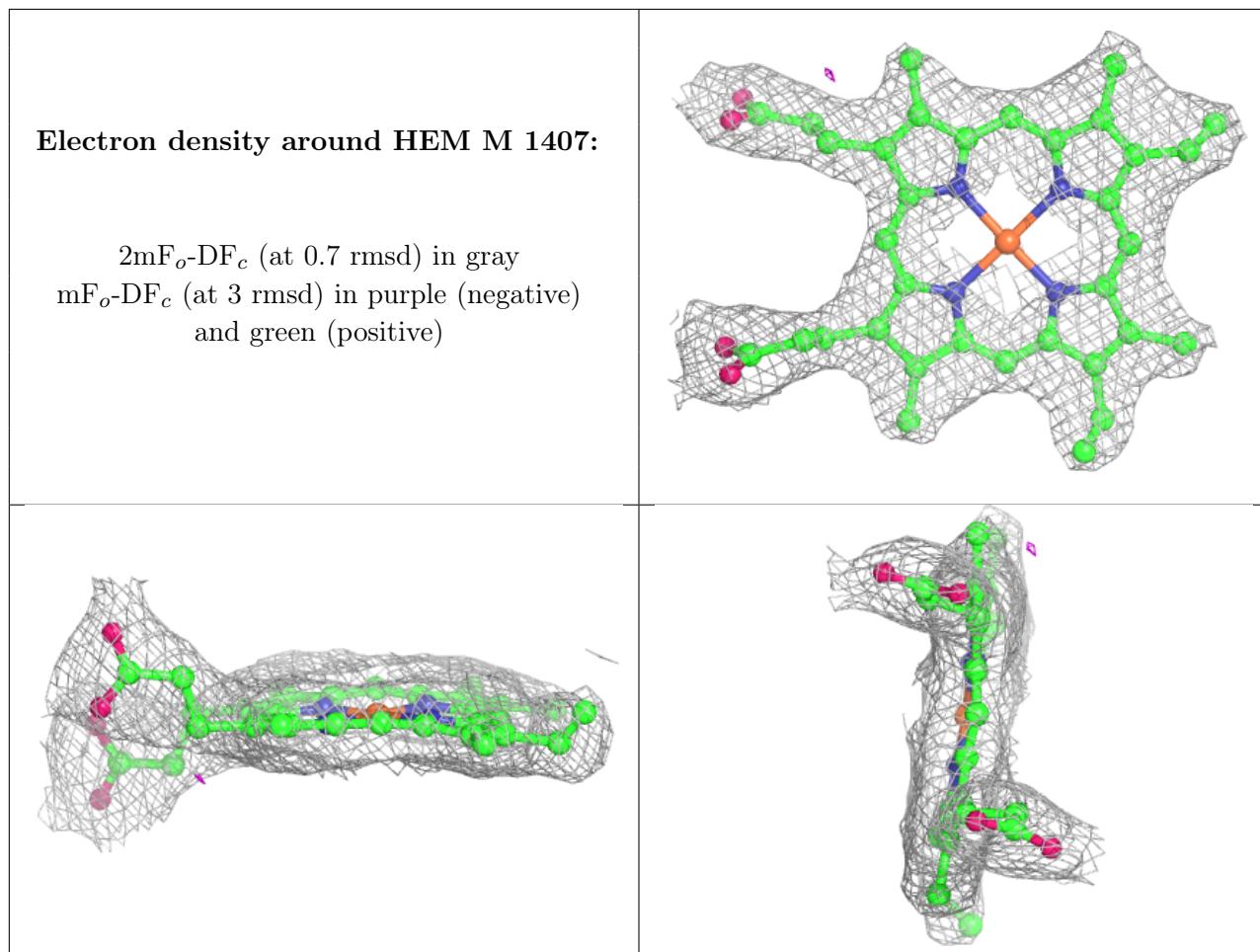


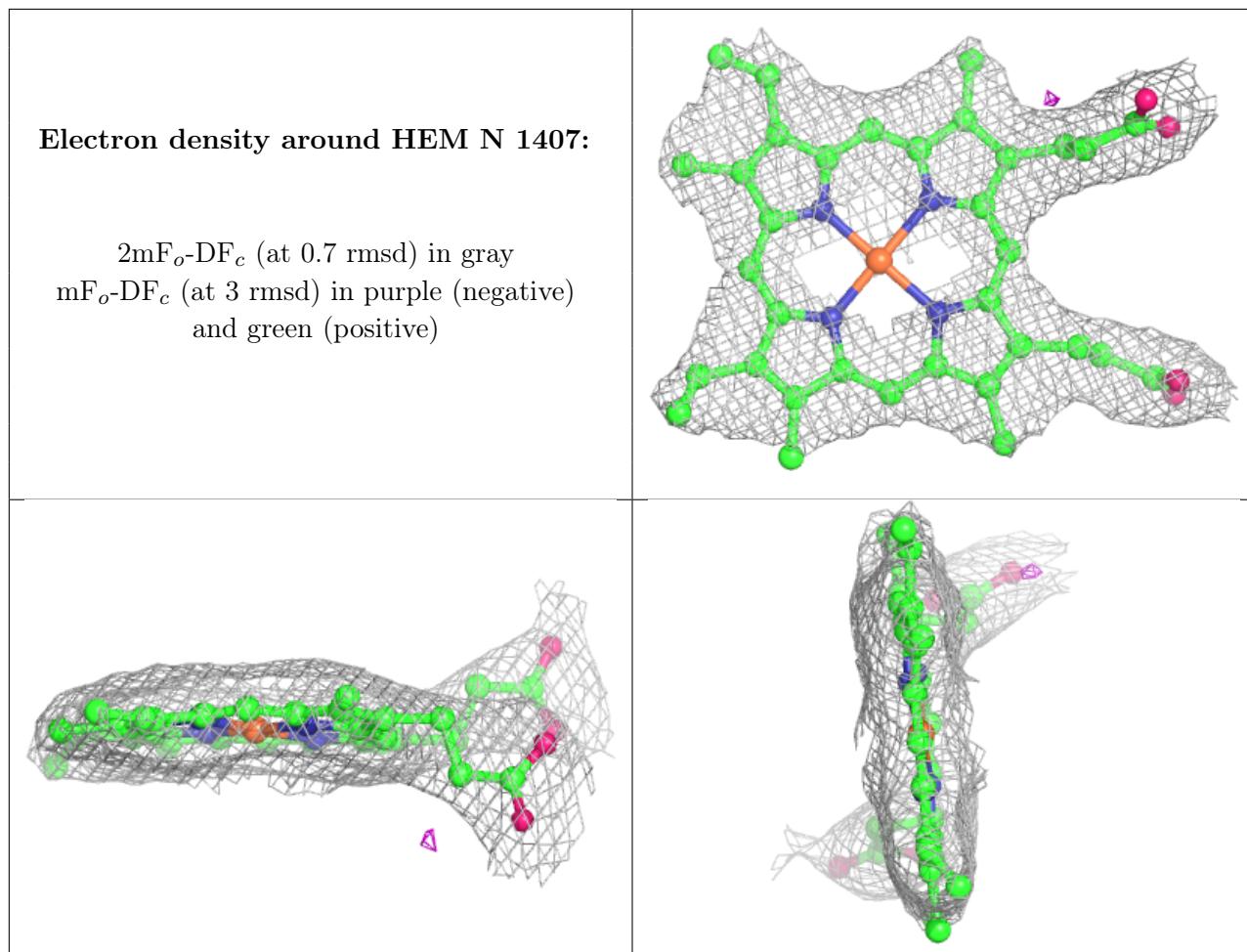


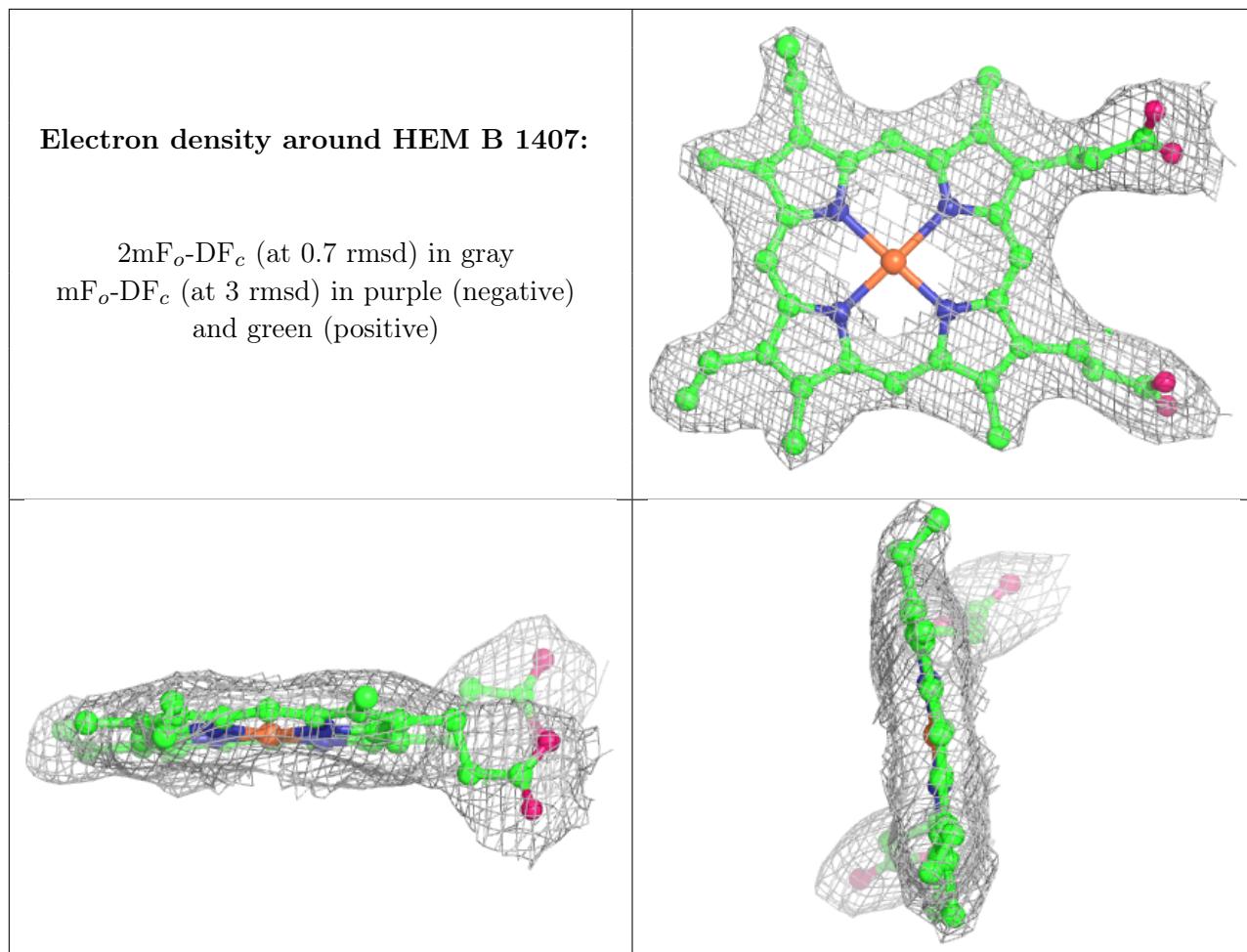


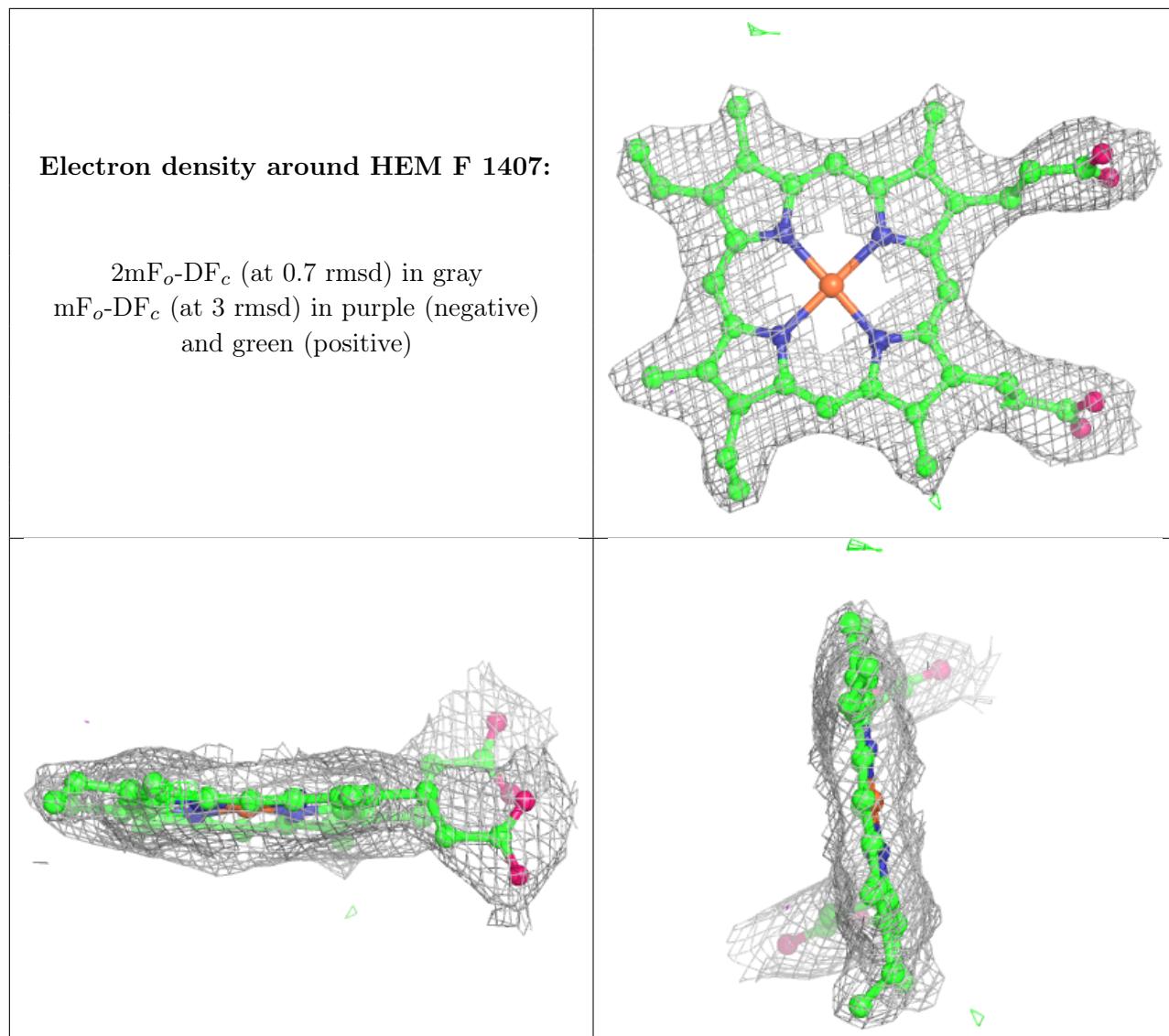


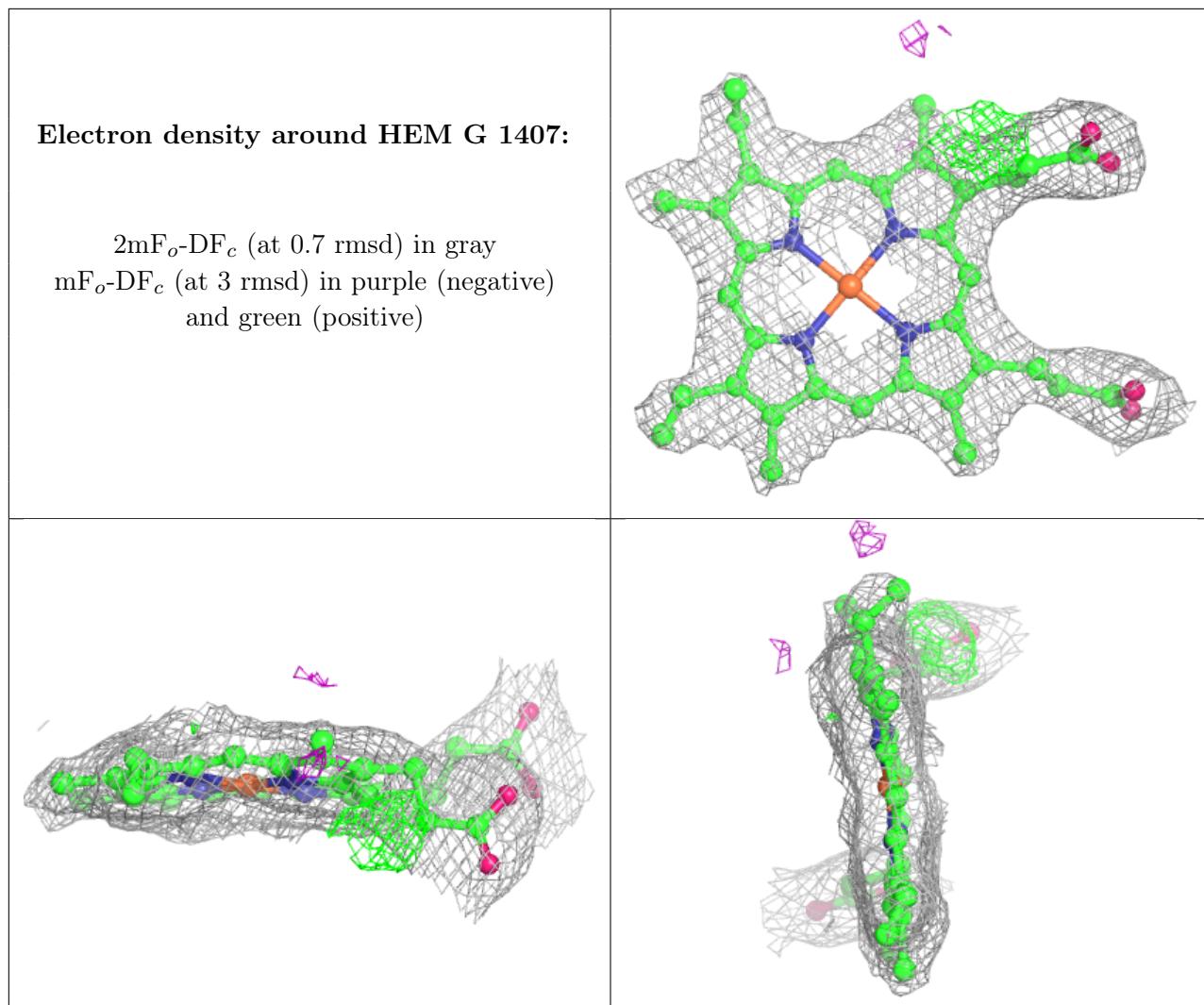


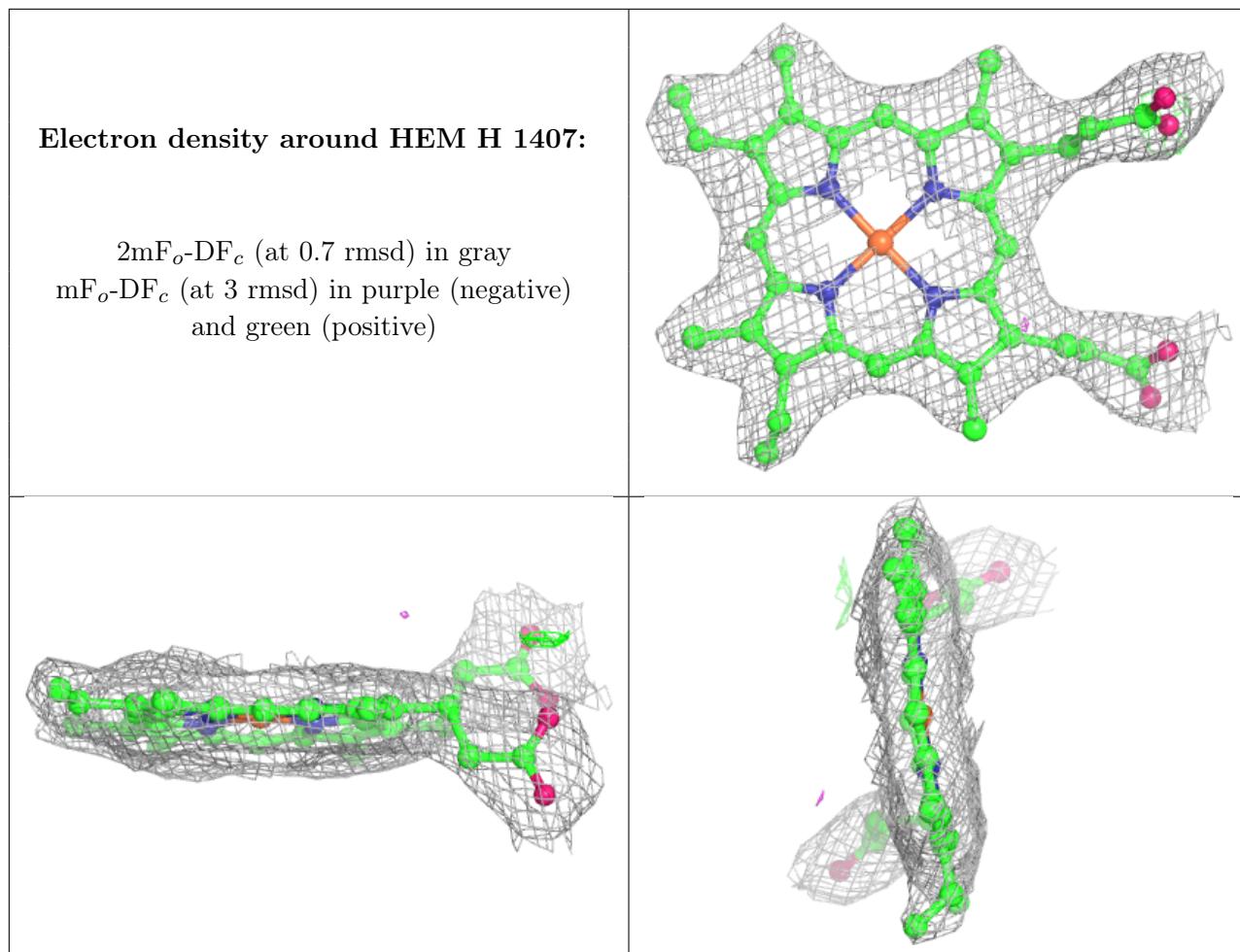


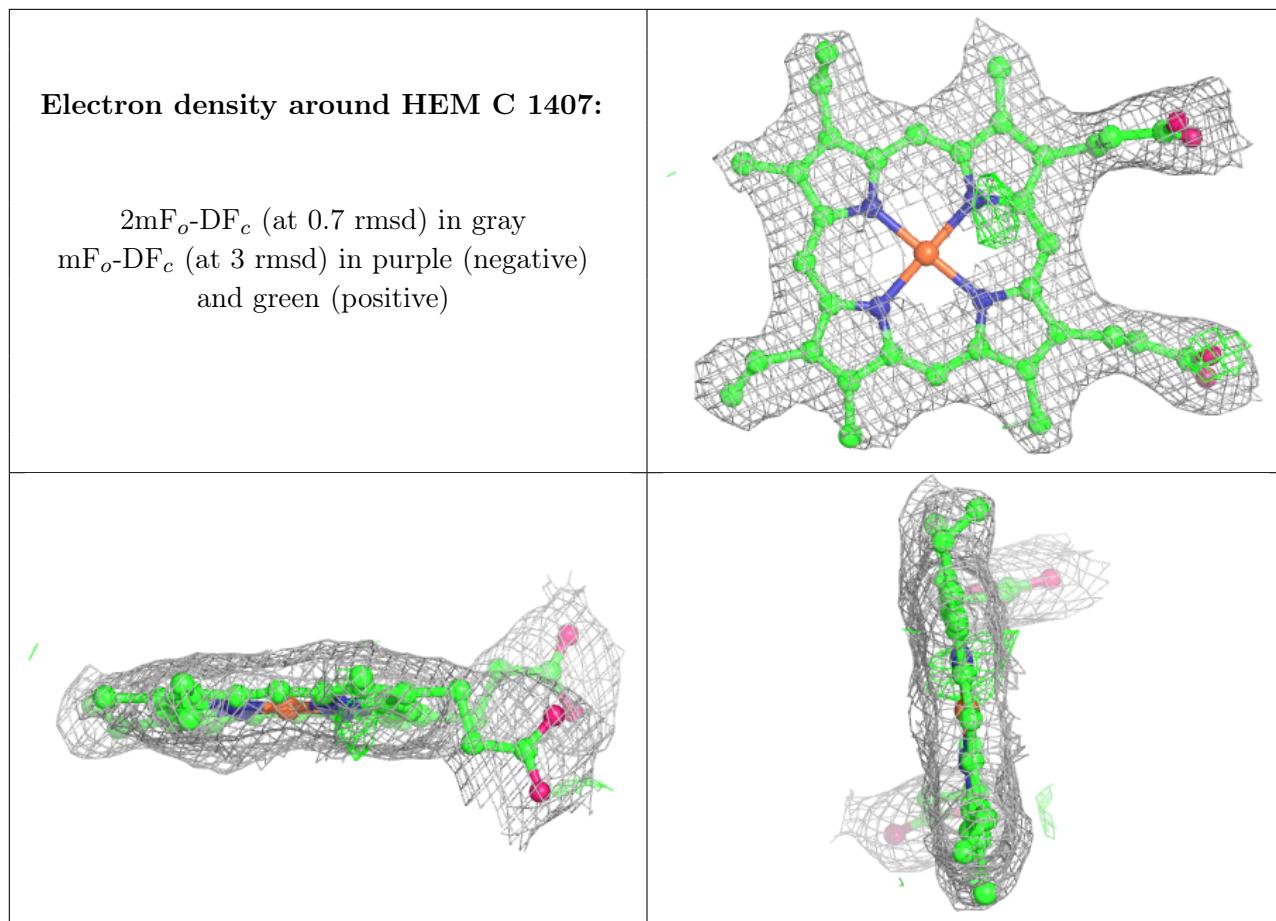


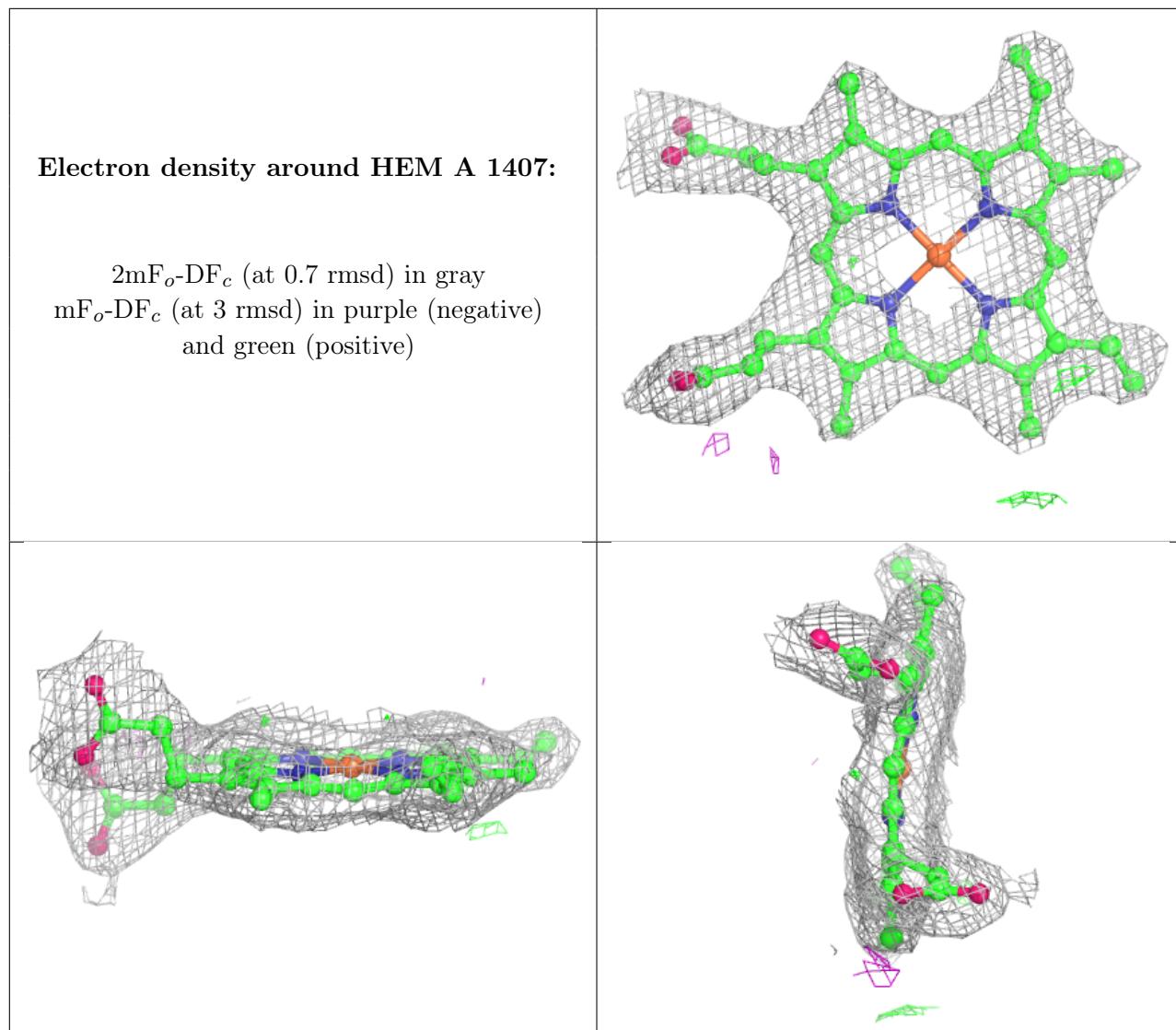












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.