



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 11:37 AM BST

PDB ID : 3UOI
Title : Mycobacterium tuberculosis bacterioferritin, BfrA
Authors : McMath, L.M.; Goulding, C.W.; TB Structural Genomics Consortium (TB-SGC)
Deposited on : 2011-11-16
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

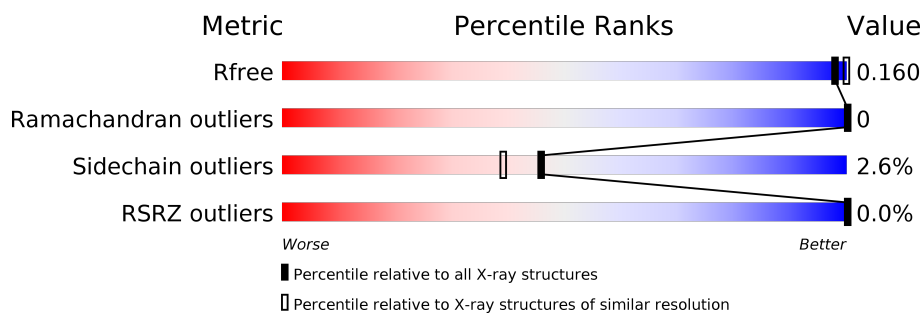
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



















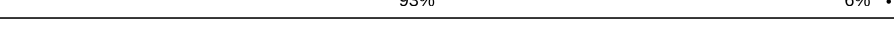
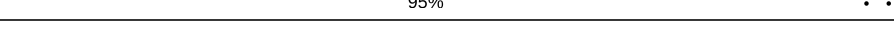

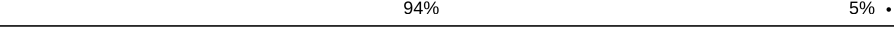
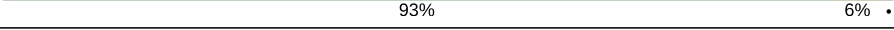
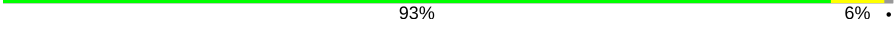
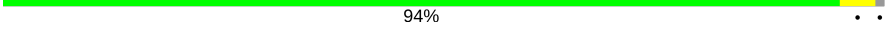

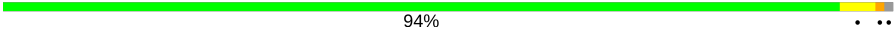
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	161	92% 6% ..
1	B	161	96% ...
1	C	161	92% 7% .
1	D	161	93% 6% .
1	E	161	89% 9% .
1	F	161	92% 7% .
1	G	161	92% 7% .




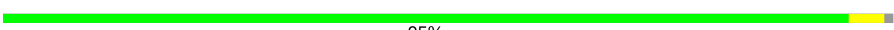








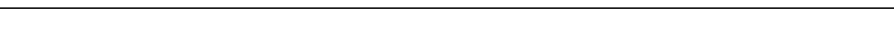



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Mol	Chain	Length	Quality of chain
1	H	161	 93% 6% .
1	I	161	 94% 5% .
1	J	161	 89% 10% .
1	K	161	 92% 6% ..
1	L	161	 94% . .
1	M	161	 91% 7% ..
1	N	161	 89% 9% .
1	O	161	 94% . .
1	P	161	 91% 7% ..
1	Q	161	 91% 7% ..
1	R	161	 88% 9% ..
1	S	161	 92% 6% ..
1	T	161	 90% 9% .
1	U	161	 88% 11% .
1	V	161	 90% 9% .
1	W	161	 93% 6% .
1	X	161	 95% . .
1	a	161	 89% 10% .
1	b	161	 94% 5% .
1	c	161	 93% 6% .
1	d	161	 93% 6% .
1	e	161	 94% . .
1	f	161	 94% . .
1	g	161	 94% . .
1	h	161	 94% . .

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Mol	Chain	Length	Quality of chain
1	i	161	 93% 6% .
1	j	161	 91% 8% .
1	k	161	 90% 9% .
1	l	161	 95% . .
1	m	161	 89% 9% .
1	n	161	 88% 11% .
1	o	161	 93% 6% .
1	p	161	 92% 7% .
1	q	161	 93% 5% ..
1	r	161	 92% 7% .
1	s	161	 93% 6% .
1	t	161	 88% 11% .
1	u	161	 91% 7% .
1	v	161	 89% 9% ..
1	w	161	 90% 9% .
1	x	161	 92% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 67560 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 Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	B	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	C	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	D	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	E	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	F	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	G	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	H	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	I	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	J	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	K	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	L	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	M	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	N	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	O	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	P	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	R	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	S	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	T	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	U	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	V	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	W	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	X	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	a	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	b	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	c	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	d	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	e	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	f	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	g	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	h	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	i	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	j	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	k	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	l	159	Total 1285	C 802	N 218	O 258	S 7	0	0	0
1	m	159	Total 1281	C 800	N 218	O 256	S 7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	n	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	o	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	p	159	Total	C	N	O	S	0	0	0
			1281	800	218	256	7			
1	q	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	r	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	s	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	t	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	u	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	v	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	w	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			
1	x	159	Total	C	N	O	S	0	0	0
			1285	802	218	258	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P63697
A	0	GLY	-	EXPRESSION TAG	UNP P63697
B	-1	MET	-	EXPRESSION TAG	UNP P63697
B	0	GLY	-	EXPRESSION TAG	UNP P63697
C	-1	MET	-	EXPRESSION TAG	UNP P63697
C	0	GLY	-	EXPRESSION TAG	UNP P63697
D	-1	MET	-	EXPRESSION TAG	UNP P63697
D	0	GLY	-	EXPRESSION TAG	UNP P63697
E	-1	MET	-	EXPRESSION TAG	UNP P63697
E	0	GLY	-	EXPRESSION TAG	UNP P63697
F	-1	MET	-	EXPRESSION TAG	UNP P63697
F	0	GLY	-	EXPRESSION TAG	UNP P63697
G	-1	MET	-	EXPRESSION TAG	UNP P63697
G	0	GLY	-	EXPRESSION TAG	UNP P63697
H	-1	MET	-	EXPRESSION TAG	UNP P63697
H	0	GLY	-	EXPRESSION TAG	UNP P63697
I	-1	MET	-	EXPRESSION TAG	UNP P63697

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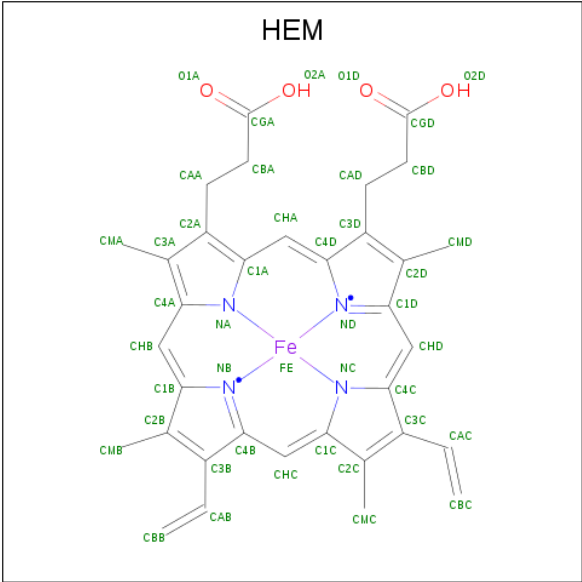
Chain	Residue	Modelled	Actual	Comment	Reference
I	0	GLY	-	EXPRESSION TAG	UNP P63697
J	-1	MET	-	EXPRESSION TAG	UNP P63697
J	0	GLY	-	EXPRESSION TAG	UNP P63697
K	-1	MET	-	EXPRESSION TAG	UNP P63697
K	0	GLY	-	EXPRESSION TAG	UNP P63697
L	-1	MET	-	EXPRESSION TAG	UNP P63697
L	0	GLY	-	EXPRESSION TAG	UNP P63697
M	-1	MET	-	EXPRESSION TAG	UNP P63697
M	0	GLY	-	EXPRESSION TAG	UNP P63697
N	-1	MET	-	EXPRESSION TAG	UNP P63697
N	0	GLY	-	EXPRESSION TAG	UNP P63697
O	-1	MET	-	EXPRESSION TAG	UNP P63697
O	0	GLY	-	EXPRESSION TAG	UNP P63697
P	-1	MET	-	EXPRESSION TAG	UNP P63697
P	0	GLY	-	EXPRESSION TAG	UNP P63697
Q	-1	MET	-	EXPRESSION TAG	UNP P63697
Q	0	GLY	-	EXPRESSION TAG	UNP P63697
R	-1	MET	-	EXPRESSION TAG	UNP P63697
R	0	GLY	-	EXPRESSION TAG	UNP P63697
S	-1	MET	-	EXPRESSION TAG	UNP P63697
S	0	GLY	-	EXPRESSION TAG	UNP P63697
T	-1	MET	-	EXPRESSION TAG	UNP P63697
T	0	GLY	-	EXPRESSION TAG	UNP P63697
U	-1	MET	-	EXPRESSION TAG	UNP P63697
U	0	GLY	-	EXPRESSION TAG	UNP P63697
V	-1	MET	-	EXPRESSION TAG	UNP P63697
V	0	GLY	-	EXPRESSION TAG	UNP P63697
W	-1	MET	-	EXPRESSION TAG	UNP P63697
W	0	GLY	-	EXPRESSION TAG	UNP P63697
X	-1	MET	-	EXPRESSION TAG	UNP P63697
X	0	GLY	-	EXPRESSION TAG	UNP P63697
a	-1	MET	-	EXPRESSION TAG	UNP P63697
a	0	GLY	-	EXPRESSION TAG	UNP P63697
b	-1	MET	-	EXPRESSION TAG	UNP P63697
b	0	GLY	-	EXPRESSION TAG	UNP P63697
c	-1	MET	-	EXPRESSION TAG	UNP P63697
c	0	GLY	-	EXPRESSION TAG	UNP P63697
d	-1	MET	-	EXPRESSION TAG	UNP P63697
d	0	GLY	-	EXPRESSION TAG	UNP P63697
e	-1	MET	-	EXPRESSION TAG	UNP P63697
e	0	GLY	-	EXPRESSION TAG	UNP P63697
f	-1	MET	-	EXPRESSION TAG	UNP P63697

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Chain	Residue	Modelled	Actual	Comment	Reference
f	0	GLY	-	EXPRESSION TAG	UNP P63697
g	-1	MET	-	EXPRESSION TAG	UNP P63697
g	0	GLY	-	EXPRESSION TAG	UNP P63697
h	-1	MET	-	EXPRESSION TAG	UNP P63697
h	0	GLY	-	EXPRESSION TAG	UNP P63697
i	-1	MET	-	EXPRESSION TAG	UNP P63697
i	0	GLY	-	EXPRESSION TAG	UNP P63697
j	-1	MET	-	EXPRESSION TAG	UNP P63697
j	0	GLY	-	EXPRESSION TAG	UNP P63697
k	-1	MET	-	EXPRESSION TAG	UNP P63697
k	0	GLY	-	EXPRESSION TAG	UNP P63697
l	-1	MET	-	EXPRESSION TAG	UNP P63697
l	0	GLY	-	EXPRESSION TAG	UNP P63697
m	-1	MET	-	EXPRESSION TAG	UNP P63697
m	0	GLY	-	EXPRESSION TAG	UNP P63697
n	-1	MET	-	EXPRESSION TAG	UNP P63697
n	0	GLY	-	EXPRESSION TAG	UNP P63697
o	-1	MET	-	EXPRESSION TAG	UNP P63697
o	0	GLY	-	EXPRESSION TAG	UNP P63697
p	-1	MET	-	EXPRESSION TAG	UNP P63697
p	0	GLY	-	EXPRESSION TAG	UNP P63697
q	-1	MET	-	EXPRESSION TAG	UNP P63697
q	0	GLY	-	EXPRESSION TAG	UNP P63697
r	-1	MET	-	EXPRESSION TAG	UNP P63697
r	0	GLY	-	EXPRESSION TAG	UNP P63697
s	-1	MET	-	EXPRESSION TAG	UNP P63697
s	0	GLY	-	EXPRESSION TAG	UNP P63697
t	-1	MET	-	EXPRESSION TAG	UNP P63697
t	0	GLY	-	EXPRESSION TAG	UNP P63697
u	-1	MET	-	EXPRESSION TAG	UNP P63697
u	0	GLY	-	EXPRESSION TAG	UNP P63697
v	-1	MET	-	EXPRESSION TAG	UNP P63697
v	0	GLY	-	EXPRESSION TAG	UNP P63697
w	-1	MET	-	EXPRESSION TAG	UNP P63697
w	0	GLY	-	EXPRESSION TAG	UNP P63697
x	-1	MET	-	EXPRESSION TAG	UNP P63697
x	0	GLY	-	EXPRESSION TAG	UNP P63697

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	S	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	a	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	c	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	g	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	j	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	k	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	n	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	o	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	t	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	x	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	120	Total 120	O 120	0	0
3	C	89	Total 89	O 89	0	0
3	D	105	Total 105	O 105	0	0
3	E	104	Total 104	O 104	0	0
3	F	102	Total 102	O 102	0	0
3	G	115	Total 115	O 115	0	0
3	H	135	Total 135	O 135	0	0
3	I	127	Total 127	O 127	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	142	Total 142	O 142	0	0
3	K	115	Total 115	O 115	0	0
3	L	116	Total 116	O 116	0	0
3	M	115	Total 115	O 115	0	0
3	N	122	Total 122	O 122	0	0
3	O	127	Total 127	O 127	0	0
3	P	127	Total 127	O 127	0	0
3	Q	108	Total 108	O 108	0	0
3	R	104	Total 104	O 104	0	0
3	S	73	Total 73	O 73	0	0
3	T	136	Total 136	O 136	0	0
3	U	151	Total 151	O 151	0	0
3	V	119	Total 119	O 119	0	0
3	W	91	Total 91	O 91	0	0
3	X	131	Total 131	O 131	0	0
3	a	65	Total 65	O 65	0	0
3	b	59	Total 59	O 59	0	0
3	c	94	Total 94	O 94	0	0
3	d	57	Total 57	O 57	0	0
3	e	103	Total 103	O 103	0	0
3	f	105	Total 105	O 105	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	g	59	Total 59	O 59	0	0
3	h	63	Total 63	O 63	0	0
3	i	128	Total 128	O 128	0	0
3	j	74	Total 74	O 74	0	0
3	k	102	Total 102	O 102	0	0
3	l	120	Total 120	O 120	0	0
3	m	58	Total 58	O 58	0	0
3	n	41	Total 41	O 41	0	0
3	o	106	Total 106	O 106	0	0
3	p	69	Total 69	O 69	0	0
3	q	91	Total 91	O 91	0	0
3	r	96	Total 96	O 96	0	0
3	s	65	Total 65	O 65	0	0
3	t	69	Total 69	O 69	0	0
3	u	131	Total 131	O 131	0	0
3	v	74	Total 74	O 74	0	0
3	w	100	Total 100	O 100	0	0
3	x	122	Total 122	O 122	0	0

3 Residue-property plots [i](#)

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

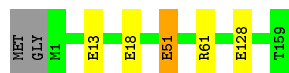
- Molecule 1: Bacterioferritin

Chain A: 



- Molecule 1: Bacterioferritin

Chain B: 



- Molecule 1: Bacterioferritin

Chain C: 



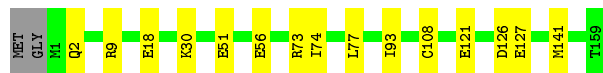
- Molecule 1: Bacterioferritin

Chain D: 



- Molecule 1: Bacterioferritin

Chain E: 



- Molecule 1: Bacterioferritin

Chain F: 



- Molecule 1: Bacterioferritin

Chain G: 92% 7% .



- Molecule 1: Bacterioferritin

Chain H: 93% 6% .



- Molecule 1: Bacterioferritin

Chain I: 94% 5% .



- Molecule 1: Bacterioferritin

Chain J: 89% 10% .



- Molecule 1: Bacterioferritin

Chain K: 92% 6% ..



- Molecule 1: Bacterioferritin

Chain L: 94% . .



- Molecule 1: Bacterioferritin

Chain M: 91% 7% ..



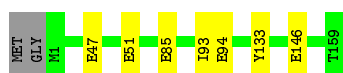
- Molecule 1: Bacterioferritin

Chain N: 89% 9% .



- Molecule 1: Bacterioferritin

Chain O: 94% . .



- Molecule 1: Bacterioferritin

Chain P: 91% 7% ..



- Molecule 1: Bacterioferritin

Chain Q: 91% 7% ..



- Molecule 1: Bacterioferritin

Chain R: 88% 9% ..



- Molecule 1: Bacterioferritin

Chain S: 92% 6% ..



- Molecule 1: Bacterioferritin

Chain T: 90% 9% .



- Molecule 1: Bacterioferritin

Chain U: 88% 11%



- Molecule 1: Bacterioferritin

Chain V: 90% 9%



- Molecule 1: Bacterioferritin

Chain W: 93% 6%



- Molecule 1: Bacterioferritin

Chain X: 95%



- Molecule 1: Bacterioferritin

Chain a: 89% 10%



- Molecule 1: Bacterioferritin

Chain b: 94% 5%



- Molecule 1: Bacterioferritin

Chain c: 93% 6%



- Molecule 1: Bacterioferritin

Chain d: 93% 6%



- Molecule 1: Bacterioferritin

Chain e: 94%



- Molecule 1: Bacterioferritin

Chain f: 94%



- Molecule 1: Bacterioferritin

Chain g: 94%



- Molecule 1: Bacterioferritin

Chain h: 94%



- Molecule 1: Bacterioferritin

Chain i: 93% 6%



- Molecule 1: Bacterioferritin

Chain j: 91% 8%



- Molecule 1: Bacterioferritin

Chain k: 90% 9% .



- Molecule 1: Bacterioferritin

Chain l: 95% . .



- Molecule 1: Bacterioferritin

Chain m: 89% 9% .



- Molecule 1: Bacterioferritin

Chain n: 88% 11% .



- Molecule 1: Bacterioferritin

Chain o: 93% 6% .



- Molecule 1: Bacterioferritin

Chain p: 92% 7% .



- Molecule 1: Bacterioferritin

Chain q: 93% 5% ..



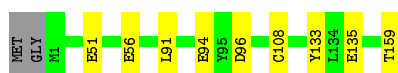
- Molecule 1: Bacterioferritin

Chain r: 92% 7% .



- Molecule 1: Bacterioferritin

Chain s: 93% 6% .



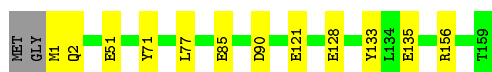
- Molecule 1: Bacterioferritin

Chain t: 88% 11% .



- Molecule 1: Bacterioferritin

Chain u: 91% 7% .



- Molecule 1: Bacterioferritin

Chain v: 89% 9% ..



- Molecule 1: Bacterioferritin

Chain w: 90% 9% .



- Molecule 1: Bacterioferritin

Chain x: 92% 7% .

MET	GLY	MI	Q2	S29	Y71	L77	R78	I93	D96	L119	Y149	C153	V154	T159
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.96Å 123.22Å 175.45Å 89.95° 89.95° 90.00°	Depositor
Resolution (Å)	32.56 – 1.90 32.56 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.4 (32.56-1.90) 86.6 (32.56-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.148 , 0.194 0.162 , 0.160	Depositor DCC
R_{free} test set	35667 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.459 for k,-h,l 0.459 for -k,h,l 0.087 for h,-k,-l 0.087 for -h,k,-l 0.470 for -h,-k,l 0.087 for k,h,-l 0.087 for -k,-h,-l	Xtriage
Reported twinning fraction	0.315 for 1.000H, 1.000K, L 0.208 for -1.000H, -1.000K, L 0.232 for 1.000K, -1.000H, L 0.245 for -1.000K, 1.000H, L	Depositor
Outliers	0 of 718164 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	67560	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 53.20 % 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 4.3586e-05.*

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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.58	6/1304 (0.5%)	0.95	3/1763 (0.2%)
1	B	1.60	3/1304 (0.2%)	0.98	1/1763 (0.1%)
1	C	1.60	4/1304 (0.3%)	1.01	1/1763 (0.1%)
1	D	1.63	5/1304 (0.4%)	0.96	0/1763
1	E	1.56	7/1304 (0.5%)	1.05	4/1763 (0.2%)
1	F	1.62	6/1304 (0.5%)	0.98	1/1763 (0.1%)
1	G	1.67	9/1304 (0.7%)	0.99	1/1763 (0.1%)
1	H	1.64	6/1304 (0.5%)	0.96	1/1763 (0.1%)
1	I	1.57	2/1304 (0.2%)	1.00	4/1763 (0.2%)
1	J	1.66	10/1304 (0.8%)	1.02	7/1763 (0.4%)
1	K	1.57	7/1304 (0.5%)	0.94	3/1763 (0.2%)
1	L	1.60	4/1304 (0.3%)	1.00	3/1763 (0.2%)
1	M	1.64	7/1304 (0.5%)	0.96	1/1763 (0.1%)
1	N	1.71	8/1304 (0.6%)	0.98	4/1763 (0.2%)
1	O	1.62	6/1304 (0.5%)	0.98	1/1763 (0.1%)
1	P	1.69	11/1304 (0.8%)	0.95	3/1763 (0.2%)
1	Q	1.66	12/1304 (0.9%)	0.97	1/1763 (0.1%)
1	R	1.57	10/1304 (0.8%)	1.04	6/1763 (0.3%)
1	S	1.63	6/1304 (0.5%)	1.04	4/1763 (0.2%)
1	T	1.71	10/1304 (0.8%)	1.00	3/1763 (0.2%)
1	U	1.77	13/1304 (1.0%)	0.98	2/1763 (0.1%)
1	V	1.61	5/1304 (0.4%)	0.98	4/1763 (0.2%)
1	W	1.61	4/1304 (0.3%)	0.97	2/1763 (0.1%)
1	X	1.66	3/1304 (0.2%)	0.98	1/1763 (0.1%)
1	a	1.71	15/1304 (1.2%)	0.97	2/1763 (0.1%)
1	b	1.66	6/1304 (0.5%)	0.98	2/1763 (0.1%)
1	c	1.56	3/1304 (0.2%)	0.99	3/1763 (0.2%)
1	d	1.56	7/1304 (0.5%)	0.96	2/1763 (0.1%)
1	e	1.48	2/1304 (0.2%)	0.96	2/1763 (0.1%)
1	f	1.58	5/1304 (0.4%)	1.01	4/1763 (0.2%)
1	g	1.60	4/1304 (0.3%)	0.97	2/1763 (0.1%)
1	h	1.53	3/1304 (0.2%)	0.95	0/1763

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	1.59	8/1304 (0.6%)	0.98	3/1763 (0.2%)
1	j	1.65	7/1304 (0.5%)	1.01	3/1763 (0.2%)
1	k	1.62	7/1304 (0.5%)	0.99	2/1763 (0.1%)
1	l	1.62	5/1304 (0.4%)	0.96	0/1763
1	m	1.67	9/1300 (0.7%)	0.97	3/1758 (0.2%)
1	n	1.69	9/1304 (0.7%)	1.02	3/1763 (0.2%)
1	o	1.71	8/1304 (0.6%)	0.97	0/1763
1	p	1.59	6/1300 (0.5%)	0.95	2/1758 (0.1%)
1	q	1.56	5/1304 (0.4%)	0.96	1/1763 (0.1%)
1	r	1.60	7/1304 (0.5%)	0.99	2/1763 (0.1%)
1	s	1.60	7/1304 (0.5%)	0.96	2/1763 (0.1%)
1	t	1.77	14/1304 (1.1%)	0.99	2/1763 (0.1%)
1	u	1.72	10/1304 (0.8%)	1.01	2/1763 (0.1%)
1	v	1.67	8/1304 (0.6%)	0.99	2/1763 (0.1%)
1	w	1.61	5/1304 (0.4%)	1.05	6/1763 (0.3%)
1	x	1.68	6/1304 (0.5%)	0.94	1/1763 (0.1%)
All	All	1.63	330/62584 (0.5%)	0.98	112/84614 (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	q	0	1

The worst 5 of 330 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	108	CYS	CB-SG	-10.43	1.64	1.82
1	W	108	CYS	CB-SG	-9.99	1.65	1.82
1	k	108	CYS	CB-SG	-9.76	1.65	1.82
1	N	93	ILE	C-N	9.53	1.55	1.34
1	M	153	CYS	CB-SG	-9.14	1.66	1.82

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	9	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	f	9	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	q	94	GLU	O-C-N	-8.12	109.70	122.70
1	w	45	ARG	NE-CZ-NH2	8.01	124.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	94	GLU	O-C-N	-8.00	109.91	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	q	94	GLU	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	B	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	C	157/161 (98%)	157 (100%)	0	0	100	100
1	D	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	E	157/161 (98%)	157 (100%)	0	0	100	100
1	F	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	G	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	H	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	I	157/161 (98%)	157 (100%)	0	0	100	100
1	J	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	K	157/161 (98%)	157 (100%)	0	0	100	100
1	L	157/161 (98%)	156 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	N	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	O	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	P	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	Q	157/161 (98%)	157 (100%)	0	0	100	100
1	R	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	S	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	T	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	U	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	V	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	W	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	X	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	a	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	b	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	c	157/161 (98%)	157 (100%)	0	0	100	100
1	d	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	e	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	f	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	g	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	h	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	i	157/161 (98%)	157 (100%)	0	0	100	100
1	j	157/161 (98%)	157 (100%)	0	0	100	100
1	k	157/161 (98%)	157 (100%)	0	0	100	100
1	l	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	m	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	n	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	o	157/161 (98%)	157 (100%)	0	0	100	100
1	p	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	q	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	r	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	s	157/161 (98%)	156 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	t	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	u	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	v	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
1	w	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
1	x	157/161 (98%)	156 (99%)	1 (1%)	0	100	100
All	All	7536/7728 (98%)	7492 (99%)	44 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	B	142/143 (99%)	140 (99%)	2 (1%)	67	65
1	C	142/143 (99%)	136 (96%)	6 (4%)	30	20
1	D	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	E	142/143 (99%)	135 (95%)	7 (5%)	25	15
1	F	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	G	142/143 (99%)	140 (99%)	2 (1%)	67	65
1	H	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	I	142/143 (99%)	139 (98%)	3 (2%)	53	48
1	J	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	K	142/143 (99%)	137 (96%)	5 (4%)	36	27
1	L	142/143 (99%)	142 (100%)	0	100	100
1	M	142/143 (99%)	136 (96%)	6 (4%)	30	20
1	N	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	O	142/143 (99%)	142 (100%)	0	100	100
1	P	142/143 (99%)	139 (98%)	3 (2%)	53	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	R	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	S	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	T	142/143 (99%)	137 (96%)	5 (4%)	36	27
1	U	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	V	142/143 (99%)	136 (96%)	6 (4%)	30	20
1	W	142/143 (99%)	137 (96%)	5 (4%)	36	27
1	X	142/143 (99%)	140 (99%)	2 (1%)	67	65
1	a	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	b	142/143 (99%)	140 (99%)	2 (1%)	67	65
1	c	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	d	142/143 (99%)	140 (99%)	2 (1%)	67	65
1	e	142/143 (99%)	139 (98%)	3 (2%)	53	48
1	f	142/143 (99%)	141 (99%)	1 (1%)	84	84
1	g	142/143 (99%)	139 (98%)	3 (2%)	53	48
1	h	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	i	142/143 (99%)	140 (99%)	2 (1%)	67	65
1	j	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	k	142/143 (99%)	135 (95%)	7 (5%)	25	15
1	l	142/143 (99%)	141 (99%)	1 (1%)	84	84
1	m	141/143 (99%)	136 (96%)	5 (4%)	36	27
1	n	142/143 (99%)	135 (95%)	7 (5%)	25	15
1	o	142/143 (99%)	141 (99%)	1 (1%)	84	84
1	p	141/143 (99%)	137 (97%)	4 (3%)	43	36
1	q	142/143 (99%)	139 (98%)	3 (2%)	53	48
1	r	142/143 (99%)	139 (98%)	3 (2%)	53	48
1	s	142/143 (99%)	141 (99%)	1 (1%)	84	84
1	t	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	u	142/143 (99%)	138 (97%)	4 (3%)	43	36
1	v	142/143 (99%)	135 (95%)	7 (5%)	25	15
1	w	142/143 (99%)	136 (96%)	6 (4%)	30	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	142/143 (99%)	137 (96%)	5 (4%)	36	27
All	All	6814/6864 (99%)	6635 (97%)	179 (3%)	46	39

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	2	GLN
1	c	91	LEU
1	v	115	THR
1	V	77	LEU
1	X	2	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	112	GLN
1	f	24	GLN
1	w	70	ASN
1	b	34	ASN
1	d	137	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](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	t	200	1	27,50,50	2.79	11 (40%)	17,82,82	2.11	6 (35%)
2	HEM	q	200	1	27,50,50	2.11	5 (18%)	17,82,82	1.84	7 (41%)
2	HEM	S	200	1	27,50,50	2.80	10 (37%)	17,82,82	3.13	9 (52%)
2	HEM	P	200	1	27,50,50	2.74	10 (37%)	17,82,82	3.39	10 (58%)
2	HEM	n	200	1	27,50,50	2.76	8 (29%)	17,82,82	2.08	6 (35%)
2	HEM	k	200	1	27,50,50	2.80	8 (29%)	17,82,82	1.99	5 (29%)
2	HEM	H	200	1	27,50,50	1.96	7 (25%)	17,82,82	2.95	10 (58%)
2	HEM	x	200	1	27,50,50	2.49	7 (25%)	17,82,82	2.92	8 (47%)
2	HEM	M	200	1	27,50,50	2.32	9 (33%)	17,82,82	2.18	8 (47%)
2	HEM	e	200	1	27,50,50	2.38	10 (37%)	17,82,82	2.37	5 (29%)
2	HEM	c	200	1	27,50,50	2.19	7 (25%)	17,82,82	3.03	8 (47%)
2	HEM	R	200	1	27,50,50	2.17	6 (22%)	17,82,82	1.78	7 (41%)
2	HEM	X	200	1	27,50,50	2.29	11 (40%)	17,82,82	2.25	6 (35%)
2	HEM	U	200	1	27,50,50	2.48	6 (22%)	17,82,82	3.13	9 (52%)
2	HEM	j	200	1	27,50,50	2.71	8 (29%)	17,82,82	3.45	10 (58%)
2	HEM	B	200	1	27,50,50	2.16	7 (25%)	17,82,82	2.66	10 (58%)
2	HEM	L	200	1	27,50,50	2.28	8 (29%)	17,82,82	2.69	4 (23%)
2	HEM	g	200	1	27,50,50	2.32	9 (33%)	17,82,82	2.54	8 (47%)
2	HEM	a	200	1	27,50,50	2.01	7 (25%)	17,82,82	4.04	10 (58%)
2	HEM	F	200	1	27,50,50	2.40	4 (14%)	17,82,82	2.25	8 (47%)
2	HEM	C	200	1	27,50,50	2.38	8 (29%)	17,82,82	2.85	7 (41%)
2	HEM	v	200	1	27,50,50	2.77	9 (33%)	17,82,82	2.73	9 (52%)
2	HEM	o	200	1	27,50,50	2.40	6 (22%)	17,82,82	1.82	4 (23%)
2	HEM	I	200	1	27,50,50	2.87	11 (40%)	17,82,82	3.45	6 (35%)

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	t	200	1	-	6/6/54/54	-
2	HEM	q	200	1	-	0/6/54/54	-
2	HEM	S	200	1	-	0/6/54/54	-
2	HEM	P	200	1	-	2/6/54/54	-
2	HEM	n	200	1	-	0/6/54/54	-
2	HEM	k	200	1	-	6/6/54/54	-
2	HEM	H	200	1	-	0/6/54/54	-
2	HEM	x	200	1	-	0/6/54/54	-
2	HEM	M	200	1	-	3/6/54/54	-
2	HEM	e	200	1	-	0/6/54/54	-
2	HEM	c	200	1	-	0/6/54/54	-
2	HEM	R	200	1	-	5/6/54/54	-
2	HEM	X	200	1	-	4/6/54/54	-
2	HEM	U	200	1	-	0/6/54/54	-
2	HEM	j	200	1	-	1/6/54/54	-
2	HEM	B	200	1	-	1/6/54/54	-
2	HEM	L	200	1	-	3/6/54/54	-
2	HEM	g	200	1	-	3/6/54/54	-
2	HEM	a	200	1	-	0/6/54/54	-
2	HEM	F	200	1	-	1/6/54/54	-
2	HEM	C	200	1	-	4/6/54/54	-
2	HEM	v	200	1	-	1/6/54/54	-
2	HEM	o	200	1	-	4/6/54/54	-
2	HEM	I	200	1	-	0/6/54/54	-

The worst 5 of 192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	n	200	HEM	C3C-C2C	-8.80	1.28	1.40
2	k	200	HEM	C3B-C2B	-8.47	1.28	1.40
2	I	200	HEM	C3C-C2C	-8.42	1.28	1.40
2	v	200	HEM	C3B-C2B	-8.28	1.28	1.40
2	t	200	HEM	C3B-C2B	-8.24	1.28	1.40

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	200	HEM	CBA-CAA-C2A	-8.03	97.67	112.49
2	a	200	HEM	C4C-C3C-C2C	7.93	112.44	106.90
2	a	200	HEM	CAA-CBA-CGA	-7.88	99.45	112.67
2	P	200	HEM	CBD-CAD-C3D	-7.38	98.89	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	200	HEM	CBD-CAD-C3D	-7.34	98.96	112.48

There are no chirality outliers.

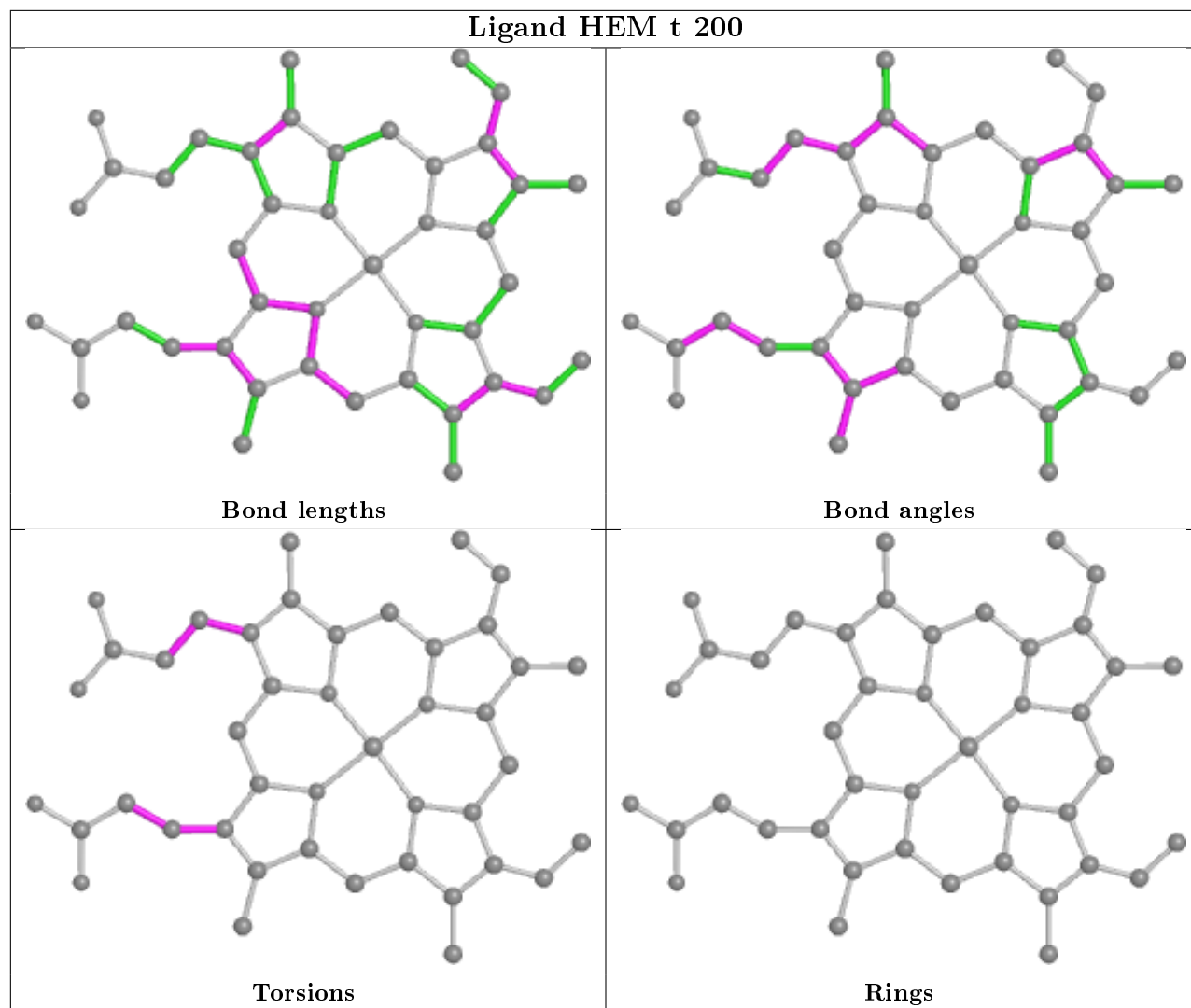
5 of 44 torsion outliers are listed below:

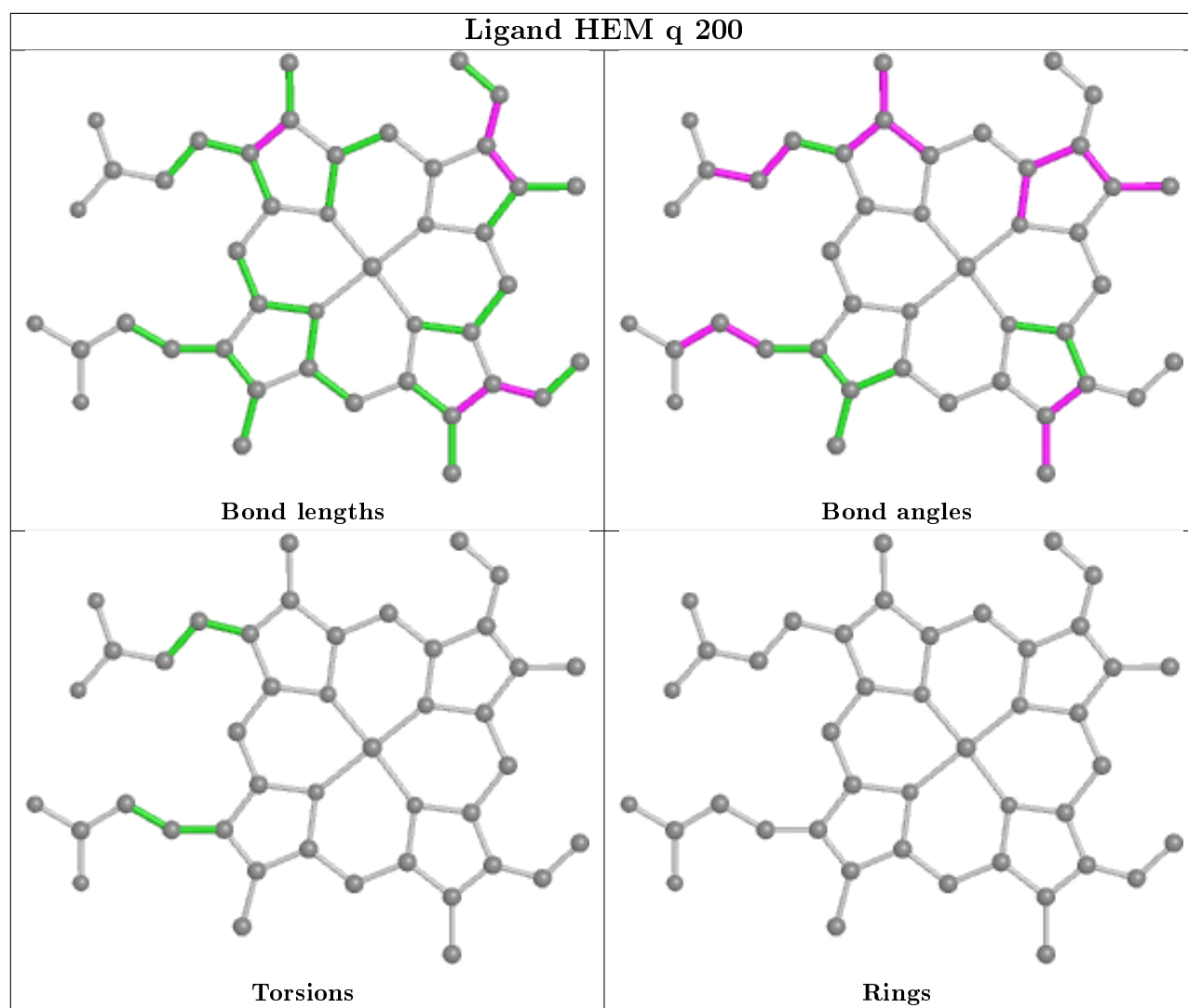
Mol	Chain	Res	Type	Atoms
2	t	200	HEM	C2D-C3D-CAD-CBD
2	t	200	HEM	C4D-C3D-CAD-CBD
2	P	200	HEM	C1A-C2A-CAA-CBA
2	P	200	HEM	C3A-C2A-CAA-CBA
2	k	200	HEM	C2A-CAA-CBA-CGA

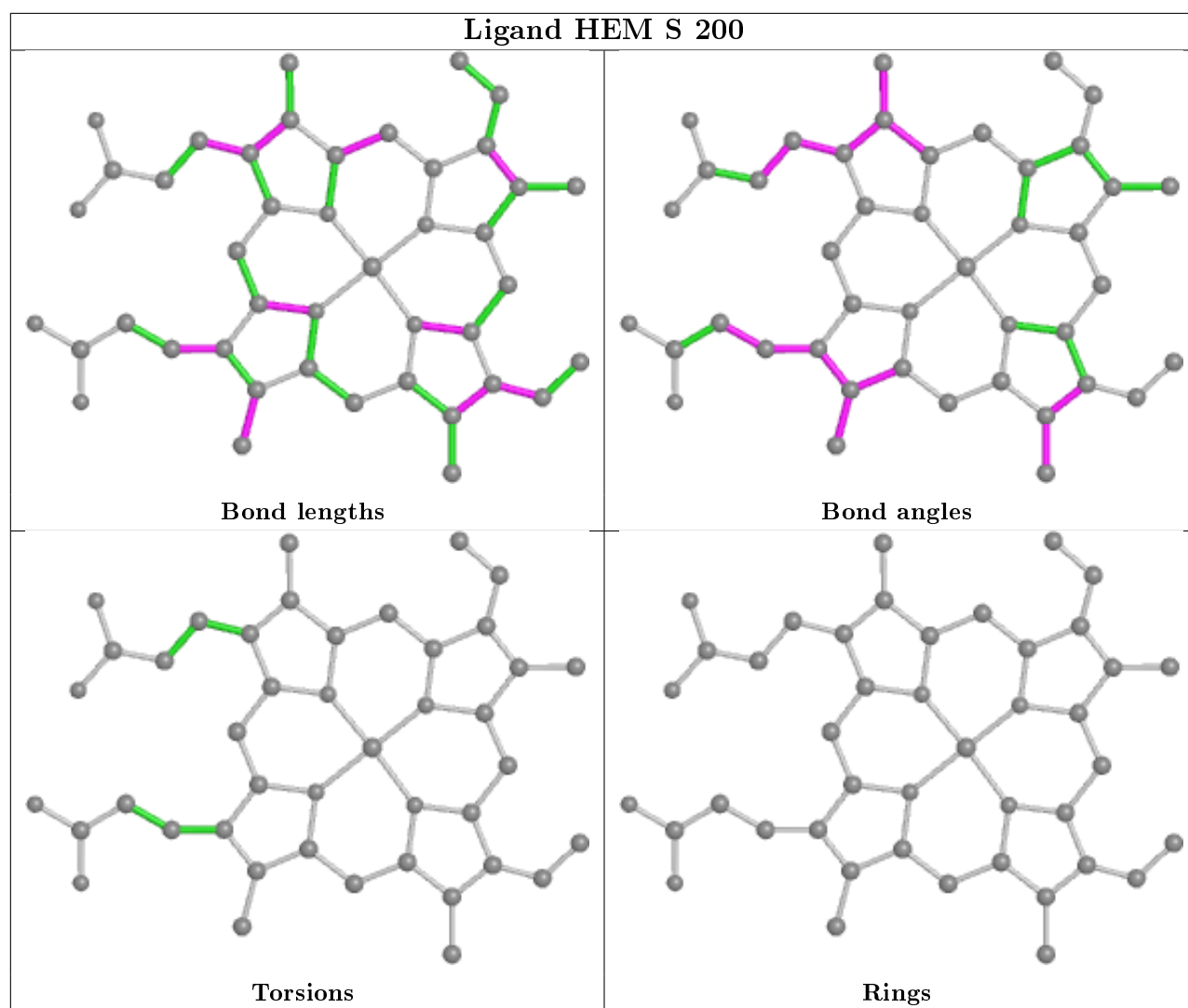
There are no ring outliers.

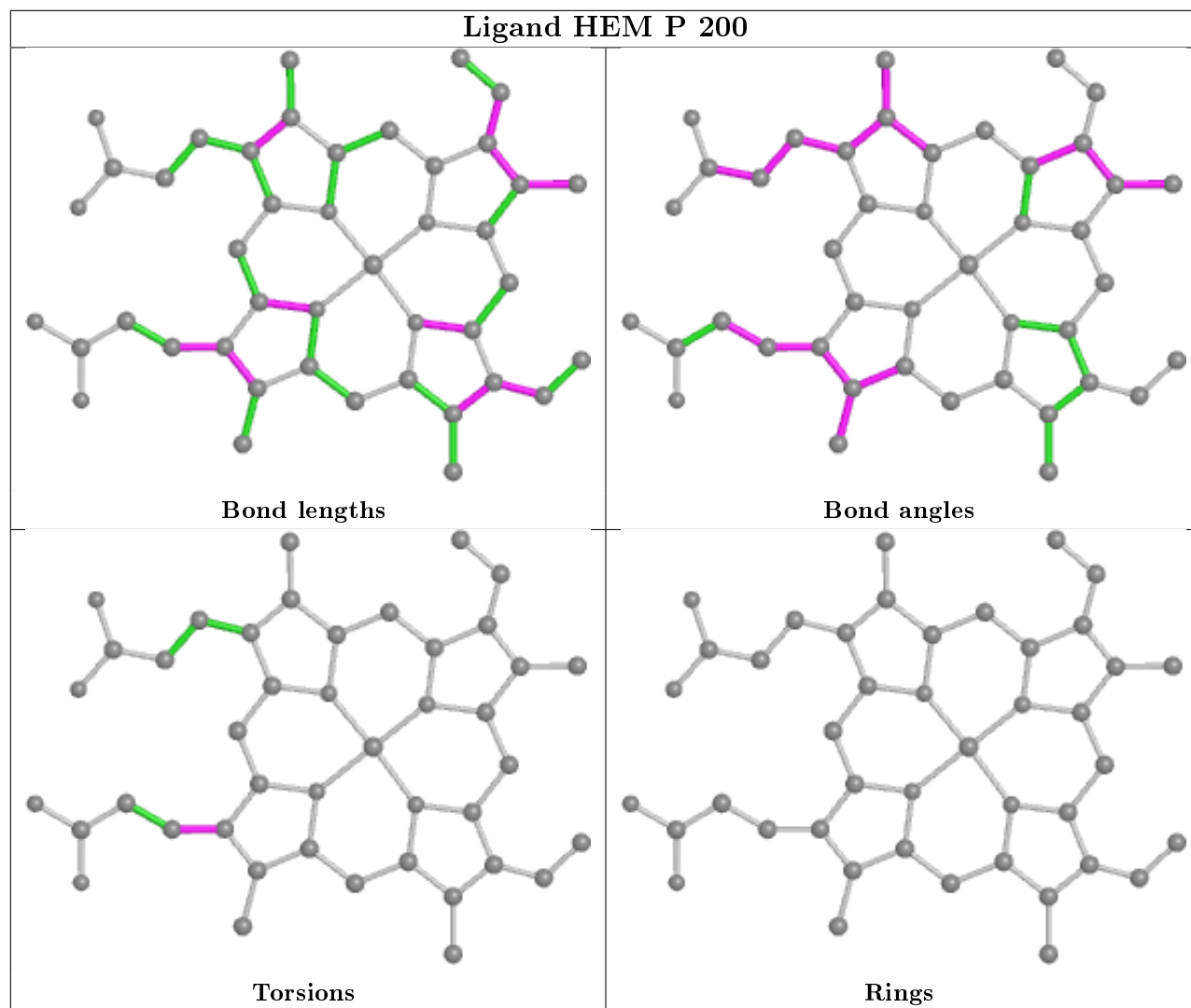
No monomer is involved in short contacts.

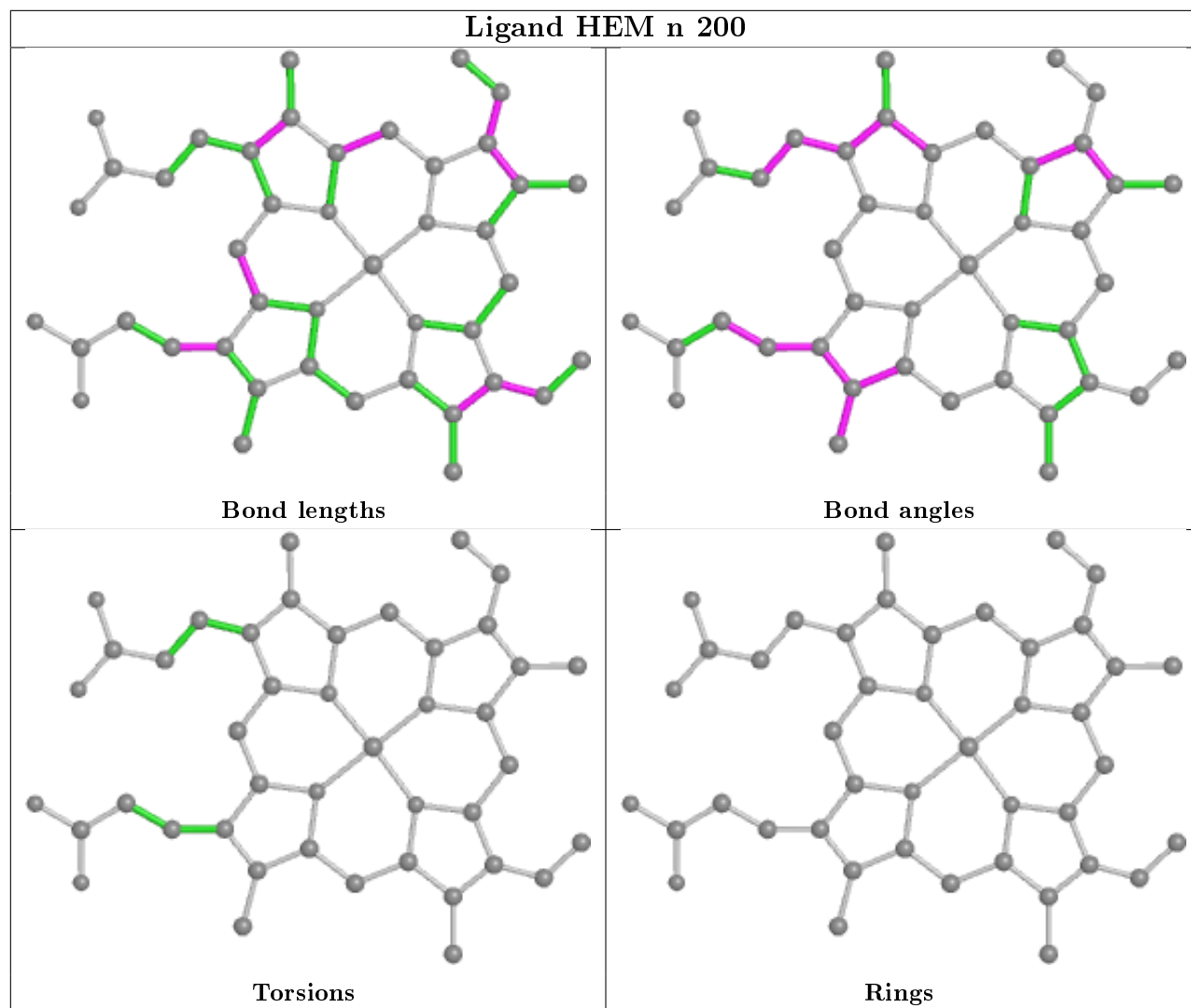
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

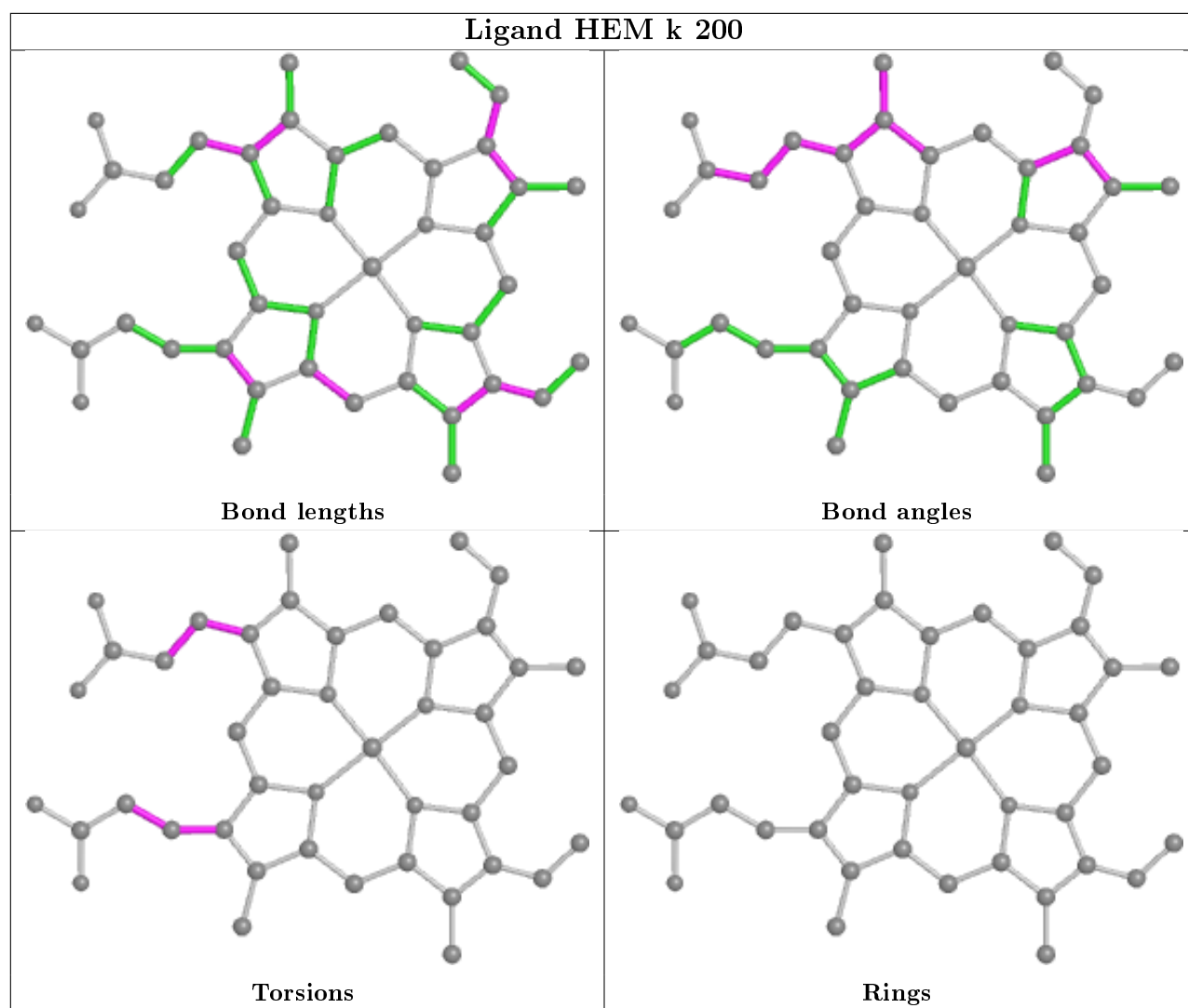


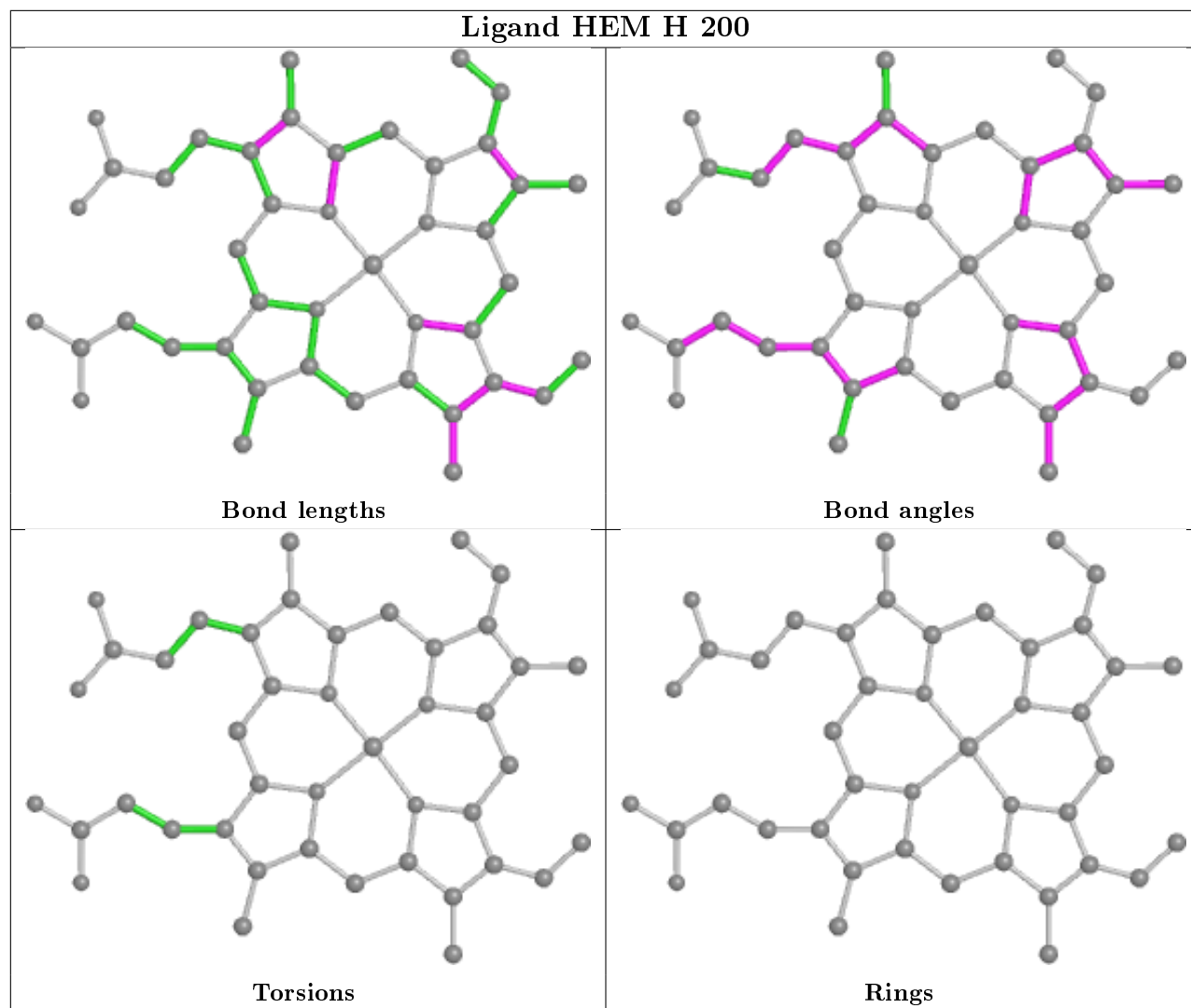


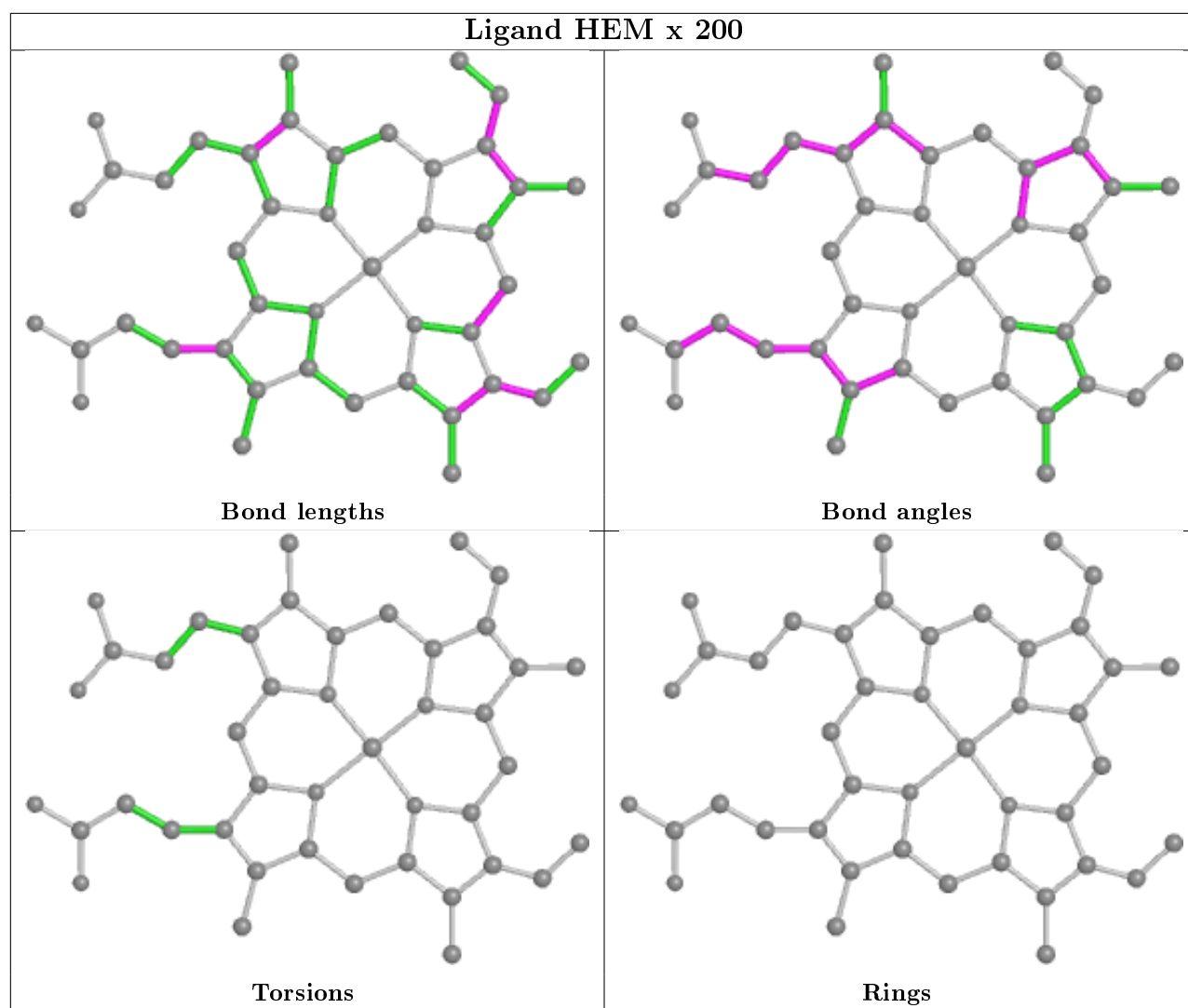


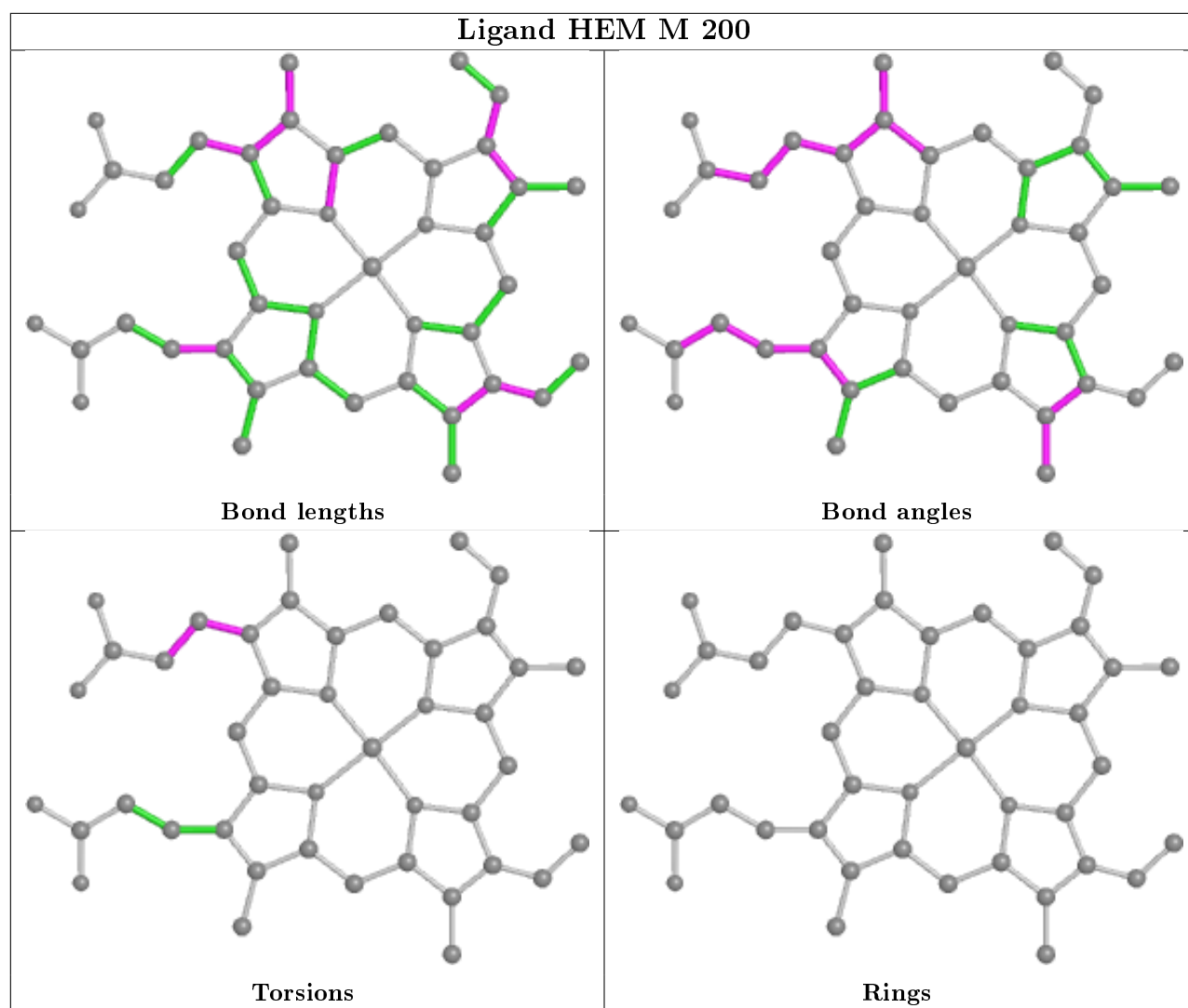


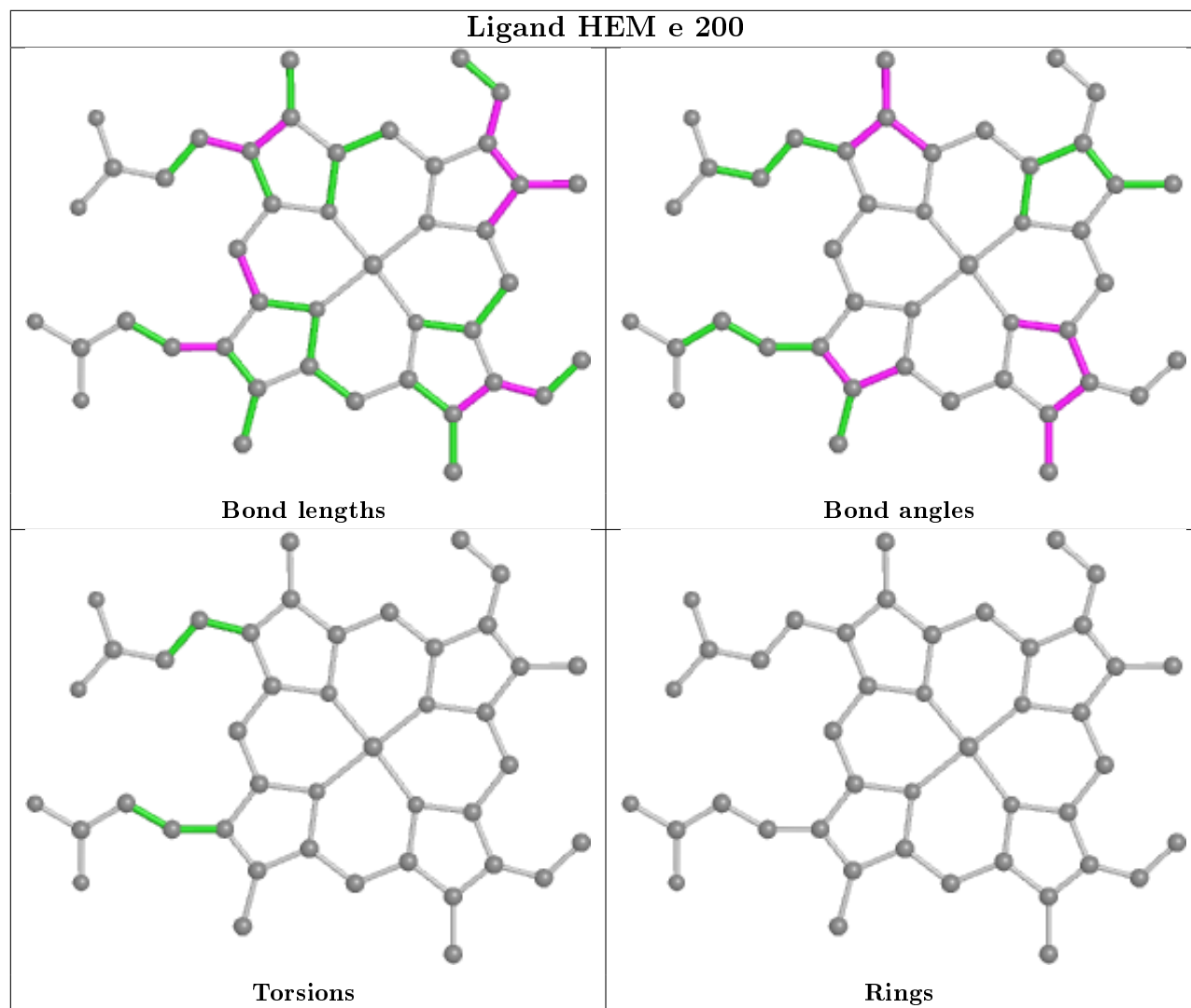


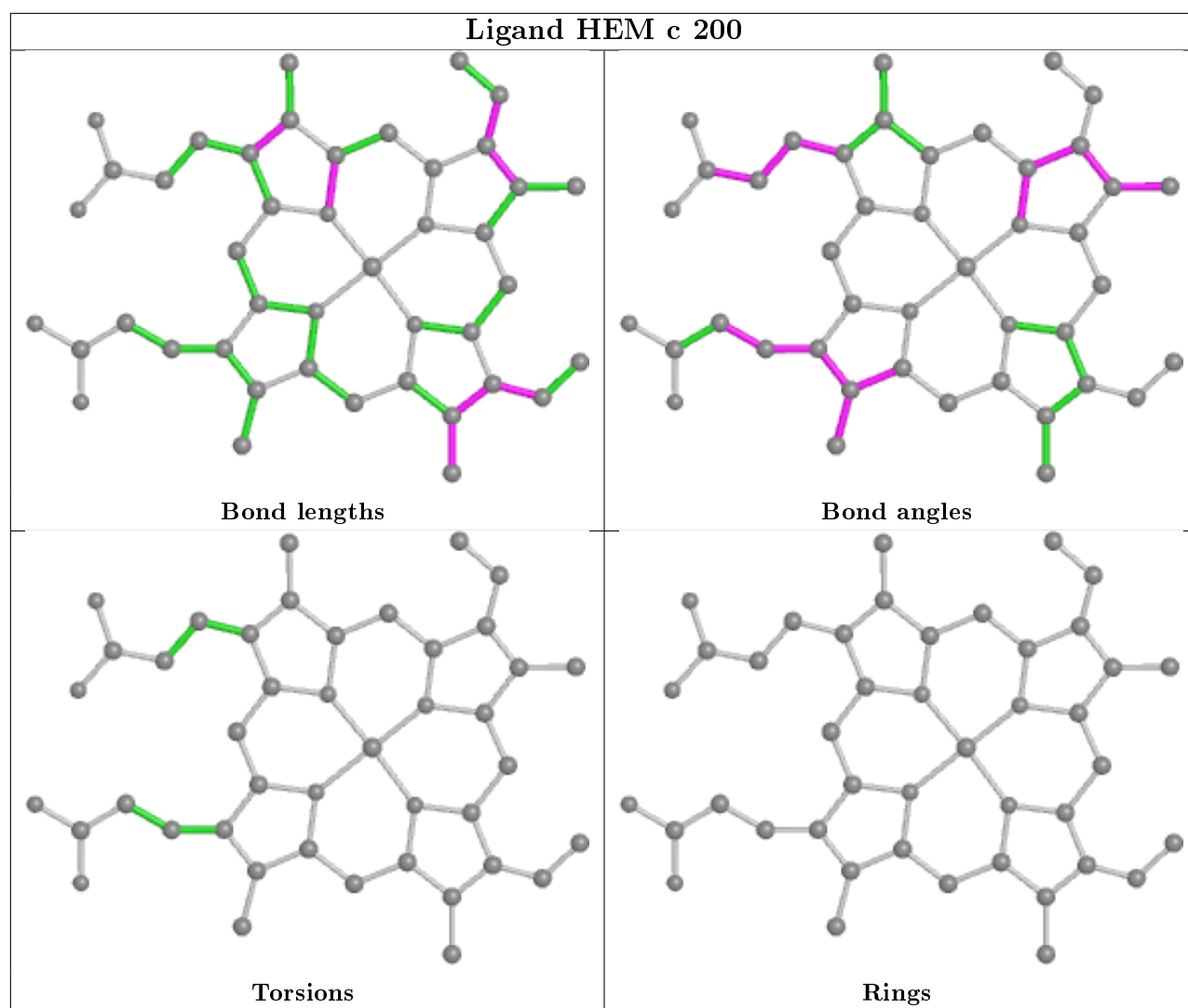


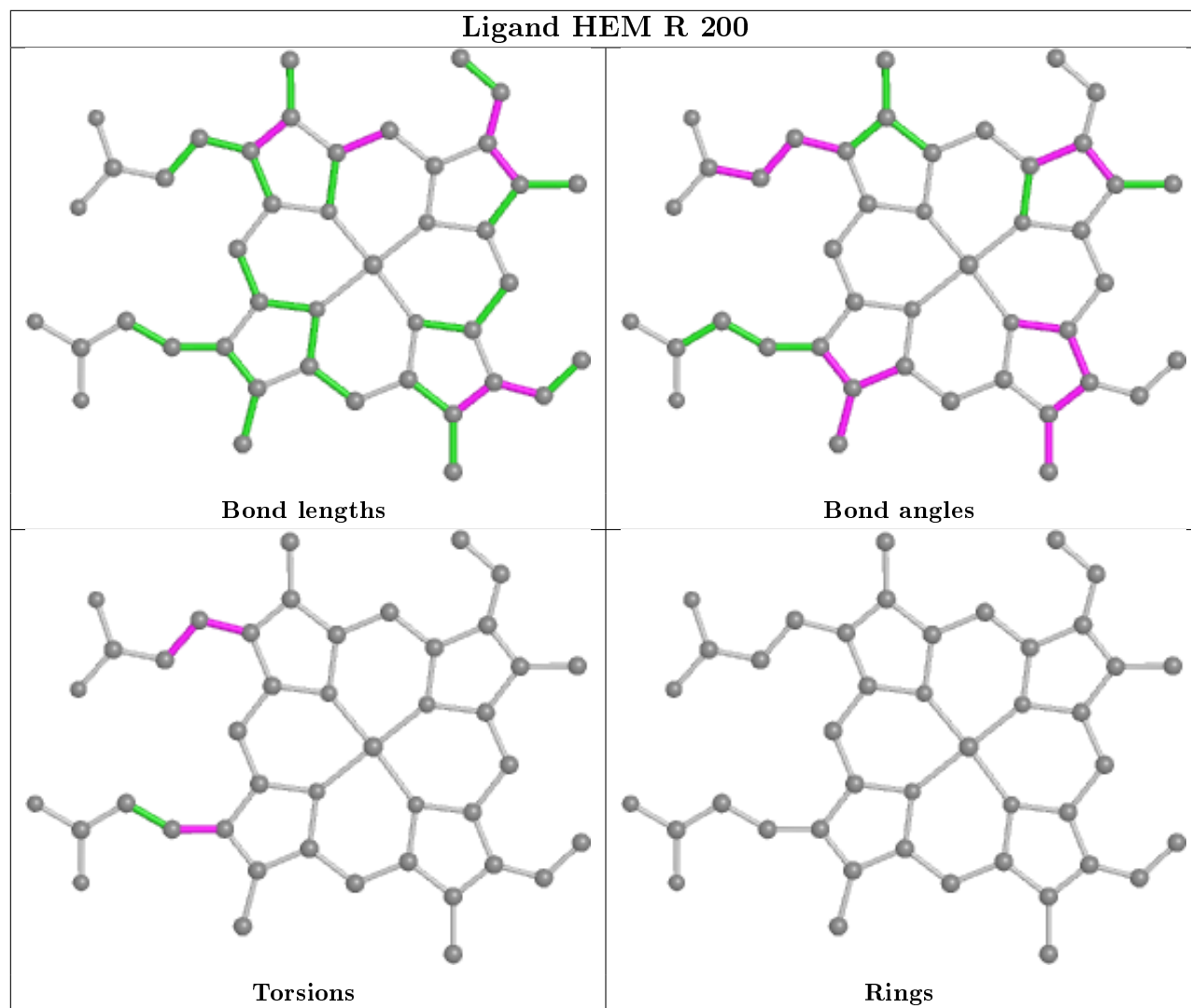


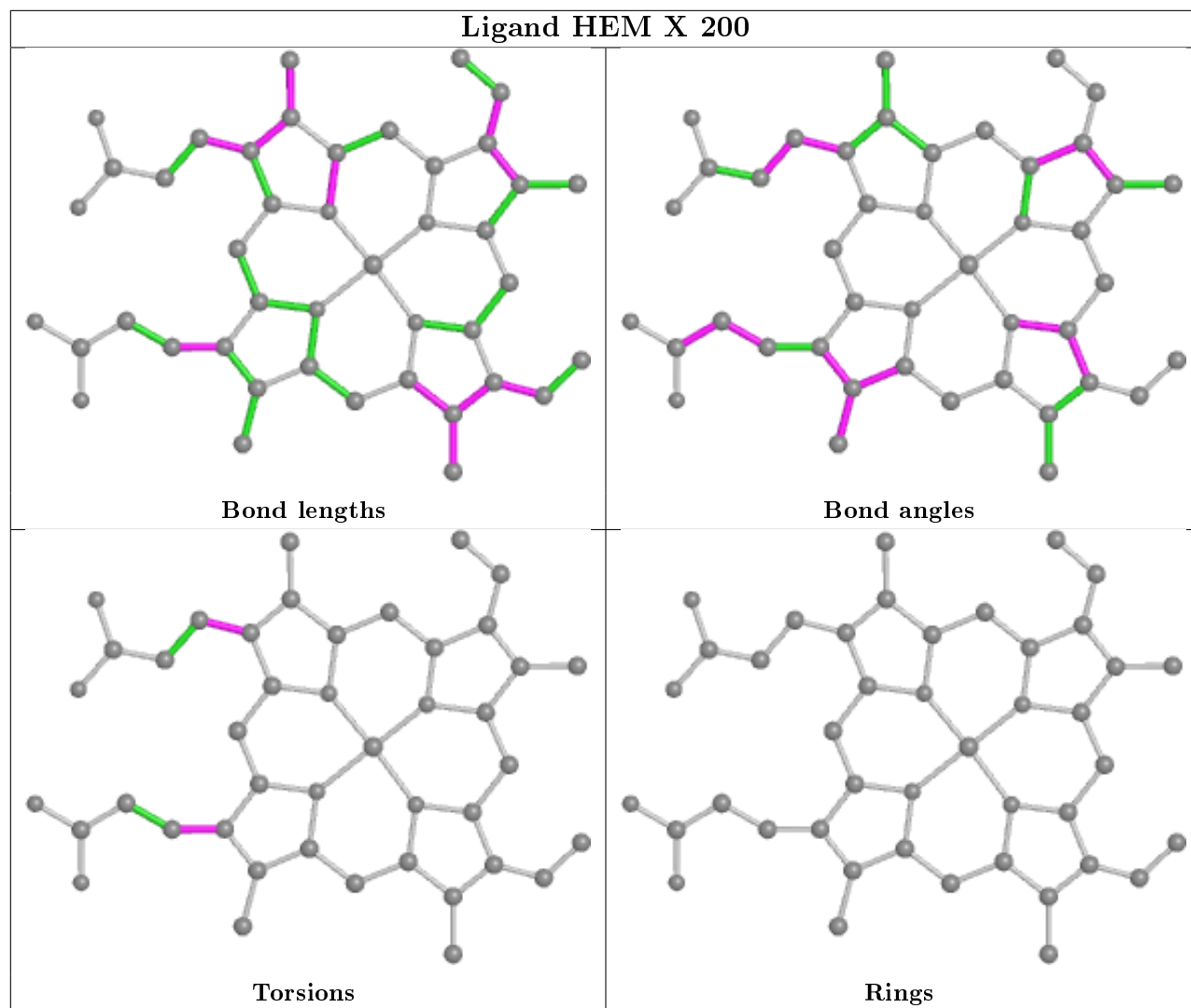


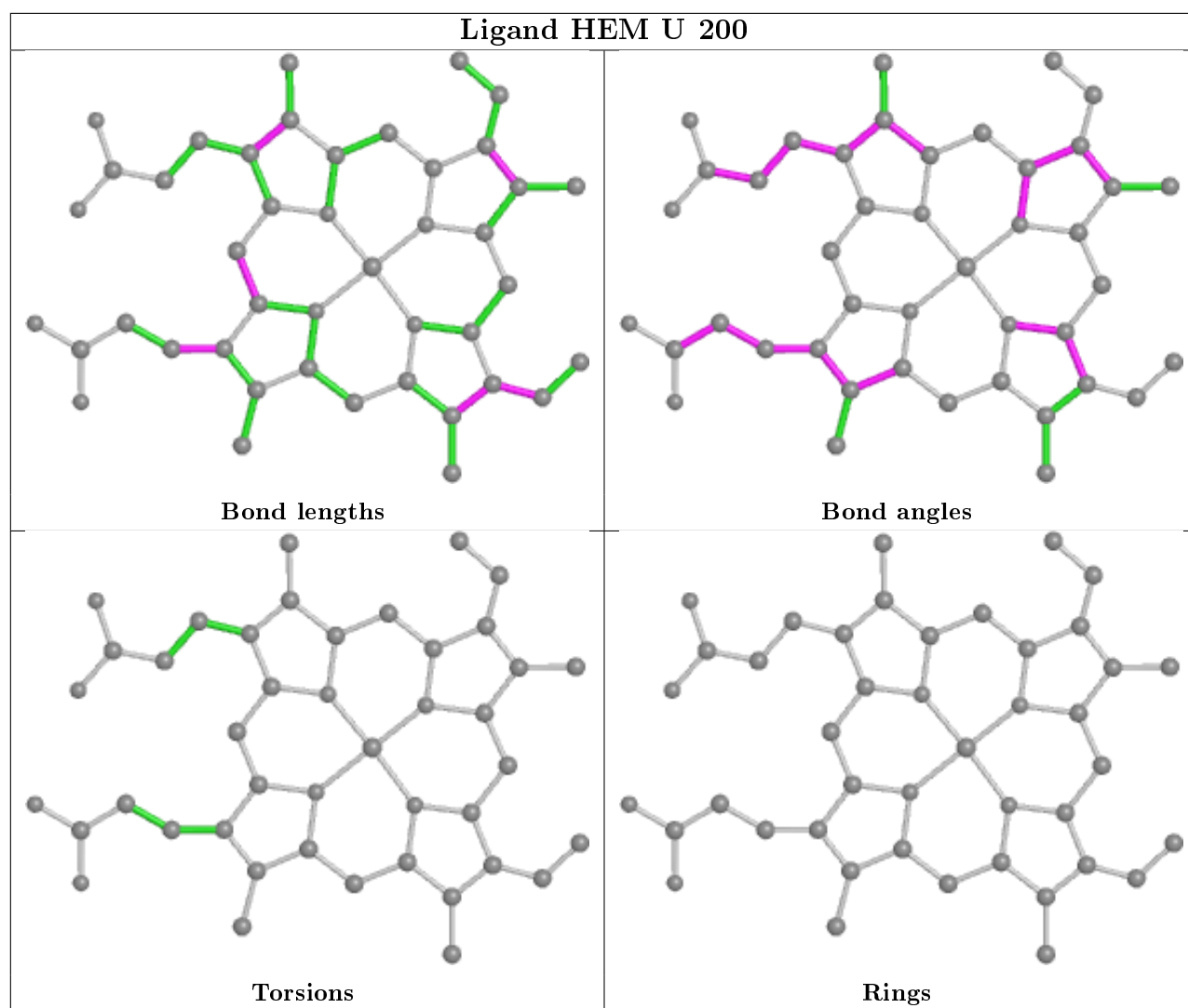


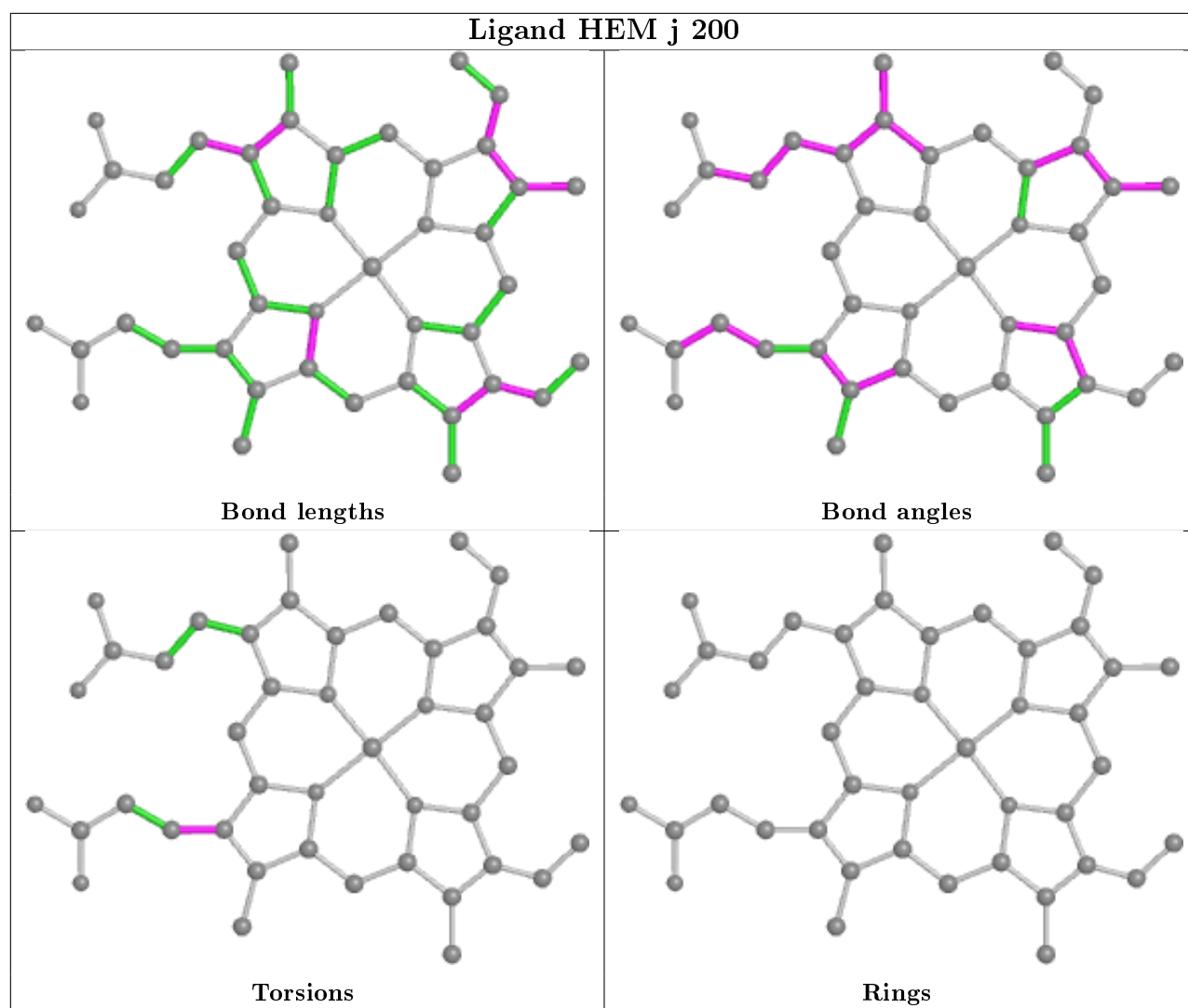


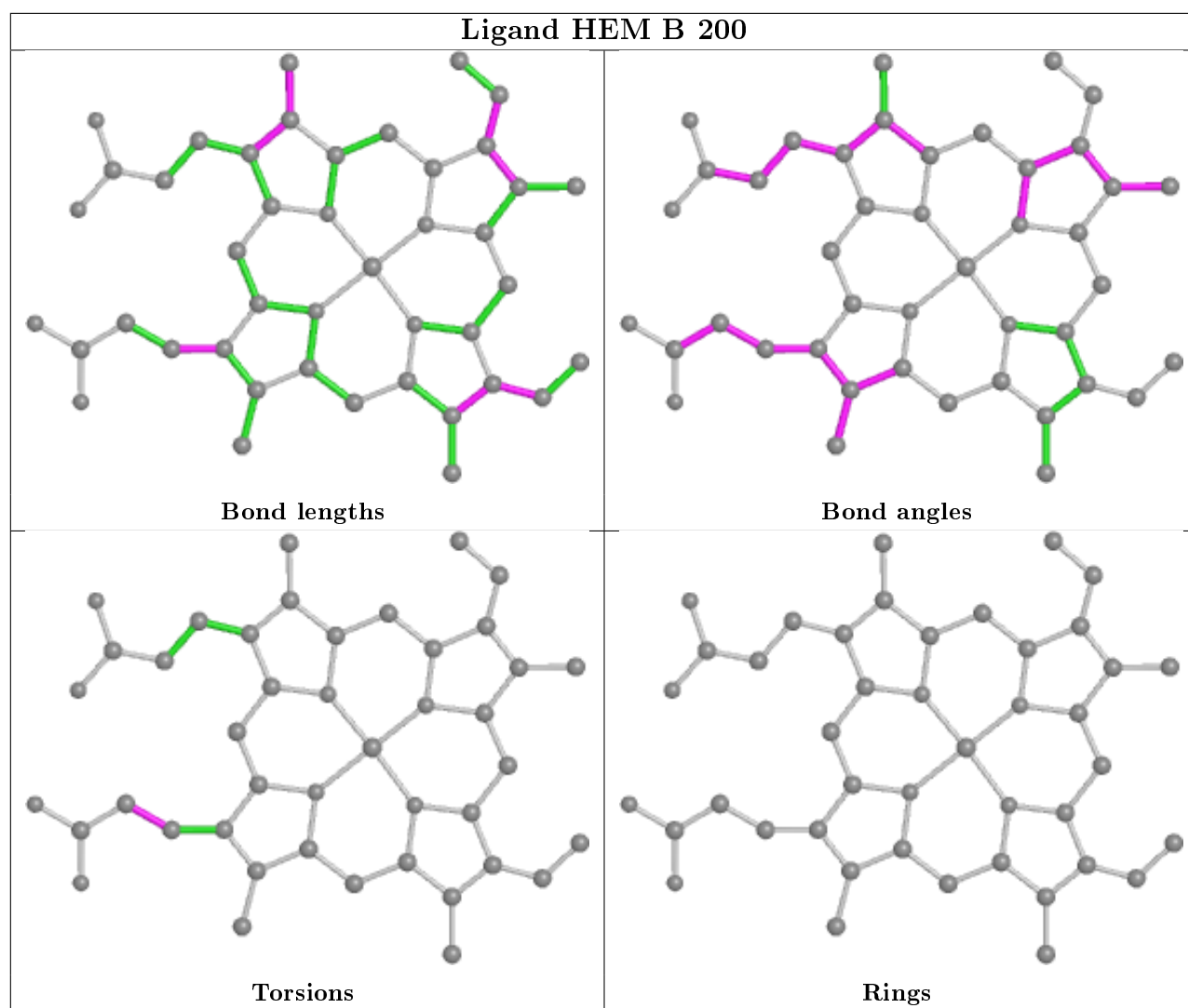


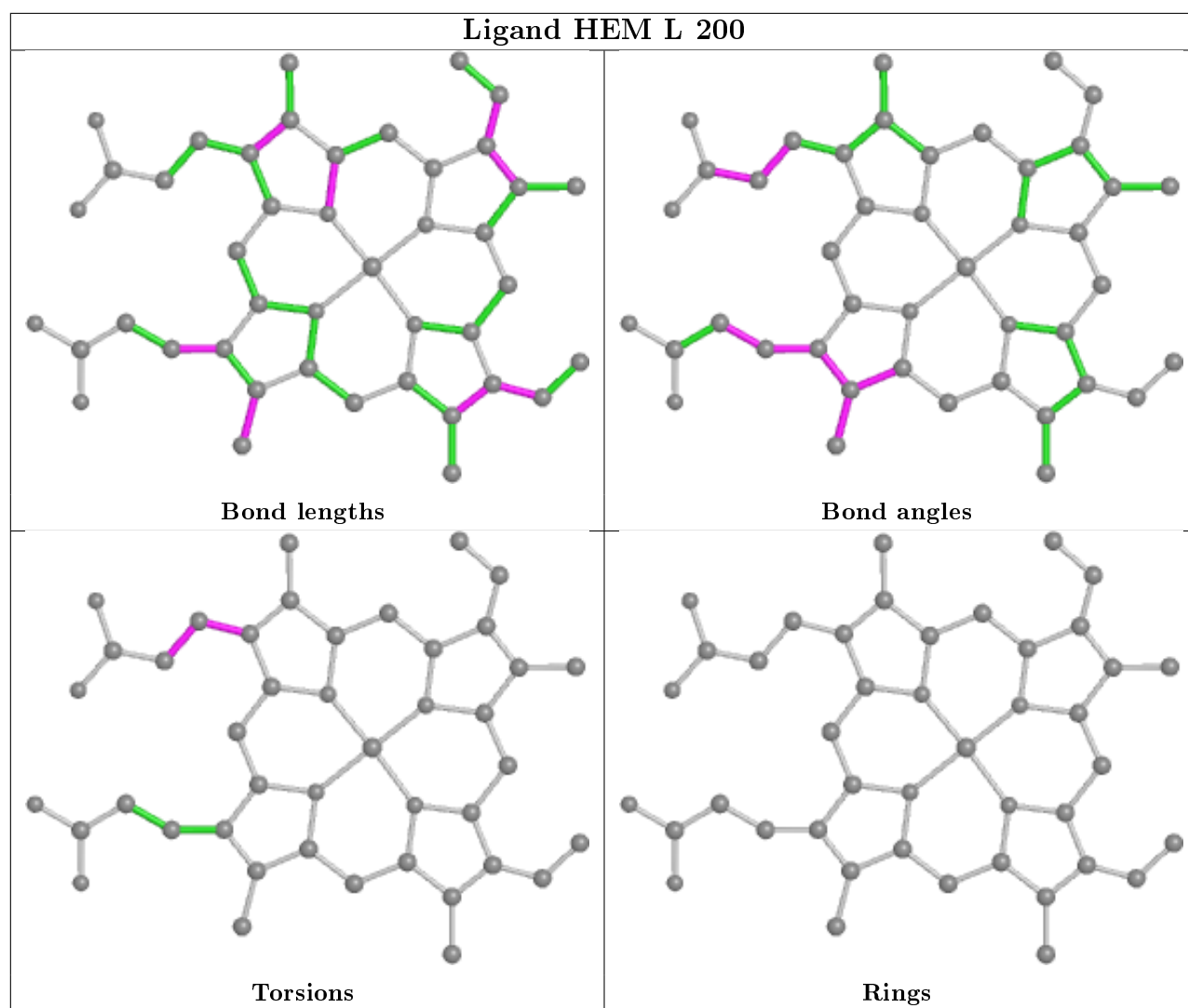


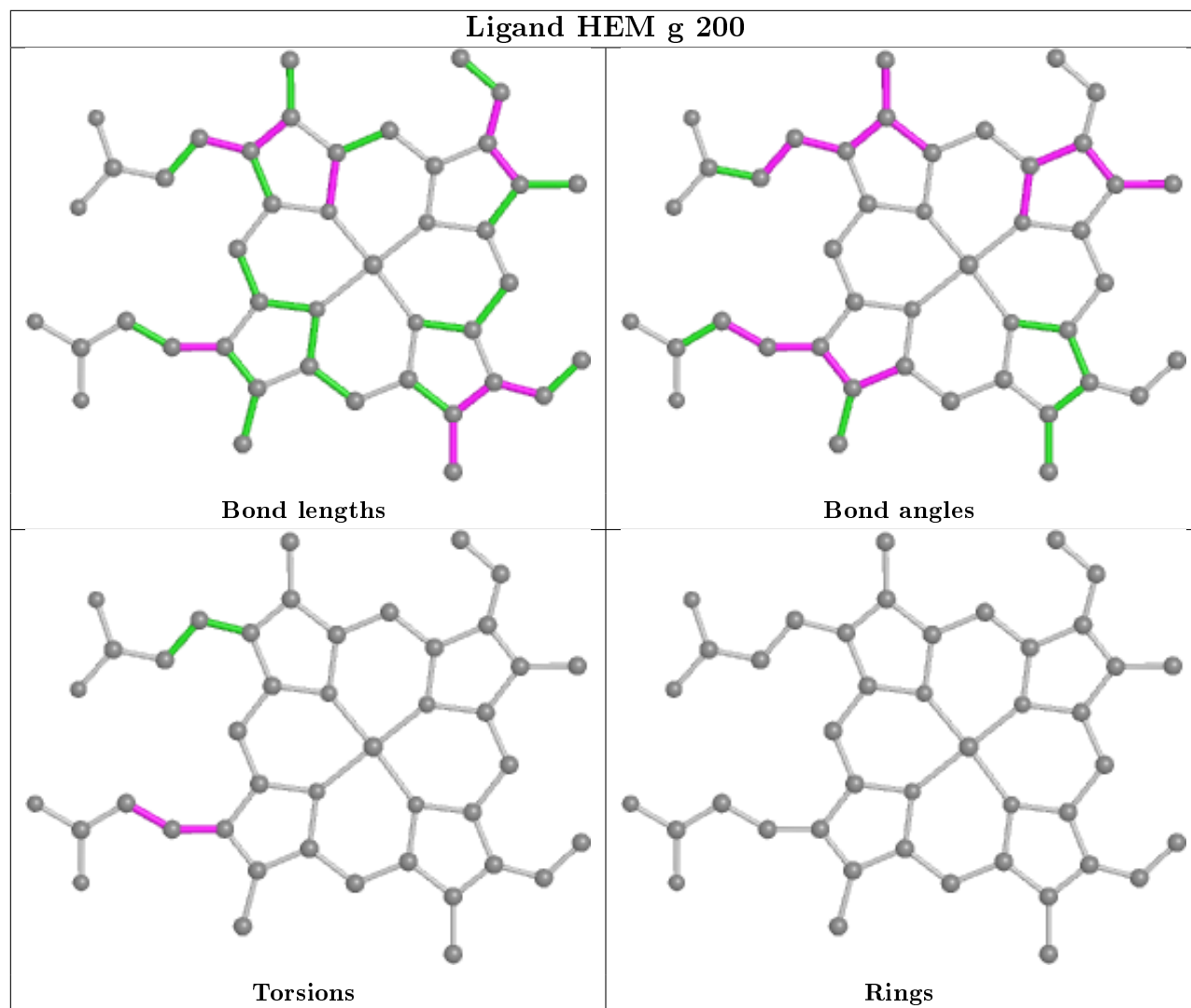


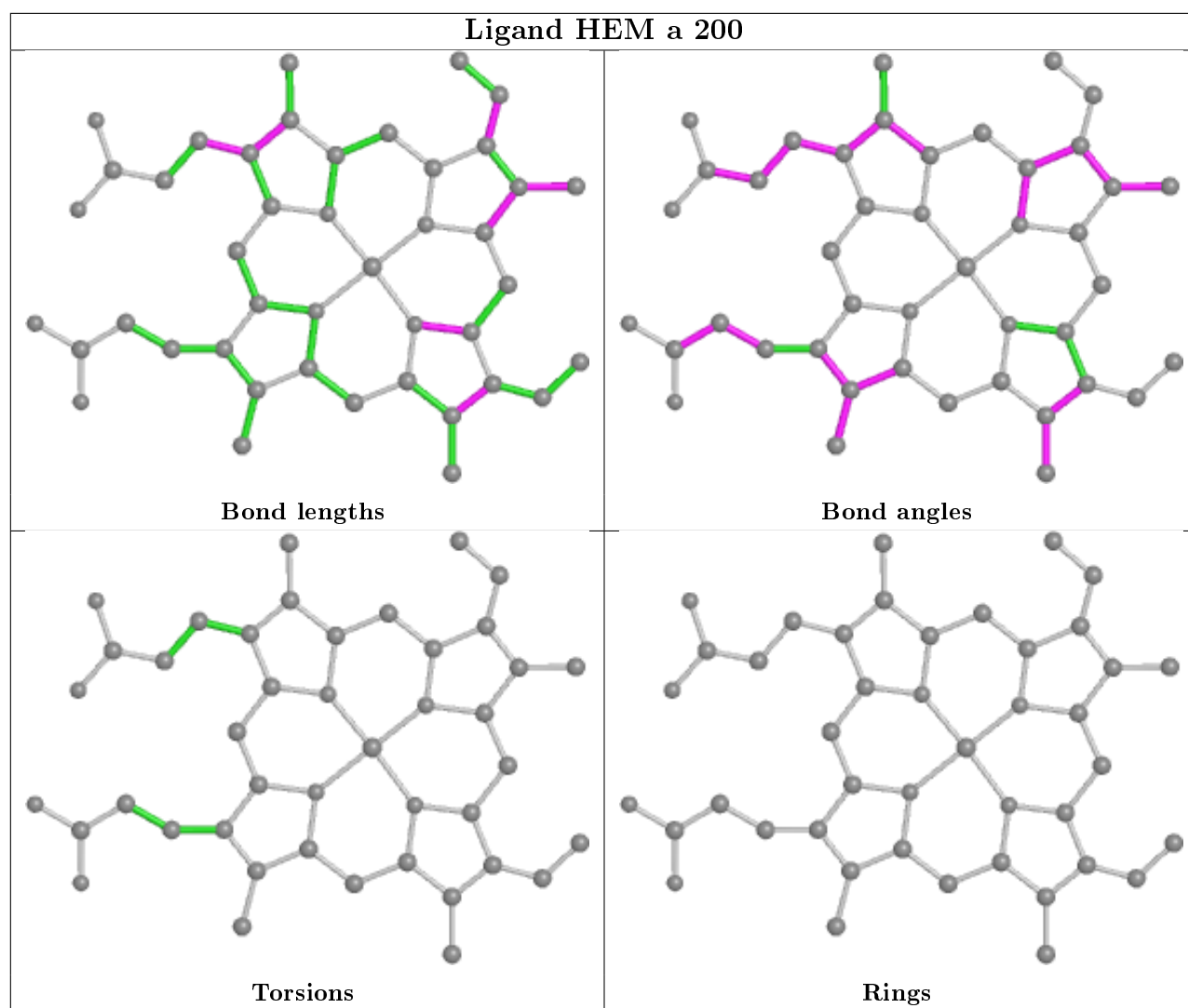


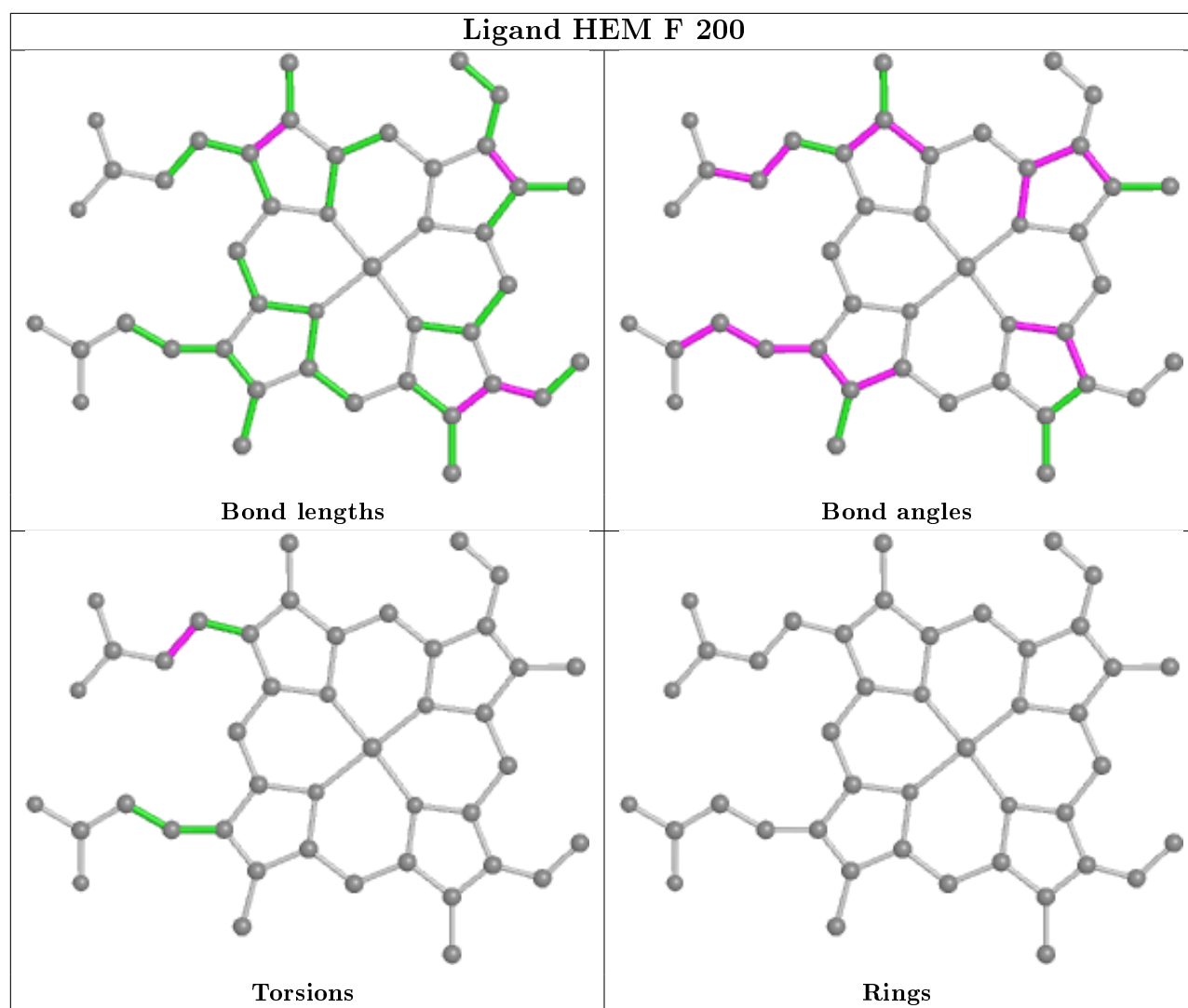


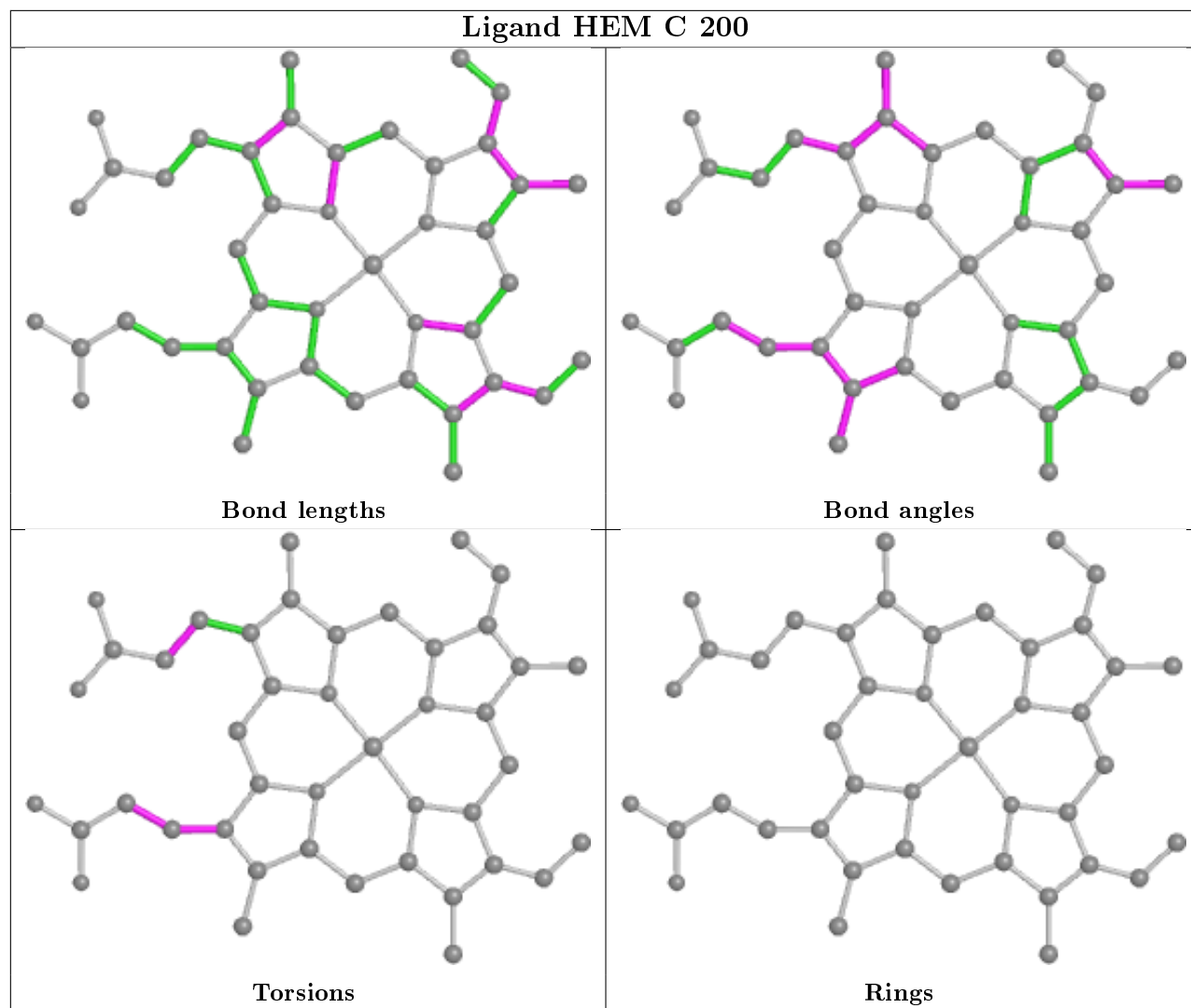


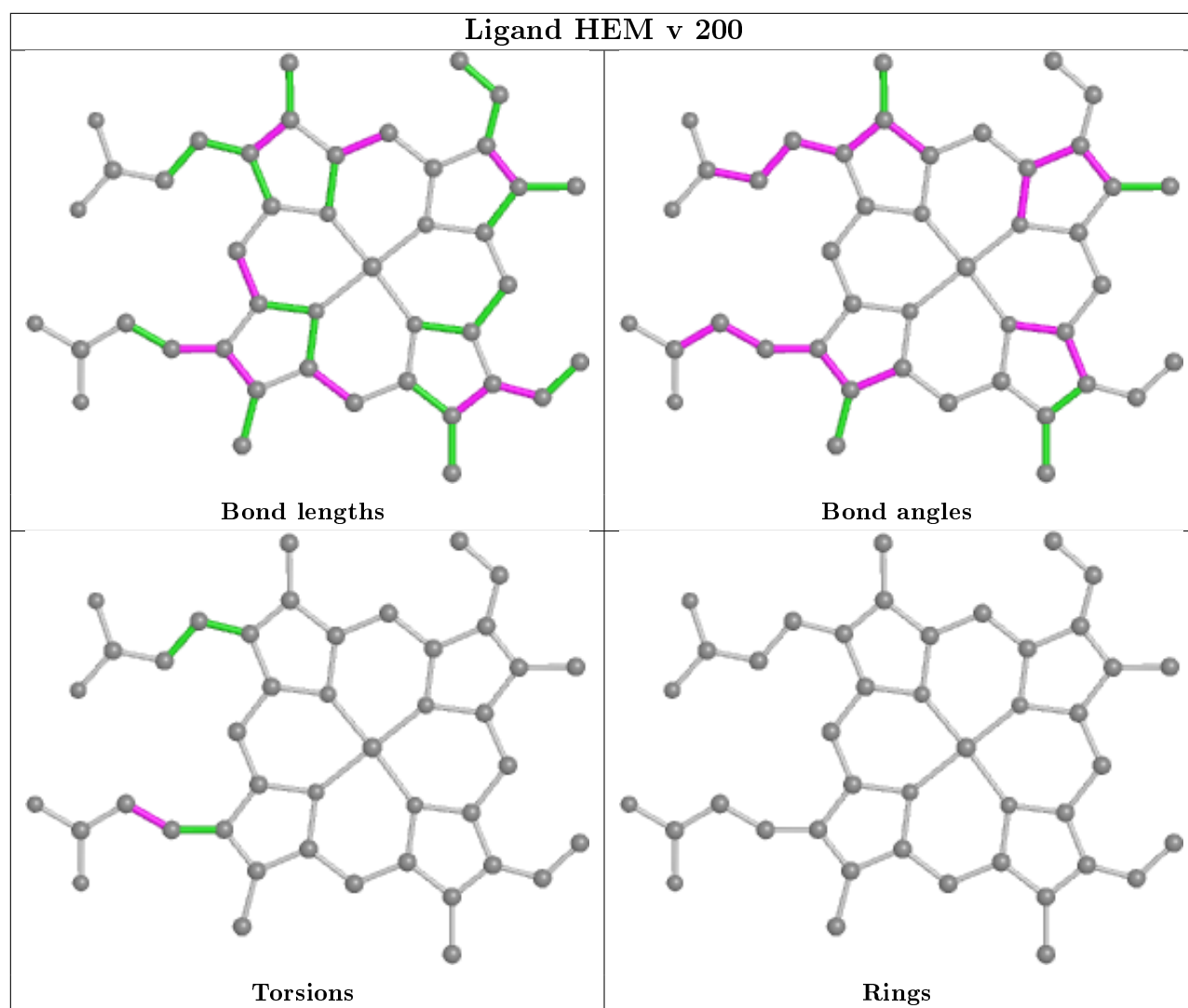


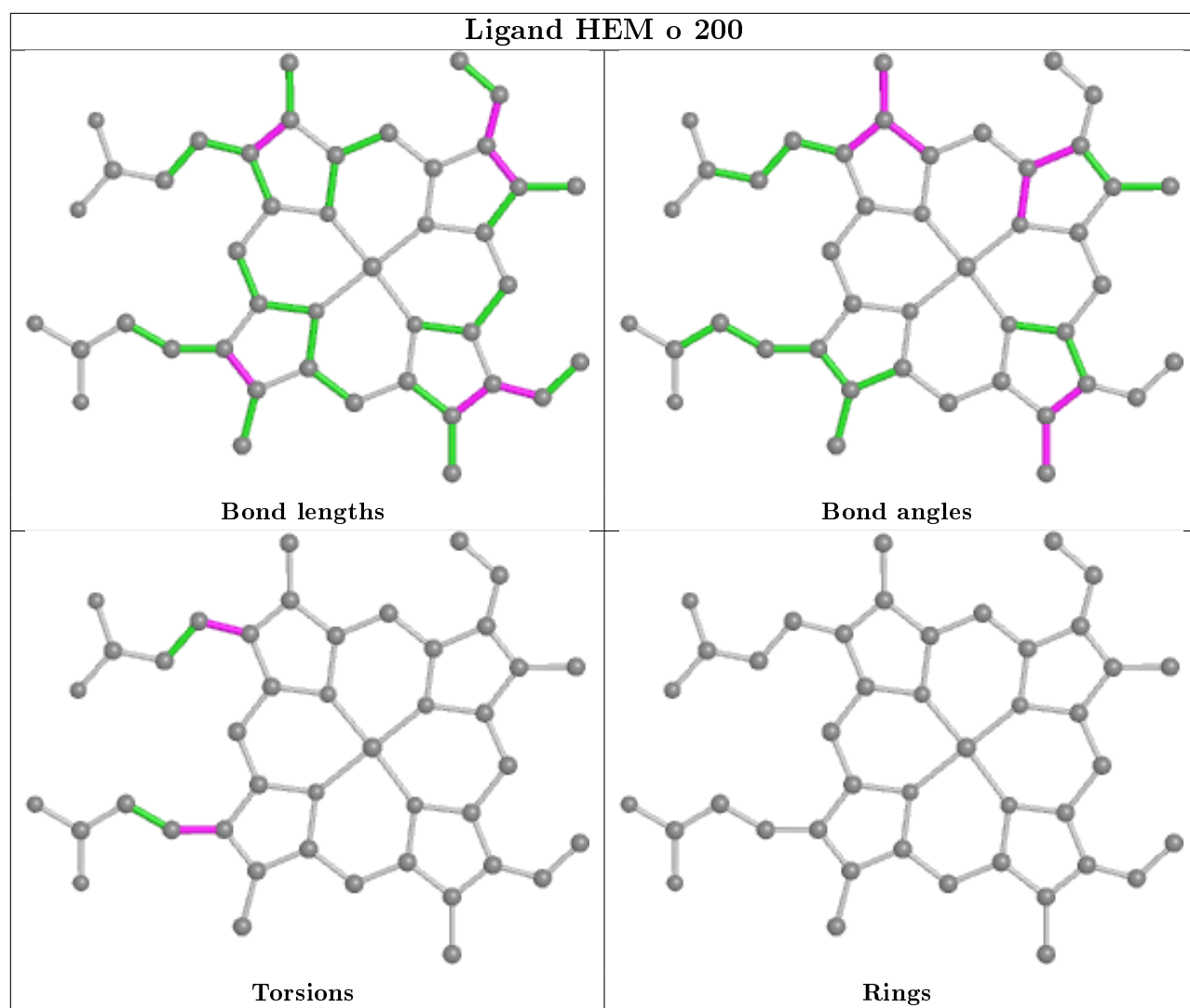


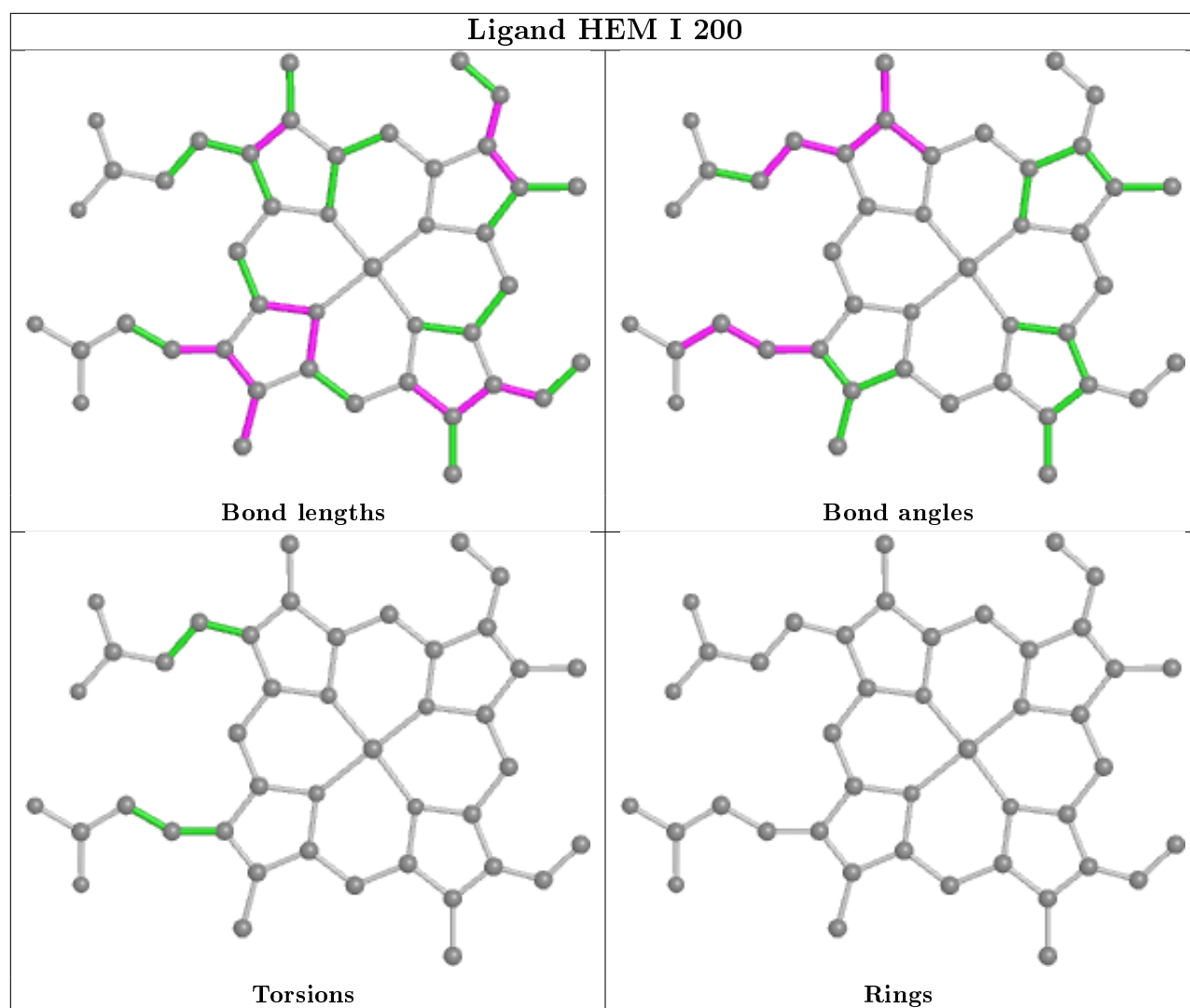












5.7 Other polymers [i](#)

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(Å²)	Q<0.9	
1	A	159/161 (98%)	-0.32	0	100	100	16, 24, 32, 39	0
1	B	159/161 (98%)	-0.32	0	100	100	15, 25, 33, 41	0
1	C	159/161 (98%)	-0.24	0	100	100	16, 25, 33, 39	0
1	D	159/161 (98%)	-0.28	0	100	100	16, 24, 33, 43	0
1	E	159/161 (98%)	-0.14	0	100	100	16, 25, 34, 42	0
1	F	159/161 (98%)	-0.23	0	100	100	16, 24, 32, 39	0
1	G	159/161 (98%)	-0.26	0	100	100	16, 23, 32, 36	0
1	H	159/161 (98%)	-0.27	0	100	100	12, 22, 30, 41	0
1	I	159/161 (98%)	-0.37	0	100	100	14, 22, 31, 36	0
1	J	159/161 (98%)	-0.35	0	100	100	14, 22, 30, 41	0
1	K	159/161 (98%)	-0.31	0	100	100	15, 25, 33, 37	0
1	L	159/161 (98%)	-0.32	0	100	100	14, 24, 33, 42	0
1	M	159/161 (98%)	-0.29	0	100	100	17, 26, 34, 45	0
1	N	159/161 (98%)	-0.31	0	100	100	17, 24, 34, 39	0
1	O	159/161 (98%)	-0.27	0	100	100	16, 22, 31, 40	0
1	P	159/161 (98%)	-0.30	0	100	100	13, 23, 31, 38	0
1	Q	159/161 (98%)	-0.14	0	100	100	16, 26, 36, 44	0
1	R	159/161 (98%)	-0.17	0	100	100	16, 24, 32, 46	0
1	S	159/161 (98%)	-0.27	0	100	100	13, 20, 29, 35	0
1	T	159/161 (98%)	-0.29	0	100	100	12, 20, 28, 42	0
1	U	159/161 (98%)	-0.28	0	100	100	13, 21, 30, 39	0
1	V	159/161 (98%)	-0.37	0	100	100	15, 22, 30, 36	0
1	W	159/161 (98%)	-0.22	0	100	100	17, 26, 35, 42	0
1	X	159/161 (98%)	-0.33	0	100	100	14, 23, 31, 44	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	159/161 (98%)	-0.29	0 100 100	13, 22, 31, 38	0
1	b	159/161 (98%)	-0.25	0 100 100	14, 23, 32, 40	0
1	c	159/161 (98%)	-0.32	0 100 100	17, 25, 34, 40	0
1	d	159/161 (98%)	-0.27	0 100 100	17, 25, 34, 43	0
1	e	159/161 (98%)	-0.28	0 100 100	20, 28, 36, 46	0
1	f	159/161 (98%)	-0.28	1 (0%) 89 90	17, 25, 34, 42	0
1	g	159/161 (98%)	-0.24	0 100 100	15, 24, 32, 39	0
1	h	159/161 (98%)	-0.35	0 100 100	16, 23, 32, 42	0
1	i	159/161 (98%)	-0.36	0 100 100	15, 22, 34, 38	0
1	j	159/161 (98%)	-0.34	0 100 100	14, 22, 30, 39	0
1	k	159/161 (98%)	-0.22	0 100 100	14, 23, 33, 38	0
1	l	159/161 (98%)	-0.32	0 100 100	14, 23, 32, 39	0
1	m	159/161 (98%)	-0.26	0 100 100	15, 22, 33, 38	0
1	n	159/161 (98%)	-0.25	0 100 100	15, 23, 32, 42	0
1	o	159/161 (98%)	-0.29	0 100 100	16, 24, 30, 36	0
1	p	159/161 (98%)	-0.32	0 100 100	18, 24, 31, 41	0
1	q	159/161 (98%)	-0.22	0 100 100	20, 28, 36, 43	0
1	r	159/161 (98%)	-0.22	0 100 100	18, 27, 36, 43	0
1	s	159/161 (98%)	-0.34	0 100 100	14, 23, 31, 37	0
1	t	159/161 (98%)	-0.33	0 100 100	14, 21, 30, 34	0
1	u	159/161 (98%)	-0.29	0 100 100	13, 21, 29, 37	0
1	v	159/161 (98%)	-0.38	0 100 100	14, 22, 32, 39	0
1	w	159/161 (98%)	-0.28	0 100 100	16, 25, 34, 44	0
1	x	159/161 (98%)	-0.26	0 100 100	14, 21, 29, 38	0
All	All	7632/7728 (98%)	-0.28	1 (0%) 100 100	12, 24, 33, 46	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	f	144	LEU	2.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

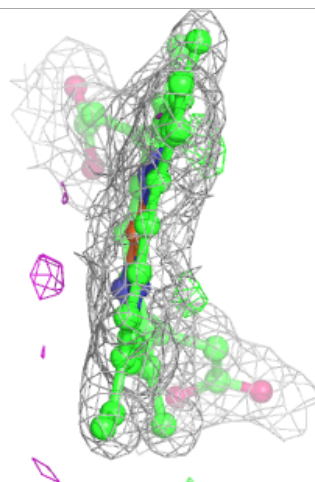
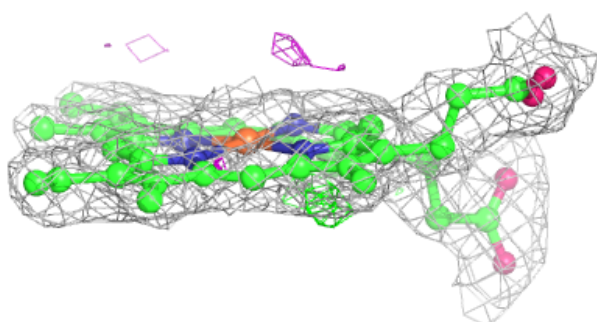
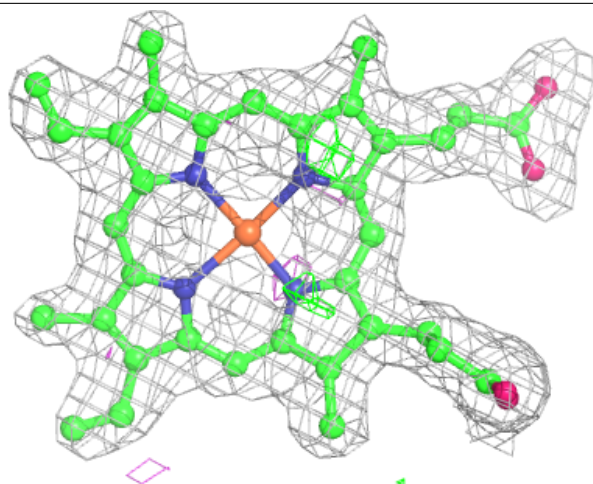
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	q	200	43/43	0.96	0.10	25,32,42,45	0
2	HEM	P	200	43/43	0.96	0.14	12,25,37,39	0
2	HEM	n	200	43/43	0.96	0.13	10,21,34,37	0
2	HEM	x	200	43/43	0.96	0.12	10,22,34,38	0
2	HEM	R	200	43/43	0.96	0.15	21,28,38,40	0
2	HEM	C	200	43/43	0.96	0.15	18,31,44,47	0
2	HEM	v	200	43/43	0.96	0.12	14,24,33,35	0
2	HEM	e	200	43/43	0.97	0.14	19,31,38,40	0
2	HEM	c	200	43/43	0.97	0.12	17,27,40,43	0
2	HEM	k	200	43/43	0.97	0.12	10,21,34,37	0
2	HEM	X	200	43/43	0.97	0.10	13,24,37,41	0
2	HEM	B	200	43/43	0.97	0.11	18,27,38,45	0
2	HEM	L	200	43/43	0.97	0.11	14,21,42,48	0
2	HEM	g	200	43/43	0.97	0.14	17,29,40,42	0
2	HEM	a	200	43/43	0.97	0.11	13,22,29,33	0
2	HEM	F	200	43/43	0.97	0.12	16,28,46,52	0
2	HEM	H	200	43/43	0.97	0.10	14,24,32,35	0
2	HEM	t	200	43/43	0.97	0.12	10,21,34,37	0
2	HEM	o	200	43/43	0.97	0.11	12,22,37,44	0
2	HEM	S	200	43/43	0.98	0.12	8,16,30,33	0
2	HEM	M	200	43/43	0.98	0.11	14,24,43,53	0
2	HEM	U	200	43/43	0.98	0.10	10,20,26,33	0
2	HEM	j	200	43/43	0.98	0.11	6,18,36,37	0
2	HEM	I	200	43/43	0.98	0.11	10,21,34,37	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.

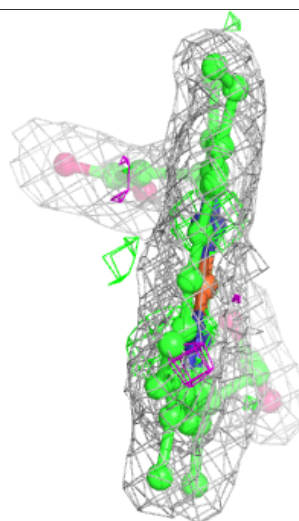
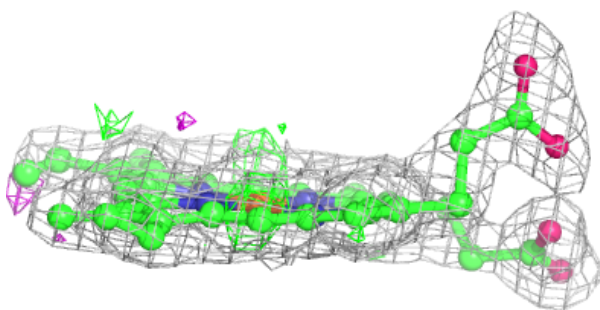
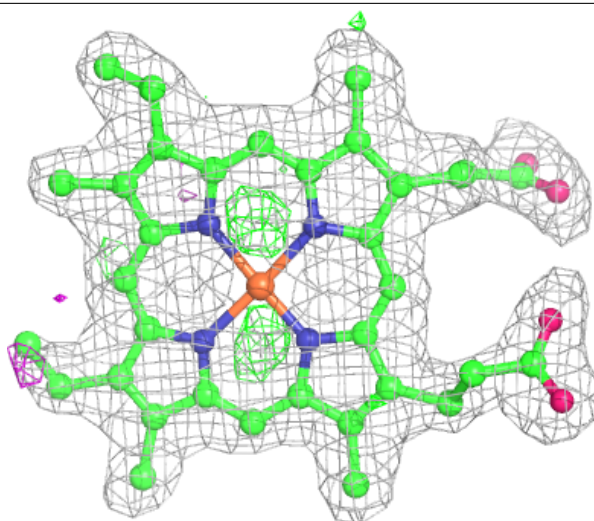
Electron density around HEM q 200:

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



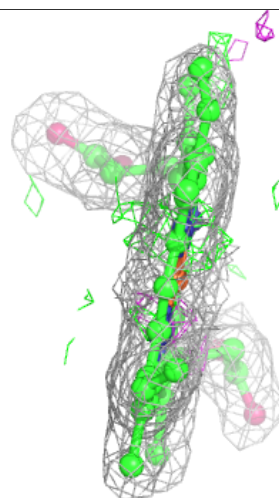
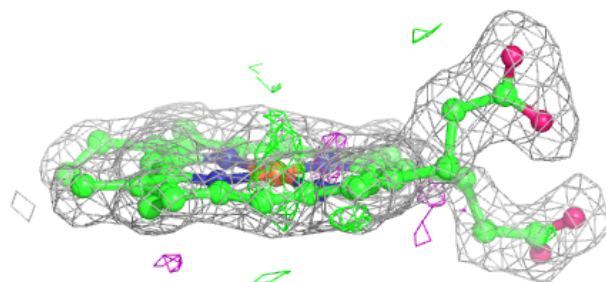
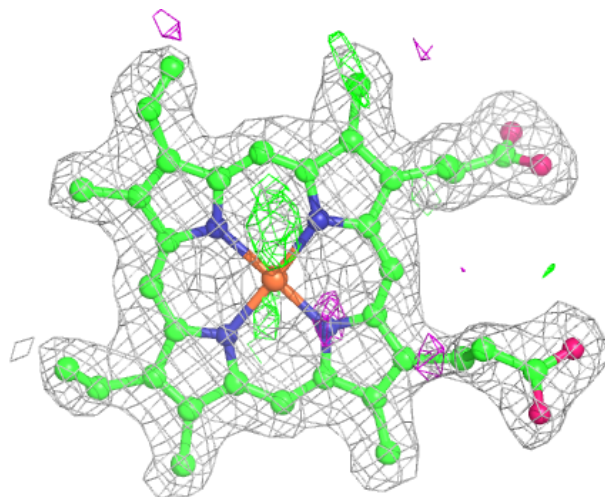
Electron density around HEM P 200:

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



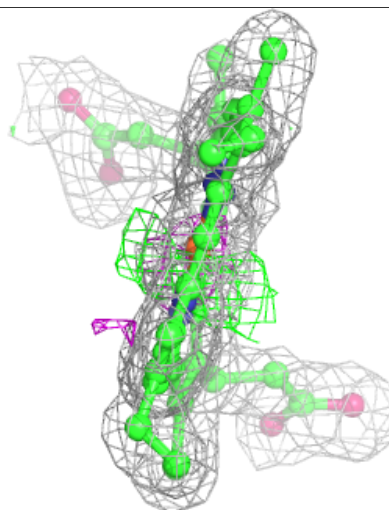
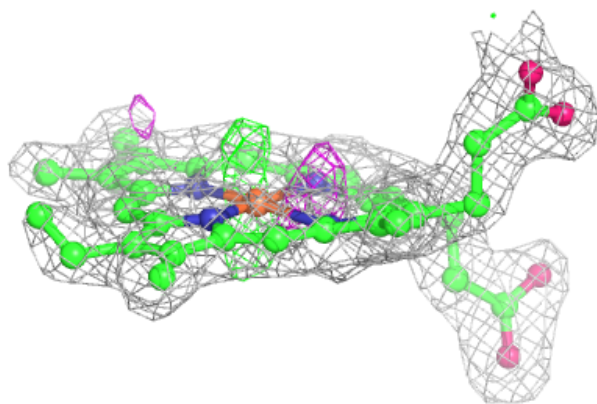
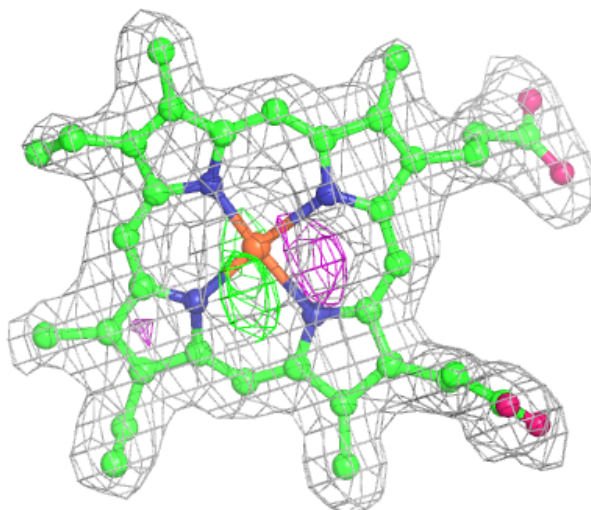
Electron density around HEM n 200:

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



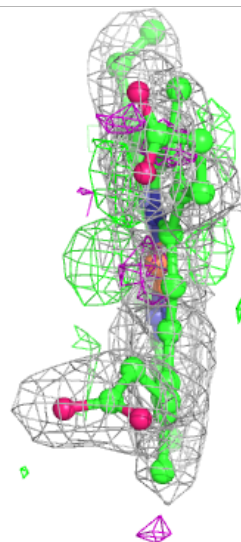
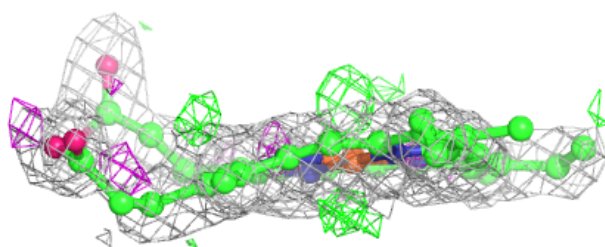
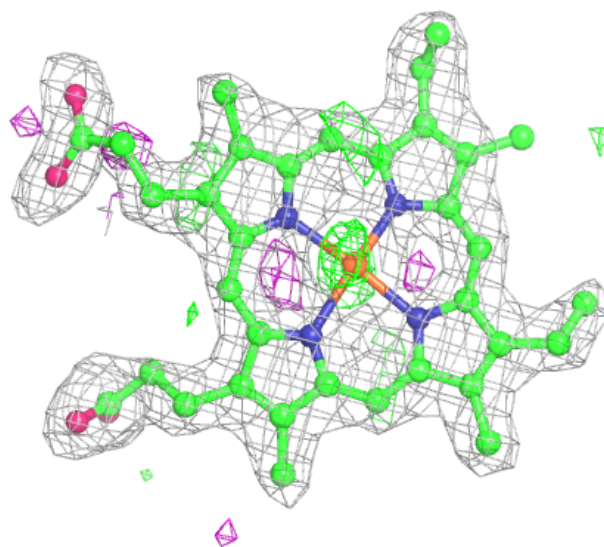
Electron density around HEM x 200:

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



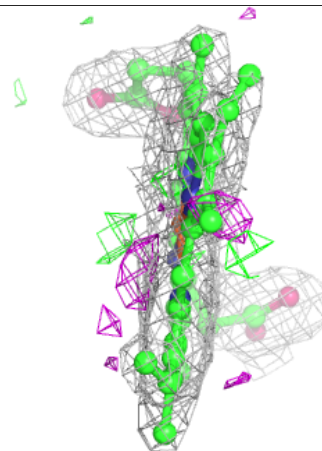
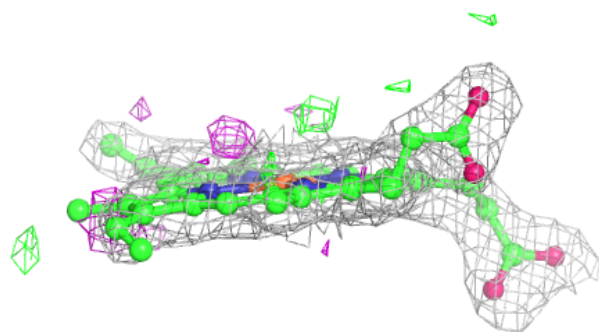
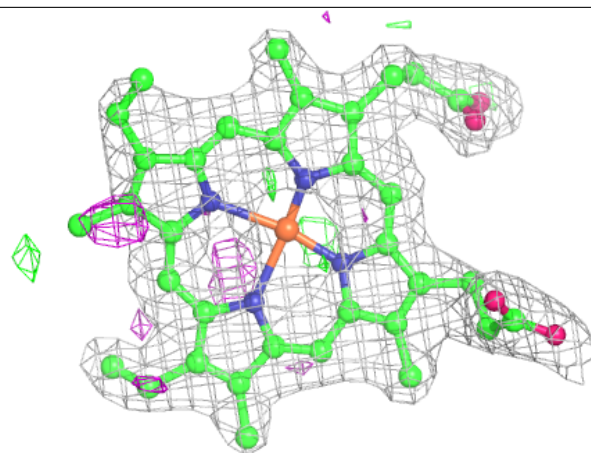
Electron density around HEM R 200:

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



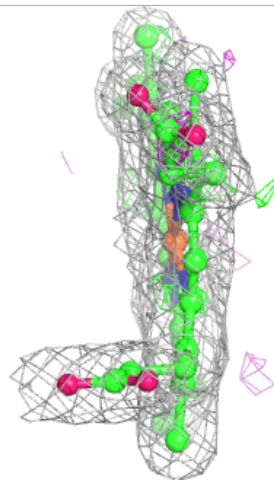
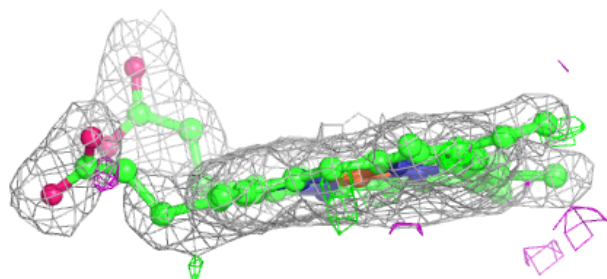
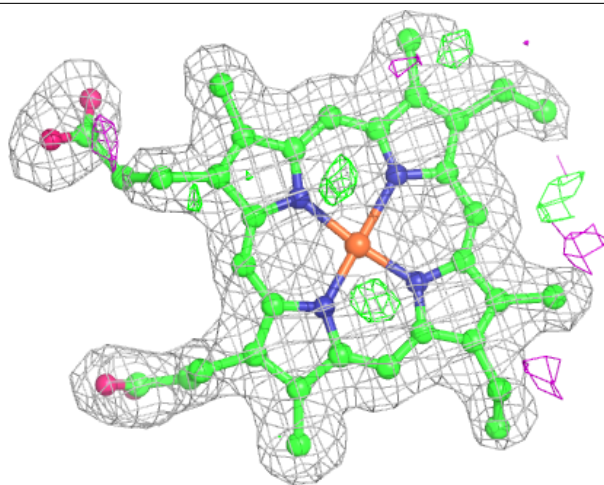
Electron density around HEM C 200:

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



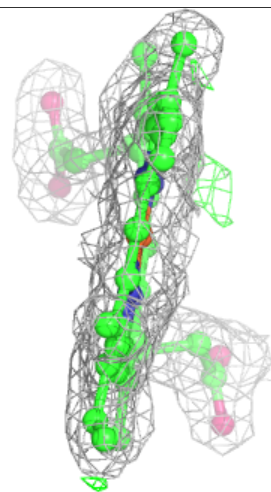
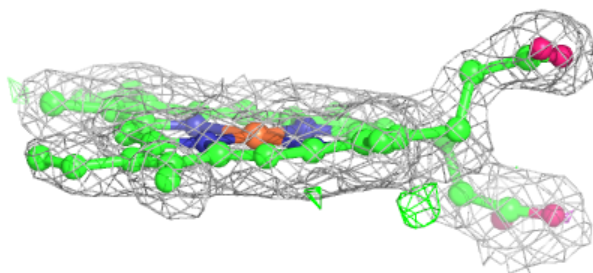
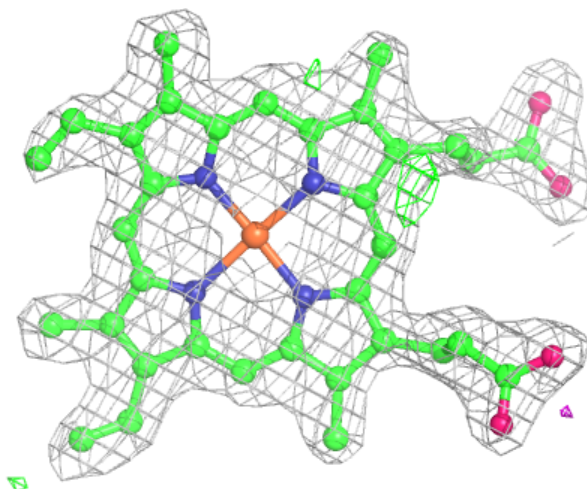
Electron density around HEM v 200:

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



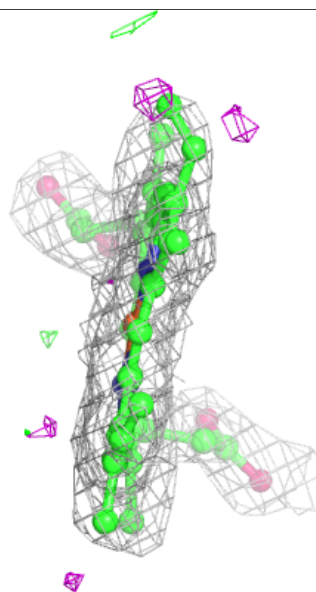
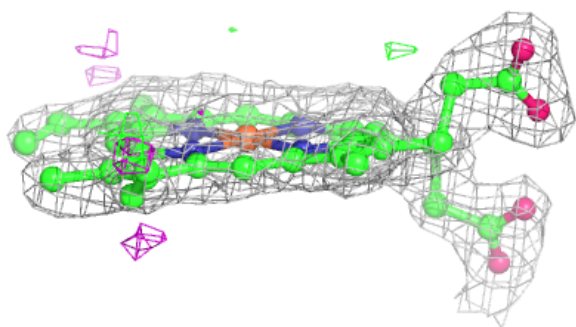
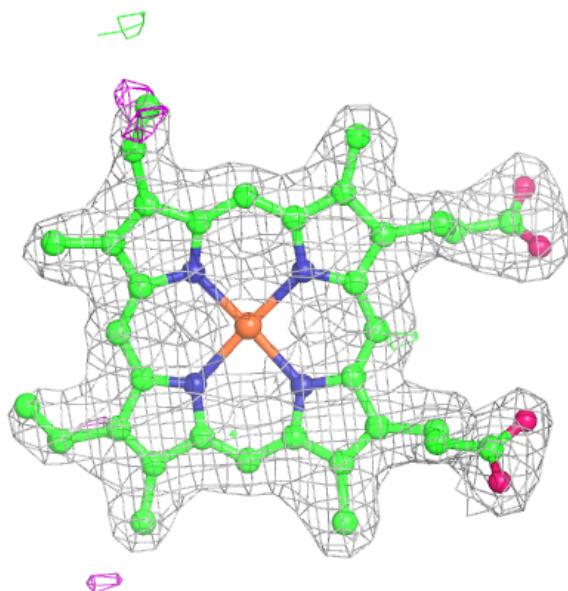
Electron density around HEM e 200:

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



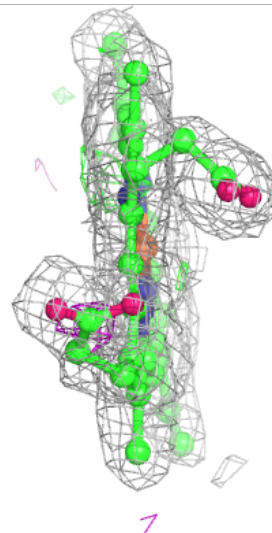
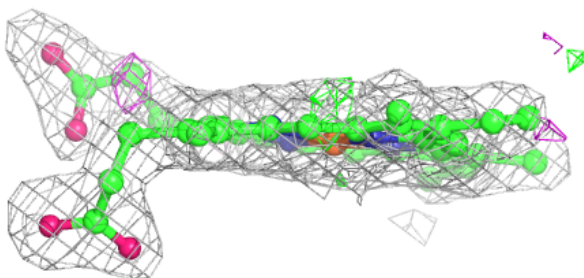
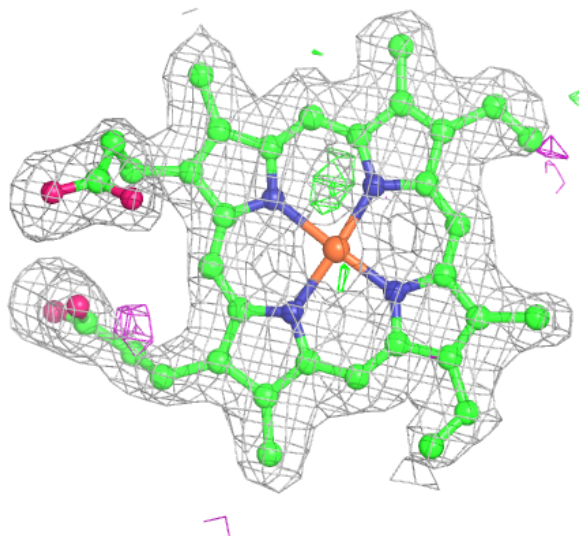
Electron density around HEM c 200:

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



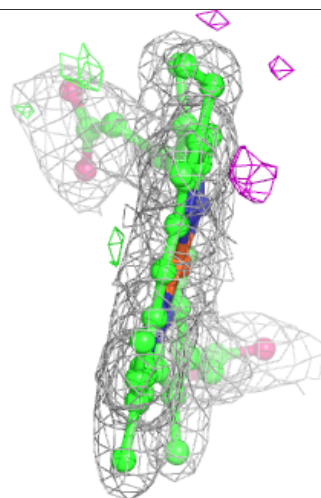
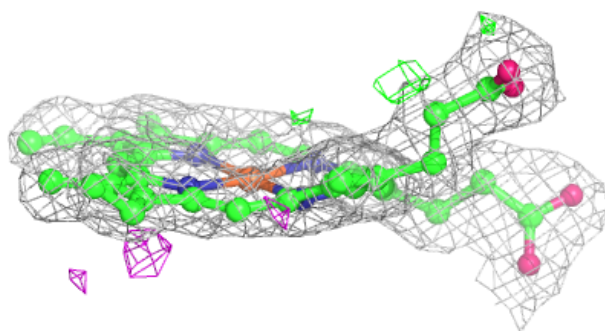
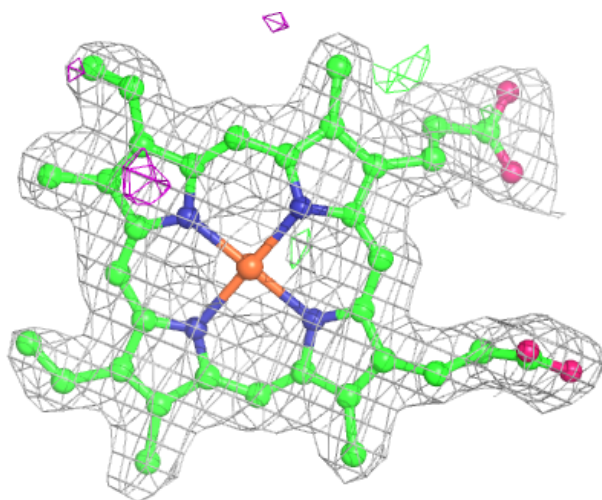
Electron density around HEM k 200:

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



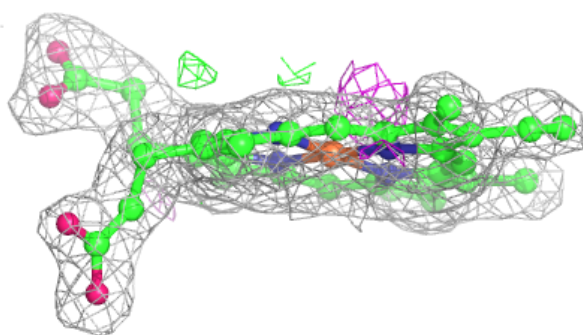
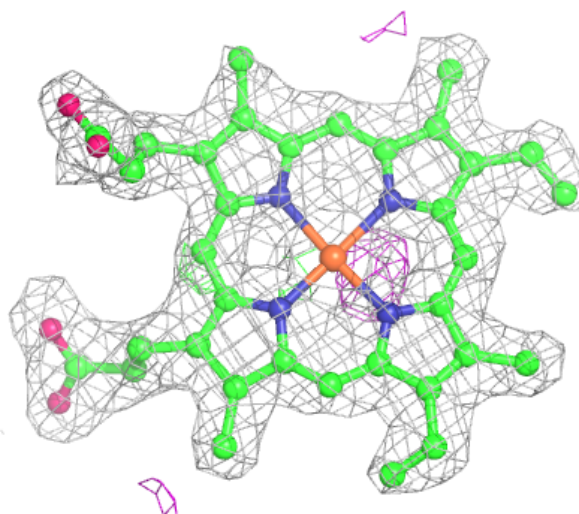
Electron density around HEM X 200:

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



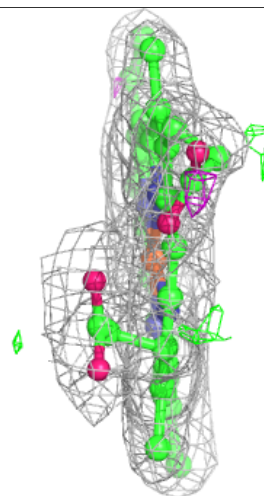
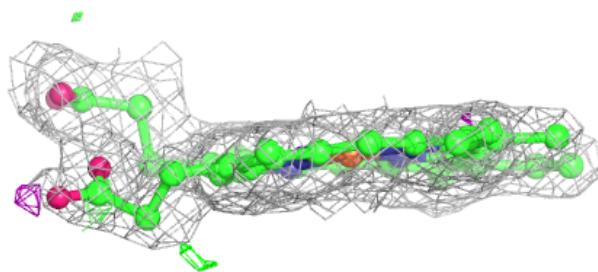
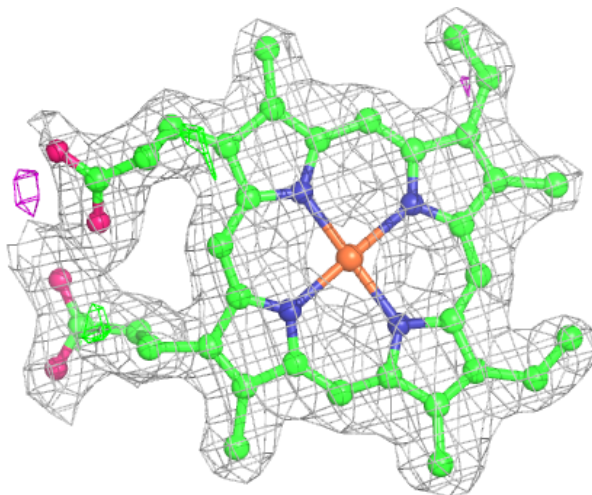
Electron density around HEM B 200:

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



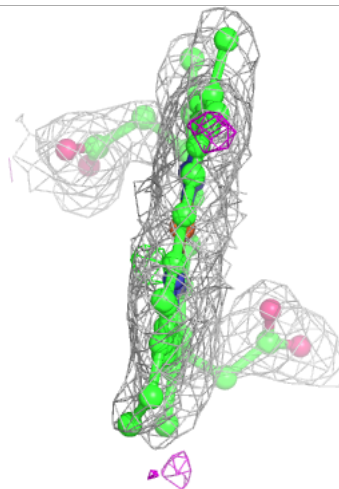
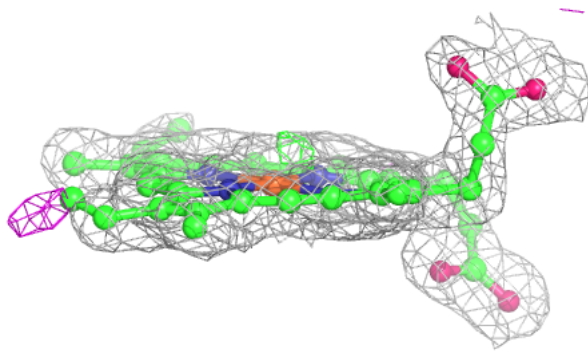
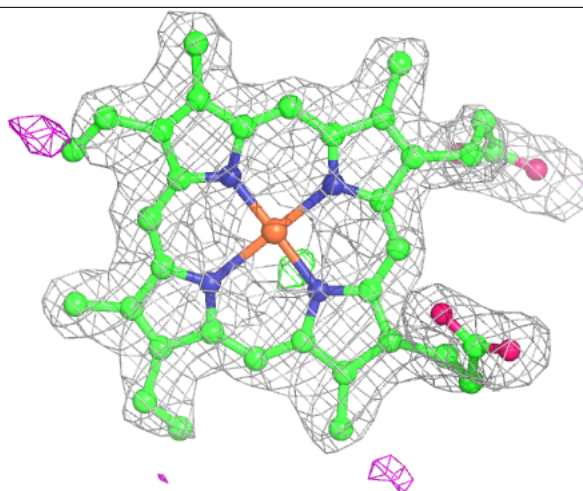
Electron density around HEM L 200:

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



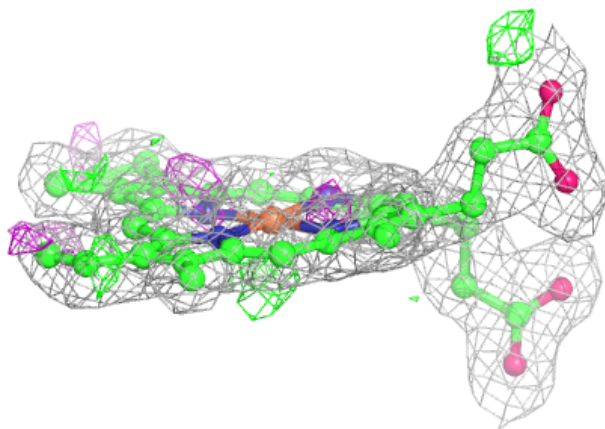
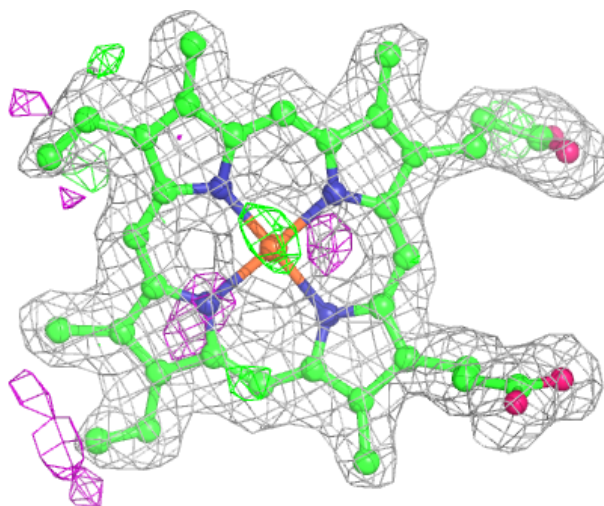
Electron density around HEM g 200:

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



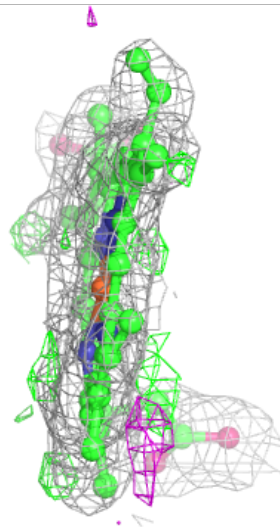
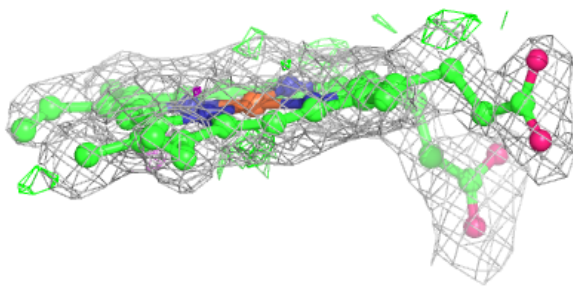
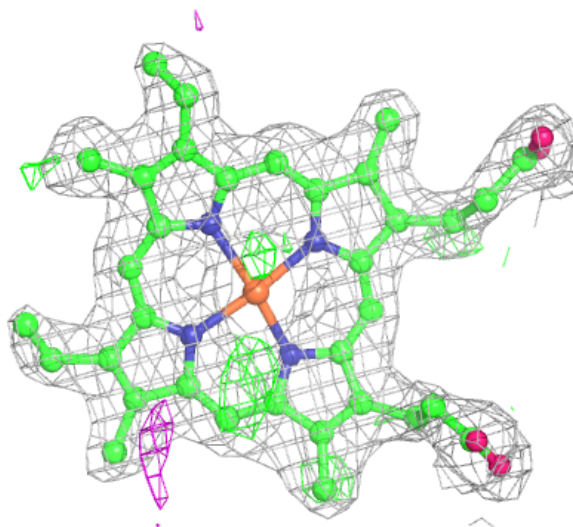
Electron density around HEM a 200:

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



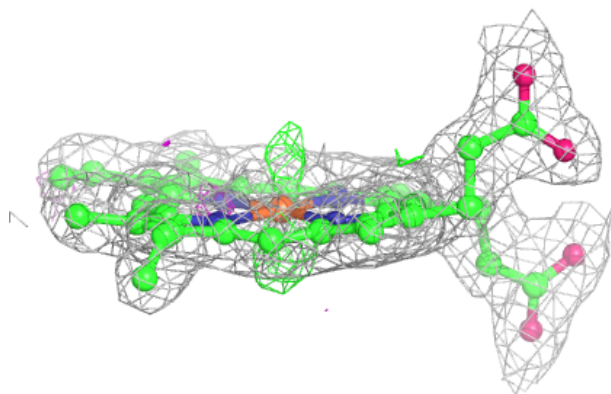
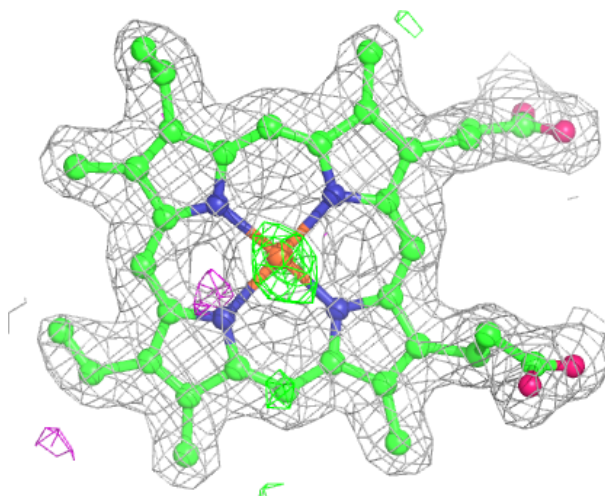
Electron density around HEM F 200:

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



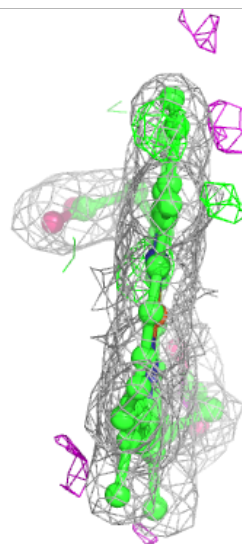
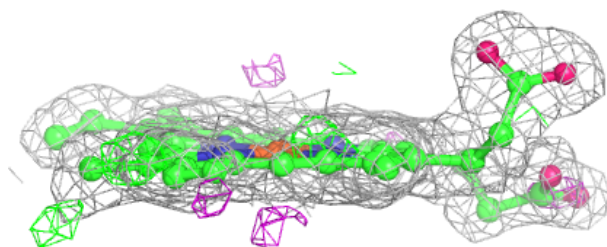
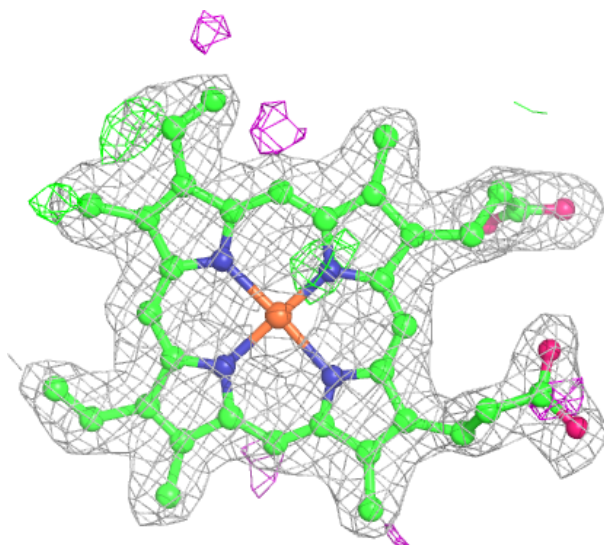
Electron density around HEM H 200:

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



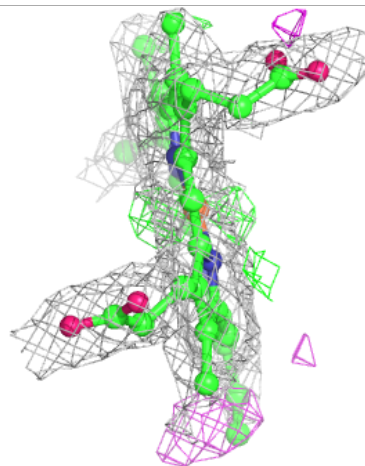
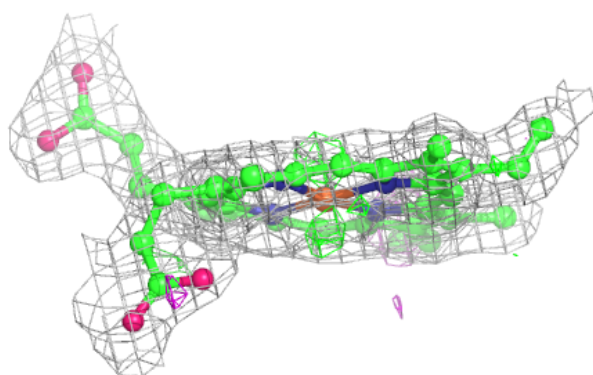
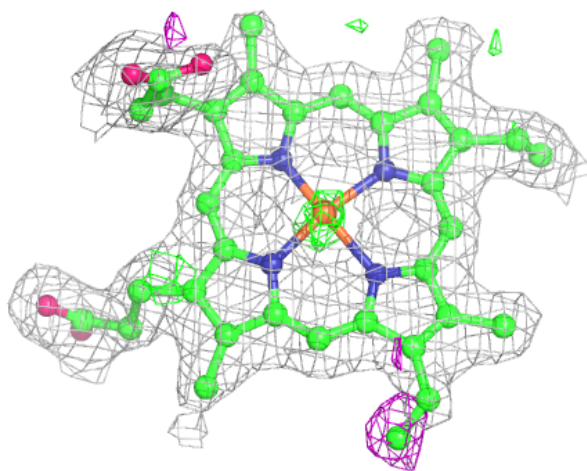
Electron density around HEM t 200:

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



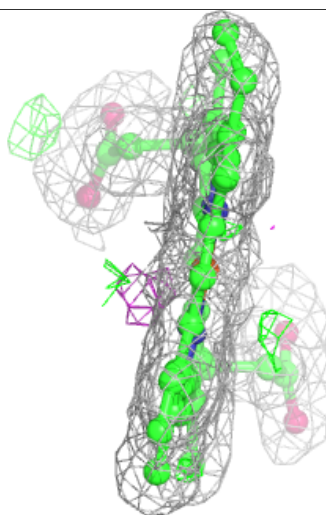
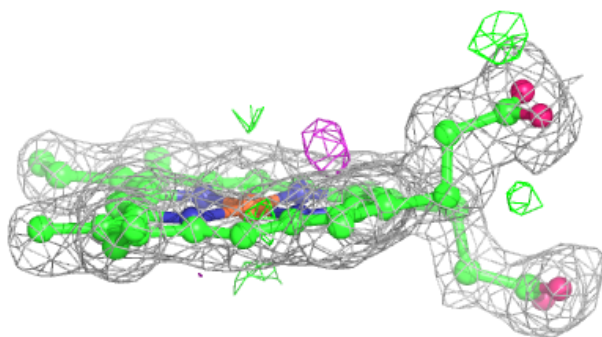
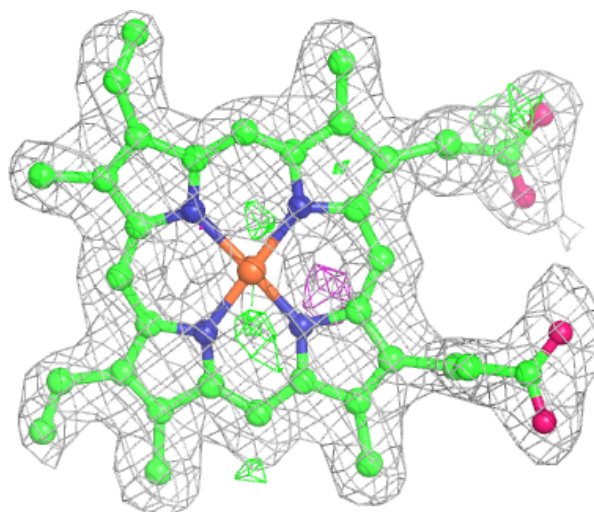
Electron density around HEM o 200:

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



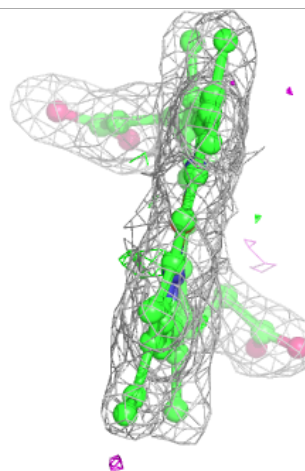
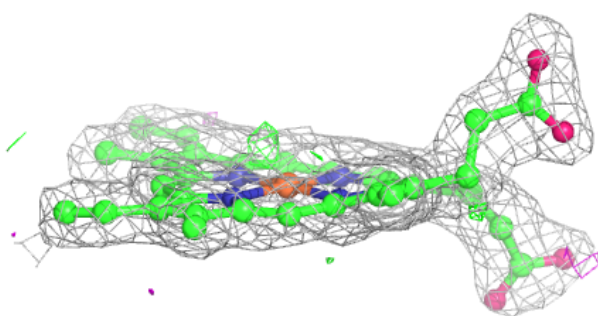
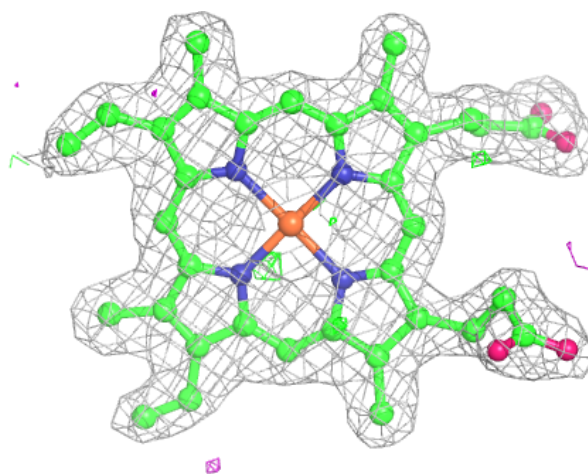
Electron density around HEM S 200:

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



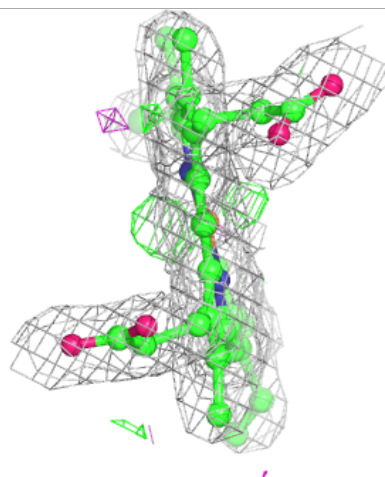
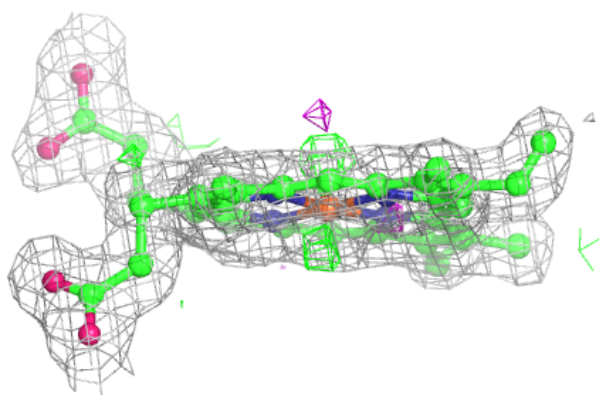
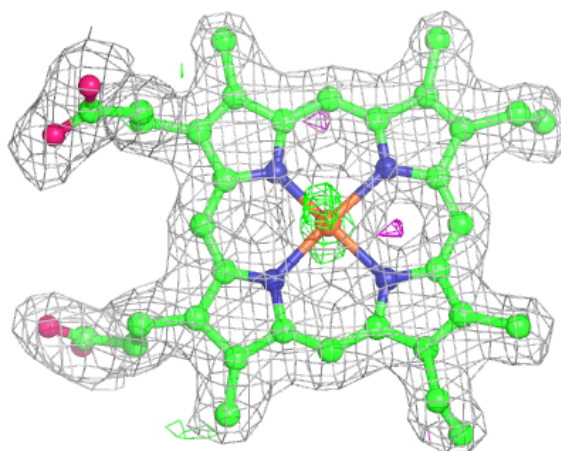
Electron density around HEM M 200:

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



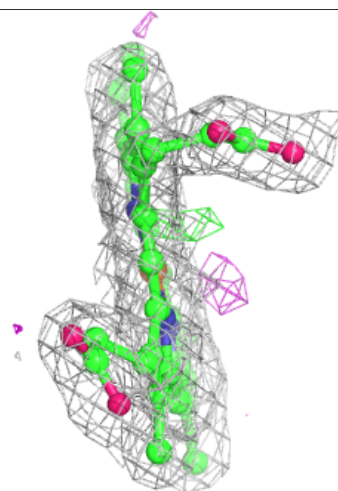
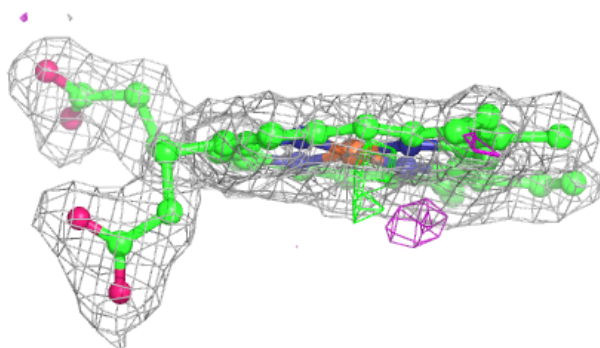
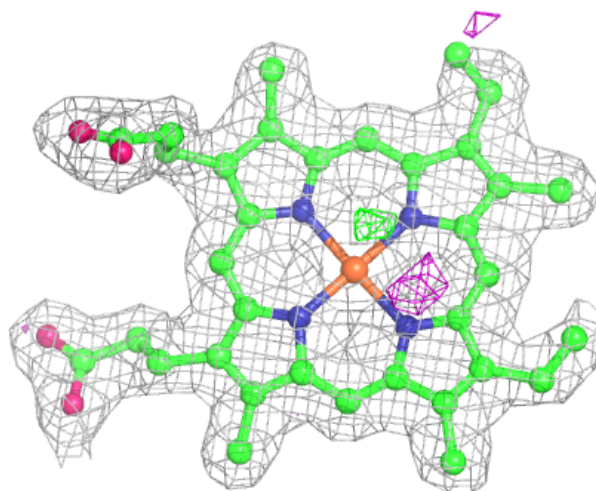
Electron density around HEM U 200:

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



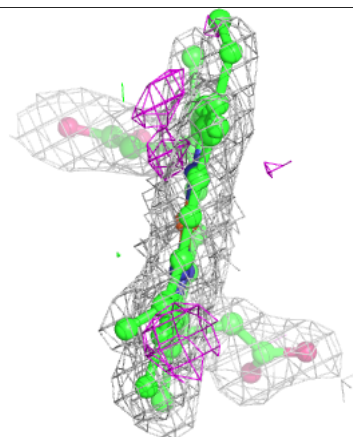
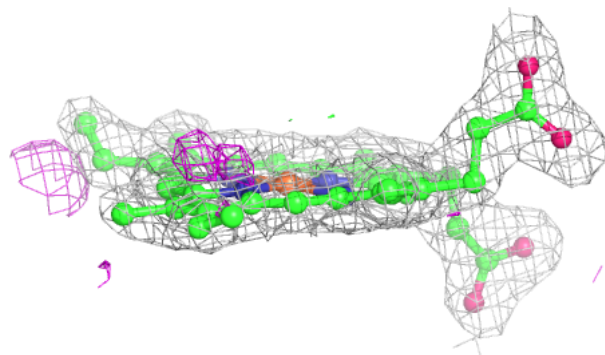
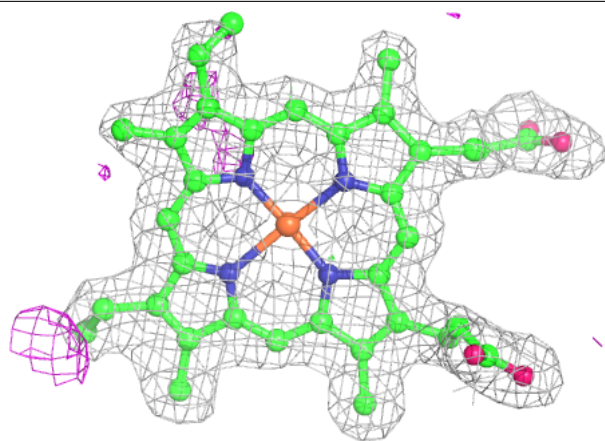
Electron density around HEM j 200:

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



Electron density around HEM I 200:

$2mF_o-DF_c$ (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.