



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:44 pm BST

PDB ID : 1YHU  
Title : Crystal structure of Riftia pachyptila C1 hemoglobin reveals novel assembly of 24 subunits.  
Authors : Flores, J.F.; Fisher, C.R.; Carney, S.L.; Green, B.N.; Freytag, J.K.; Schaeffer, S.W.; Royer, W.E.  
Deposited on : 2005-01-10  
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

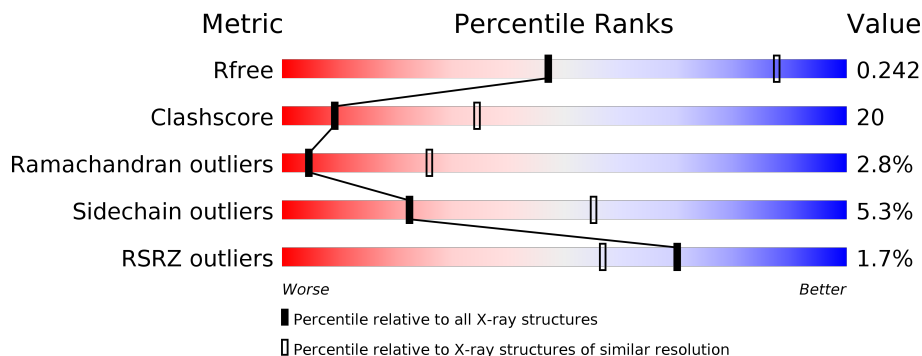
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	145	 71% 27%
1	E	145	 70% 28%
1	I	145	 71% 27%
1	M	145	 68% 30%
1	Q	145	 70% 28%
1	U	145	 68% 28%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	144	<p>% 67% 28% 5%</p>
2	F	144	<p>% 67% 28% 5%</p>
2	J	144	<p>67% 29% .</p>
2	N	144	<p>2% 67% 28% .</p>
2	R	144	<p>% 66% 30% .</p>
2	V	144	<p>% 69% 27% .</p>
3	C	148	<p>7% 62% 34% .</p>
3	G	148	<p>3% 61% 34% .</p>
3	K	148	<p>2% 60% 36% .</p>
3	O	148	<p>% 61% 36% .</p>
3	S	148	<p>3% 62% 34% .</p>
3	W	148	<p>7% 62% 34% .</p>
4	D	149	<p>% 56% 42% .</p>
4	H	149	<p>58% 41% .</p>
4	L	149	<p>3% 57% 42% .</p>
4	P	149	<p>4% 54% 45% .</p>
4	T	149	<p>3% 56% 43% .</p>
4	X	149	<p>% 58% 42% .</p>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 27804 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 hemoglobin A1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	145	1111	705	197	203	6	0	0	0
1	E	145	1111	705	197	203	6	0	0	0
1	I	145	1111	705	197	203	6	0	0	0
1	M	145	1111	705	197	203	6	0	0	0
1	Q	145	1111	705	197	203	6	0	0	0
1	U	145	1111	705	197	203	6	0	0	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	-	SEE REMARK 999	UNP Q8IFK4
A	4	CYS	-	SEE REMARK 999	UNP Q8IFK4
A	5	ALA	-	SEE REMARK 999	UNP Q8IFK4
A	6	MET	-	SEE REMARK 999	UNP Q8IFK4
A	7	LEU	-	SEE REMARK 999	UNP Q8IFK4
A	8	GLU	-	SEE REMARK 999	UNP Q8IFK4
A	9	ARG	-	SEE REMARK 999	UNP Q8IFK4
A	10	ALA	-	SEE REMARK 999	UNP Q8IFK4
A	11	LYS	-	SEE REMARK 999	UNP Q8IFK4
A	12	VAL	-	SEE REMARK 999	UNP Q8IFK4
A	13	LYS	-	SEE REMARK 999	UNP Q8IFK4
A	14	ASP	-	SEE REMARK 999	UNP Q8IFK4
A	15	GLU	-	SEE REMARK 999	UNP Q8IFK4
A	131	GLN	-	SEE REMARK 999	UNP Q8IFK4
A	132	GLY	-	SEE REMARK 999	UNP Q8IFK4
A	133	CYS	-	SEE REMARK 999	UNP Q8IFK4
A	134	TYR	-	SEE REMARK 999	UNP Q8IFK4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	ASN	-	SEE REMARK 999	UNP Q8IFK4
A	136	ILE	-	SEE REMARK 999	UNP Q8IFK4
A	137	ILE	-	SEE REMARK 999	UNP Q8IFK4
A	138	ALA	-	SEE REMARK 999	UNP Q8IFK4
A	139	LYS	-	SEE REMARK 999	UNP Q8IFK4
A	140	GLY	-	SEE REMARK 999	UNP Q8IFK4
A	141	ILE	-	SEE REMARK 999	UNP Q8IFK4
A	142	THR	-	SEE REMARK 999	UNP Q8IFK4
A	143	GLY	-	SEE REMARK 999	UNP Q8IFK4
A	144	SER	-	SEE REMARK 999	UNP Q8IFK4
A	145	ASP	-	SEE REMARK 999	UNP Q8IFK4
A	146	ALA	-	SEE REMARK 999	UNP Q8IFK4
A	147	ALA	-	SEE REMARK 999	UNP Q8IFK4
E	3	ALA	-	SEE REMARK 999	UNP Q8IFK4
E	4	CYS	-	SEE REMARK 999	UNP Q8IFK4
E	5	ALA	-	SEE REMARK 999	UNP Q8IFK4
E	6	MET	-	SEE REMARK 999	UNP Q8IFK4
E	7	LEU	-	SEE REMARK 999	UNP Q8IFK4
E	8	GLU	-	SEE REMARK 999	UNP Q8IFK4
E	9	ARG	-	SEE REMARK 999	UNP Q8IFK4
E	10	ALA	-	SEE REMARK 999	UNP Q8IFK4
E	11	LYS	-	SEE REMARK 999	UNP Q8IFK4
E	12	VAL	-	SEE REMARK 999	UNP Q8IFK4
E	13	LYS	-	SEE REMARK 999	UNP Q8IFK4
E	14	ASP	-	SEE REMARK 999	UNP Q8IFK4
E	15	GLU	-	SEE REMARK 999	UNP Q8IFK4
E	131	GLN	-	SEE REMARK 999	UNP Q8IFK4
E	132	GLY	-	SEE REMARK 999	UNP Q8IFK4
E	133	CYS	-	SEE REMARK 999	UNP Q8IFK4
E	134	TYR	-	SEE REMARK 999	UNP Q8IFK4
E	135	ASN	-	SEE REMARK 999	UNP Q8IFK4
E	136	ILE	-	SEE REMARK 999	UNP Q8IFK4
E	137	ILE	-	SEE REMARK 999	UNP Q8IFK4
E	138	ALA	-	SEE REMARK 999	UNP Q8IFK4
E	139	LYS	-	SEE REMARK 999	UNP Q8IFK4
E	140	GLY	-	SEE REMARK 999	UNP Q8IFK4
E	141	ILE	-	SEE REMARK 999	UNP Q8IFK4
E	142	THR	-	SEE REMARK 999	UNP Q8IFK4
E	143	GLY	-	SEE REMARK 999	UNP Q8IFK4
E	144	SER	-	SEE REMARK 999	UNP Q8IFK4
E	145	ASP	-	SEE REMARK 999	UNP Q8IFK4
E	146	ALA	-	SEE REMARK 999	UNP Q8IFK4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	147	ALA	-	SEE REMARK 999	UNP Q8IFK4
I	3	ALA	-	SEE REMARK 999	UNP Q8IFK4
I	4	CYS	-	SEE REMARK 999	UNP Q8IFK4
I	5	ALA	-	SEE REMARK 999	UNP Q8IFK4
I	6	MET	-	SEE REMARK 999	UNP Q8IFK4
I	7	LEU	-	SEE REMARK 999	UNP Q8IFK4
I	8	GLU	-	SEE REMARK 999	UNP Q8IFK4
I	9	ARG	-	SEE REMARK 999	UNP Q8IFK4
I	10	ALA	-	SEE REMARK 999	UNP Q8IFK4
I	11	LYS	-	SEE REMARK 999	UNP Q8IFK4
I	12	VAL	-	SEE REMARK 999	UNP Q8IFK4
I	13	LYS	-	SEE REMARK 999	UNP Q8IFK4
I	14	ASP	-	SEE REMARK 999	UNP Q8IFK4
I	15	GLU	-	SEE REMARK 999	UNP Q8IFK4
I	131	GLN	-	SEE REMARK 999	UNP Q8IFK4
I	132	GLY	-	SEE REMARK 999	UNP Q8IFK4
I	133	CYS	-	SEE REMARK 999	UNP Q8IFK4
I	134	TYR	-	SEE REMARK 999	UNP Q8IFK4
I	135	ASN	-	SEE REMARK 999	UNP Q8IFK4
I	136	ILE	-	SEE REMARK 999	UNP Q8IFK4
I	137	ILE	-	SEE REMARK 999	UNP Q8IFK4
I	138	ALA	-	SEE REMARK 999	UNP Q8IFK4
I	139	LYS	-	SEE REMARK 999	UNP Q8IFK4
I	140	GLY	-	SEE REMARK 999	UNP Q8IFK4
I	141	ILE	-	SEE REMARK 999	UNP Q8IFK4
I	142	THR	-	SEE REMARK 999	UNP Q8IFK4
I	143	GLY	-	SEE REMARK 999	UNP Q8IFK4
I	144	SER	-	SEE REMARK 999	UNP Q8IFK4
I	145	ASP	-	SEE REMARK 999	UNP Q8IFK4
I	146	ALA	-	SEE REMARK 999	UNP Q8IFK4
I	147	ALA	-	SEE REMARK 999	UNP Q8IFK4
M	3	ALA	-	SEE REMARK 999	UNP Q8IFK4
M	4	CYS	-	SEE REMARK 999	UNP Q8IFK4
M	5	ALA	-	SEE REMARK 999	UNP Q8IFK4
M	6	MET	-	SEE REMARK 999	UNP Q8IFK4
M	7	LEU	-	SEE REMARK 999	UNP Q8IFK4
M	8	GLU	-	SEE REMARK 999	UNP Q8IFK4
M	9	ARG	-	SEE REMARK 999	UNP Q8IFK4
M	10	ALA	-	SEE REMARK 999	UNP Q8IFK4
M	11	LYS	-	SEE REMARK 999	UNP Q8IFK4
M	12	VAL	-	SEE REMARK 999	UNP Q8IFK4
M	13	LYS	-	SEE REMARK 999	UNP Q8IFK4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	14	ASP	-	SEE REMARK 999	UNP Q8IFK4
M	15	GLU	-	SEE REMARK 999	UNP Q8IFK4
M	131	GLN	-	SEE REMARK 999	UNP Q8IFK4
M	132	GLY	-	SEE REMARK 999	UNP Q8IFK4
M	133	CYS	-	SEE REMARK 999	UNP Q8IFK4
M	134	TYR	-	SEE REMARK 999	UNP Q8IFK4
M	135	ASN	-	SEE REMARK 999	UNP Q8IFK4
M	136	ILE	-	SEE REMARK 999	UNP Q8IFK4
M	137	ILE	-	SEE REMARK 999	UNP Q8IFK4
M	138	ALA	-	SEE REMARK 999	UNP Q8IFK4
M	139	LYS	-	SEE REMARK 999	UNP Q8IFK4
M	140	GLY	-	SEE REMARK 999	UNP Q8IFK4
M	141	ILE	-	SEE REMARK 999	UNP Q8IFK4
M	142	THR	-	SEE REMARK 999	UNP Q8IFK4
M	143	GLY	-	SEE REMARK 999	UNP Q8IFK4
M	144	SER	-	SEE REMARK 999	UNP Q8IFK4
M	145	ASP	-	SEE REMARK 999	UNP Q8IFK4
M	146	ALA	-	SEE REMARK 999	UNP Q8IFK4
M	147	ALA	-	SEE REMARK 999	UNP Q8IFK4
Q	3	ALA	-	SEE REMARK 999	UNP Q8IFK4
Q	4	CYS	-	SEE REMARK 999	UNP Q8IFK4
Q	5	ALA	-	SEE REMARK 999	UNP Q8IFK4
Q	6	MET	-	SEE REMARK 999	UNP Q8IFK4
Q	7	LEU	-	SEE REMARK 999	UNP Q8IFK4
Q	8	GLU	-	SEE REMARK 999	UNP Q8IFK4
Q	9	ARG	-	SEE REMARK 999	UNP Q8IFK4
Q	10	ALA	-	SEE REMARK 999	UNP Q8IFK4
Q	11	LYS	-	SEE REMARK 999	UNP Q8IFK4
Q	12	VAL	-	SEE REMARK 999	UNP Q8IFK4
Q	13	LYS	-	SEE REMARK 999	UNP Q8IFK4
Q	14	ASP	-	SEE REMARK 999	UNP Q8IFK4
Q	15	GLU	-	SEE REMARK 999	UNP Q8IFK4
Q	131	GLN	-	SEE REMARK 999	UNP Q8IFK4
Q	132	GLY	-	SEE REMARK 999	UNP Q8IFK4
Q	133	CYS	-	SEE REMARK 999	UNP Q8IFK4
Q	134	TYR	-	SEE REMARK 999	UNP Q8IFK4
Q	135	ASN	-	SEE REMARK 999	UNP Q8IFK4
Q	136	ILE	-	SEE REMARK 999	UNP Q8IFK4
Q	137	ILE	-	SEE REMARK 999	UNP Q8IFK4
Q	138	ALA	-	SEE REMARK 999	UNP Q8IFK4
Q	139	LYS	-	SEE REMARK 999	UNP Q8IFK4
Q	140	GLY	-	SEE REMARK 999	UNP Q8IFK4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
Q	141	ILE	-	SEE REMARK 999	UNP Q8IFK4
Q	142	THR	-	SEE REMARK 999	UNP Q8IFK4
Q	143	GLY	-	SEE REMARK 999	UNP Q8IFK4
Q	144	SER	-	SEE REMARK 999	UNP Q8IFK4
Q	145	ASP	-	SEE REMARK 999	UNP Q8IFK4
Q	146	ALA	-	SEE REMARK 999	UNP Q8IFK4
Q	147	ALA	-	SEE REMARK 999	UNP Q8IFK4
U	3	ALA	-	SEE REMARK 999	UNP Q8IFK4
U	4	CYS	-	SEE REMARK 999	UNP Q8IFK4
U	5	ALA	-	SEE REMARK 999	UNP Q8IFK4
U	6	MET	-	SEE REMARK 999	UNP Q8IFK4
U	7	LEU	-	SEE REMARK 999	UNP Q8IFK4
U	8	GLU	-	SEE REMARK 999	UNP Q8IFK4
U	9	ARG	-	SEE REMARK 999	UNP Q8IFK4
U	10	ALA	-	SEE REMARK 999	UNP Q8IFK4
U	11	LYS	-	SEE REMARK 999	UNP Q8IFK4
U	12	VAL	-	SEE REMARK 999	UNP Q8IFK4
U	13	LYS	-	SEE REMARK 999	UNP Q8IFK4
U	14	ASP	-	SEE REMARK 999	UNP Q8IFK4
U	15	GLU	-	SEE REMARK 999	UNP Q8IFK4
U	131	GLN	-	SEE REMARK 999	UNP Q8IFK4
U	132	GLY	-	SEE REMARK 999	UNP Q8IFK4
U	133	CYS	-	SEE REMARK 999	UNP Q8IFK4
U	134	TYR	-	SEE REMARK 999	UNP Q8IFK4
U	135	ASN	-	SEE REMARK 999	UNP Q8IFK4
U	136	ILE	-	SEE REMARK 999	UNP Q8IFK4
U	137	ILE	-	SEE REMARK 999	UNP Q8IFK4
U	138	ALA	-	SEE REMARK 999	UNP Q8IFK4
U	139	LYS	-	SEE REMARK 999	UNP Q8IFK4
U	140	GLY	-	SEE REMARK 999	UNP Q8IFK4
U	141	ILE	-	SEE REMARK 999	UNP Q8IFK4
U	142	THR	-	SEE REMARK 999	UNP Q8IFK4
U	143	GLY	-	SEE REMARK 999	UNP Q8IFK4
U	144	SER	-	SEE REMARK 999	UNP Q8IFK4
U	145	ASP	-	SEE REMARK 999	UNP Q8IFK4
U	146	ALA	-	SEE REMARK 999	UNP Q8IFK4
U	147	ALA	-	SEE REMARK 999	UNP Q8IFK4

- Molecule 2 is a protein called Giant hemoglobins B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	144	1136	711	211	207	7	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	144	Total	C	N	O	S	0	0	0
			1136	711	211	207	7			
2	J	144	Total	C	N	O	S	0	0	0
			1136	711	211	207	7			
2	N	144	Total	C	N	O	S	0	0	0
			1136	711	211	207	7			
2	R	144	Total	C	N	O	S	0	0	0
			1136	711	211	207	7			
2	V	144	Total	C	N	O	S	0	0	0
			1136	711	211	207	7			

- Molecule 3 is a protein called hemoglobin B1a chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	148	Total	C	N	O	S	0	0	0
			1072	676	183	206	7			
3	G	148	Total	C	N	O	S	0	0	0
			1072	676	183	206	7			
3	K	148	Total	C	N	O	S	0	0	0
			1072	676	183	206	7			
3	O	148	Total	C	N	O	S	0	0	0
			1072	676	183	206	7			
3	S	148	Total	C	N	O	S	0	0	0
			1072	676	183	206	7			
3	W	148	Total	C	N	O	S	0	0	0
			1072	676	183	206	7			

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	2	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	3	ASN	-	SEE REMARK 999	UNP Q8IFK2
C	4	CYS	-	SEE REMARK 999	UNP Q8IFK2
C	5	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	6	ASP	-	SEE REMARK 999	UNP Q8IFK2
C	7	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	8	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	9	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	10	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	11	ILE	-	SEE REMARK 999	UNP Q8IFK2
C	12	VAL	-	SEE REMARK 999	UNP Q8IFK2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	13	GLN	-	SEE REMARK 999	UNP Q8IFK2
C	14	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	15	GLN	-	SEE REMARK 999	UNP Q8IFK2
C	17	GLU	GLN	SEE REMARK 999	UNP Q8IFK2
C	20	TRP	SER	SEE REMARK 999	UNP Q8IFK2
C	22	ALA	PRO	SEE REMARK 999	UNP Q8IFK2
C	23	ALA	ASP	SEE REMARK 999	UNP Q8IFK2
C	27	ALA	ARG	SEE REMARK 999	UNP Q8IFK2
C	29	ARG	LYS	SEE REMARK 999	UNP Q8IFK2
C	30	VAL	LEU	SEE REMARK 999	UNP Q8IFK2
C	32	ALA	CYS	SEE REMARK 999	UNP Q8IFK2
C	34	GLU	HIS	SEE REMARK 999	UNP Q8IFK2
C	35	GLU	ALA	SEE REMARK 999	UNP Q8IFK2
C	39	ALA	GLU	SEE REMARK 999	UNP Q8IFK2
C	58	ASP	GLU	SEE REMARK 999	UNP Q8IFK2
C	65	GLN	ASN	SEE REMARK 999	UNP Q8IFK2
C	69	VAL	MET	SEE REMARK 999	UNP Q8IFK2
C	81	ALA	TYR	SEE REMARK 999	UNP Q8IFK2
C	107	GLY	LYS	SEE REMARK 999	UNP Q8IFK2
C	111	GLN	GLY	SEE REMARK 999	UNP Q8IFK2
C	112	LEU	ALA	SEE REMARK 999	UNP Q8IFK2
C	119	GLU	LYS	SEE REMARK 999	UNP Q8IFK2
C	121	LEU	MET	SEE REMARK 999	UNP Q8IFK2
C	134	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	135	SER	-	SEE REMARK 999	UNP Q8IFK2
C	136	CYS	-	SEE REMARK 999	UNP Q8IFK2
C	137	LEU	-	SEE REMARK 999	UNP Q8IFK2
C	138	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	139	GLY	-	SEE REMARK 999	UNP Q8IFK2
C	140	ILE	-	SEE REMARK 999	UNP Q8IFK2
C	141	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	142	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	143	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	144	ILE	-	SEE REMARK 999	UNP Q8IFK2
C	145	SER	-	SEE REMARK 999	UNP Q8IFK2
C	146	SER	-	SEE REMARK 999	UNP Q8IFK2
C	147	ALA	-	SEE REMARK 999	UNP Q8IFK2
C	148	LEU	-	SEE REMARK 999	UNP Q8IFK2
G	1	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	2	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	3	ASN	-	SEE REMARK 999	UNP Q8IFK2
G	4	CYS	-	SEE REMARK 999	UNP Q8IFK2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	6	ASP	-	SEE REMARK 999	UNP Q8IFK2
G	7	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	8	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	9	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	10	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	11	ILE	-	SEE REMARK 999	UNP Q8IFK2
G	12	VAL	-	SEE REMARK 999	UNP Q8IFK2
G	13	GLN	-	SEE REMARK 999	UNP Q8IFK2
G	14	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	15	GLN	-	SEE REMARK 999	UNP Q8IFK2
G	17	GLU	GLN	SEE REMARK 999	UNP Q8IFK2
G	20	TRP	SER	SEE REMARK 999	UNP Q8IFK2
G	22	ALA	PRO	SEE REMARK 999	UNP Q8IFK2
G	23	ALA	ASP	SEE REMARK 999	UNP Q8IFK2
G	27	ALA	ARG	SEE REMARK 999	UNP Q8IFK2
G	29	ARG	LYS	SEE REMARK 999	UNP Q8IFK2
G	30	VAL	LEU	SEE REMARK 999	UNP Q8IFK2
G	32	ALA	CYS	SEE REMARK 999	UNP Q8IFK2
G	34	GLU	HIS	SEE REMARK 999	UNP Q8IFK2
G	35	GLU	ALA	SEE REMARK 999	UNP Q8IFK2
G	39	ALA	GLU	SEE REMARK 999	UNP Q8IFK2
G	58	ASP	GLU	SEE REMARK 999	UNP Q8IFK2
G	65	GLN	ASN	SEE REMARK 999	UNP Q8IFK2
G	69	VAL	MET	SEE REMARK 999	UNP Q8IFK2
G	81	ALA	TYR	SEE REMARK 999	UNP Q8IFK2
G	107	GLY	LYS	SEE REMARK 999	UNP Q8IFK2
G	111	GLN	GLY	SEE REMARK 999	UNP Q8IFK2
G	112	LEU	ALA	SEE REMARK 999	UNP Q8IFK2
G	119	GLU	LYS	SEE REMARK 999	UNP Q8IFK2
G	121	LEU	MET	SEE REMARK 999	UNP Q8IFK2
G	134	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	135	SER	-	SEE REMARK 999	UNP Q8IFK2
G	136	CYS	-	SEE REMARK 999	UNP Q8IFK2
G	137	LEU	-	SEE REMARK 999	UNP Q8IFK2
G	138	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	139	GLY	-	SEE REMARK 999	UNP Q8IFK2
G	140	ILE	-	SEE REMARK 999	UNP Q8IFK2
G	141	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	142	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	143	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	144	ILE	-	SEE REMARK 999	UNP Q8IFK2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	145	SER	-	SEE REMARK 999	UNP Q8IFK2
G	146	SER	-	SEE REMARK 999	UNP Q8IFK2
G	147	ALA	-	SEE REMARK 999	UNP Q8IFK2
G	148	LEU	-	SEE REMARK 999	UNP Q8IFK2
K	1	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	2	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	3	ASN	-	SEE REMARK 999	UNP Q8IFK2
K	4	CYS	-	SEE REMARK 999	UNP Q8IFK2
K	5	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	6	ASP	-	SEE REMARK 999	UNP Q8IFK2
K	7	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	8	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	9	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	10	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	11	ILE	-	SEE REMARK 999	UNP Q8IFK2
K	12	VAL	-	SEE REMARK 999	UNP Q8IFK2
K	13	GLN	-	SEE REMARK 999	UNP Q8IFK2
K	14	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	15	GLN	-	SEE REMARK 999	UNP Q8IFK2
K	17	GLU	GLN	SEE REMARK 999	UNP Q8IFK2
K	20	TRP	SER	SEE REMARK 999	UNP Q8IFK2
K	22	ALA	PRO	SEE REMARK 999	UNP Q8IFK2
K	23	ALA	ASP	SEE REMARK 999	UNP Q8IFK2
K	27	ALA	ARG	SEE REMARK 999	UNP Q8IFK2
K	29	ARG	LYS	SEE REMARK 999	UNP Q8IFK2
K	30	VAL	LEU	SEE REMARK 999	UNP Q8IFK2
K	32	ALA	CYS	SEE REMARK 999	UNP Q8IFK2
K	34	GLU	HIS	SEE REMARK 999	UNP Q8IFK2
K	35	GLU	ALA	SEE REMARK 999	UNP Q8IFK2
K	39	ALA	GLU	SEE REMARK 999	UNP Q8IFK2
K	58	ASP	GLU	SEE REMARK 999	UNP Q8IFK2
K	65	GLN	ASN	SEE REMARK 999	UNP Q8IFK2
K	69	VAL	MET	SEE REMARK 999	UNP Q8IFK2
K	81	ALA	TYR	SEE REMARK 999	UNP Q8IFK2
K	107	GLY	LYS	SEE REMARK 999	UNP Q8IFK2
K	111	GLN	GLY	SEE REMARK 999	UNP Q8IFK2
K	112	LEU	ALA	SEE REMARK 999	UNP Q8IFK2
K	119	GLU	LYS	SEE REMARK 999	UNP Q8IFK2
K	121	LEU	MET	SEE REMARK 999	UNP Q8IFK2
K	134	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	135	SER	-	SEE REMARK 999	UNP Q8IFK2
K	136	CYS	-	SEE REMARK 999	UNP Q8IFK2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
K	137	LEU	-	SEE REMARK 999	UNP Q8IFK2
K	138	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	139	GLY	-	SEE REMARK 999	UNP Q8IFK2
K	140	ILE	-	SEE REMARK 999	UNP Q8IFK2
K	141	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	142	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	143	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	144	ILE	-	SEE REMARK 999	UNP Q8IFK2
K	145	SER	-	SEE REMARK 999	UNP Q8IFK2
K	146	SER	-	SEE REMARK 999	UNP Q8IFK2
K	147	ALA	-	SEE REMARK 999	UNP Q8IFK2
K	148	LEU	-	SEE REMARK 999	UNP Q8IFK2
O	1	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	2	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	3	ASN	-	SEE REMARK 999	UNP Q8IFK2
O	4	CYS	-	SEE REMARK 999	UNP Q8IFK2
O	5	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	6	ASP	-	SEE REMARK 999	UNP Q8IFK2
O	7	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	8	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	9	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	10	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	11	ILE	-	SEE REMARK 999	UNP Q8IFK2
O	12	VAL	-	SEE REMARK 999	UNP Q8IFK2
O	13	GLN	-	SEE REMARK 999	UNP Q8IFK2
O	14	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	15	GLN	-	SEE REMARK 999	UNP Q8IFK2
O	17	GLU	GLN	SEE REMARK 999	UNP Q8IFK2
O	20	TRP	SER	SEE REMARK 999	UNP Q8IFK2
O	22	ALA	PRO	SEE REMARK 999	UNP Q8IFK2
O	23	ALA	ASP	SEE REMARK 999	UNP Q8IFK2
O	27	ALA	ARG	SEE REMARK 999	UNP Q8IFK2
O	29	ARG	LYS	SEE REMARK 999	UNP Q8IFK2
O	30	VAL	LEU	SEE REMARK 999	UNP Q8IFK2
O	32	ALA	CYS	SEE REMARK 999	UNP Q8IFK2
O	34	GLU	HIS	SEE REMARK 999	UNP Q8IFK2
O	35	GLU	ALA	SEE REMARK 999	UNP Q8IFK2
O	39	ALA	GLU	SEE REMARK 999	UNP Q8IFK2
O	58	ASP	GLU	SEE REMARK 999	UNP Q8IFK2
O	65	GLN	ASN	SEE REMARK 999	UNP Q8IFK2
O	69	VAL	MET	SEE REMARK 999	UNP Q8IFK2
O	81	ALA	TYR	SEE REMARK 999	UNP Q8IFK2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
O	107	GLY	LYS	SEE REMARK 999	UNP Q8IFK2
O	111	GLN	GLY	SEE REMARK 999	UNP Q8IFK2
O	112	LEU	ALA	SEE REMARK 999	UNP Q8IFK2
O	119	GLU	LYS	SEE REMARK 999	UNP Q8IFK2
O	121	LEU	MET	SEE REMARK 999	UNP Q8IFK2
O	134	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	135	SER	-	SEE REMARK 999	UNP Q8IFK2
O	136	CYS	-	SEE REMARK 999	UNP Q8IFK2
O	137	LEU	-	SEE REMARK 999	UNP Q8IFK2
O	138	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	139	GLY	-	SEE REMARK 999	UNP Q8IFK2
O	140	ILE	-	SEE REMARK 999	UNP Q8IFK2
O	141	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	142	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	143	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	144	ILE	-	SEE REMARK 999	UNP Q8IFK2
O	145	SER	-	SEE REMARK 999	UNP Q8IFK2
O	146	SER	-	SEE REMARK 999	UNP Q8IFK2
O	147	ALA	-	SEE REMARK 999	UNP Q8IFK2
O	148	LEU	-	SEE REMARK 999	UNP Q8IFK2
S	1	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	2	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	3	ASN	-	SEE REMARK 999	UNP Q8IFK2
S	4	CYS	-	SEE REMARK 999	UNP Q8IFK2
S	5	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	6	ASP	-	SEE REMARK 999	UNP Q8IFK2
S	7	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	8	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	9	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	10	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	11	ILE	-	SEE REMARK 999	UNP Q8IFK2
S	12	VAL	-	SEE REMARK 999	UNP Q8IFK2
S	13	GLN	-	SEE REMARK 999	UNP Q8IFK2
S	14	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	15	GLN	-	SEE REMARK 999	UNP Q8IFK2
S	17	GLU	GLN	SEE REMARK 999	UNP Q8IFK2
S	20	TRP	SER	SEE REMARK 999	UNP Q8IFK2
S	22	ALA	PRO	SEE REMARK 999	UNP Q8IFK2
S	23	ALA	ASP	SEE REMARK 999	UNP Q8IFK2
S	27	ALA	ARG	SEE REMARK 999	UNP Q8IFK2
S	29	ARG	LYS	SEE REMARK 999	UNP Q8IFK2
S	30	VAL	LEU	SEE REMARK 999	UNP Q8IFK2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
S	32	ALA	CYS	SEE REMARK 999	UNP Q8IFK2
S	34	GLU	HIS	SEE REMARK 999	UNP Q8IFK2
S	35	GLU	ALA	SEE REMARK 999	UNP Q8IFK2
S	39	ALA	GLU	SEE REMARK 999	UNP Q8IFK2
S	58	ASP	GLU	SEE REMARK 999	UNP Q8IFK2
S	65	GLN	ASN	SEE REMARK 999	UNP Q8IFK2
S	69	VAL	MET	SEE REMARK 999	UNP Q8IFK2
S	81	ALA	TYR	SEE REMARK 999	UNP Q8IFK2
S	107	GLY	LYS	SEE REMARK 999	UNP Q8IFK2
S	111	GLN	GLY	SEE REMARK 999	UNP Q8IFK2
S	112	LEU	ALA	SEE REMARK 999	UNP Q8IFK2
S	119	GLU	LYS	SEE REMARK 999	UNP Q8IFK2
S	121	LEU	MET	SEE REMARK 999	UNP Q8IFK2
S	134	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	135	SER	-	SEE REMARK 999	UNP Q8IFK2
S	136	CYS	-	SEE REMARK 999	UNP Q8IFK2
S	137	LEU	-	SEE REMARK 999	UNP Q8IFK2
S	138	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	139	GLY	-	SEE REMARK 999	UNP Q8IFK2
S	140	ILE	-	SEE REMARK 999	UNP Q8IFK2
S	141	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	142	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	143	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	144	ILE	-	SEE REMARK 999	UNP Q8IFK2
S	145	SER	-	SEE REMARK 999	UNP Q8IFK2
S	146	SER	-	SEE REMARK 999	UNP Q8IFK2
S	147	ALA	-	SEE REMARK 999	UNP Q8IFK2
S	148	LEU	-	SEE REMARK 999	UNP Q8IFK2
W	1	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	2	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	3	ASN	-	SEE REMARK 999	UNP Q8IFK2
W	4	CYS	-	SEE REMARK 999	UNP Q8IFK2
W	5	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	6	ASP	-	SEE REMARK 999	UNP Q8IFK2
W	7	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	8	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	9	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	10	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	11	ILE	-	SEE REMARK 999	UNP Q8IFK2
W	12	VAL	-	SEE REMARK 999	UNP Q8IFK2
W	13	GLN	-	SEE REMARK 999	UNP Q8IFK2
W	14	ALA	-	SEE REMARK 999	UNP Q8IFK2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
W	15	GLN	-	SEE REMARK 999	UNP Q8IFK2
W	17	GLU	GLN	SEE REMARK 999	UNP Q8IFK2
W	20	TRP	SER	SEE REMARK 999	UNP Q8IFK2
W	22	ALA	PRO	SEE REMARK 999	UNP Q8IFK2
W	23	ALA	ASP	SEE REMARK 999	UNP Q8IFK2
W	27	ALA	ARG	SEE REMARK 999	UNP Q8IFK2
W	29	ARG	LYS	SEE REMARK 999	UNP Q8IFK2
W	30	VAL	LEU	SEE REMARK 999	UNP Q8IFK2
W	32	ALA	CYS	SEE REMARK 999	UNP Q8IFK2
W	34	GLU	HIS	SEE REMARK 999	UNP Q8IFK2
W	35	GLU	ALA	SEE REMARK 999	UNP Q8IFK2
W	39	ALA	GLU	SEE REMARK 999	UNP Q8IFK2
W	58	ASP	GLU	SEE REMARK 999	UNP Q8IFK2
W	65	GLN	ASN	SEE REMARK 999	UNP Q8IFK2
W	69	VAL	MET	SEE REMARK 999	UNP Q8IFK2
W	81	ALA	TYR	SEE REMARK 999	UNP Q8IFK2
W	107	GLY	LYS	SEE REMARK 999	UNP Q8IFK2
W	111	GLN	GLY	SEE REMARK 999	UNP Q8IFK2
W	112	LEU	ALA	SEE REMARK 999	UNP Q8IFK2
W	119	GLU	LYS	SEE REMARK 999	UNP Q8IFK2
W	121	LEU	MET	SEE REMARK 999	UNP Q8IFK2
W	134	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	135	SER	-	SEE REMARK 999	UNP Q8IFK2
W	136	CYS	-	SEE REMARK 999	UNP Q8IFK2
W	137	LEU	-	SEE REMARK 999	UNP Q8IFK2
W	138	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	139	GLY	-	SEE REMARK 999	UNP Q8IFK2
W	140	ILE	-	SEE REMARK 999	UNP Q8IFK2
W	141	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	142	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	143	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	144	ILE	-	SEE REMARK 999	UNP Q8IFK2
W	145	SER	-	SEE REMARK 999	UNP Q8IFK2
W	146	SER	-	SEE REMARK 999	UNP Q8IFK2
W	147	ALA	-	SEE REMARK 999	UNP Q8IFK2
W	148	LEU	-	SEE REMARK 999	UNP Q8IFK2

- Molecule 4 is a protein called hemoglobin B2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	149	1133	708	205	212	8	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	149	1133	708	205	212	8	0	0	0
4	L	149	1133	708	205	212	8	0	0	0
4	P	149	1133	708	205	212	8	0	0	0
4	T	149	1133	708	205	212	8	0	0	0
4	X	149	1133	708	205	212	8	0	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	SEE REMARK 999	UNP Q8IFJ9
D	2	ALA	-	SEE REMARK 999	UNP Q8IFJ9
D	3	SER	-	SEE REMARK 999	UNP Q8IFJ9
D	4	CYS	-	SEE REMARK 999	UNP Q8IFJ9
D	5	THR	-	SEE REMARK 999	UNP Q8IFJ9
D	6	THR	-	SEE REMARK 999	UNP Q8IFJ9
D	7	GLU	-	SEE REMARK 999	UNP Q8IFJ9
D	8	ASP	-	SEE REMARK 999	UNP Q8IFJ9
D	9	ARG	-	SEE REMARK 999	UNP Q8IFJ9
D	10	ARG	-	SEE REMARK 999	UNP Q8IFJ9
D	11	GLU	-	SEE REMARK 999	UNP Q8IFJ9
D	12	MET	-	SEE REMARK 999	UNP Q8IFJ9
D	13	GLN	-	SEE REMARK 999	UNP Q8IFJ9
D	14	LEU	-	SEE REMARK 999	UNP Q8IFJ9
D	15	MET	-	SEE REMARK 999	UNP Q8IFJ9
D	133	SER	-	SEE REMARK 999	UNP Q8IFJ9
D	134	ARG	-	SEE REMARK 999	UNP Q8IFJ9
D	135	CYS	-	SEE REMARK 999	UNP Q8IFJ9
D	136	PHE	-	SEE REMARK 999	UNP Q8IFJ9
D	137	ASN	-	SEE REMARK 999	UNP Q8IFJ9
D	138	ARG	-	SEE REMARK 999	UNP Q8IFJ9
D	139	ILE	-	SEE REMARK 999	UNP Q8IFJ9
D	140	THR	-	SEE REMARK 999	UNP Q8IFJ9
D	141	THR	-	SEE REMARK 999	UNP Q8IFJ9
D	142	GLY	-	SEE REMARK 999	UNP Q8IFJ9
D	143	MET	-	SEE REMARK 999	UNP Q8IFJ9
D	144	THR	-	SEE REMARK 999	UNP Q8IFJ9
D	145	GLU	-	SEE REMARK 999	UNP Q8IFJ9
D	146	PRO	-	SEE REMARK 999	UNP Q8IFJ9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	147	LEU	-	SEE REMARK 999	UNP Q8IFJ9
D	148	PRO	-	SEE REMARK 999	UNP Q8IFJ9
D	149	ALA	-	SEE REMARK 999	UNP Q8IFJ9
H	1	ALA	-	SEE REMARK 999	UNP Q8IFJ9
H	2	ALA	-	SEE REMARK 999	UNP Q8IFJ9
H	3	SER	-	SEE REMARK 999	UNP Q8IFJ9
H	4	CYS	-	SEE REMARK 999	UNP Q8IFJ9
H	5	THR	-	SEE REMARK 999	UNP Q8IFJ9
H	6	THR	-	SEE REMARK 999	UNP Q8IFJ9
H	7	GLU	-	SEE REMARK 999	UNP Q8IFJ9
H	8	ASP	-	SEE REMARK 999	UNP Q8IFJ9
H	9	ARG	-	SEE REMARK 999	UNP Q8IFJ9
H	10	ARG	-	SEE REMARK 999	UNP Q8IFJ9
H	11	GLU	-	SEE REMARK 999	UNP Q8IFJ9
H	12	MET	-	SEE REMARK 999	UNP Q8IFJ9
H	13	GLN	-	SEE REMARK 999	UNP Q8IFJ9
H	14	LEU	-	SEE REMARK 999	UNP Q8IFJ9
H	15	MET	-	SEE REMARK 999	UNP Q8IFJ9
H	133	SER	-	SEE REMARK 999	UNP Q8IFJ9
H	134	ARG	-	SEE REMARK 999	UNP Q8IFJ9
H	135	CYS	-	SEE REMARK 999	UNP Q8IFJ9
H	136	PHE	-	SEE REMARK 999	UNP Q8IFJ9
H	137	ASN	-	SEE REMARK 999	UNP Q8IFJ9
H	138	ARG	-	SEE REMARK 999	UNP Q8IFJ9
H	139	ILE	-	SEE REMARK 999	UNP Q8IFJ9
H	140	THR	-	SEE REMARK 999	UNP Q8IFJ9
H	141	THR	-	SEE REMARK 999	UNP Q8IFJ9
H	142	GLY	-	SEE REMARK 999	UNP Q8IFJ9
H	143	MET	-	SEE REMARK 999	UNP Q8IFJ9
H	144	THR	-	SEE REMARK 999	UNP Q8IFJ9
H	145	GLU	-	SEE REMARK 999	UNP Q8IFJ9
H	146	PRO	-	SEE REMARK 999	UNP Q8IFJ9
H	147	LEU	-	SEE REMARK 999	UNP Q8IFJ9
H	148	PRO	-	SEE REMARK 999	UNP Q8IFJ9
H	149	ALA	-	SEE REMARK 999	UNP Q8IFJ9
L	1	ALA	-	SEE REMARK 999	UNP Q8IFJ9
L	2	ALA	-	SEE REMARK 999	UNP Q8IFJ9
L	3	SER	-	SEE REMARK 999	UNP Q8IFJ9
L	4	CYS	-	SEE REMARK 999	UNP Q8IFJ9
L	5	THR	-	SEE REMARK 999	UNP Q8IFJ9
L	6	THR	-	SEE REMARK 999	UNP Q8IFJ9
L	7	GLU	-	SEE REMARK 999	UNP Q8IFJ9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
L	8	ASP	-	SEE REMARK 999	UNP Q8IFJ9
L	9	ARG	-	SEE REMARK 999	UNP Q8IFJ9
L	10	ARG	-	SEE REMARK 999	UNP Q8IFJ9
L	11	GLU	-	SEE REMARK 999	UNP Q8IFJ9
L	12	MET	-	SEE REMARK 999	UNP Q8IFJ9
L	13	GLN	-	SEE REMARK 999	UNP Q8IFJ9
L	14	LEU	-	SEE REMARK 999	UNP Q8IFJ9
L	15	MET	-	SEE REMARK 999	UNP Q8IFJ9
L	133	SER	-	SEE REMARK 999	UNP Q8IFJ9
L	134	ARG	-	SEE REMARK 999	UNP Q8IFJ9
L	135	CYS	-	SEE REMARK 999	UNP Q8IFJ9
L	136	PHE	-	SEE REMARK 999	UNP Q8IFJ9
L	137	ASN	-	SEE REMARK 999	UNP Q8IFJ9
L	138	ARG	-	SEE REMARK 999	UNP Q8IFJ9
L	139	ILE	-	SEE REMARK 999	UNP Q8IFJ9
L	140	THR	-	SEE REMARK 999	UNP Q8IFJ9
L	141	THR	-	SEE REMARK 999	UNP Q8IFJ9
L	142	GLY	-	SEE REMARK 999	UNP Q8IFJ9
L	143	MET	-	SEE REMARK 999	UNP Q8IFJ9
L	144	THR	-	SEE REMARK 999	UNP Q8IFJ9
L	145	GLU	-	SEE REMARK 999	UNP Q8IFJ9
L	146	PRO	-	SEE REMARK 999	UNP Q8IFJ9
L	147	LEU	-	SEE REMARK 999	UNP Q8IFJ9
L	148	PRO	-	SEE REMARK 999	UNP Q8IFJ9
L	149	ALA	-	SEE REMARK 999	UNP Q8IFJ9
P	1	ALA	-	SEE REMARK 999	UNP Q8IFJ9
P	2	ALA	-	SEE REMARK 999	UNP Q8IFJ9
P	3	SER	-	SEE REMARK 999	UNP Q8IFJ9
P	4	CYS	-	SEE REMARK 999	UNP Q8IFJ9
P	5	THR	-	SEE REMARK 999	UNP Q8IFJ9
P	6	THR	-	SEE REMARK 999	UNP Q8IFJ9
P	7	GLU	-	SEE REMARK 999	UNP Q8IFJ9
P	8	ASP	-	SEE REMARK 999	UNP Q8IFJ9
P	9	ARG	-	SEE REMARK 999	UNP Q8IFJ9
P	10	ARG	-	SEE REMARK 999	UNP Q8IFJ9
P	11	GLU	-	SEE REMARK 999	UNP Q8IFJ9
P	12	MET	-	SEE REMARK 999	UNP Q8IFJ9
P	13	GLN	-	SEE REMARK 999	UNP Q8IFJ9
P	14	LEU	-	SEE REMARK 999	UNP Q8IFJ9
P	15	MET	-	SEE REMARK 999	UNP Q8IFJ9
P	133	SER	-	SEE REMARK 999	UNP Q8IFJ9
P	134	ARG	-	SEE REMARK 999	UNP Q8IFJ9

*Continued on next page...*

*Continued from previous page...*

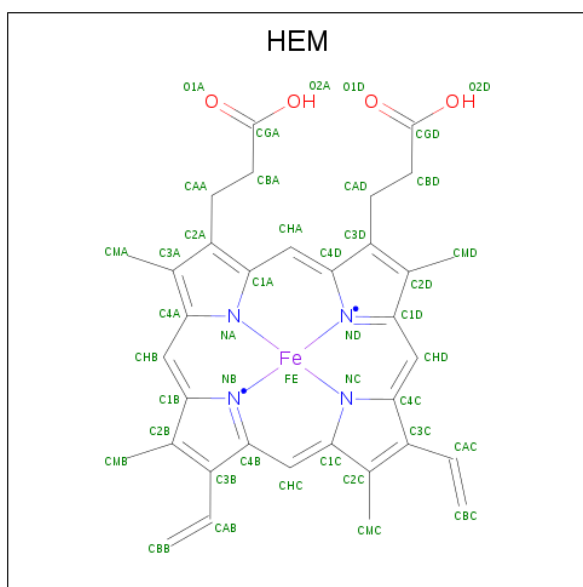
Chain	Residue	Modelled	Actual	Comment	Reference
P	135	CYS	-	SEE REMARK 999	UNP Q8IFJ9
P	136	PHE	-	SEE REMARK 999	UNP Q8IFJ9
P	137	ASN	-	SEE REMARK 999	UNP Q8IFJ9
P	138	ARG	-	SEE REMARK 999	UNP Q8IFJ9
P	139	ILE	-	SEE REMARK 999	UNP Q8IFJ9
P	140	THR	-	SEE REMARK 999	UNP Q8IFJ9
P	141	THR	-	SEE REMARK 999	UNP Q8IFJ9
P	142	GLY	-	SEE REMARK 999	UNP Q8IFJ9
P	143	MET	-	SEE REMARK 999	UNP Q8IFJ9
P	144	THR	-	SEE REMARK 999	UNP Q8IFJ9
P	145	GLU	-	SEE REMARK 999	UNP Q8IFJ9
P	146	PRO	-	SEE REMARK 999	UNP Q8IFJ9
P	147	LEU	-	SEE REMARK 999	UNP Q8IFJ9
P	148	PRO	-	SEE REMARK 999	UNP Q8IFJ9
P	149	ALA	-	SEE REMARK 999	UNP Q8IFJ9
T	1	ALA	-	SEE REMARK 999	UNP Q8IFJ9
T	2	ALA	-	SEE REMARK 999	UNP Q8IFJ9
T	3	SER	-	SEE REMARK 999	UNP Q8IFJ9
T	4	CYS	-	SEE REMARK 999	UNP Q8IFJ9
T	5	THR	-	SEE REMARK 999	UNP Q8IFJ9
T	6	THR	-	SEE REMARK 999	UNP Q8IFJ9
T	7	GLU	-	SEE REMARK 999	UNP Q8IFJ9
T	8	ASP	-	SEE REMARK 999	UNP Q8IFJ9
T	9	ARG	-	SEE REMARK 999	UNP Q8IFJ9
T	10	ARG	-	SEE REMARK 999	UNP Q8IFJ9
T	11	GLU	-	SEE REMARK 999	UNP Q8IFJ9
T	12	MET	-	SEE REMARK 999	UNP Q8IFJ9
T	13	GLN	-	SEE REMARK 999	UNP Q8IFJ9
T	14	LEU	-	SEE REMARK 999	UNP Q8IFJ9
T	15	MET	-	SEE REMARK 999	UNP Q8IFJ9
T	133	SER	-	SEE REMARK 999	UNP Q8IFJ9
T	134	ARG	-	SEE REMARK 999	UNP Q8IFJ9
T	135	CYS	-	SEE REMARK 999	UNP Q8IFJ9
T	136	PHE	-	SEE REMARK 999	UNP Q8IFJ9
T	137	ASN	-	SEE REMARK 999	UNP Q8IFJ9
T	138	ARG	-	SEE REMARK 999	UNP Q8IFJ9
T	139	ILE	-	SEE REMARK 999	UNP Q8IFJ9
T	140	THR	-	SEE REMARK 999	UNP Q8IFJ9
T	141	THR	-	SEE REMARK 999	UNP Q8IFJ9
T	142	GLY	-	SEE REMARK 999	UNP Q8IFJ9
T	143	MET	-	SEE REMARK 999	UNP Q8IFJ9
T	144	THR	-	SEE REMARK 999	UNP Q8IFJ9

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
T	145	GLU	-	SEE REMARK 999	UNP Q8IFJ9
T	146	PRO	-	SEE REMARK 999	UNP Q8IFJ9
T	147	LEU	-	SEE REMARK 999	UNP Q8IFJ9
T	148	PRO	-	SEE REMARK 999	UNP Q8IFJ9
T	149	ALA	-	SEE REMARK 999	UNP Q8IFJ9
X	1	ALA	-	SEE REMARK 999	UNP Q8IFJ9
X	2	ALA	-	SEE REMARK 999	UNP Q8IFJ9
X	3	SER	-	SEE REMARK 999	UNP Q8IFJ9
X	4	CYS	-	SEE REMARK 999	UNP Q8IFJ9
X	5	THR	-	SEE REMARK 999	UNP Q8IFJ9
X	6	THR	-	SEE REMARK 999	UNP Q8IFJ9
X	7	GLU	-	SEE REMARK 999	UNP Q8IFJ9
X	8	ASP	-	SEE REMARK 999	UNP Q8IFJ9
X	9	ARG	-	SEE REMARK 999	UNP Q8IFJ9
X	10	ARG	-	SEE REMARK 999	UNP Q8IFJ9
X	11	GLU	-	SEE REMARK 999	UNP Q8IFJ9
X	12	MET	-	SEE REMARK 999	UNP Q8IFJ9
X	13	GLN	-	SEE REMARK 999	UNP Q8IFJ9
X	14	LEU	-	SEE REMARK 999	UNP Q8IFJ9
X	15	MET	-	SEE REMARK 999	UNP Q8IFJ9
X	133	SER	-	SEE REMARK 999	UNP Q8IFJ9
X	134	ARG	-	SEE REMARK 999	UNP Q8IFJ9
X	135	CYS	-	SEE REMARK 999	UNP Q8IFJ9
X	136	PHE	-	SEE REMARK 999	UNP Q8IFJ9
X	137	ASN	-	SEE REMARK 999	UNP Q8IFJ9
X	138	ARG	-	SEE REMARK 999	UNP Q8IFJ9
X	139	ILE	-	SEE REMARK 999	UNP Q8IFJ9
X	140	THR	-	SEE REMARK 999	UNP Q8IFJ9
X	141	THR	-	SEE REMARK 999	UNP Q8IFJ9
X	142	GLY	-	SEE REMARK 999	UNP Q8IFJ9
X	143	MET	-	SEE REMARK 999	UNP Q8IFJ9
X	144	THR	-	SEE REMARK 999	UNP Q8IFJ9
X	145	GLU	-	SEE REMARK 999	UNP Q8IFJ9
X	146	PRO	-	SEE REMARK 999	UNP Q8IFJ9
X	147	LEU	-	SEE REMARK 999	UNP Q8IFJ9
X	148	PRO	-	SEE REMARK 999	UNP Q8IFJ9
X	149	ALA	-	SEE REMARK 999	UNP Q8IFJ9

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



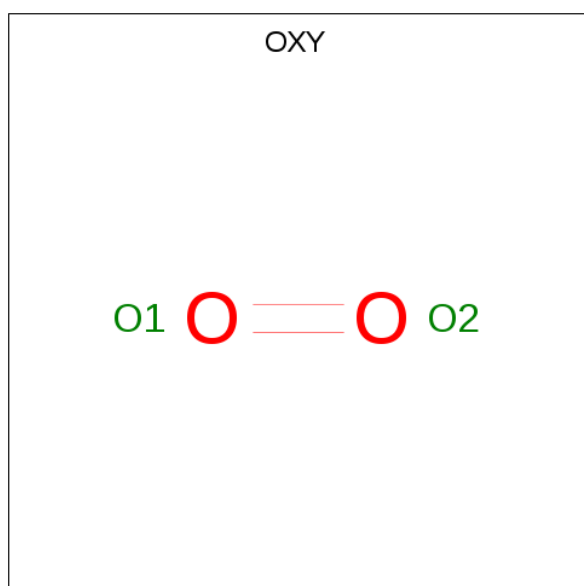
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	N	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	
5	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			2	2		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 2 2	0	0
6	C	1	Total O 2 2	0	0
6	D	1	Total O 2 2	0	0
6	E	1	Total O 2 2	0	0
6	F	1	Total O 2 2	0	0
6	G	1	Total O 2 2	0	0
6	H	1	Total O 2 2	0	0
6	I	1	Total O 2 2	0	0
6	J	1	Total O 2 2	0	0
6	K	1	Total O 2 2	0	0
6	L	1	Total O 2 2	0	0
6	M	1	Total O 2 2	0	0
6	N	1	Total O 2 2	0	0
6	O	1	Total O 2 2	0	0
6	P	1	Total O 2 2	0	0
6	Q	1	Total O 2 2	0	0
6	R	1	Total O 2 2	0	0
6	S	1	Total O 2 2	0	0
6	T	1	Total O 2 2	0	0
6	U	1	Total O 2 2	0	0
6	V	1	Total O 2 2	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	W	1	Total O 2 2	0	0
6	X	1	Total O 2 2	0	0

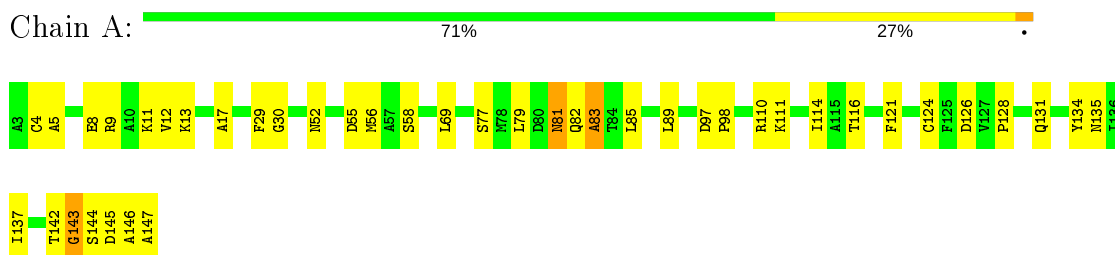
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	2	Total Zn 2 2	0	0
7	B	2	Total Zn 2 2	0	0
7	V	2	Total Zn 2 2	0	0
7	N	2	Total Zn 2 2	0	0
7	R	2	Total Zn 2 2	0	0
7	F	2	Total Zn 2 2	0	0

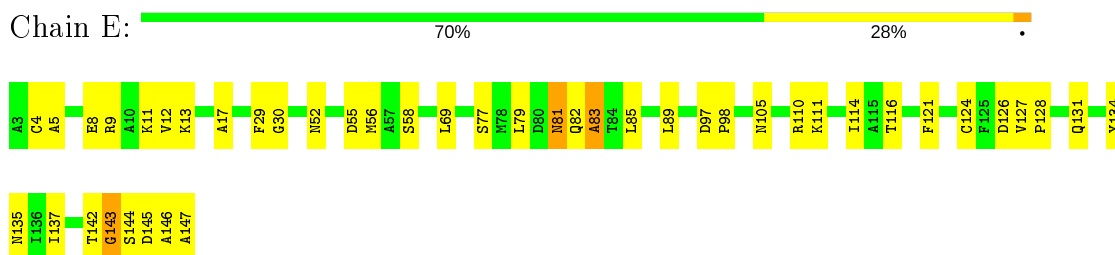
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

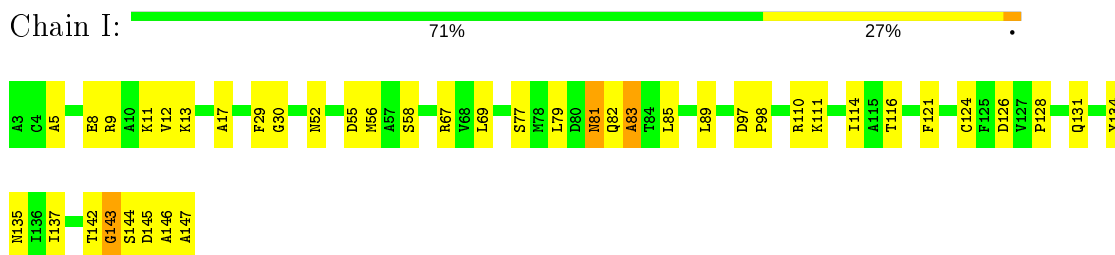
- Molecule 1: hemoglobin A1 chain



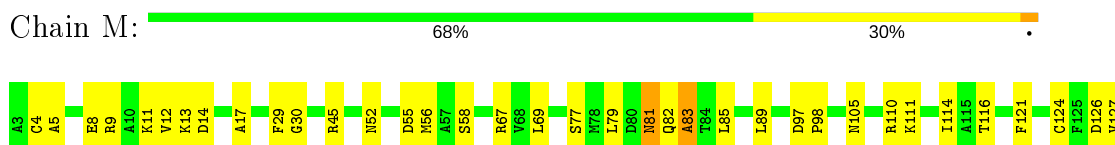
- Molecule 1: hemoglobin A1 chain



- Molecule 1: hemoglobin A1 chain

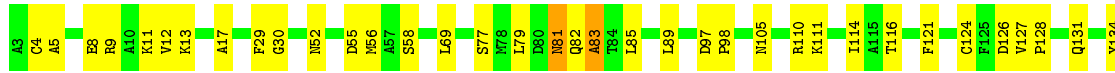


- Molecule 1: hemoglobin A1 chain

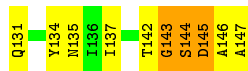




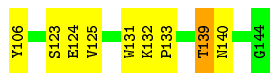
• Molecule 1: hemoglobin A1 chain



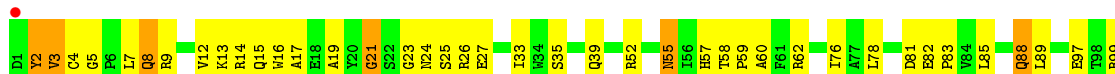
• Molecule 1: hemoglobin A1 chain



• Molecule 2: Giant hemoglobins B chain

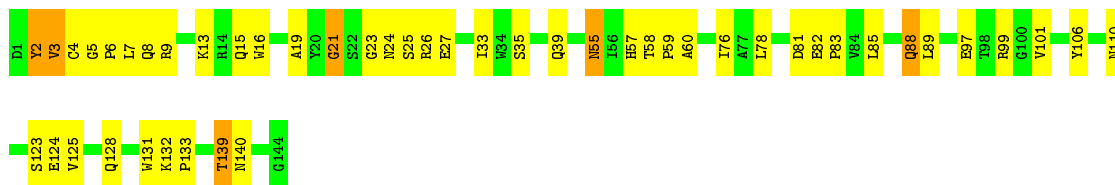


• Molecule 2: Giant hemoglobins B chain

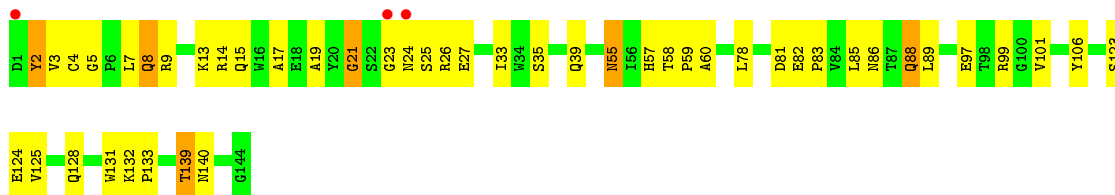


• Molecule 2: Giant hemoglobins B chain

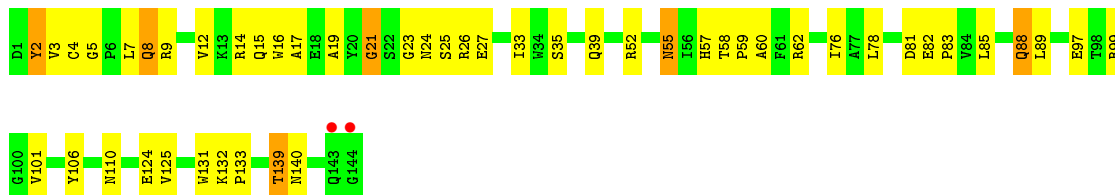




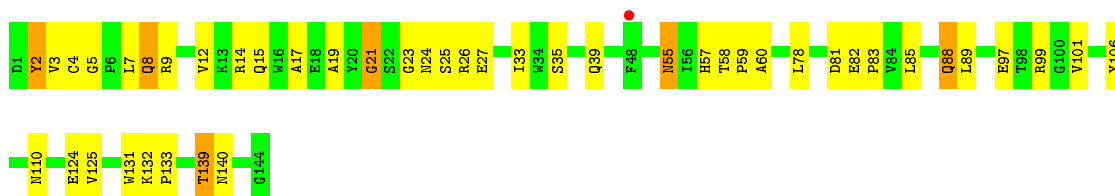
• Molecule 2: Giant hemoglobins B chain



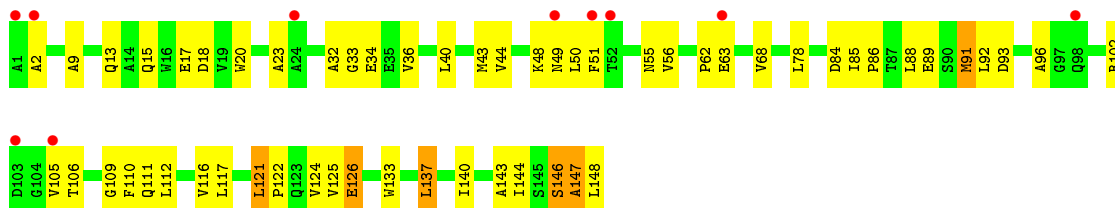
• Molecule 2: Giant hemoglobins B chain



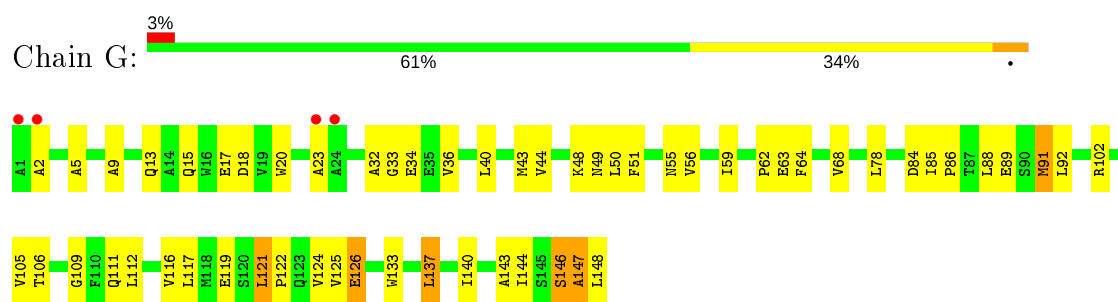
• Molecule 2: Giant hemoglobins B chain



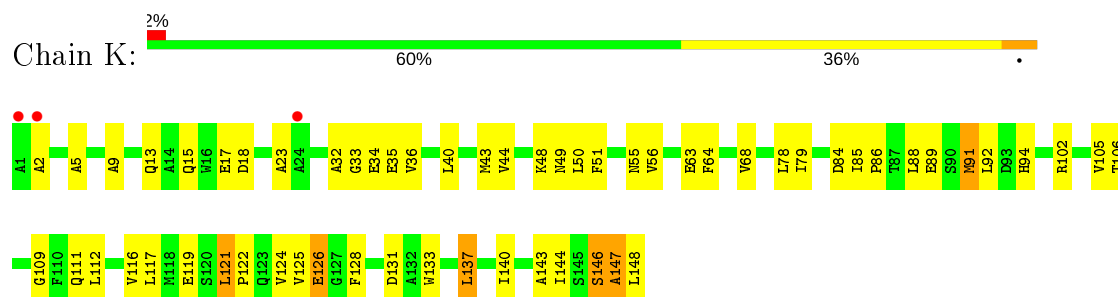
• Molecule 3: hemoglobin B1a chain



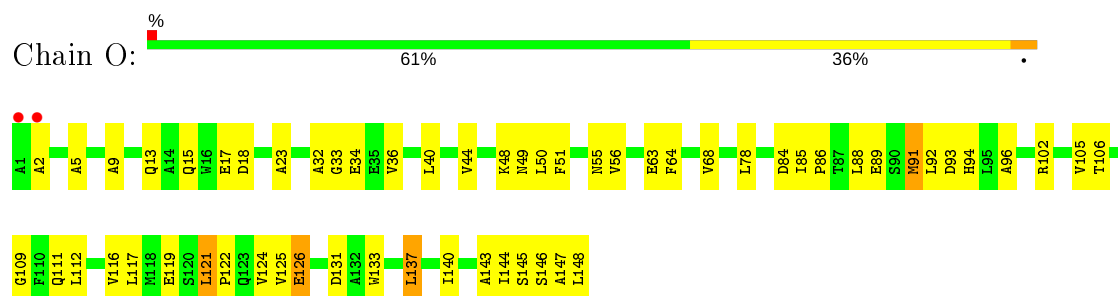
• Molecule 3: hemoglobin B1a chain



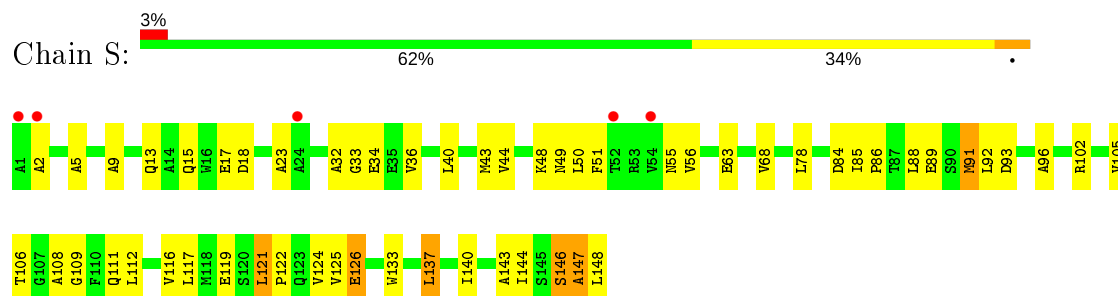
- Molecule 3: hemoglobin B1a chain



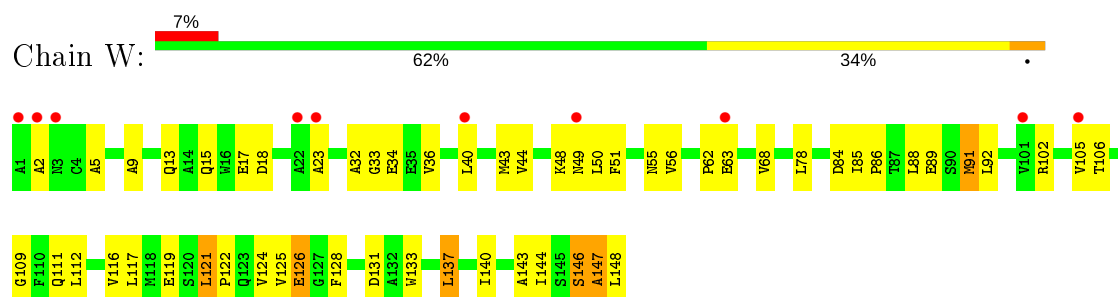
- Molecule 3: hemoglobin B1a chain



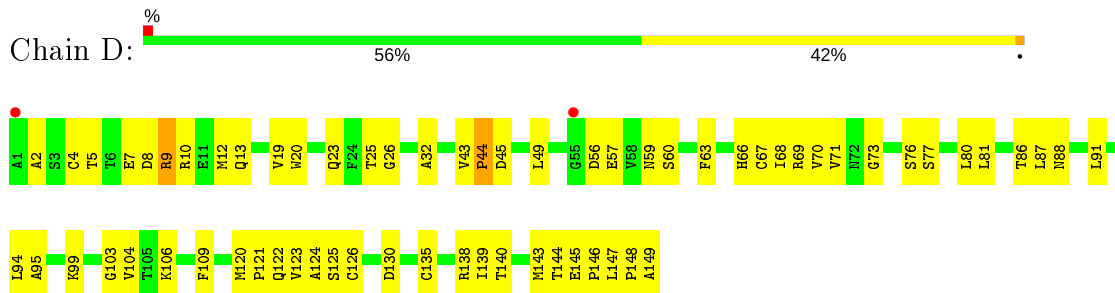
- Molecule 3: hemoglobin B1a chain



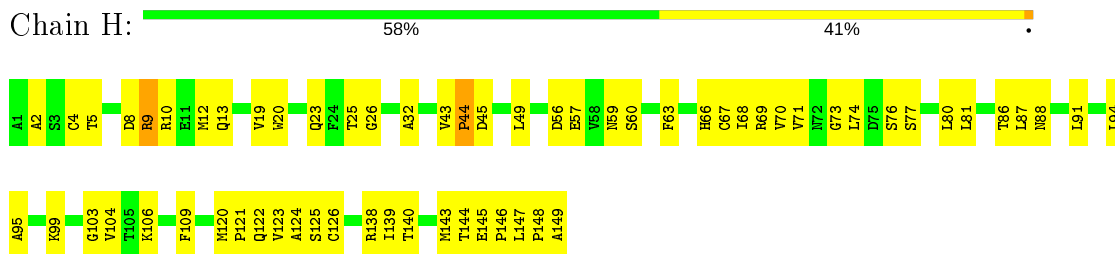
- Molecule 3: hemoglobin B1a chain



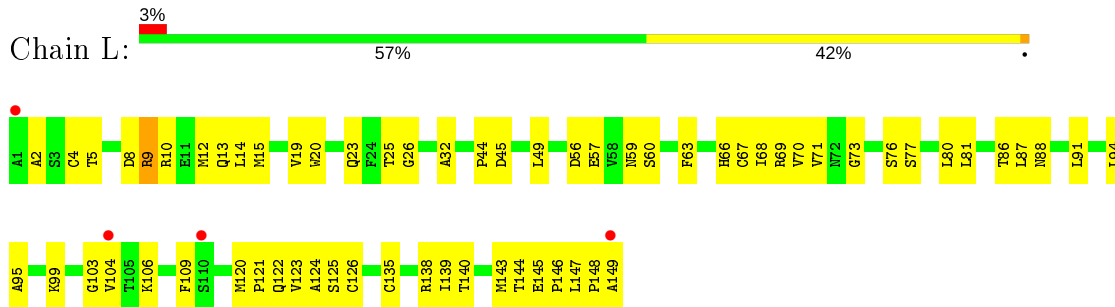
• Molecule 4: hemoglobin B2 chain



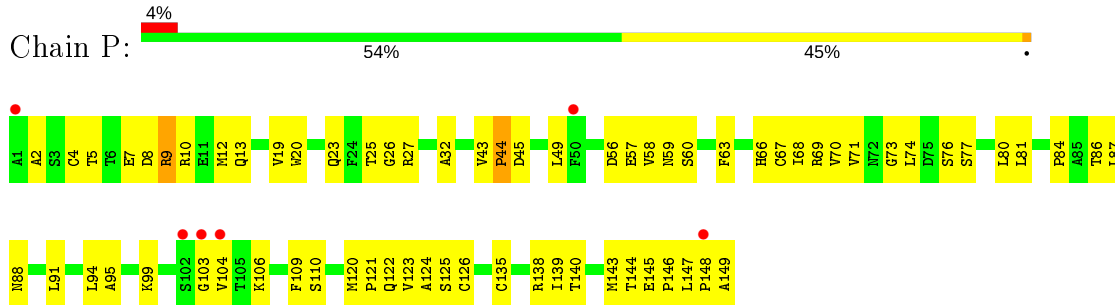
• Molecule 4: hemoglobin B2 chain



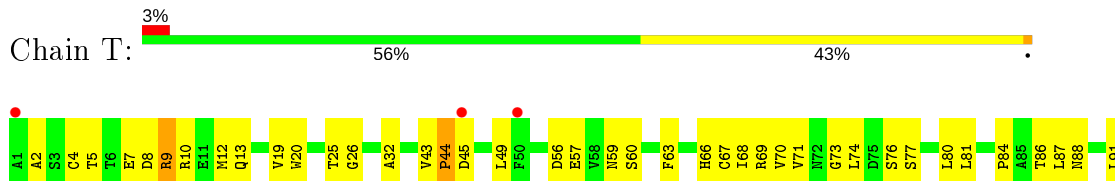
• Molecule 4: hemoglobin B2 chain



• Molecule 4: hemoglobin B2 chain



• Molecule 4: hemoglobin B2 chain





- Molecule 4: hemoglobin B2 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.84Å 195.84Å 308.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.15 49.85 – 3.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.15) 94.9 (49.85-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.97 (at 3.12Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.271 0.219 , 0.242	Depositor DCC
$R_{free}$ test set	5273 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.8	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	27804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.43	0/1135	0.59	0/1536
1	E	0.43	0/1135	0.58	0/1536
1	I	0.44	0/1135	0.58	0/1536
1	M	0.41	0/1135	0.59	0/1536
1	Q	0.42	0/1135	0.58	0/1536
1	U	0.43	0/1135	0.59	0/1536
2	B	0.38	0/1164	0.57	0/1576
2	F	0.41	0/1164	0.57	0/1576
2	J	0.42	0/1164	0.56	0/1576
2	N	0.42	0/1164	0.57	0/1576
2	R	0.39	0/1164	0.56	0/1576
2	V	0.41	0/1164	0.57	0/1576
3	C	0.46	0/1091	0.60	0/1488
3	G	0.46	0/1091	0.61	0/1488
3	K	0.48	0/1091	0.61	0/1488
3	O	0.45	0/1091	0.61	0/1488
3	S	0.45	0/1091	0.60	0/1488
3	W	0.49	0/1091	0.60	0/1488
4	D	0.38	0/1156	0.56	0/1565
4	H	0.37	0/1156	0.56	0/1565
4	L	0.40	0/1156	0.55	0/1565
4	P	0.39	0/1156	0.57	0/1565
4	T	0.38	0/1156	0.56	0/1565
4	X	0.41	0/1156	0.57	0/1565
All	All	0.42	0/27276	0.58	0/36990

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	1111	0	1095	33	0
1	E	1111	0	1095	33	0
1	I	1111	0	1095	30	0
1	M	1111	0	1095	35	0
1	Q	1111	0	1095	33	0
1	U	1111	0	1095	34	0
2	B	1136	0	1090	42	0
2	F	1136	0	1090	45	1
2	J	1136	0	1090	40	0
2	N	1136	0	1090	42	0
2	R	1136	0	1090	45	0
2	V	1136	0	1090	42	0
3	C	1072	0	1053	60	0
3	G	1072	0	1053	63	0
3	K	1072	0	1053	65	0
3	O	1072	0	1053	62	1
3	S	1072	0	1053	63	0
3	W	1072	0	1053	64	0
4	D	1133	0	1112	62	0
4	H	1133	0	1112	57	0
4	L	1133	0	1112	57	0
4	P	1133	0	1112	63	0
4	T	1133	0	1112	64	0
4	X	1133	0	1112	57	0
5	A	43	0	30	0	0
5	B	43	0	30	0	0
5	C	43	0	30	0	0
5	D	43	0	30	6	0
5	E	43	0	30	0	0
5	F	43	0	30	0	0
5	G	43	0	30	0	0
5	H	43	0	30	7	0
5	I	43	0	30	0	0
5	J	43	0	30	0	0
5	K	43	0	30	0	0
5	L	43	0	30	6	0
5	M	43	0	30	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	43	0	30	0	0
5	O	43	0	30	0	0
5	P	43	0	30	7	0
5	Q	43	0	30	0	0
5	R	43	0	30	0	0
5	S	43	0	30	0	0
5	T	43	0	30	7	0
5	U	43	0	30	0	0
5	V	43	0	30	0	0
5	W	43	0	30	0	0
5	X	43	0	30	7	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
6	M	2	0	0	0	0
6	N	2	0	0	0	0
6	O	2	0	0	0	0
6	P	2	0	0	0	0
6	Q	2	0	0	0	0
6	R	2	0	0	0	0
6	S	2	0	0	0	0
6	T	2	0	0	0	0
6	U	2	0	0	0	0
6	V	2	0	0	0	0
6	W	2	0	0	0	0
6	X	2	0	0	0	0
7	B	2	0	0	0	0
7	F	2	0	0	0	0
7	J	2	0	0	0	0
7	N	2	0	0	0	0
7	R	2	0	0	0	0
7	V	2	0	0	0	0
All	All	27804	0	26820	1073	1

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 20.

The worst 5 of 1073 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:M:124:CYS:HG	4:P:126:CYS:HG	1.04	1.02
3:W:88:LEU:O	3:W:92:LEU:HG	1.66	0.95
3:O:2:ALA:HB2	3:O:92:LEU:HD11	1.49	0.94
3:C:88:LEU:O	3:C:92:LEU:HG	1.66	0.94
3:G:88:LEU:O	3:G:92:LEU:HG	1.69	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:TYR:OH	3:O:145:SER:O[5_545]	2.00	0.20

## 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	143/145 (99%)	127 (89%)	14 (10%)	2 (1%)	11	43
1	E	143/145 (99%)	128 (90%)	13 (9%)	2 (1%)	11	43
1	I	143/145 (99%)	128 (90%)	13 (9%)	2 (1%)	11	43
1	M	143/145 (99%)	127 (89%)	14 (10%)	2 (1%)	11	43
1	Q	143/145 (99%)	128 (90%)	13 (9%)	2 (1%)	11	43
1	U	143/145 (99%)	128 (90%)	13 (9%)	2 (1%)	11	43
2	B	142/144 (99%)	120 (84%)	16 (11%)	6 (4%)	3	17
2	F	142/144 (99%)	122 (86%)	14 (10%)	6 (4%)	3	17
2	J	142/144 (99%)	120 (84%)	16 (11%)	6 (4%)	3	17

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	142/144 (99%)	121 (85%)	15 (11%)	6 (4%)	3	17
2	R	142/144 (99%)	120 (84%)	16 (11%)	6 (4%)	3	17
2	V	142/144 (99%)	120 (84%)	16 (11%)	6 (4%)	3	17
3	C	146/148 (99%)	124 (85%)	19 (13%)	3 (2%)	7	33
3	G	146/148 (99%)	126 (86%)	17 (12%)	3 (2%)	7	33
3	K	146/148 (99%)	124 (85%)	19 (13%)	3 (2%)	7	33
3	O	146/148 (99%)	126 (86%)	17 (12%)	3 (2%)	7	33
3	S	146/148 (99%)	125 (86%)	18 (12%)	3 (2%)	7	33
3	W	146/148 (99%)	124 (85%)	19 (13%)	3 (2%)	7	33
4	D	147/149 (99%)	132 (90%)	10 (7%)	5 (3%)	3	21
4	H	147/149 (99%)	131 (89%)	11 (8%)	5 (3%)	3	21
4	L	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3	21
4	P	147/149 (99%)	131 (89%)	11 (8%)	5 (3%)	3	21
4	T	147/149 (99%)	133 (90%)	9 (6%)	5 (3%)	3	21
4	X	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3	21
All	All	3468/3516 (99%)	3025 (87%)	347 (10%)	96 (3%)	5	26

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	GLY
4	D	148	PRO
1	E	143	GLY
4	H	125	SER
4	H	148	PRO

### 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	112/112 (100%)	107 (96%)	5 (4%)	27	61

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	112/112 (100%)	107 (96%)	5 (4%)	27	61
1	I	112/112 (100%)	107 (96%)	5 (4%)	27	61
1	M	112/112 (100%)	107 (96%)	5 (4%)	27	61
1	Q	112/112 (100%)	107 (96%)	5 (4%)	27	61
1	U	112/112 (100%)	107 (96%)	5 (4%)	27	61
2	B	118/118 (100%)	112 (95%)	6 (5%)	24	56
2	F	118/118 (100%)	112 (95%)	6 (5%)	24	56
2	J	118/118 (100%)	112 (95%)	6 (5%)	24	56
2	N	118/118 (100%)	112 (95%)	6 (5%)	24	56
2	R	118/118 (100%)	112 (95%)	6 (5%)	24	56
2	V	118/118 (100%)	112 (95%)	6 (5%)	24	56
3	C	106/106 (100%)	98 (92%)	8 (8%)	13	42
3	G	106/106 (100%)	98 (92%)	8 (8%)	13	42
3	K	106/106 (100%)	99 (93%)	7 (7%)	16	47
3	O	106/106 (100%)	99 (93%)	7 (7%)	16	47
3	S	106/106 (100%)	99 (93%)	7 (7%)	16	47
3	W	106/106 (100%)	99 (93%)	7 (7%)	16	47
4	D	120/120 (100%)	114 (95%)	6 (5%)	24	57
4	H	120/120 (100%)	114 (95%)	6 (5%)	24	57
4	L	120/120 (100%)	114 (95%)	6 (5%)	24	57
4	P	120/120 (100%)	114 (95%)	6 (5%)	24	57
4	T	120/120 (100%)	114 (95%)	6 (5%)	24	57
4	X	120/120 (100%)	114 (95%)	6 (5%)	24	57
All	All	2736/2736 (100%)	2590 (95%)	146 (5%)	22	55

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	146	SER
2	N	27	GLU
3	W	91	MET
3	K	148	LEU
1	M	52	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
3	K	15	GLN
2	N	24	ASN
2	V	110	ASN
4	L	18	ASN
1	M	39	ASN

### 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 carbohydrates in this entry.

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

Of 60 ligands modelled in this entry, 12 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	OXY	D	161	5	1,1,1	0.04	0	-		
5	HEM	G	160	3,6	27,50,50	1.75	6 (22%)	17,82,82	0.85	0
5	HEM	E	160	1,6	27,50,50	1.50	6 (22%)	17,82,82	1.29	1 (5%)
5	HEM	T	160	4,6	27,50,50	2.08	6 (22%)	17,82,82	1.27	2 (11%)
6	OXY	L	161	5	1,1,1	0.05	0	-		
5	HEM	M	160	1,6	27,50,50	1.57	5 (18%)	17,82,82	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEM	R	160	2,6	27,50,50	1.81	6 (22%)	17,82,82	0.91	1 (5%)
5	HEM	U	160	1,6	27,50,50	1.62	5 (18%)	17,82,82	1.00	1 (5%)
6	OXY	X	161	5	1,1,1	0.02	0	-		
5	HEM	A	160	1,6	27,50,50	1.63	6 (22%)	17,82,82	0.97	1 (5%)
6	OXY	R	161	5	1,1,1	0.03	0	-		
6	OXY	S	161	5	1,1,1	0.03	0	-		
6	OXY	N	161	5	1,1,1	0.03	0	-		
5	HEM	I	160	1,6	27,50,50	1.72	6 (22%)	17,82,82	1.08	1 (5%)
6	OXY	U	161	5	1,1,1	0.03	0	-		
6	OXY	H	161	5	1,1,1	0.07	0	-		
6	OXY	K	161	5	1,1,1	0.05	0	-		
6	OXY	W	161	5	1,1,1	0.01	0	-		
6	OXY	M	161	5	1,1,1	0.00	0	-		
5	HEM	D	160	4,6	27,50,50	2.05	6 (22%)	17,82,82	1.47	2 (11%)
6	OXY	E	161	5	1,1,1	0.02	0	-		
6	OXY	V	161	5	1,1,1	0.03	0	-		
5	HEM	L	160	4,6	27,50,50	2.18	6 (22%)	17,82,82	1.43	2 (11%)
5	HEM	B	160	2,6	27,50,50	1.58	6 (22%)	17,82,82	1.03	2 (11%)
5	HEM	J	160	2,6	27,50,50	1.85	5 (18%)	17,82,82	1.26	1 (5%)
5	HEM	H	160	4,6	27,50,50	2.14	6 (22%)	17,82,82	1.36	2 (11%)
5	HEM	N	160	2,6	27,50,50	1.66	7 (25%)	17,82,82	0.87	1 (5%)
6	OXY	F	161	5	1,1,1	0.02	0	-		
6	OXY	G	161	5	1,1,1	0.02	0	-		
5	HEM	W	160	3,6	27,50,50	1.55	5 (18%)	17,82,82	0.78	1 (5%)
5	HEM	P	160	4,6	27,50,50	2.01	6 (22%)	17,82,82	1.26	2 (11%)
5	HEM	X	160	4,6	27,50,50	1.88	5 (18%)	17,82,82	1.22	2 (11%)
5	HEM	C	160	3,6	27,50,50	1.79	7 (25%)	17,82,82	0.80	1 (5%)
6	OXY	Q	161	5	1,1,1	0.03	0	-		
6	OXY	T	161	5	1,1,1	0.03	0	-		
5	HEM	F	160	2,6	27,50,50	1.72	6 (22%)	17,82,82	1.16	1 (5%)
5	HEM	K	160	3,6	27,50,50	2.03	5 (18%)	17,82,82	0.92	0
6	OXY	I	161	5	1,1,1	0.03	0	-		
6	OXY	O	161	5	1,1,1	0.03	0	-		
5	HEM	O	160	3,6	27,50,50	1.71	6 (22%)	17,82,82	0.87	0
6	OXY	C	161	5	1,1,1	0.00	0	-		
5	HEM	S	160	3,6	27,50,50	1.70	7 (25%)	17,82,82	0.97	1 (5%)
6	OXY	A	161	5	1,1,1	0.03	0	-		
5	HEM	Q	160	1,6	27,50,50	1.54	5 (18%)	17,82,82	1.35	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	OXY	P	161	5	1,1,1	0.02	0	-		
6	OXY	B	161	5	1,1,1	0.03	0	-		
5	HEM	V	160	2,6	27,50,50	1.63	5 (18%)	17,82,82	1.06	1 (5%)
6	OXY	J	161	5	1,1,1	0.04	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
5	HEM	G	160	3,6	-	0/6/54/54	-
5	HEM	E	160	1,6	-	0/6/54/54	-
5	HEM	T	160	4,6	-	0/6/54/54	-
5	HEM	M	160	1,6	-	0/6/54/54	-
5	HEM	R	160	2,6	-	0/6/54/54	-
5	HEM	U	160	1,6	-	0/6/54/54	-
5	HEM	A	160	1,6	-	0/6/54/54	-
5	HEM	I	160	1,6	-	0/6/54/54	-
5	HEM	D	160	4,6	-	0/6/54/54	-
5	HEM	L	160	4,6	-	0/6/54/54	-
5	HEM	B	160	2,6	-	0/6/54/54	-
5	HEM	J	160	2,6	-	0/6/54/54	-
5	HEM	H	160	4,6	-	0/6/54/54	-
5	HEM	N	160	2,6	-	0/6/54/54	-
5	HEM	W	160	3,6	-	0/6/54/54	-
5	HEM	P	160	4,6	-	0/6/54/54	-
5	HEM	X	160	4,6	-	0/6/54/54	-
5	HEM	C	160	3,6	-	0/6/54/54	-
5	HEM	F	160	2,6	-	0/6/54/54	-
5	HEM	K	160	3,6	-	0/6/54/54	-
5	HEM	O	160	3,6	-	0/6/54/54	-
5	HEM	S	160	3,6	-	0/6/54/54	-
5	HEM	Q	160	1,6	-	0/6/54/54	-
5	HEM	V	160	2,6	-	0/6/54/54	-

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	160	HEM	C3B-CAB	-5.53	1.36	1.47
5	L	160	HEM	C3B-C2B	-5.46	1.32	1.40
5	H	160	HEM	C3B-CAB	-5.40	1.36	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	160	HEM	C3B-CAB	-5.18	1.37	1.47
5	H	160	HEM	C3C-CAC	-5.14	1.37	1.47

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	160	HEM	C4C-C3C-C2C	4.60	110.11	106.90
5	D	160	HEM	C4C-C3C-C2C	4.49	110.04	106.90
5	J	160	HEM	C4C-C3C-C2C	-4.16	103.99	106.90
5	H	160	HEM	C4C-C3C-C2C	4.07	109.74	106.90
5	T	160	HEM	C4C-C3C-C2C	4.01	109.70	106.90

There are no chirality outliers.

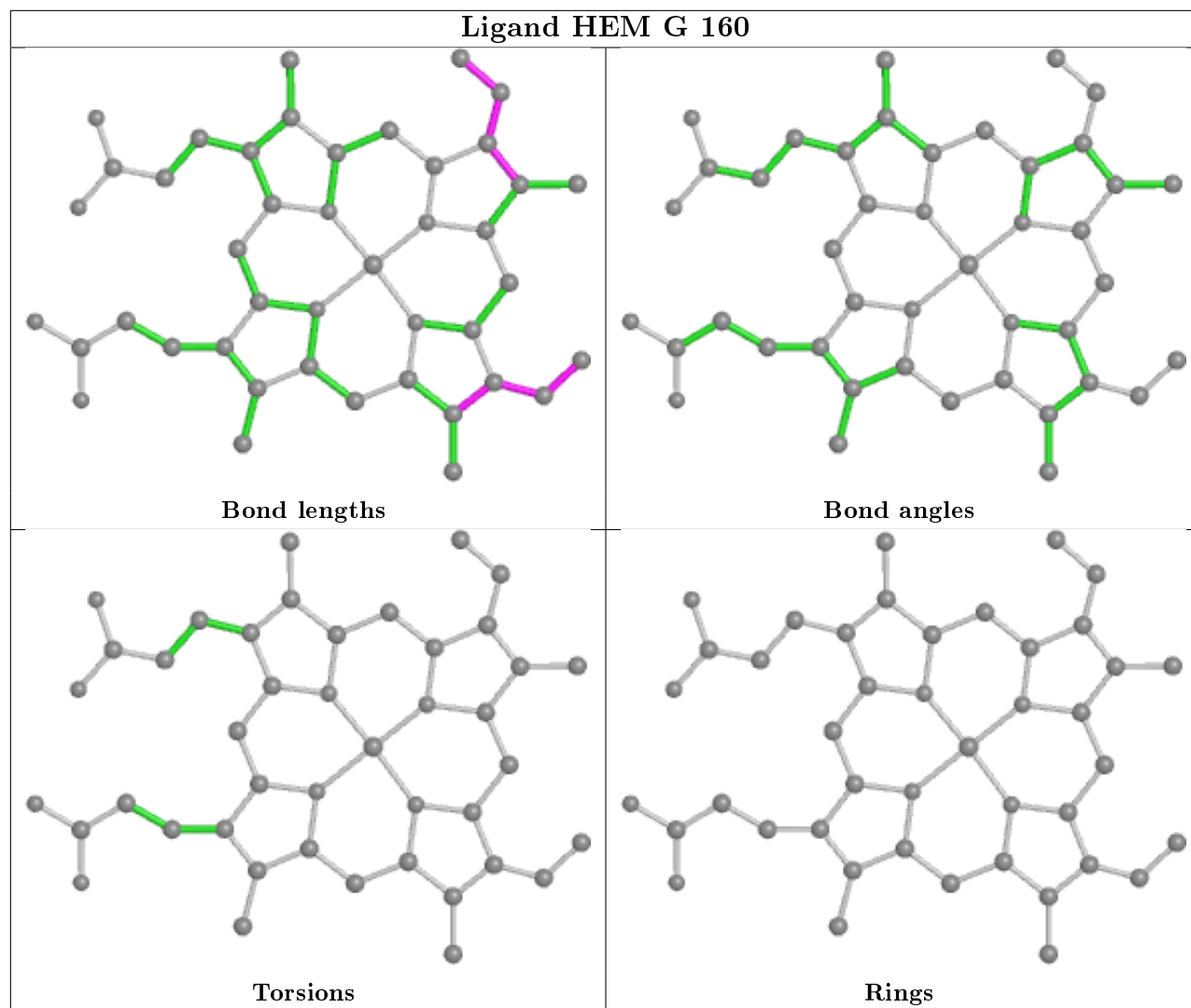
There are no torsion outliers.

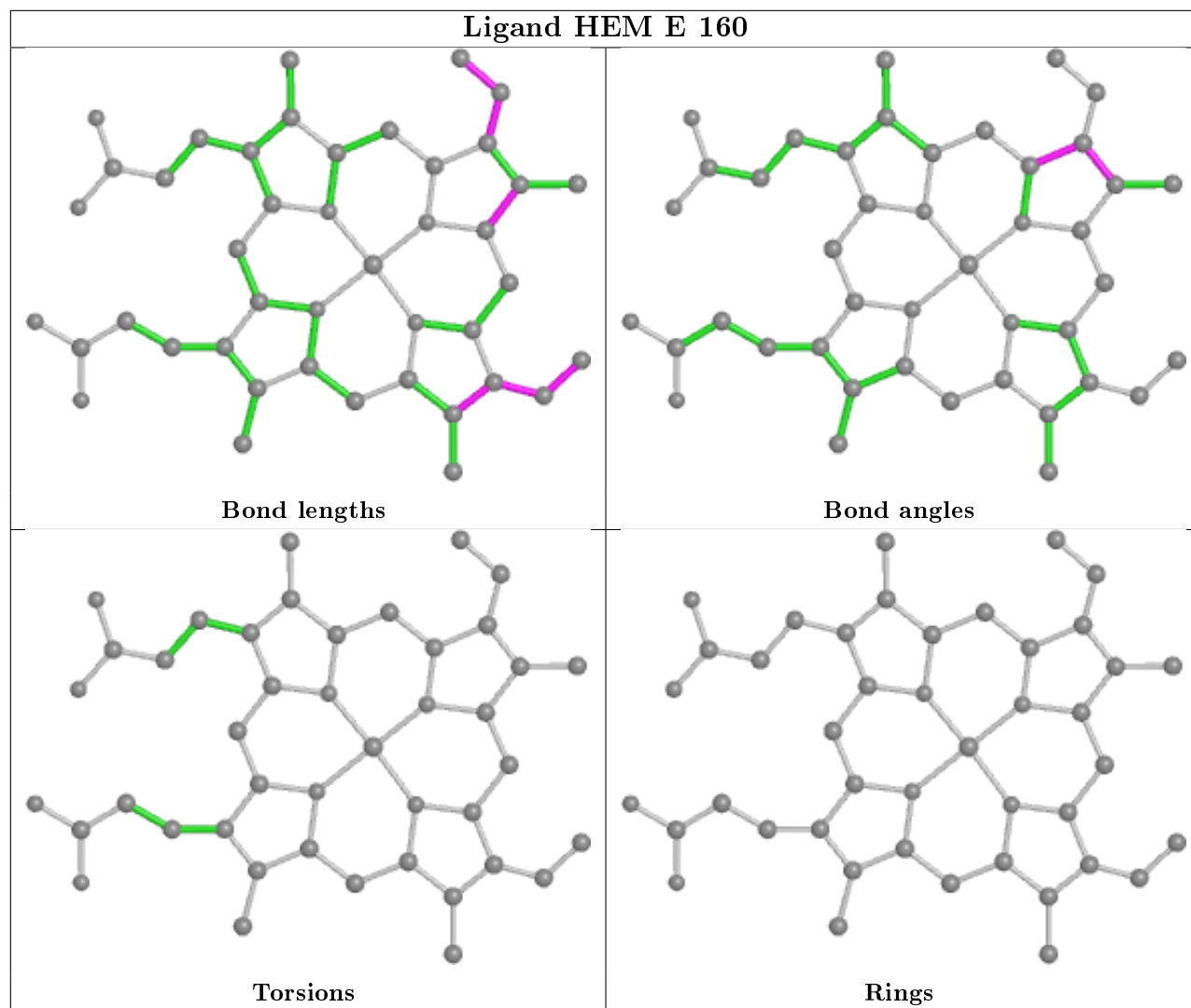
There are no ring outliers.

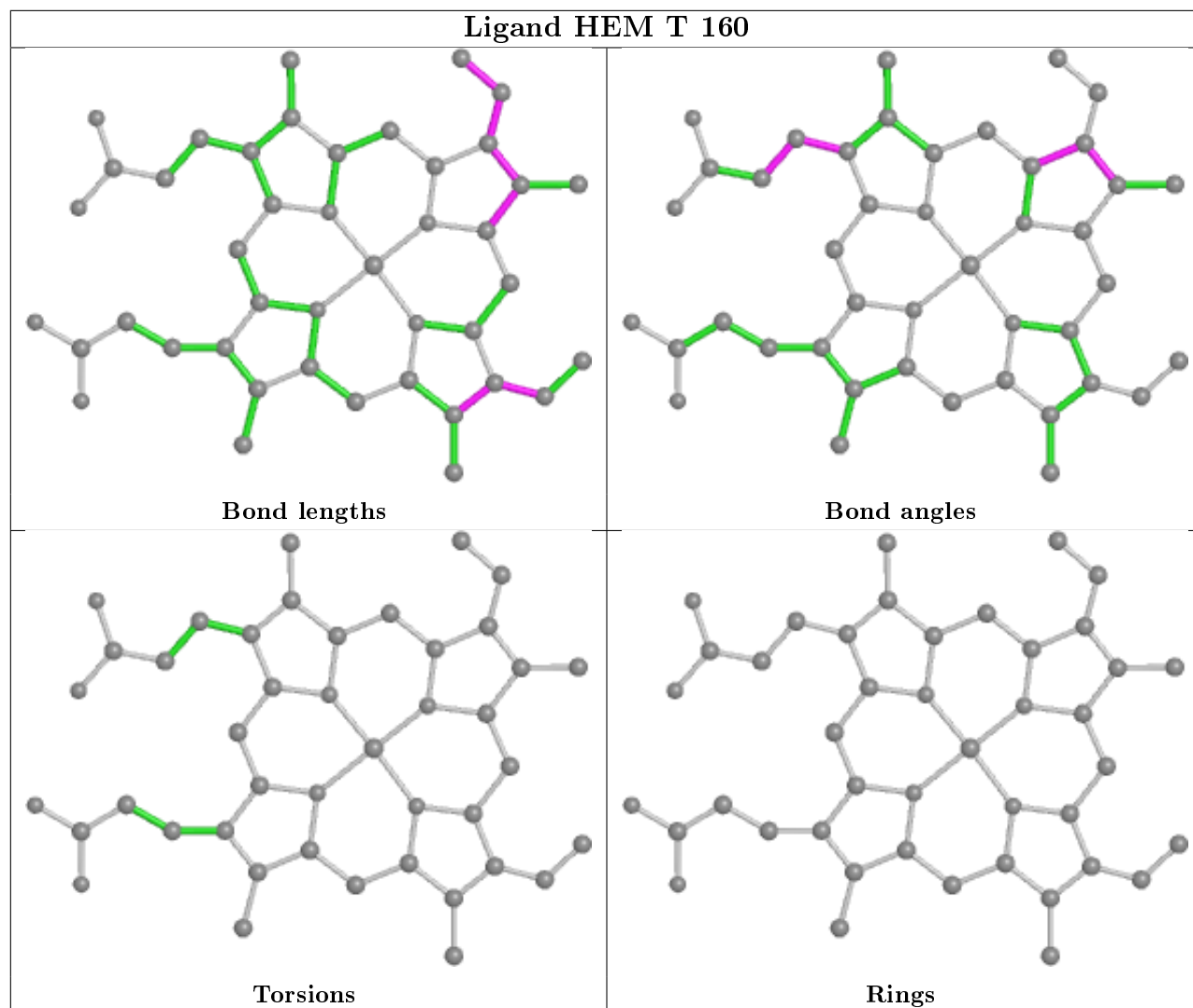
6 monomers are involved in 40 short contacts:

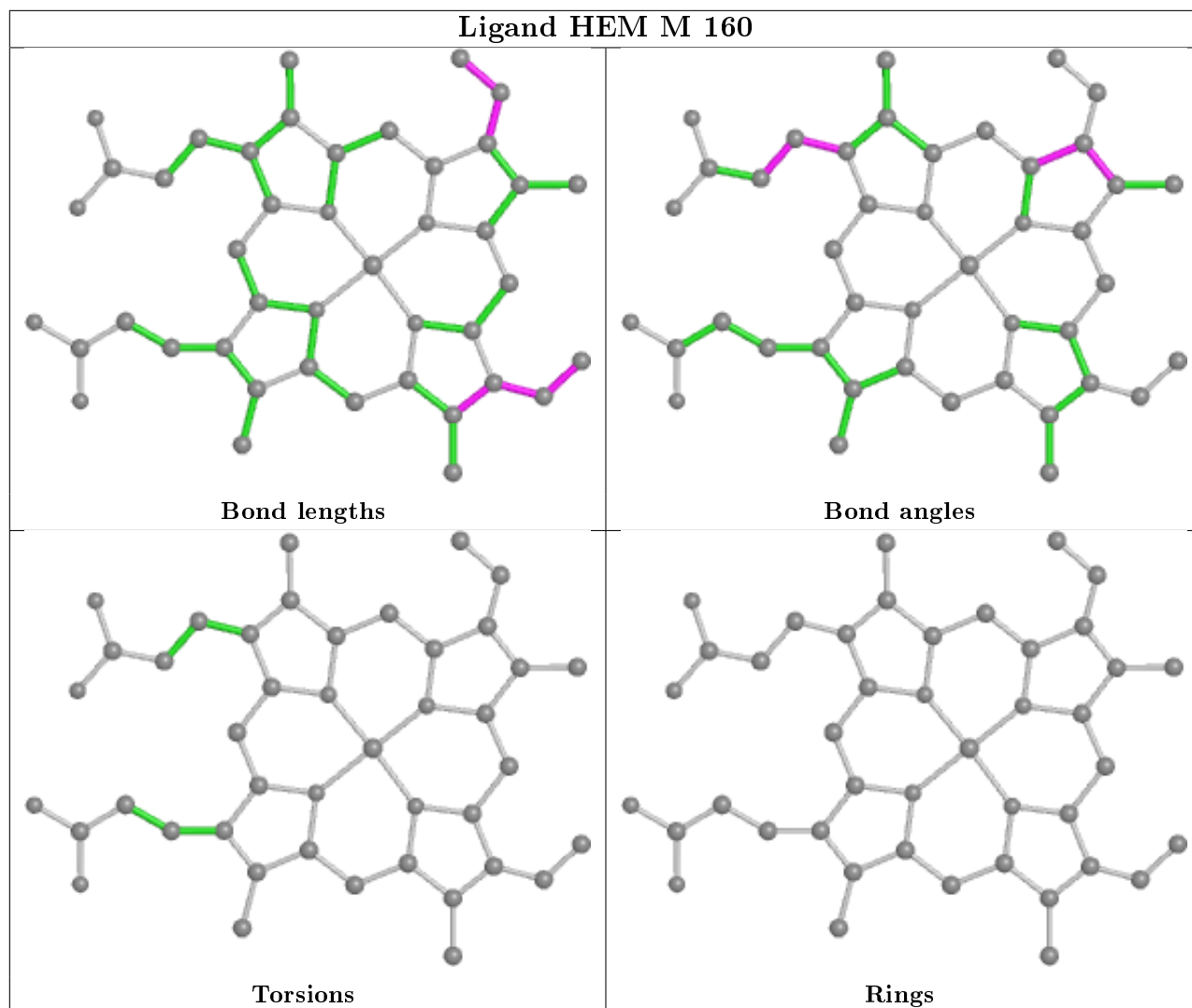
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	160	HEM	7	0
5	D	160	HEM	6	0
5	L	160	HEM	6	0
5	H	160	HEM	7	0
5	P	160	HEM	7	0
5	X	160	HEM	7	0

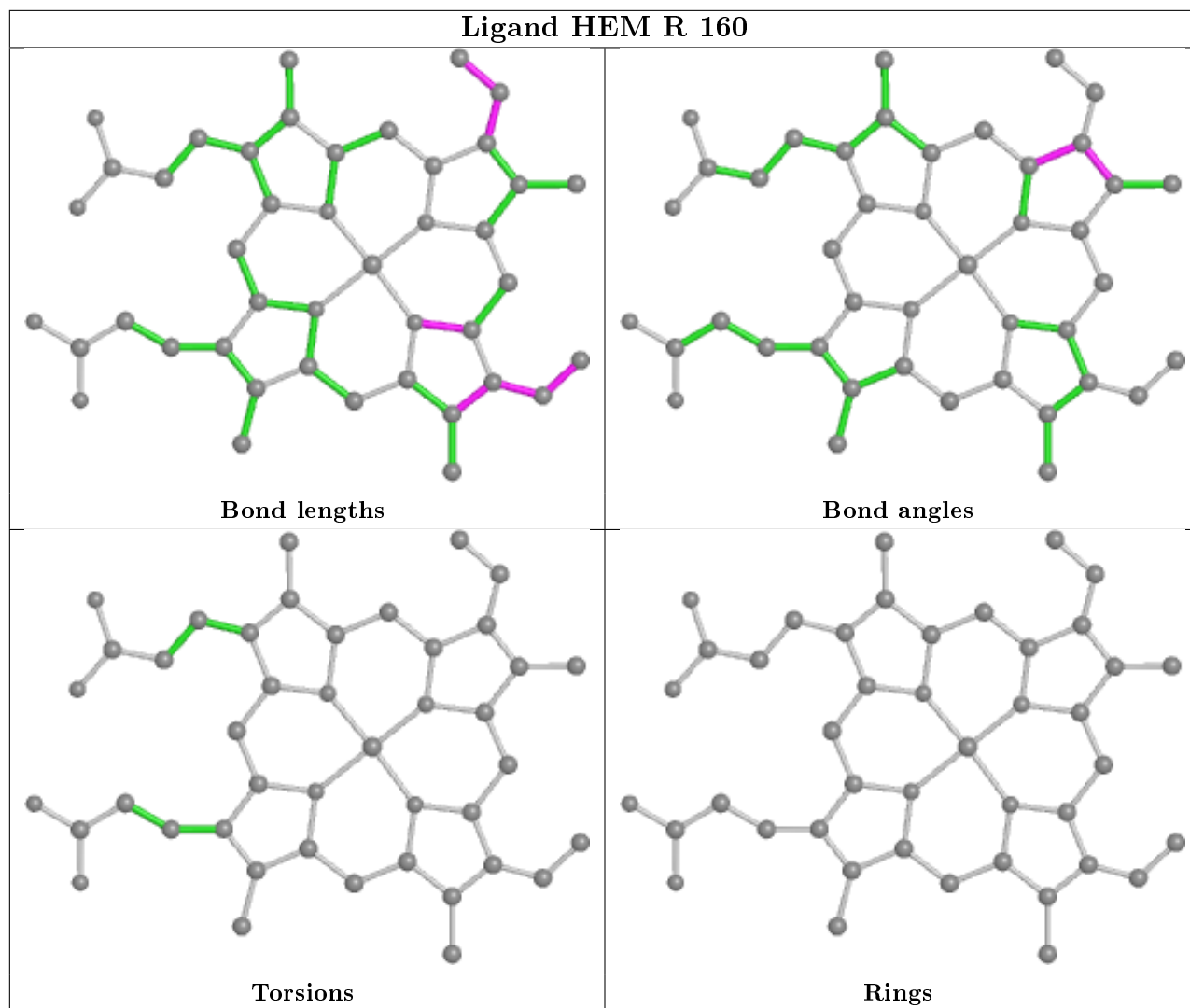
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

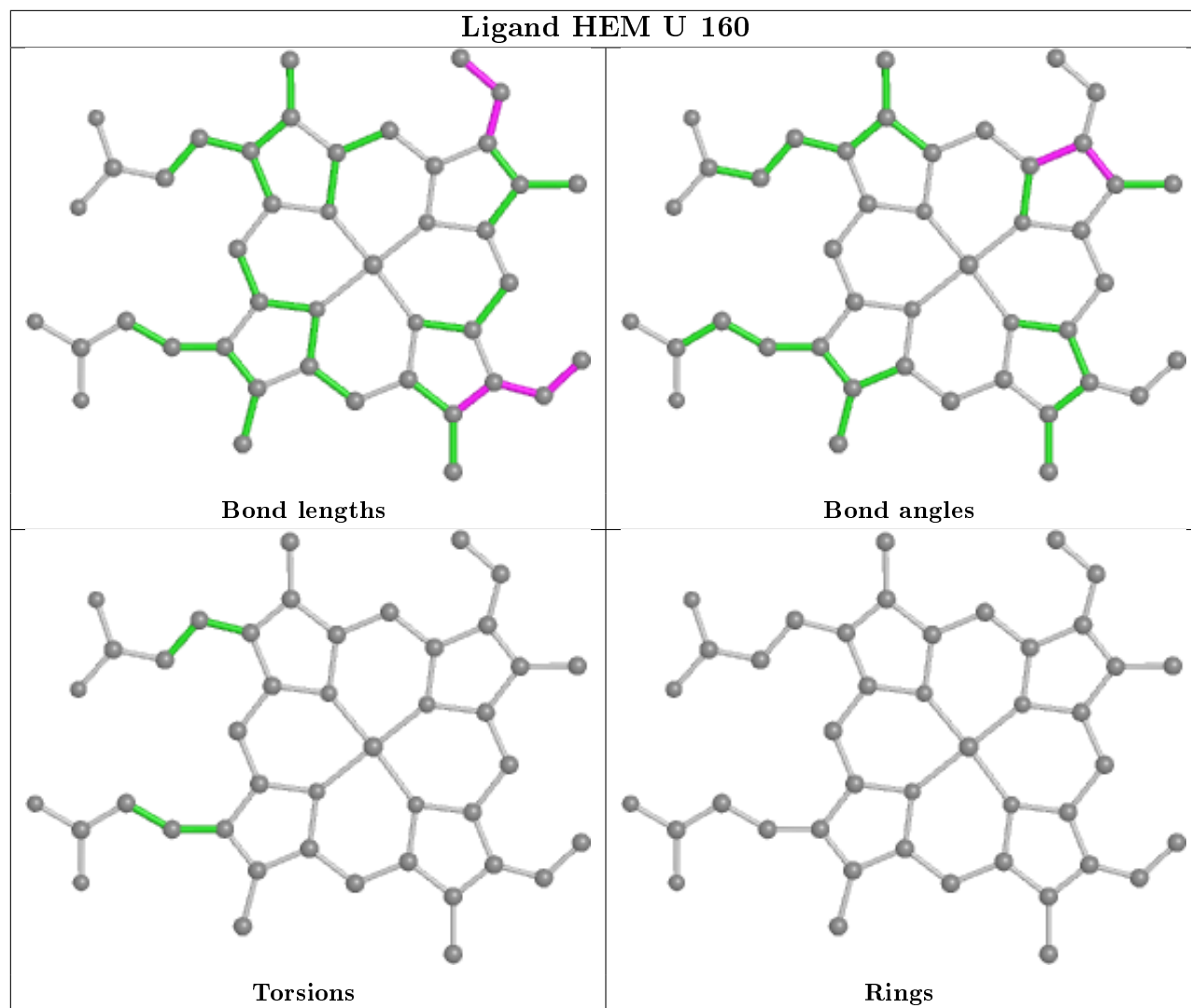




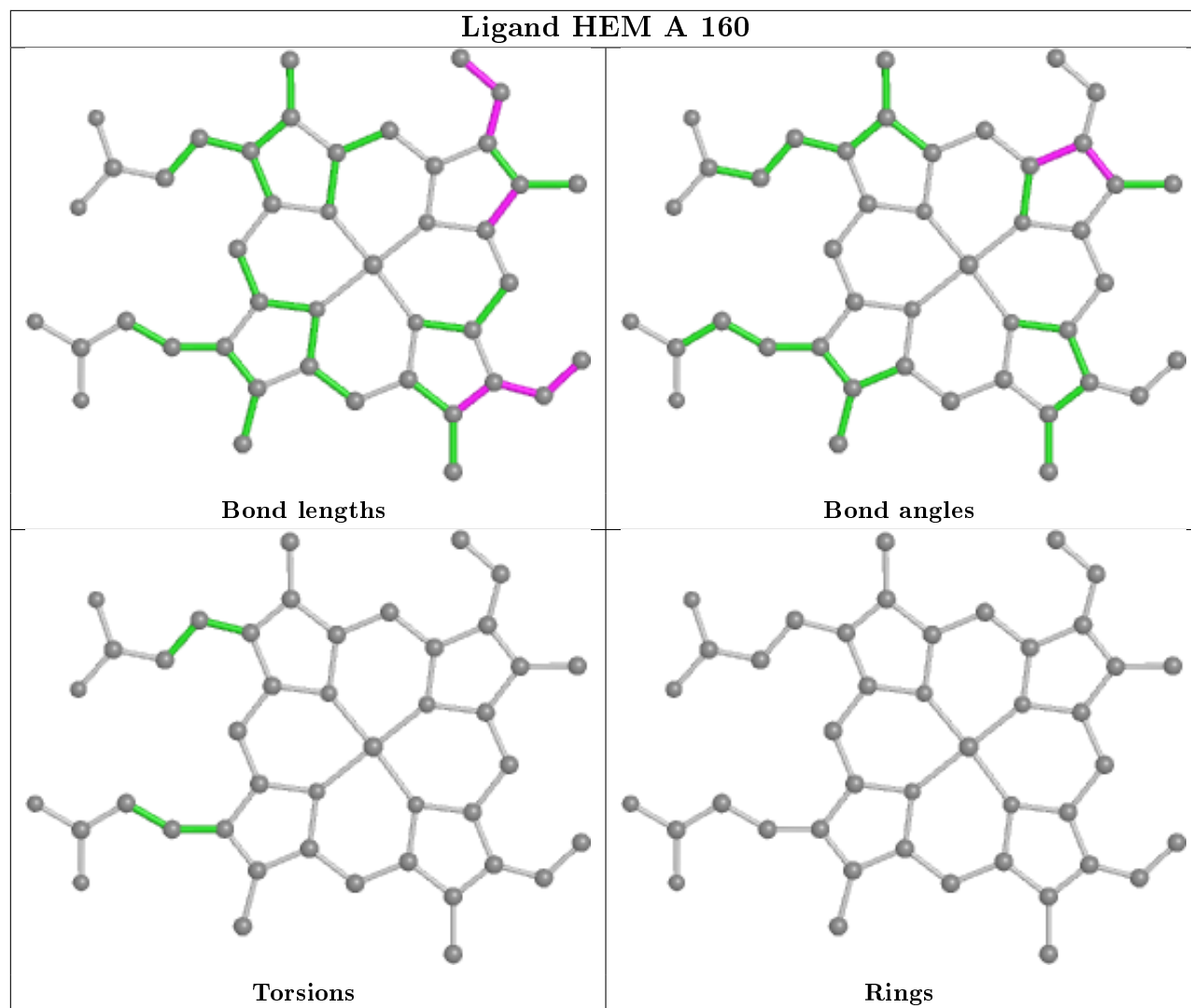


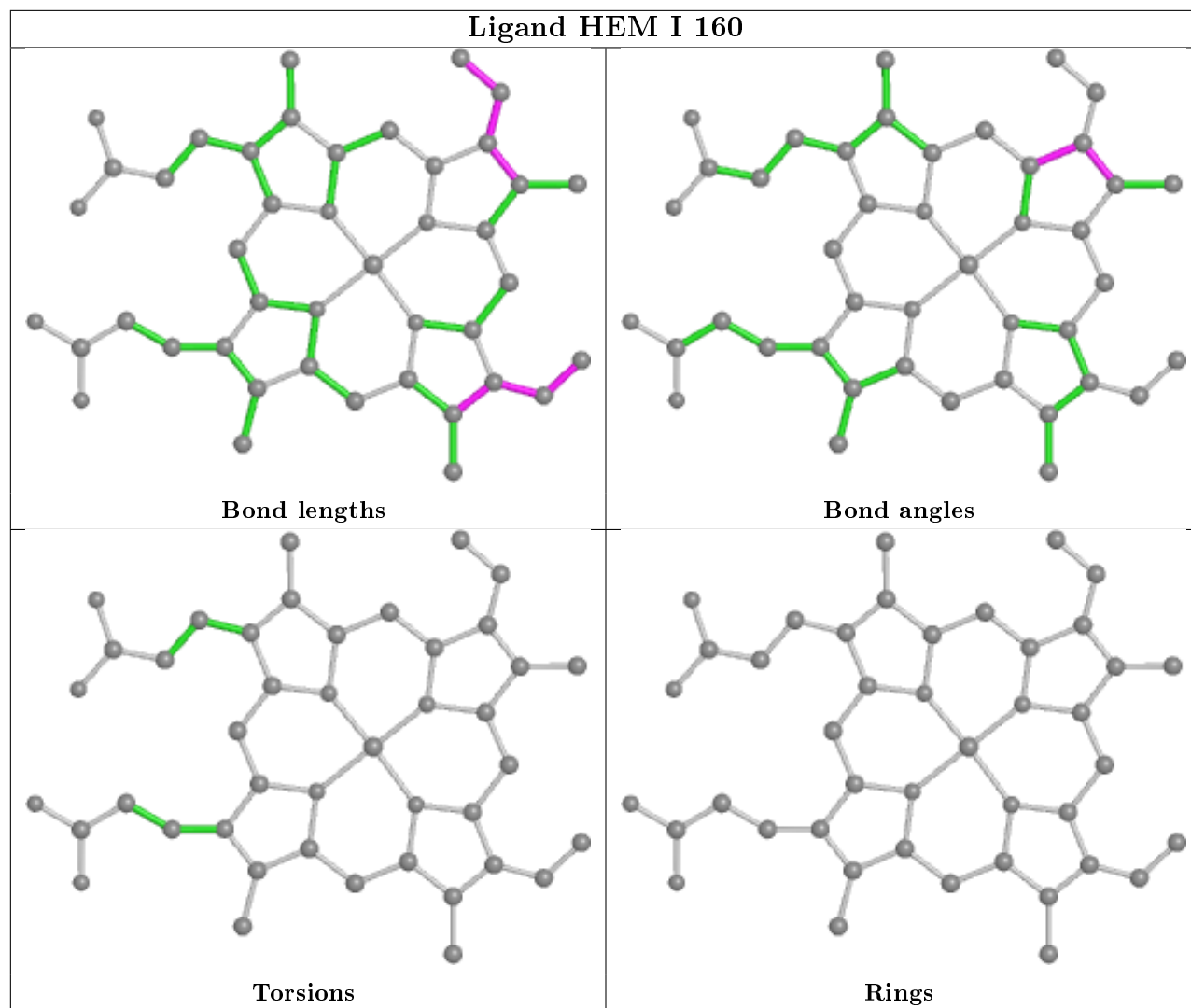


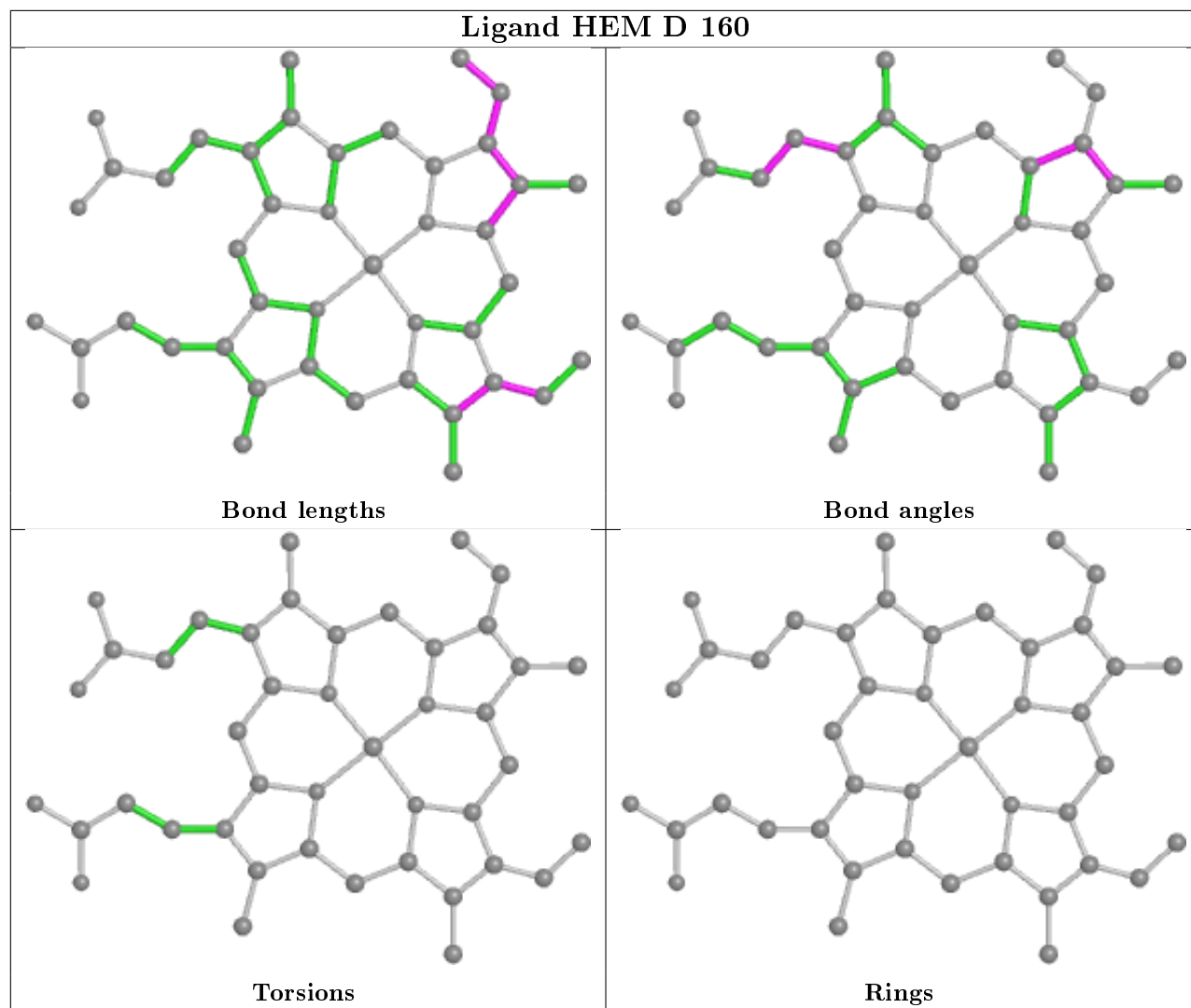


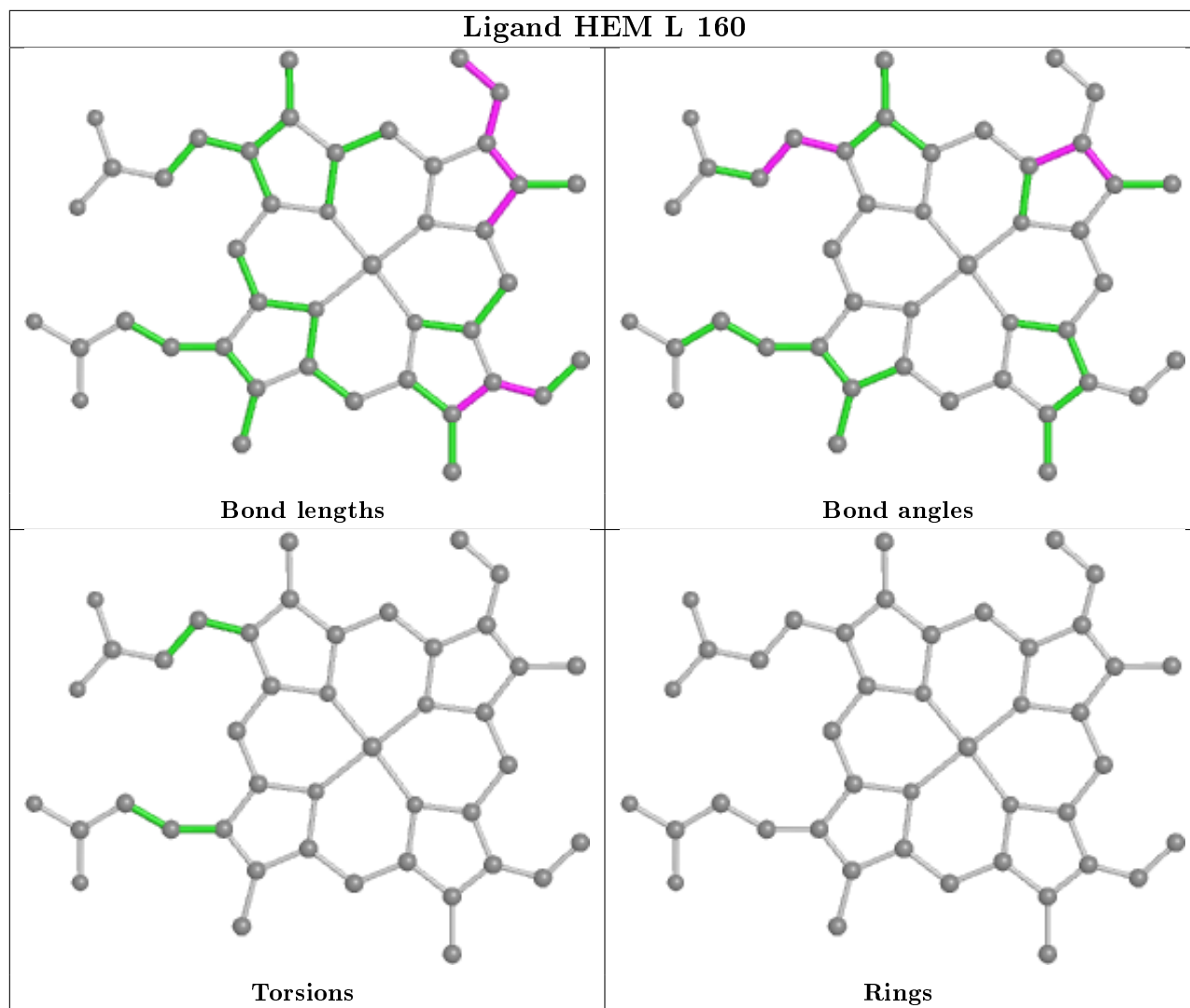


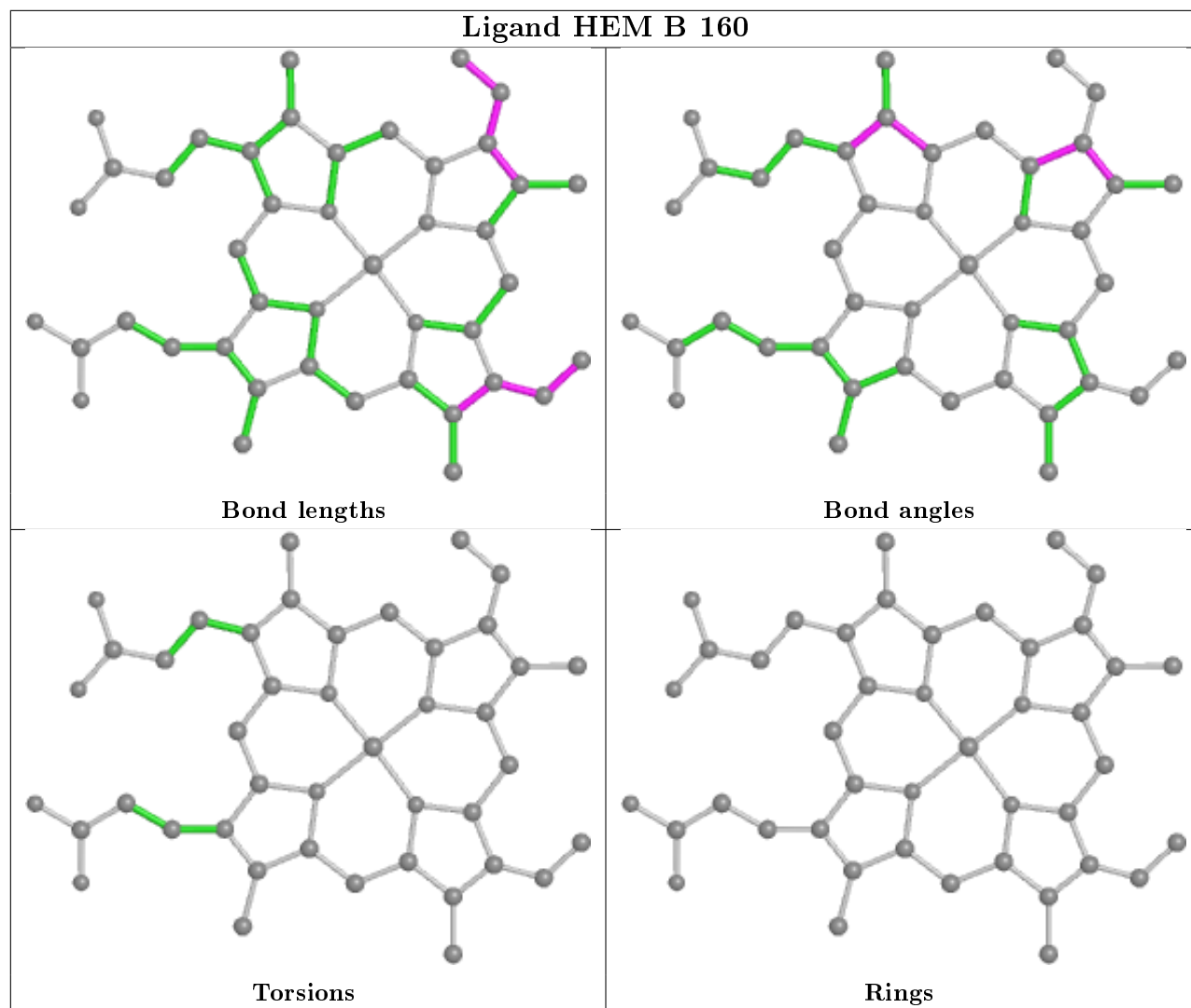


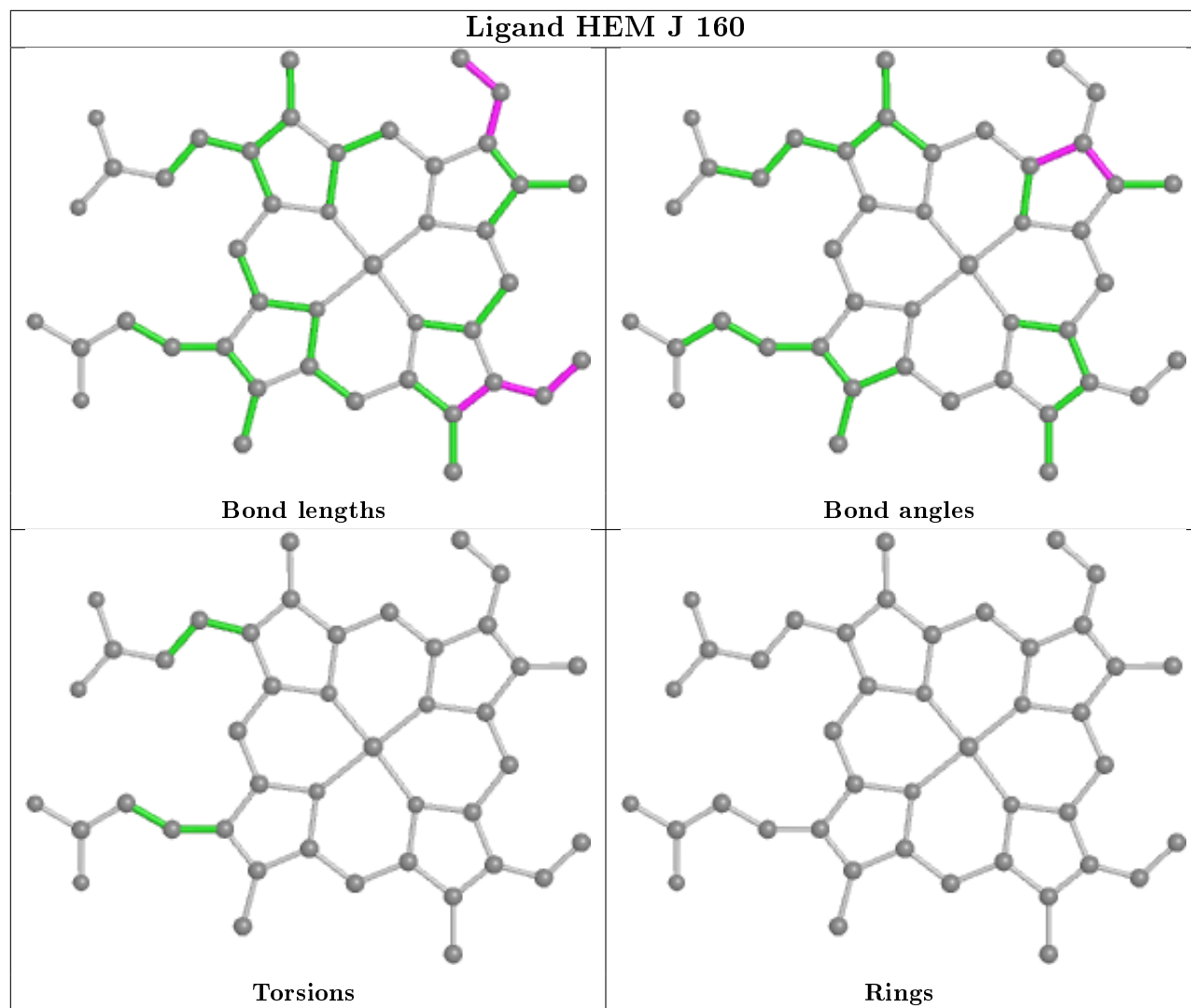


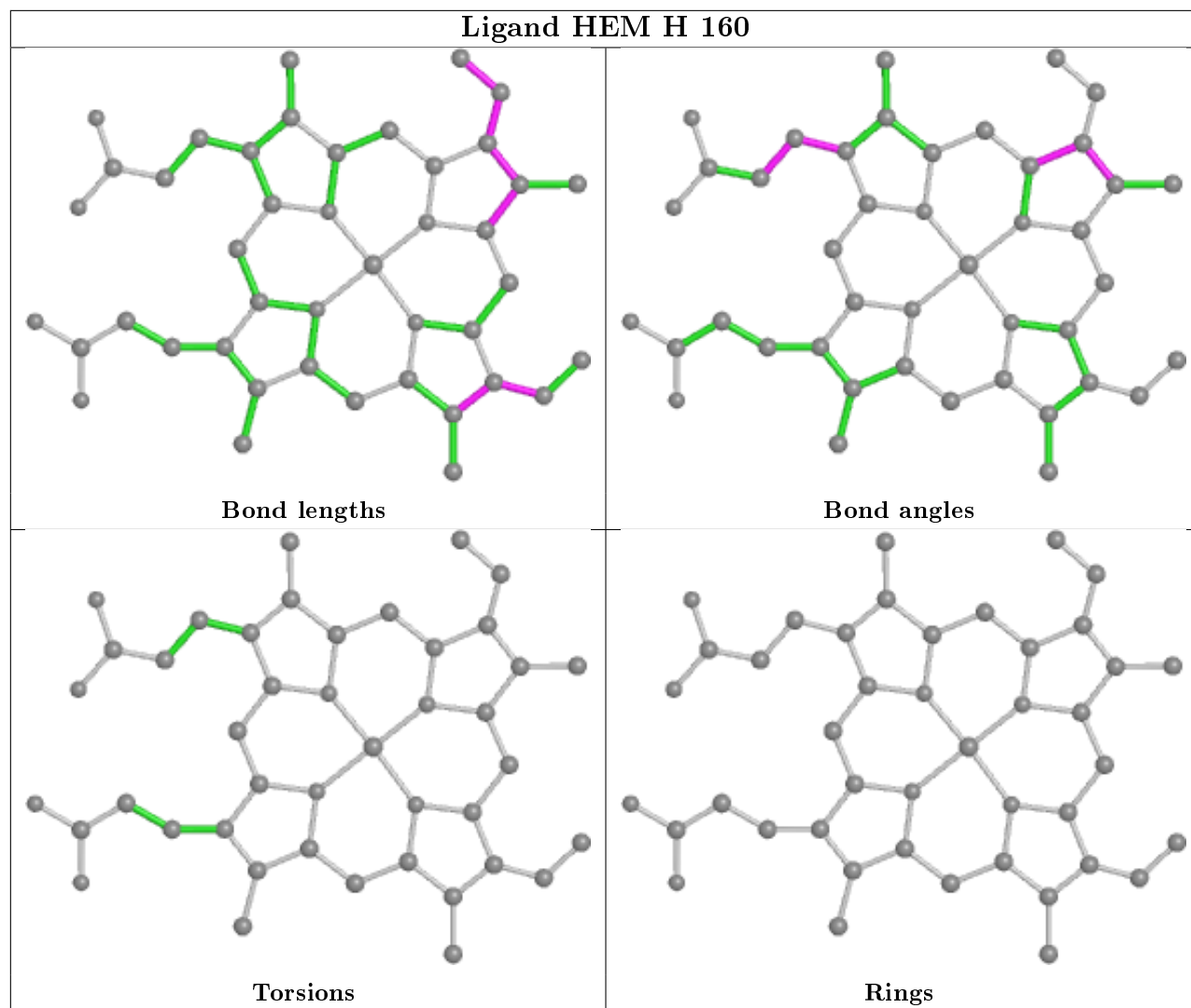


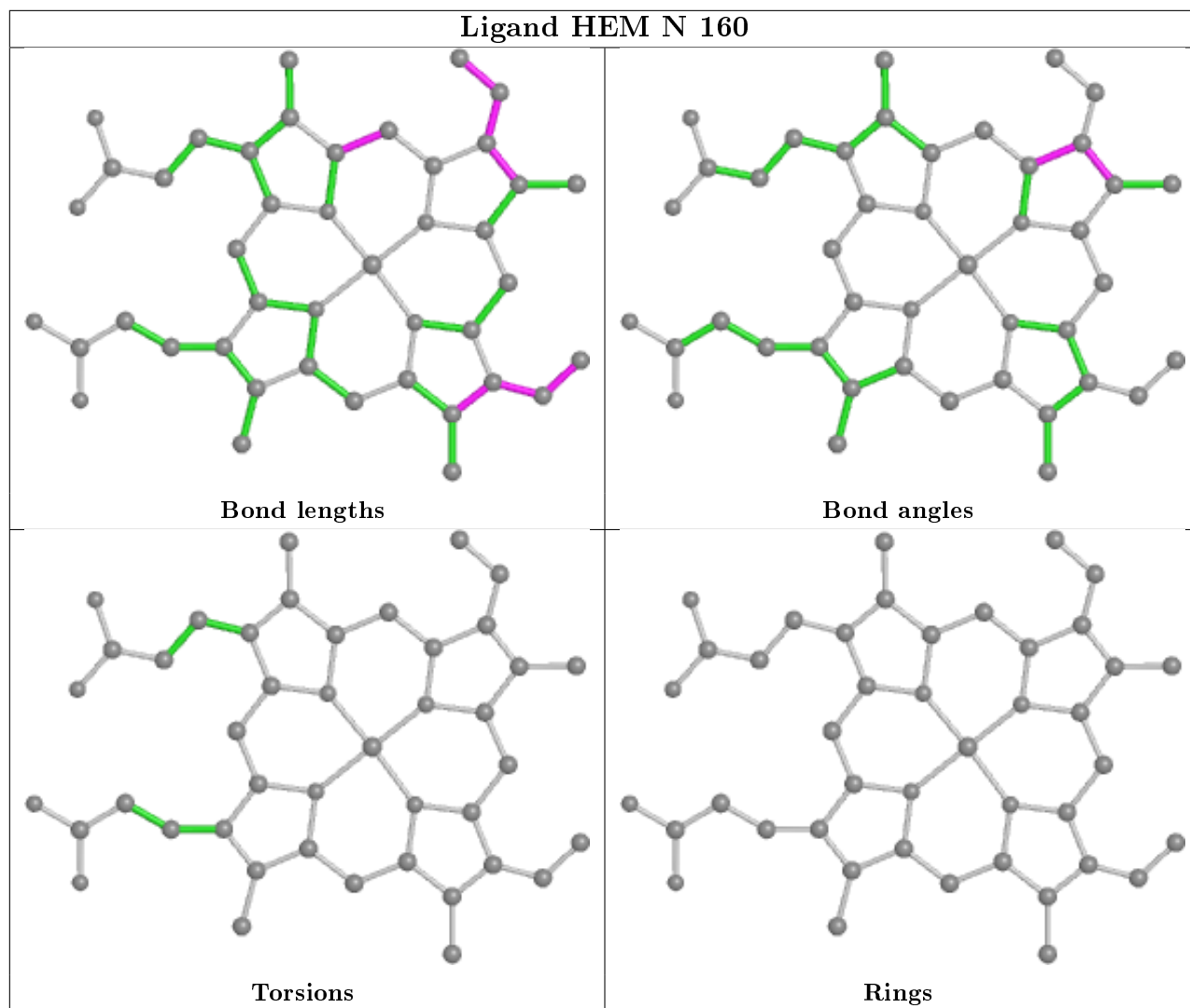




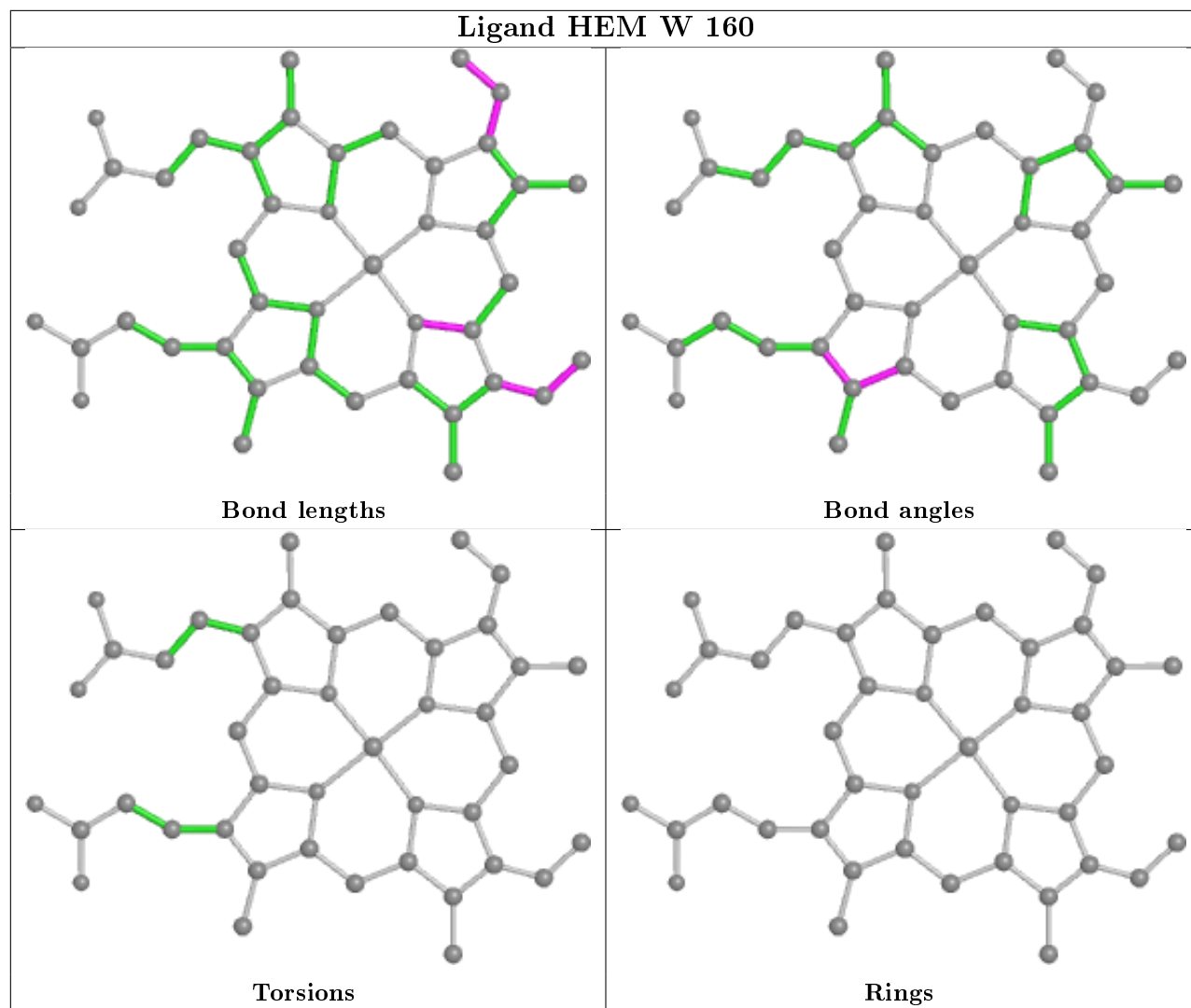


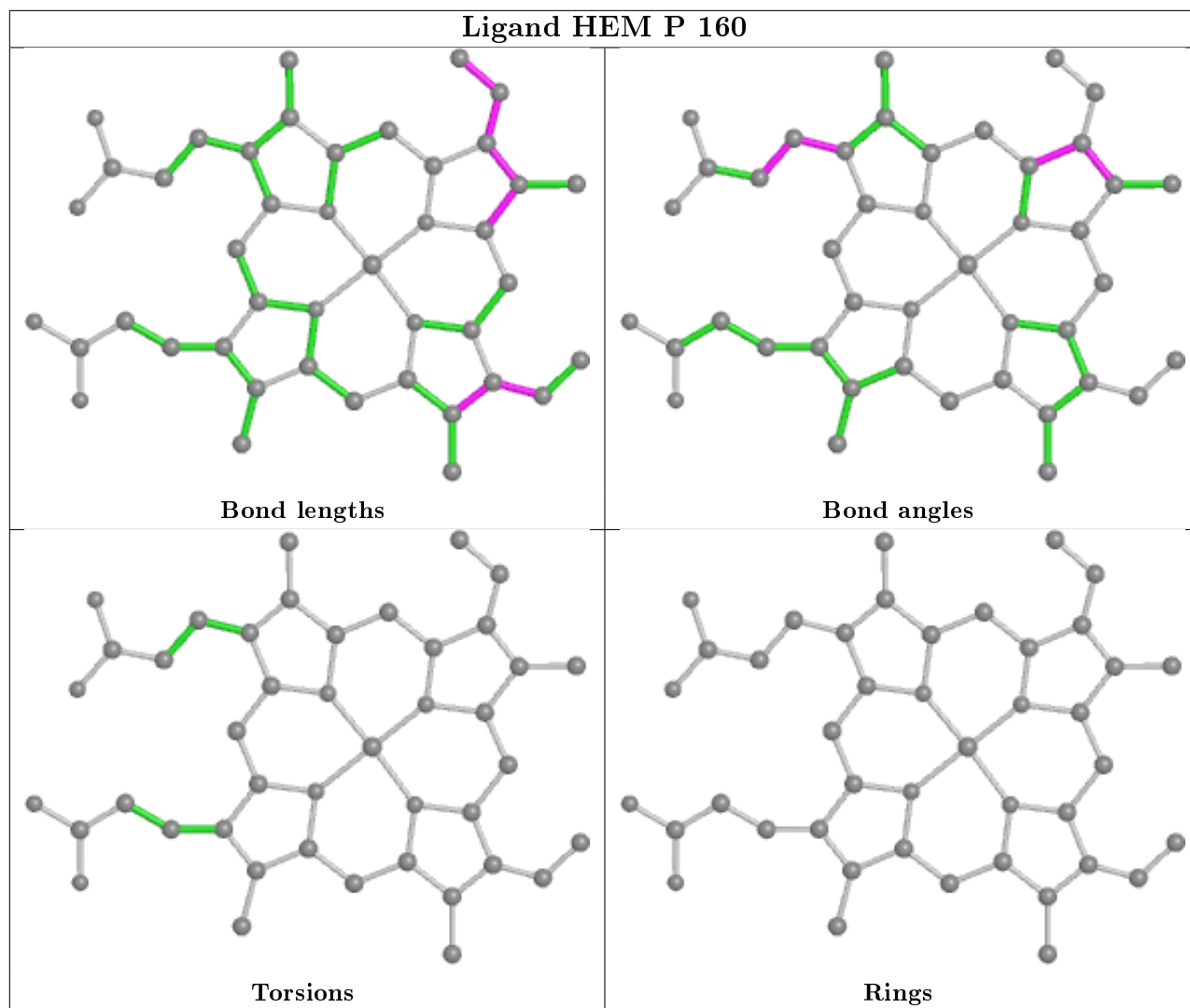


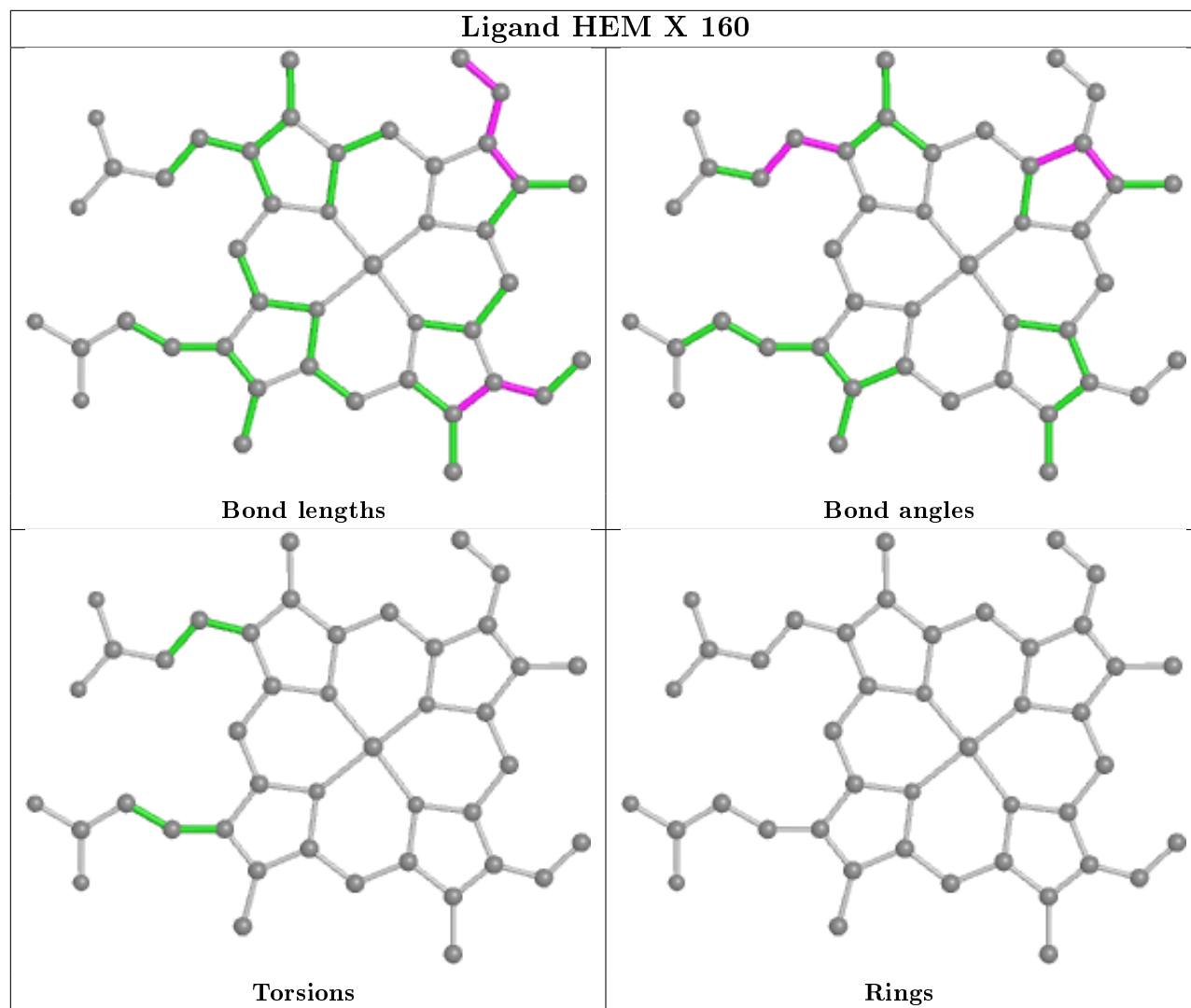


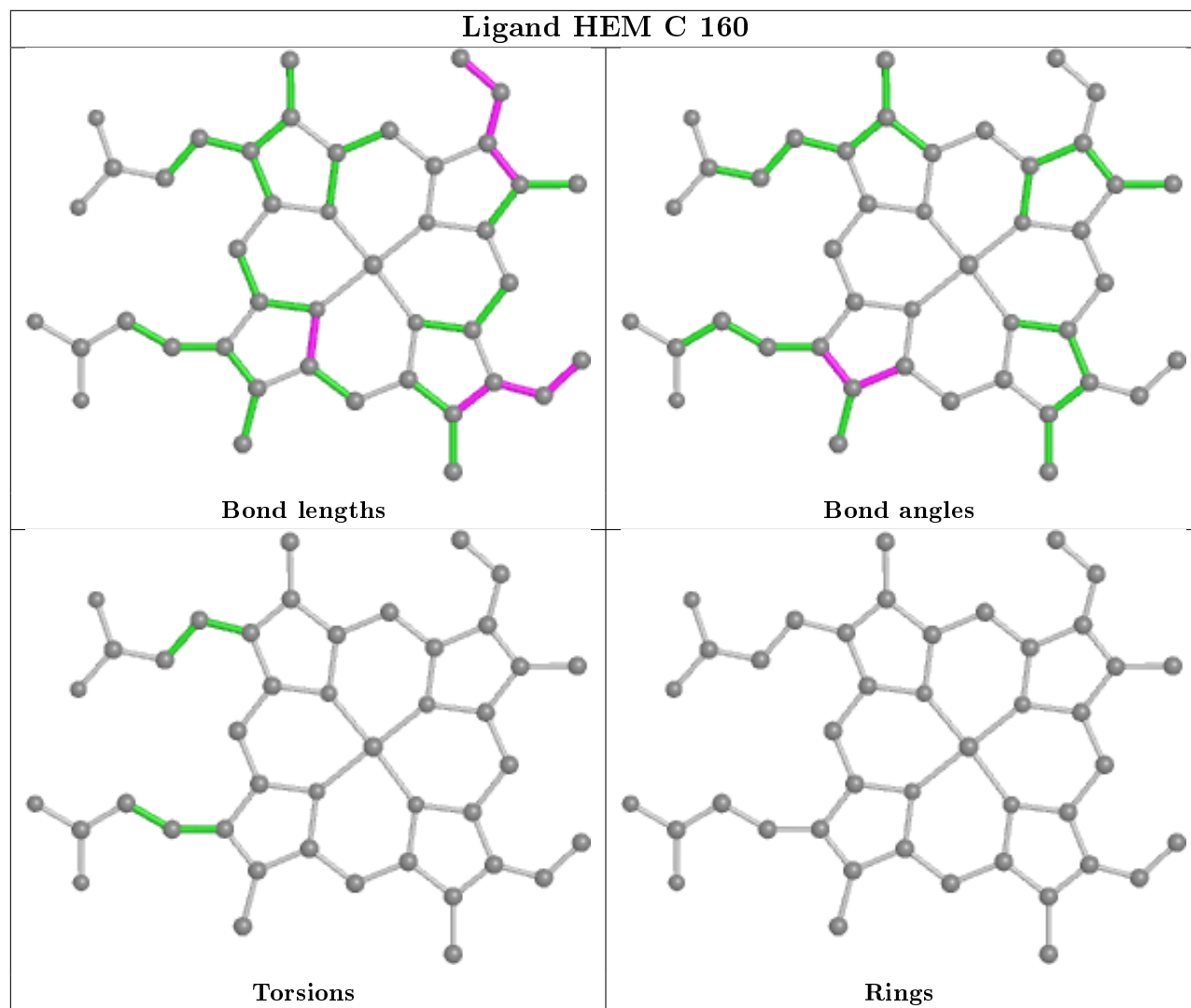


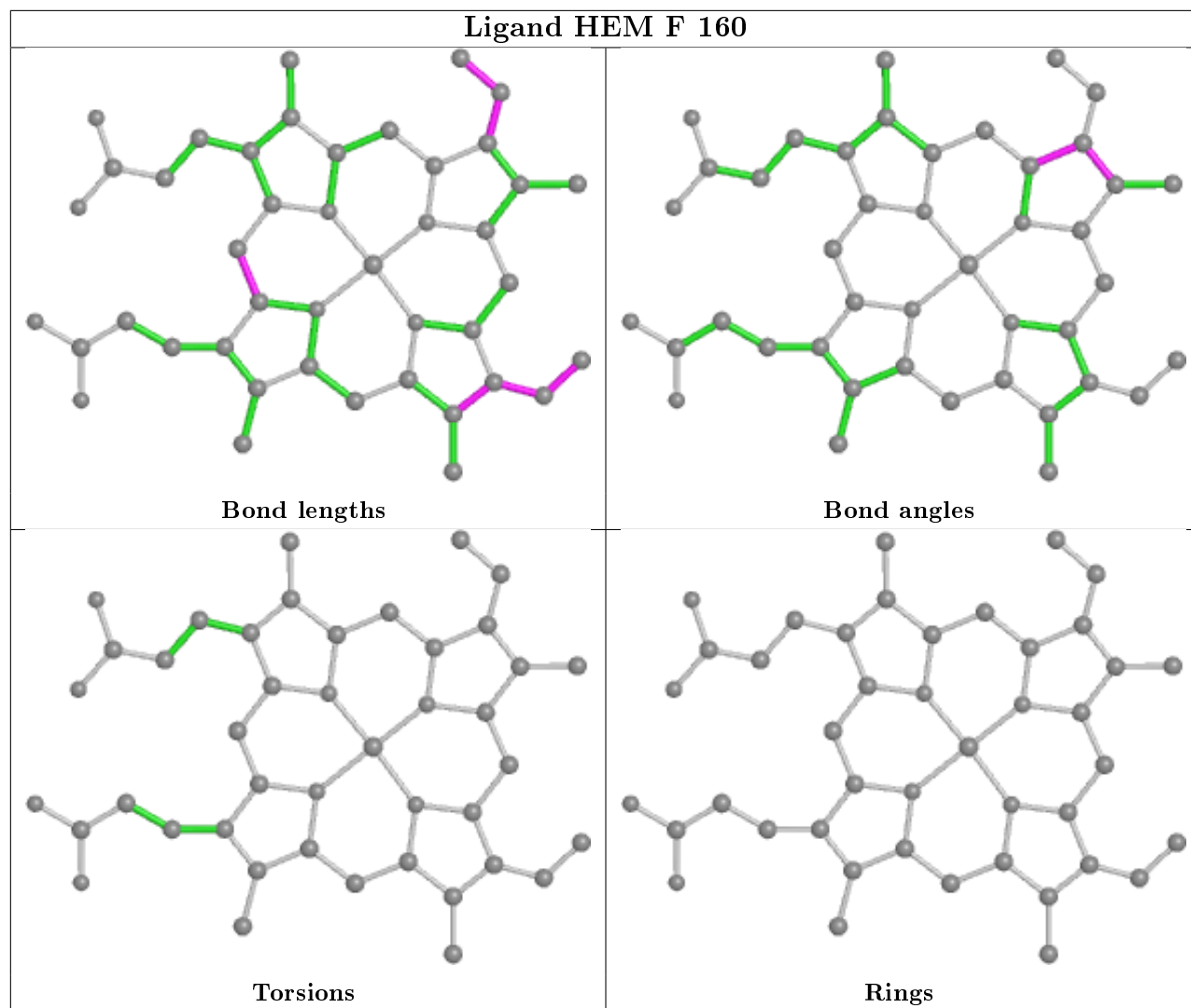


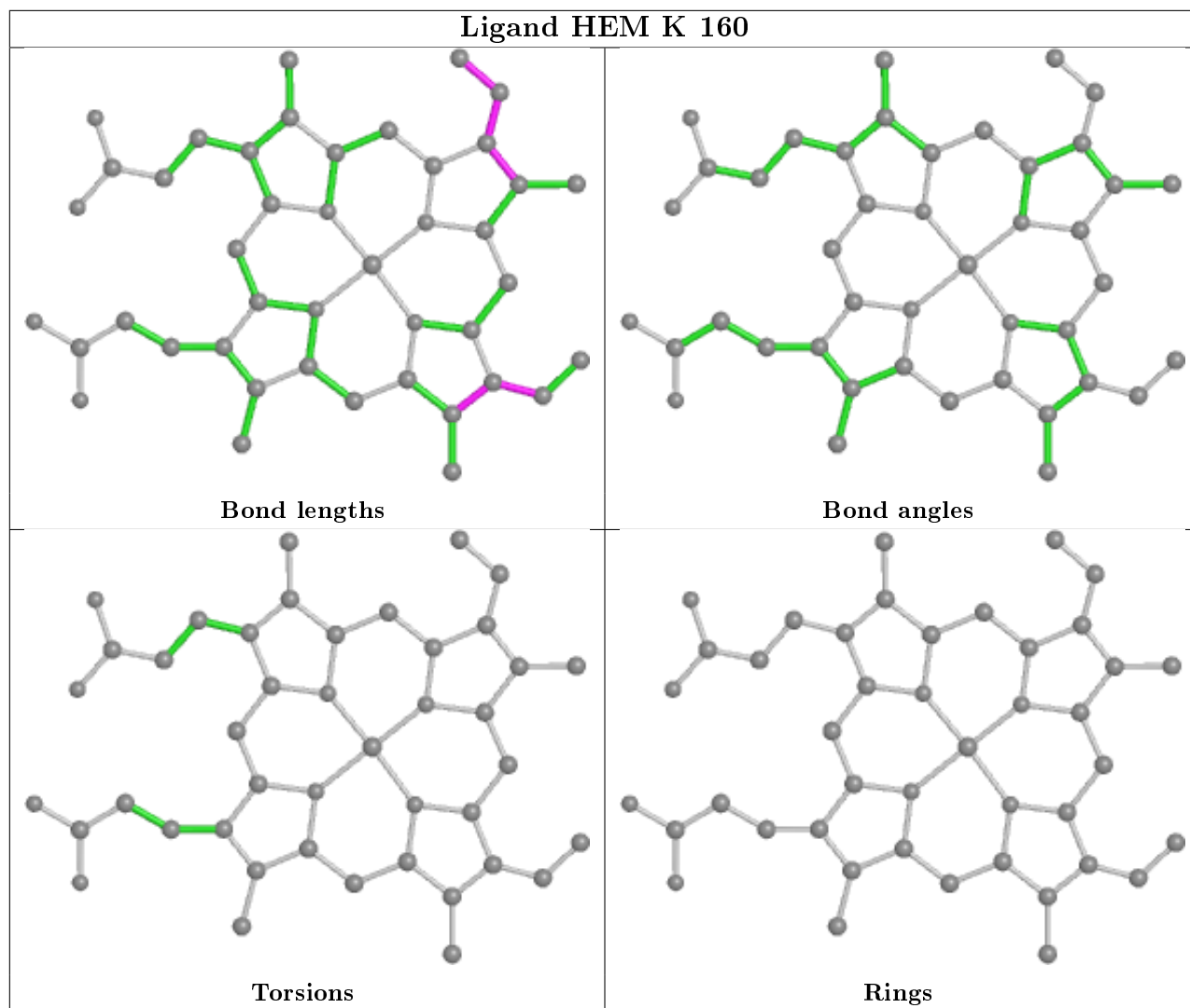


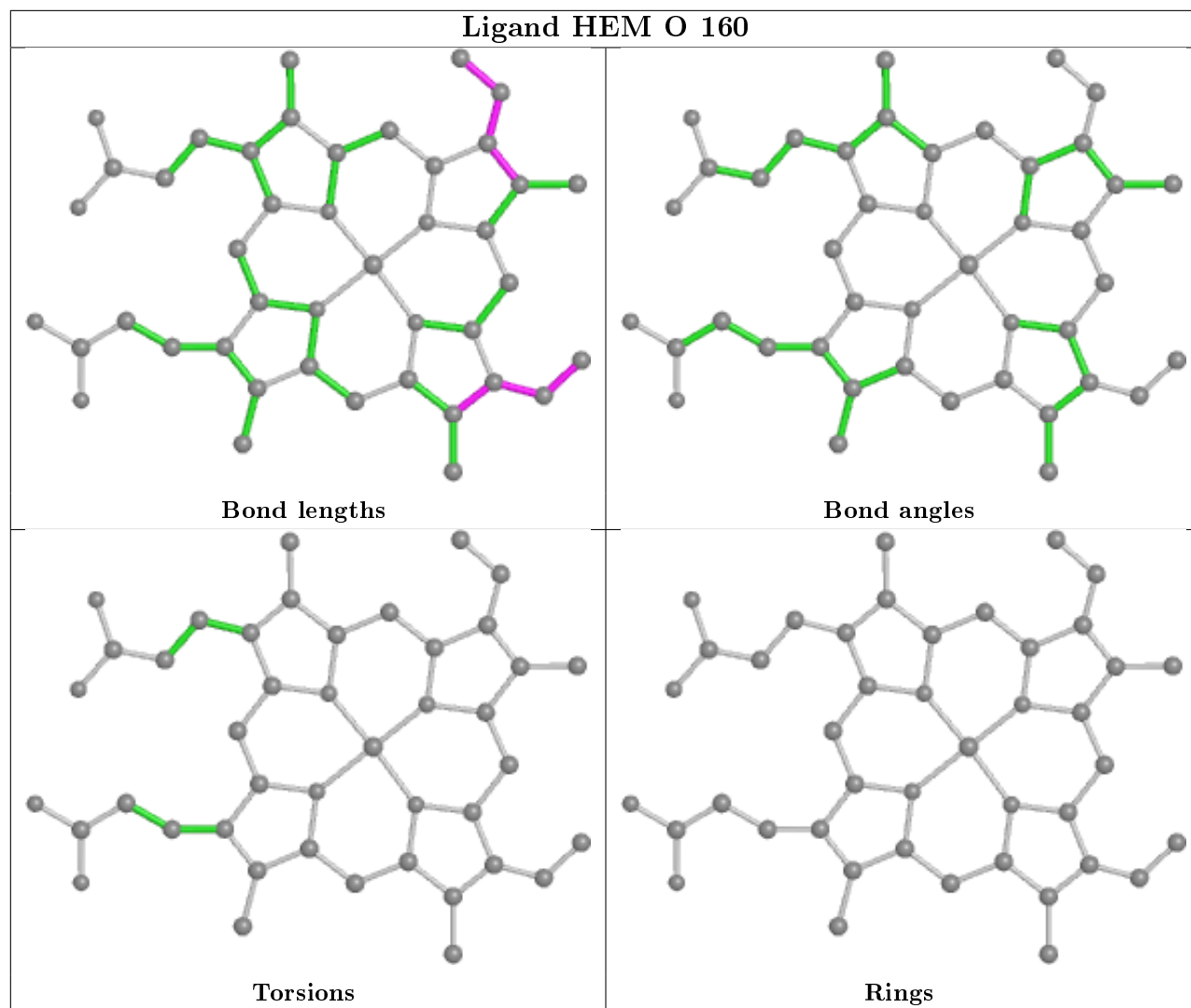


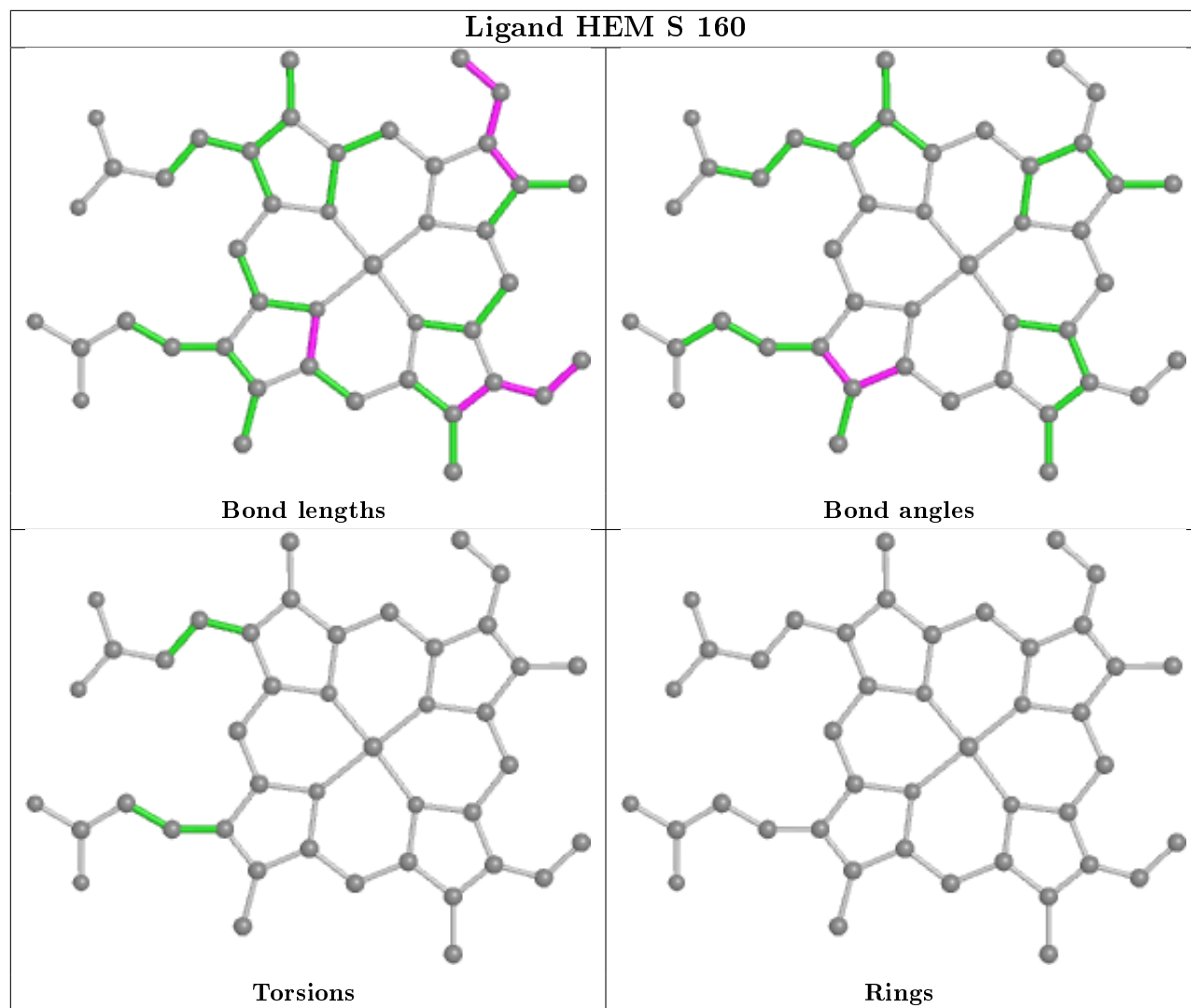




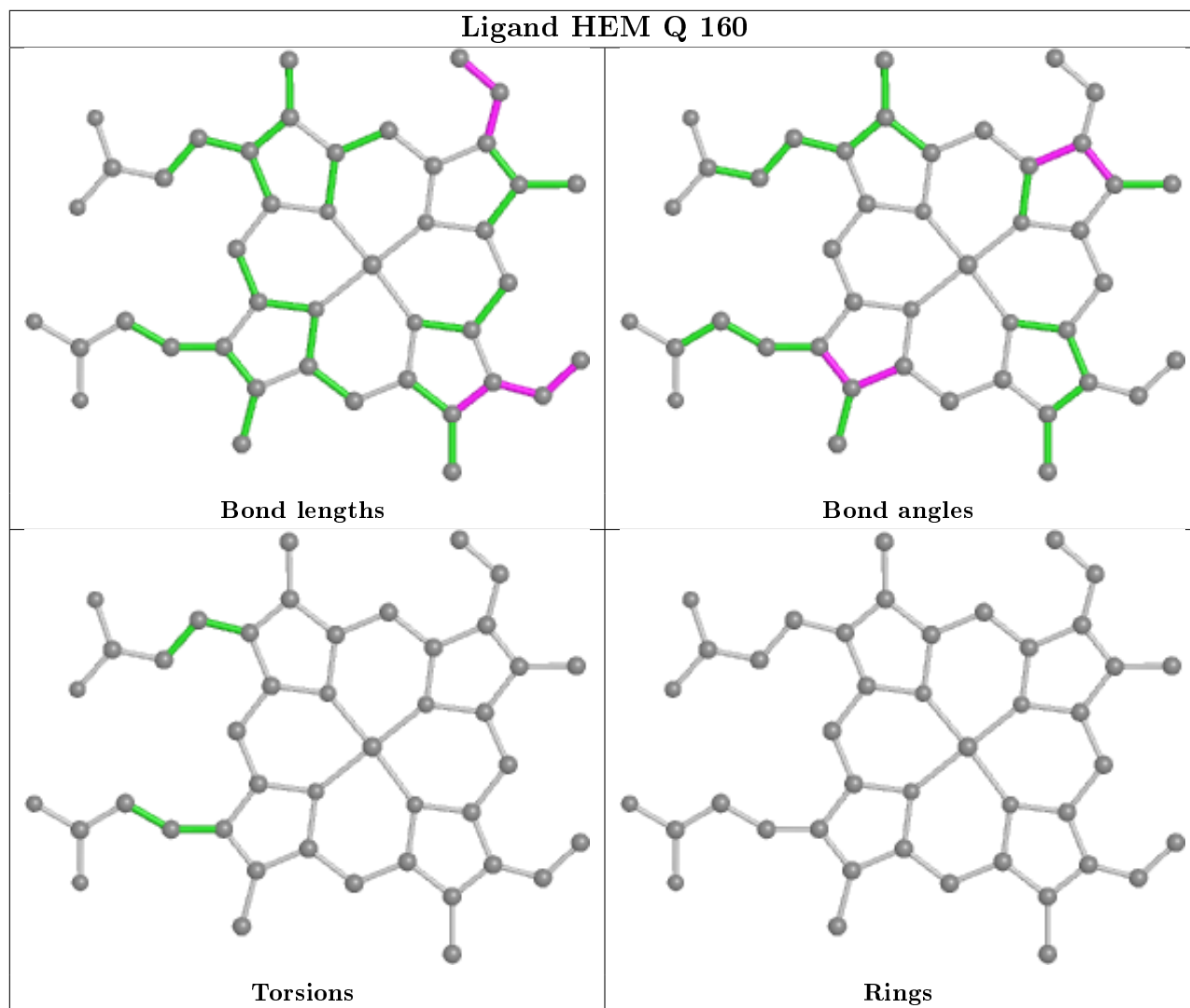


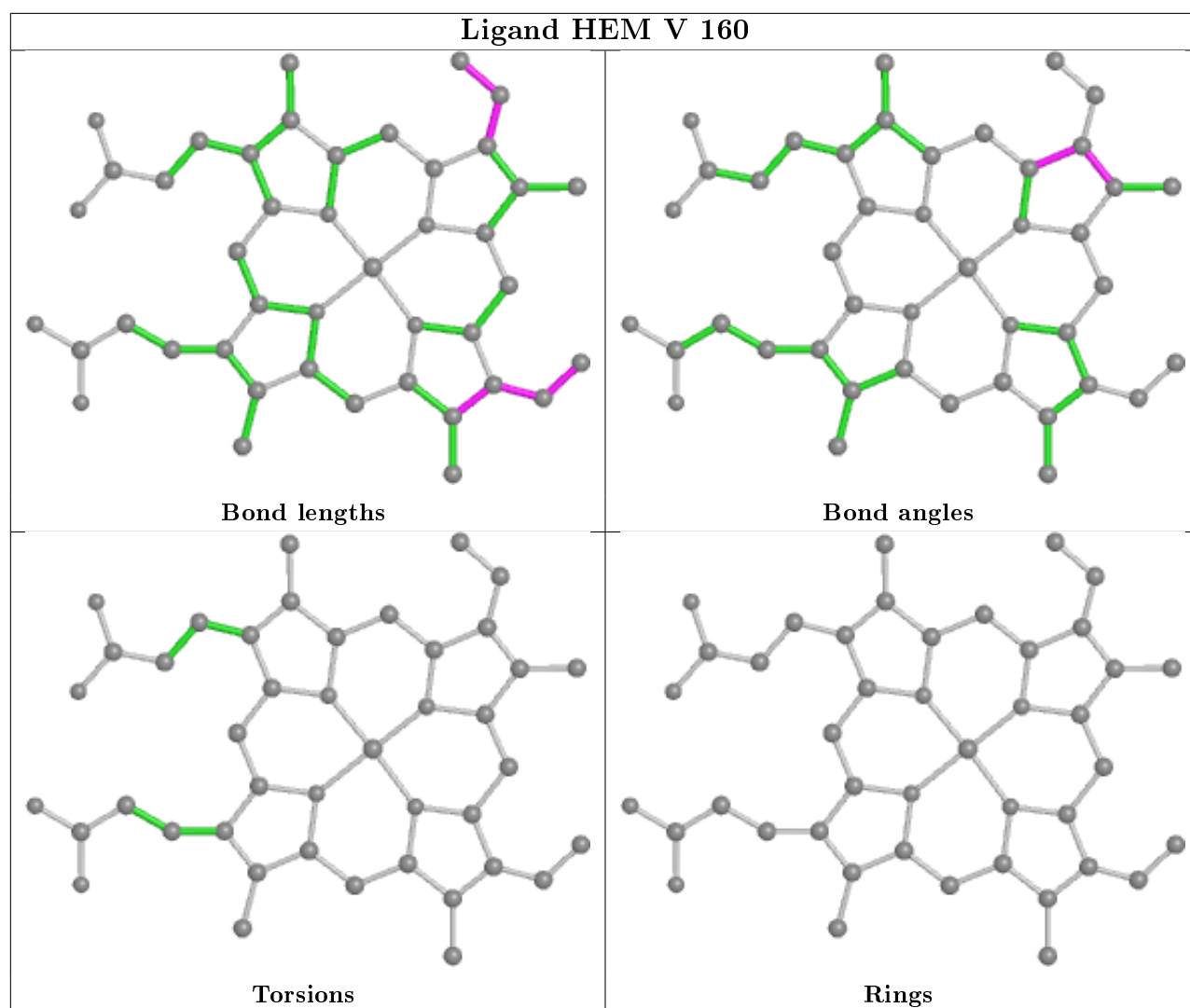












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	145/145 (100%)	-0.45	0 100 100	21, 53, 86, 95	0
1	E	145/145 (100%)	-0.43	0 100 100	25, 50, 85, 100	0
1	I	145/145 (100%)	-0.53	0 100 100	8, 31, 64, 99	0
1	M	145/145 (100%)	-0.43	0 100 100	19, 45, 74, 97	0
1	Q	145/145 (100%)	-0.57	0 100 100	16, 40, 72, 95	0
1	U	145/145 (100%)	-0.45	0 100 100	29, 55, 84, 100	0
2	B	144/144 (100%)	-0.20	1 (0%) 87 81	15, 44, 87, 100	0
2	F	144/144 (100%)	-0.42	1 (0%) 87 81	11, 37, 81, 100	0
2	J	144/144 (100%)	-0.44	0 100 100	9, 34, 85, 100	0
2	N	144/144 (100%)	-0.21	3 (2%) 63 49	23, 57, 97, 100	0
2	R	144/144 (100%)	-0.19	2 (1%) 75 63	30, 55, 99, 100	0
2	V	144/144 (100%)	-0.19	1 (0%) 87 81	31, 62, 99, 100	0
3	C	148/148 (100%)	0.10	10 (6%) 17 9	24, 65, 98, 100	0
3	G	148/148 (100%)	-0.15	4 (2%) 54 38	17, 55, 90, 100	0
3	K	148/148 (100%)	-0.22	3 (2%) 65 50	15, 43, 79, 100	0
3	O	148/148 (100%)	-0.14	2 (1%) 75 63	17, 50, 80, 100	0
3	S	148/148 (100%)	-0.00	5 (3%) 45 28	25, 67, 95, 100	0
3	W	148/148 (100%)	0.26	10 (6%) 17 9	42, 73, 98, 100	0
4	D	149/149 (100%)	-0.17	2 (1%) 77 66	22, 51, 93, 100	0
4	H	149/149 (100%)	-0.27	0 100 100	13, 39, 83, 100	0
4	L	149/149 (100%)	-0.18	4 (2%) 54 38	8, 35, 80, 100	0
4	P	149/149 (100%)	-0.06	6 (4%) 38 23	31, 64, 99, 100	0
4	T	149/149 (100%)	-0.18	4 (2%) 54 38	20, 56, 93, 100	0
4	X	149/149 (100%)	-0.18	2 (1%) 77 66	35, 69, 100, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3516/3516 (100%)	-0.24	60 (1%) 70 57	8, 52, 93, 100	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	W	2	ALA	5.6
3	W	1	ALA	5.5
3	G	2	ALA	4.6
3	O	1	ALA	4.5
4	L	1	ALA	4.4

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	HEM	P	160	43/43	0.93	0.32	61,61,61,61	0
5	HEM	W	160	43/43	0.95	0.34	78,78,78,78	0
5	HEM	C	160	43/43	0.95	0.36	66,66,66,66	0
5	HEM	B	160	43/43	0.96	0.22	27,27,27,27	0
5	HEM	H	160	43/43	0.96	0.28	42,42,42,42	0
7	ZN	R	191	1/1	0.96	0.08	48,48,48,48	0
5	HEM	D	160	43/43	0.96	0.26	59,59,59,59	0
5	HEM	L	160	43/43	0.96	0.24	17,17,17,17	0
5	HEM	O	160	43/43	0.96	0.23	39,39,39,39	0
5	HEM	S	160	43/43	0.96	0.25	63,63,63,63	0
5	HEM	V	160	43/43	0.96	0.26	45,45,45,45	0
6	OXY	E	161	2/2	0.97	0.22	65,65,65,65	0
5	HEM	T	160	43/43	0.97	0.23	61,61,61,61	0

Continued on next page...

*Continued from previous page...*

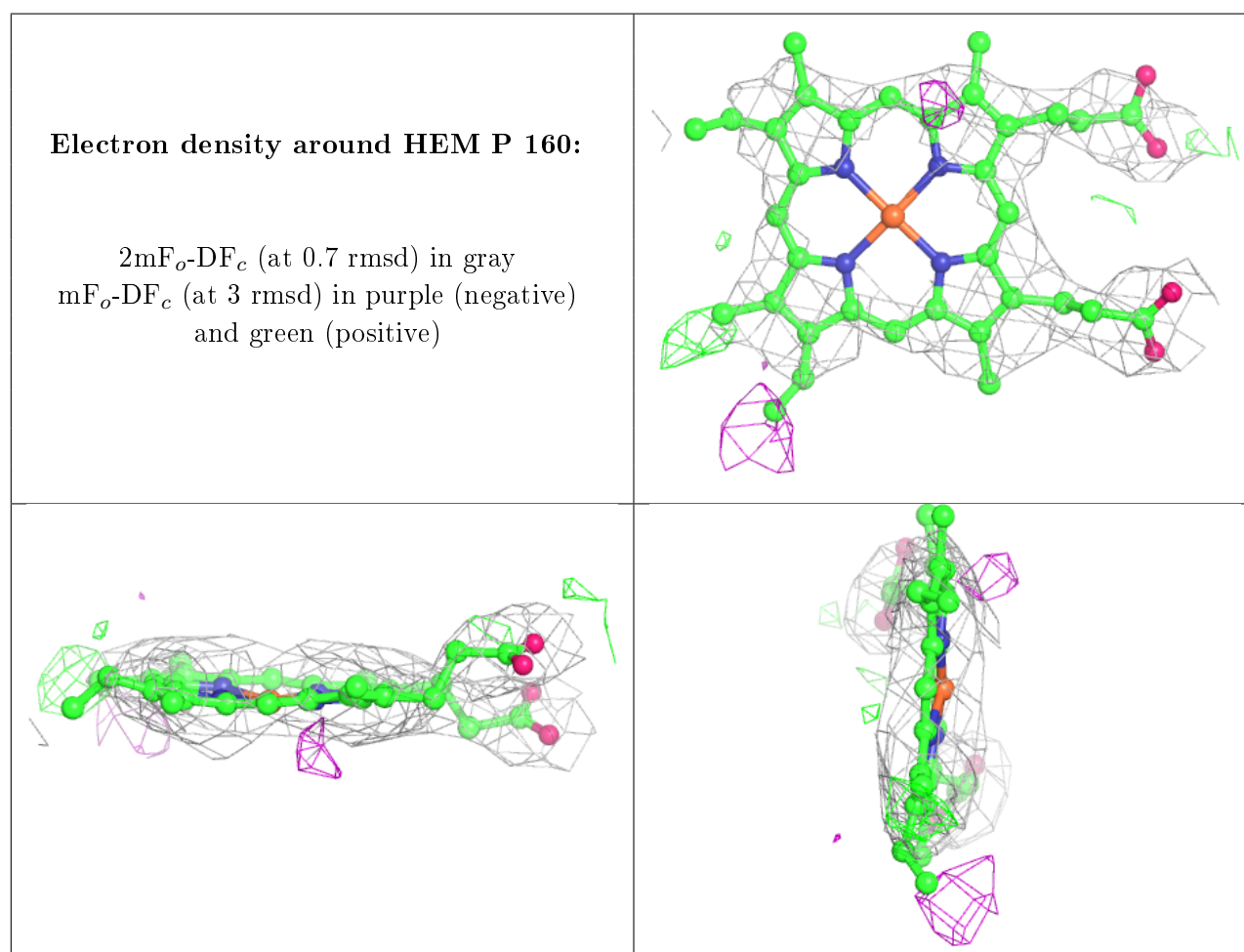
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	HEM	M	160	43/43	0.97	0.18	28,28,28,28	0
5	HEM	J	160	43/43	0.97	0.23	27,27,27,27	0
5	HEM	R	160	43/43	0.97	0.22	49,49,49,49	0
5	HEM	N	160	43/43	0.97	0.24	42,42,42,42	0
5	HEM	U	160	43/43	0.97	0.20	54,54,54,54	0
5	HEM	G	160	43/43	0.97	0.24	48,48,48,48	0
5	HEM	X	160	43/43	0.97	0.27	73,73,73,73	0
5	HEM	A	160	43/43	0.97	0.22	55,55,55,55	0
7	ZN	N	191	1/1	0.97	0.10	52,52,52,52	0
6	OXY	W	161	2/2	0.97	0.16	78,78,78,78	0
5	HEM	E	160	43/43	0.97	0.22	37,37,37,37	0
7	ZN	J	191	1/1	0.98	0.08	29,29,29,29	0
5	HEM	F	160	43/43	0.98	0.24	19,19,19,19	0
5	HEM	K	160	43/43	0.98	0.22	18,18,18,18	0
7	ZN	V	191	1/1	0.98	0.11	60,60,60,60	0
5	HEM	I	160	43/43	0.98	0.26	25,25,25,25	0
5	HEM	Q	160	43/43	0.98	0.20	28,28,28,28	0
7	ZN	F	190	1/1	0.98	0.10	27,27,27,27	0
7	ZN	V	190	1/1	0.98	0.09	46,46,46,46	0
6	OXY	U	161	2/2	0.99	0.29	65,65,65,65	0
6	OXY	H	161	2/2	0.99	0.15	58,58,58,58	0
7	ZN	J	190	1/1	0.99	0.10	28,28,28,28	0
6	OXY	G	161	2/2	0.99	0.17	78,78,78,78	0
6	OXY	K	161	2/2	0.99	0.34	78,78,78,78	0
7	ZN	B	190	1/1	0.99	0.10	22,22,22,22	0
7	ZN	N	190	1/1	0.99	0.07	45,45,45,45	0
7	ZN	F	191	1/1	0.99	0.08	35,35,35,35	0
6	OXY	L	161	2/2	0.99	0.22	58,58,58,58	0
6	OXY	Q	161	2/2	0.99	0.13	65,65,65,65	0
6	OXY	T	161	2/2	0.99	0.10	58,58,58,58	0
6	OXY	D	161	2/2	0.99	0.12	58,58,58,58	0
6	OXY	S	161	2/2	0.99	0.12	78,78,78,78	0
6	OXY	C	161	2/2	0.99	0.25	78,78,78,78	0
6	OXY	O	161	2/2	0.99	0.15	78,78,78,78	0
6	OXY	V	161	2/2	0.99	0.46	73,73,73,73	0
6	OXY	J	161	2/2	0.99	0.19	73,73,73,73	0
6	OXY	N	161	2/2	0.99	0.28	73,73,73,73	0
6	OXY	P	161	2/2	0.99	0.24	58,58,58,58	0
6	OXY	B	161	2/2	0.99	0.20	73,73,73,73	0
7	ZN	R	190	1/1	0.99	0.10	44,44,44,44	0
7	ZN	B	191	1/1	0.99	0.08	37,37,37,37	0
6	OXY	I	161	2/2	0.99	0.22	65,65,65,65	0

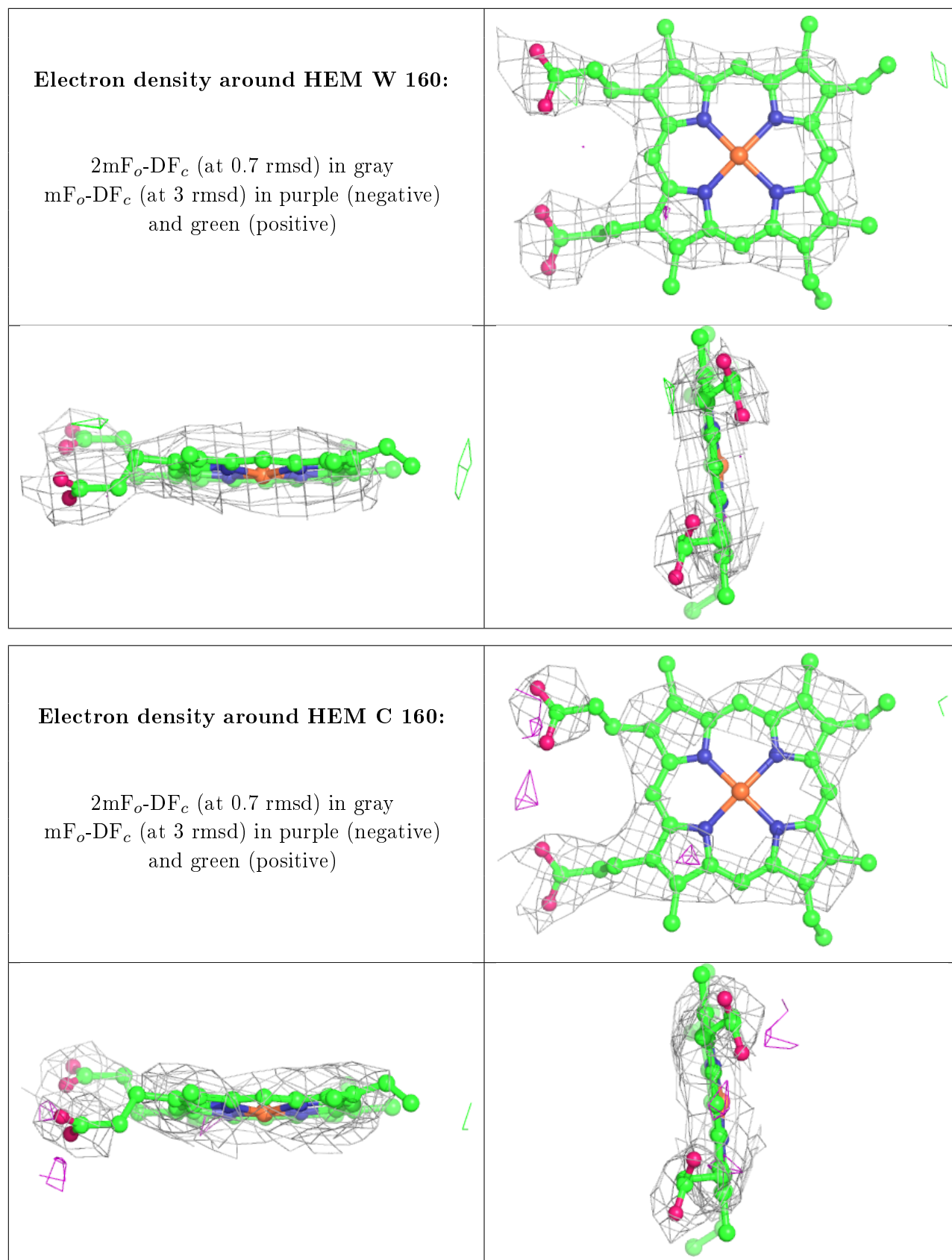
*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	OXY	X	161	2/2	1.00	0.14	58,58,58,58	0
6	OXY	M	161	2/2	1.00	0.10	65,65,65,65	0
6	OXY	R	161	2/2	1.00	0.14	73,73,73,73	0
6	OXY	A	161	2/2	1.00	0.10	65,65,65,65	0
6	OXY	F	161	2/2	1.00	0.33	73,73,73,73	0

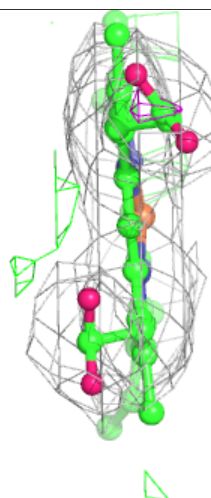
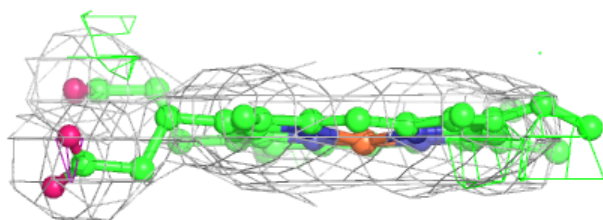
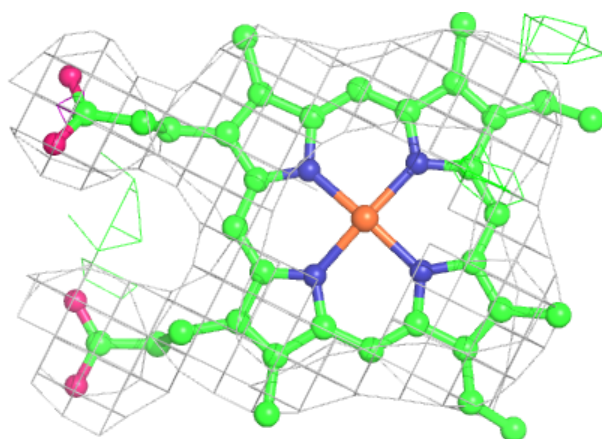
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



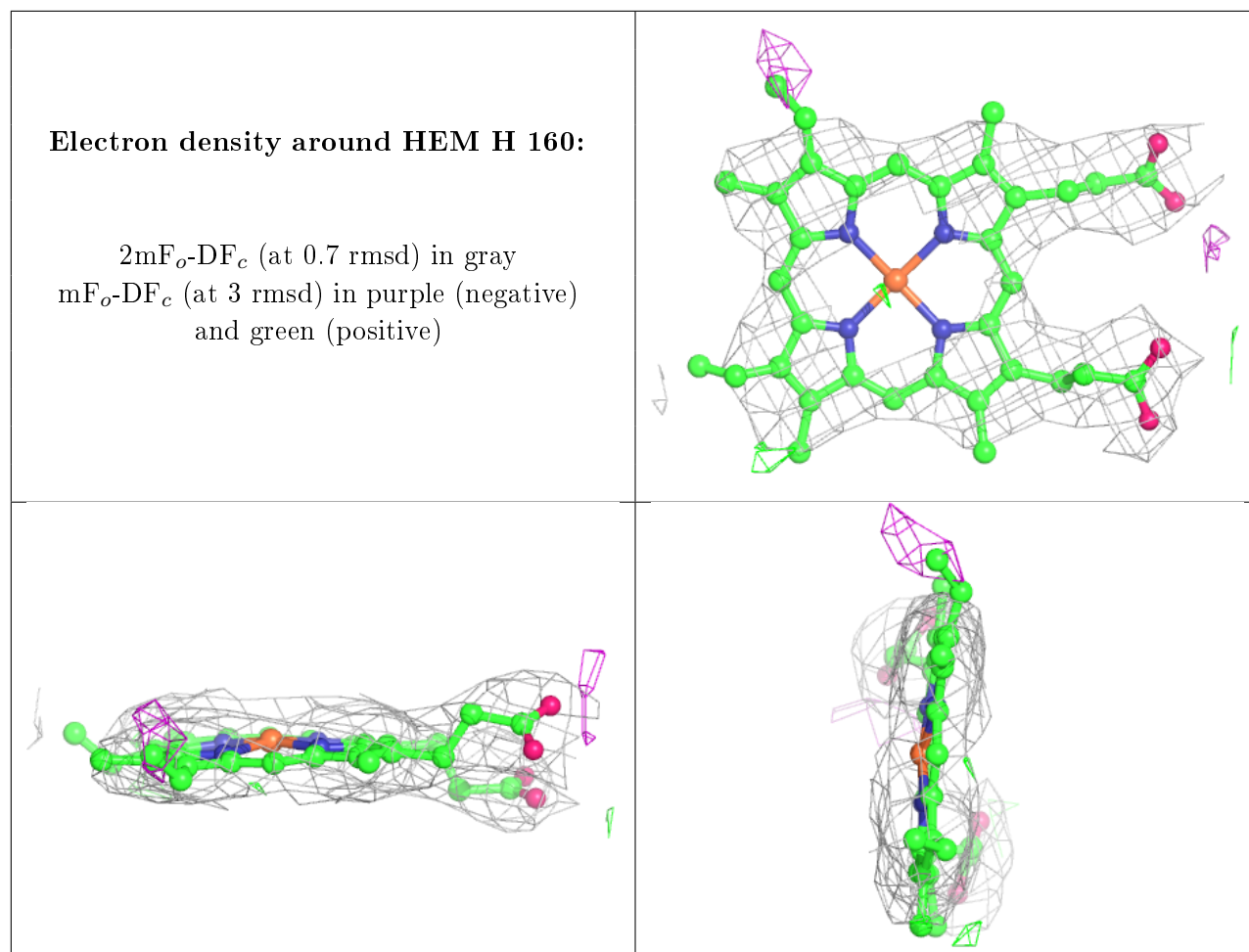


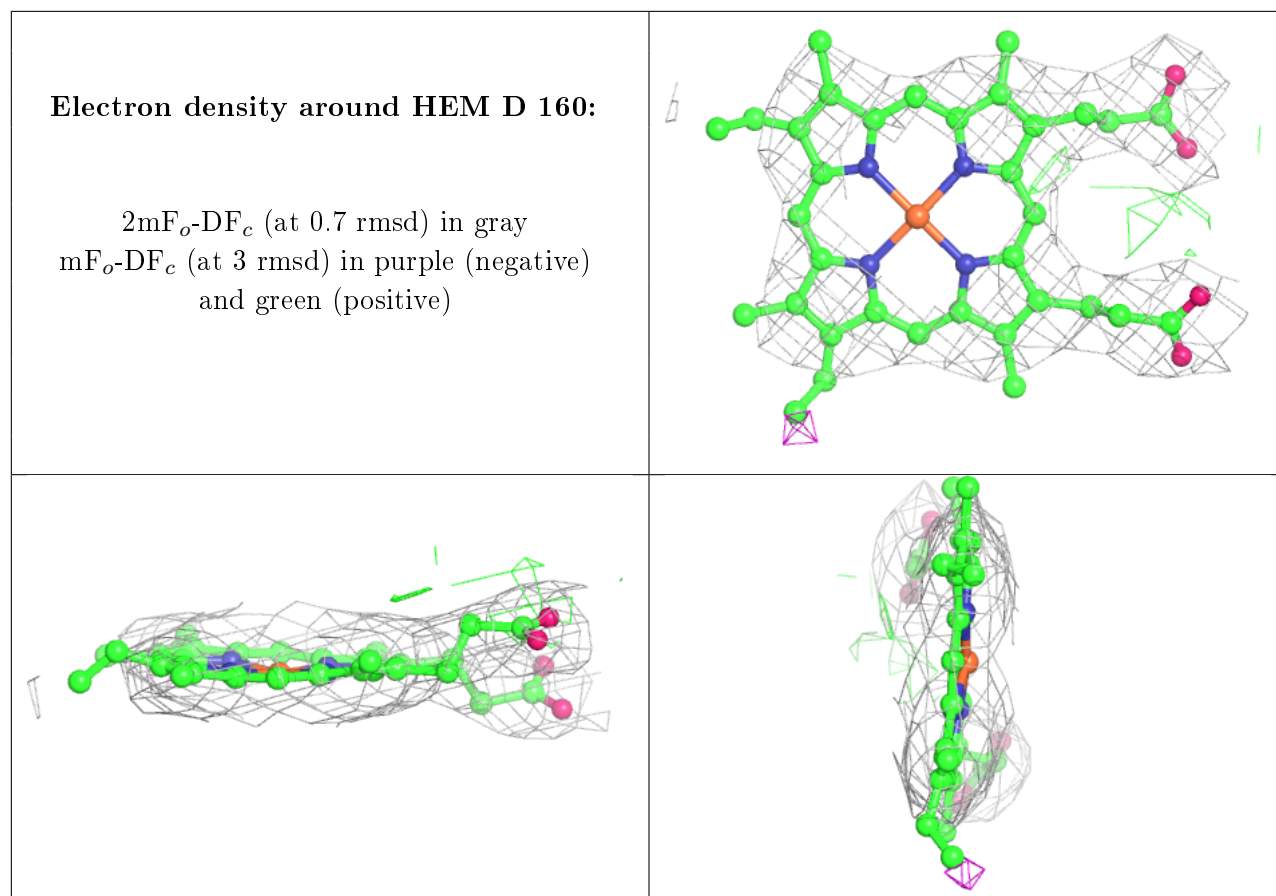
**Electron density around HEM B 160:**

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



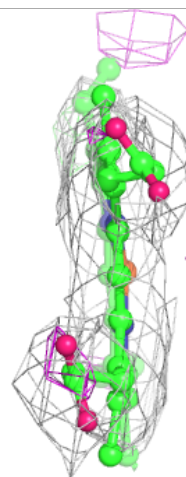
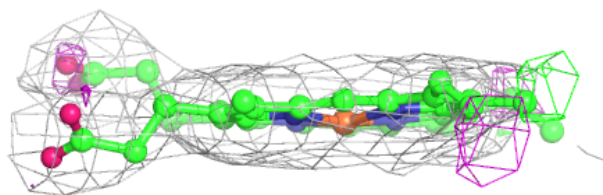
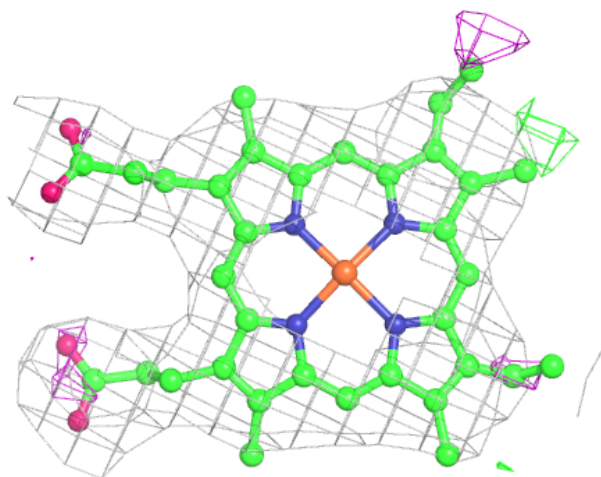


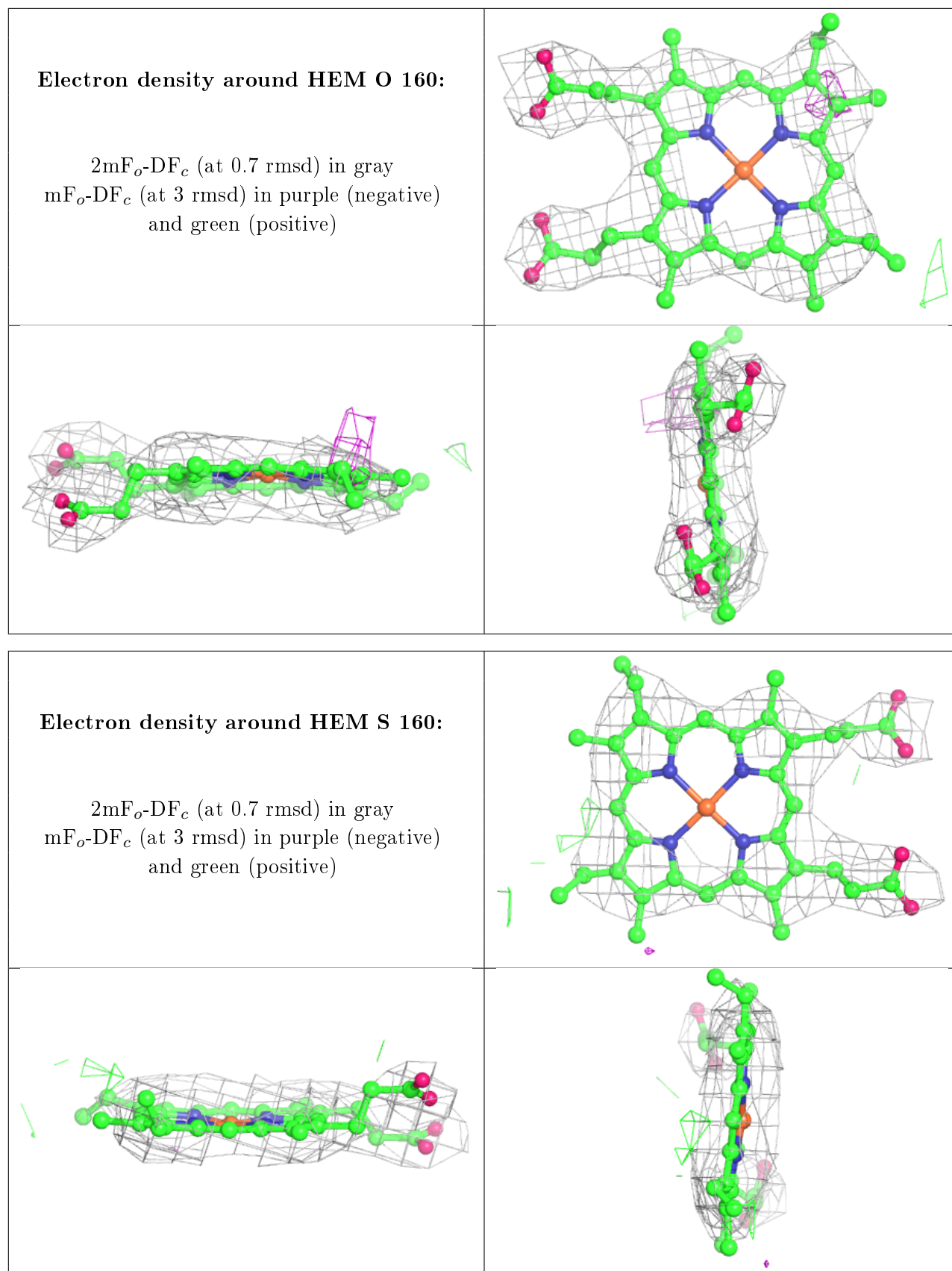




**Electron density around HEM L 160:**

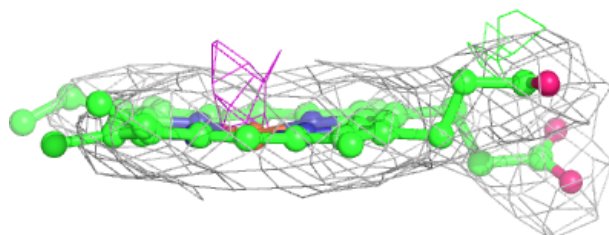
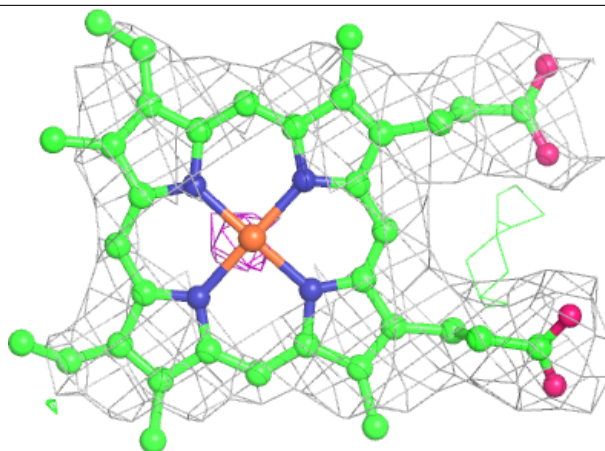
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



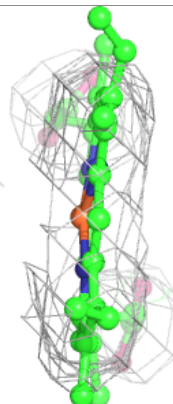
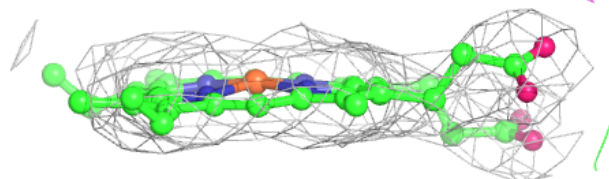
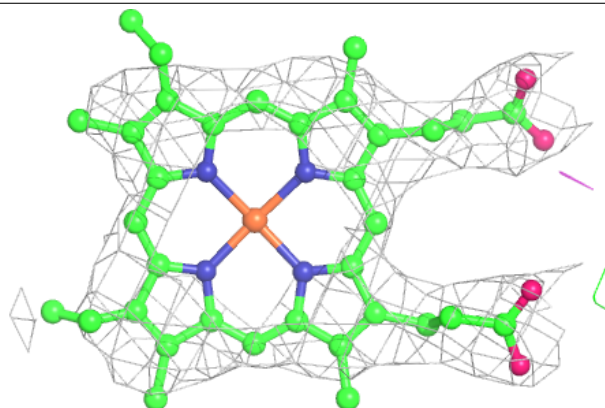


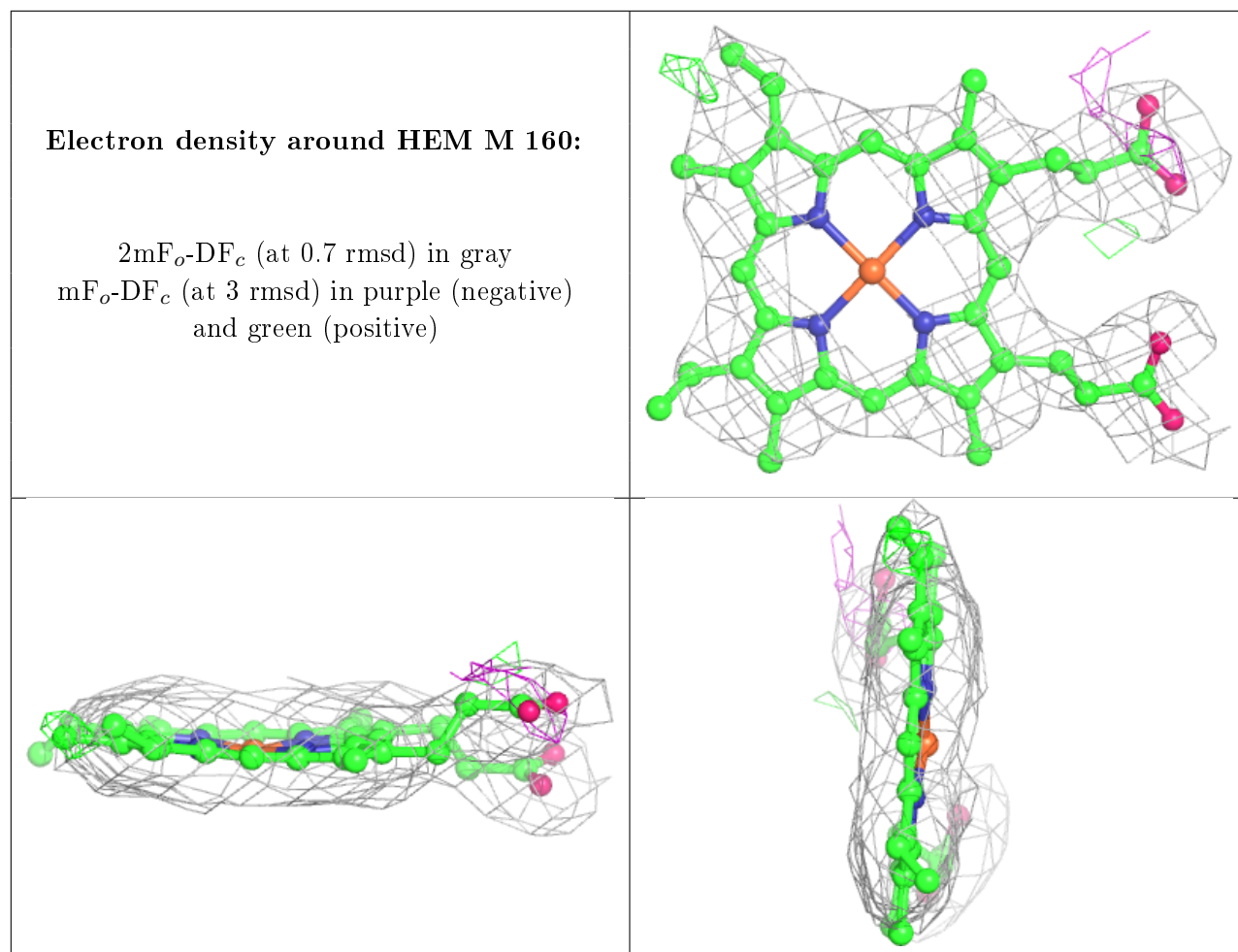
**Electron density around HEM V 160:**

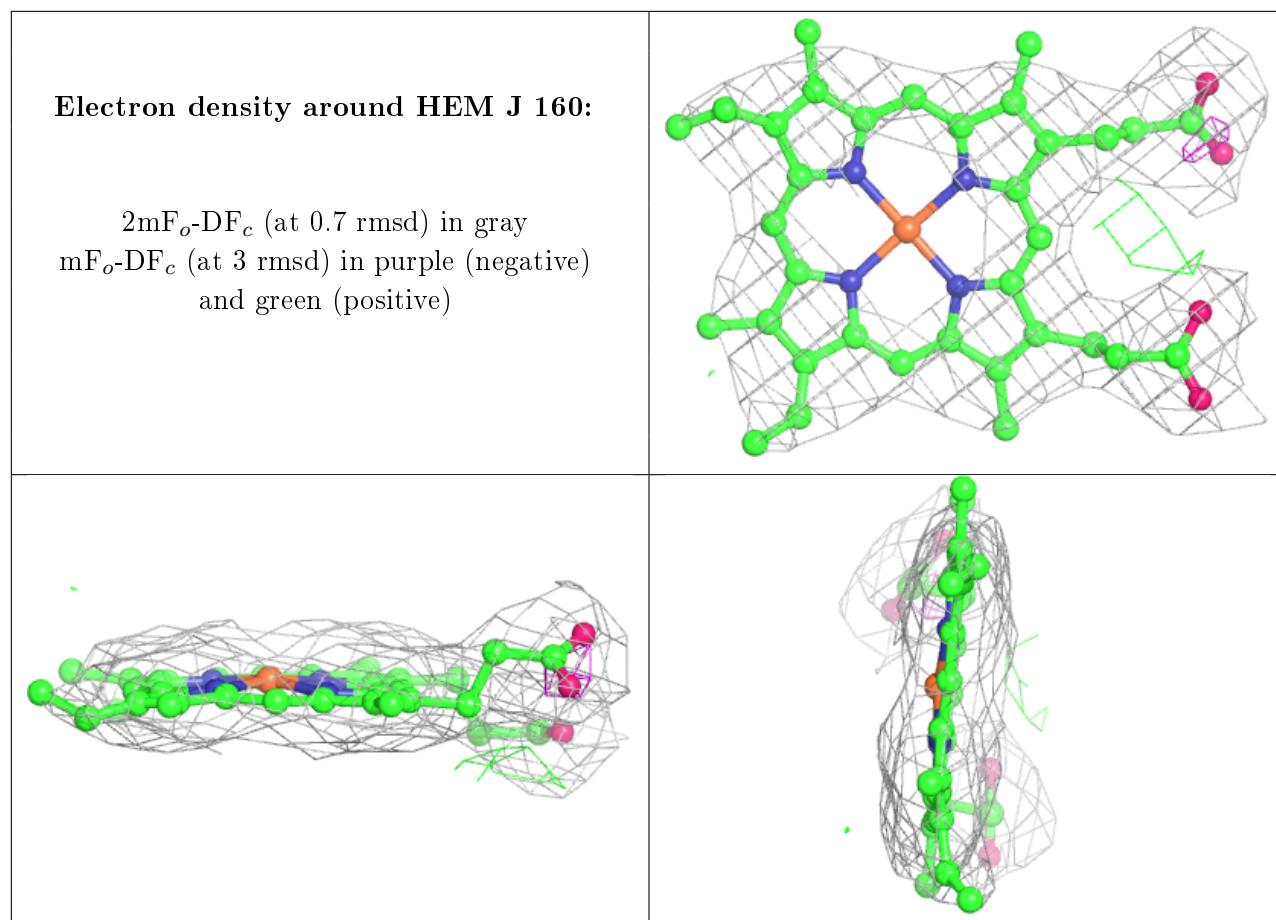
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

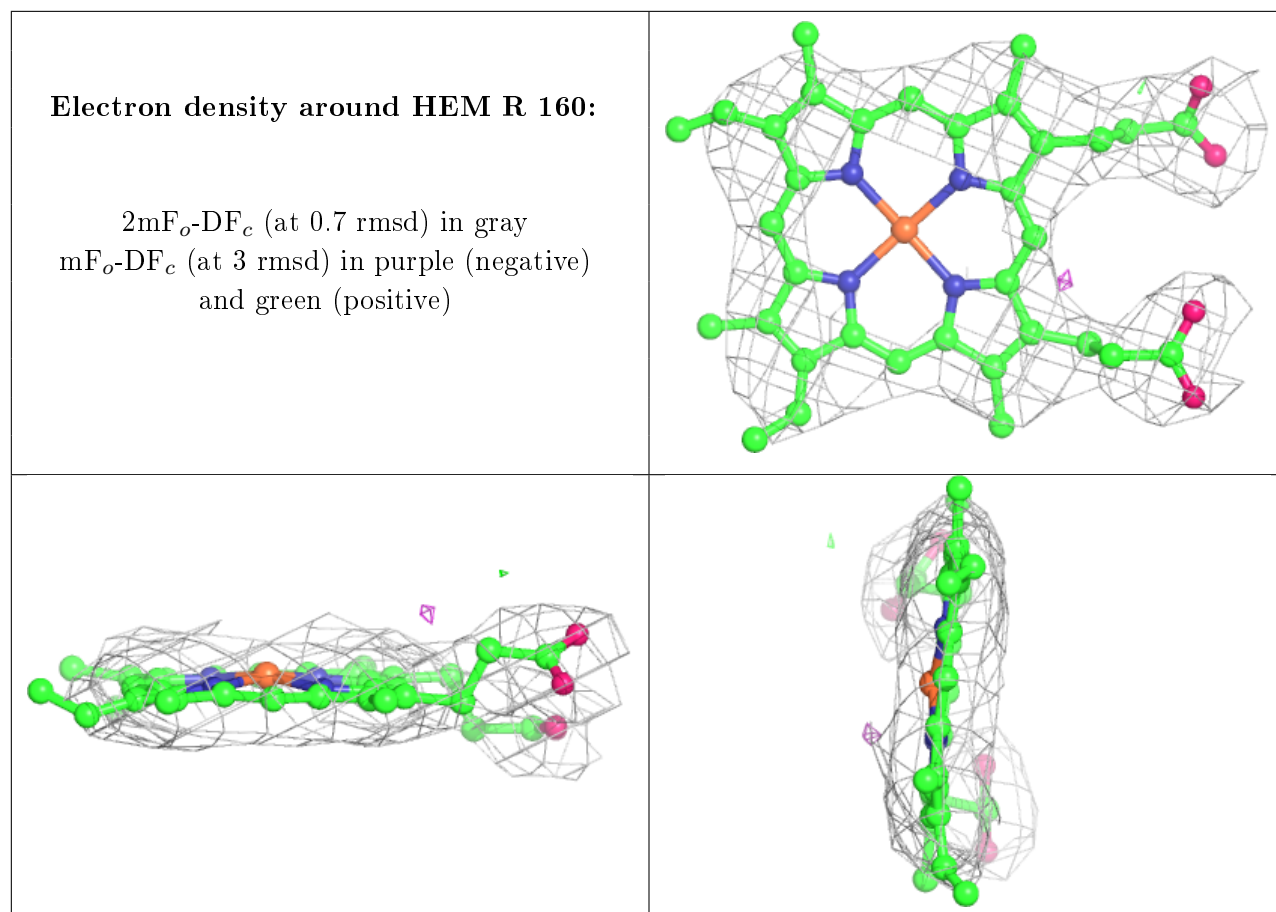
**Electron density around HEM T 160:**

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

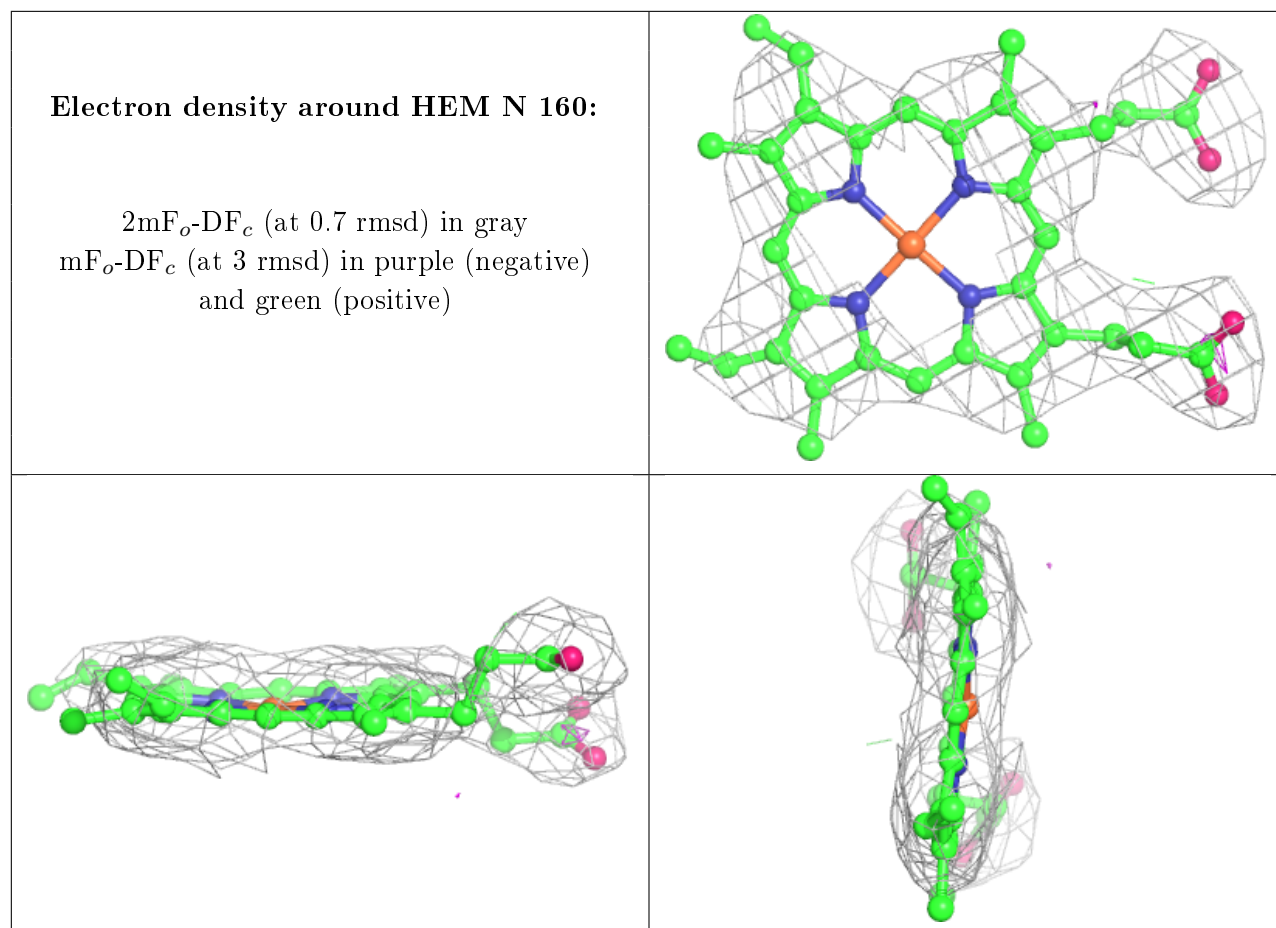


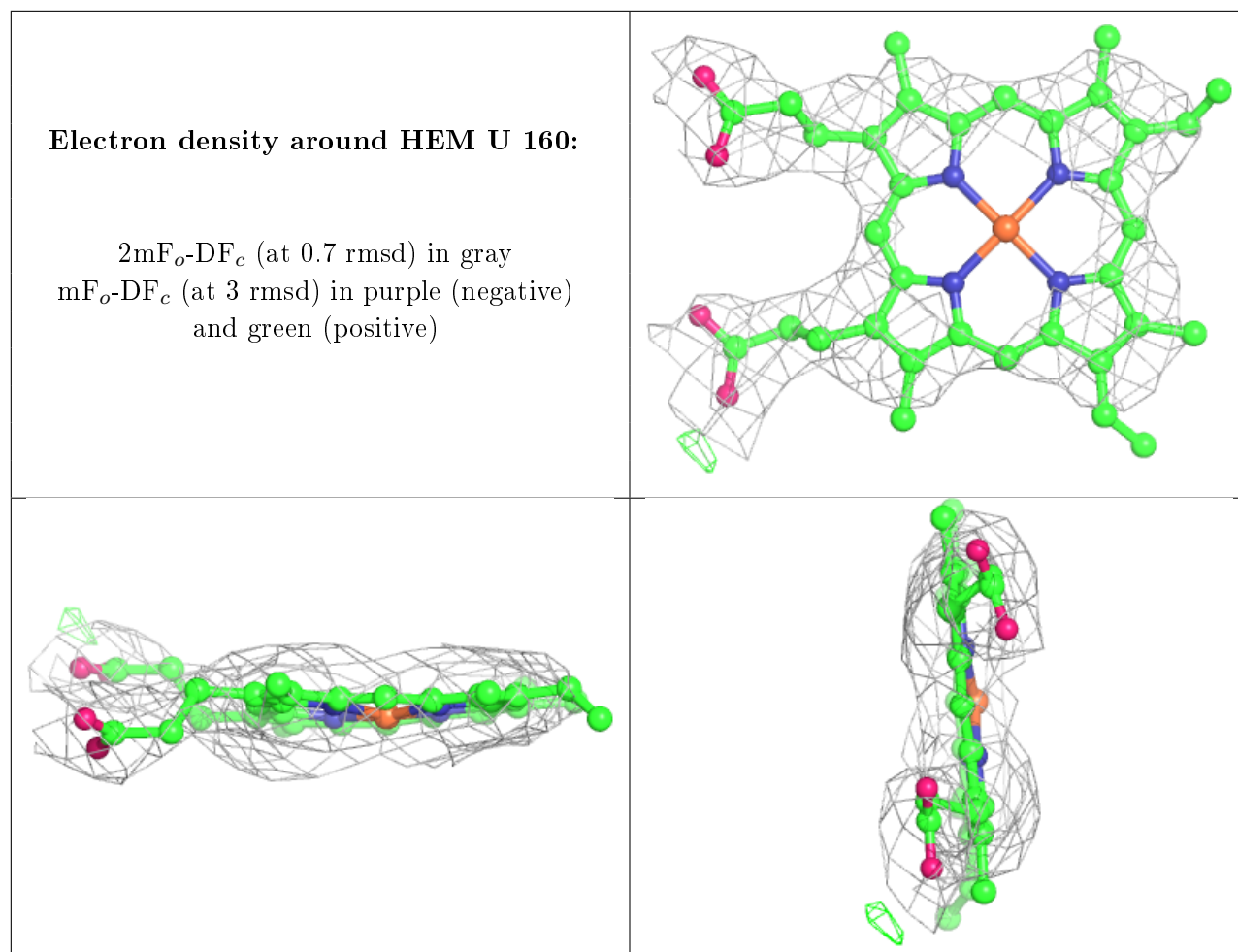


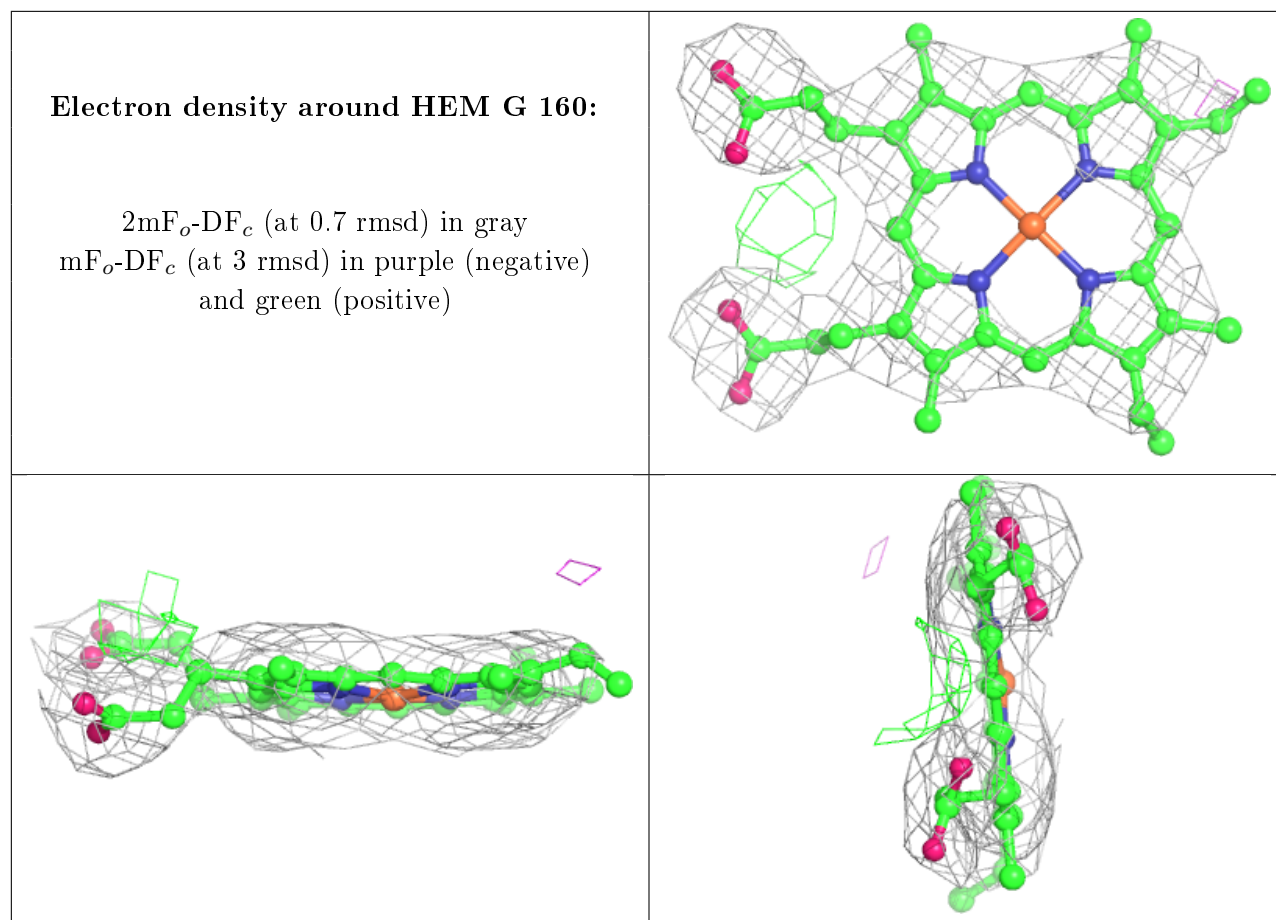


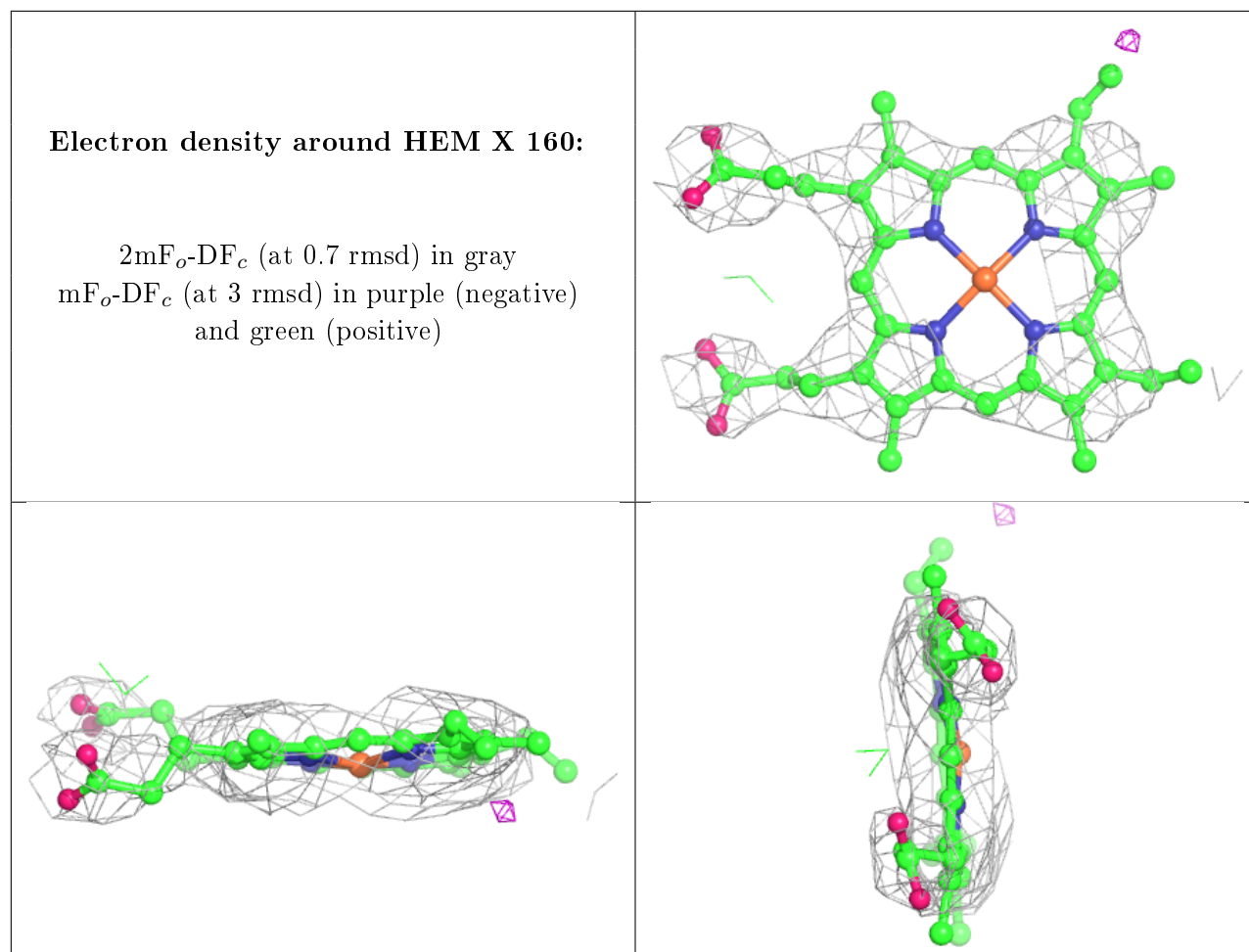


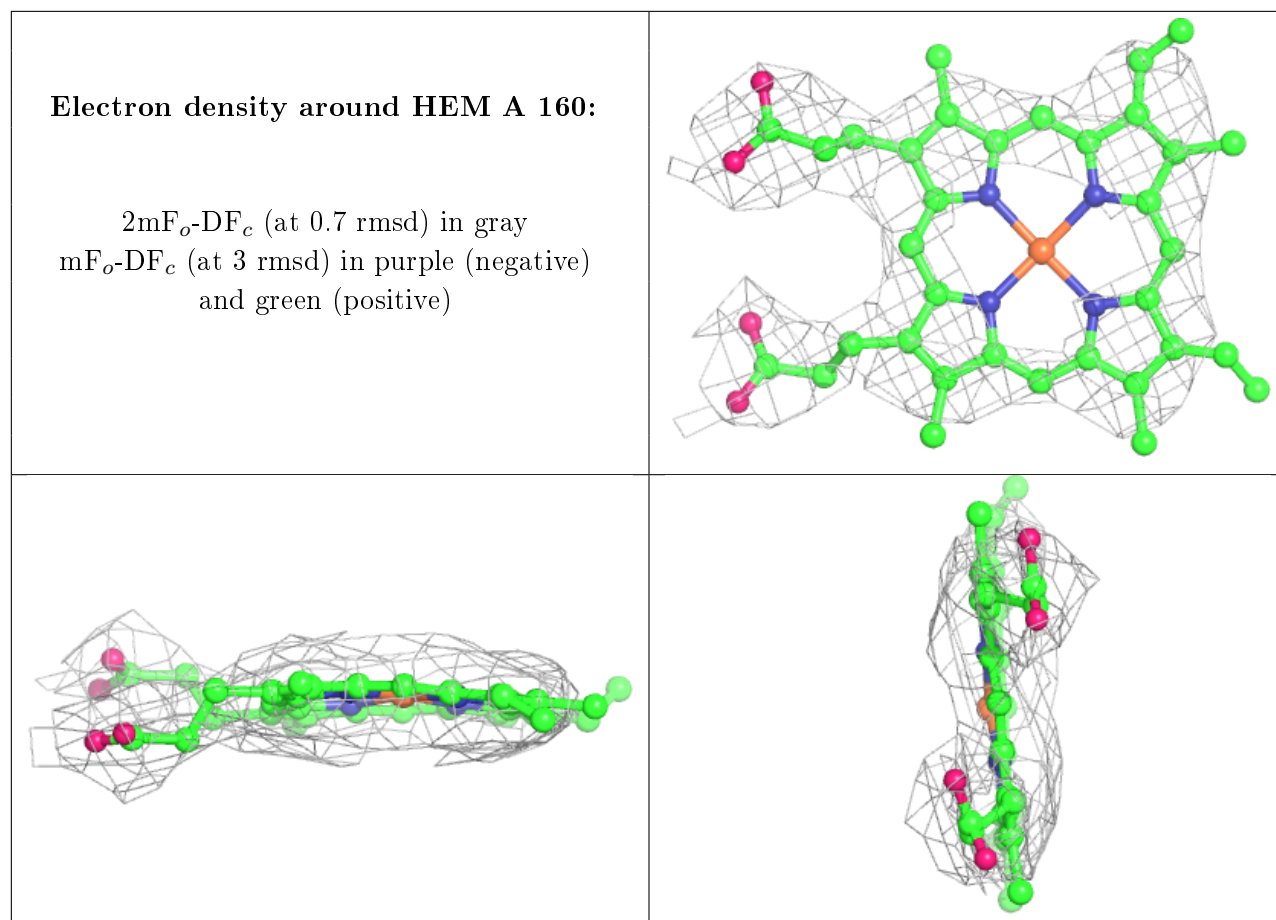






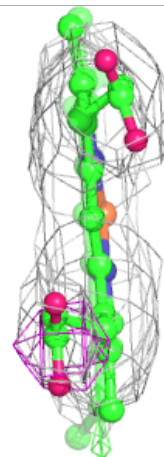
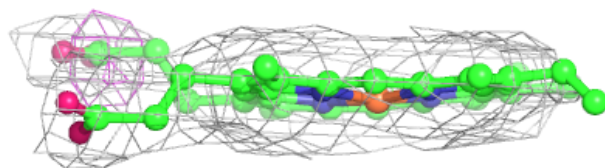
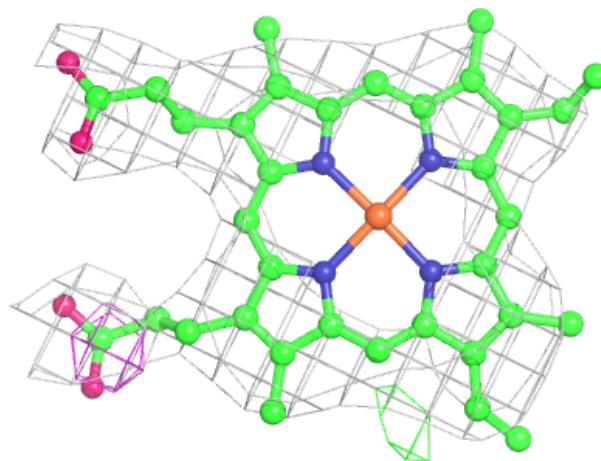






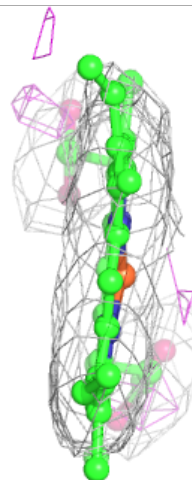
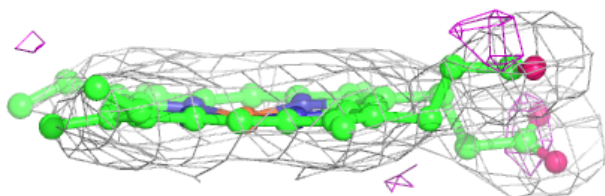
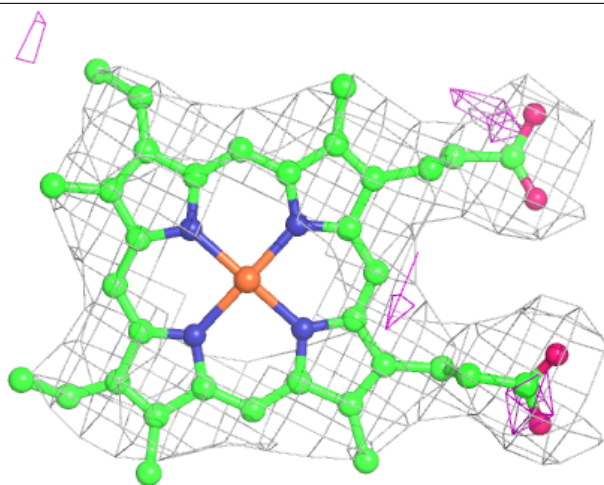
**Electron density around HEM E 160:**

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



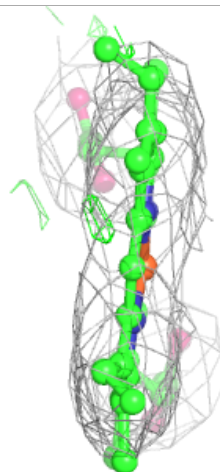
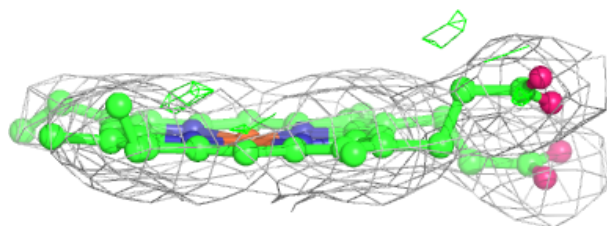
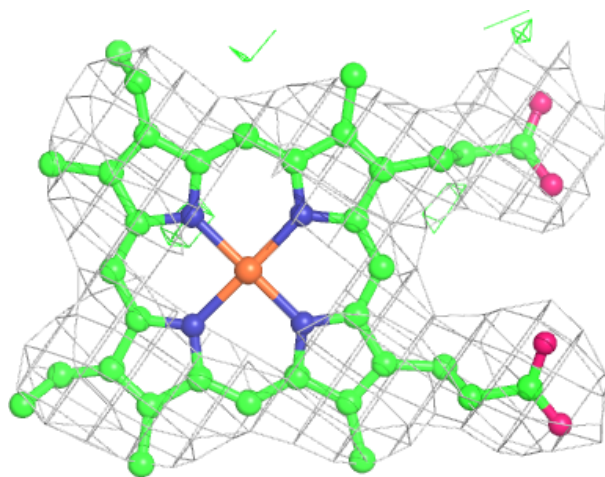
**Electron density around HEM F 160:**

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



**Electron density around HEM K 160:**

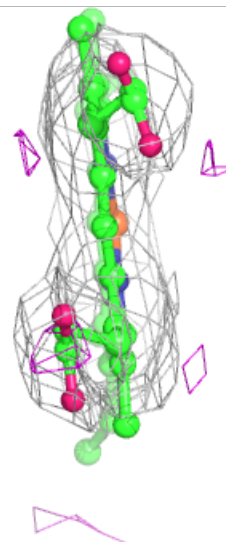
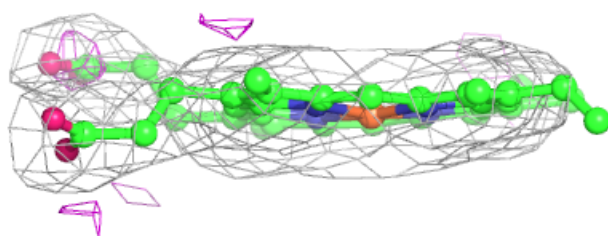
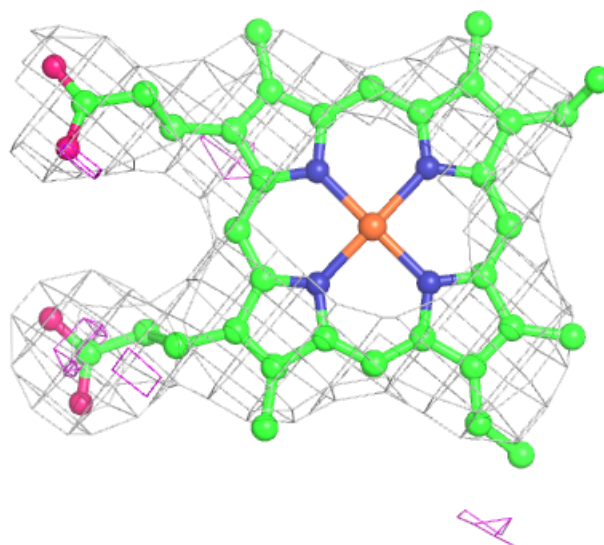
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

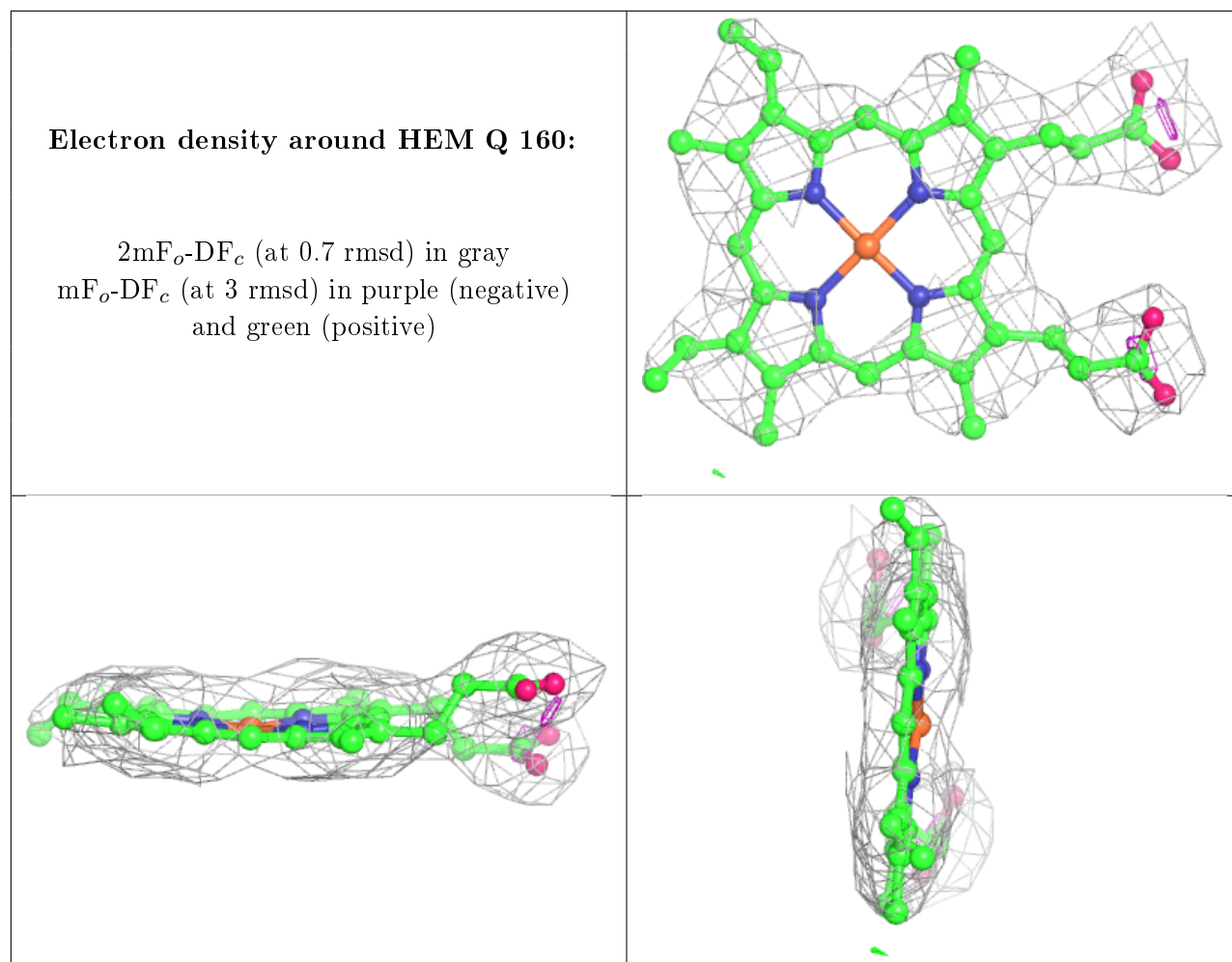




**Electron density around HEM I 160:**

$2mF_o-DF_c$  (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.