

Continued from previous page...

Mol	Chain	Res	Type
1	A	328	GLU
1	A	341	HIS
1	A	349	ARG
1	A	353	GLN
1	A	370	LYS
1	A	375	LYS
1	A	469	LYS
1	A	508	GLN
1	A	511	LYS
1	A	523	LEU
1	A	547	ARG
1	A	552	ASP
1	A	555	LYS
1	A	645	LYS
1	A	663	GLU
1	A	713	THR
1	A	715	VAL
1	B	341	HIS
1	B	351	LYS
1	B	352	ASP
1	B	353	GLN
1	B	360	GLU
1	B	390	SER
1	B	392	SER
1	B	535	GLN
1	B	547	ARG
1	B	645	LYS
1	B	699	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

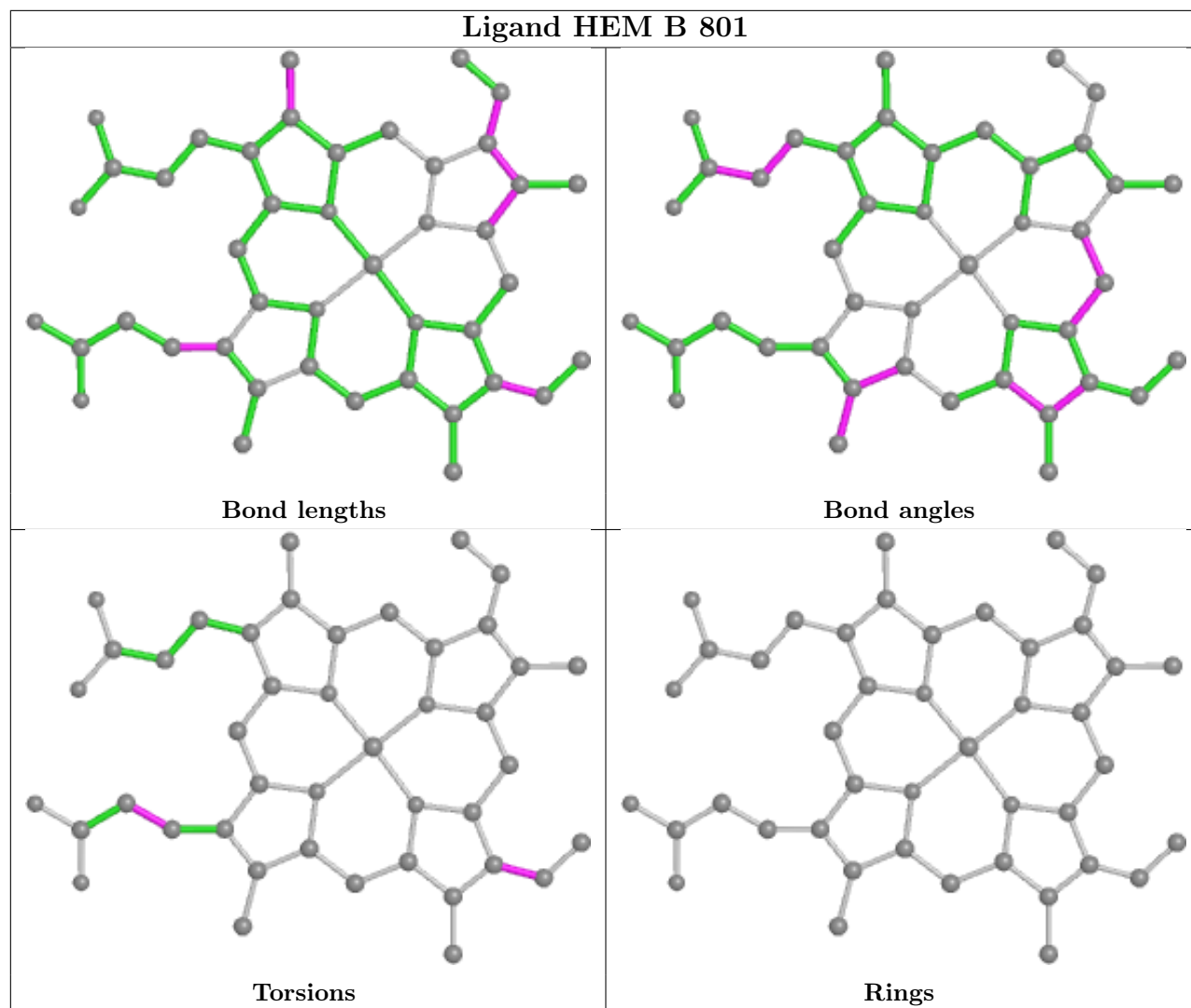
There are no RNA molecules in this entry.

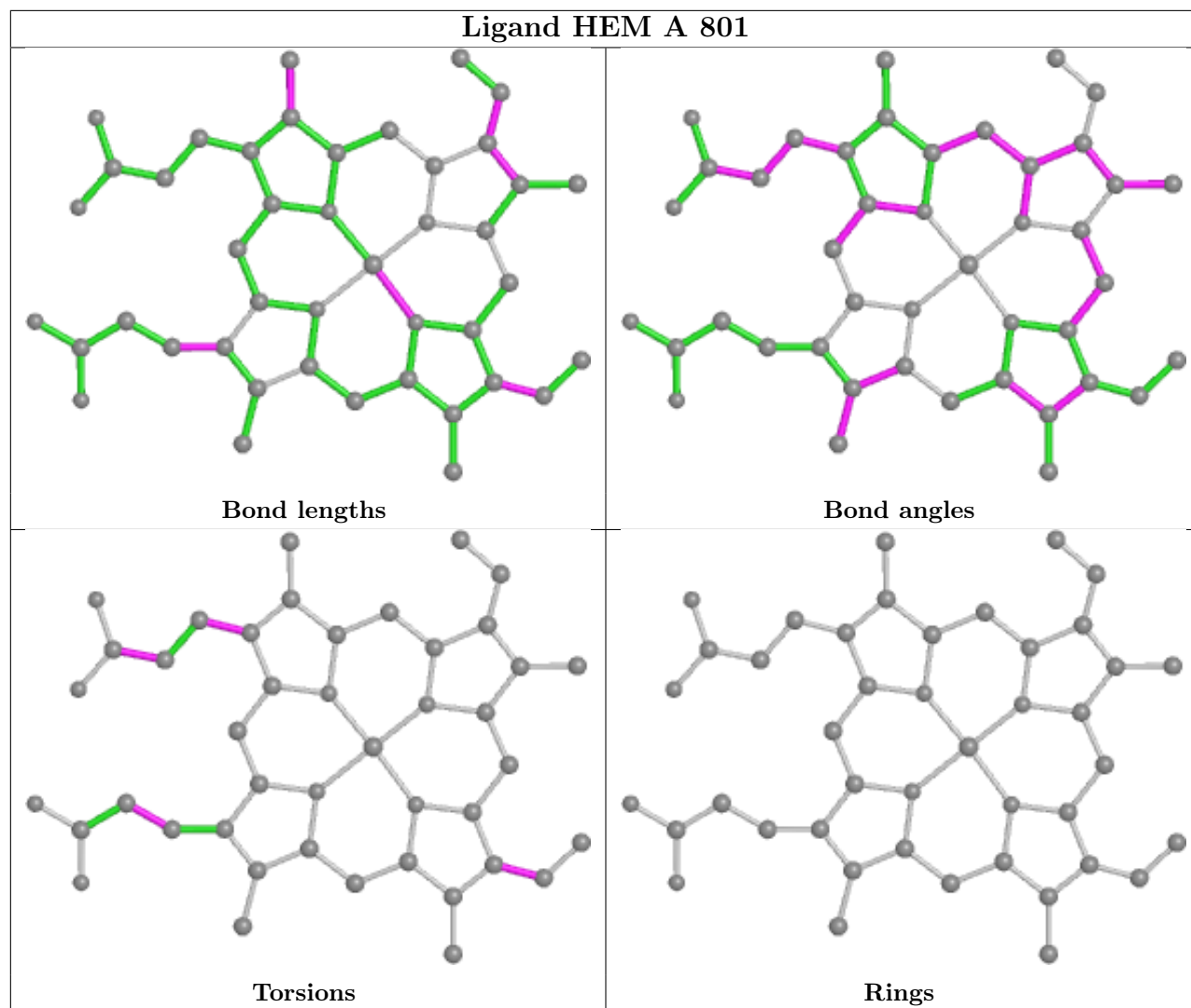
5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

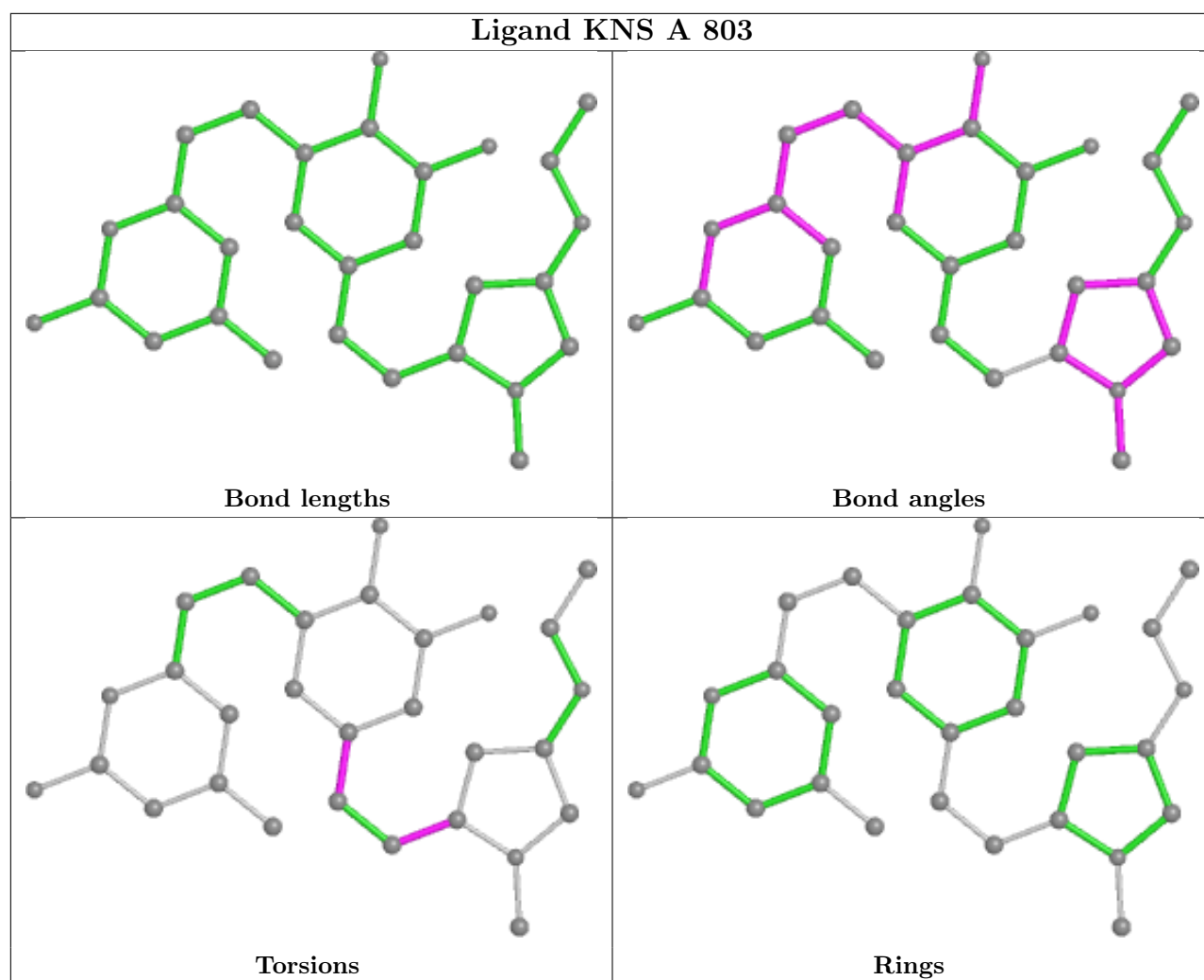
There are no non-standard protein/DNA/RNA residues in this entry.

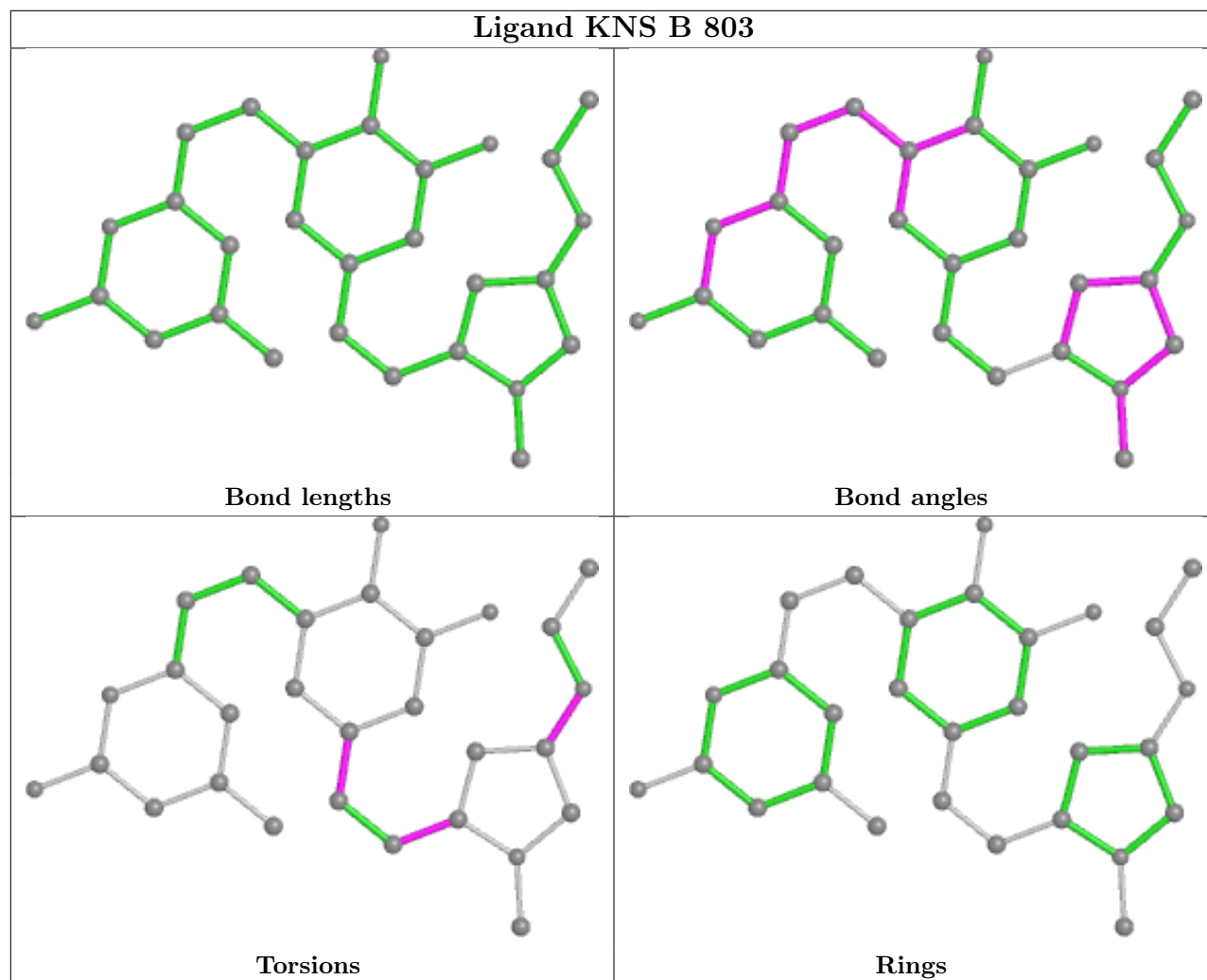
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	2	0
2	A	801	HEM	2	0
4	A	803	KNS	1	0
4	B	803	KNS	1	0

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









5.7 Other polymers [i](#)

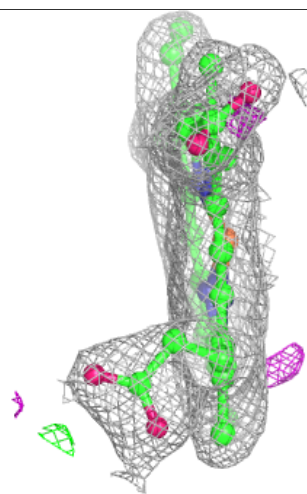
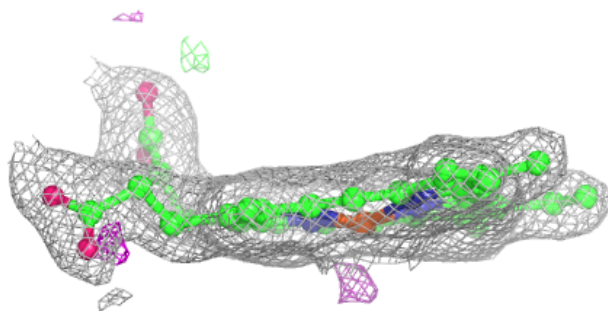
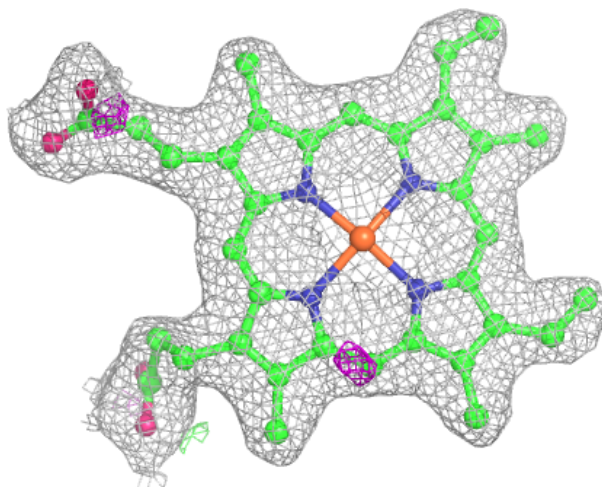
There are no such residues in this entry.

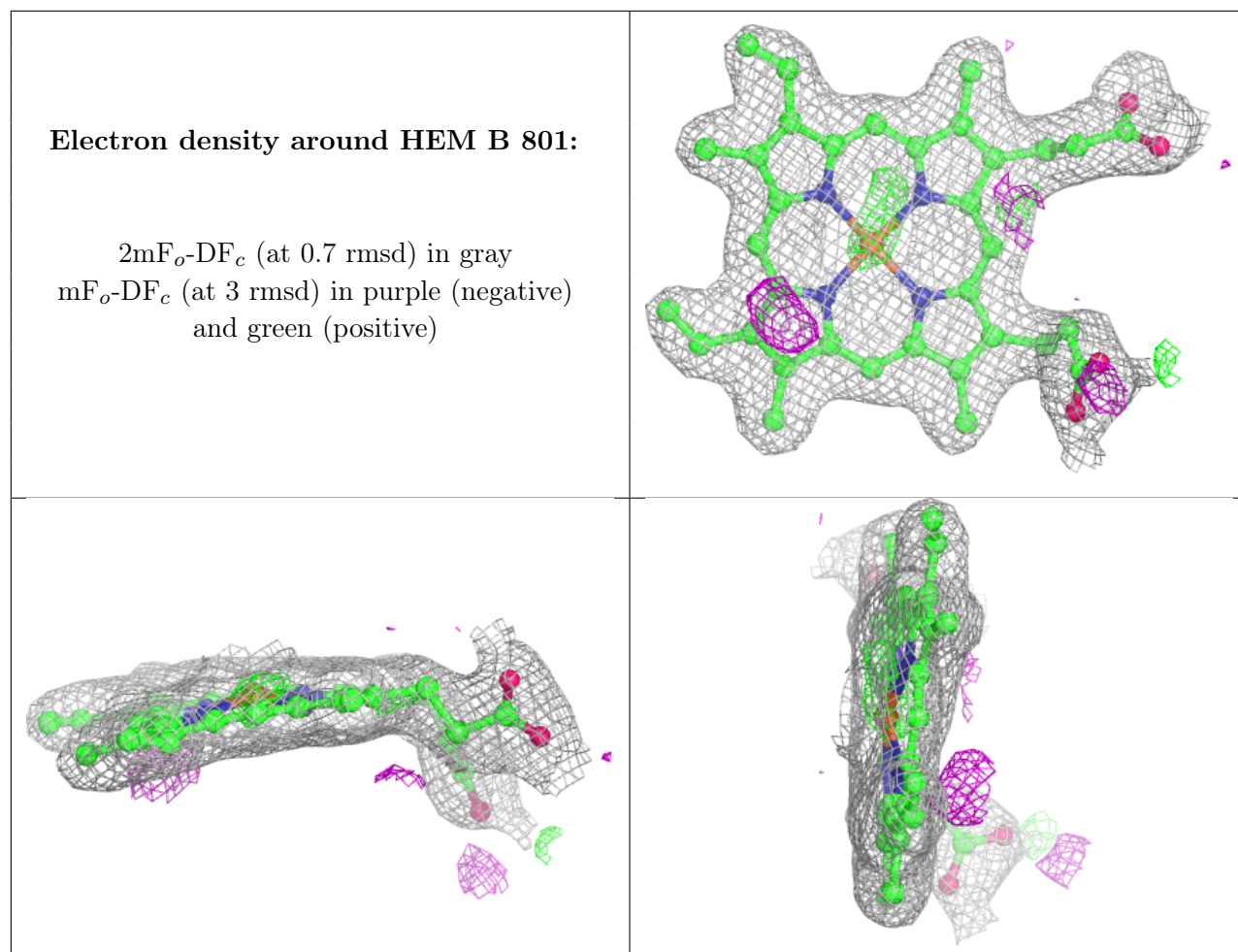
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

Electron density around HEM A 801:

$2mF_o-DF_c$ (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.