



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2026 – 08:49 am BST

PDB ID : 6R2Q / pdb_00006r2q
Title : Structure of the Mtr complex
Authors : Clarke, T.A.; Edwards, M.J.
Deposited on : 2019-03-18
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

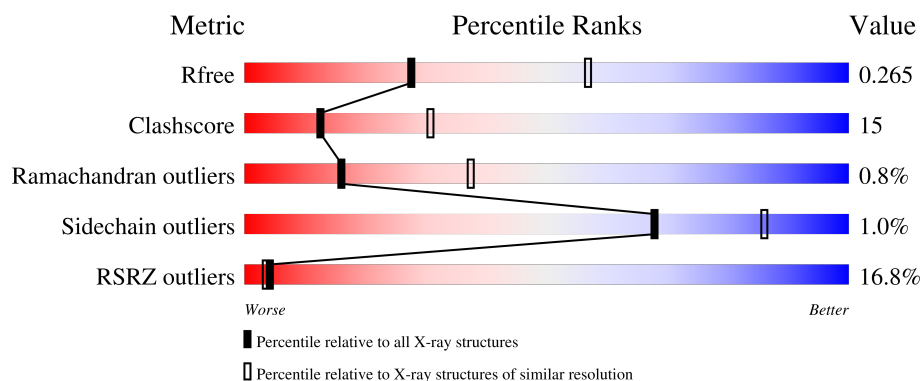
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	333	
2	B	695	
3	C	650	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HEC	A	901	X	-	-	-
4	HEC	A	904	X	-	-	-
4	HEC	A	905	X	-	-	-
4	HEC	A	906	X	-	-	-
4	HEC	A	907	X	-	-	-
4	HEC	A	908	X	-	-	-
4	HEC	A	909	X	-	-	-
4	HEC	A	910	X	-	-	-
4	HEC	C	801	X	-	-	-
4	HEC	C	802	X	-	-	-
4	HEC	C	803	X	-	-	-
4	HEC	C	804	X	-	-	-
4	HEC	C	805	X	-	-	-
4	HEC	C	806	X	-	-	-
4	HEC	C	807	X	-	-	-
4	HEC	C	808	X	-	-	-
4	HEC	C	809	X	-	-	-
4	HEC	C	810	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24030 atoms, of which 11567 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	265	Total	C	H	N	O	S	0	0	0
			3844	1190	1856	381	387	30			

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	649	Total	C	H	N	O	S	0	0	0
			9901	3165	4796	867	1057	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	GLU	ASP	conflict	UNP A0A165K351

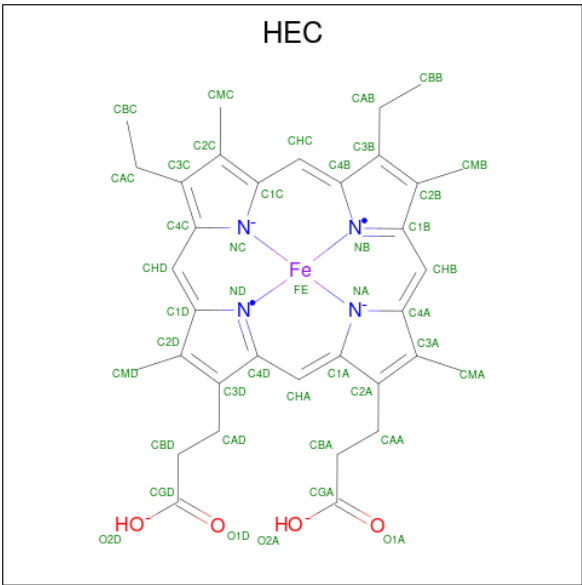
- Molecule 3 is a protein called Decaheme c-type cytochrome, OmcA/MtrC family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	608	Total	C	H	N	O	S	0	0	0
			8767	2772	4283	781	896	35			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	23	THR	ALA	conflict	UNP A0A379ZX38
C	48	ILE	THR	conflict	UNP A0A379ZX38
C	408	ALA	ASP	conflict	UNP A0A379ZX38

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

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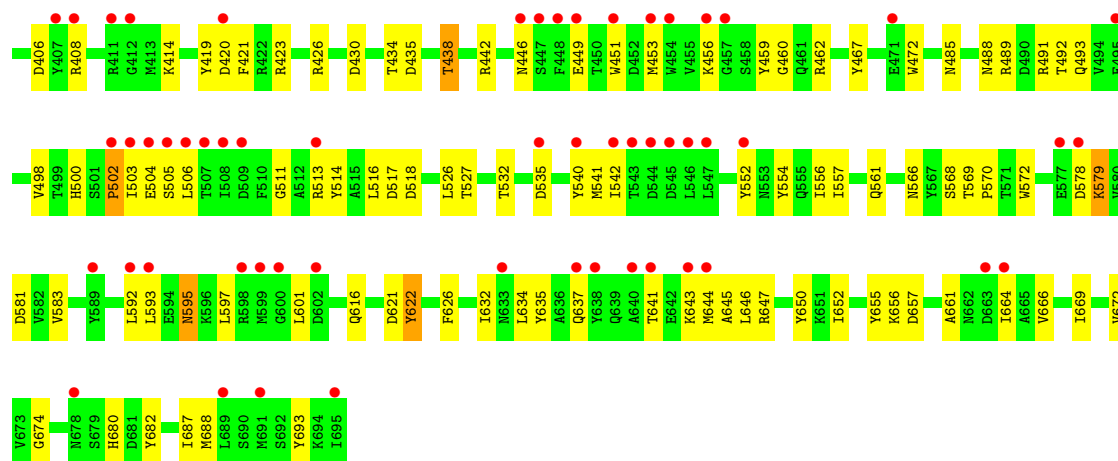
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

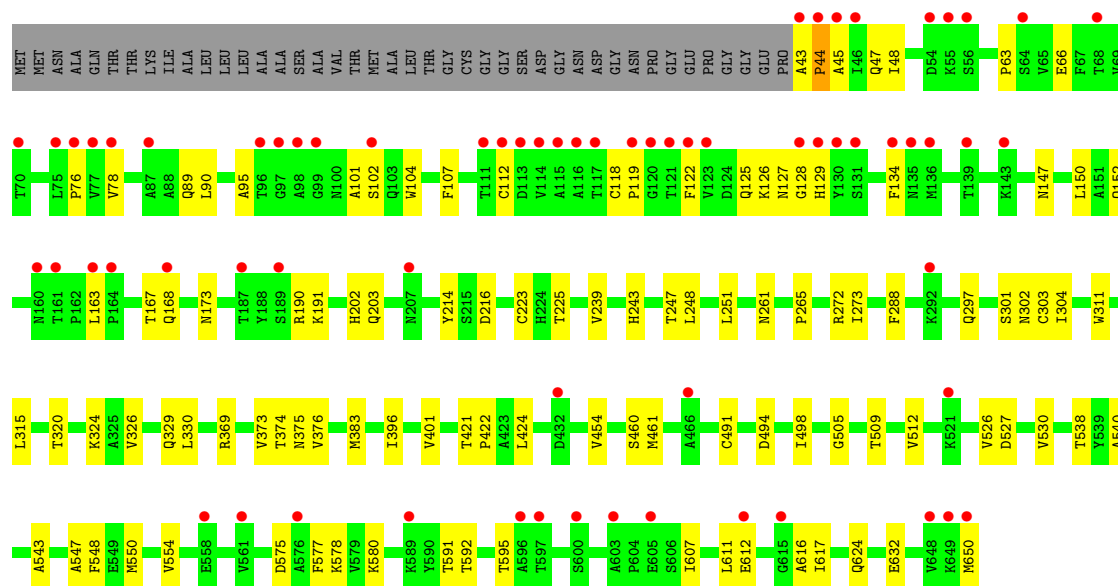
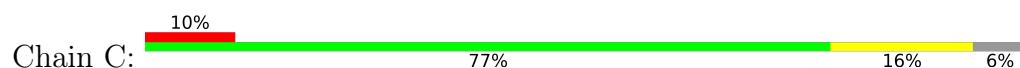
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	C	2	Total	Ca	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	13	Total	O	0	0
			13	13		
6	C	8	Total	O	0	0
			8	8		



● Molecule 3: Decaheme c-type cytochrome, OmcA/MtrC family



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.04Å 234.16Å 99.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.25 – 2.70 73.25 – 2.70	Depositor EDS
% Data completeness (in resolution range)	72.8 (73.25-2.70) 72.9 (73.25-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.257 0.230 , 0.265	Depositor DCC
R_{free} test set	2472 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	24030	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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: HEC, CA

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	0.48	0/2030	0.94	4/2735 (0.1%)
2	B	0.45	0/5202	0.90	3/7055 (0.0%)
3	C	0.43	1/4575 (0.0%)	0.84	1/6225 (0.0%)
All	All	0.45	1/11807 (0.0%)	0.89	8/16015 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	538	THR	CA-C	7.38	1.57	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	GLN	N-CA-C	8.05	122.41	112.58
2	B	211	LYS	CA-CB-CG	-6.45	101.20	114.10
2	B	176	GLU	CA-CB-CG	5.59	125.27	114.10
3	C	66	GLU	CB-CA-C	-5.52	99.71	109.70
1	A	128	SER	N-CA-C	5.38	121.00	110.56

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	1988	1856	1856	94	0
2	B	5105	4796	4796	175	0
3	C	4484	4283	4280	76	0
4	A	430	315	307	43	0
4	C	430	317	312	33	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	A	1	0	0	0	0
6	B	13	0	0	3	0
6	C	8	0	0	0	0
All	All	12463	11567	11551	368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 368 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)
3:C:617:ILE:HD13	3:C:624:GLN:HG2	1.42	1.01
1:A:253:GLU:OE1	2:B:426:ARG:NH2	2.00	0.94
2:B:113:VAL:HG22	2:B:125:VAL:HG22	1.48	0.93
1:A:188:THR:HG21	2:B:535:ASP:OD2	1.72	0.90
2:B:361:SER:OG	2:B:402:LYS:HG3	1.70	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	259/333 (78%)	216 (83%)	35 (14%)	8 (3%)	3 8
2	B	647/695 (93%)	614 (95%)	30 (5%)	3 (0%)	24 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	606/650 (93%)	583 (96%)	22 (4%)	1 (0%)	43	68
All	All	1512/1678 (90%)	1413 (94%)	87 (6%)	12 (1%)	16	37

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	A	169	ALA
1	A	274	ALA
1	A	99	GLN
1	A	123	LYS

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	226/282 (80%)	224 (99%)	2 (1%)	70	87
2	B	552/586 (94%)	544 (99%)	8 (1%)	59	82
3	C	483/511 (94%)	481 (100%)	2 (0%)	84	93
All	All	1261/1379 (91%)	1249 (99%)	12 (1%)	68	86

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	438	THR
2	B	579	LYS
3	C	454	VAL
2	B	622	TYR
2	B	64	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	100	ASN
3	C	149	GLN
3	C	302	ASN
3	C	168	GLN
2	B	129	GLN

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.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\# Z > 2$
4	HEC	A	905	1	50,50,50	1.85	6 (12%)	68,82,82	1.42	7 (10%)
4	HEC	C	802	3	50,50,50	1.83	4 (8%)	68,82,82	1.99	17 (25%)
4	HEC	C	801	3	50,50,50	1.70	6 (12%)	68,82,82	2.22	25 (36%)
4	HEC	C	809	3	50,50,50	2.25	6 (12%)	68,82,82	1.66	15 (22%)
4	HEC	C	808	3	50,50,50	1.76	6 (12%)	68,82,82	1.89	17 (25%)
4	HEC	C	810	3	50,50,50	1.76	5 (10%)	68,82,82	1.76	20 (29%)
4	HEC	A	901	1	50,50,50	2.05	6 (12%)	68,82,82	1.63	12 (17%)
4	HEC	C	803	3	50,50,50	1.62	4 (8%)	68,82,82	1.46	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEC	C	804	3	50,50,50	1.53	3 (6%)	68,82,82	1.77	16 (23%)
4	HEC	A	903	1	50,50,50	2.28	4 (8%)	68,82,82	1.89	14 (20%)
4	HEC	A	907	1	50,50,50	1.73	4 (8%)	68,82,82	1.68	16 (23%)
4	HEC	A	902	1	50,50,50	2.02	7 (14%)	68,82,82	1.94	18 (26%)
4	HEC	A	908	1	50,50,50	1.74	3 (6%)	68,82,82	1.68	15 (22%)
4	HEC	A	904	1	50,50,50	2.06	8 (16%)	68,82,82	2.03	14 (20%)
4	HEC	C	805	3	50,50,50	1.72	8 (16%)	68,82,82	2.11	16 (23%)
4	HEC	C	806	3	50,50,50	1.69	5 (10%)	68,82,82	1.59	13 (19%)
4	HEC	A	906	1	50,50,50	1.66	4 (8%)	68,82,82	1.85	11 (16%)
4	HEC	A	910	1	50,50,50	1.83	6 (12%)	68,82,82	1.68	12 (17%)
4	HEC	A	909	1	50,50,50	1.74	5 (10%)	68,82,82	1.88	12 (17%)
4	HEC	C	807	3	50,50,50	1.71	5 (10%)	68,82,82	1.57	11 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	A	905	1	1/1/7/7	8/14/54/54	-
4	HEC	C	802	3	1/1/7/7	11/14/54/54	-
4	HEC	C	801	3	1/1/7/7	9/14/54/54	-
4	HEC	C	809	3	1/1/7/7	9/14/54/54	-
4	HEC	C	808	3	1/1/7/7	8/14/54/54	-
4	HEC	C	810	3	1/1/7/7	9/14/54/54	-
4	HEC	A	901	1	1/1/7/7	6/14/54/54	-
4	HEC	C	803	3	1/1/7/7	6/14/54/54	-
4	HEC	C	804	3	1/1/7/7	11/14/54/54	-
4	HEC	A	903	1	-	5/14/54/54	-
4	HEC	A	907	1	1/1/7/7	6/14/54/54	-
4	HEC	A	902	1	-	11/14/54/54	-
4	HEC	A	908	1	1/1/7/7	8/14/54/54	-
4	HEC	A	904	1	1/1/7/7	12/14/54/54	-
4	HEC	C	805	3	1/1/7/7	7/14/54/54	-
4	HEC	C	806	3	1/1/7/7	12/14/54/54	-
4	HEC	A	906	1	1/1/7/7	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEC	A	910	1	1/1/7/7	8/14/54/54	-
4	HEC	A	909	1	1/1/7/7	6/14/54/54	-
4	HEC	C	807	3	1/1/7/7	8/14/54/54	-

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	HEC	FE-NA	8.89	2.25	1.95
4	C	809	HEC	FE-ND	8.89	2.22	1.94
4	A	904	HEC	C3D-C2D	8.23	1.54	1.36
4	C	806	HEC	C3D-C2D	8.13	1.54	1.36
4	A	903	HEC	FE-ND	8.09	2.19	1.94

The worst 5 of 290 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	909	HEC	CAC-C3C-C4C	7.63	135.51	124.92
4	A	904	HEC	CAB-C3B-C4B	-6.49	116.39	124.81
4	A	902	HEC	C1D-ND-C4D	6.34	111.62	105.07
4	A	904	HEC	C1D-ND-C4D	6.33	111.61	105.07
4	A	903	HEC	C1D-ND-C4D	6.26	111.54	105.07

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	901	HEC	NA
4	A	904	HEC	NA
4	A	905	HEC	NA
4	A	906	HEC	NA
4	A	907	HEC	NA

5 of 167 torsion outliers are listed below:

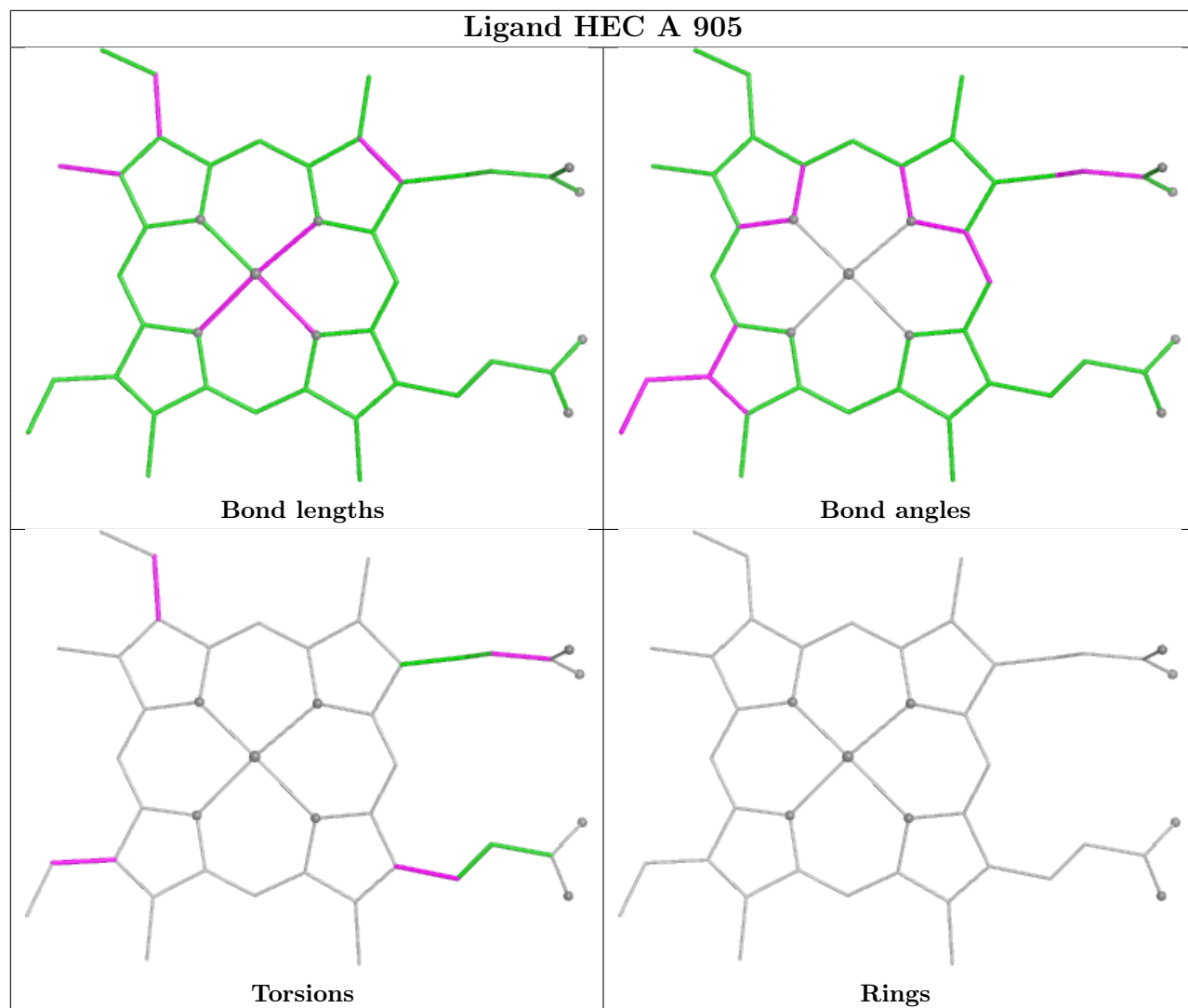
Mol	Chain	Res	Type	Atoms
4	A	901	HEC	C2C-C3C-CAC-CBC
4	A	907	HEC	C2C-C3C-CAC-CBC
4	A	908	HEC	C2C-C3C-CAC-CBC
4	A	910	HEC	C2C-C3C-CAC-CBC
4	C	802	HEC	C3D-CAD-CBD-CGD

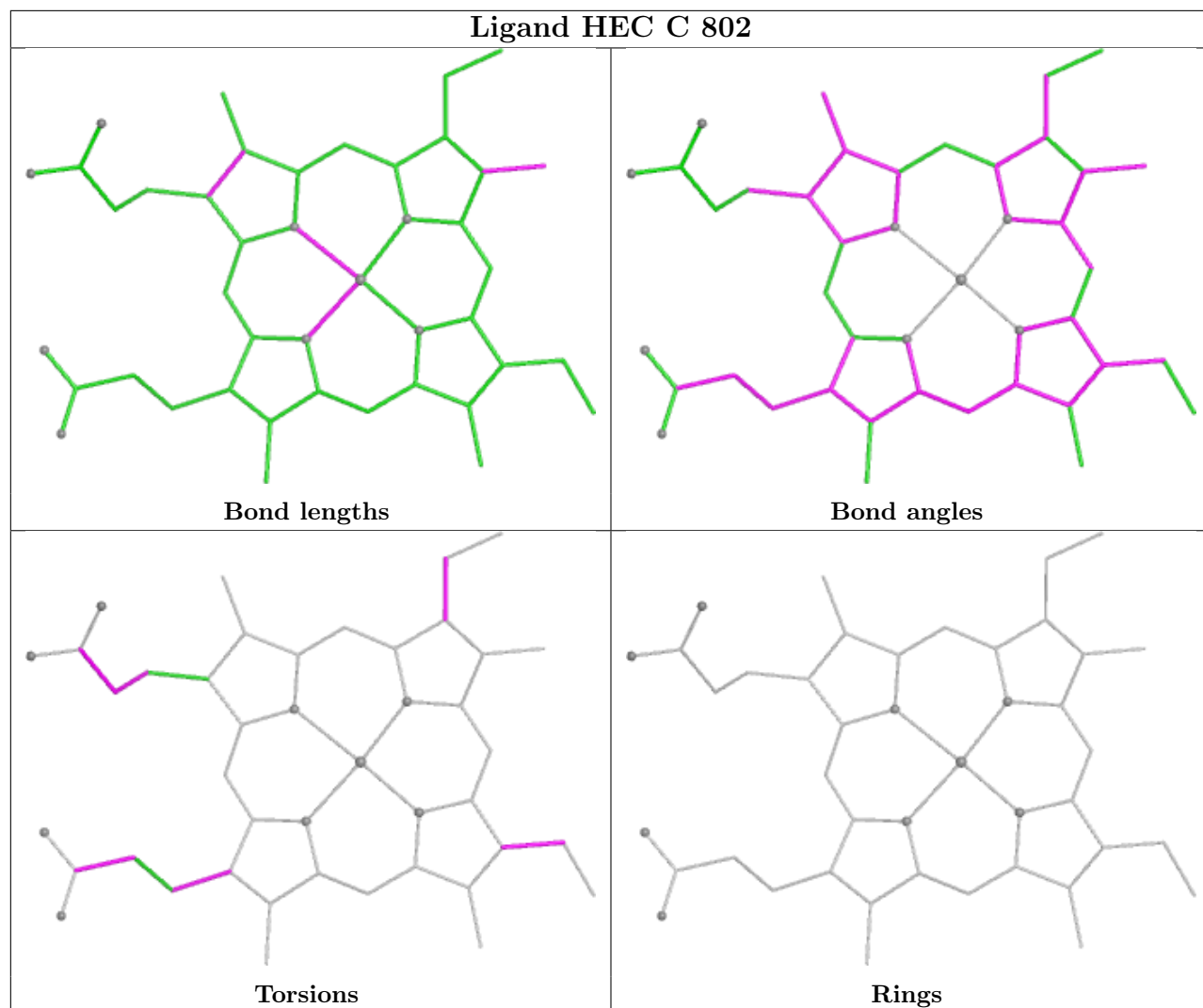
There are no ring outliers.

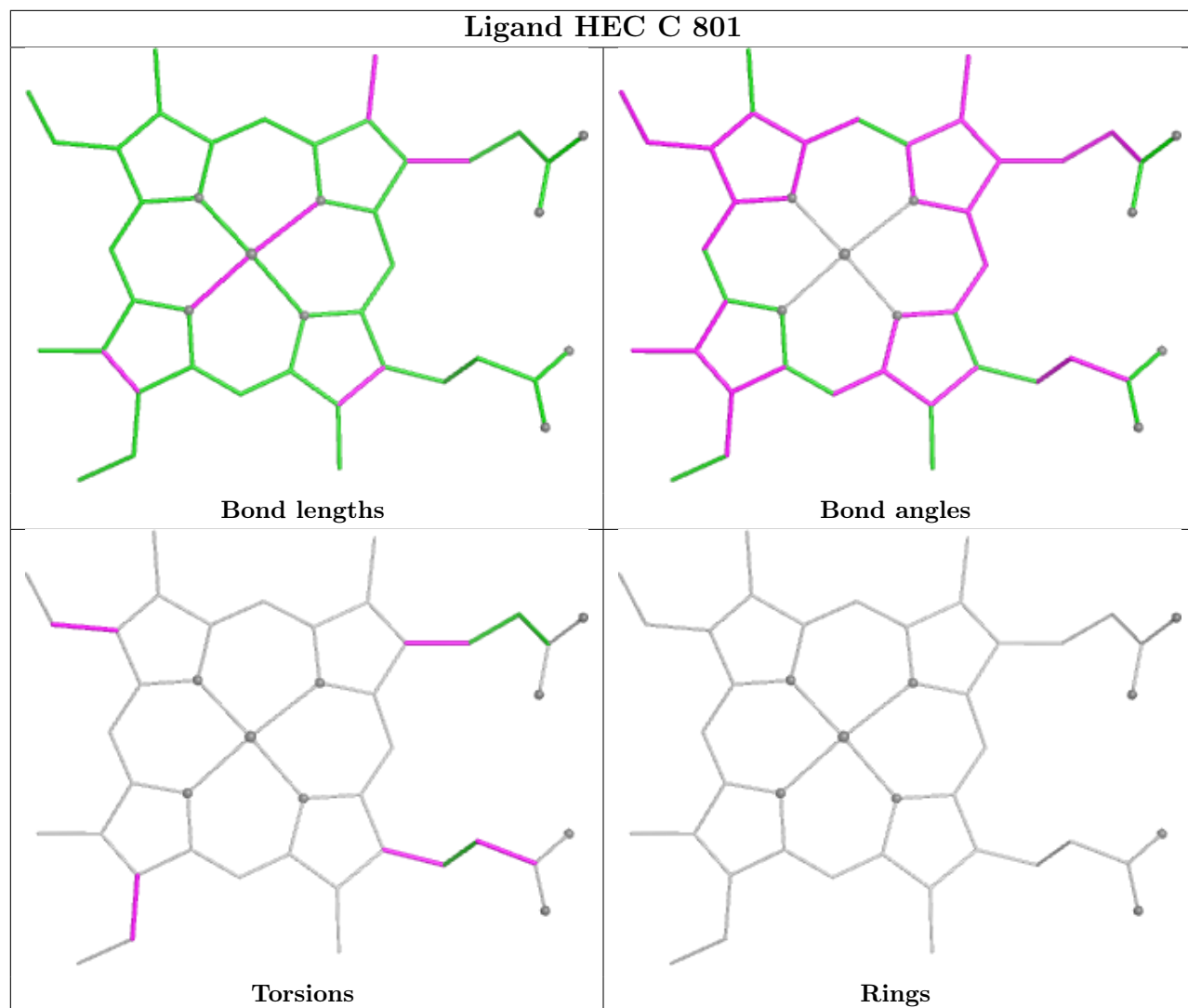
20 monomers are involved in 76 short contacts:

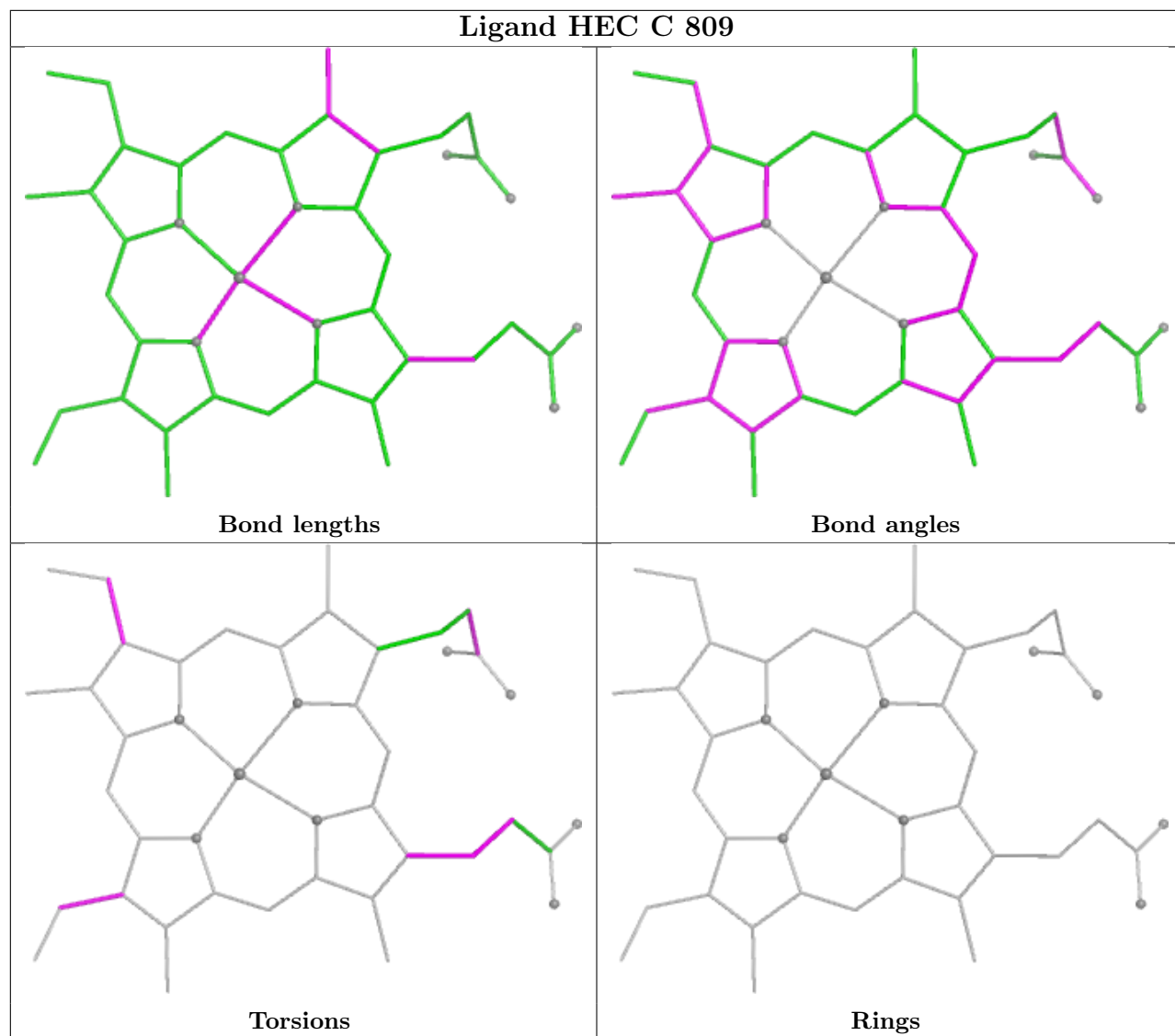
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	905	HEC	2	0
4	C	802	HEC	4	0
4	C	801	HEC	2	0
4	C	809	HEC	1	0
4	C	808	HEC	2	0
4	C	810	HEC	2	0
4	A	901	HEC	3	0
4	C	803	HEC	2	0
4	C	804	HEC	2	0
4	A	903	HEC	2	0
4	A	907	HEC	6	0
4	A	902	HEC	4	0
4	A	908	HEC	9	0
4	A	904	HEC	7	0
4	C	805	HEC	8	0
4	C	806	HEC	5	0
4	A	906	HEC	2	0
4	A	910	HEC	4	0
4	A	909	HEC	4	0
4	C	807	HEC	5	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.

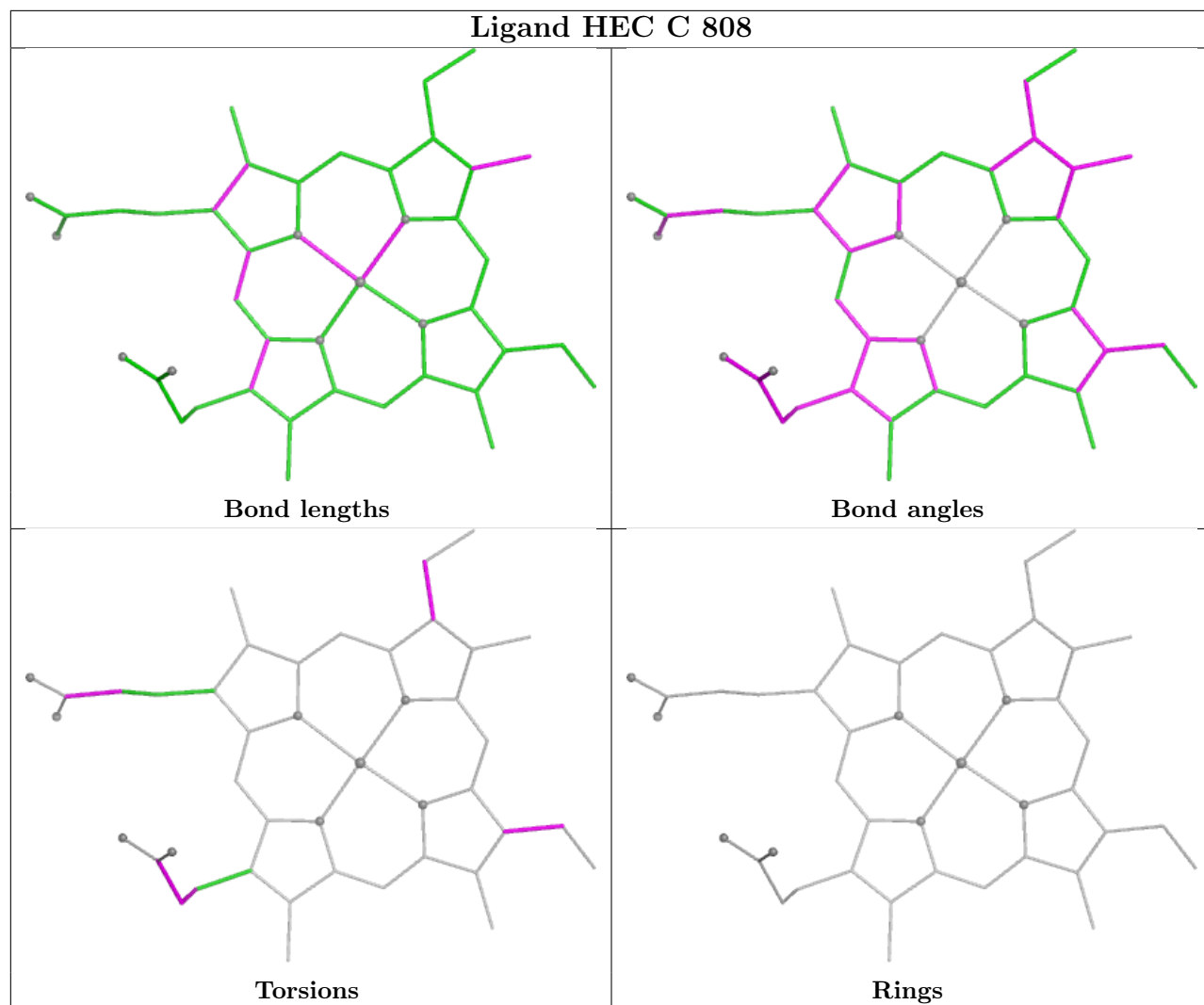


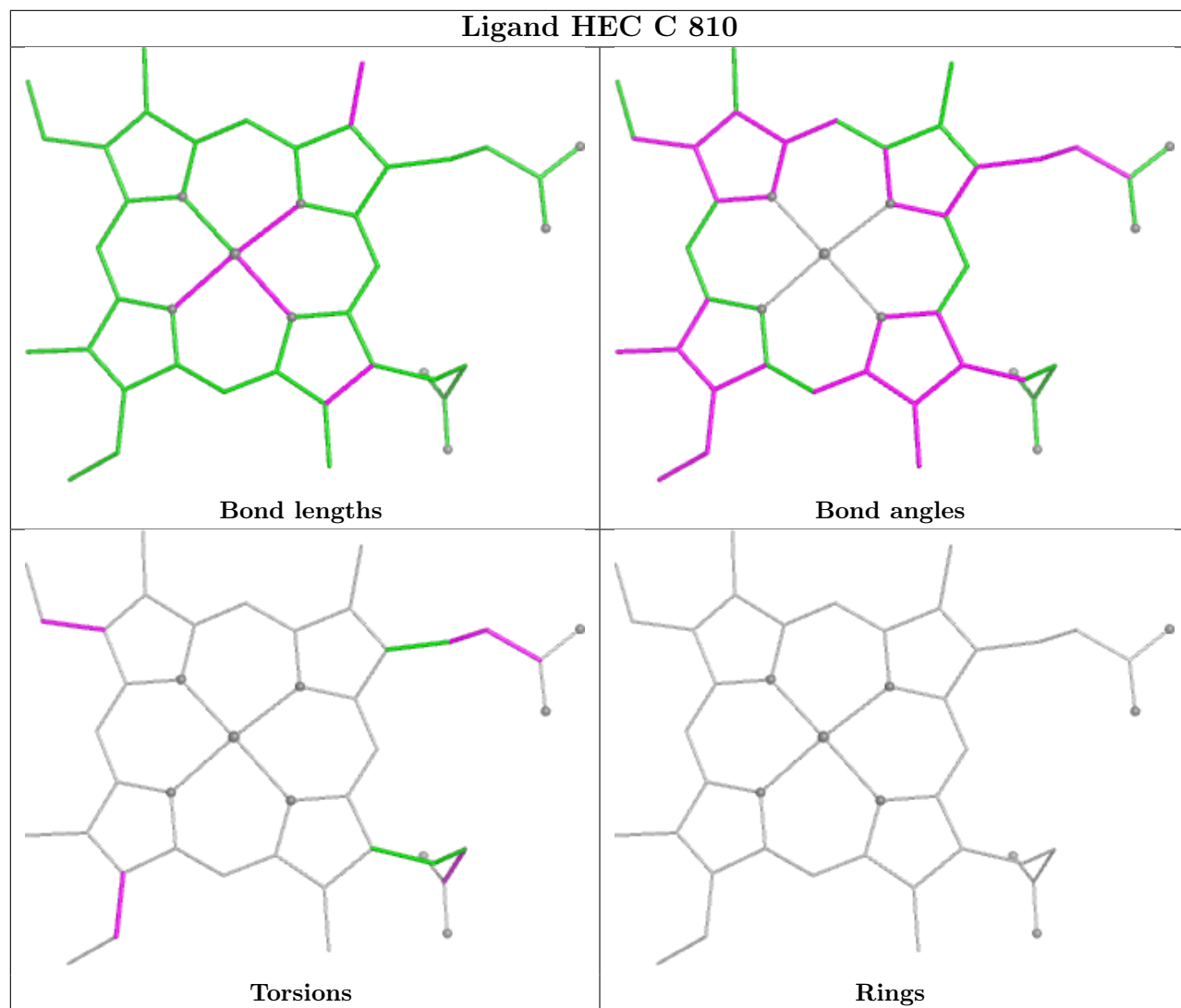


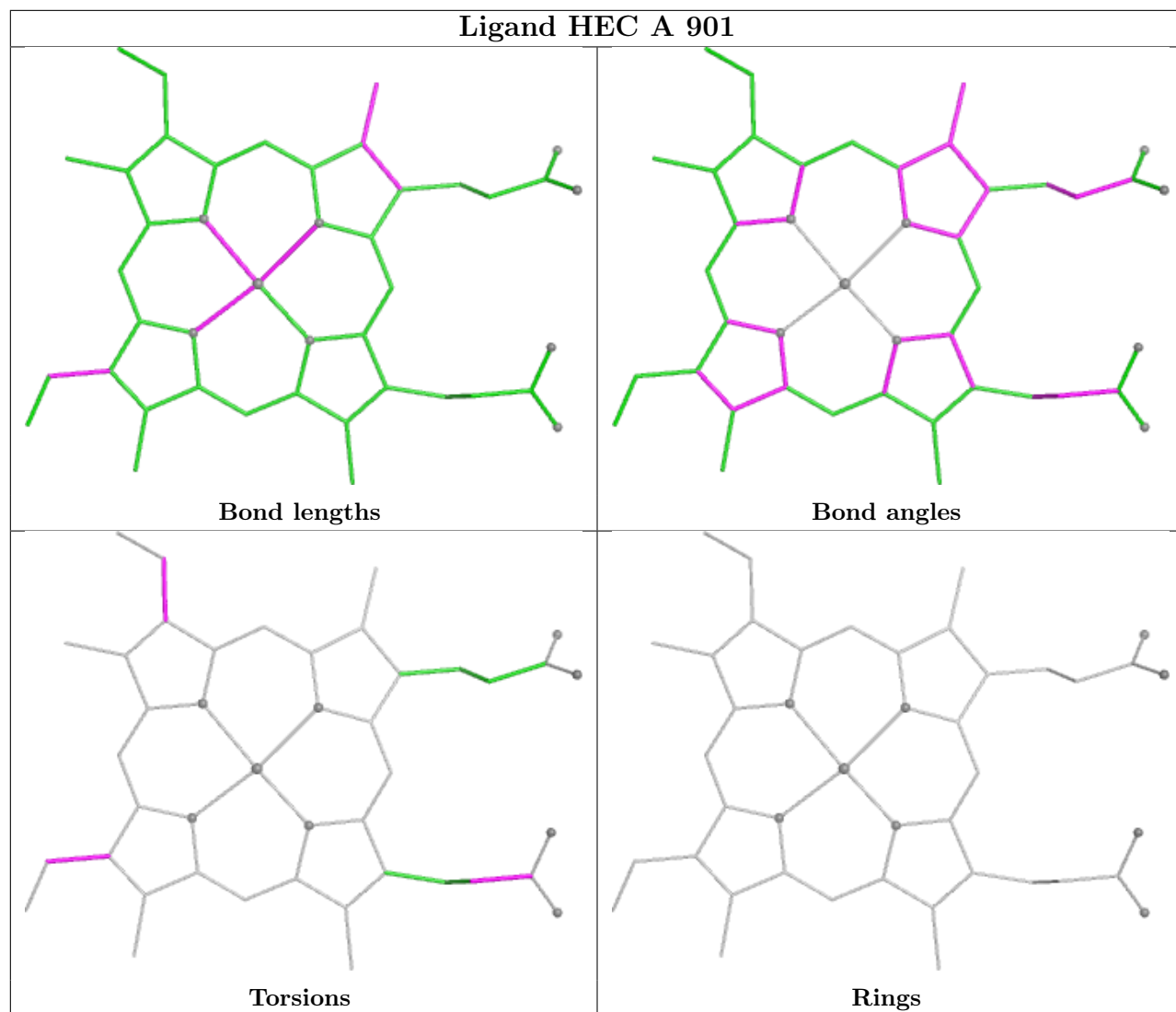




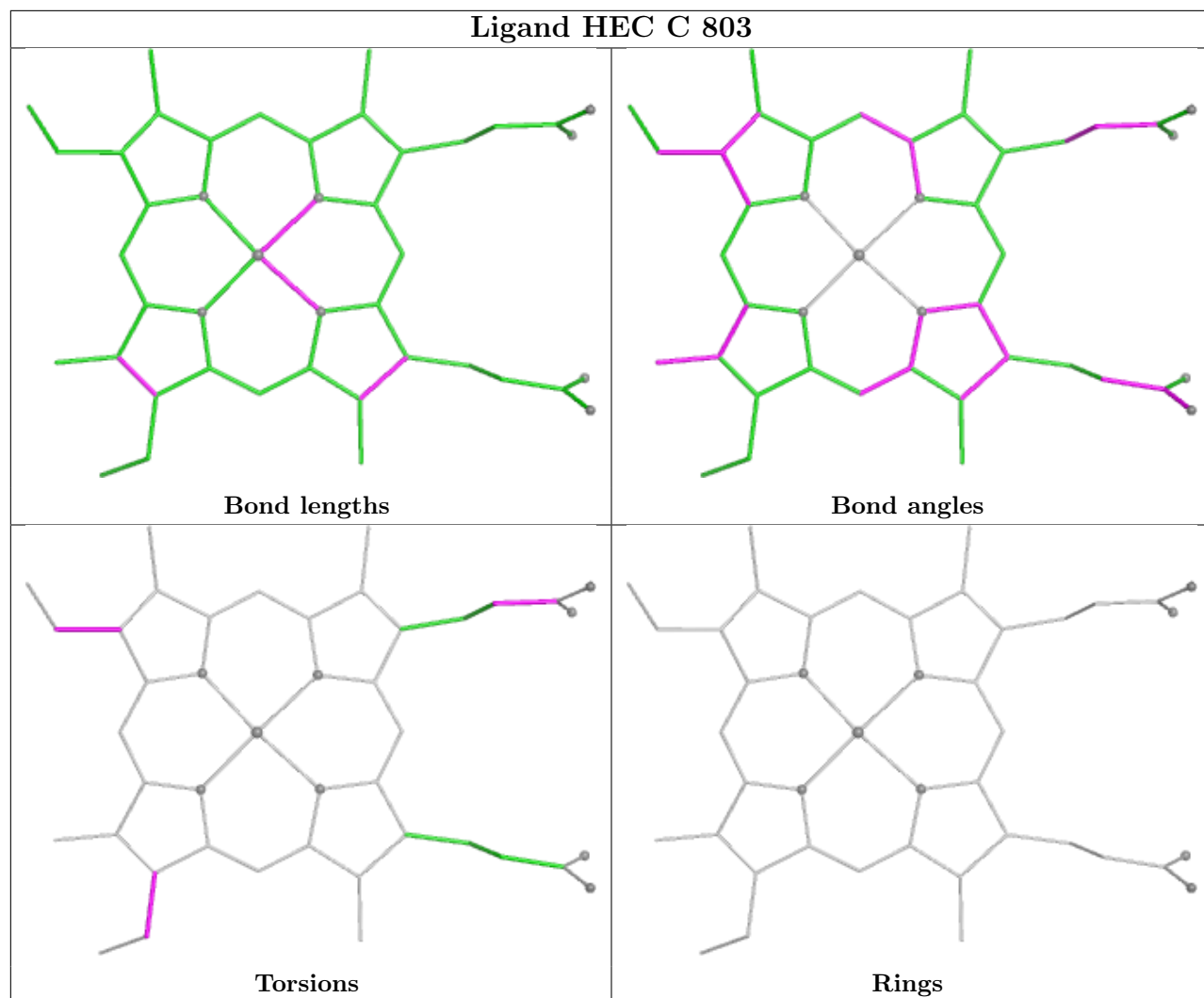
Ligand HEC C 808

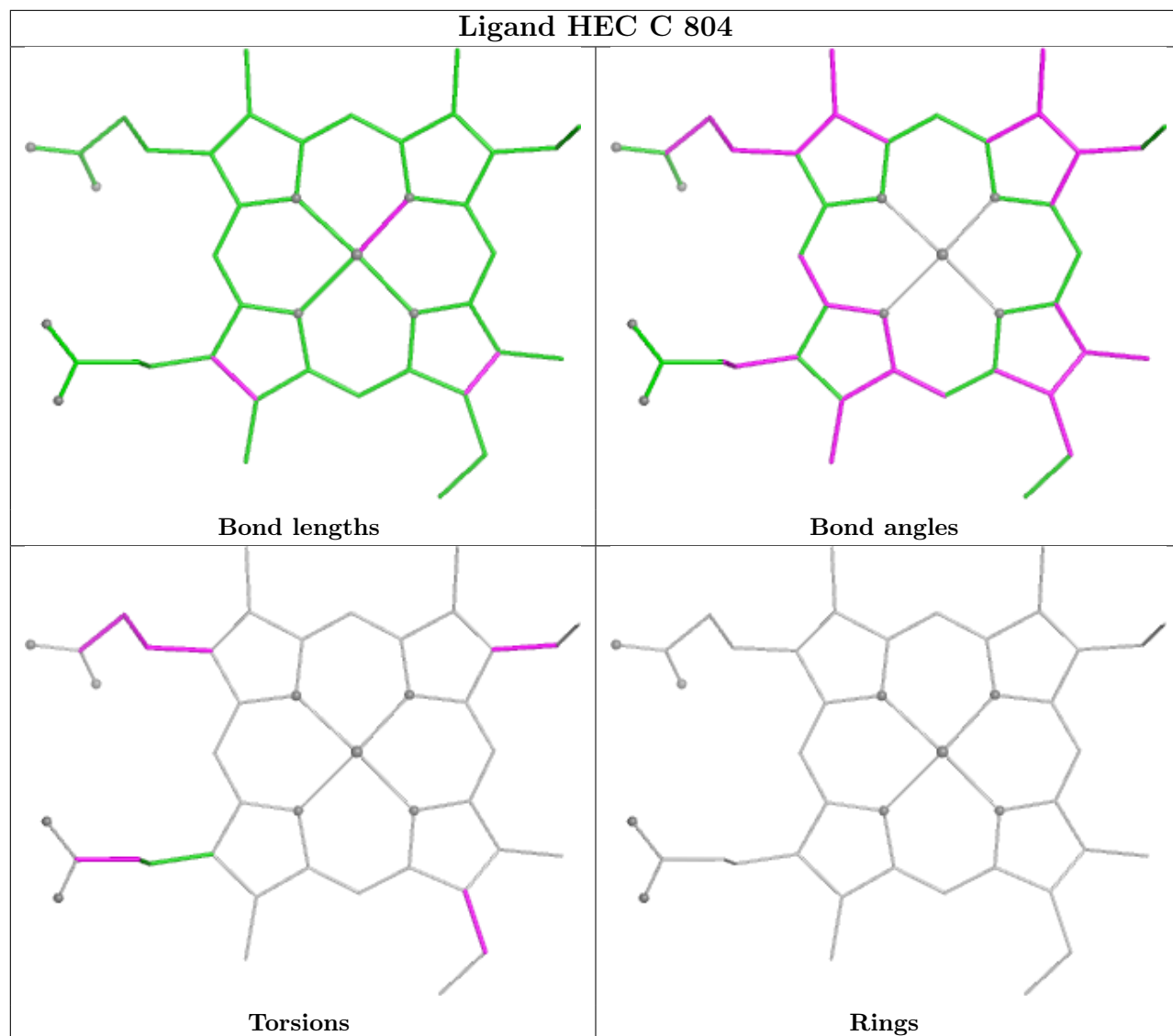


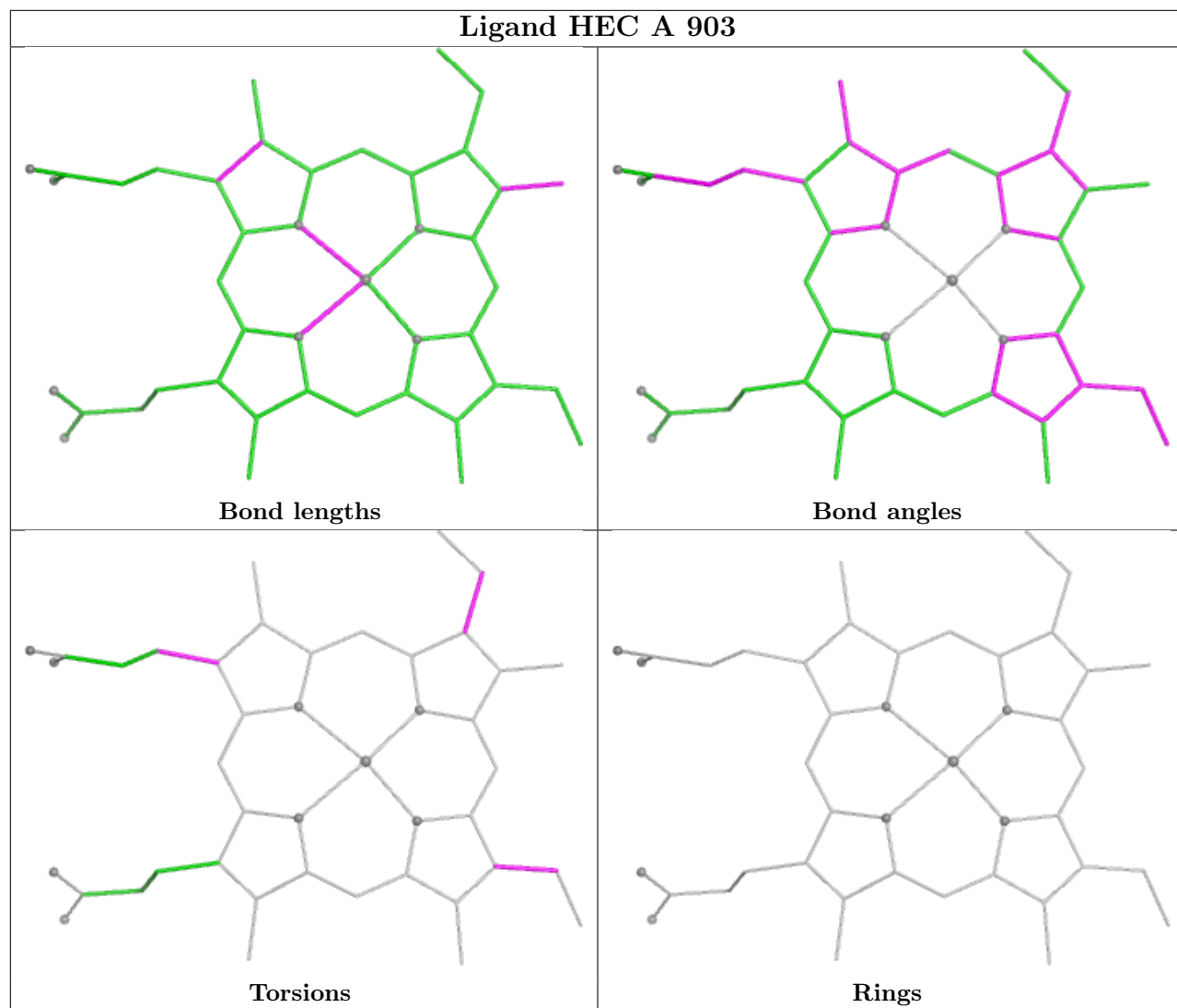


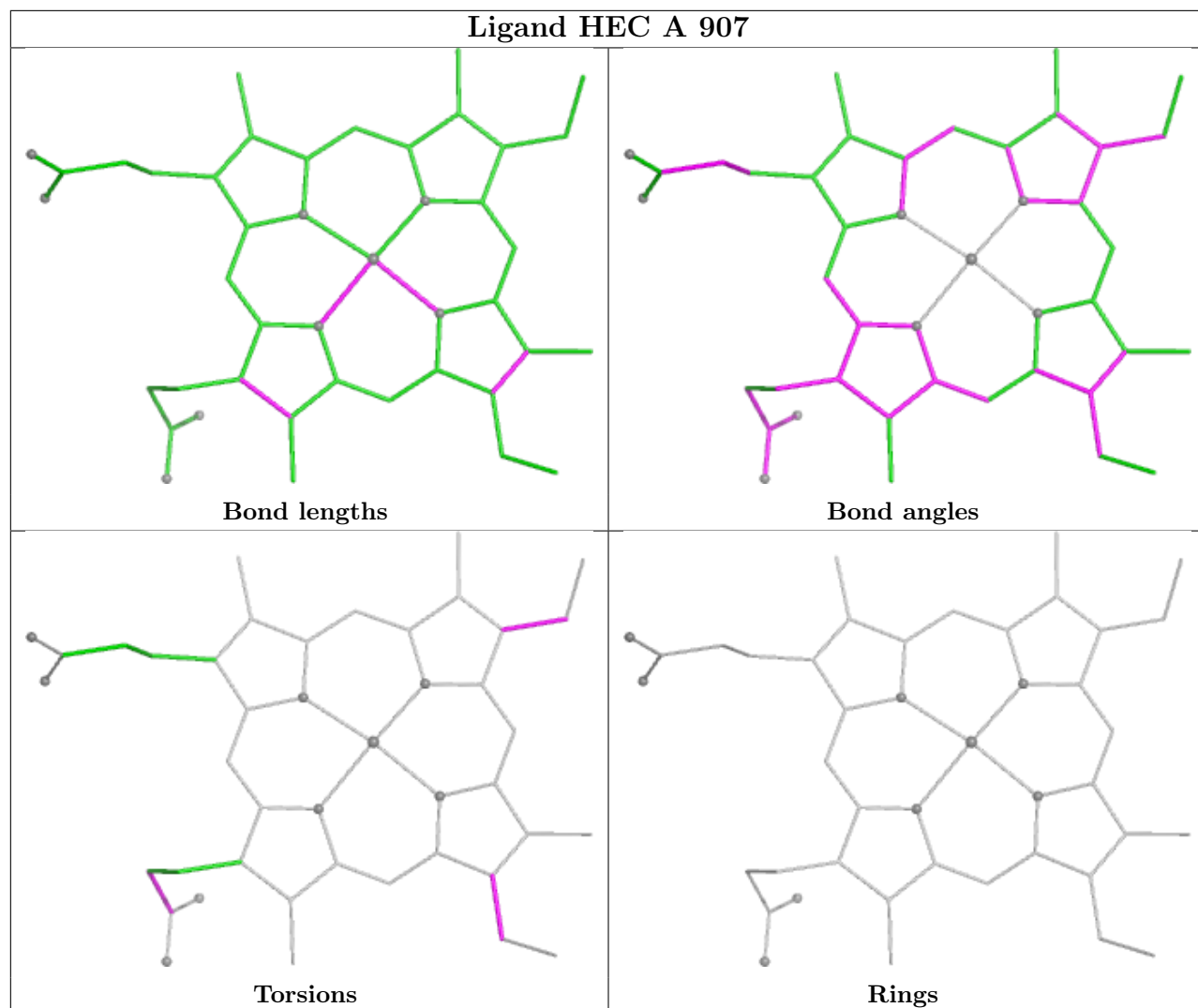


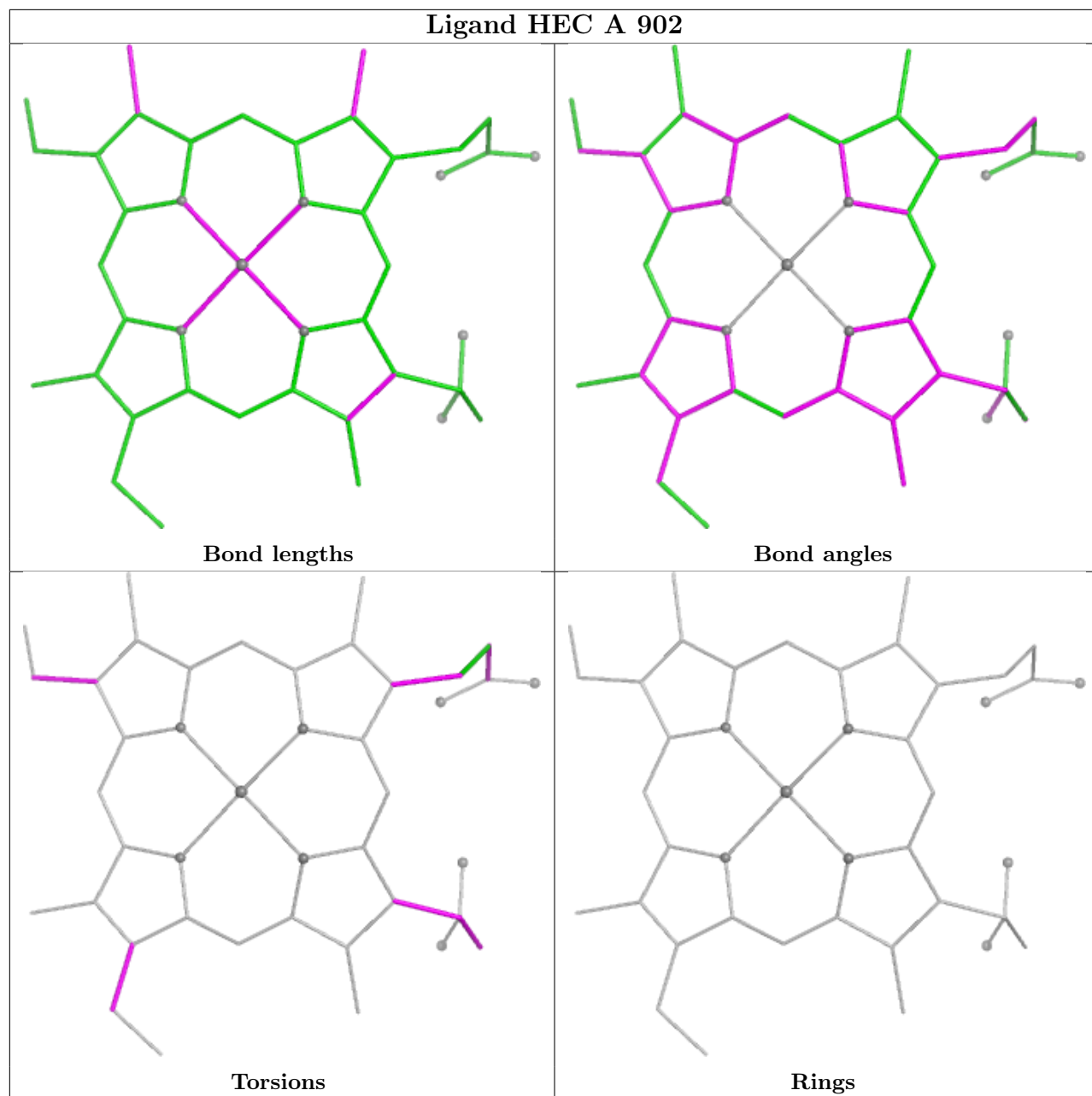
Ligand HEC C 803

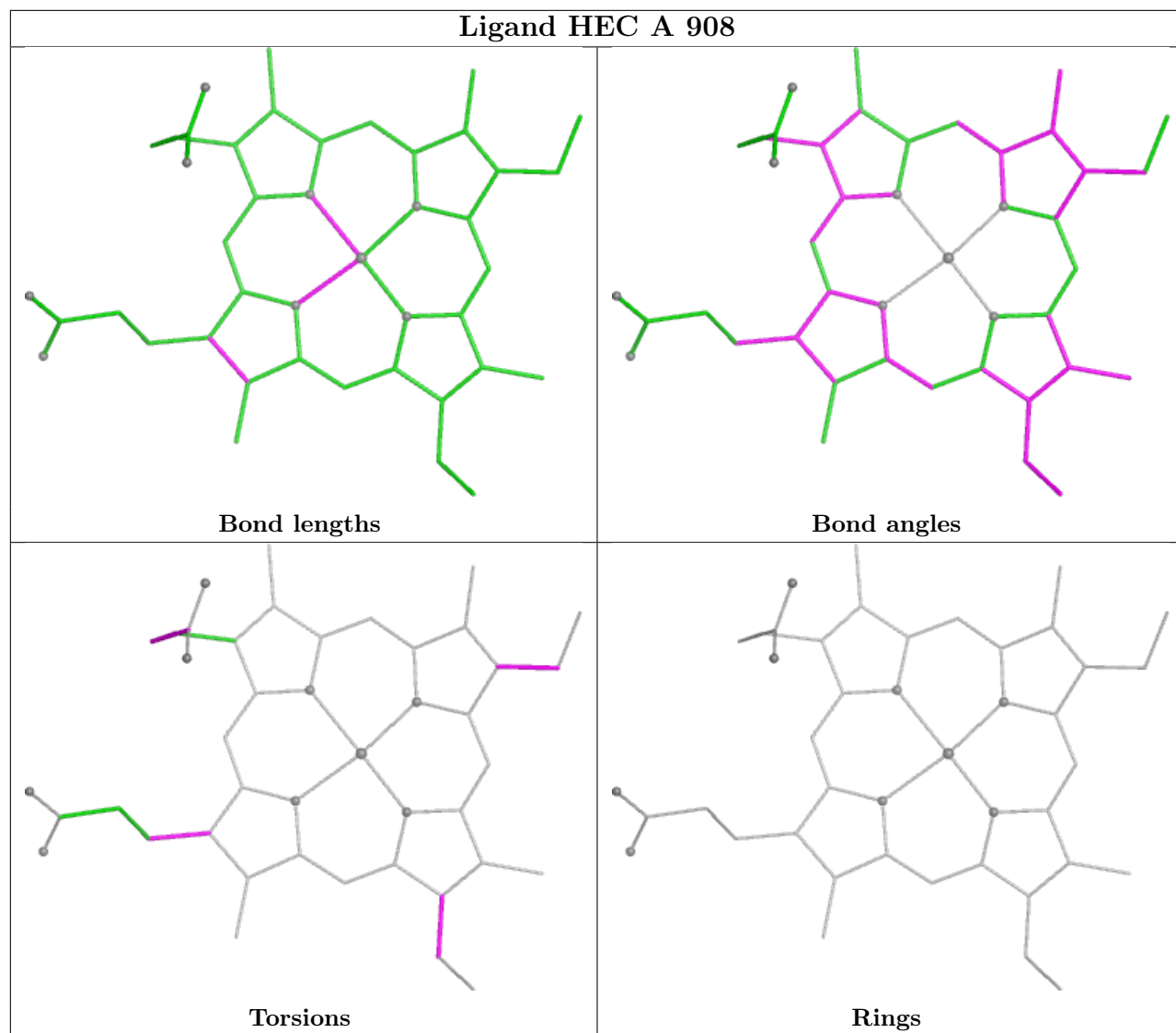


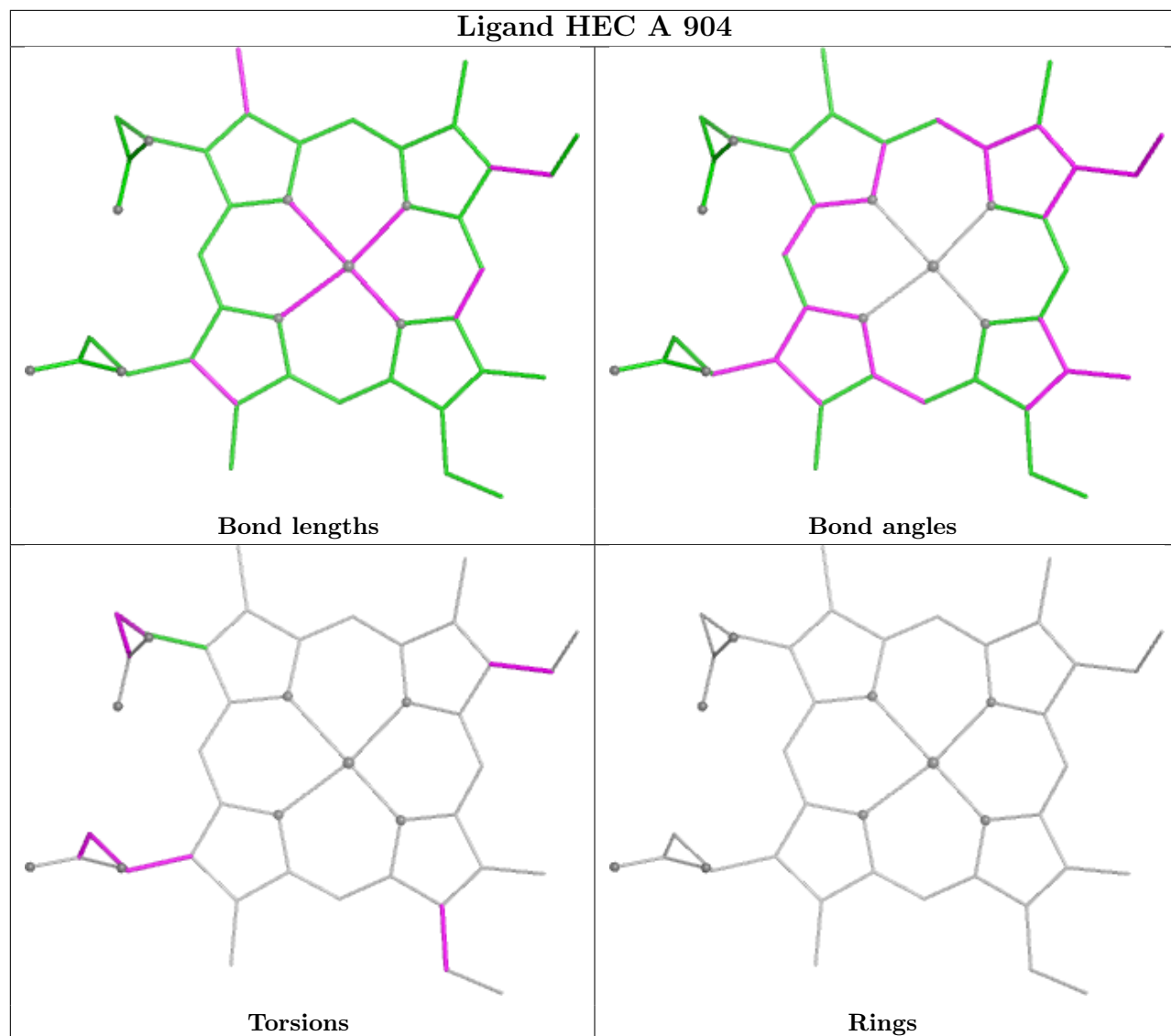


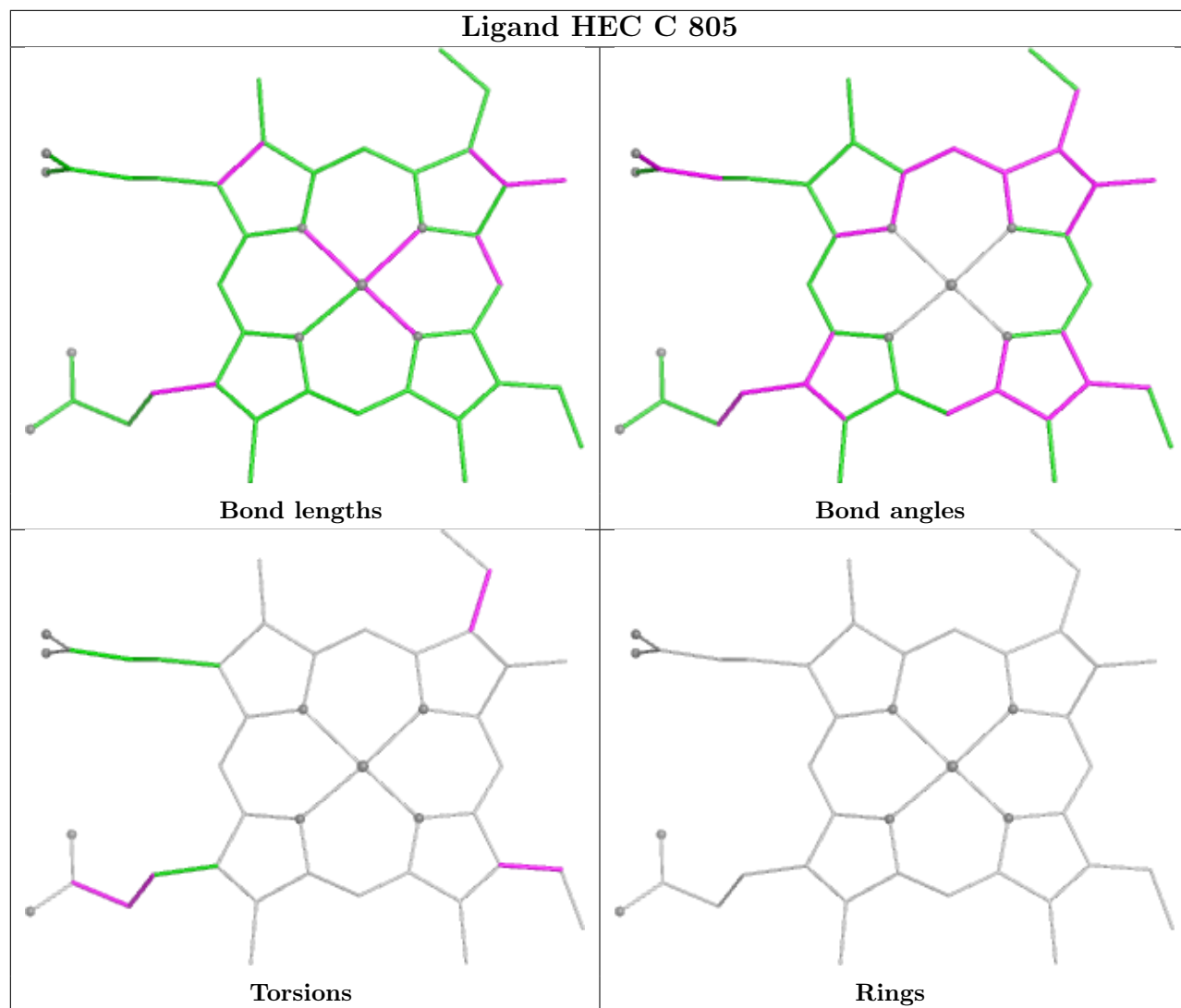




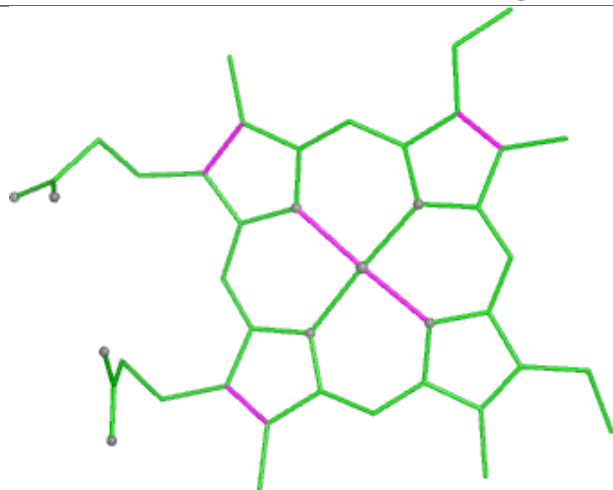




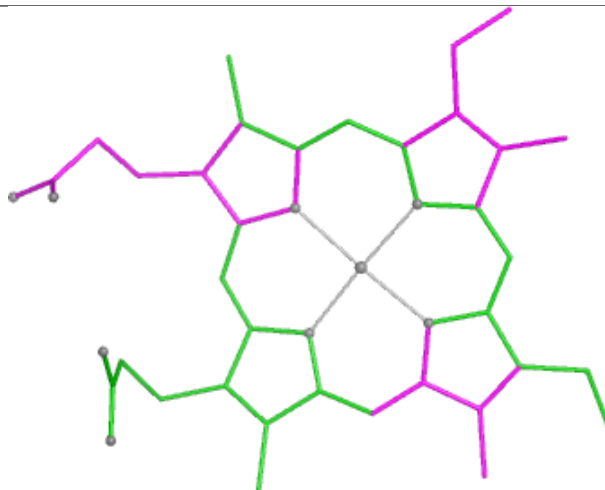




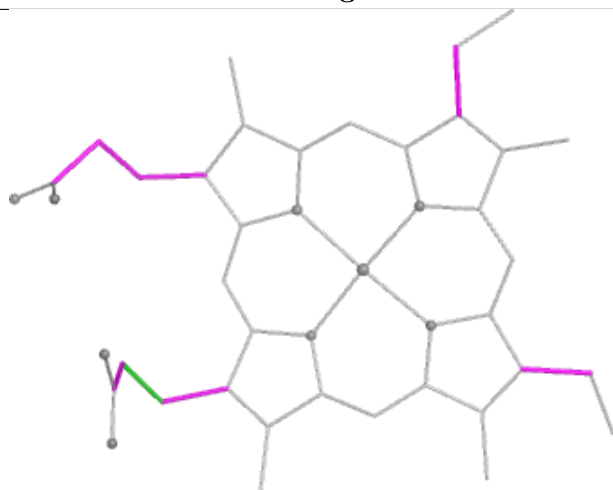
Ligand HEC C 806



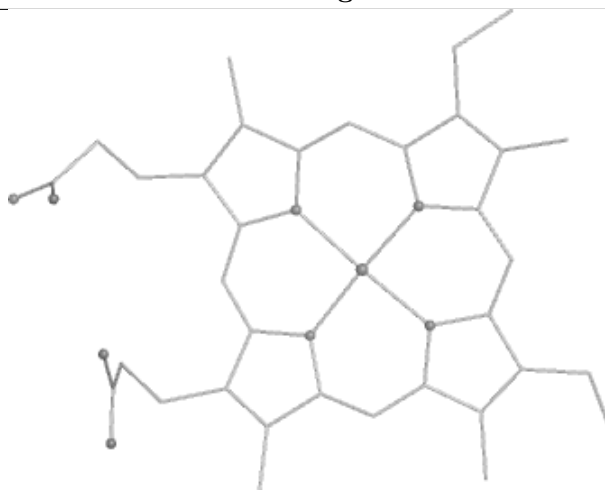
Bond lengths



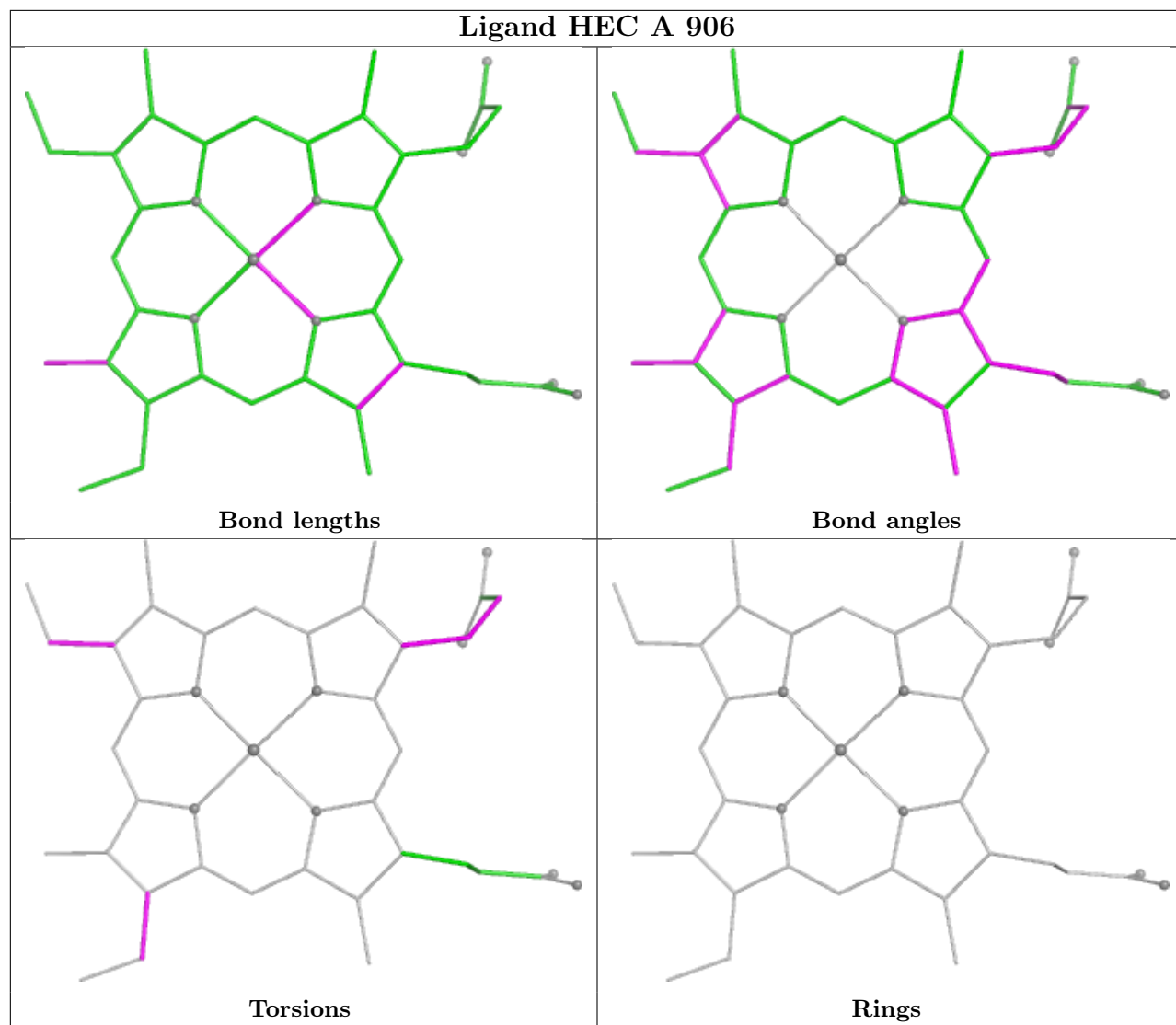
Bond angles

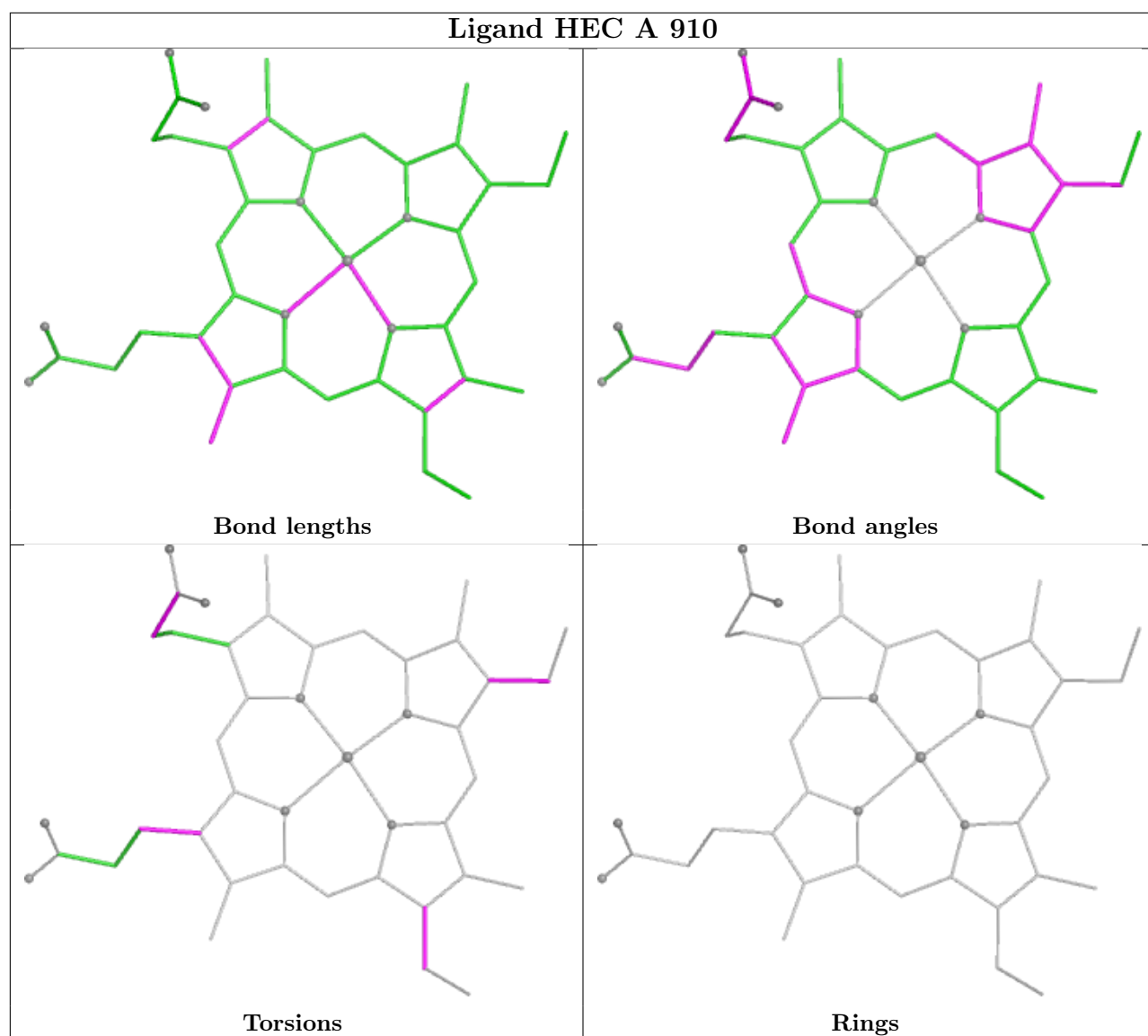


Torsions

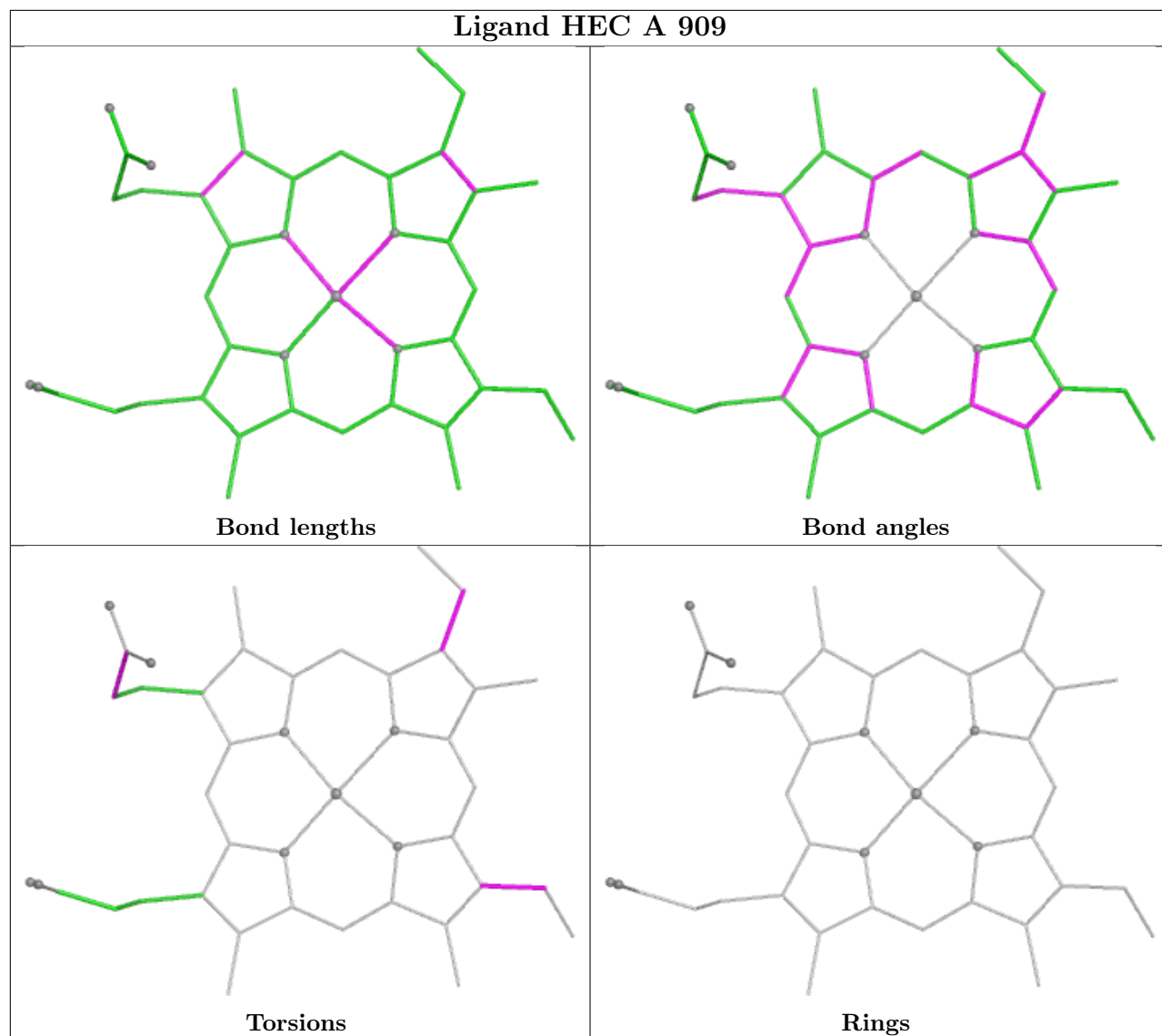


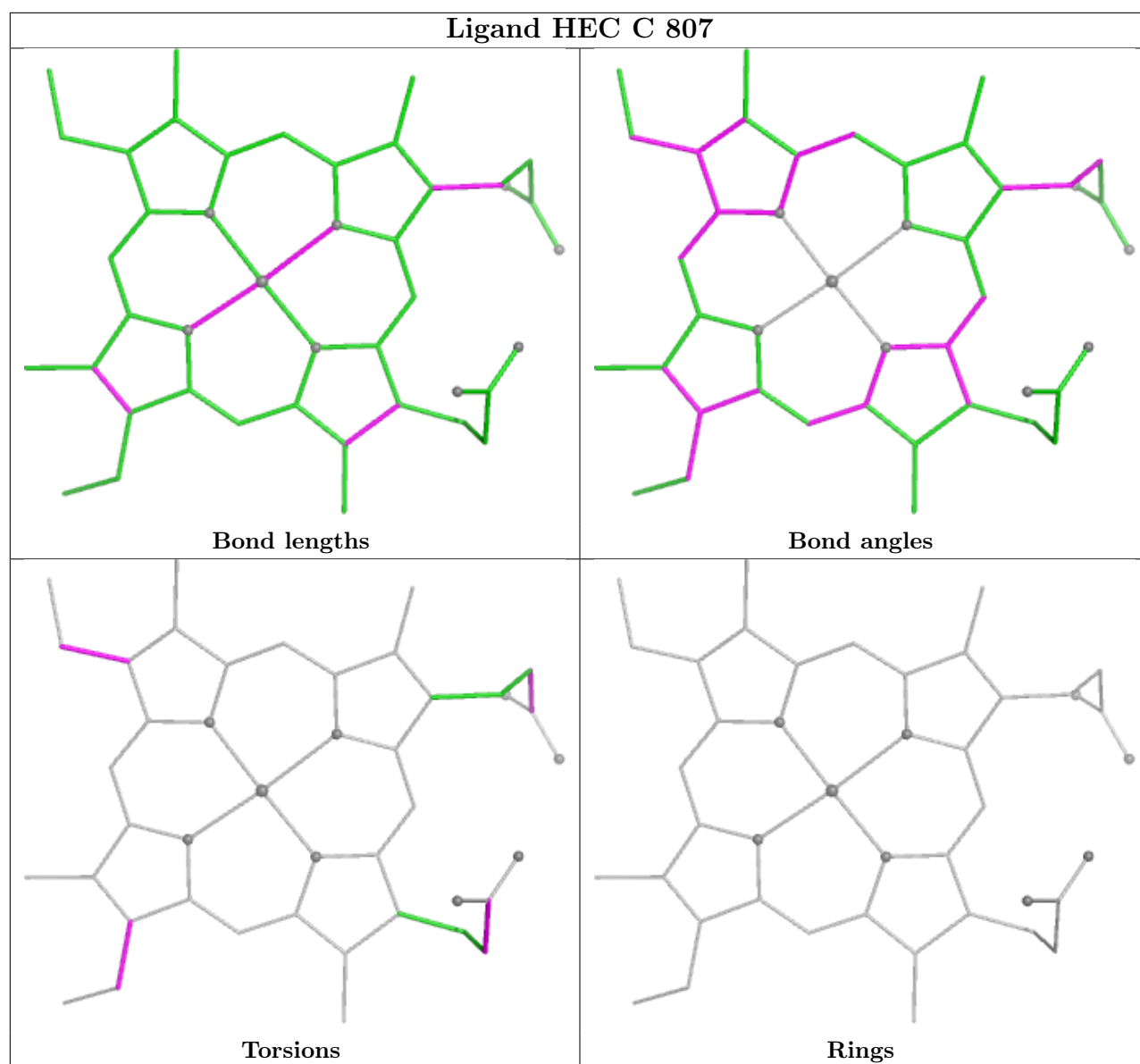
Rings





Ligand HEC A 909





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/333 (79%)	1.49	95 (35%) 1 0	19, 59, 150, 185	0
2	B	649/695 (93%)	0.86	94 (14%) 6 5	25, 58, 108, 175	0
3	C	608/650 (93%)	0.77	67 (11%) 10 9	22, 52, 102, 139	0
All	All	1522/1678 (90%)	0.93	256 (16%) 4 3	19, 56, 118, 185	0

The worst 5 of 256 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	PHE	7.2
1	A	121	PHE	6.9
1	A	165	GLN	6.5
2	B	542	ILE	6.5
1	A	107	LEU	6.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

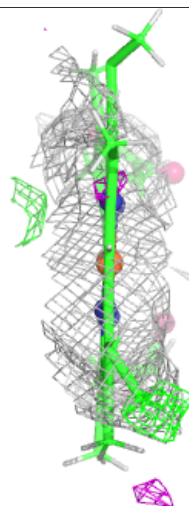
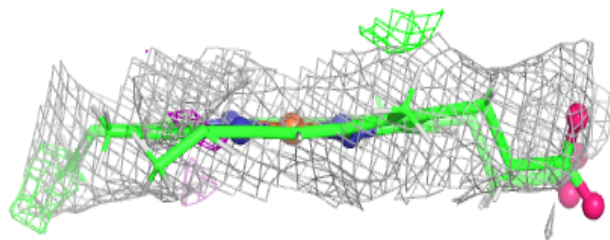
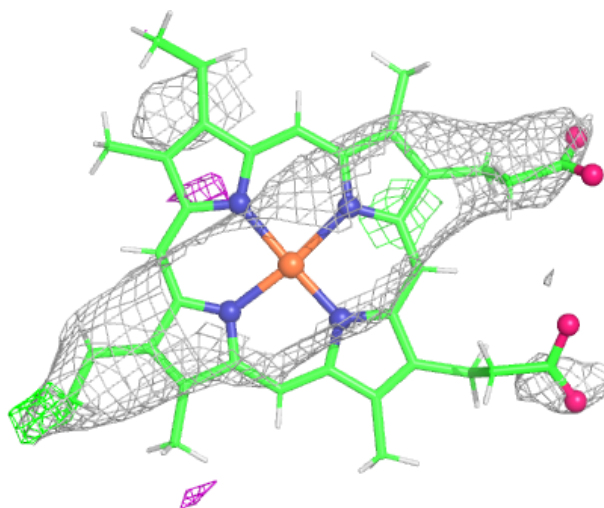
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HEC	A	901	43/43	0.75	0.24	107,155,190,192	0
4	HEC	A	902	43/43	0.87	0.19	73,116,143,154	0
4	HEC	A	903	43/43	0.91	0.18	58,100,125,126	0
4	HEC	A	904	43/43	0.93	0.15	50,77,110,115	0
4	HEC	C	809	43/43	0.94	0.15	29,53,104,130	0
4	HEC	C	810	43/43	0.94	0.15	46,67,101,116	0
5	CA	C	812	1/1	0.94	0.12	52,52,52,52	0
4	HEC	A	905	43/43	0.95	0.14	39,56,72,90	0
4	HEC	C	804	43/43	0.96	0.10	10,26,49,71	0
4	HEC	C	805	43/43	0.96	0.10	10,23,43,59	0
4	HEC	C	806	43/43	0.96	0.13	18,33,56,97	0
4	HEC	A	906	43/43	0.96	0.12	29,43,73,87	0
4	HEC	A	907	43/43	0.96	0.11	20,35,59,71	0
5	CA	B	701	1/1	0.96	0.14	47,47,47,47	0
5	CA	C	811	1/1	0.96	0.08	52,52,52,52	0
4	HEC	C	801	43/43	0.96	0.11	12,31,51,94	0
4	HEC	A	910	43/43	0.97	0.10	11,29,45,48	0
4	HEC	C	807	43/43	0.97	0.11	16,30,57,100	0
4	HEC	C	808	43/43	0.97	0.09	16,35,55,56	0
4	HEC	A	908	43/43	0.97	0.10	13,31,57,64	0
4	HEC	C	802	43/43	0.98	0.09	22,39,52,72	0
4	HEC	C	803	43/43	0.98	0.07	12,27,37,44	0
4	HEC	A	909	43/43	0.98	0.08	16,30,45,50	0
5	CA	B	702	1/1	0.99	0.04	28,28,28,28	0

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

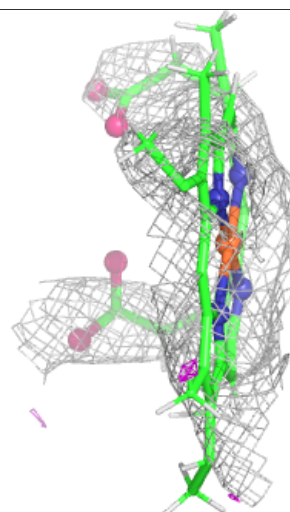
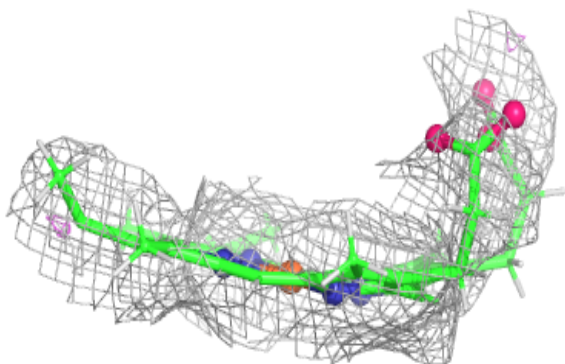
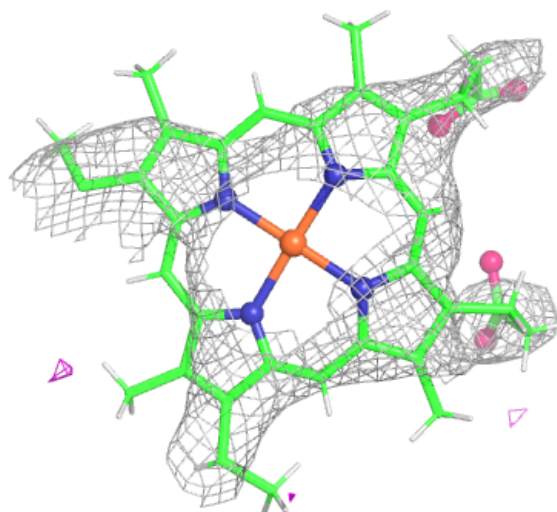
Electron density around HEC A 901:

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



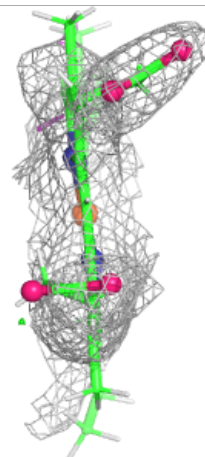
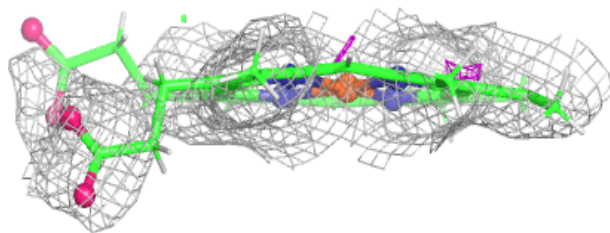
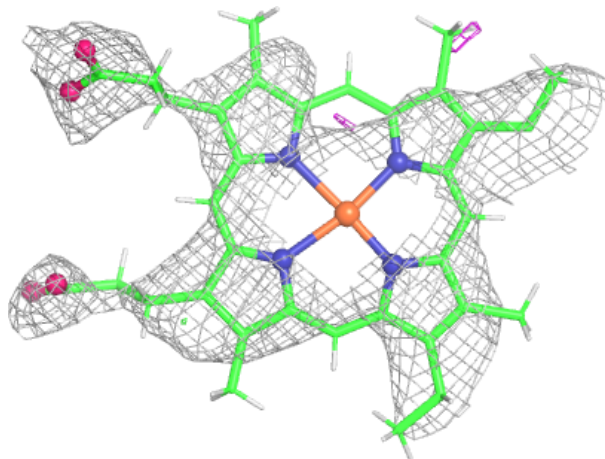
Electron density around HEC A 902:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



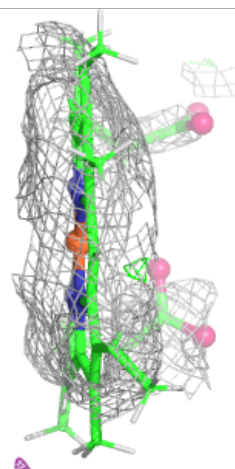
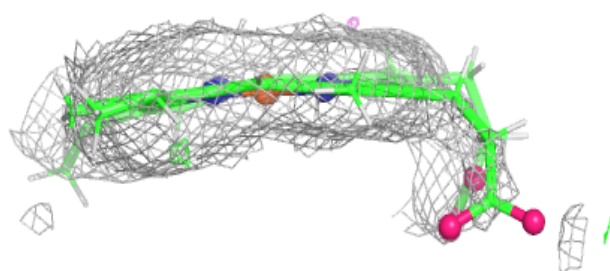
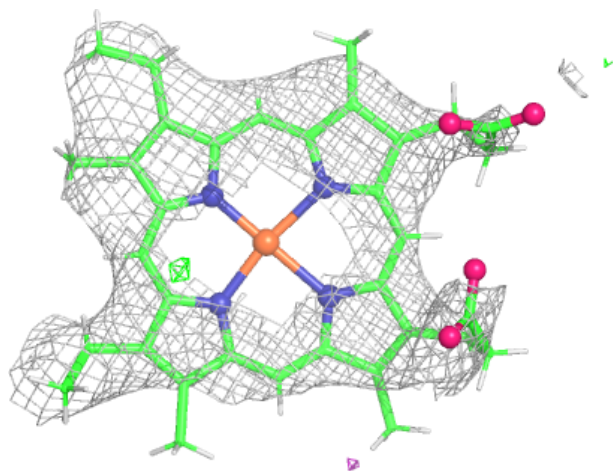
Electron density around HEC A 903:

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



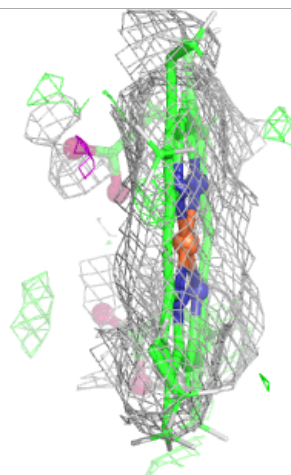
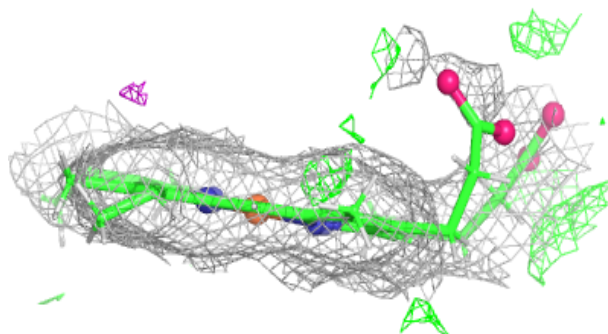
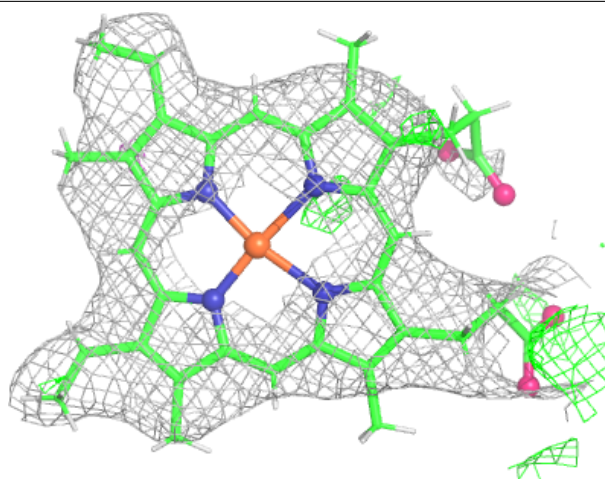
Electron density around HEC A 904:

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and green (positive)



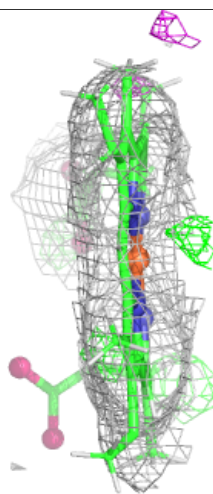
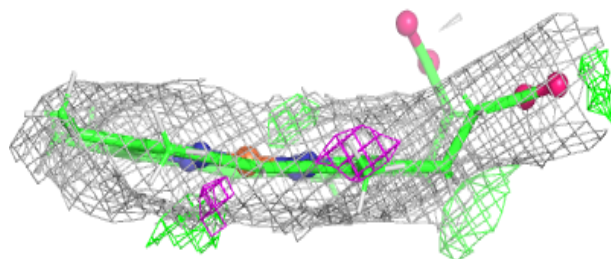
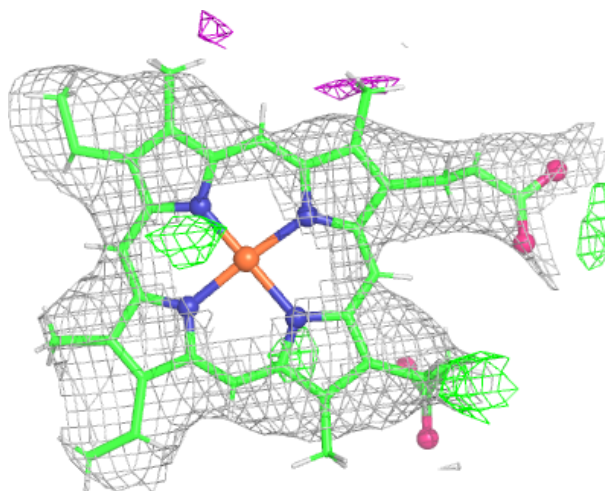
Electron density around HEC C 809:

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and green (positive)



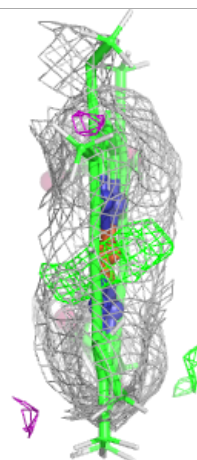
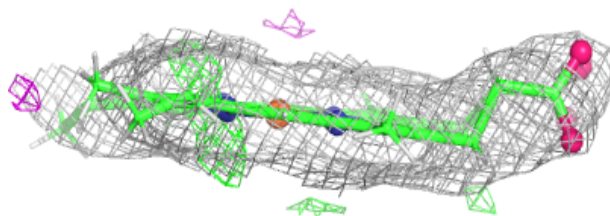
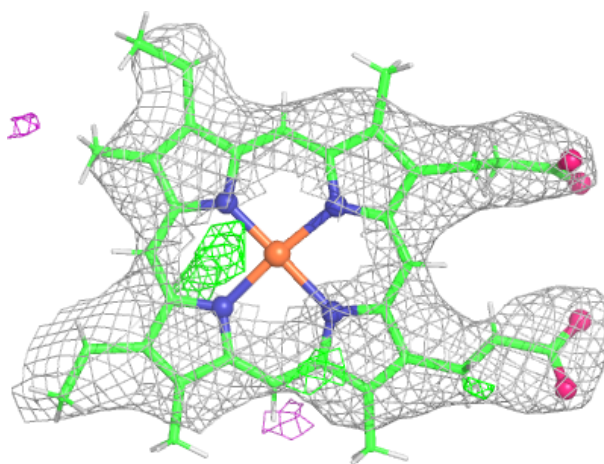
Electron density around HEC C 810:

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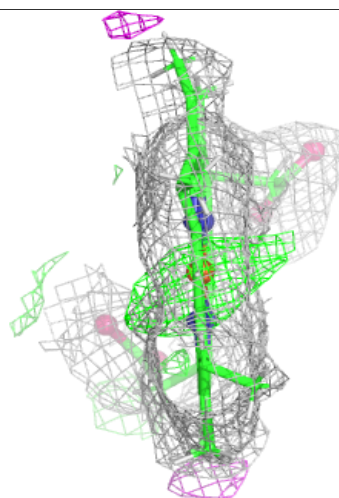
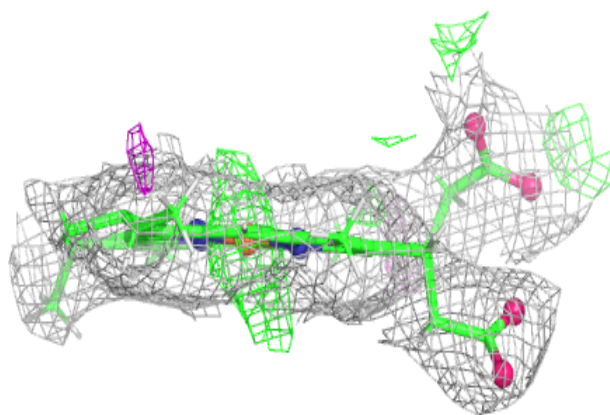
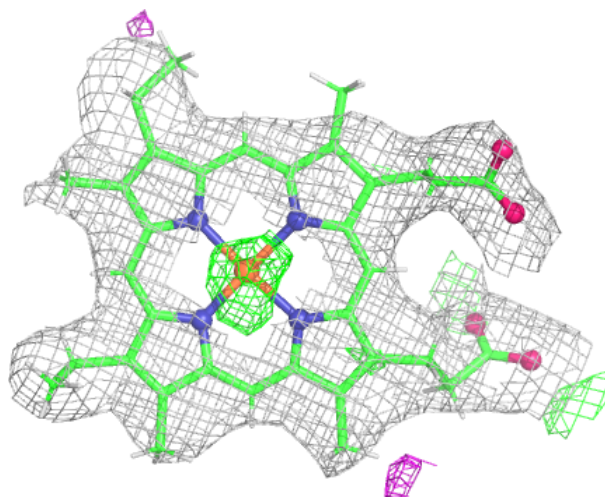
Electron density around HEC A 905:

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and green (positive)



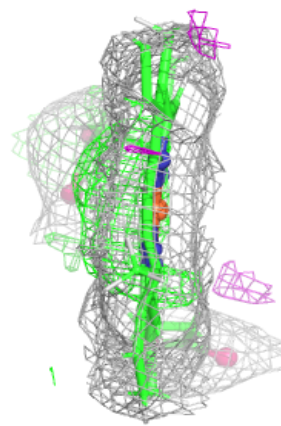
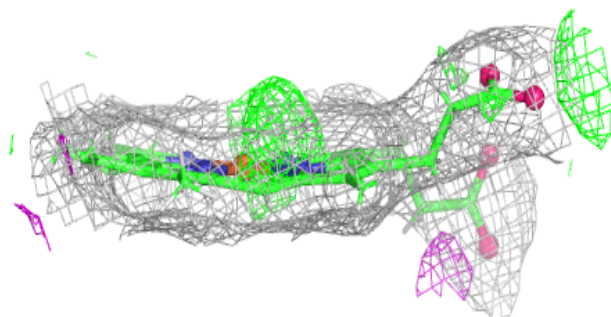
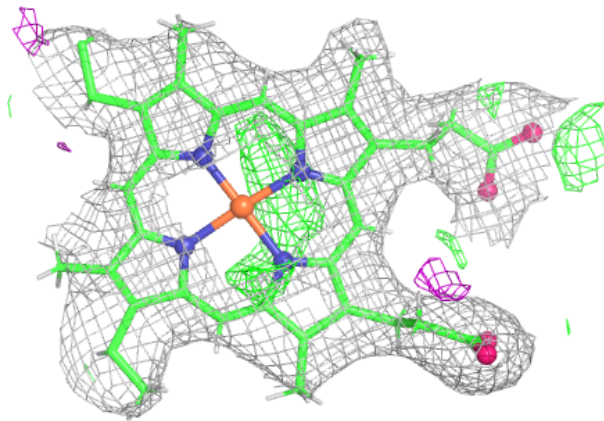
Electron density around HEC C 804:

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and green (positive)



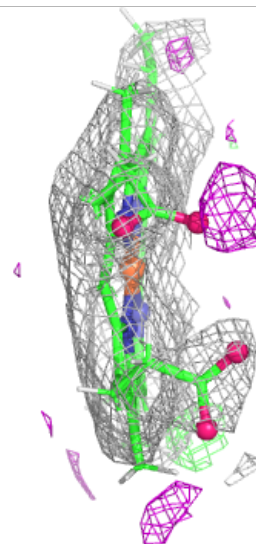
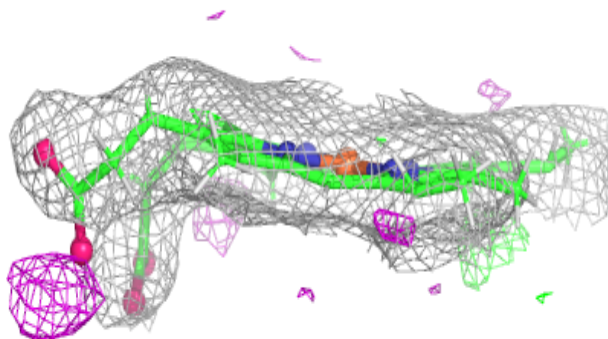
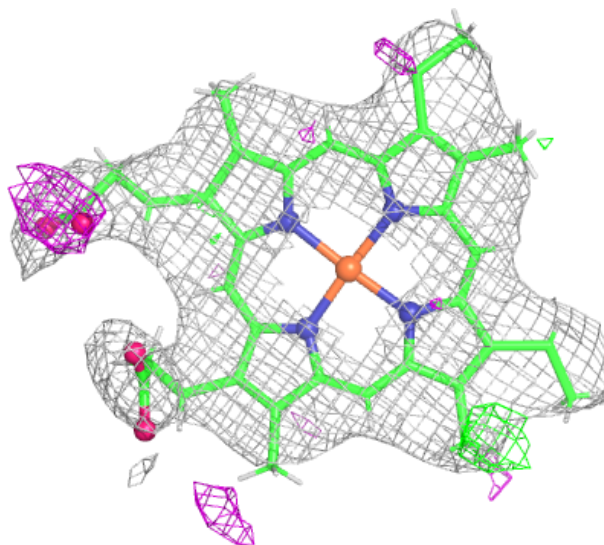
Electron density around HEC C 805:

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and green (positive)



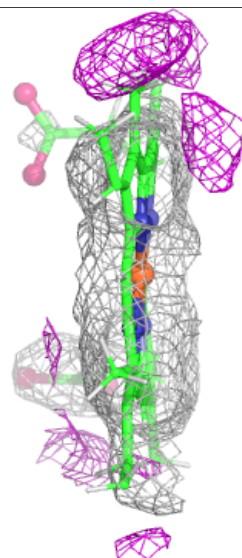
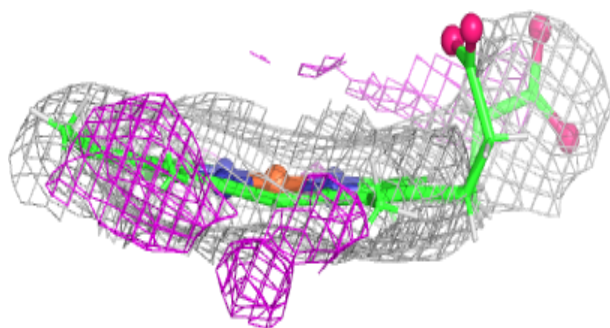
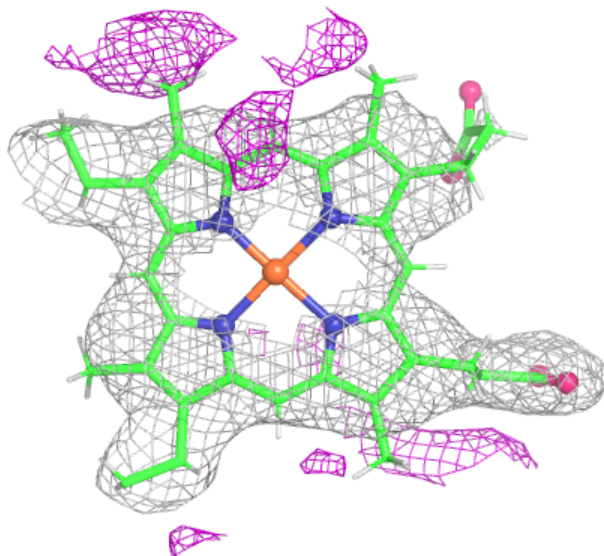
Electron density around HEC C 806:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



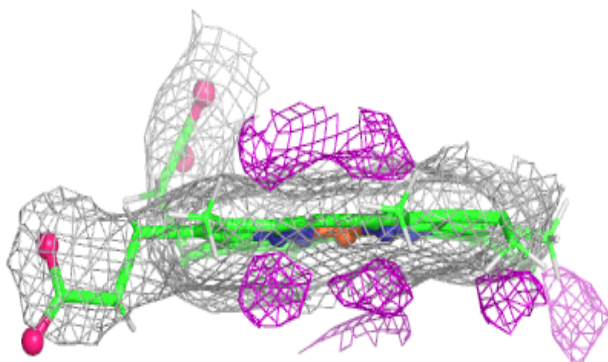
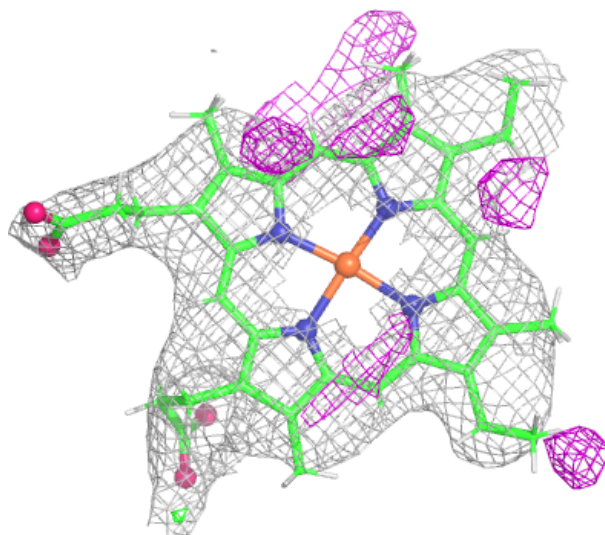
Electron density around HEC A 906:

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



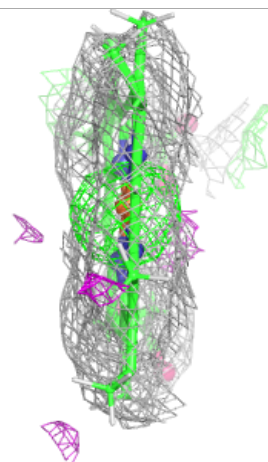
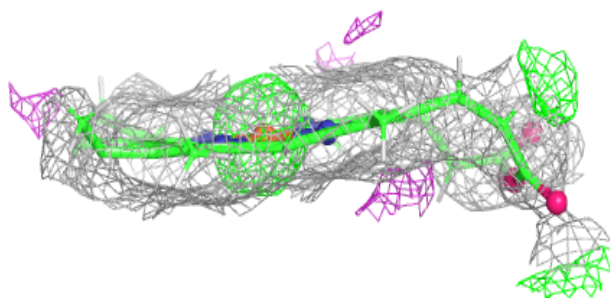
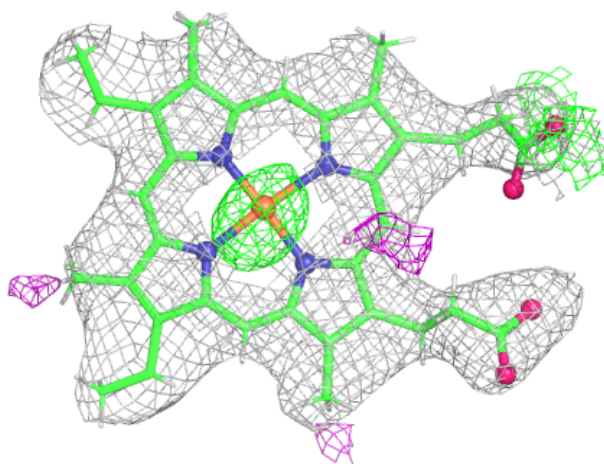
Electron density around HEC A 907:

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and green (positive)



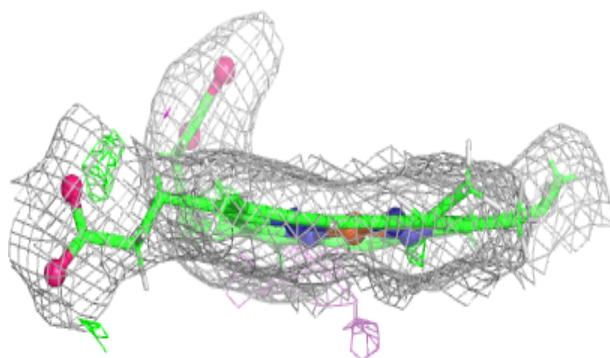
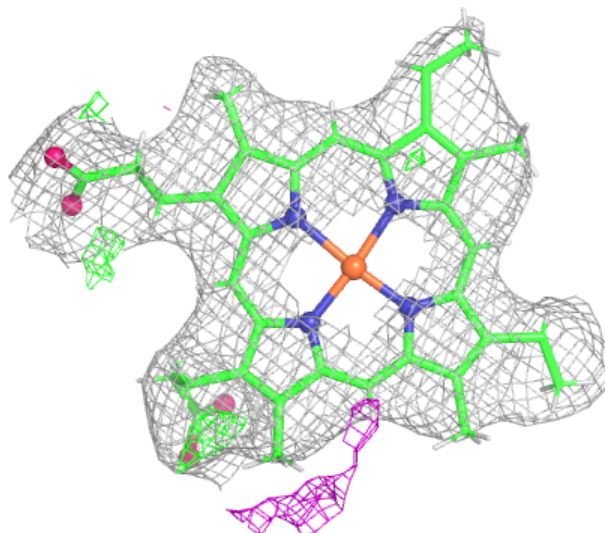
Electron density around HEC C 801:

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and green (positive)



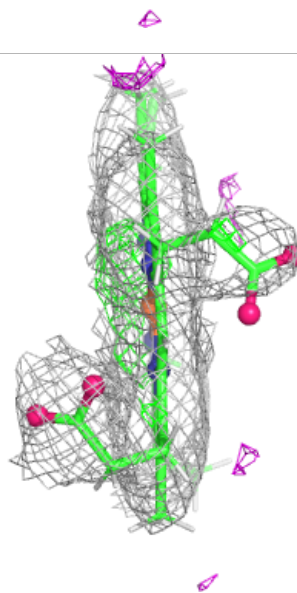
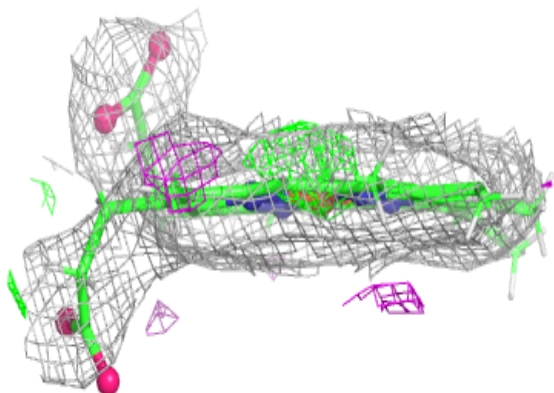
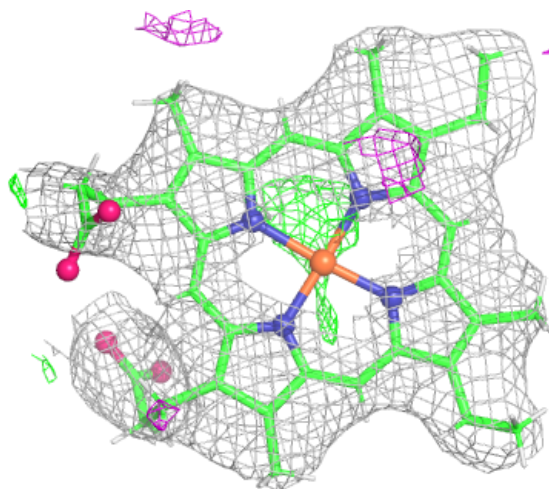
Electron density around HEC A 910:

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



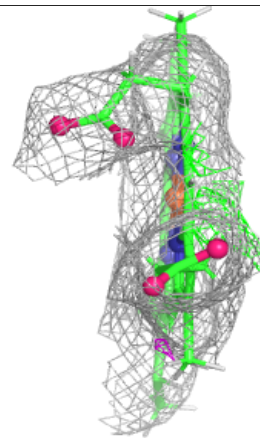
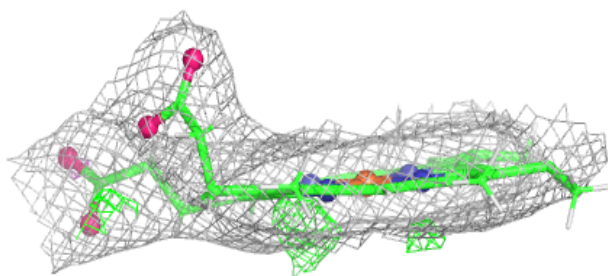
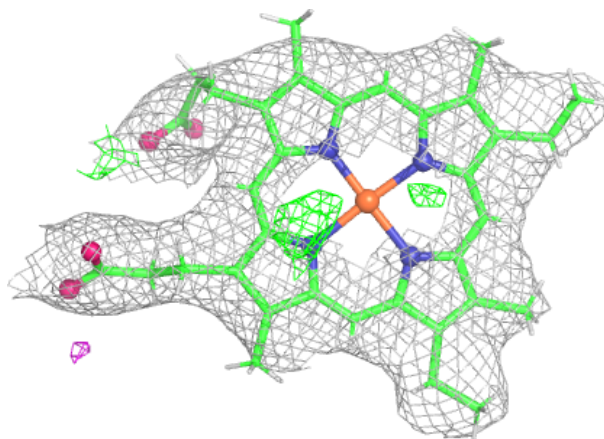
Electron density around HEC C 807:

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



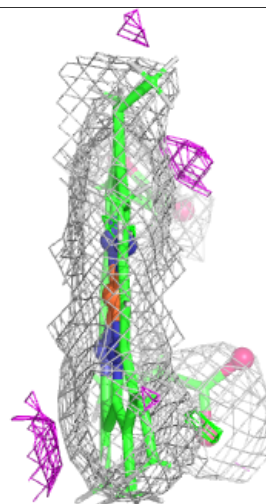
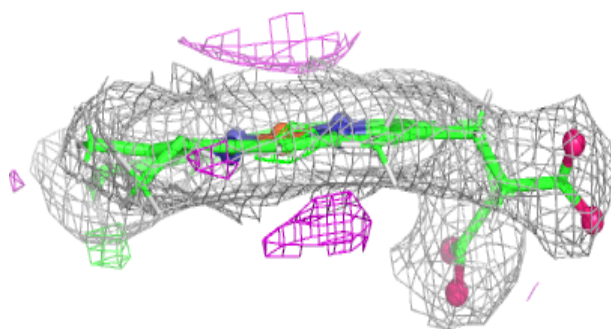
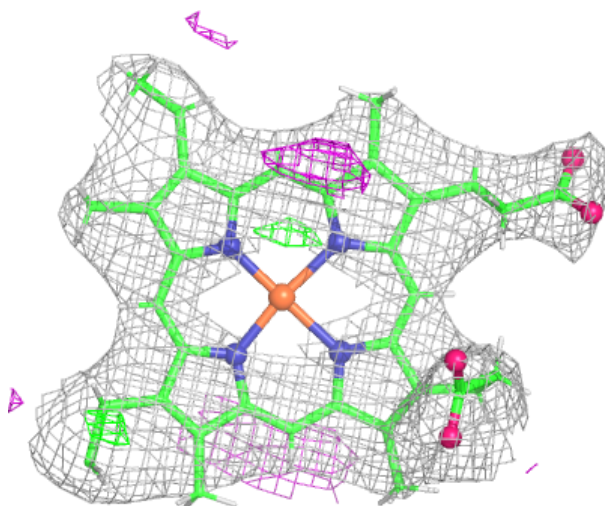
Electron density around HEC C 808:

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



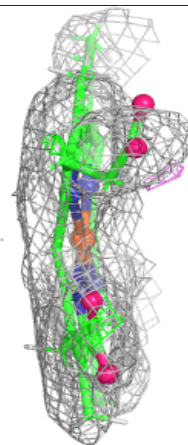
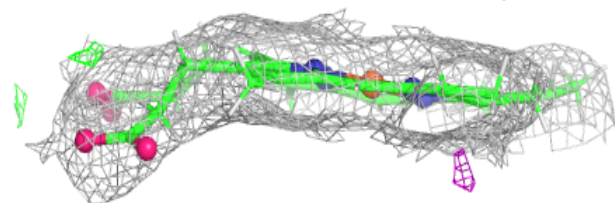
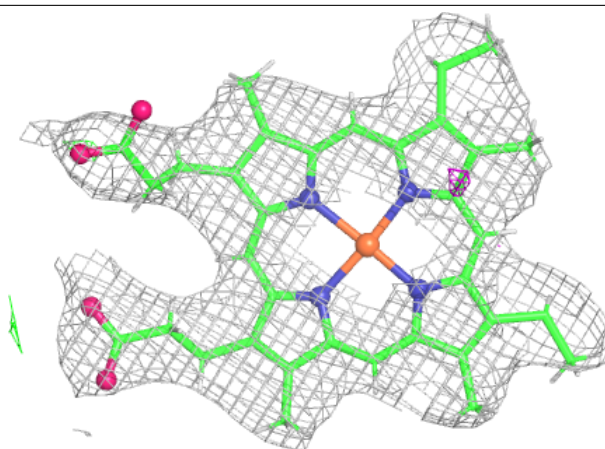
Electron density around HEC A 908:

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



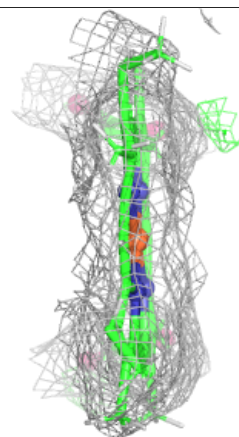
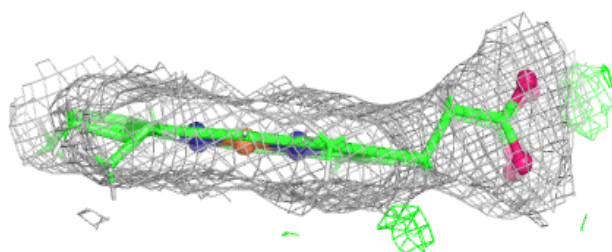
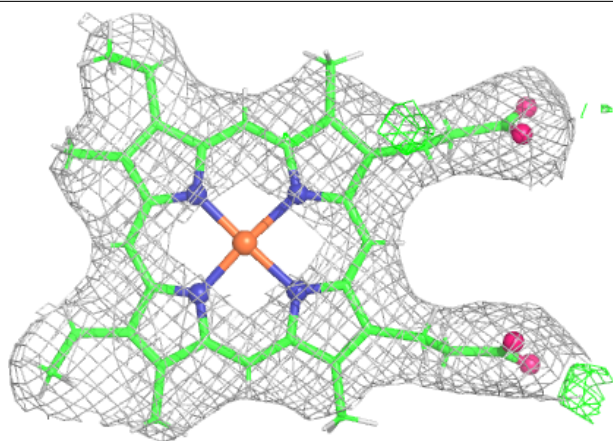
Electron density around HEC C 802:

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



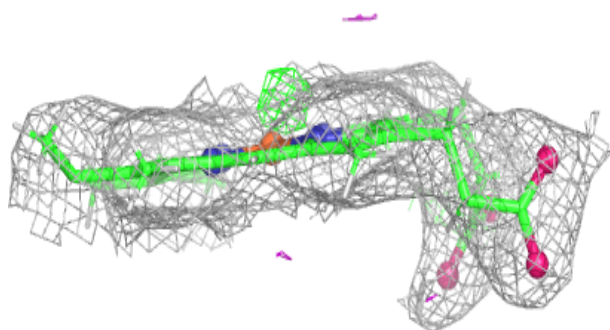
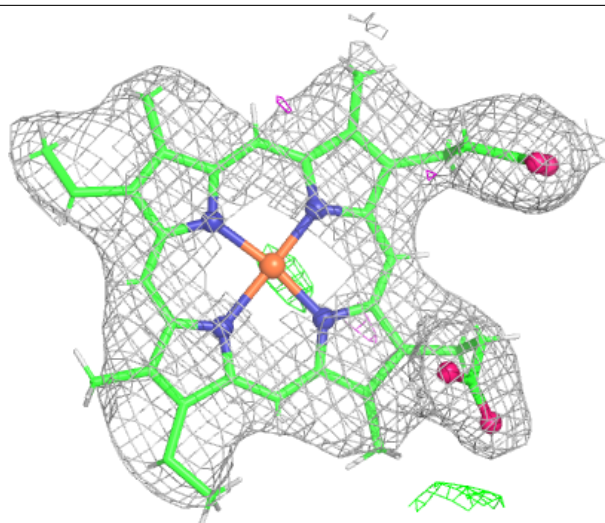
Electron density around HEC C 803:

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



Electron density around HEC A 909:

$2mF_o-DF_c$ (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.