



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:16 PM EDT

PDB ID : 4RKN / pdb_00004rkn
Title : Wolinella succinogenes octaheme sulfite reductase MccA, form II
Authors : Hermann, B.; Kern, M.; La Pietra, L.; Simon, J.; Einsle, O.
Deposited on : 2014-10-13
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	2022.3.0, CSD as543be (2022)
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

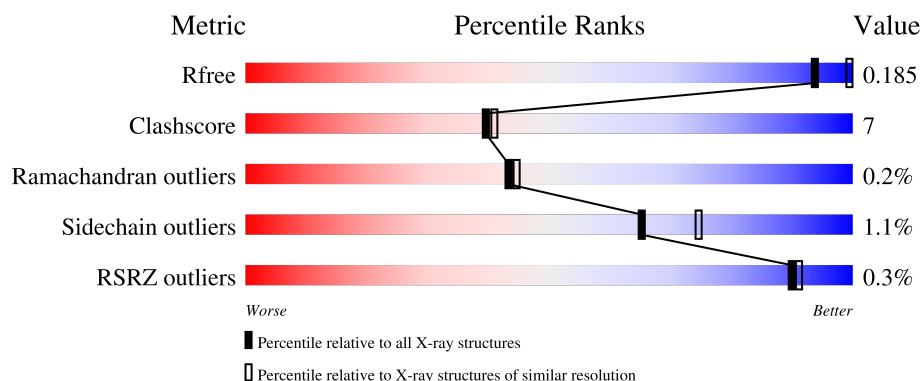
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	732	 83% 7% 10%
1	B	732	 85% 5% 10%
1	C	732	 84% 6% 10%
1	D	732	 82% 7% 10%

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
5	SO3	D	912	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23997 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 MccA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	3	0
			5250	3299	923	991	37			
1	B	660	Total	C	N	O	S	0	3	0
			5246	3295	923	991	37			
1	C	659	Total	C	N	O	S	0	3	0
			5240	3292	922	989	37			
1	D	660	Total	C	N	O	S	0	2	0
			5240	3291	922	990	37			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	691	SER	-	expression tag	UNP Q7MSJ8
A	692	ALA	-	expression tag	UNP Q7MSJ8
A	693	TRP	-	expression tag	UNP Q7MSJ8
A	694	SER	-	expression tag	UNP Q7MSJ8
A	695	HIS	-	expression tag	UNP Q7MSJ8
A	696	PRO	-	expression tag	UNP Q7MSJ8
A	697	GLN	-	expression tag	UNP Q7MSJ8
A	698	PHE	-	expression tag	UNP Q7MSJ8
A	699	GLU	-	expression tag	UNP Q7MSJ8
A	700	LYS	-	expression tag	UNP Q7MSJ8
A	701	GLY	-	expression tag	UNP Q7MSJ8
A	702	GLY	-	expression tag	UNP Q7MSJ8
A	703	GLY	-	expression tag	UNP Q7MSJ8
A	704	SER	-	expression tag	UNP Q7MSJ8
A	705	GLY	-	expression tag	UNP Q7MSJ8
A	706	GLY	-	expression tag	UNP Q7MSJ8
A	707	GLY	-	expression tag	UNP Q7MSJ8
A	708	SER	-	expression tag	UNP Q7MSJ8
A	709	GLY	-	expression tag	UNP Q7MSJ8
A	710	GLY	-	expression tag	UNP Q7MSJ8
A	711	SER	-	expression tag	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	712	ALA	-	expression tag	UNP Q7MSJ8
A	713	TRP	-	expression tag	UNP Q7MSJ8
A	714	SER	-	expression tag	UNP Q7MSJ8
A	715	HIS	-	expression tag	UNP Q7MSJ8
A	716	PRO	-	expression tag	UNP Q7MSJ8
A	717	GLN	-	expression tag	UNP Q7MSJ8
A	718	PHE	-	expression tag	UNP Q7MSJ8
A	719	GLU	-	expression tag	UNP Q7MSJ8
A	720	LYS	-	expression tag	UNP Q7MSJ8
B	691	SER	-	expression tag	UNP Q7MSJ8
B	692	ALA	-	expression tag	UNP Q7MSJ8
B	693	TRP	-	expression tag	UNP Q7MSJ8
B	694	SER	-	expression tag	UNP Q7MSJ8
B	695	HIS	-	expression tag	UNP Q7MSJ8
B	696	PRO	-	expression tag	UNP Q7MSJ8
B	697	GLN	-	expression tag	UNP Q7MSJ8
B	698	PHE	-	expression tag	UNP Q7MSJ8
B	699	GLU	-	expression tag	UNP Q7MSJ8
B	700	LYS	-	expression tag	UNP Q7MSJ8
B	701	GLY	-	expression tag	UNP Q7MSJ8
B	702	GLY	-	expression tag	UNP Q7MSJ8
B	703	GLY	-	expression tag	UNP Q7MSJ8
B	704	SER	-	expression tag	UNP Q7MSJ8
B	705	GLY	-	expression tag	UNP Q7MSJ8
B	706	GLY	-	expression tag	UNP Q7MSJ8
B	707	GLY	-	expression tag	UNP Q7MSJ8
B	708	SER	-	expression tag	UNP Q7MSJ8
B	709	GLY	-	expression tag	UNP Q7MSJ8
B	710	GLY	-	expression tag	UNP Q7MSJ8
B	711	SER	-	expression tag	UNP Q7MSJ8
B	712	ALA	-	expression tag	UNP Q7MSJ8
B	713	TRP	-	expression tag	UNP Q7MSJ8
B	714	SER	-	expression tag	UNP Q7MSJ8
B	715	HIS	-	expression tag	UNP Q7MSJ8
B	716	PRO	-	expression tag	UNP Q7MSJ8
B	717	GLN	-	expression tag	UNP Q7MSJ8
B	718	PHE	-	expression tag	UNP Q7MSJ8
B	719	GLU	-	expression tag	UNP Q7MSJ8
B	720	LYS	-	expression tag	UNP Q7MSJ8
C	691	SER	-	expression tag	UNP Q7MSJ8
C	692	ALA	-	expression tag	UNP Q7MSJ8
C	693	TRP	-	expression tag	UNP Q7MSJ8

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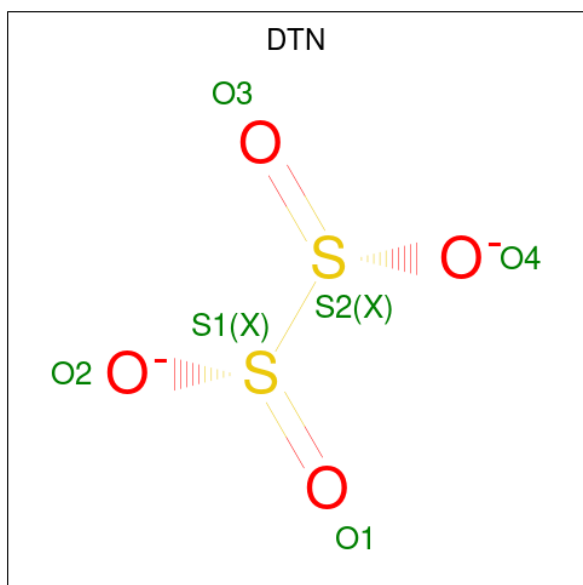
Chain	Residue	Modelled	Actual	Comment	Reference
C	694	SER	-	expression tag	UNP Q7MSJ8
C	695	HIS	-	expression tag	UNP Q7MSJ8
C	696	PRO	-	expression tag	UNP Q7MSJ8
C	697	GLN	-	expression tag	UNP Q7MSJ8
C	698	PHE	-	expression tag	UNP Q7MSJ8
C	699	GLU	-	expression tag	UNP Q7MSJ8
C	700	LYS	-	expression tag	UNP Q7MSJ8
C	701	GLY	-	expression tag	UNP Q7MSJ8
C	702	GLY	-	expression tag	UNP Q7MSJ8
C	703	GLY	-	expression tag	UNP Q7MSJ8
C	704	SER	-	expression tag	UNP Q7MSJ8
C	705	GLY	-	expression tag	UNP Q7MSJ8
C	706	GLY	-	expression tag	UNP Q7MSJ8
C	707	GLY	-	expression tag	UNP Q7MSJ8
C	708	SER	-	expression tag	UNP Q7MSJ8
C	709	GLY	-	expression tag	UNP Q7MSJ8
C	710	GLY	-	expression tag	UNP Q7MSJ8
C	711	SER	-	expression tag	UNP Q7MSJ8
C	712	ALA	-	expression tag	UNP Q7MSJ8
C	713	TRP	-	expression tag	UNP Q7MSJ8
C	714	SER	-	expression tag	UNP Q7MSJ8
C	715	HIS	-	expression tag	UNP Q7MSJ8
C	716	PRO	-	expression tag	UNP Q7MSJ8
C	717	GLN	-	expression tag	UNP Q7MSJ8
C	718	PHE	-	expression tag	UNP Q7MSJ8
C	719	GLU	-	expression tag	UNP Q7MSJ8
C	720	LYS	-	expression tag	UNP Q7MSJ8
D	691	SER	-	expression tag	UNP Q7MSJ8
D	692	ALA	-	expression tag	UNP Q7MSJ8
D	693	TRP	-	expression tag	UNP Q7MSJ8
D	694	SER	-	expression tag	UNP Q7MSJ8
D	695	HIS	-	expression tag	UNP Q7MSJ8
D	696	PRO	-	expression tag	UNP Q7MSJ8
D	697	GLN	-	expression tag	UNP Q7MSJ8
D	698	PHE	-	expression tag	UNP Q7MSJ8
D	699	GLU	-	expression tag	UNP Q7MSJ8
D	700	LYS	-	expression tag	UNP Q7MSJ8
D	701	GLY	-	expression tag	UNP Q7MSJ8
D	702	GLY	-	expression tag	UNP Q7MSJ8
D	703	GLY	-	expression tag	UNP Q7MSJ8
D	704	SER	-	expression tag	UNP Q7MSJ8
D	705	GLY	-	expression tag	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	706	GLY	-	expression tag	UNP Q7MSJ8
D	707	GLY	-	expression tag	UNP Q7MSJ8
D	708	SER	-	expression tag	UNP Q7MSJ8
D	709	GLY	-	expression tag	UNP Q7MSJ8
D	710	GLY	-	expression tag	UNP Q7MSJ8
D	711	SER	-	expression tag	UNP Q7MSJ8
D	712	ALA	-	expression tag	UNP Q7MSJ8
D	713	TRP	-	expression tag	UNP Q7MSJ8
D	714	SER	-	expression tag	UNP Q7MSJ8
D	715	HIS	-	expression tag	UNP Q7MSJ8
D	716	PRO	-	expression tag	UNP Q7MSJ8
D	717	GLN	-	expression tag	UNP Q7MSJ8
D	718	PHE	-	expression tag	UNP Q7MSJ8
D	719	GLU	-	expression tag	UNP Q7MSJ8
D	720	LYS	-	expression tag	UNP Q7MSJ8

- Molecule 2 is DITHIONITE (CCD ID: DTN) (formula: O₄S₂).



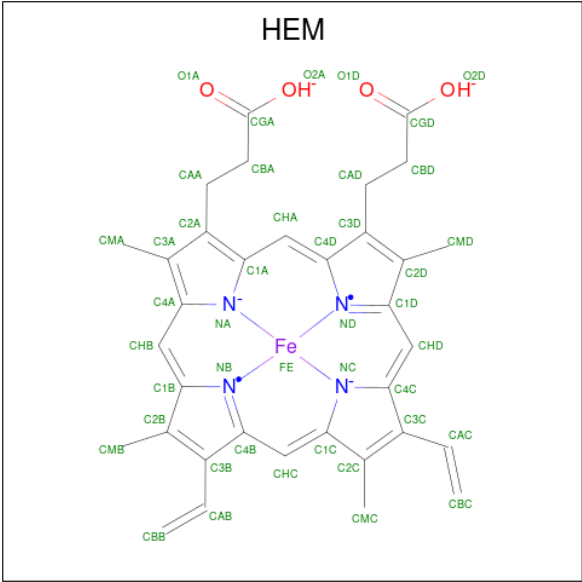
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			6	4	2		
2	A	1	Total	O	S	0	0
			6	4	2		
2	B	1	Total	O	S	0	0
			6	4	2		
2	C	1	Total	O	S	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			6	4	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 86	C 68	Fe 2	N 8	O 8	0	1
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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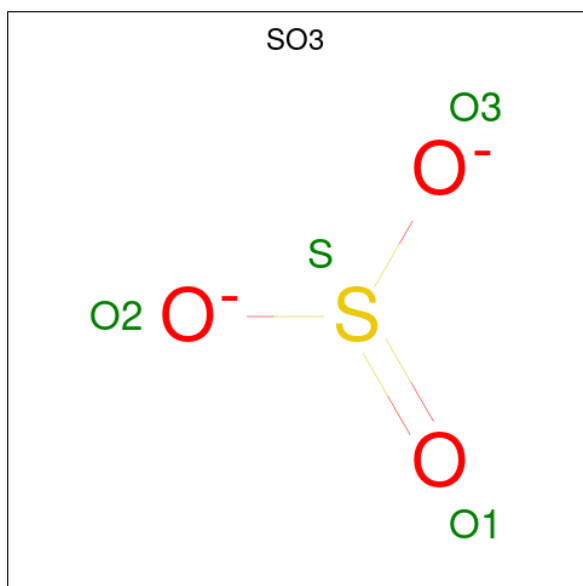
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		
4	B	1	Total	Cu	0	0
			1	1		
4	C	1	Total	Cu	0	0
			1	1		
4	D	1	Total	Cu	0	0
			1	1		

- Molecule 5 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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

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

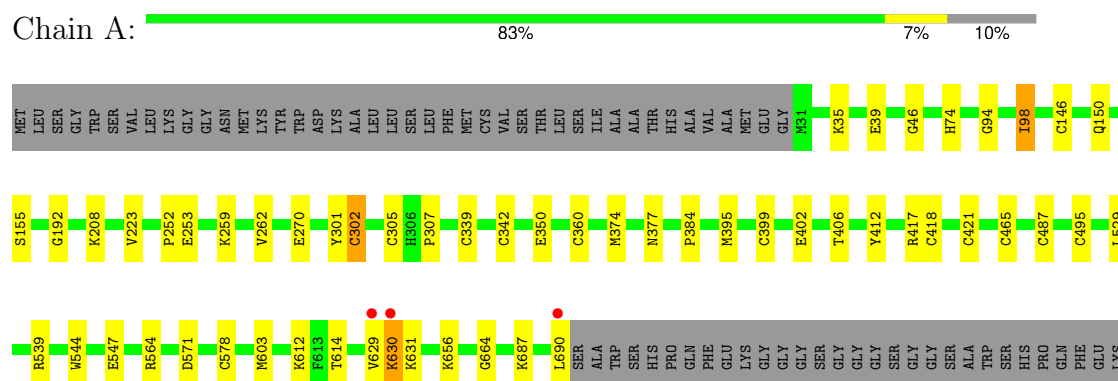
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	335	Total	O	0	0
			335	335		
6	B	355	Total	O	0	0
			355	355		
6	C	312	Total	O	0	0
			312	312		
6	D	417	Total	O	0	0
			417	417		

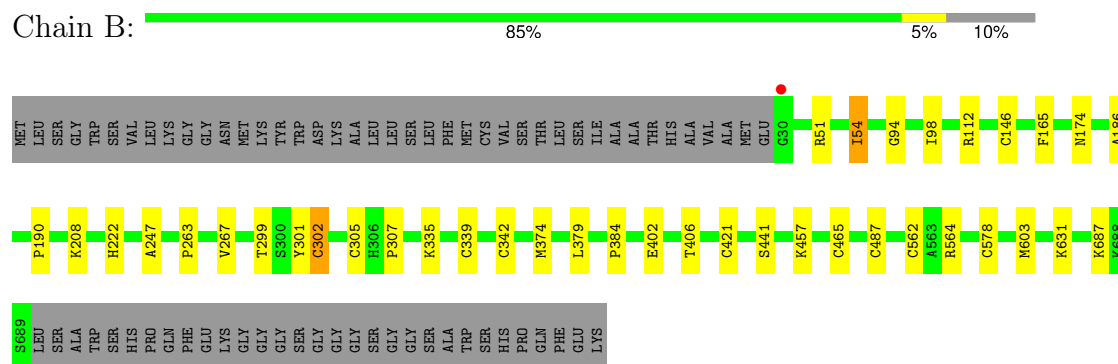
3 Residue-property plots

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

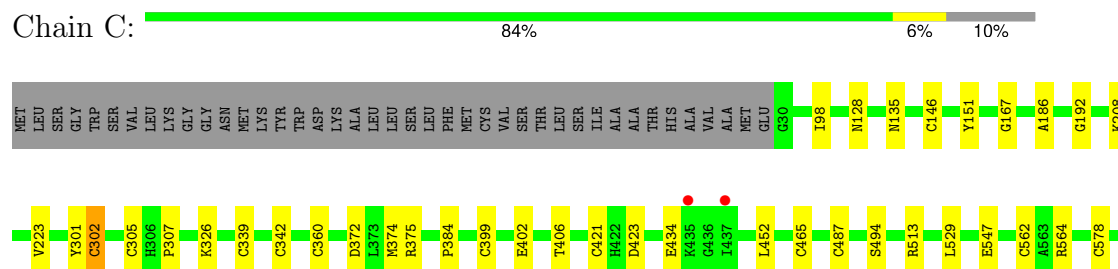
• Molecule 1: MccA

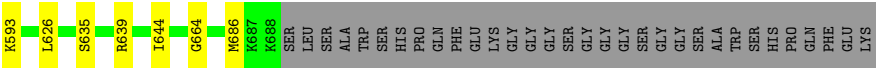


• Molecule 1: MccA

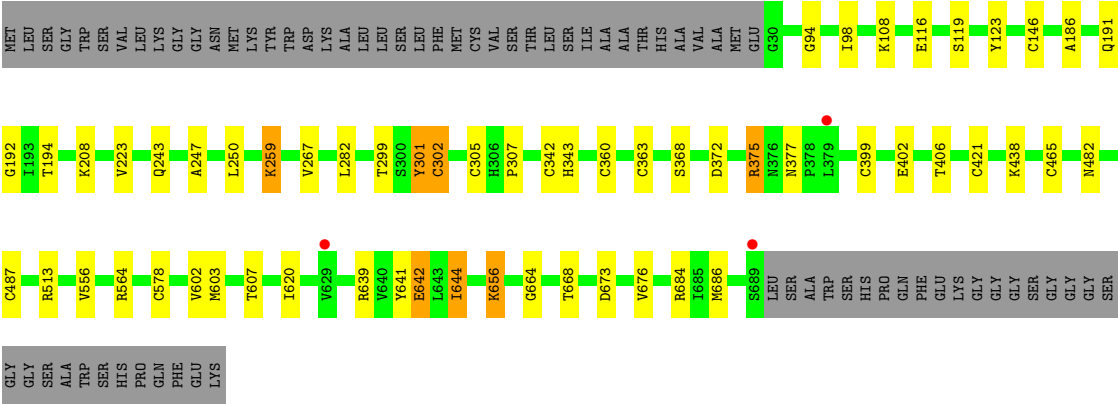
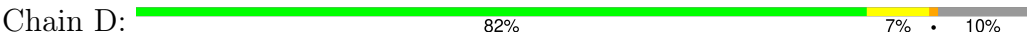


• Molecule 1: MccA





● Molecule 1: MccA



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	186.47Å 186.47Å 232.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.26 – 2.10 47.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.26-2.10) 99.8 (47.26-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.135 , 0.175 0.150 , 0.185	Depositor DCC
R_{free} test set	8789 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.009 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.009 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.011 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.011 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.015 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.019 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: HEM, CU, DTN, SO3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.14	6/5383 (0.1%)	1.05	5/7251 (0.1%)
1	B	1.15	1/5379 (0.0%)	1.06	4/7245 (0.1%)
1	C	1.15	2/5373 (0.0%)	1.06	6/7237 (0.1%)
1	D	1.25	12/5370 (0.2%)	1.09	7/7233 (0.1%)
All	All	1.18	21/21505 (0.1%)	1.06	22/28966 (0.1%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	635	SER	CA-C	6.50	1.61	1.52
1	A	614	THR	C-O	-6.15	1.17	1.24
1	D	607	THR	C-O	-6.00	1.18	1.24
1	D	641	TYR	CA-C	-5.97	1.45	1.52
1	D	267	VAL	C-O	-5.74	1.16	1.24
1	D	375	ARG	C-O	-5.72	1.17	1.24
1	A	155	SER	C-O	-5.72	1.16	1.24
1	B	247	ALA	C-O	5.67	1.30	1.24
1	D	119	SER	C-O	5.61	1.30	1.23
1	A	98	ILE	N-CA	5.59	1.51	1.46
1	D	642	GLU	N-CA	-5.56	1.39	1.46
1	A	150	GLN	C-O	-5.38	1.17	1.24
1	C	494	SER	CA-C	-5.37	1.46	1.52
1	D	602	VAL	CA-C	5.31	1.59	1.52
1	D	191	GLN	CA-C	-5.25	1.46	1.52
1	A	46	GLY	C-O	-5.21	1.18	1.23
1	A	571	ASP	N-CA	5.10	1.52	1.46
1	D	482	ASN	CG-ND2	5.10	1.44	1.33
1	D	556	VAL	CA-C	5.04	1.59	1.52
1	D	368	SER	C-O	-5.01	1.18	1.23
1	D	243	GLN	C-O	5.00	1.29	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	644	ILE	CB-CA-C	-6.96	102.62	112.22
1	A	74	HIS	CA-C-N	6.66	127.19	119.47
1	A	74	HIS	C-N-CA	6.66	127.19	119.47
1	C	186	ALA	N-CA-C	6.50	120.09	110.48
1	C	98	ILE	CB-CA-C	-5.94	105.76	111.05
1	C	423	ASP	N-CA-C	-5.75	102.53	109.83
1	B	299	THR	N-CA-C	5.63	119.66	112.34
1	D	299	THR	N-CA-C	5.38	118.94	112.38
1	D	668	THR	N-CA-C	-5.30	105.58	111.36
1	B	267	VAL	N-CA-C	5.27	116.09	111.56
1	B	186	ALA	N-CA-C	5.25	118.26	110.48
1	D	194	THR	CA-C-N	5.25	125.05	119.28
1	D	194	THR	C-N-CA	5.25	125.05	119.28
1	C	167	GLY	N-CA-C	-5.19	107.38	114.64
1	D	644	ILE	CB-CA-C	-5.18	105.15	112.14
1	C	639	ARG	CG-CD-NE	-5.16	100.66	112.00
1	B	174	ASN	N-CA-C	5.15	118.55	111.54
1	A	377	ASN	CA-C-N	5.07	124.73	119.56
1	A	377	ASN	C-N-CA	5.07	124.73	119.56
1	A	539	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	D	247	ALA	N-CA-C	5.06	116.80	111.28
1	D	259	LYS	N-CA-C	5.05	117.52	111.71

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	5250	0	5072	74	0
1	B	5246	0	5063	69	0
1	C	5240	0	5059	65	0
1	D	5240	0	5054	74	0
2	A	12	0	0	0	0
2	B	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	387	0	270	54	0
3	B	387	0	270	55	0
3	C	387	0	270	58	0
3	D	387	0	270	57	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
5	D	8	0	0	3	0
6	A	335	0	0	5	0
6	B	355	0	0	4	0
6	C	312	0	0	3	0
6	D	417	0	0	5	0
All	All	23997	0	21328	296	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 7.

All (296) 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:B:562:CYS:SG	3:B:909:HEM:CAB	2.01	1.48
1:D:578:CYS:SG	3:D:909:HEM:CAC	2.03	1.47
1:B:339:CYS:SG	3:B:904[A]:HEM:CAB	2.03	1.47
1:C:562:CYS:SG	3:C:909:HEM:CAB	2.02	1.47
1:D:305:CYS:SG	3:D:903:HEM:CAC	2.03	1.47
1:D:360:CYS:SG	3:D:905:HEM:CAB	2.02	1.46
1:C:339:CYS:SG	3:C:904[A]:HEM:CAB	2.03	1.46
1:A:339:CYS:SG	3:A:904[A]:HEM:CAB	2.04	1.45
1:B:339:CYS:SG	3:B:904[B]:HEM:CAB	2.05	1.44
1:D:487:CYS:SG	3:D:908:HEM:CAC	2.06	1.44
1:B:578:CYS:SG	3:B:909:HEM:CAC	2.07	1.43
1:A:360:CYS:SG	3:A:905:HEM:CAB	2.07	1.42
1:D:363:CYS:SG	3:D:905:HEM:CAC	2.08	1.42
1:A:421:CYS:SG	3:A:906:HEM:CAC	2.07	1.41
1:C:487:CYS:SG	3:C:908:HEM:CAC	2.08	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:CYS:SG	3:A:904[B]:HEM:CAB	2.07	1.39
1:D:146:CYS:SG	3:D:902:HEM:CAC	2.11	1.39
1:D:421:CYS:SG	3:D:906:HEM:CAC	2.10	1.39
1:A:487:CYS:SG	3:A:908:HEM:CAC	2.09	1.38
1:B:305:CYS:SG	3:B:903:HEM:CAC	2.12	1.38
1:C:360:CYS:SG	3:C:905:HEM:CAB	2.11	1.37
1:C:305:CYS:SG	3:C:903:HEM:CAC	2.13	1.37
1:A:578:CYS:SG	3:A:909:HEM:CAC	2.12	1.36
1:C:421:CYS:SG	3:C:906:HEM:CAC	2.13	1.36
1:C:146:CYS:SG	3:C:902:HEM:CAC	2.13	1.36
1:D:342:CYS:SG	3:D:904[B]:HEM:CAC	2.13	1.36
1:B:487:CYS:SG	3:B:908:HEM:CAC	2.13	1.36
1:D:465:CYS:SG	3:D:907:HEM:CAC	2.14	1.35
1:A:305:CYS:SG	3:A:903:HEM:CAC	2.14	1.35
1:C:578:CYS:SG	3:C:909:HEM:CAC	2.15	1.35
1:D:342:CYS:SG	3:D:904[A]:HEM:CAC	2.15	1.34
1:B:421:CYS:SG	3:B:906:HEM:CAC	2.16	1.32
1:B:146:CYS:SG	3:B:902:HEM:CAC	2.18	1.30
1:C:342:CYS:SG	3:C:904[A]:HEM:CAC	2.20	1.30
1:A:342:CYS:SG	3:A:904[B]:HEM:CAC	2.19	1.29
1:A:146:CYS:SG	3:A:902:HEM:CAC	2.19	1.29
1:B:342:CYS:SG	3:B:904[B]:HEM:CAC	2.21	1.29
1:B:342:CYS:SG	3:B:904[A]:HEM:CAC	2.21	1.27
1:C:342:CYS:SG	3:C:904[B]:HEM:CAC	2.22	1.27
1:A:465:CYS:SG	3:A:907:HEM:CAC	2.21	1.27
1:A:342:CYS:SG	3:A:904[A]:HEM:CAC	2.23	1.26
1:B:465:CYS:SG	3:B:907:HEM:CAC	2.25	1.24
1:D:302:CYS:SG	3:D:903:HEM:CAB	2.28	1.22
1:C:465:CYS:SG	3:C:907:HEM:CAC	2.28	1.20
1:A:360:CYS:HG	3:A:905:HEM:CAB	1.52	1.17
1:B:302:CYS:SG	3:B:903:HEM:CAB	2.33	1.14
1:B:339:CYS:SG	3:B:904[B]:HEM:HAB	1.85	1.14
1:D:360:CYS:SG	3:D:905:HEM:HAB	1.87	1.14
1:A:302:CYS:SG	3:A:903:HEM:CAB	2.36	1.14
1:B:562:CYS:SG	3:B:909:HEM:HAB	1.88	1.14
1:C:562:CYS:SG	3:C:909:HEM:HAB	1.82	1.08
1:D:487:CYS:SG	3:D:908:HEM:HAC	1.91	1.08
1:C:302:CYS:SG	3:C:903:HEM:CAB	2.42	1.07
1:A:421:CYS:SG	3:A:906:HEM:HAC	1.92	1.06
1:A:339:CYS:SG	3:A:904[A]:HEM:HAB	1.90	1.06
1:B:339:CYS:SG	3:B:904[A]:HEM:HAB	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:CYS:SG	3:D:905:HEM:HAC	1.94	1.04
1:C:360:CYS:HG	3:C:905:HEM:CAB	1.62	1.03
1:D:342:CYS:SG	3:D:904[B]:HEM:CBC	2.46	1.03
1:B:578:CYS:SG	3:B:909:HEM:HAC	1.96	1.01
1:D:578:CYS:SG	3:D:909:HEM:HAC	1.98	1.01
1:B:305:CYS:SG	3:B:903:HEM:CBC	2.48	1.01
1:B:146:CYS:SG	3:B:902:HEM:CBC	2.48	1.00
1:A:487:CYS:SG	3:A:908:HEM:HAC	1.99	0.99
1:D:259:LYS:HE3	6:D:1403:HOH:O	1.63	0.99
1:D:305:CYS:SG	3:D:903:HEM:HAC	2.04	0.97
1:D:305:CYS:SG	3:D:903:HEM:C3C	2.59	0.96
1:C:339:CYS:SG	3:C:904[A]:HEM:HAB	1.85	0.96
1:B:562:CYS:SG	3:B:909:HEM:CBB	2.53	0.96
1:A:339:CYS:SG	3:A:904[B]:HEM:HAB	1.91	0.95
1:A:360:CYS:SG	3:A:905:HEM:HAB	2.02	0.95
1:C:487:CYS:SG	3:C:908:HEM:HAC	2.06	0.95
1:D:342:CYS:SG	3:D:904[A]:HEM:CBC	2.47	0.95
1:B:302:CYS:HG	3:B:903:HEM:CAB	1.80	0.95
1:D:421:CYS:SG	3:D:906:HEM:CBC	2.54	0.95
1:A:578:CYS:SG	3:A:909:HEM:HAC	2.04	0.95
1:A:339:CYS:SG	3:A:904[A]:HEM:CBB	2.57	0.92
1:A:305:CYS:SG	3:A:903:HEM:CBC	2.58	0.92
1:C:305:CYS:SG	3:C:903:HEM:C3C	2.62	0.92
1:B:487:CYS:SG	3:B:908:HEM:HAC	2.09	0.91
1:D:578:CYS:SG	3:D:909:HEM:CBC	2.58	0.91
1:A:339:CYS:SG	3:A:904[B]:HEM:CBB	2.57	0.91
1:C:578:CYS:SG	3:C:909:HEM:CBC	2.58	0.91
1:C:146:CYS:SG	3:C:902:HEM:HAC	2.11	0.91
1:C:421:CYS:SG	3:C:906:HEM:CBC	2.59	0.90
1:A:342:CYS:SG	3:A:904[B]:HEM:CBC	2.60	0.89
1:C:305:CYS:SG	3:C:903:HEM:CBC	2.59	0.89
1:C:360:CYS:SG	3:C:905:HEM:CBB	2.61	0.89
1:C:487:CYS:SG	3:C:908:HEM:CBC	2.60	0.89
1:C:360:CYS:SG	3:C:905:HEM:HAB	2.12	0.89
1:D:146:CYS:SG	3:D:902:HEM:HAC	2.11	0.89
1:A:146:CYS:SG	3:A:902:HEM:CBC	2.62	0.88
1:B:305:CYS:SG	3:B:903:HEM:C3C	2.67	0.88
1:B:487:CYS:SG	3:B:908:HEM:CBC	2.61	0.88
1:D:302:CYS:SG	3:D:903:HEM:C3B	2.65	0.88
1:A:301:TYR:OH	6:A:1327:HOH:O	1.89	0.88
1:B:339:CYS:SG	3:B:904[A]:HEM:CBB	2.61	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:CYS:SG	3:C:909:HEM:CBB	2.62	0.87
1:D:302:CYS:HG	3:D:903:HEM:CAB	1.84	0.87
1:D:146:CYS:SG	3:D:902:HEM:CBC	2.62	0.87
1:B:421:CYS:SG	3:B:906:HEM:HAC	2.15	0.87
1:C:578:CYS:SG	3:C:909:HEM:HAC	2.14	0.87
1:D:578:CYS:SG	3:D:909:HEM:C3C	2.67	0.87
1:D:305:CYS:SG	3:D:903:HEM:CBC	2.62	0.86
1:C:302:CYS:HG	3:C:903:HEM:CAB	1.88	0.85
1:C:421:CYS:SG	3:C:906:HEM:HAC	2.16	0.85
1:D:465:CYS:SG	3:D:907:HEM:HAC	2.16	0.85
1:A:421:CYS:SG	3:A:906:HEM:C3C	2.70	0.85
1:C:342:CYS:SG	3:C:904[A]:HEM:CBC	2.65	0.85
1:D:465:CYS:SG	3:D:907:HEM:C3C	2.70	0.85
1:D:421:CYS:SG	3:D:906:HEM:HAC	2.15	0.84
1:B:578:CYS:SG	3:B:909:HEM:CBC	2.65	0.84
1:A:487:CYS:SG	3:A:908:HEM:CBC	2.66	0.84
1:B:342:CYS:SG	3:B:904[B]:HEM:CBC	2.65	0.83
1:C:146:CYS:SG	3:C:902:HEM:CBC	2.66	0.83
1:A:305:CYS:SG	3:A:903:HEM:C3C	2.71	0.83
1:B:342:CYS:SG	3:B:904[B]:HEM:HAC	2.18	0.83
1:D:360:CYS:SG	3:D:905:HEM:C3B	2.71	0.83
1:D:360:CYS:SG	3:D:905:HEM:CBB	2.67	0.82
1:D:465:CYS:SG	3:D:907:HEM:CBC	2.66	0.82
1:A:302:CYS:SG	3:A:903:HEM:C3B	2.71	0.82
1:B:421:CYS:SG	3:B:906:HEM:CBC	2.67	0.82
1:D:342:CYS:SG	3:D:904[B]:HEM:HAC	2.20	0.82
1:D:146:CYS:SG	3:D:902:HEM:C3C	2.72	0.82
1:C:302:CYS:SG	3:C:903:HEM:C3B	2.72	0.81
1:D:363:CYS:SG	3:D:905:HEM:C3C	2.72	0.81
1:C:146:CYS:SG	3:C:902:HEM:C3C	2.72	0.81
1:A:465:CYS:SG	3:A:907:HEM:CBC	2.68	0.81
1:A:578:CYS:SG	3:A:909:HEM:CBC	2.68	0.81
1:D:421:CYS:SG	3:D:906:HEM:C3C	2.73	0.81
1:C:421:CYS:SG	3:C:906:HEM:C3C	2.73	0.81
1:A:302:CYS:HG	3:A:903:HEM:CAB	1.90	0.80
1:B:578:CYS:SG	3:B:909:HEM:C3C	2.75	0.80
1:A:146:CYS:SG	3:A:902:HEM:C3C	2.74	0.79
1:A:360:CYS:SG	3:A:905:HEM:CBB	2.69	0.79
1:B:301:TYR:OH	6:B:1351:HOH:O	1.99	0.79
1:C:487:CYS:SG	3:C:908:HEM:C3C	2.76	0.79
1:A:305:CYS:SG	3:A:903:HEM:HAC	2.21	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:CYS:SG	3:D:908:HEM:C3C	2.76	0.78
1:D:487:CYS:SG	3:D:908:HEM:CBC	2.72	0.78
1:A:465:CYS:SG	3:A:907:HEM:C3C	2.76	0.78
1:B:342:CYS:SG	3:B:904[A]:HEM:HAC	2.18	0.78
1:C:342:CYS:SG	3:C:904[A]:HEM:HAC	2.23	0.78
4:D:910:CU:CU	5:D:912:SO3:O3	1.32	0.78
1:D:363:CYS:SG	3:D:905:HEM:CBC	2.71	0.78
1:B:421:CYS:SG	3:B:906:HEM:C3C	2.77	0.77
1:C:305:CYS:SG	3:C:903:HEM:HAC	2.24	0.77
1:C:360:CYS:SG	3:C:905:HEM:C3B	2.71	0.77
1:B:302:CYS:SG	3:B:903:HEM:C3B	2.75	0.77
1:A:578:CYS:SG	3:A:909:HEM:C3C	2.77	0.76
1:B:465:CYS:SG	3:B:907:HEM:CBC	2.73	0.76
1:C:465:CYS:SG	3:C:907:HEM:C3C	2.78	0.76
1:A:487:CYS:SG	3:A:908:HEM:C3C	2.79	0.75
1:B:146:CYS:SG	3:B:902:HEM:C3C	2.79	0.75
1:A:421:CYS:SG	3:A:906:HEM:CBC	2.75	0.75
1:B:465:CYS:SG	3:B:907:HEM:C3C	2.79	0.75
1:C:339:CYS:SG	3:C:904[A]:HEM:CBB	2.54	0.75
1:C:342:CYS:SG	3:C:904[A]:HEM:C3C	2.80	0.75
1:B:487:CYS:SG	3:B:908:HEM:C3C	2.80	0.74
1:A:342:CYS:SG	3:A:904[A]:HEM:CBC	2.63	0.74
1:B:562:CYS:SG	3:B:909:HEM:C3B	2.81	0.74
1:A:146:CYS:SG	3:A:902:HEM:HAC	2.28	0.74
1:A:342:CYS:SG	3:A:904[B]:HEM:HAC	2.23	0.74
1:C:342:CYS:SG	3:C:904[B]:HEM:CBC	2.66	0.73
1:A:360:CYS:SG	3:A:905:HEM:C3B	2.66	0.73
1:B:342:CYS:SG	3:B:904[A]:HEM:CBC	2.67	0.73
1:C:465:CYS:SG	3:C:907:HEM:CBC	2.76	0.73
1:B:339:CYS:SG	3:B:904[A]:HEM:C3B	2.82	0.72
1:C:302:CYS:SG	3:C:903:HEM:CBB	2.78	0.72
1:C:578:CYS:SG	3:C:909:HEM:C3C	2.82	0.72
1:D:342:CYS:SG	3:D:904[B]:HEM:C3C	2.84	0.71
1:A:342:CYS:SG	3:A:904[B]:HEM:C3C	2.83	0.71
1:A:339:CYS:SG	3:A:904[A]:HEM:C3B	2.83	0.70
1:B:305:CYS:SG	3:B:903:HEM:HAC	2.27	0.70
1:B:339:CYS:SG	3:B:904[B]:HEM:CBB	2.62	0.70
1:B:342:CYS:SG	3:B:904[A]:HEM:C3C	2.85	0.69
1:B:146:CYS:SG	3:B:902:HEM:HAC	2.31	0.69
1:C:593:LYS:NZ	6:C:1287:HOH:O	2.26	0.69
1:C:562:CYS:SG	3:C:909:HEM:C3B	2.84	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:CYS:SG	3:B:903:HEM:CBB	2.82	0.68
1:A:465:CYS:SG	3:A:907:HEM:HAC	2.30	0.68
1:D:302:CYS:SG	3:D:903:HEM:CBB	2.80	0.68
1:B:465:CYS:SG	3:B:907:HEM:HAC	2.28	0.68
3:C:904[A]:HEM:HBA2	3:C:904[A]:HEM:HHB	1.74	0.68
3:A:907:HEM:O2D	6:A:1332:HOH:O	2.13	0.66
1:A:302:CYS:SG	3:A:903:HEM:CBB	2.84	0.65
1:D:684:ARG:HG2	1:D:684:ARG:HH11	1.61	0.65
5:D:912:SO3:O1	6:D:1404:HOH:O	2.14	0.64
1:D:208:LYS:HG3	3:D:903:HEM:HMA2	1.81	0.61
1:D:399[A]:CYS:SG	5:D:912:SO3:O3	2.58	0.61
3:B:903:HEM:HMD1	3:B:903:HEM:CGD	2.31	0.60
3:A:903:HEM:HMD1	3:A:903:HEM:CGD	2.30	0.60
1:C:465:CYS:SG	3:C:907:HEM:HAC	2.35	0.59
3:D:903:HEM:HMD1	3:D:903:HEM:CGD	2.33	0.58
1:D:402:GLU:O	1:D:406:THR:HG23	2.04	0.58
1:C:342:CYS:SG	3:C:904[B]:HEM:C3C	2.80	0.57
1:A:252:PRO:HG2	1:A:253:GLU:OE1	2.04	0.57
1:A:687:LYS:O	1:A:690:LEU:HG	2.05	0.57
1:A:612:LYS:HG3	6:A:1234:HOH:O	2.05	0.56
1:A:342:CYS:SG	3:A:904[A]:HEM:C3C	2.84	0.56
1:C:301:TYR:OH	6:C:1308:HOH:O	2.17	0.55
1:A:690:LEU:HD12	1:A:690:LEU:C	2.32	0.55
1:D:684:ARG:HG2	1:D:684:ARG:NH1	2.21	0.55
1:D:377:ASN:HB2	6:D:1326:HOH:O	2.06	0.55
1:C:301:TYR:CD2	3:C:903:HEM:HAB	2.42	0.55
1:B:402:GLU:O	1:B:406:THR:HG23	2.07	0.55
3:C:903:HEM:CGD	3:C:903:HEM:HMD1	2.37	0.54
1:C:192:GLY:HA3	1:C:223:VAL:HB	1.89	0.54
1:B:54:ILE:CG2	6:B:1199:HOH:O	2.55	0.54
1:C:402:GLU:O	1:C:406:THR:HG23	2.07	0.54
1:C:305:CYS:CB	3:C:903:HEM:C3C	2.90	0.54
1:A:35:LYS:O	1:A:39:GLU:HG2	2.08	0.53
1:A:208:LYS:HG3	3:A:903:HEM:HMA2	1.90	0.53
1:B:305:CYS:CB	3:B:903:HEM:C3C	2.91	0.53
1:D:302:CYS:SG	3:D:903:HEM:HAB	2.41	0.53
5:B:911:SO3:O3	6:B:1351:HOH:O	2.19	0.52
1:A:402:GLU:O	1:A:406:THR:HG23	2.10	0.52
1:D:305:CYS:CB	3:D:903:HEM:C3C	2.93	0.51
1:C:374:MET:CE	1:C:384:PRO:HA	2.40	0.51
1:C:626:LEU:HD13	1:C:686:MET:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:CYS:SG	3:B:903:HEM:HAB	2.42	0.51
1:B:305:CYS:C	1:B:307:PRO:HD3	2.36	0.50
1:D:603:MET:HE1	6:D:1361:HOH:O	2.11	0.50
1:C:146:CYS:CB	3:C:902:HEM:C3C	2.94	0.50
1:A:253:GLU:CD	1:A:253:GLU:H	2.20	0.49
1:A:350:GLU:HG3	1:C:128:ASN:CG	2.37	0.49
1:A:305:CYS:C	1:A:307:PRO:HD3	2.38	0.49
3:C:903:HEM:HBB2	3:C:903:HEM:HMB2	1.94	0.49
3:D:904[A]:HEM:HBC2	3:D:904[A]:HEM:CMC	2.43	0.49
1:B:165:PHE:CZ	1:B:335:LYS:HD3	2.48	0.48
1:B:342:CYS:SG	3:B:904[B]:HEM:C3C	2.87	0.48
1:C:208:LYS:HG3	3:C:903:HEM:HMA2	1.95	0.48
1:D:146:CYS:CB	3:D:902:HEM:C3C	2.95	0.48
1:A:146:CYS:CB	3:A:902:HEM:C3C	2.96	0.48
1:A:612:LYS:CG	6:A:1234:HOH:O	2.61	0.48
3:C:909:HEM:HMC1	3:C:909:HEM:HBC2	1.96	0.48
1:B:374:MET:CE	1:B:384:PRO:HA	2.44	0.48
1:D:123:TYR:CE1	3:D:903:HEM:HBC2	2.49	0.48
3:D:904[B]:HEM:HBC2	3:D:904[B]:HEM:CMC	2.44	0.47
1:B:94:GLY:O	1:B:98:ILE:HB	2.14	0.47
1:A:629:VAL:C	1:A:630:LYS:O	2.57	0.47
1:B:305:CYS:HB2	3:B:903:HEM:C3C	2.50	0.47
1:B:562:CYS:CB	3:B:909:HEM:CAB	2.90	0.47
1:D:94:GLY:O	1:D:98:ILE:HB	2.14	0.47
1:D:305:CYS:C	1:D:307:PRO:HD3	2.40	0.47
1:A:94:GLY:O	1:A:98:ILE:HB	2.14	0.47
1:D:342:CYS:SG	3:D:904[A]:HEM:C3C	2.84	0.47
1:C:305:CYS:C	1:C:307:PRO:HD3	2.40	0.46
1:D:620:ILE:HG23	1:D:644:ILE:HG23	1.96	0.46
1:A:342:CYS:SG	3:A:904[A]:HEM:HAC	2.28	0.46
1:B:146:CYS:CB	3:B:902:HEM:C3C	2.98	0.46
1:C:372:ASP:OD1	1:C:375:ARG:NH2	2.45	0.46
1:B:208:LYS:HG3	3:B:903:HEM:HMA2	1.98	0.45
1:D:639:ARG:NH1	1:D:642:GLU:OE1	2.45	0.45
1:D:603:MET:HA	1:D:603:MET:HE2	1.99	0.45
1:A:421:CYS:CB	3:A:906:HEM:C3C	3.00	0.45
1:C:434:GLU:HG2	1:C:452:LEU:HG	1.98	0.45
1:A:192:GLY:HA3	1:A:223:VAL:HB	1.98	0.45
1:D:305:CYS:HB2	3:D:903:HEM:C3C	2.52	0.44
1:D:343:HIS:CE1	3:D:904[A]:HEM:ND	2.86	0.44
1:B:112:ARG:HB2	1:C:151:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:MET:HE2	1:B:603:MET:HA	2.00	0.43
1:A:374:MET:CE	1:A:384:PRO:HA	2.49	0.43
1:D:656:LYS:HD2	1:D:656:LYS:HA	1.86	0.43
1:A:259:LYS:HA	1:A:262:VAL:O	2.19	0.42
3:C:904[A]:HEM:HBC1	3:C:905:HEM:CHC	2.50	0.42
1:D:399[B]:CYS:SG	1:D:513:ARG:HG3	2.59	0.42
1:D:186:ALA:HB1	1:D:282:LEU:HG	2.01	0.42
1:D:259:LYS:CE	6:D:1403:HOH:O	2.43	0.42
5:C:911:SO3:O3	6:C:1308:HOH:O	2.22	0.42
3:C:904[B]:HEM:HBC1	3:C:905:HEM:CHC	2.50	0.42
1:D:301:TYR:CE2	3:D:903:HEM:HHC	2.55	0.42
1:D:363:CYS:CB	3:D:905:HEM:C3C	3.03	0.42
1:A:305:CYS:CB	3:A:903:HEM:C3C	3.02	0.42
1:B:687:LYS:HB2	1:B:687:LYS:HE3	1.88	0.42
1:B:190:PRO:HB2	1:B:222:HIS:HB3	2.02	0.42
1:A:417:ARG:O	1:A:418:CYS:C	2.63	0.41
5:A:912:SO3:O1	6:A:1327:HOH:O	2.21	0.41
1:A:603:MET:HA	1:A:603:MET:HE2	2.02	0.41
1:D:108:LYS:NZ	1:D:116:GLU:OE1	2.46	0.41
1:B:263:PRO:HD2	6:B:1318:HOH:O	2.21	0.41
1:B:51:ARG:NH2	1:C:135:ASN:OD1	2.53	0.41
1:A:395:MET:HG2	1:A:544:TRP:CE2	2.55	0.41
1:A:399[B]:CYS:SG	1:A:495[B]:CYS:N	2.93	0.41
1:B:54:ILE:CG2	1:B:54:ILE:O	2.69	0.41
1:B:562:CYS:HB3	3:B:909:HEM:C3B	2.55	0.41
1:D:208:LYS:HE3	3:D:903:HEM:C3A	2.55	0.41
1:D:673:ASP:HA	1:D:676:VAL:HG22	2.03	0.41
1:D:192:GLY:HA3	1:D:223:VAL:HB	2.02	0.41
1:D:372:ASP:OD1	1:D:375:ARG:NH1	2.54	0.41
1:A:406:THR:O	1:A:412:TYR:HB2	2.20	0.40
1:A:630:LYS:O	1:A:631:LYS:HB2	2.20	0.40
1:C:305:CYS:HB2	3:C:903:HEM:C3C	2.56	0.40
1:D:421:CYS:CB	3:D:906:HEM:C3C	3.04	0.40
1:B:374:MET:HE1	1:B:384:PRO:HA	2.03	0.40
1:C:399[B]:CYS:SG	1:C:513:ARG:HG3	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	661/732 (90%)	631 (96%)	28 (4%)	2 (0%)	36	36
1	B	661/732 (90%)	635 (96%)	26 (4%)	0	100	100
1	C	660/732 (90%)	629 (95%)	30 (4%)	1 (0%)	43	44
1	D	660/732 (90%)	633 (96%)	25 (4%)	2 (0%)	36	36
All	All	2642/2928 (90%)	2528 (96%)	109 (4%)	5 (0%)	43	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	630	LYS
1	D	301	TYR
1	A	664	GLY
1	C	664	GLY
1	D	664	GLY

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	563/613 (92%)	557 (99%)	6 (1%)	65	74
1	B	562/613 (92%)	555 (99%)	7 (1%)	63	72
1	C	561/613 (92%)	556 (99%)	5 (1%)	70	78
1	D	561/613 (92%)	555 (99%)	6 (1%)	65	74
All	All	2247/2452 (92%)	2223 (99%)	24 (1%)	65	74

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	GLU
1	A	302	CYS
1	A	529	LEU
1	A	547	GLU
1	A	564	ARG
1	A	656	LYS
1	B	54	ILE
1	B	302	CYS
1	B	379	LEU
1	B	441	SER
1	B	457	LYS
1	B	564	ARG
1	B	631	LYS
1	C	302	CYS
1	C	326	LYS
1	C	529	LEU
1	C	547	GLU
1	C	564	ARG
1	D	250	LEU
1	D	302	CYS
1	D	438	LYS
1	D	564	ARG
1	D	656	LYS
1	D	686	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	243	GLN
1	A	376	ASN
1	A	377	ASN
1	A	497	ASN
1	B	648	GLN
1	C	43	HIS
1	C	621	GLN
1	D	377	ASN
1	D	446	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 50 ligands modelled in this entry, 4 are monoatomic - leaving 46 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	$\# Z > 2$
3	HEM	A	903	5,1	50,50,50	1.64	11 (22%)	67,82,82	1.73	15 (22%)
3	HEM	B	902	1	50,50,50	1.51	10 (20%)	67,82,82	1.68	13 (19%)
3	HEM	B	904[A]	1	50,50,50	1.51	9 (18%)	67,82,82	1.78	17 (25%)
3	HEM	C	908	1	50,50,50	1.36	8 (16%)	67,82,82	1.67	12 (17%)
3	HEM	B	907	1	50,50,50	1.61	10 (20%)	67,82,82	1.75	16 (23%)
3	HEM	D	906	1	50,50,50	1.36	4 (8%)	67,82,82	1.67	12 (17%)
3	HEM	C	904[A]	1	50,50,50	1.49	10 (20%)	67,82,82	1.79	16 (23%)
3	HEM	B	904[B]	1	50,50,50	1.53	9 (18%)	67,82,82	1.75	15 (22%)
3	HEM	B	903	5,1	50,50,50	1.65	9 (18%)	67,82,82	1.65	16 (23%)
3	HEM	C	907	1	50,50,50	1.46	8 (16%)	67,82,82	1.78	19 (28%)
3	HEM	C	904[B]	1	50,50,50	1.47	8 (16%)	67,82,82	1.70	15 (22%)
3	HEM	D	903	5,1	50,50,50	1.83	12 (24%)	67,82,82	1.57	15 (22%)
3	HEM	B	906	1	50,50,50	1.51	9 (18%)	67,82,82	1.86	15 (22%)
2	DTN	A	901	-	0,5,5	-	-	0,6,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO3	D	912	3	1,3,3	6.54	1 (100%)	0,3,3	-	-
3	HEM	A	908	1	50,50,50	1.55	6 (12%)	67,82,82	1.62	15 (22%)
3	HEM	C	909	1	50,50,50	1.55	9 (18%)	67,82,82	1.78	17 (25%)
3	HEM	B	905	1	50,50,50	1.46	7 (14%)	67,82,82	1.56	9 (13%)
2	DTN	D	901	-	0,5,5	-	-	0,6,6	-	-
2	DTN	A	911	-	0,5,5	-	-	0,6,6	-	-
3	HEM	C	905	1	50,50,50	1.70	9 (18%)	67,82,82	1.49	9 (13%)
3	HEM	A	902	1	50,50,50	1.57	9 (18%)	67,82,82	1.81	16 (23%)
3	HEM	D	905	1	50,50,50	1.59	9 (18%)	67,82,82	1.38	9 (13%)
3	HEM	D	907	1	50,50,50	1.56	5 (10%)	67,82,82	1.97	19 (28%)
3	HEM	A	909	1	50,50,50	1.48	8 (16%)	67,82,82	1.96	19 (28%)
3	HEM	D	908	1	50,50,50	1.48	6 (12%)	67,82,82	1.81	17 (25%)
2	DTN	B	901	-	0,5,5	-	-	0,6,6	-	-
5	SO3	B	911	4,3	1,3,3	5.15	1 (100%)	0,3,3	-	-
3	HEM	A	904[A]	1	50,50,50	1.53	12 (24%)	67,82,82	1.79	17 (25%)
2	DTN	C	901	-	0,5,5	-	-	0,6,6	-	-
3	HEM	A	905	1	50,50,50	1.63	7 (14%)	67,82,82	1.57	14 (20%)
5	SO3	C	911	3	1,3,3	5.90	1 (100%)	0,3,3	-	-
5	SO3	A	912	4,3	1,3,3	7.78	1 (100%)	0,3,3	-	-
3	HEM	D	902	1	50,50,50	1.68	9 (18%)	67,82,82	1.72	13 (19%)
3	HEM	A	904[B]	1	50,50,50	1.56	12 (24%)	67,82,82	1.83	19 (28%)
3	HEM	D	909	1	50,50,50	1.49	10 (20%)	67,82,82	1.97	18 (26%)
3	HEM	C	903	5,1	50,50,50	1.69	9 (18%)	67,82,82	1.66	18 (26%)
3	HEM	B	909	1	50,50,50	1.55	7 (14%)	67,82,82	1.76	16 (23%)
3	HEM	C	906	1	50,50,50	1.64	9 (18%)	67,82,82	1.72	16 (23%)
3	HEM	C	902	1	50,50,50	1.64	11 (22%)	67,82,82	1.80	17 (25%)
3	HEM	A	907	1	50,50,50	1.60	9 (18%)	67,82,82	1.86	18 (26%)
3	HEM	D	904[A]	1	50,50,50	1.41	5 (10%)	67,82,82	1.72	17 (25%)
5	SO3	D	911	-	1,3,3	9.03	1 (100%)	0,3,3	-	-
3	HEM	A	906	1	50,50,50	1.62	11 (22%)	67,82,82	1.59	13 (19%)
3	HEM	D	904[B]	1	50,50,50	1.50	6 (12%)	67,82,82	1.70	15 (22%)
3	HEM	B	908	1	50,50,50	1.43	10 (20%)	67,82,82	1.70	13 (19%)

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
3	HEM	A	903	5,1	-	2/14/54/54	-
3	HEM	B	902	1	-	3/14/54/54	-
3	HEM	B	904[A]	1	-	3/14/54/54	-
3	HEM	C	908	1	-	5/14/54/54	-
3	HEM	B	907	1	-	3/14/54/54	-
3	HEM	D	906	1	-	3/14/54/54	-
3	HEM	C	904[A]	1	-	4/14/54/54	-
3	HEM	B	904[B]	1	-	3/14/54/54	-
3	HEM	B	903	5,1	-	2/14/54/54	-
3	HEM	C	907	1	-	3/14/54/54	-
3	HEM	C	904[B]	1	-	3/14/54/54	-
3	HEM	D	903	5,1	-	3/14/54/54	-
3	HEM	B	906	1	-	3/14/54/54	-
2	DTN	A	901	-	-	0/0/4/4	-
3	HEM	A	908	1	-	5/14/54/54	-
3	HEM	C	909	1	-	5/14/54/54	-
3	HEM	B	905	1	-	2/14/54/54	-
2	DTN	D	901	-	-	0/0/4/4	-
2	DTN	A	911	-	-	0/0/4/4	-
3	HEM	C	905	1	-	2/14/54/54	-
3	HEM	A	902	1	-	2/14/54/54	-
3	HEM	D	905	1	-	2/14/54/54	-
3	HEM	D	907	1	-	3/14/54/54	-
3	HEM	A	909	1	-	5/14/54/54	-
3	HEM	D	908	1	-	7/14/54/54	-
2	DTN	B	901	-	-	0/0/4/4	-
3	HEM	A	904[A]	1	-	2/14/54/54	-
2	DTN	C	901	-	-	0/0/4/4	-
3	HEM	A	905	1	-	2/14/54/54	-
3	HEM	D	902	1	-	2/14/54/54	-
3	HEM	A	904[B]	1	-	2/14/54/54	-
3	HEM	D	909	1	-	7/14/54/54	-
3	HEM	C	903	5,1	-	2/14/54/54	-
3	HEM	B	909	1	-	7/14/54/54	-
3	HEM	C	906	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	902	1	-	2/14/54/54	-
3	HEM	A	907	1	-	3/14/54/54	-
3	HEM	D	904[A]	1	-	4/14/54/54	-
3	HEM	A	906	1	-	4/14/54/54	-
3	HEM	D	904[B]	1	-	2/14/54/54	-
3	HEM	B	908	1	-	6/14/54/54	-

All (317) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	911	SO3	O1-S	9.03	1.83	1.44
5	A	912	SO3	O1-S	7.78	1.77	1.44
5	D	912	SO3	O1-S	6.54	1.72	1.44
3	A	905	HEM	FE-NB	6.12	2.13	1.94
5	C	911	SO3	O1-S	5.90	1.69	1.44
3	C	905	HEM	FE-NB	5.70	2.12	1.94
5	B	911	SO3	O1-S	5.15	1.66	1.44
3	D	907	HEM	C1B-NB	-4.91	1.31	1.40
3	A	902	HEM	FE-NB	4.87	2.09	1.94
3	D	905	HEM	C1B-NB	-4.74	1.32	1.40
3	A	907	HEM	C1B-NB	-4.72	1.32	1.40
3	B	907	HEM	C1B-NB	-4.70	1.32	1.40
3	D	903	HEM	FE-NC	4.67	2.10	1.95
3	A	908	HEM	C1B-NB	-4.60	1.32	1.40
3	C	906	HEM	FE-NC	4.56	2.10	1.95
3	B	904[B]	HEM	FE-NB	4.54	2.08	1.94
3	B	905	HEM	FE-NC	4.52	2.10	1.95
3	B	904[A]	HEM	FE-NB	4.43	2.08	1.94
3	C	907	HEM	C1B-NB	-4.43	1.32	1.40
3	D	907	HEM	FE-NC	4.39	2.09	1.95
3	D	909	HEM	FE-NC	4.37	2.09	1.95
3	B	908	HEM	C1B-NB	-4.32	1.32	1.40
3	B	905	HEM	FE-NB	4.32	2.08	1.94
3	B	909	HEM	C1B-NB	-4.30	1.32	1.40
3	C	905	HEM	C1B-NB	-4.25	1.32	1.40
3	A	906	HEM	FE-NC	4.24	2.09	1.95
3	D	905	HEM	FE-NB	4.23	2.07	1.94
3	D	903	HEM	C4D-ND	-4.16	1.33	1.40
3	C	903	HEM	FE-NB	4.16	2.07	1.94
3	C	907	HEM	FE-NB	4.13	2.07	1.94
3	D	908	HEM	FE-NC	4.12	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	HEM	C1B-NB	-4.12	1.33	1.40
3	C	904[A]	HEM	C1B-NB	-4.11	1.33	1.40
3	B	909	HEM	FE-NC	4.08	2.08	1.95
3	B	903	HEM	FE-NB	4.05	2.07	1.94
3	C	905	HEM	FE-NC	4.02	2.08	1.95
3	D	904[B]	HEM	FE-NB	4.00	2.07	1.94
3	B	904[A]	HEM	C4B-NB	-3.99	1.31	1.38
3	C	904[B]	HEM	C1B-NB	-3.99	1.33	1.40
3	C	902	HEM	CBA-CGA	3.99	1.59	1.50
3	C	903	HEM	C1B-NB	-3.98	1.33	1.40
3	D	903	HEM	C3B-C4B	3.96	1.52	1.44
3	D	904[A]	HEM	FE-NB	3.96	2.07	1.94
3	B	903	HEM	C1B-NB	-3.95	1.33	1.40
3	D	904[B]	HEM	O1A-CGA	3.92	1.34	1.22
3	A	904[B]	HEM	C1B-NB	-3.90	1.33	1.40
3	B	903	HEM	C3B-C4B	3.89	1.52	1.44
3	D	903	HEM	C1B-NB	-3.88	1.33	1.40
3	A	907	HEM	FE-NB	3.87	2.06	1.94
3	C	907	HEM	FE-NC	3.85	2.07	1.95
3	A	905	HEM	C4D-C3D	3.85	1.51	1.45
3	A	909	HEM	FE-NC	3.84	2.07	1.95
3	A	904[A]	HEM	C1B-NB	-3.82	1.33	1.40
3	A	906	HEM	C1B-NB	-3.80	1.33	1.40
3	C	902	HEM	FE-NB	3.80	2.06	1.94
3	A	903	HEM	C1C-C2C	-3.77	1.37	1.45
3	C	906	HEM	C1B-NB	-3.74	1.33	1.40
3	C	906	HEM	FE-NB	3.74	2.06	1.94
3	D	902	HEM	FE-NB	3.72	2.06	1.94
3	B	906	HEM	FE-NC	3.71	2.07	1.95
3	D	902	HEM	FE-NC	3.70	2.07	1.95
3	B	903	HEM	FE-NC	3.68	2.07	1.95
3	D	908	HEM	C1B-NB	-3.67	1.33	1.40
3	A	908	HEM	FE-NC	3.66	2.07	1.95
3	A	905	HEM	C1B-NB	-3.66	1.33	1.40
3	A	903	HEM	C1B-NB	-3.66	1.33	1.40
3	C	908	HEM	FE-NB	3.65	2.06	1.94
3	C	904[B]	HEM	FE-NB	3.63	2.06	1.94
3	A	909	HEM	FE-NB	3.63	2.06	1.94
3	D	904[B]	HEM	FE-NC	3.61	2.07	1.95
3	A	903	HEM	FE-NB	3.60	2.06	1.94
3	B	902	HEM	FE-NC	3.60	2.07	1.95
3	C	904[A]	HEM	FE-NB	3.59	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	906	HEM	O2D-CGD	-3.58	1.19	1.30
3	C	903	HEM	C3B-C4B	3.56	1.51	1.44
3	A	906	HEM	FE-NB	3.54	2.05	1.94
3	B	907	HEM	FE-NC	3.53	2.06	1.95
3	D	904[A]	HEM	C1B-NB	-3.51	1.34	1.40
3	C	903	HEM	C4D-C3D	3.51	1.51	1.45
3	A	905	HEM	C4D-ND	-3.50	1.34	1.40
3	C	903	HEM	FE-NC	3.50	2.06	1.95
3	D	904[B]	HEM	C1B-NB	-3.50	1.34	1.40
3	A	904[B]	HEM	FE-NC	3.49	2.06	1.95
3	C	909	HEM	FE-NC	3.48	2.06	1.95
3	D	908	HEM	C4B-NB	-3.47	1.32	1.38
3	B	903	HEM	C4D-ND	-3.46	1.34	1.40
3	B	904[B]	HEM	C4B-NB	-3.45	1.32	1.38
3	D	904[A]	HEM	FE-NC	3.45	2.06	1.95
3	C	909	HEM	FE-NB	3.42	2.05	1.94
3	A	904[B]	HEM	FE-NB	3.40	2.05	1.94
3	C	902	HEM	FE-NC	3.39	2.06	1.95
3	A	904[A]	HEM	FE-NB	3.38	2.05	1.94
3	B	905	HEM	C1B-NB	-3.35	1.34	1.40
3	A	902	HEM	FE-NC	3.35	2.06	1.95
3	C	902	HEM	C4B-NB	-3.34	1.32	1.38
3	A	902	HEM	CBA-CGA	3.33	1.58	1.50
3	B	902	HEM	FE-NB	3.33	2.05	1.94
3	D	902	HEM	CBA-CGA	3.32	1.58	1.50
3	D	903	HEM	FE-NB	3.32	2.05	1.94
3	C	904[B]	HEM	C4B-NB	-3.29	1.32	1.38
3	C	908	HEM	FE-NC	3.29	2.06	1.95
3	D	902	HEM	C4B-NB	-3.29	1.32	1.38
3	B	908	HEM	FE-NC	3.28	2.06	1.95
3	A	902	HEM	FE-NA	3.27	2.05	1.95
3	D	906	HEM	C1B-NB	-3.26	1.34	1.40
3	B	909	HEM	C4B-NB	-3.26	1.32	1.38
3	A	904[A]	HEM	FE-NC	3.25	2.05	1.95
3	B	909	HEM	FE-NB	3.24	2.04	1.94
3	A	903	HEM	C3B-C4B	3.23	1.51	1.44
3	D	905	HEM	C4D-ND	-3.23	1.34	1.40
3	C	903	HEM	C4A-NA	-3.22	1.33	1.39
3	C	903	HEM	C4B-NB	-3.22	1.32	1.38
3	C	905	HEM	C3B-C4B	3.22	1.51	1.44
3	B	904[B]	HEM	FE-NC	3.20	2.05	1.95
3	C	909	HEM	C1B-NB	-3.19	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	909	HEM	C1B-NB	-3.19	1.34	1.40
3	D	909	HEM	C1B-C2B	-3.17	1.38	1.44
3	D	906	HEM	FE-NC	3.16	2.05	1.95
3	A	907	HEM	FE-NC	3.14	2.05	1.95
3	D	909	HEM	C4D-ND	-3.13	1.34	1.40
3	C	909	HEM	C4D-ND	-3.13	1.34	1.40
3	D	902	HEM	O1A-CGA	3.12	1.32	1.22
3	B	907	HEM	FE-NB	3.11	2.04	1.94
3	B	903	HEM	C4D-C3D	3.11	1.50	1.45
3	D	903	HEM	C4A-NA	-3.11	1.33	1.39
3	C	904[A]	HEM	C4B-NB	-3.10	1.32	1.38
3	B	906	HEM	FE-NA	3.08	2.05	1.95
3	C	909	HEM	C4A-NA	-3.07	1.33	1.39
3	D	905	HEM	C4D-C3D	3.04	1.50	1.45
3	B	904[B]	HEM	O1A-CGA	3.04	1.32	1.22
3	C	904[A]	HEM	FE-NC	3.03	2.05	1.95
3	C	904[B]	HEM	FE-NC	3.02	2.05	1.95
3	B	906	HEM	FE-NB	3.01	2.04	1.94
3	B	902	HEM	CBA-CGA	2.99	1.57	1.50
3	B	906	HEM	C1B-NB	-2.96	1.35	1.40
3	B	902	HEM	C1B-NB	-2.96	1.35	1.40
3	B	908	HEM	C4B-NB	-2.94	1.33	1.38
3	B	904[B]	HEM	C1B-NB	-2.94	1.35	1.40
3	C	902	HEM	C1B-NB	-2.93	1.35	1.40
3	C	906	HEM	C4D-ND	-2.92	1.35	1.40
3	A	903	HEM	C4D-C3D	2.90	1.50	1.45
3	B	909	HEM	C1C-NC	-2.88	1.34	1.39
3	D	903	HEM	C1C-NC	-2.84	1.34	1.39
3	C	905	HEM	C1D-C2D	2.83	1.50	1.44
3	A	905	HEM	C4B-NB	-2.82	1.33	1.38
3	A	902	HEM	O1A-CGA	2.80	1.31	1.22
3	B	904[A]	HEM	C1B-NB	-2.80	1.35	1.40
3	A	903	HEM	C4D-ND	-2.80	1.35	1.40
3	D	906	HEM	O2D-CGD	-2.80	1.21	1.30
3	A	903	HEM	FE-NC	2.79	2.04	1.95
3	B	904[A]	HEM	FE-NC	2.79	2.04	1.95
3	A	909	HEM	C1C-NC	-2.77	1.34	1.39
3	A	906	HEM	C1D-C2D	2.76	1.50	1.44
3	B	909	HEM	C4D-ND	-2.76	1.35	1.40
3	B	903	HEM	C1D-ND	-2.75	1.33	1.38
3	A	904[A]	HEM	C4C-NC	-2.73	1.34	1.39
3	D	903	HEM	C4D-C3D	2.72	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	903	HEM	C1A-NA	-2.72	1.34	1.39
3	C	906	HEM	C1D-C2D	2.71	1.50	1.44
3	D	909	HEM	C4A-NA	-2.71	1.34	1.39
3	B	908	HEM	FE-NB	2.69	2.03	1.94
3	B	908	HEM	C4D-ND	-2.68	1.35	1.40
3	B	903	HEM	C4B-NB	-2.68	1.33	1.38
3	A	904[B]	HEM	CBA-CGA	2.68	1.56	1.50
3	D	903	HEM	C4C-NC	-2.67	1.34	1.39
3	C	902	HEM	C3B-C4B	2.66	1.50	1.44
3	A	908	HEM	C4D-ND	-2.66	1.35	1.40
3	D	905	HEM	FE-NC	2.66	2.03	1.95
3	D	902	HEM	C3B-C4B	2.65	1.50	1.44
3	C	908	HEM	C4B-NB	-2.64	1.33	1.38
3	A	907	HEM	C4D-ND	-2.63	1.35	1.40
3	A	904[A]	HEM	C4B-NB	-2.63	1.33	1.38
3	D	905	HEM	C1C-C2C	-2.62	1.40	1.45
3	A	904[B]	HEM	C4D-ND	-2.61	1.35	1.40
3	C	907	HEM	C3C-C2C	2.61	1.42	1.37
3	C	907	HEM	C4B-NB	-2.61	1.33	1.38
3	A	904[B]	HEM	C1D-ND	-2.60	1.33	1.38
3	A	907	HEM	C4D-C3D	2.58	1.49	1.45
3	D	904[B]	HEM	CBA-CGA	2.58	1.56	1.50
3	A	907	HEM	CAC-C3C	2.58	1.54	1.47
3	A	902	HEM	C1B-NB	-2.58	1.35	1.40
3	A	908	HEM	FE-NB	2.57	2.02	1.94
3	A	904[B]	HEM	C4C-NC	-2.57	1.34	1.39
3	B	906	HEM	C4C-NC	-2.57	1.34	1.39
3	D	907	HEM	FE-NB	2.56	2.02	1.94
3	A	903	HEM	C1D-ND	-2.56	1.33	1.38
3	D	908	HEM	FE-NB	2.56	2.02	1.94
3	C	902	HEM	C1D-ND	-2.56	1.33	1.38
3	A	905	HEM	C3B-C4B	2.56	1.49	1.44
3	A	906	HEM	C4D-C3D	2.54	1.49	1.45
3	C	905	HEM	C3C-C2C	2.53	1.42	1.37
3	A	904[A]	HEM	C1A-NA	-2.53	1.34	1.39
3	A	902	HEM	C4D-C3D	2.53	1.49	1.45
3	A	902	HEM	C4B-NB	-2.51	1.33	1.38
3	B	904[A]	HEM	C1C-NC	-2.50	1.34	1.39
3	B	905	HEM	C3B-C4B	2.49	1.49	1.44
3	D	907	HEM	C4D-ND	-2.49	1.35	1.40
3	A	904[A]	HEM	C1D-ND	-2.48	1.34	1.38
3	A	907	HEM	CMD-C2D	2.47	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	HEM	C1D-ND	-2.45	1.34	1.38
3	B	907	HEM	C1C-NC	-2.45	1.35	1.39
3	C	909	HEM	C1A-NA	-2.44	1.35	1.39
3	C	902	HEM	C4D-ND	-2.44	1.36	1.40
3	C	909	HEM	C3C-C4C	-2.44	1.41	1.46
3	B	904[B]	HEM	C1C-NC	-2.43	1.35	1.39
3	D	905	HEM	C4B-NB	-2.43	1.34	1.38
3	B	904[A]	HEM	C1A-C2A	-2.42	1.39	1.44
3	D	909	HEM	CBB-CAB	2.42	1.42	1.30
3	C	904[A]	HEM	CBA-CGA	2.41	1.56	1.50
3	A	903	HEM	C4B-NB	-2.41	1.34	1.38
3	A	903	HEM	C1C-NC	-2.40	1.35	1.39
3	B	907	HEM	C4B-NB	-2.40	1.34	1.38
3	B	908	HEM	C4D-C3D	2.39	1.49	1.45
3	C	904[A]	HEM	C1D-ND	-2.39	1.34	1.38
3	A	904[A]	HEM	C4D-C3D	2.38	1.49	1.45
3	C	908	HEM	C1B-NB	-2.37	1.36	1.40
3	B	907	HEM	C4C-NC	-2.37	1.35	1.39
3	A	909	HEM	C1C-C2C	-2.37	1.40	1.45
3	A	905	HEM	FE-NC	2.37	2.03	1.95
3	B	902	HEM	O1A-CGA	2.36	1.29	1.22
3	D	904[A]	HEM	C3C-C4C	-2.35	1.41	1.46
3	C	905	HEM	C4B-NB	-2.35	1.34	1.38
3	D	906	HEM	FE-NB	2.34	2.02	1.94
3	C	904[B]	HEM	C1D-ND	-2.33	1.34	1.38
3	B	905	HEM	FE-NA	2.33	2.02	1.95
3	D	904[B]	HEM	C3C-C4C	-2.33	1.42	1.46
3	A	904[B]	HEM	C4B-NB	-2.32	1.34	1.38
3	C	906	HEM	FE-NA	2.31	2.02	1.95
3	A	906	HEM	C4D-ND	-2.31	1.36	1.40
3	A	907	HEM	FE-NA	2.31	2.02	1.95
3	C	905	HEM	C4D-ND	-2.30	1.36	1.40
3	B	904[A]	HEM	C1D-ND	-2.30	1.34	1.38
3	A	904[A]	HEM	C4D-ND	-2.30	1.36	1.40
3	C	903	HEM	C4D-ND	-2.29	1.36	1.40
3	D	908	HEM	C1C-C2C	-2.28	1.40	1.45
3	C	907	HEM	C4D-ND	-2.28	1.36	1.40
3	C	904[B]	HEM	C1D-C2D	2.28	1.49	1.44
3	D	908	HEM	C1D-C2D	2.27	1.49	1.44
3	A	904[A]	HEM	C1D-C2D	2.27	1.49	1.44
3	D	909	HEM	FE-NB	2.27	2.01	1.94
3	A	906	HEM	C3B-C4B	2.27	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	HEM	C1D-C2D	2.25	1.49	1.44
3	D	909	HEM	C1B-NB	-2.24	1.36	1.40
3	D	904[A]	HEM	C4B-NB	-2.24	1.34	1.38
3	B	902	HEM	C4D-C3D	2.24	1.48	1.45
3	A	908	HEM	C1A-NA	-2.24	1.35	1.39
3	D	902	HEM	C4C-NC	-2.24	1.35	1.39
3	C	904[A]	HEM	C1D-C2D	2.24	1.49	1.44
3	A	904[B]	HEM	C1D-C2D	2.23	1.49	1.44
3	A	909	HEM	C1D-ND	-2.23	1.34	1.38
3	B	906	HEM	C4D-ND	-2.23	1.36	1.40
3	B	909	HEM	O2A-CGA	-2.23	1.23	1.30
3	B	907	HEM	C1D-ND	-2.23	1.34	1.38
3	A	907	HEM	C4B-NB	-2.21	1.34	1.38
3	B	908	HEM	C1C-NC	-2.21	1.35	1.39
3	B	904[B]	HEM	C1D-ND	-2.21	1.34	1.38
3	A	909	HEM	C1B-C2B	-2.20	1.40	1.44
3	D	905	HEM	CBA-CGA	2.20	1.55	1.50
3	A	906	HEM	O2D-CGD	-2.20	1.23	1.30
3	D	909	HEM	C4B-NB	-2.20	1.34	1.38
3	A	904[A]	HEM	C1C-C2C	-2.19	1.41	1.45
3	C	907	HEM	FE-NA	2.18	2.02	1.95
3	C	909	HEM	C1C-C2C	-2.18	1.41	1.45
3	C	908	HEM	C4D-ND	-2.17	1.36	1.40
3	B	907	HEM	C4D-ND	-2.15	1.36	1.40
3	A	904[B]	HEM	C4D-C3D	2.15	1.48	1.45
3	B	902	HEM	C4C-NC	-2.14	1.35	1.39
3	C	908	HEM	O2A-CGA	-2.14	1.23	1.30
3	D	903	HEM	CAB-C3B	2.14	1.53	1.47
3	B	908	HEM	C3B-C4B	2.14	1.49	1.44
3	B	906	HEM	C4B-NB	-2.13	1.34	1.38
3	B	908	HEM	CBB-CAB	2.13	1.40	1.30
3	B	902	HEM	C4B-NB	-2.13	1.34	1.38
3	D	903	HEM	O1A-CGA	2.12	1.29	1.22
3	D	909	HEM	FE-ND	-2.12	1.88	1.94
3	B	906	HEM	CHA-C4D	2.12	1.42	1.38
3	B	904[A]	HEM	C4C-NC	-2.12	1.35	1.39
3	C	904[A]	HEM	C4D-ND	-2.11	1.36	1.40
3	C	904[A]	HEM	C4C-NC	-2.11	1.35	1.39
3	B	904[A]	HEM	C1C-C2C	-2.11	1.41	1.45
3	B	904[B]	HEM	C1C-C2C	-2.11	1.41	1.45
3	C	903	HEM	FE-NA	2.11	2.02	1.95
3	C	904[B]	HEM	C4C-NC	-2.11	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	906	HEM	C1C-NC	-2.10	1.35	1.39
3	A	904[B]	HEM	C1C-C2C	-2.10	1.41	1.45
3	C	909	HEM	CBB-CAB	2.10	1.40	1.30
3	B	906	HEM	C1A-C2A	-2.09	1.40	1.44
3	B	908	HEM	O2D-CGD	-2.09	1.23	1.30
3	C	904[B]	HEM	C1C-C2C	-2.09	1.41	1.45
3	C	908	HEM	FE-NA	2.09	2.02	1.95
3	C	905	HEM	C1C-C2C	-2.09	1.41	1.45
3	B	905	HEM	C4D-C3D	2.09	1.48	1.45
3	A	906	HEM	CHA-C1A	-2.08	1.34	1.39
3	D	905	HEM	C3D-C2D	-2.08	1.32	1.36
3	B	907	HEM	C1C-C2C	-2.08	1.41	1.45
3	C	908	HEM	CHA-C4D	2.08	1.42	1.38
3	B	905	HEM	O1D-CGD	2.07	1.28	1.22
3	A	902	HEM	C1B-C2B	-2.06	1.40	1.44
3	C	902	HEM	C1C-NC	-2.06	1.35	1.39
3	C	904[A]	HEM	C1C-C2C	-2.06	1.41	1.45
3	A	908	HEM	CBB-CAB	2.05	1.40	1.30
3	D	907	HEM	CBB-CAB	2.05	1.40	1.30
3	A	903	HEM	C4C-NC	-2.05	1.35	1.39
3	A	904[B]	HEM	C1A-NA	-2.05	1.35	1.39
3	A	906	HEM	C4B-NB	-2.04	1.34	1.38
3	A	906	HEM	CBB-CAB	2.04	1.40	1.30
3	C	907	HEM	C1D-ND	-2.04	1.34	1.38
3	B	904[B]	HEM	CBA-CGA	2.04	1.55	1.50
3	D	909	HEM	C2A-C3A	-2.03	1.33	1.38
3	B	903	HEM	C3C-C2C	2.03	1.41	1.37
3	B	907	HEM	O2A-CGA	-2.02	1.24	1.30
3	C	902	HEM	C1C-C2C	-2.02	1.41	1.45
3	A	904[A]	HEM	C3B-C4B	2.01	1.48	1.44
3	C	902	HEM	FE-NA	2.01	2.01	1.95
3	B	902	HEM	C4D-ND	-2.01	1.36	1.40
3	C	906	HEM	O2A-CGA	-2.01	1.24	1.30
3	A	909	HEM	C4B-NB	-2.00	1.34	1.38

All (550) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	907	HEM	CHC-C4B-NB	5.91	130.78	124.42
3	A	904[B]	HEM	CHC-C4B-NB	5.80	130.66	124.42
3	A	909	HEM	CHC-C4B-NB	5.79	130.65	124.42
3	B	909	HEM	CHC-C4B-NB	5.74	130.60	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	907	HEM	C1B-NB-C4B	5.71	111.97	105.21
3	A	902	HEM	C1B-NB-C4B	5.63	111.87	105.21
3	A	907	HEM	C1B-NB-C4B	5.56	111.79	105.21
3	A	902	HEM	CHC-C4B-NB	5.40	130.24	124.42
3	D	902	HEM	CHC-C4B-NB	5.38	130.22	124.42
3	B	906	HEM	CHC-C4B-NB	5.25	130.07	124.42
3	B	907	HEM	CHC-C4B-NB	5.25	130.07	124.42
3	C	902	HEM	CHC-C4B-NB	5.24	130.06	124.42
3	A	904[B]	HEM	C1B-NB-C4B	5.21	111.37	105.21
3	D	909	HEM	CHC-C4B-NB	5.20	130.02	124.42
3	A	904[A]	HEM	CHC-C4B-NB	5.19	130.01	124.42
3	D	909	HEM	CAA-CBA-CGA	-5.13	100.06	113.67
3	B	904[B]	HEM	CHC-C4B-NB	5.12	129.93	124.42
3	C	908	HEM	CHD-C1D-ND	4.91	129.71	124.42
3	D	908	HEM	CHC-C4B-NB	4.83	129.62	124.42
3	A	909	HEM	C1B-NB-C4B	4.79	110.88	105.21
3	D	906	HEM	CHC-C4B-NB	4.78	129.57	124.42
3	A	908	HEM	CHC-C4B-NB	4.78	129.56	124.42
3	B	902	HEM	CHC-C4B-NB	4.75	129.54	124.42
3	C	904[A]	HEM	C1B-NB-C4B	4.74	110.82	105.21
3	B	908	HEM	CHC-C4B-NB	4.73	129.52	124.42
3	B	906	HEM	C1B-NB-C4B	4.72	110.80	105.21
3	A	902	HEM	C3B-C4B-NB	-4.72	106.08	109.47
3	B	904[A]	HEM	CHC-C4B-NB	4.67	129.45	124.42
3	C	902	HEM	C1B-NB-C4B	4.66	110.73	105.21
3	C	907	HEM	CHD-C1D-ND	4.63	129.41	124.42
3	A	904[A]	HEM	C1B-NB-C4B	4.62	110.68	105.21
3	A	903	HEM	C1B-NB-C4B	4.60	110.66	105.21
3	B	905	HEM	C3B-C2B-C1B	4.55	109.83	106.41
3	C	908	HEM	C1B-NB-C4B	4.55	110.60	105.21
3	C	907	HEM	CHC-C4B-NB	4.55	129.31	124.42
3	D	908	HEM	C1B-NB-C4B	4.54	110.59	105.21
3	D	907	HEM	C1B-NB-C4B	4.52	110.56	105.21
3	C	904[B]	HEM	C1B-NB-C4B	4.52	110.55	105.21
3	C	909	HEM	CHC-C4B-NB	4.51	129.28	124.42
3	D	909	HEM	CHD-C1D-ND	4.50	129.26	124.42
3	B	903	HEM	C1B-NB-C4B	4.48	110.52	105.21
3	C	903	HEM	C1B-NB-C4B	4.43	110.45	105.21
3	C	909	HEM	CHD-C1D-ND	4.42	129.18	124.42
3	D	904[B]	HEM	CHC-C4B-NB	4.42	129.18	124.42
3	D	904[B]	HEM	CHD-C1D-ND	4.41	129.17	124.42
3	D	904[B]	HEM	C1B-NB-C4B	4.40	110.42	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	907	HEM	CHA-C4D-ND	4.36	129.76	124.37
3	D	904[A]	HEM	CHD-C1D-ND	4.35	129.10	124.42
3	B	904[B]	HEM	C1B-NB-C4B	4.32	110.32	105.21
3	C	905	HEM	C1B-NB-C4B	4.30	110.30	105.21
3	D	907	HEM	CHD-C1D-ND	4.25	129.00	124.42
3	B	902	HEM	C1B-NB-C4B	4.25	110.24	105.21
3	C	903	HEM	CHD-C1D-C2D	-4.22	118.37	125.03
3	B	905	HEM	CHD-C1D-ND	4.21	128.96	124.42
3	C	906	HEM	C1B-NB-C4B	4.20	110.18	105.21
3	C	906	HEM	CHC-C4B-NB	4.18	128.92	124.42
3	B	907	HEM	CHD-C1D-ND	4.17	128.91	124.42
3	A	903	HEM	CHC-C4B-NB	4.15	128.89	124.42
3	D	902	HEM	CHD-C1D-ND	4.15	128.89	124.42
3	C	906	HEM	O2D-CGD-O1D	-4.14	112.69	123.33
3	C	909	HEM	C1B-NB-C4B	4.12	110.09	105.21
3	B	904[A]	HEM	C1B-NB-C4B	4.10	110.07	105.21
3	B	908	HEM	CHA-C4D-ND	4.09	129.43	124.37
3	A	907	HEM	CHC-C4B-NB	4.09	128.82	124.42
3	D	909	HEM	CHD-C1D-C2D	-4.08	118.59	125.03
3	A	906	HEM	CHD-C1D-ND	4.08	128.81	124.42
3	D	902	HEM	C1B-NB-C4B	4.08	110.03	105.21
3	C	905	HEM	C4B-C3B-C2B	-4.06	103.55	107.28
3	D	903	HEM	C4B-C3B-C2B	-4.06	103.55	107.28
3	B	907	HEM	C3B-C4B-NB	-4.04	106.57	109.47
3	B	902	HEM	CHD-C1D-ND	4.03	128.76	124.42
3	C	904[A]	HEM	CHC-C4B-NB	4.03	128.76	124.42
3	C	904[B]	HEM	CAD-C3D-C4D	4.00	131.67	124.70
3	D	903	HEM	CHD-C1D-C2D	-3.99	118.73	125.03
3	B	906	HEM	C3B-C4B-NB	-3.99	106.60	109.47
3	A	902	HEM	CHD-C1D-ND	3.97	128.69	124.42
3	D	909	HEM	C3B-C4B-NB	-3.96	106.62	109.47
3	B	908	HEM	C1B-NB-C4B	3.94	109.87	105.21
3	D	904[A]	HEM	C1B-NB-C4B	3.93	109.86	105.21
3	C	907	HEM	O2D-CGD-CBD	3.92	126.40	114.00
3	D	904[A]	HEM	CHC-C4B-NB	3.92	128.64	124.42
3	A	906	HEM	CHC-C4B-NB	3.91	128.63	124.42
3	B	909	HEM	C1B-NB-C4B	3.88	109.80	105.21
3	B	908	HEM	CHD-C1D-ND	3.85	128.56	124.42
3	B	904[A]	HEM	CHA-C1A-NA	3.85	130.83	123.86
3	B	905	HEM	C4B-C3B-C2B	-3.84	103.75	107.28
3	D	908	HEM	C4C-C3C-C2C	-3.84	103.48	106.81
3	B	903	HEM	CHD-C1D-C2D	-3.83	118.98	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	904[B]	HEM	CHC-C4B-NB	3.82	128.53	124.42
3	A	909	HEM	O2D-CGD-O1D	-3.81	113.52	123.33
3	B	905	HEM	C1B-NB-C4B	3.81	109.72	105.21
3	D	907	HEM	O2D-CGD-CBD	3.81	126.04	114.00
3	A	903	HEM	CHD-C1D-C2D	-3.79	119.05	125.03
3	C	909	HEM	CHD-C1D-C2D	-3.79	119.05	125.03
3	D	908	HEM	CHD-C1D-ND	3.78	128.49	124.42
3	B	905	HEM	CHC-C4B-NB	3.78	128.49	124.42
3	C	908	HEM	CHC-C4B-NB	3.78	128.49	124.42
3	C	902	HEM	CHD-C1D-ND	3.76	128.47	124.42
3	C	904[A]	HEM	CAD-C3D-C4D	3.76	131.24	124.70
3	A	903	HEM	C4B-C3B-C2B	-3.74	103.84	107.28
3	D	909	HEM	CMD-C2D-C1D	3.74	130.88	125.03
3	A	909	HEM	CHD-C4C-NC	3.74	128.52	124.45
3	C	908	HEM	CHD-C1D-C2D	-3.73	119.14	125.03
3	C	907	HEM	C1B-NB-C4B	3.71	109.61	105.21
3	A	906	HEM	O2D-CGD-O1D	-3.70	113.80	123.33
3	A	905	HEM	C4B-C3B-C2B	-3.70	103.88	107.28
3	B	904[B]	HEM	CHD-C1D-ND	3.70	128.40	124.42
3	A	907	HEM	CHD-C1D-C2D	-3.70	119.19	125.03
3	A	908	HEM	CHB-C1B-NB	3.70	128.94	124.37
3	A	902	HEM	CHA-C4D-ND	3.70	128.94	124.37
3	B	903	HEM	CHD-C1D-ND	3.69	128.40	124.42
3	A	903	HEM	CHD-C1D-ND	3.69	128.39	124.42
3	C	909	HEM	O2A-CGA-CBA	3.64	125.49	114.00
3	A	905	HEM	C1B-NB-C4B	3.64	109.51	105.21
3	D	909	HEM	CHA-C4D-ND	3.62	128.85	124.37
3	B	903	HEM	C3B-C4B-NB	-3.61	106.88	109.47
3	D	905	HEM	CHD-C1D-C2D	-3.61	119.33	125.03
3	D	905	HEM	C1B-NB-C4B	3.58	109.44	105.21
3	B	906	HEM	O2A-CGA-CBA	3.57	125.29	114.00
3	C	905	HEM	CHD-C1D-ND	3.57	128.27	124.42
3	C	902	HEM	O2A-CGA-CBA	3.56	125.25	114.00
3	D	903	HEM	CHD-C1D-ND	3.55	128.25	124.42
3	C	907	HEM	CHA-C4D-ND	3.53	128.73	124.37
3	D	906	HEM	C1B-NB-C4B	3.52	109.37	105.21
3	C	904[A]	HEM	CHD-C4C-NC	3.51	128.28	124.45
3	C	906	HEM	CHB-C1B-NB	3.51	128.71	124.37
3	B	909	HEM	CAA-CBA-CGA	-3.48	104.42	113.67
3	D	906	HEM	CHD-C4C-NC	3.48	128.25	124.45
3	C	903	HEM	CHD-C1D-ND	3.48	128.16	124.42
3	D	903	HEM	C3D-C4D-ND	3.47	113.97	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	906	HEM	CHA-C4D-ND	3.46	128.65	124.37
3	B	905	HEM	CHD-C1D-C2D	-3.46	119.56	125.03
3	D	908	HEM	O2D-CGD-CBD	3.46	124.93	114.00
3	B	906	HEM	CHD-C1D-ND	3.45	128.14	124.42
3	C	908	HEM	CHA-C4D-ND	3.45	128.63	124.37
3	A	905	HEM	CHD-C1D-C2D	-3.45	119.59	125.03
3	A	907	HEM	CHD-C1D-ND	3.41	128.09	124.42
3	A	906	HEM	C1B-NB-C4B	3.40	109.23	105.21
3	B	904[A]	HEM	C1A-CHA-C4D	-3.37	118.33	126.25
3	C	904[B]	HEM	CHD-C4C-NC	3.36	128.11	124.45
3	C	908	HEM	CHD-C4C-NC	3.35	128.10	124.45
3	C	906	HEM	C3B-C2B-C1B	3.35	108.92	106.41
3	D	909	HEM	C1B-NB-C4B	3.34	109.16	105.21
3	D	907	HEM	CHD-C4C-NC	3.33	128.08	124.45
3	A	909	HEM	C3B-C4B-NB	-3.31	107.09	109.47
3	A	909	HEM	CHD-C1D-ND	3.31	127.99	124.42
3	B	902	HEM	CAD-C3D-C4D	3.31	130.47	124.70
3	B	904[A]	HEM	C3B-C4B-NB	-3.30	107.10	109.47
3	C	907	HEM	O1D-CGD-CBD	-3.28	112.68	123.09
3	D	902	HEM	CHD-C1D-C2D	-3.28	119.86	125.03
3	A	904[B]	HEM	CHD-C1D-ND	3.27	127.95	124.42
3	C	905	HEM	CHC-C4B-NB	3.27	127.94	124.42
3	C	909	HEM	O2A-CGA-O1A	-3.27	114.93	123.33
3	D	907	HEM	O2A-CGA-CBA	3.26	124.29	114.00
3	C	905	HEM	CHD-C1D-C2D	-3.25	119.90	125.03
3	B	906	HEM	CHB-C1B-NB	3.24	128.38	124.37
3	A	904[A]	HEM	CHD-C1D-ND	3.24	127.91	124.42
3	B	902	HEM	CHD-C1D-C2D	-3.23	119.93	125.03
3	D	902	HEM	CHA-C4D-C3D	-3.23	119.28	125.23
3	B	904[A]	HEM	CHD-C1D-ND	3.23	127.89	124.42
3	A	907	HEM	C4C-CHD-C1D	-3.22	119.17	126.02
3	A	903	HEM	C1A-CHA-C4D	-3.21	118.70	126.25
3	C	906	HEM	CHA-C4D-C3D	-3.21	119.31	125.23
3	D	906	HEM	O2D-CGD-O1D	-3.21	115.08	123.33
3	B	904[B]	HEM	CAA-CBA-CGA	3.19	122.13	113.67
3	B	906	HEM	CHA-C4D-C3D	-3.19	119.34	125.23
3	A	906	HEM	O2D-CGD-CBD	3.18	124.06	114.00
3	A	904[A]	HEM	CHD-C1D-C2D	-3.17	120.02	125.03
3	B	908	HEM	CAD-C3D-C4D	3.17	130.23	124.70
3	B	909	HEM	CHD-C1D-ND	3.17	127.83	124.42
3	C	906	HEM	C3D-C4D-ND	3.17	113.64	110.17
3	B	906	HEM	O2D-CGD-O1D	-3.15	115.24	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	907	HEM	C4C-CHD-C1D	-3.14	119.34	126.02
3	C	903	HEM	CHB-C1B-NB	3.14	128.25	124.37
3	D	907	HEM	O2D-CGD-O1D	-3.13	115.27	123.33
3	B	903	HEM	CHC-C4B-NB	3.13	127.79	124.42
3	D	902	HEM	CHA-C4D-ND	3.13	128.24	124.37
3	D	903	HEM	C1B-NB-C4B	3.12	108.90	105.21
3	A	904[B]	HEM	CAA-CBA-CGA	3.12	121.94	113.67
3	B	904[B]	HEM	CHD-C1D-C2D	-3.12	120.11	125.03
3	D	908	HEM	CHB-C1B-NB	3.11	128.22	124.37
3	C	902	HEM	C4B-C3B-C2B	-3.10	104.43	107.28
3	D	907	HEM	C4B-C3B-C2B	-3.09	104.44	107.28
3	D	907	HEM	CHD-C1D-C2D	-3.09	120.15	125.03
3	A	904[B]	HEM	CHD-C1D-C2D	-3.08	120.16	125.03
3	B	907	HEM	CHD-C4C-NC	3.08	127.81	124.45
3	A	905	HEM	C2D-C1D-ND	3.08	113.46	109.90
3	A	908	HEM	C1B-NB-C4B	3.08	108.85	105.21
3	A	902	HEM	CHA-C4D-C3D	-3.06	119.58	125.23
3	D	902	HEM	CAA-CBA-CGA	3.06	121.78	113.67
3	D	908	HEM	CHA-C4D-C3D	-3.05	119.60	125.23
3	B	909	HEM	CHA-C4D-ND	3.05	128.14	124.37
3	A	904[B]	HEM	C3B-C4B-NB	-3.05	107.28	109.47
3	B	904[A]	HEM	CHD-C1D-C2D	-3.04	120.22	125.03
3	D	904[A]	HEM	CHA-C1A-NA	3.04	129.37	123.86
3	A	904[A]	HEM	C3B-C4B-NB	-3.03	107.29	109.47
3	B	904[A]	HEM	CHD-C4C-NC	3.03	127.75	124.45
3	B	907	HEM	O2D-CGD-CBD	3.03	123.57	114.00
3	B	908	HEM	CHA-C4D-C3D	-3.01	119.67	125.23
3	D	906	HEM	O2A-CGA-CBA	3.00	123.47	114.00
3	D	907	HEM	CAD-CBD-CGD	-3.00	105.72	113.67
3	A	904[A]	HEM	CHB-C4A-NA	2.99	129.28	123.86
3	C	903	HEM	C2D-C1D-ND	2.99	113.36	109.90
3	D	906	HEM	CHB-C1B-NB	2.97	128.04	124.37
3	B	904[B]	HEM	C1A-CHA-C4D	-2.96	119.28	126.25
3	D	908	HEM	C3B-C4B-NB	-2.96	107.34	109.47
3	A	908	HEM	CHA-C4D-C3D	-2.95	119.79	125.23
3	B	902	HEM	CHA-C4D-C3D	-2.95	119.79	125.23
3	A	905	HEM	CMD-C2D-C1D	2.94	129.63	125.03
3	B	909	HEM	C4C-C3C-C2C	-2.94	104.27	106.81
3	C	903	HEM	O2D-CGD-O1D	-2.93	115.80	123.33
3	D	907	HEM	CMA-C3A-C4A	-2.92	120.97	125.42
3	B	908	HEM	O2A-CGA-CBA	2.91	123.20	114.00
3	A	902	HEM	CHD-C1D-C2D	-2.91	120.44	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	909	HEM	CHD-C1D-C2D	-2.90	120.44	125.03
3	C	902	HEM	CHA-C4D-ND	2.90	127.95	124.37
3	C	904[A]	HEM	O2A-CGA-O1A	-2.90	115.89	123.33
3	D	906	HEM	C3B-C4B-NB	-2.89	107.39	109.47
3	C	903	HEM	C4B-C3B-C2B	-2.89	104.62	107.28
3	D	908	HEM	C1A-CHA-C4D	-2.89	119.45	126.25
3	C	904[A]	HEM	C4C-NC-C1C	2.89	110.53	105.82
3	A	905	HEM	C1D-C2D-C3D	-2.88	103.95	106.98
3	D	905	HEM	CHB-C1B-NB	2.88	127.93	124.37
3	A	909	HEM	O2A-CGA-O1A	-2.88	115.93	123.33
3	B	904[B]	HEM	C3B-C4B-NB	-2.88	107.40	109.47
3	B	904[B]	HEM	C4A-C3A-C2A	2.87	110.11	106.82
3	A	904[A]	HEM	CAD-C3D-C4D	2.87	129.70	124.70
3	C	902	HEM	CHB-C1B-NB	2.86	127.91	124.37
3	A	903	HEM	CHA-C4D-ND	2.86	127.91	124.37
3	A	906	HEM	CHD-C1D-C2D	-2.86	120.52	125.03
3	C	903	HEM	CHC-C4B-NB	2.86	127.50	124.42
3	A	908	HEM	C4B-C3B-C2B	-2.85	104.66	107.28
3	D	904[A]	HEM	CHD-C1D-C2D	-2.85	120.52	125.03
3	A	904[B]	HEM	CHD-C4C-NC	2.85	127.56	124.45
3	B	902	HEM	CHA-C4D-ND	2.84	127.89	124.37
3	D	909	HEM	C4C-C3C-C2C	-2.84	104.35	106.81
3	B	902	HEM	CBB-CAB-C3B	-2.84	113.34	127.53
3	C	908	HEM	C1A-CHA-C4D	-2.84	119.58	126.25
3	A	904[A]	HEM	CHD-C4C-NC	2.83	127.54	124.45
3	A	909	HEM	O2A-CGA-CBA	2.83	122.95	114.00
3	D	902	HEM	C1A-CHA-C4D	-2.83	119.59	126.25
3	D	909	HEM	CAD-CBD-CGD	-2.83	106.17	113.67
3	B	903	HEM	CAD-C3D-C2D	2.82	133.15	127.87
3	C	904[B]	HEM	C4C-NC-C1C	2.82	110.41	105.82
3	D	908	HEM	CHA-C4D-ND	2.81	127.84	124.37
3	D	904[B]	HEM	CHD-C1D-C2D	-2.81	120.60	125.03
3	B	908	HEM	C1A-CHA-C4D	-2.80	119.65	126.25
3	C	903	HEM	C1D-C2D-C3D	-2.80	104.03	106.98
3	A	906	HEM	O2A-CGA-CBA	2.80	122.84	114.00
3	C	909	HEM	C4C-CHD-C1D	-2.80	120.07	126.02
3	A	906	HEM	CHA-C4D-ND	2.80	127.83	124.37
3	A	903	HEM	C3B-C2B-C1B	2.80	108.51	106.41
3	A	902	HEM	CHB-C1B-NB	2.80	127.83	124.37
3	A	907	HEM	CHA-C4D-C3D	-2.79	120.08	125.23
3	A	909	HEM	C2A-C1A-NA	-2.78	107.07	110.15
3	A	907	HEM	C3B-C4B-NB	-2.77	107.47	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	908	HEM	CAD-C3D-C4D	2.77	129.53	124.70
3	A	907	HEM	O1D-CGD-CBD	-2.77	114.32	123.09
3	C	904[A]	HEM	C3B-C4B-NB	-2.76	107.49	109.47
3	C	904[B]	HEM	C3B-C4B-NB	-2.76	107.49	109.47
3	D	904[B]	HEM	CHA-C4D-C3D	-2.76	120.14	125.23
3	A	909	HEM	CAD-C3D-C4D	2.76	129.50	124.70
3	D	904[A]	HEM	CHD-C4C-NC	2.75	127.45	124.45
3	D	907	HEM	CHB-C1B-NB	2.75	127.77	124.37
3	A	908	HEM	C3B-C2B-C1B	2.75	108.47	106.41
3	C	907	HEM	CAD-C3D-C4D	2.74	129.47	124.70
3	A	904[B]	HEM	O2A-CGA-CBA	2.73	122.63	114.00
3	D	904[A]	HEM	C2A-C1A-NA	-2.73	107.12	110.15
3	A	903	HEM	CHB-C1B-NB	2.73	127.75	124.37
3	D	904[B]	HEM	CHD-C4C-NC	2.73	127.42	124.45
3	C	908	HEM	CMA-C3A-C4A	2.72	129.56	125.42
3	B	904[A]	HEM	CBB-CAB-C3B	-2.72	113.93	127.53
3	D	908	HEM	O1D-CGD-CBD	-2.72	114.47	123.09
3	A	907	HEM	O2D-CGD-CBD	2.71	122.58	114.00
3	C	909	HEM	CHD-C4C-NC	2.71	127.41	124.45
3	D	903	HEM	C2D-C1D-ND	2.70	113.03	109.90
3	D	905	HEM	C2D-C1D-ND	2.70	113.03	109.90
3	D	909	HEM	C1D-C2D-C3D	-2.70	104.14	106.98
3	C	903	HEM	CHA-C4D-ND	2.69	127.70	124.37
3	B	903	HEM	CMA-C3A-C4A	-2.69	121.32	125.42
3	A	908	HEM	C3D-C4D-ND	2.69	113.12	110.17
3	D	904[A]	HEM	CAD-C3D-C4D	2.69	129.38	124.70
3	B	904[A]	HEM	C2A-C1A-NA	-2.68	107.17	110.15
3	C	908	HEM	C3B-C4B-NB	-2.67	107.55	109.47
3	B	908	HEM	CBB-CAB-C3B	-2.66	114.21	127.53
3	C	904[B]	HEM	C3D-C4D-ND	2.66	113.09	110.17
3	D	905	HEM	CHC-C4B-NB	2.66	127.29	124.42
3	D	908	HEM	CHD-C1D-C2D	-2.66	120.83	125.03
3	D	905	HEM	C4B-C3B-C2B	-2.66	104.84	107.28
3	D	904[A]	HEM	C1A-CHA-C4D	-2.65	120.00	126.25
3	C	904[A]	HEM	C4C-CHD-C1D	-2.64	120.40	126.02
3	D	904[A]	HEM	C4C-CHD-C1D	-2.64	120.40	126.02
3	B	904[A]	HEM	CAD-C3D-C4D	2.64	129.30	124.70
3	A	904[A]	HEM	C4C-NC-C1C	2.63	110.11	105.82
3	C	904[A]	HEM	C3D-C4D-ND	2.63	113.06	110.17
3	B	904[B]	HEM	CBB-CAB-C3B	-2.63	114.39	127.53
3	B	906	HEM	CHD-C1D-C2D	-2.63	120.88	125.03
3	B	906	HEM	O2A-CGA-O1A	-2.63	116.57	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	907	HEM	CHD-C4C-NC	2.63	127.31	124.45
3	D	902	HEM	O2D-CGD-CBD	2.63	122.30	114.00
3	D	904[A]	HEM	C3B-C4B-NB	-2.62	107.58	109.47
3	A	909	HEM	CHD-C1D-C2D	-2.62	120.89	125.03
3	C	904[A]	HEM	CHD-C1D-C2D	-2.62	120.89	125.03
3	C	904[B]	HEM	CHD-C1D-C2D	-2.62	120.90	125.03
3	B	902	HEM	CHB-C1B-NB	2.62	127.60	124.37
3	C	907	HEM	CHD-C1D-C2D	-2.62	120.90	125.03
3	B	904[B]	HEM	CHA-C4D-ND	2.61	127.60	124.37
3	A	904[A]	HEM	C2A-C1A-NA	-2.61	107.25	110.15
3	C	906	HEM	C4B-C3B-C2B	-2.61	104.88	107.28
3	C	903	HEM	C3B-C4B-NB	-2.61	107.59	109.47
3	B	907	HEM	CHD-C1D-C2D	-2.61	120.91	125.03
3	C	904[B]	HEM	CHB-C1B-NB	2.60	127.58	124.37
3	D	904[B]	HEM	C4C-CHD-C1D	-2.59	120.52	126.02
3	B	906	HEM	C1A-CHA-C4D	-2.59	120.16	126.25
3	A	906	HEM	CMD-C2D-C1D	2.58	129.07	125.03
3	C	907	HEM	CHA-C4D-C3D	-2.58	120.46	125.23
3	C	905	HEM	CHD-C4C-NC	2.58	127.27	124.45
3	C	904[B]	HEM	C4C-CHD-C1D	-2.58	120.53	126.02
3	A	909	HEM	C4C-NC-C1C	2.58	110.03	105.82
3	C	904[A]	HEM	O2A-CGA-CBA	2.57	122.13	114.00
3	B	906	HEM	O2D-CGD-CBD	2.57	122.13	114.00
3	A	907	HEM	CHB-C1B-NB	2.57	127.55	124.37
3	C	907	HEM	O2A-CGA-O1A	-2.57	116.73	123.33
3	A	908	HEM	CHD-C1D-ND	2.57	127.19	124.42
3	A	903	HEM	O2A-CGA-O1A	-2.57	116.73	123.33
3	C	904[A]	HEM	CHA-C4D-C3D	-2.56	120.51	125.23
3	C	906	HEM	O2A-CGA-CBA	2.55	122.07	114.00
3	B	904[B]	HEM	CHD-C4C-NC	2.55	127.23	124.45
3	C	902	HEM	O2A-CGA-O1A	-2.55	116.77	123.33
3	D	905	HEM	C1A-CHA-C4D	-2.55	120.26	126.25
3	C	902	HEM	CHA-C4D-C3D	-2.54	120.54	125.23
3	B	908	HEM	CHD-C1D-C2D	-2.54	121.01	125.03
3	A	904[B]	HEM	C4C-NC-C1C	2.54	109.97	105.82
3	C	904[A]	HEM	CAD-CBD-CGD	-2.54	106.93	113.67
3	D	905	HEM	CHD-C1D-ND	2.53	127.15	124.42
3	B	906	HEM	CAD-C3D-C4D	2.53	129.11	124.70
3	C	907	HEM	CHB-C1B-NB	2.53	127.50	124.37
3	C	904[A]	HEM	CHB-C1B-NB	2.53	127.49	124.37
3	D	904[B]	HEM	CHA-C4D-ND	2.52	127.49	124.37
3	B	909	HEM	O1D-CGD-CBD	-2.52	115.10	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	909	HEM	CHA-C4D-C3D	-2.52	120.58	125.23
3	C	907	HEM	O2A-CGA-CBA	2.51	121.92	114.00
3	B	904[A]	HEM	CHB-C4A-NA	2.51	128.41	123.86
3	A	907	HEM	C3B-C2B-C1B	2.50	108.29	106.41
3	D	904[B]	HEM	C3B-C4B-NB	-2.50	107.67	109.47
3	A	907	HEM	C4B-C3B-C2B	-2.49	104.99	107.28
3	B	903	HEM	CHB-C1B-NB	2.49	127.45	124.37
3	B	907	HEM	CHB-C1B-NB	2.49	127.45	124.37
3	C	909	HEM	CMD-C2D-C1D	2.49	128.92	125.03
3	C	907	HEM	C1A-CHA-C4D	-2.49	120.39	126.25
3	B	903	HEM	C4B-C3B-C2B	-2.48	105.00	107.28
3	C	906	HEM	CHD-C1D-ND	2.48	127.10	124.42
3	A	902	HEM	CHD-C4C-NC	2.48	127.16	124.45
3	D	907	HEM	CBA-CAA-C2A	-2.48	105.68	112.53
3	D	904[B]	HEM	C1A-CHA-C4D	-2.47	120.44	126.25
3	B	904[B]	HEM	CAD-C3D-C4D	2.47	129.00	124.70
3	B	903	HEM	CMA-C3A-C2A	2.46	130.85	125.62
3	A	905	HEM	CHB-C4A-NA	2.46	128.33	123.86
3	B	904[B]	HEM	CHA-C4D-C3D	-2.46	120.69	125.23
3	C	907	HEM	CHD-C4C-NC	2.46	127.13	124.45
3	A	906	HEM	CAD-C3D-C4D	2.45	128.97	124.70
3	C	903	HEM	C1A-CHA-C4D	-2.45	120.49	126.25
3	C	909	HEM	CAD-CBD-CGD	-2.45	107.18	113.67
3	D	908	HEM	CBB-CAB-C3B	-2.44	115.36	127.53
3	C	904[A]	HEM	CHD-C1D-ND	2.43	127.04	124.42
3	B	905	HEM	CMB-C2B-C1B	-2.43	121.23	125.03
3	D	906	HEM	O1A-CGA-CBA	-2.43	115.38	123.09
3	D	903	HEM	CBD-CAD-C3D	2.43	119.25	112.53
3	C	906	HEM	O2D-CGD-CBD	2.43	121.67	114.00
3	B	909	HEM	CMA-C3A-C4A	-2.43	121.72	125.42
3	C	903	HEM	O2A-CGA-CBA	2.43	121.67	114.00
3	C	904[B]	HEM	CHA-C4D-C3D	-2.42	120.76	125.23
3	B	902	HEM	C4D-C3D-C2D	-2.42	103.36	106.89
3	A	907	HEM	O2A-CGA-CBA	2.42	121.66	114.00
3	D	907	HEM	C3B-C2B-C1B	2.42	108.23	106.41
3	D	903	HEM	C1A-CHA-C4D	-2.42	120.55	126.25
3	C	904[B]	HEM	CHD-C1D-ND	2.42	127.03	124.42
3	B	903	HEM	CHA-C4D-C3D	-2.42	120.77	125.23
3	A	902	HEM	CAD-C3D-C4D	2.42	128.91	124.70
3	D	908	HEM	O2A-CGA-CBA	2.41	121.63	114.00
3	C	902	HEM	CAD-C3D-C4D	2.41	128.90	124.70
3	C	902	HEM	O2D-CGD-CBD	2.41	121.60	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	907	HEM	C2D-C1D-ND	2.41	112.68	109.90
3	C	906	HEM	CBB-CAB-C3B	-2.40	115.51	127.53
3	D	906	HEM	CHD-C1D-C2D	-2.40	121.24	125.03
3	D	903	HEM	O2D-CGD-CBD	2.40	121.58	114.00
3	D	905	HEM	CHA-C4D-ND	2.40	127.33	124.37
3	A	908	HEM	C4C-C3C-C2C	-2.39	104.74	106.81
3	C	903	HEM	C4C-C3C-C2C	-2.38	104.75	106.81
3	B	904[B]	HEM	CMA-C3A-C4A	-2.38	121.79	125.42
3	C	906	HEM	O2A-CGA-O1A	-2.38	117.20	123.33
3	D	908	HEM	C3C-C2C-C1C	2.38	109.30	107.05
3	D	902	HEM	C3B-C4B-NB	-2.38	107.76	109.47
3	D	909	HEM	C1A-CHA-C4D	-2.38	120.66	126.25
3	B	908	HEM	C4B-C3B-C2B	-2.37	105.10	107.28
3	A	904[B]	HEM	CAD-C3D-C4D	2.37	128.83	124.70
3	A	902	HEM	C2B-C1B-NB	-2.37	107.11	109.84
3	D	906	HEM	CBB-CAB-C3B	-2.37	115.68	127.53
3	D	909	HEM	C4C-CHD-C1D	-2.37	120.99	126.02
3	A	904[A]	HEM	CHB-C1B-NB	2.36	127.29	124.37
3	A	904[B]	HEM	CHB-C4A-NA	2.36	128.14	123.86
3	A	909	HEM	CHA-C4D-C3D	-2.35	120.89	125.23
3	A	909	HEM	CHA-C4D-ND	2.35	127.28	124.37
3	D	909	HEM	C3C-C2C-C1C	2.35	109.27	107.05
3	A	905	HEM	CAD-C3D-C4D	2.35	128.78	124.70
3	B	909	HEM	CAB-C3B-C2B	2.34	136.05	128.43
3	C	909	HEM	O2D-CGD-CBD	2.34	121.40	114.00
3	D	909	HEM	CHA-C4D-C3D	-2.34	120.92	125.23
3	C	902	HEM	C4A-CHB-C1B	-2.33	120.77	126.25
3	B	907	HEM	O2A-CGA-CBA	2.32	121.34	114.00
3	D	907	HEM	CMA-C3A-C2A	2.32	130.55	125.62
3	A	904[A]	HEM	O2D-CGD-CBD	2.32	121.33	114.00
3	B	909	HEM	CHB-C4A-NA	2.31	128.06	123.86
3	A	909	HEM	C1A-CHA-C4D	-2.31	120.81	126.25
3	B	905	HEM	O2A-CGA-CBA	2.31	121.30	114.00
3	C	909	HEM	C3B-C4B-NB	-2.30	107.81	109.47
3	C	905	HEM	C4C-NC-C1C	2.30	109.57	105.82
3	D	904[A]	HEM	CHB-C1B-NB	2.30	127.21	124.37
3	D	902	HEM	CHD-C4C-NC	2.30	126.95	124.45
3	D	904[A]	HEM	CHA-C4D-C3D	-2.30	121.00	125.23
3	B	902	HEM	C4C-CHD-C1D	-2.29	121.14	126.02
3	A	905	HEM	CHD-C1D-ND	2.29	126.89	124.42
3	A	904[B]	HEM	CHA-C4D-C3D	-2.29	121.00	125.23
3	C	902	HEM	C4C-CHD-C1D	-2.29	121.16	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	904[B]	HEM	CAD-C3D-C4D	2.28	128.68	124.70
3	C	907	HEM	C4C-NC-C1C	2.28	109.54	105.82
3	D	909	HEM	CHD-C4C-NC	2.28	126.93	124.45
3	B	903	HEM	CHA-C4D-ND	2.28	127.18	124.37
3	D	907	HEM	CHA-C4D-C3D	-2.27	121.04	125.23
3	D	904[B]	HEM	CAA-CBA-CGA	2.27	119.69	113.67
3	A	902	HEM	C3B-C2B-C1B	2.27	108.11	106.41
3	C	902	HEM	CHD-C1D-C2D	-2.26	121.45	125.03
3	C	909	HEM	C2A-C1A-NA	-2.26	107.65	110.15
3	C	909	HEM	C1D-C2D-C3D	-2.26	104.61	106.98
3	B	904[B]	HEM	CHA-C1A-NA	2.25	127.94	123.86
3	C	906	HEM	CHD-C1D-C2D	-2.25	121.48	125.03
3	B	904[A]	HEM	CHA-C4D-C3D	-2.25	121.08	125.23
3	C	903	HEM	CAD-CBD-CGD	2.24	119.61	113.67
3	D	903	HEM	C4C-NC-C1C	2.24	109.48	105.82
3	A	909	HEM	O2D-CGD-CBD	2.24	121.08	114.00
3	B	907	HEM	CAD-CBD-CGD	-2.24	107.72	113.67
3	A	903	HEM	O2A-CGA-CBA	2.23	121.06	114.00
3	C	902	HEM	O2D-CGD-O1D	-2.23	117.59	123.33
3	B	909	HEM	CMA-C3A-C2A	2.23	130.34	125.62
3	B	908	HEM	CHB-C1B-NB	2.22	127.12	124.37
3	A	903	HEM	C1C-CHC-C4B	-2.22	121.30	126.02
3	B	907	HEM	CHA-C4D-C3D	-2.22	121.14	125.23
3	D	903	HEM	CAD-C3D-C2D	2.21	132.01	127.87
3	B	909	HEM	C4B-C3B-C2B	-2.21	105.25	107.28
3	A	904[A]	HEM	CBB-CAB-C3B	-2.21	116.47	127.53
3	D	904[B]	HEM	CMA-C3A-C4A	-2.21	122.06	125.42
3	A	908	HEM	CHA-C4D-ND	2.20	127.09	124.37
3	B	903	HEM	CMD-C2D-C3D	2.20	132.10	126.15
3	B	904[A]	HEM	C4A-NA-C1A	2.20	109.40	105.82
3	C	907	HEM	C3B-C4B-NB	-2.19	107.89	109.47
3	D	903	HEM	CHA-C4D-C3D	-2.19	121.19	125.23
3	C	908	HEM	CHA-C4D-C3D	-2.19	121.19	125.23
3	A	906	HEM	C3B-C4B-NB	-2.19	107.90	109.47
3	A	903	HEM	CMA-C3A-C2A	2.19	130.26	125.62
3	A	903	HEM	CBD-CAD-C3D	2.18	118.56	112.53
3	A	904[A]	HEM	C4C-CHD-C1D	-2.18	121.39	126.02
3	A	904[A]	HEM	CHA-C1A-NA	2.18	127.81	123.86
3	B	902	HEM	C4B-C3B-C2B	-2.18	105.28	107.28
3	C	904[B]	HEM	CAD-CBD-CGD	-2.18	107.89	113.67
3	D	904[A]	HEM	C4C-NC-C1C	2.18	109.37	105.82
3	A	908	HEM	C4C-NC-C1C	2.17	109.36	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	906	HEM	CHA-C4D-C3D	-2.17	121.22	125.23
3	D	903	HEM	CHC-C4B-NB	2.17	126.76	124.42
3	D	903	HEM	C4D-ND-C1D	-2.17	102.64	105.21
3	B	904[A]	HEM	C4C-NC-C1C	2.16	109.35	105.82
3	C	906	HEM	CHA-C4D-ND	2.16	127.04	124.37
3	C	906	HEM	CAA-CBA-CGA	-2.16	107.94	113.67
3	A	902	HEM	CAA-CBA-CGA	2.16	119.39	113.67
3	A	905	HEM	CHC-C4B-NB	2.16	126.75	124.42
3	A	902	HEM	O2A-CGA-CBA	2.16	120.82	114.00
3	C	909	HEM	CHB-C4A-NA	2.16	127.77	123.86
3	A	909	HEM	CHB-C1B-NB	2.16	127.04	124.37
3	B	904[A]	HEM	C3B-C2B-C1B	-2.16	104.79	106.41
3	A	907	HEM	C2B-C1B-NB	-2.15	107.36	109.84
3	A	905	HEM	C1A-CHA-C4D	-2.15	121.19	126.25
3	A	904[B]	HEM	C4C-CHD-C1D	-2.15	121.46	126.02
3	D	904[A]	HEM	C4D-C3D-C2D	-2.14	103.77	106.89
3	C	908	HEM	O2D-CGD-CBD	2.14	120.77	114.00
3	D	909	HEM	CAD-C3D-C2D	-2.13	123.87	127.87
3	B	907	HEM	CHA-C4D-ND	2.13	127.00	124.37
3	A	909	HEM	CHB-C4A-NA	2.13	127.72	123.86
3	C	904[A]	HEM	CMA-C3A-C4A	-2.13	122.18	125.42
3	D	908	HEM	C3D-C4D-ND	2.13	112.50	110.17
3	A	909	HEM	C4C-CHD-C1D	-2.12	121.50	126.02
3	D	908	HEM	CHD-C4C-NC	2.12	126.76	124.45
3	A	904[B]	HEM	CHB-C1B-NB	2.12	126.99	124.37
3	B	905	HEM	CHB-C1B-NB	2.12	126.98	124.37
3	B	907	HEM	C1A-CHA-C4D	-2.11	121.28	126.25
3	B	903	HEM	C2D-C1D-ND	2.11	112.34	109.90
3	A	904[A]	HEM	C4A-CHB-C1B	-2.11	121.28	126.25
3	A	904[A]	HEM	O2D-CGD-O1D	-2.11	117.90	123.33
3	D	902	HEM	O2A-CGA-CBA	2.11	120.67	114.00
3	C	904[B]	HEM	C4A-CHB-C1B	-2.11	121.29	126.25
3	C	905	HEM	C1A-CHA-C4D	-2.11	121.29	126.25
3	D	904[B]	HEM	CHB-C1B-NB	2.11	126.97	124.37
3	A	904[B]	HEM	O2D-CGD-CBD	2.10	120.64	114.00
3	B	902	HEM	C1A-CHA-C4D	-2.10	121.31	126.25
3	D	904[A]	HEM	CHB-C4A-NA	2.10	127.67	123.86
3	D	904[A]	HEM	C3D-C4D-ND	2.10	112.47	110.17
3	C	907	HEM	CBB-CAB-C3B	-2.09	117.06	127.53
3	A	905	HEM	CAD-C3D-C2D	-2.09	123.95	127.87
3	D	909	HEM	O1D-CGD-CBD	-2.09	116.46	123.09
3	D	907	HEM	CHA-C4D-ND	2.09	126.95	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	904[B]	HEM	CHA-C1A-NA	2.09	127.65	123.86
3	B	909	HEM	C1A-CHA-C4D	-2.09	121.34	126.25
3	B	903	HEM	CMD-C2D-C1D	-2.08	121.78	125.03
3	C	908	HEM	CBB-CAB-C3B	-2.08	117.11	127.53
3	D	906	HEM	CHD-C1D-ND	2.08	126.67	124.42
3	B	903	HEM	C1A-CHA-C4D	-2.08	121.36	126.25
3	A	903	HEM	CMA-C3A-C4A	-2.08	122.26	125.42
3	D	902	HEM	O1A-CGA-CBA	-2.07	116.53	123.09
3	B	904[A]	HEM	CBA-CAA-C2A	-2.07	106.81	112.53
3	C	902	HEM	CMA-C3A-C4A	-2.06	122.28	125.42
3	C	907	HEM	CAC-C3C-C4C	-2.06	119.91	124.82
3	B	908	HEM	CMB-C2B-C1B	2.06	128.25	125.03
3	A	904[B]	HEM	CBB-CAB-C3B	-2.06	117.25	127.53
3	C	907	HEM	C4C-CHD-C1D	-2.06	121.65	126.02
3	B	906	HEM	CAA-CBA-CGA	-2.05	108.22	113.67
3	B	907	HEM	CBB-CAB-C3B	-2.05	117.28	127.53
3	A	904[B]	HEM	CMA-C3A-C4A	-2.05	122.30	125.42
3	A	908	HEM	CHC-C4B-C3B	-2.05	120.98	125.07
3	C	904[B]	HEM	CHB-C4A-NA	2.05	127.58	123.86
3	C	902	HEM	CHD-C4C-NC	2.05	126.68	124.45
3	A	904[B]	HEM	O2A-CGA-O1A	-2.05	118.06	123.33
3	A	907	HEM	CBB-CAB-C3B	-2.05	117.30	127.53
3	D	907	HEM	CHC-C4B-C3B	-2.05	120.99	125.07
3	C	909	HEM	CAA-CBA-CGA	-2.04	108.24	113.67
3	C	909	HEM	CAD-C3D-C2D	-2.04	124.04	127.87
3	A	905	HEM	C3C-C2C-C1C	2.04	108.98	107.05
3	D	903	HEM	C3B-C2B-C1B	2.04	107.94	106.41
3	C	905	HEM	C3B-C2B-C1B	2.04	107.94	106.41
3	B	909	HEM	CHC-C4B-C3B	-2.03	121.01	125.07
3	A	905	HEM	O2D-CGD-CBD	2.03	120.41	114.00
3	A	904[B]	HEM	CHA-C4D-ND	2.03	126.88	124.37
3	D	906	HEM	CHA-C4D-C3D	-2.03	121.49	125.23
3	A	906	HEM	C4B-C3B-C2B	-2.02	105.42	107.28
3	A	908	HEM	CBB-CAB-C3B	-2.02	117.42	127.53
3	B	907	HEM	C2B-C1B-NB	-2.01	107.53	109.84
3	C	903	HEM	CMD-C2D-C3D	2.01	131.59	126.15
3	A	902	HEM	C1A-CHA-C4D	-2.01	121.53	126.25
3	B	907	HEM	O2A-CGA-O1A	-2.01	118.17	123.33
3	A	902	HEM	C4C-CHD-C1D	-2.00	121.76	126.02
3	C	903	HEM	CHB-C1B-C2B	-2.00	121.25	126.95
3	A	908	HEM	C3C-C2C-C1C	2.00	108.94	107.05
3	C	903	HEM	O2D-CGD-CBD	2.00	120.32	114.00

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	903	HEM	C4D-C3D-CAD-CBD
3	C	903	HEM	C4D-C3D-CAD-CBD
3	C	904[A]	HEM	C1A-C2A-CAA-CBA
3	D	903	HEM	C4D-C3D-CAD-CBD
3	A	903	HEM	C2D-C3D-CAD-CBD
3	B	903	HEM	C2D-C3D-CAD-CBD
3	C	903	HEM	C2D-C3D-CAD-CBD
3	D	903	HEM	C2D-C3D-CAD-CBD
3	A	903	HEM	C4D-C3D-CAD-CBD
3	D	909	HEM	C2A-CAA-CBA-CGA
3	D	909	HEM	C3D-CAD-CBD-CGD
3	C	906	HEM	C4B-C3B-CAB-CBB
3	D	906	HEM	C4B-C3B-CAB-CBB
3	B	909	HEM	C3D-CAD-CBD-CGD
3	C	904[A]	HEM	C3A-C2A-CAA-CBA
3	A	902	HEM	C2A-CAA-CBA-CGA
3	B	902	HEM	C2A-CAA-CBA-CGA
3	D	902	HEM	C2A-CAA-CBA-CGA
3	A	909	HEM	C3D-CAD-CBD-CGD
3	A	902	HEM	C4B-C3B-CAB-CBB
3	B	902	HEM	C4B-C3B-CAB-CBB
3	B	906	HEM	C4B-C3B-CAB-CBB
3	C	902	HEM	C4B-C3B-CAB-CBB
3	C	904[A]	HEM	C2D-C3D-CAD-CBD
3	C	904[A]	HEM	C4D-C3D-CAD-CBD
3	A	907	HEM	CAD-CBD-CGD-O2D
3	A	907	HEM	C4B-C3B-CAB-CBB
3	A	908	HEM	C4B-C3B-CAB-CBB
3	B	907	HEM	C4B-C3B-CAB-CBB
3	C	907	HEM	C4B-C3B-CAB-CBB
3	C	908	HEM	C4B-C3B-CAB-CBB
3	D	902	HEM	C4B-C3B-CAB-CBB
3	D	908	HEM	C4B-C3B-CAB-CBB
3	D	907	HEM	CAD-CBD-CGD-O1D
3	B	907	HEM	CAD-CBD-CGD-O1D
3	C	909	HEM	CAA-CBA-CGA-O1A
3	B	904[B]	HEM	CAA-CBA-CGA-O1A
3	B	904[B]	HEM	CAA-CBA-CGA-O2A
3	B	906	HEM	CAA-CBA-CGA-O2A
3	B	909	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	C	909	HEM	CAD-CBD-CGD-O1D
3	B	905	HEM	CAD-CBD-CGD-O1D
3	D	907	HEM	CAD-CBD-CGD-O2D
3	A	907	HEM	CAD-CBD-CGD-O1D
3	A	909	HEM	CAA-CBA-CGA-O2A
3	B	908	HEM	CAD-CBD-CGD-O2D
3	B	909	HEM	CAD-CBD-CGD-O1D
3	A	905	HEM	CAD-CBD-CGD-O1D
3	C	909	HEM	CAA-CBA-CGA-O2A
3	D	904[A]	HEM	CAA-CBA-CGA-O1A
3	D	905	HEM	CAD-CBD-CGD-O1D
3	C	902	HEM	C2A-CAA-CBA-CGA
3	A	904[A]	HEM	CAA-CBA-CGA-O1A
3	B	904[A]	HEM	CAA-CBA-CGA-O1A
3	C	904[B]	HEM	CAA-CBA-CGA-O2A
3	C	905	HEM	CAD-CBD-CGD-O1D
3	D	906	HEM	CAA-CBA-CGA-O2A
3	B	907	HEM	CAD-CBD-CGD-O2D
3	B	908	HEM	CAA-CBA-CGA-O1A
3	D	909	HEM	CAD-CBD-CGD-O2D
3	A	904[B]	HEM	CAA-CBA-CGA-O1A
3	D	908	HEM	CAD-CBD-CGD-O1D
3	A	904[A]	HEM	CAA-CBA-CGA-O2A
3	D	909	HEM	CAA-CBA-CGA-O2A
3	B	904[A]	HEM	CAA-CBA-CGA-O2A
3	C	909	HEM	CAD-CBD-CGD-O2D
3	D	909	HEM	CAD-CBD-CGD-O1D
3	A	905	HEM	CAD-CBD-CGD-O2D
3	D	904[B]	HEM	CAA-CBA-CGA-O2A
3	A	908	HEM	CAD-CBD-CGD-O2D
3	B	906	HEM	CAA-CBA-CGA-O1A
3	B	908	HEM	CAA-CBA-CGA-O2A
3	A	909	HEM	CAA-CBA-CGA-O1A
3	C	908	HEM	CAD-CBD-CGD-O2D
3	C	904[B]	HEM	C2D-C3D-CAD-CBD
3	C	905	HEM	CAD-CBD-CGD-O2D
3	C	907	HEM	CAD-CBD-CGD-O2D
3	D	906	HEM	CAA-CBA-CGA-O1A
3	D	909	HEM	CAA-CBA-CGA-O1A
3	D	904[B]	HEM	CAA-CBA-CGA-O1A
3	B	909	HEM	CAA-CBA-CGA-O1A
3	C	906	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	D	905	HEM	CAD-CBD-CGD-O2D
3	B	905	HEM	CAD-CBD-CGD-O2D
3	D	904[A]	HEM	CAA-CBA-CGA-O2A
3	A	908	HEM	CAD-CBD-CGD-O1D
3	B	908	HEM	CAD-CBD-CGD-O1D
3	C	904[B]	HEM	CAA-CBA-CGA-O1A
3	A	904[B]	HEM	CAA-CBA-CGA-O2A
3	B	909	HEM	CAA-CBA-CGA-O2A
3	C	908	HEM	CAA-CBA-CGA-O2A
3	A	906	HEM	C4B-C3B-CAB-CBB
3	A	906	HEM	C4C-C3C-CAC-CBC
3	A	909	HEM	C4B-C3B-CAB-CBB
3	A	909	HEM	C4C-C3C-CAC-CBC
3	B	904[A]	HEM	C4B-C3B-CAB-CBB
3	B	904[B]	HEM	C4B-C3B-CAB-CBB
3	B	908	HEM	C4B-C3B-CAB-CBB
3	B	909	HEM	C4B-C3B-CAB-CBB
3	B	909	HEM	C4C-C3C-CAC-CBC
3	C	909	HEM	C4B-C3B-CAB-CBB
3	D	907	HEM	C4B-C3B-CAB-CBB
3	D	908	HEM	C4C-C3C-CAC-CBC
3	D	909	HEM	C4B-C3B-CAB-CBB
3	C	908	HEM	CAD-CBD-CGD-O1D
3	C	907	HEM	CAD-CBD-CGD-O1D
3	C	908	HEM	CAA-CBA-CGA-O1A
3	A	906	HEM	CAA-CBA-CGA-O2A
3	C	906	HEM	CAA-CBA-CGA-O2A
3	A	906	HEM	CAA-CBA-CGA-O1A
3	D	908	HEM	CAD-CBD-CGD-O2D
3	A	908	HEM	CAA-CBA-CGA-O2A
3	D	908	HEM	CAA-CBA-CGA-O2A
3	D	908	HEM	CAA-CBA-CGA-O1A
3	B	902	HEM	CAD-CBD-CGD-O2D
3	D	904[A]	HEM	CAD-CBD-CGD-O1D
3	A	908	HEM	CAA-CBA-CGA-O1A
3	D	904[A]	HEM	CAD-CBD-CGD-O2D
3	B	908	HEM	C2B-C3B-CAB-CBB
3	C	906	HEM	C2B-C3B-CAB-CBB
3	D	908	HEM	C2B-C3B-CAB-CBB
3	D	903	HEM	CAD-CBD-CGD-O2D

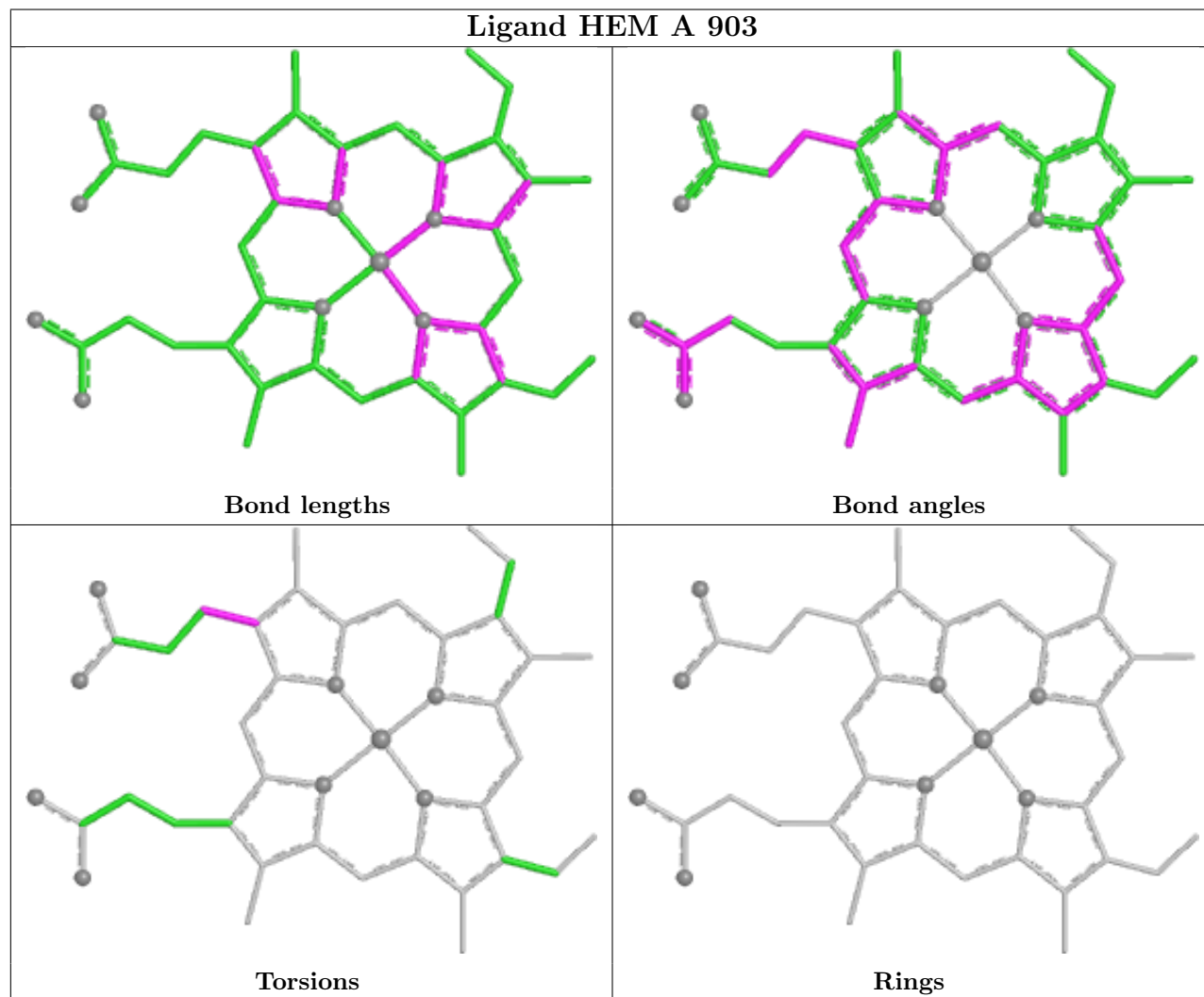
There are no ring outliers.

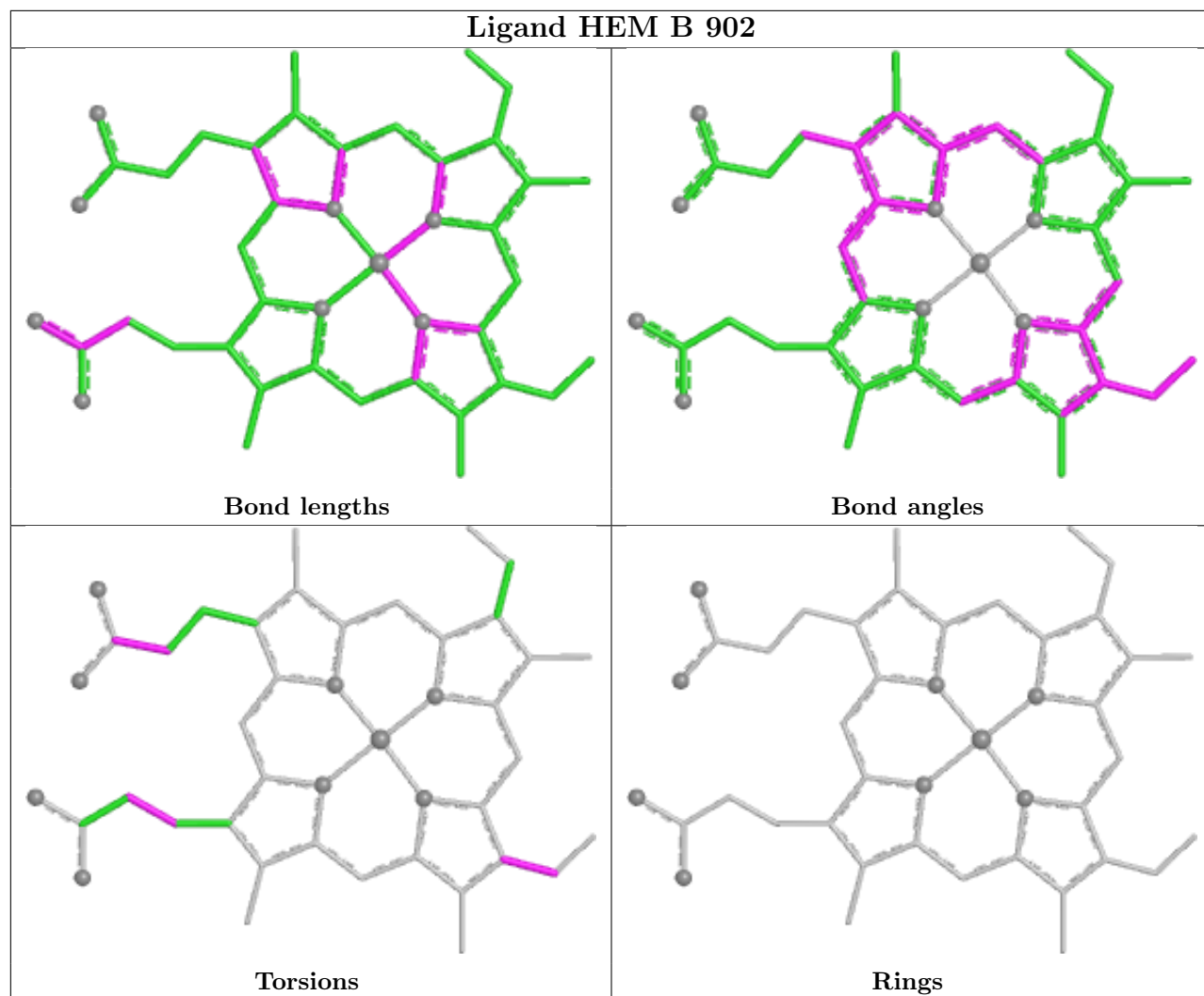
39 monomers are involved in 230 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	HEM	11	0
3	B	902	HEM	5	0
3	B	904[A]	HEM	8	0
3	C	908	HEM	4	0
3	B	907	HEM	4	0
3	D	906	HEM	5	0
3	C	904[A]	HEM	9	0
3	B	904[B]	HEM	7	0
3	B	903	HEM	13	0
3	C	907	HEM	4	0
3	C	904[B]	HEM	4	0
3	D	903	HEM	16	0
3	B	906	HEM	4	0
5	D	912	SO3	3	0
3	A	908	HEM	4	0
3	C	909	HEM	9	0
3	C	905	HEM	7	0
3	A	902	HEM	5	0
3	D	905	HEM	9	0
3	D	907	HEM	4	0
3	A	909	HEM	4	0
3	D	908	HEM	4	0
5	B	911	SO3	1	0
3	A	904[A]	HEM	8	0
3	A	905	HEM	5	0
5	C	911	SO3	1	0
5	A	912	SO3	1	0
3	D	902	HEM	5	0
3	A	904[B]	HEM	7	0
3	D	909	HEM	4	0
3	C	903	HEM	14	0
3	B	909	HEM	10	0
3	C	906	HEM	4	0
3	C	902	HEM	5	0
3	A	907	HEM	5	0
3	D	904[A]	HEM	5	0
3	A	906	HEM	5	0
3	D	904[B]	HEM	5	0
3	B	908	HEM	4	0

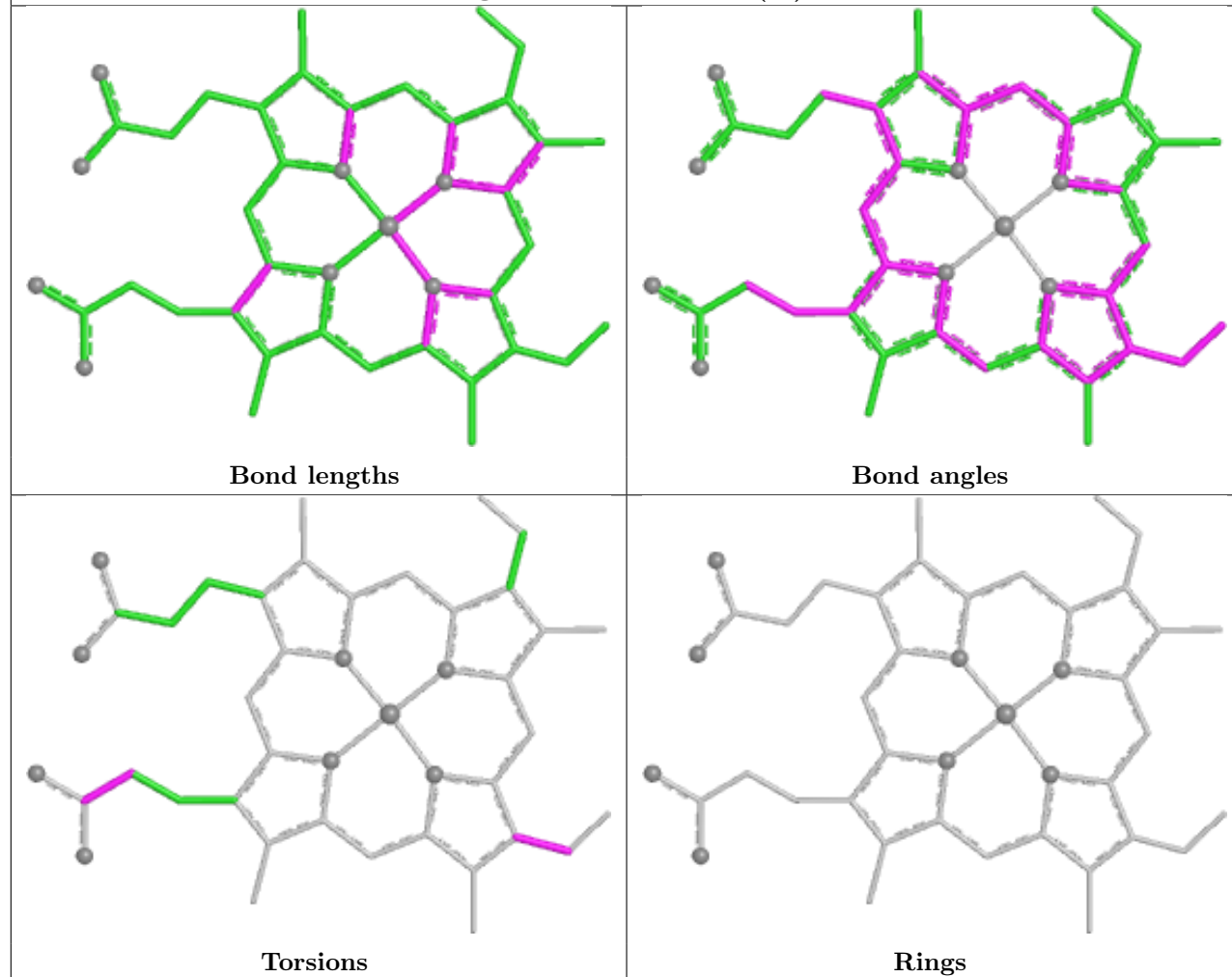
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

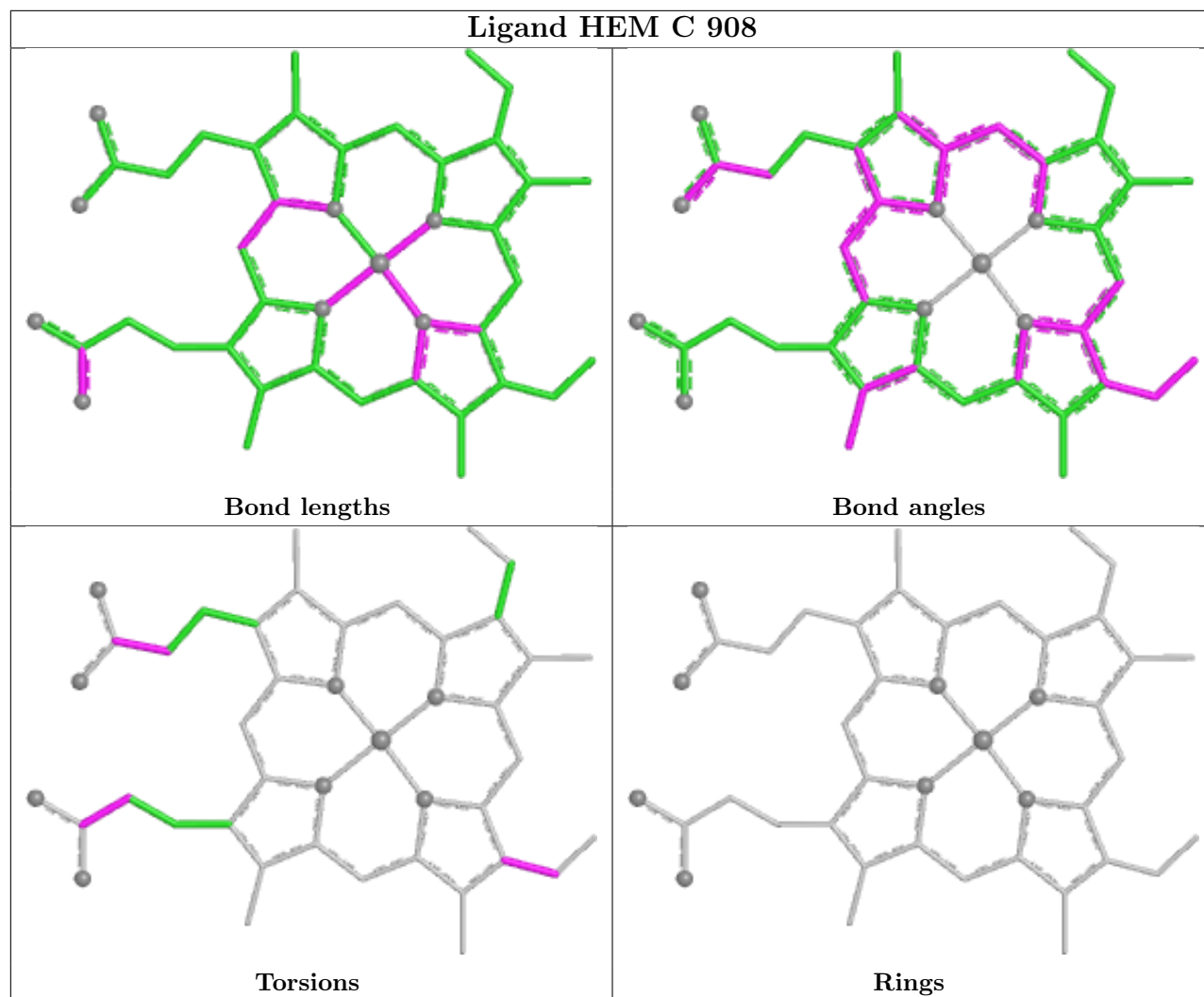
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

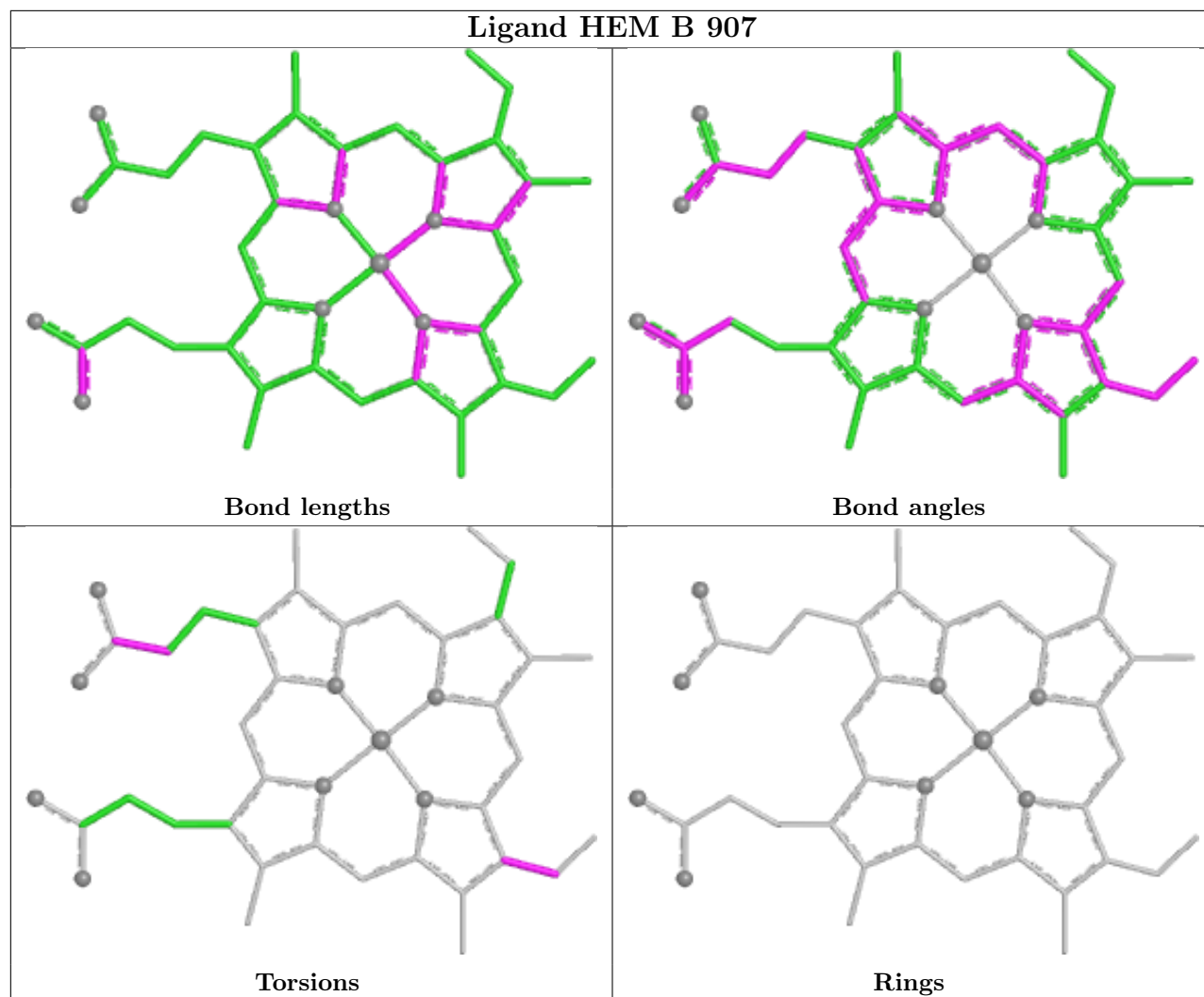


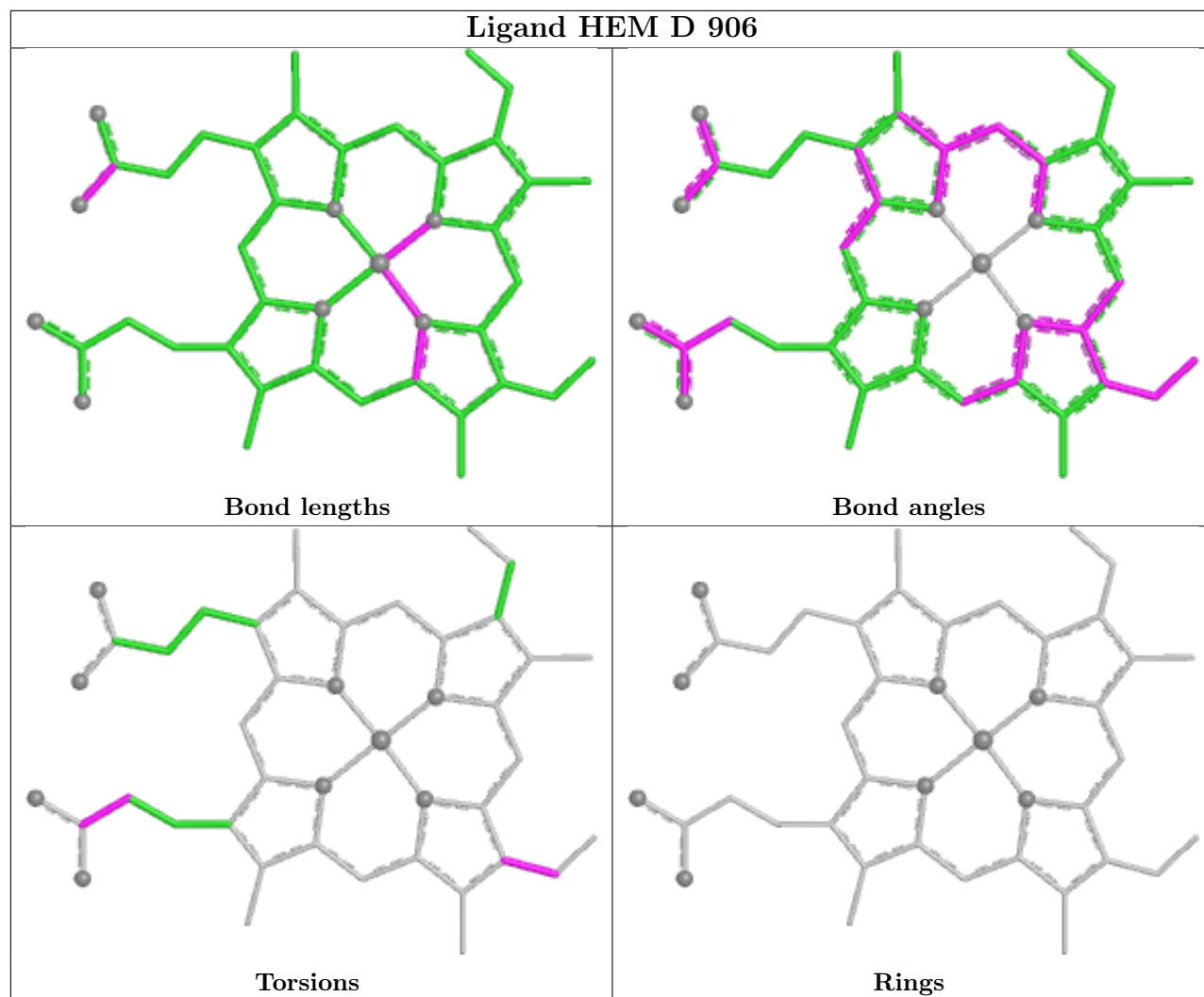


Ligand HEM B 904 (A)

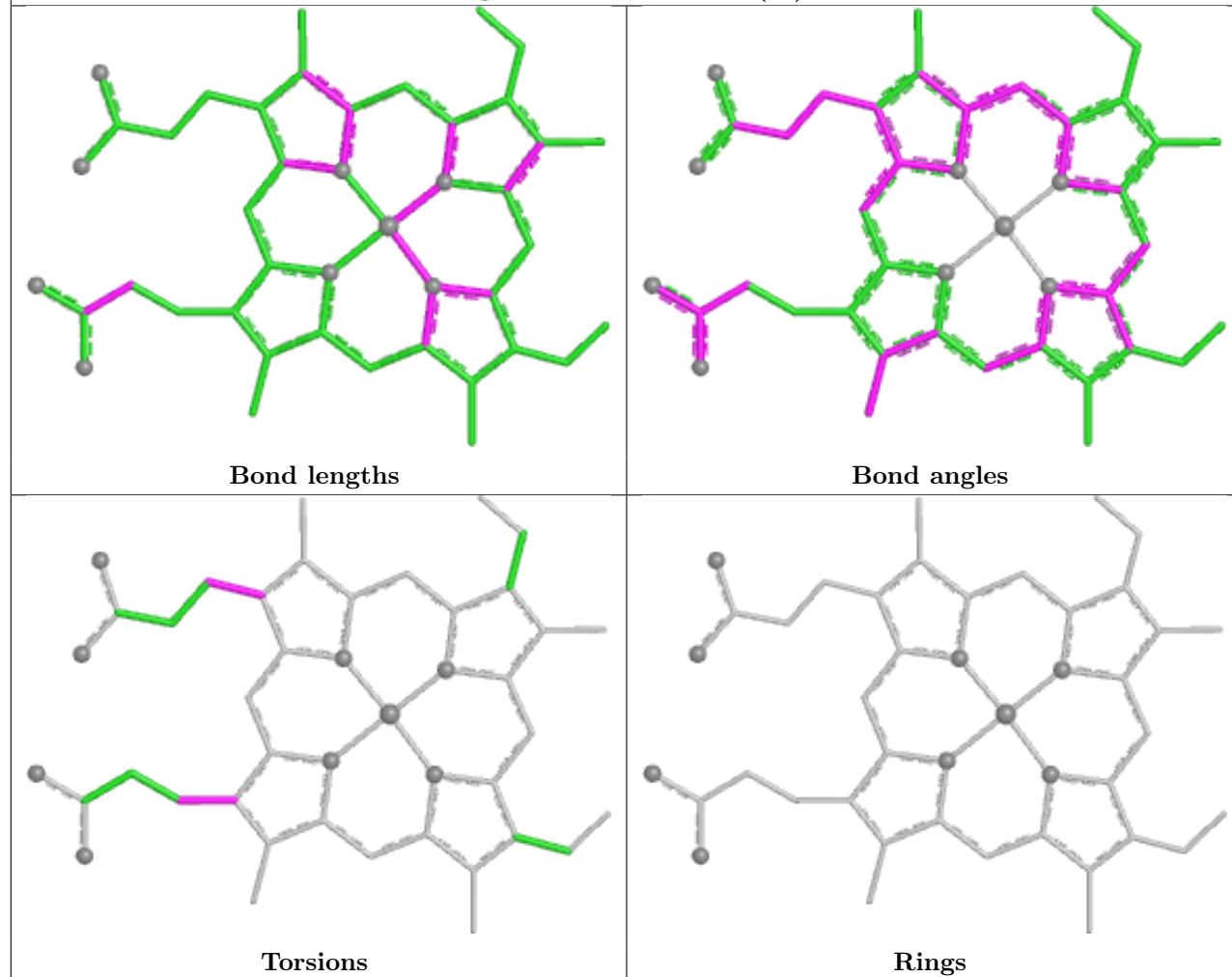




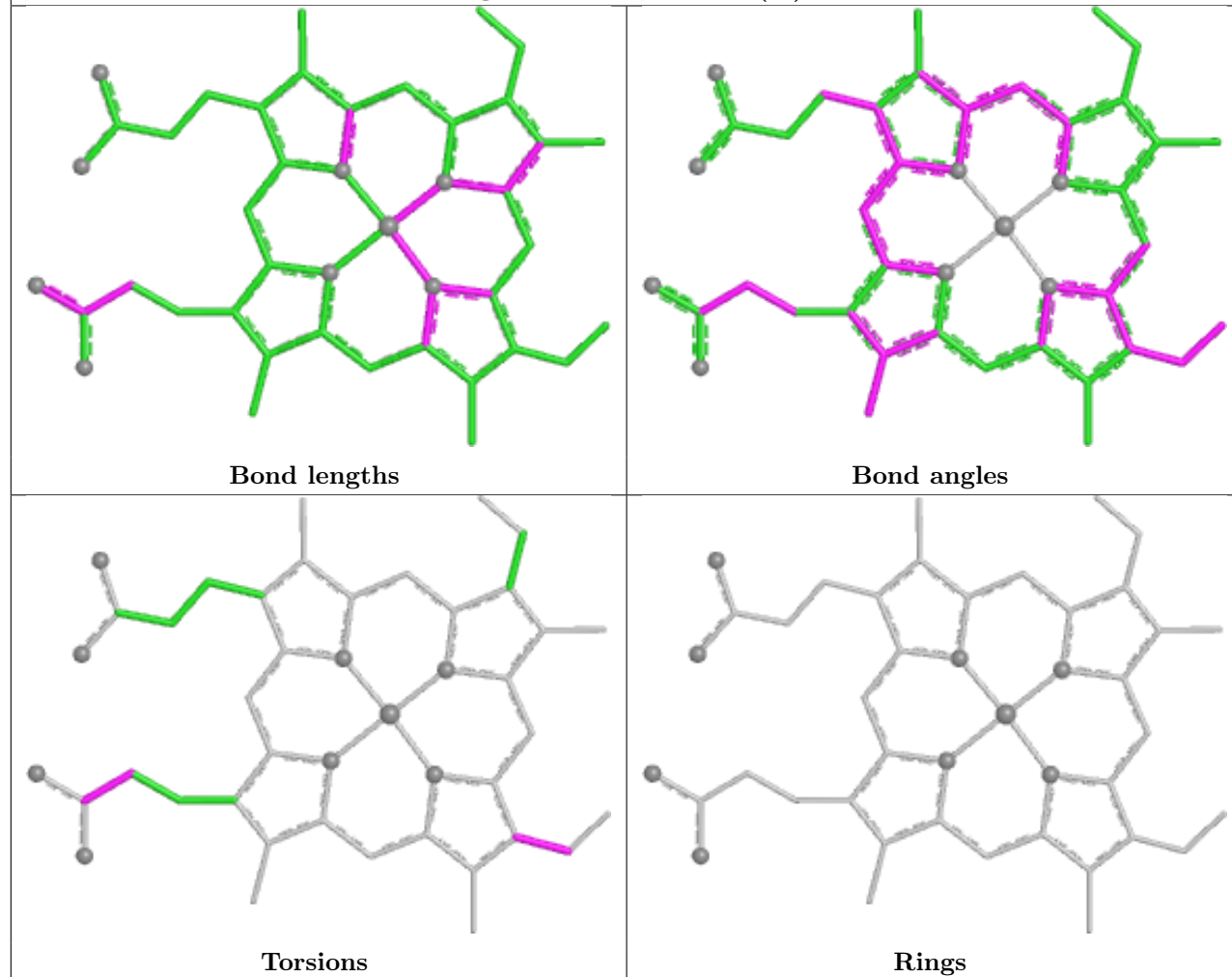


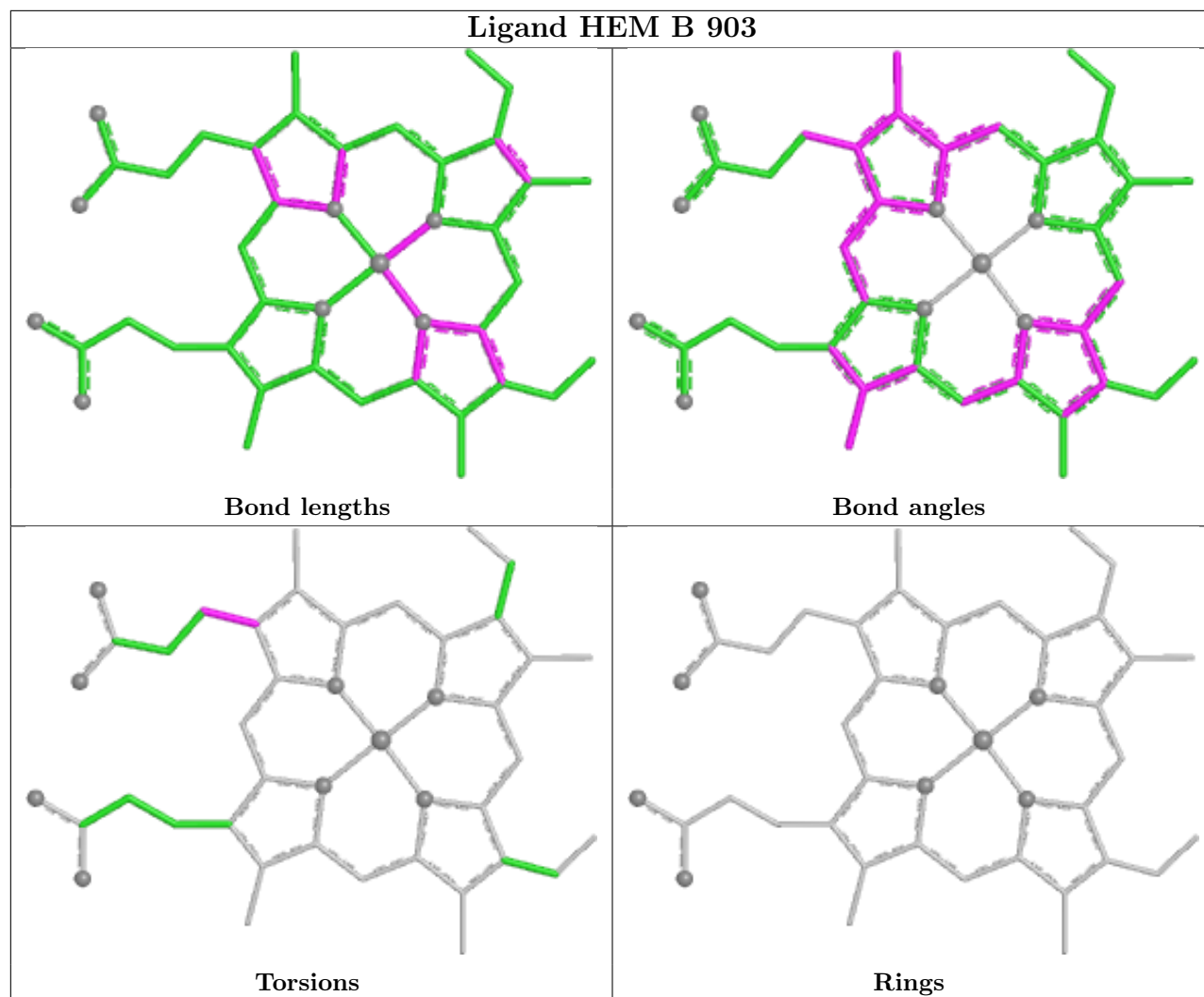


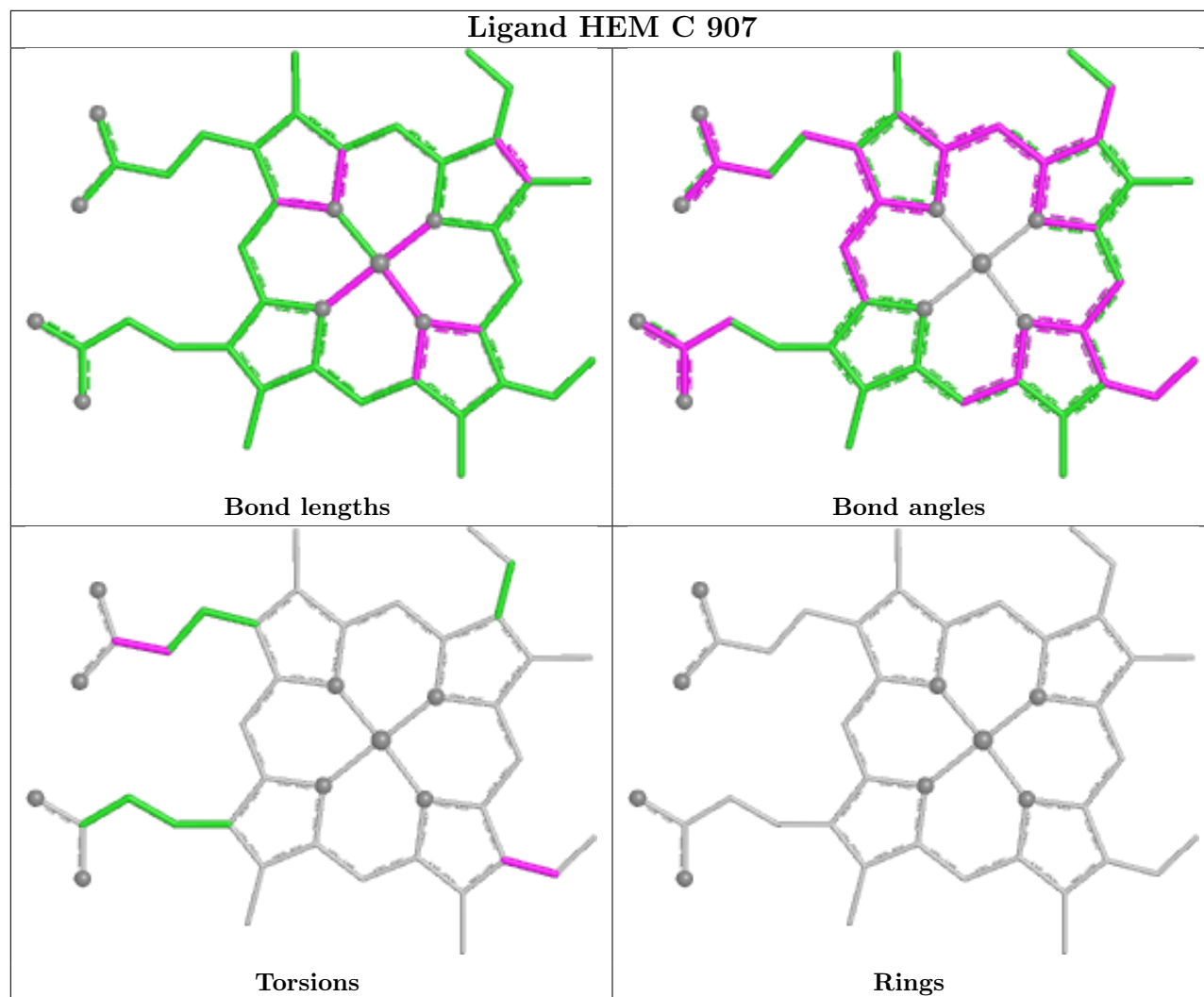
Ligand HEM C 904 (A)



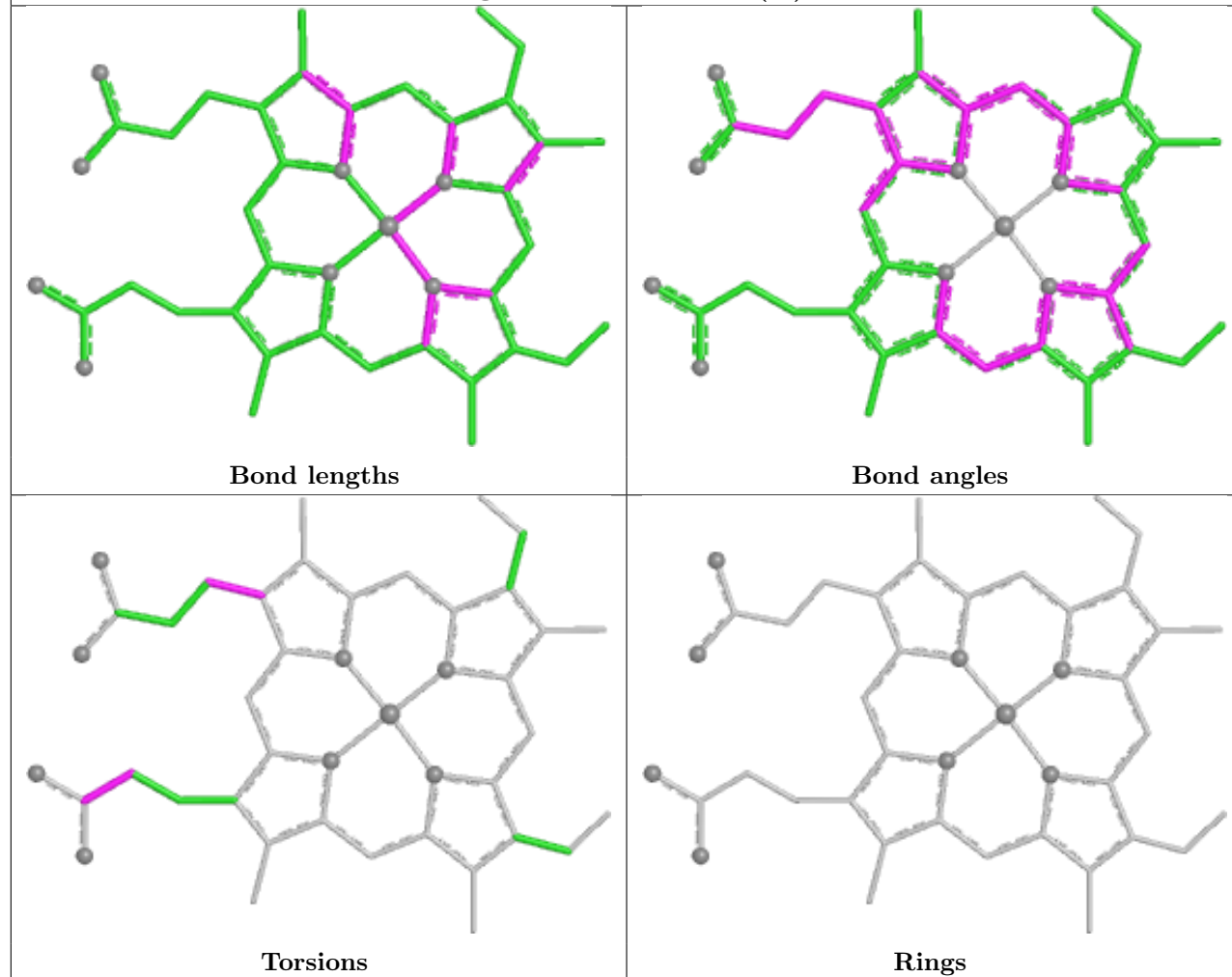
Ligand HEM B 904 (B)

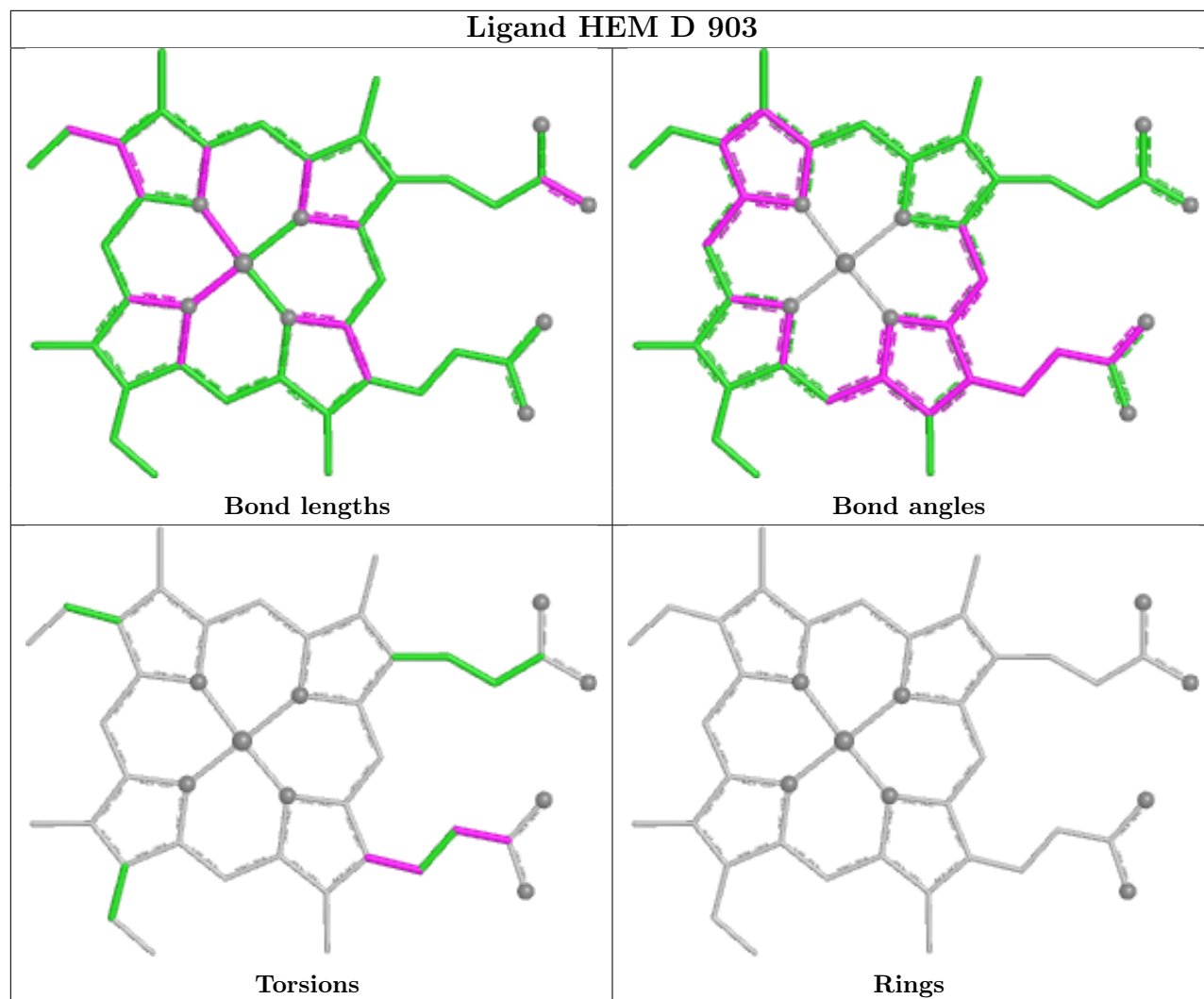


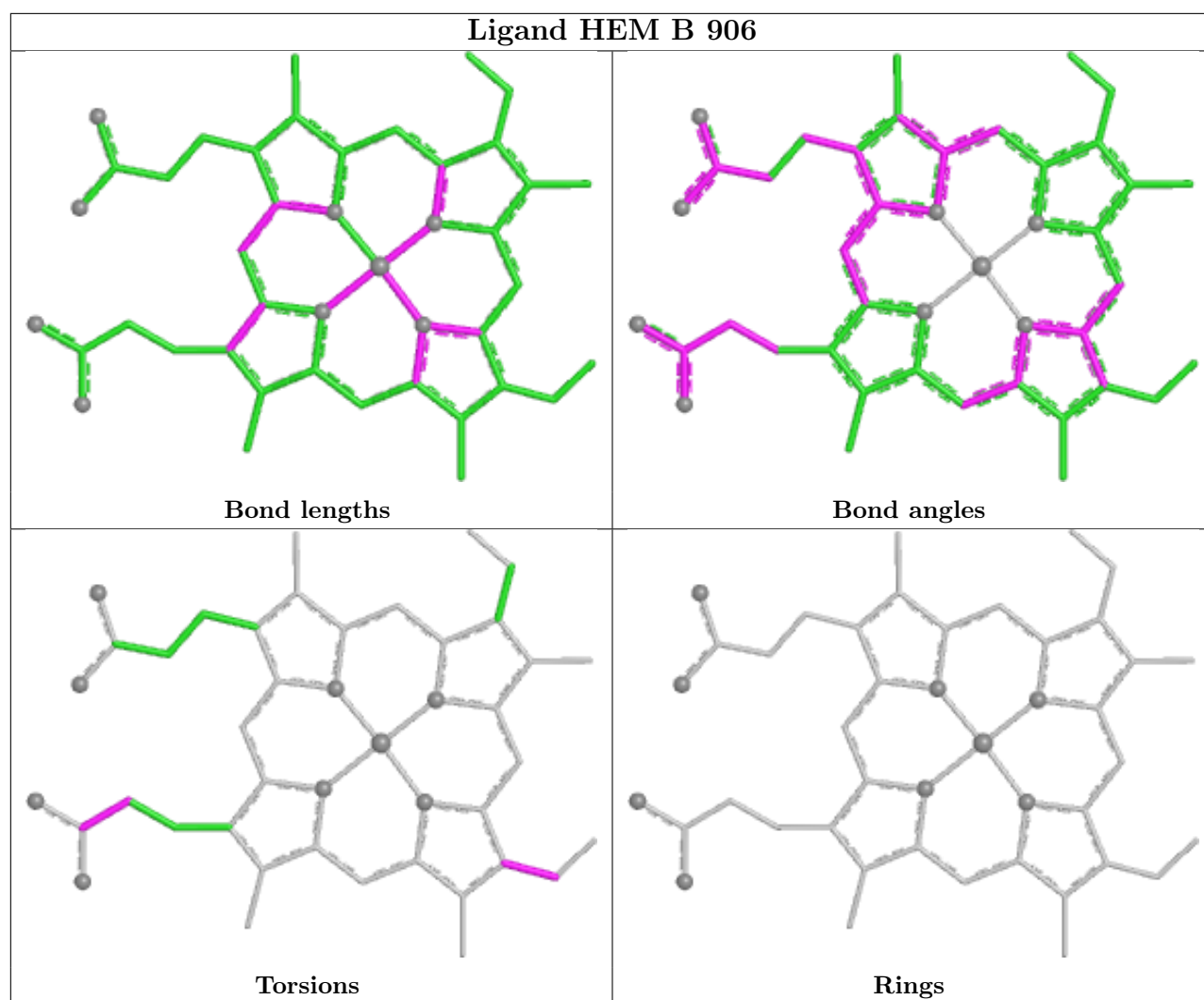


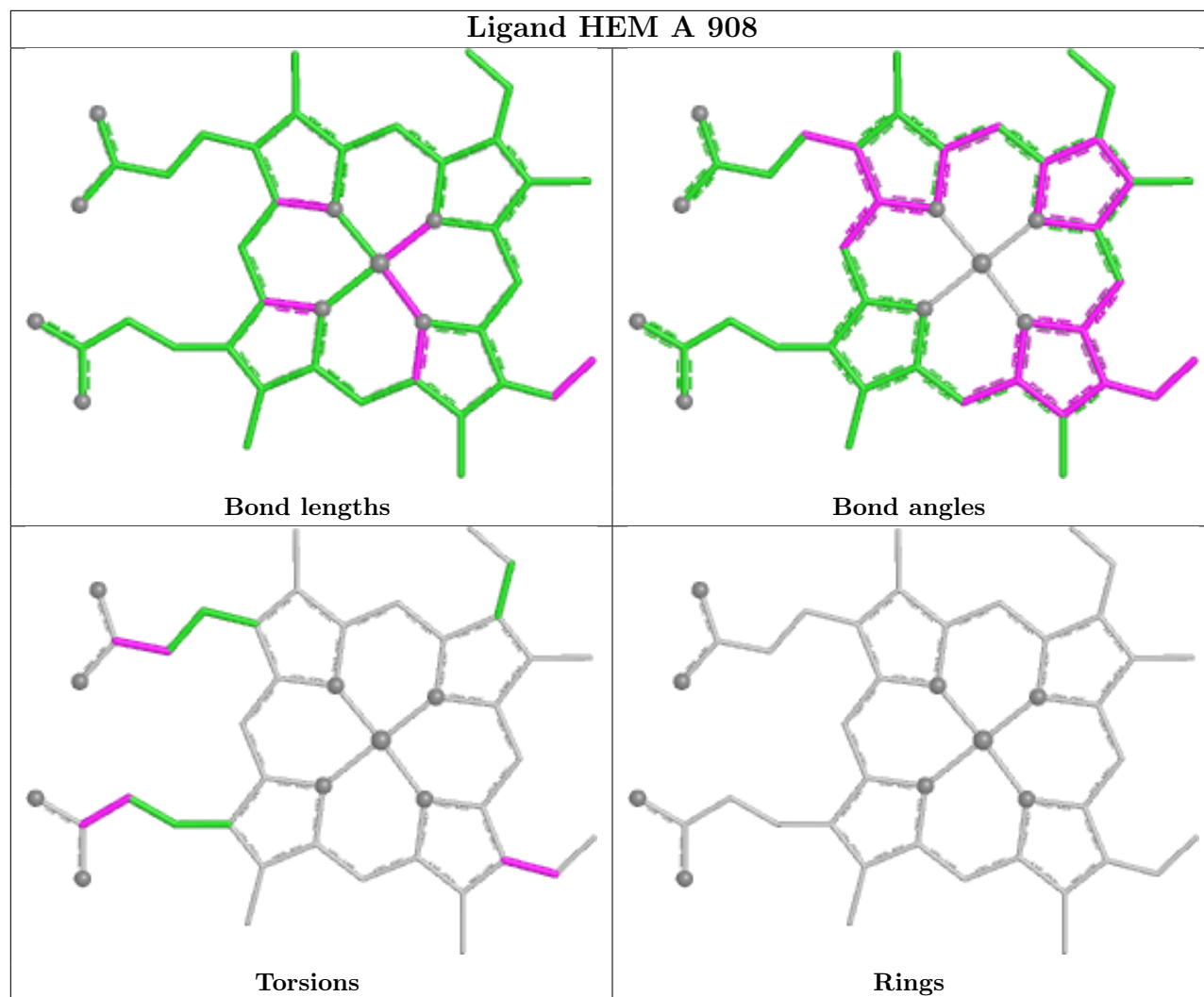


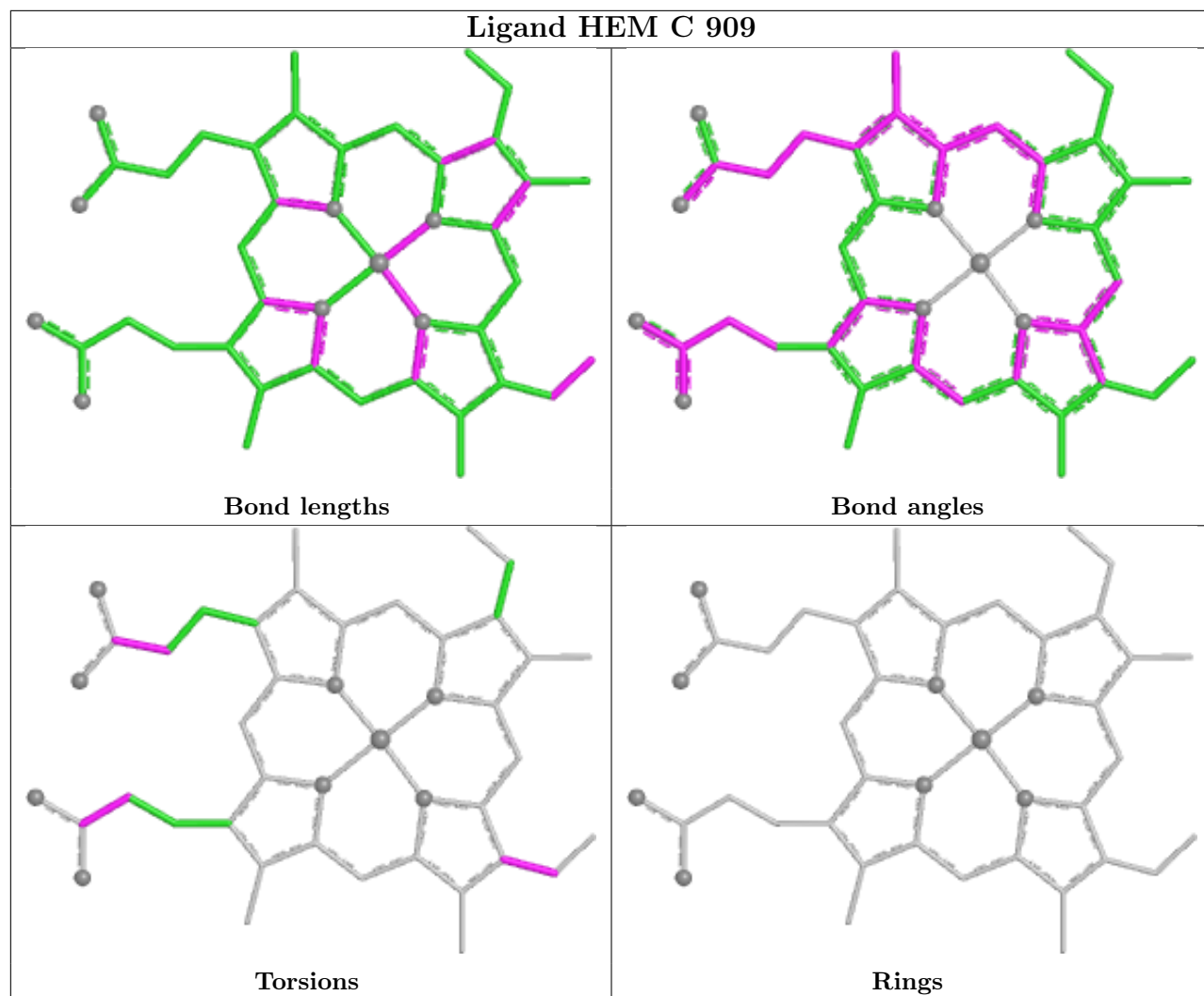
Ligand HEM C 904 (B)

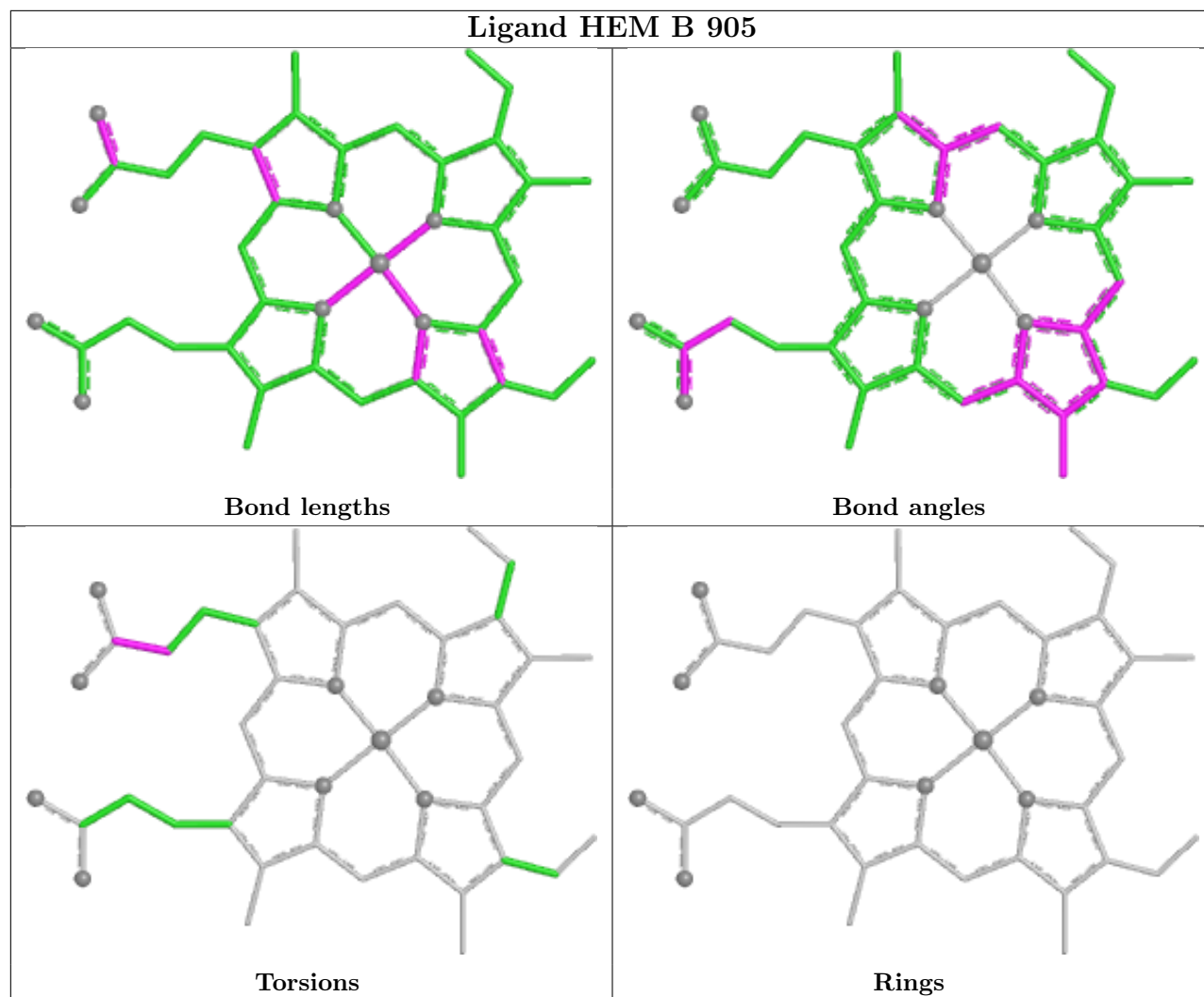


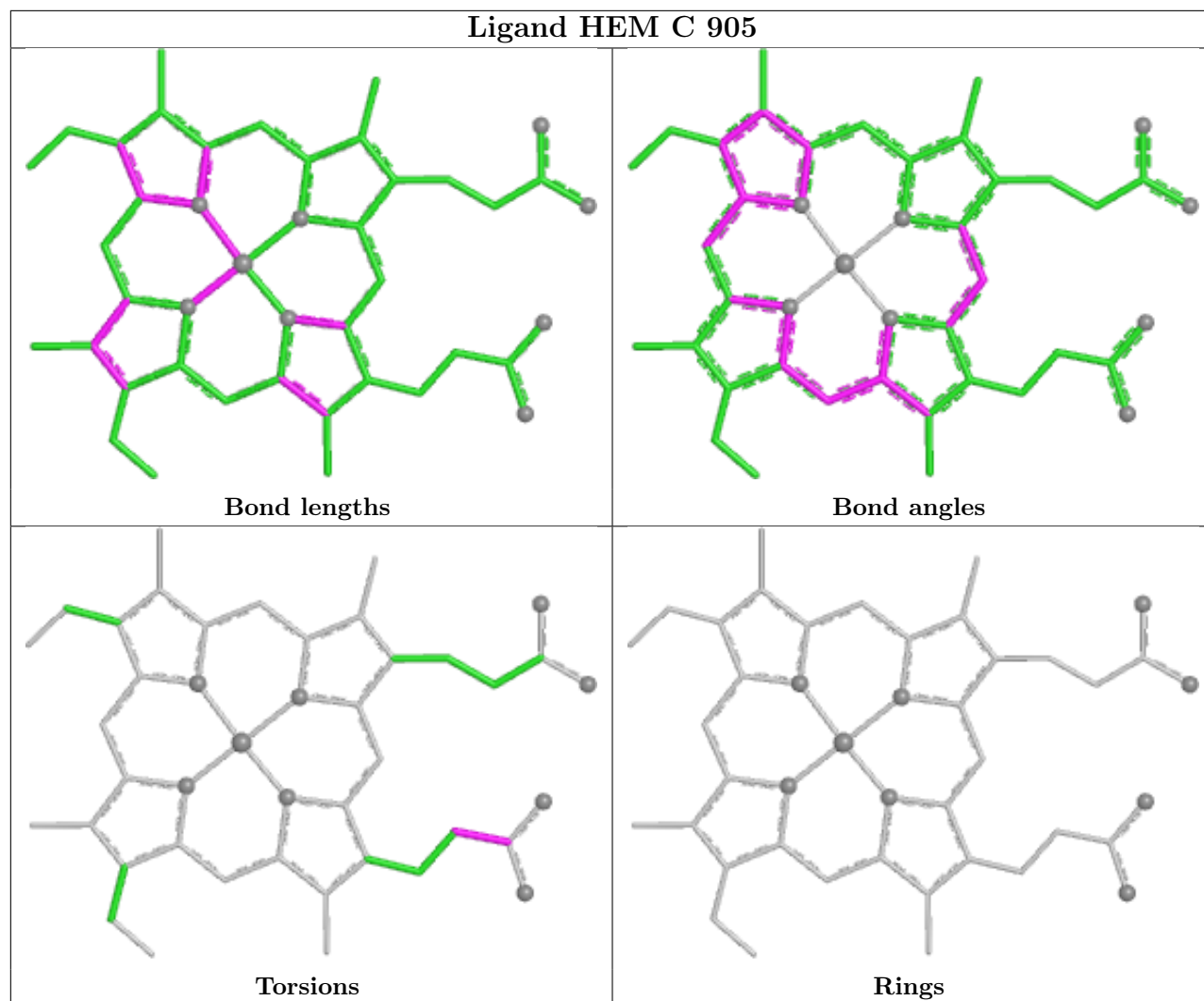


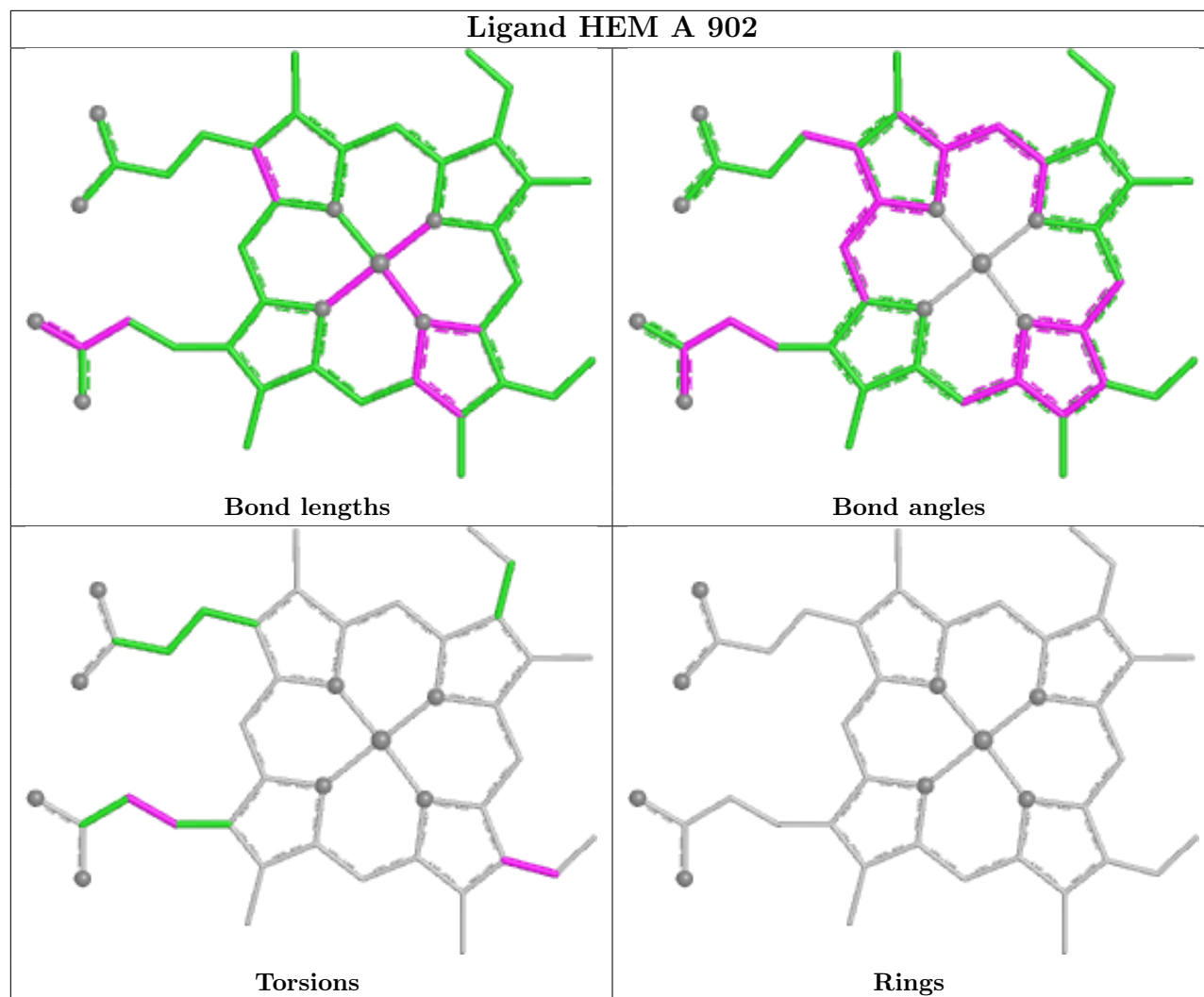


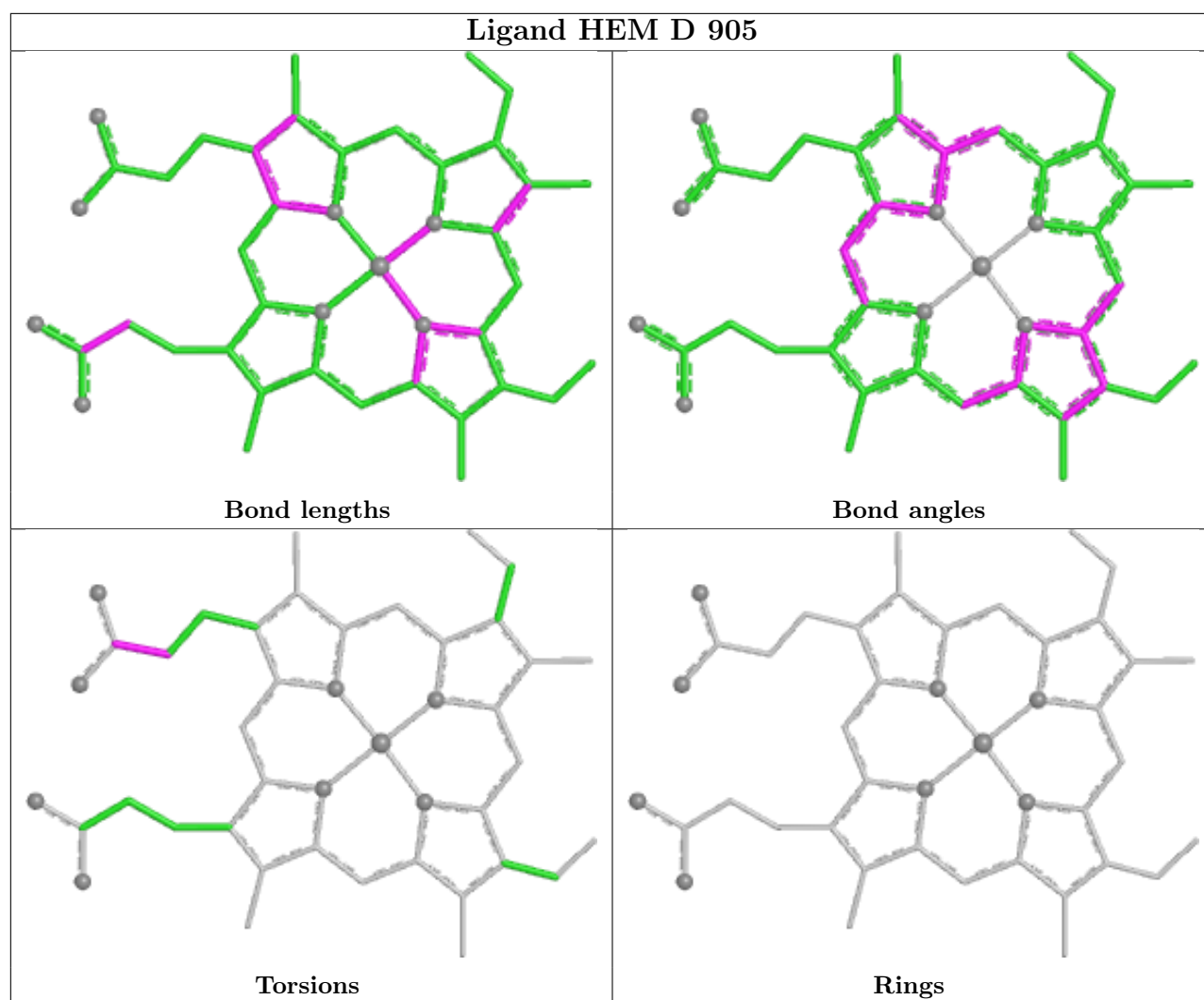


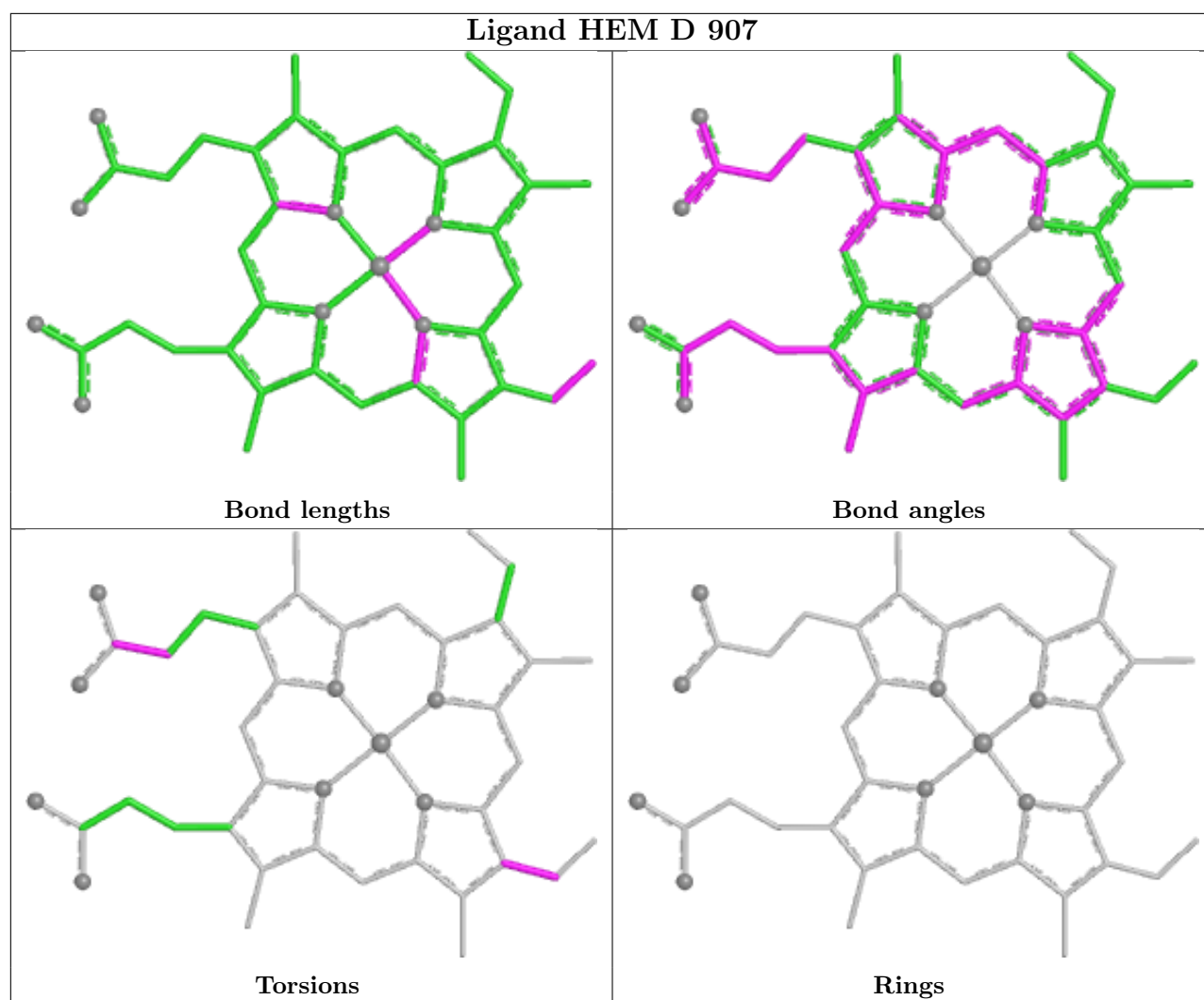


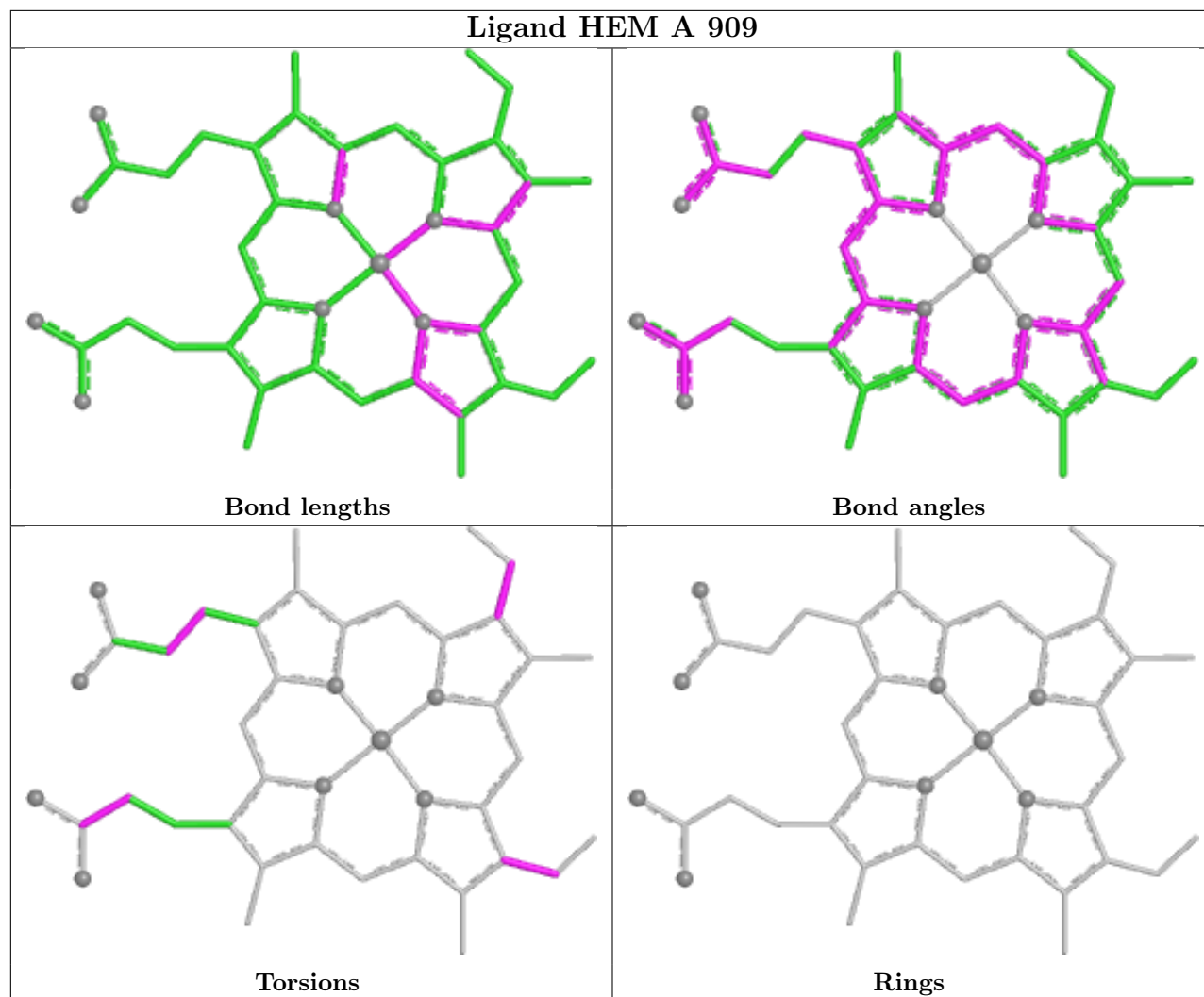


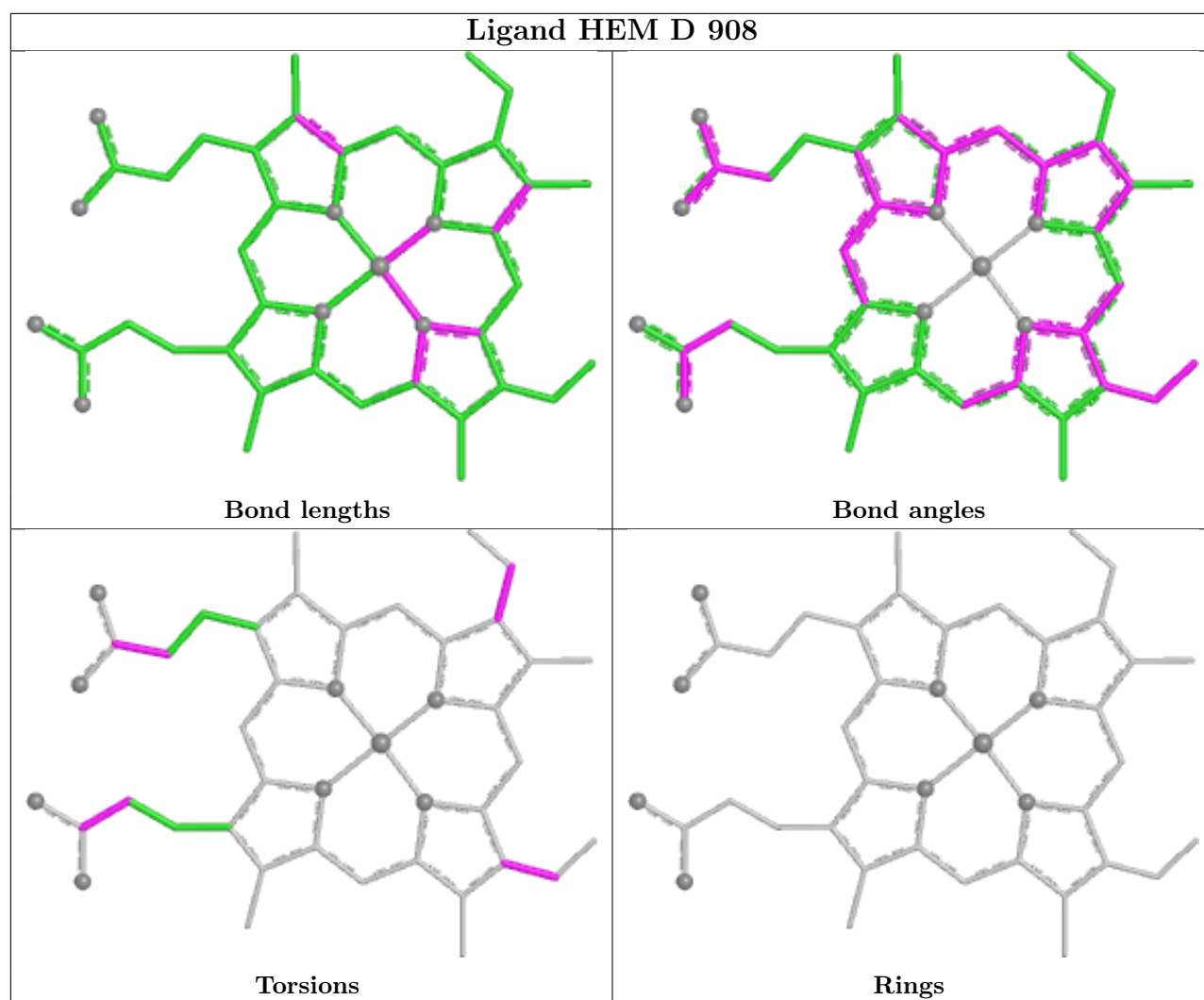




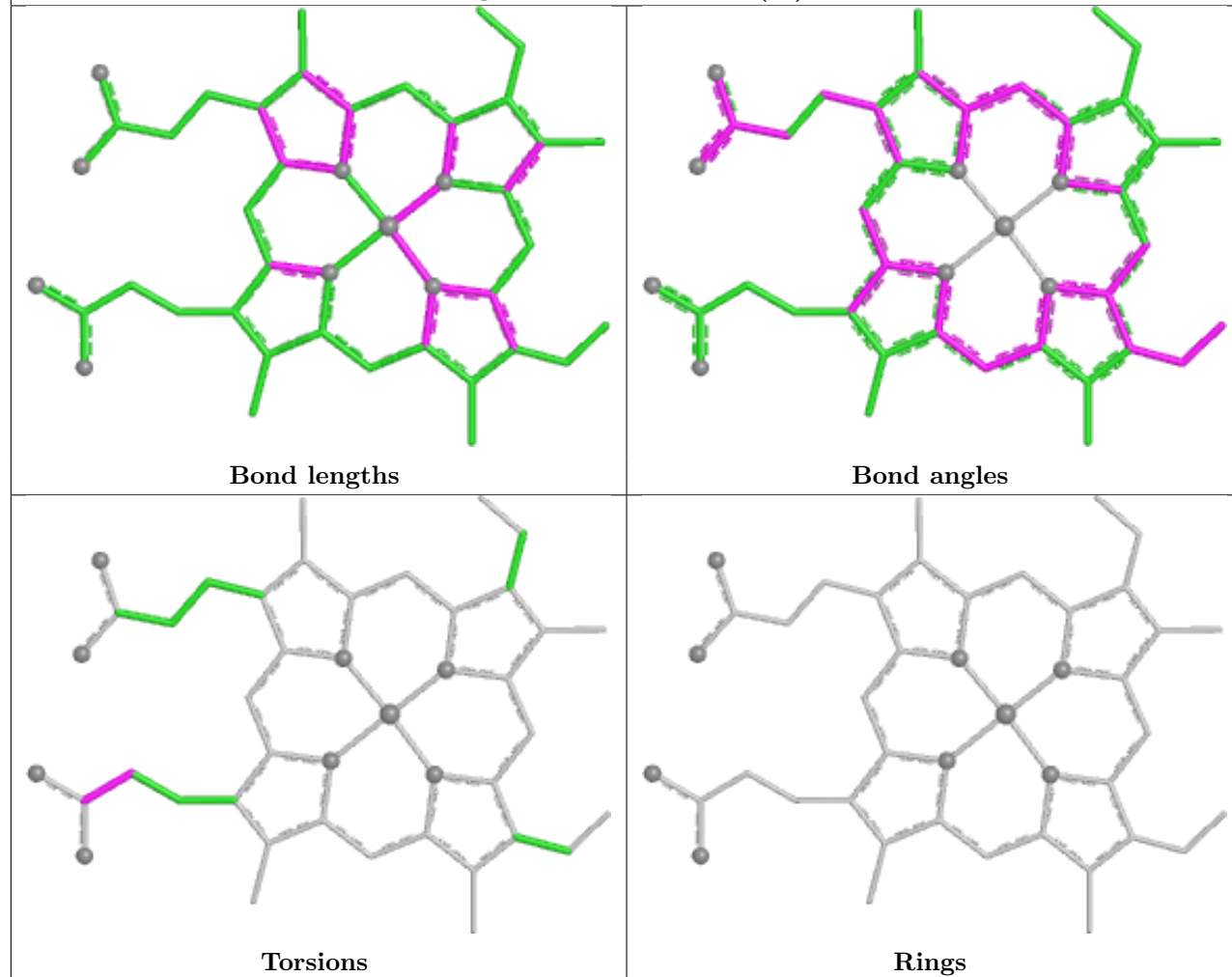


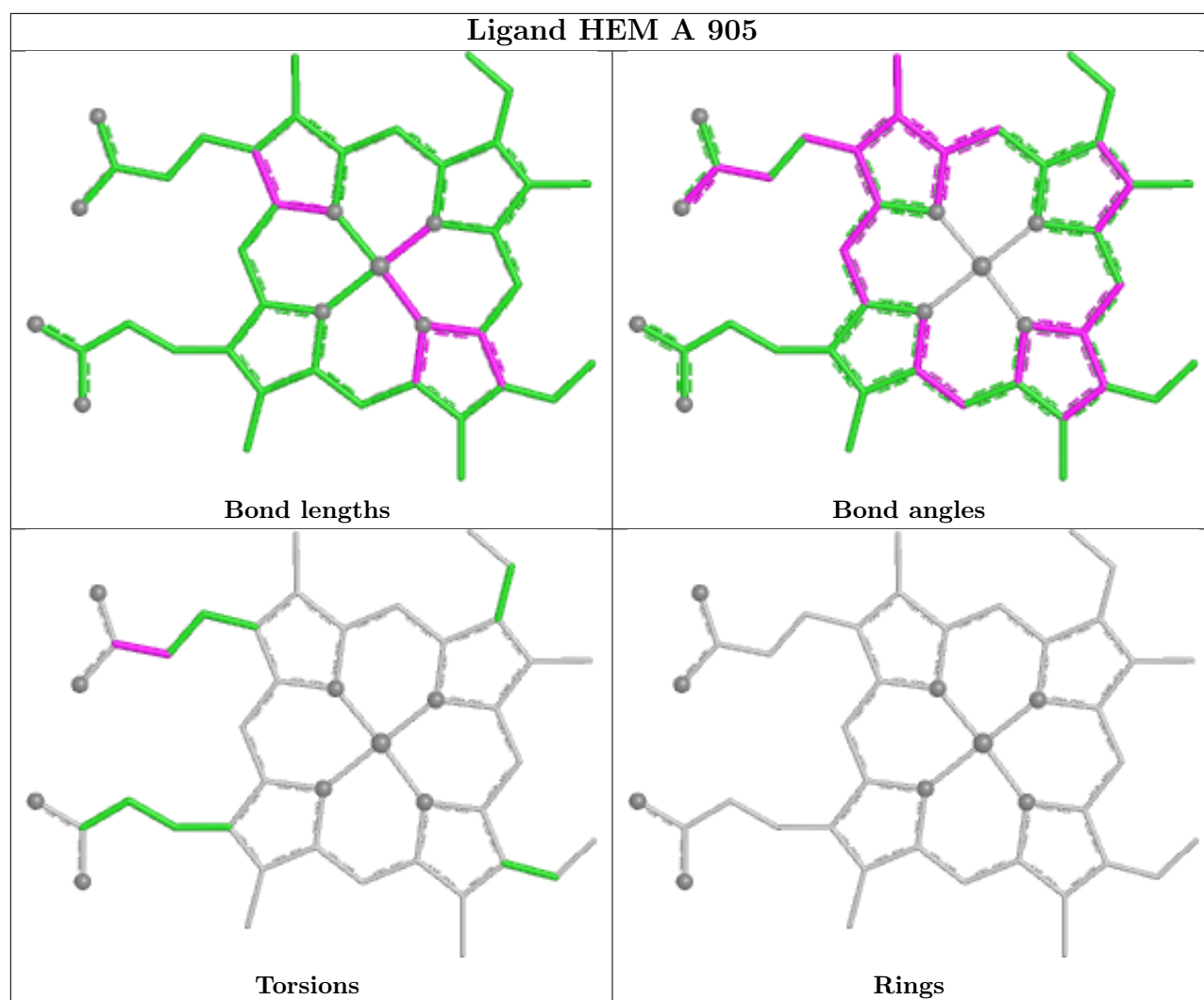


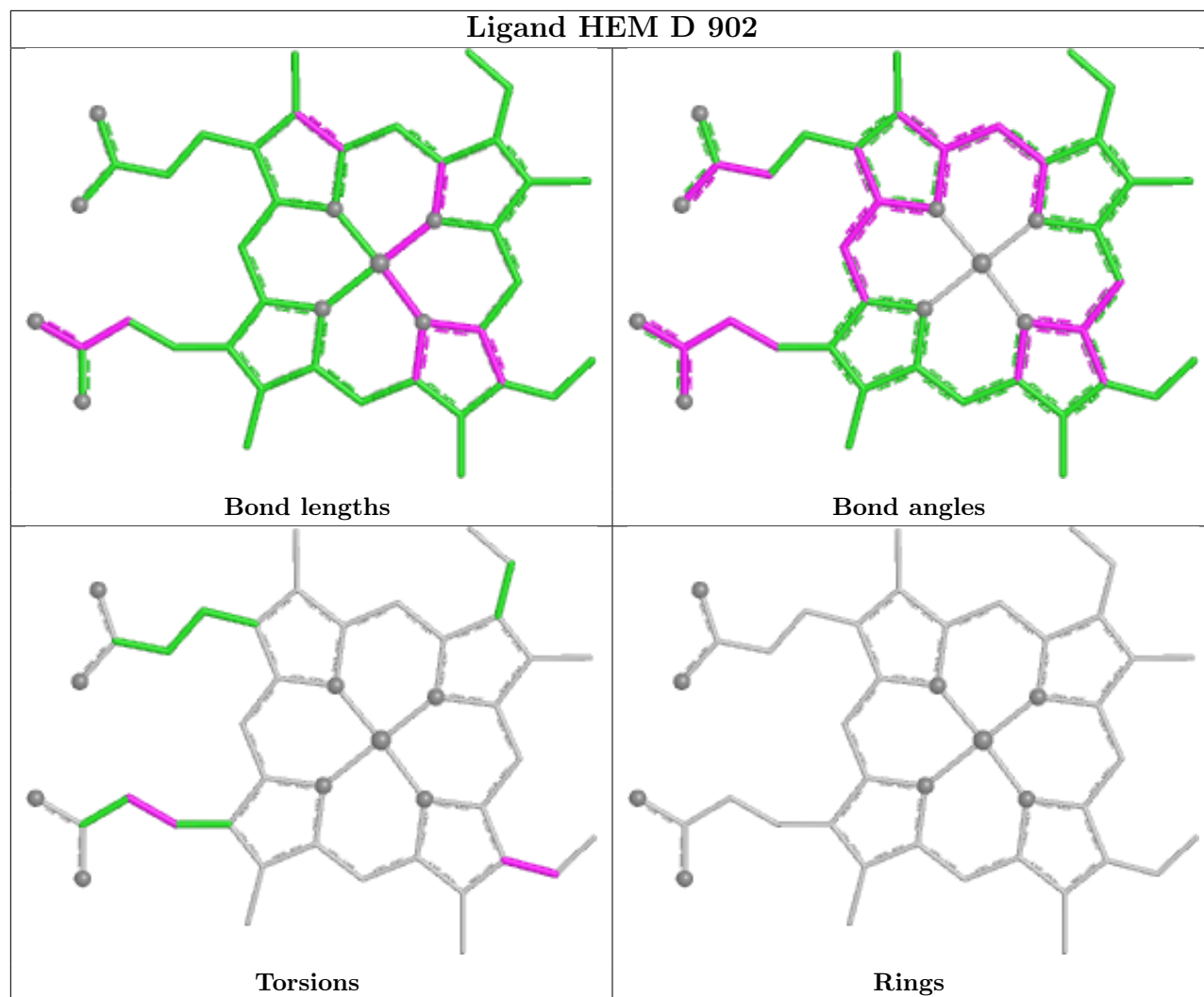




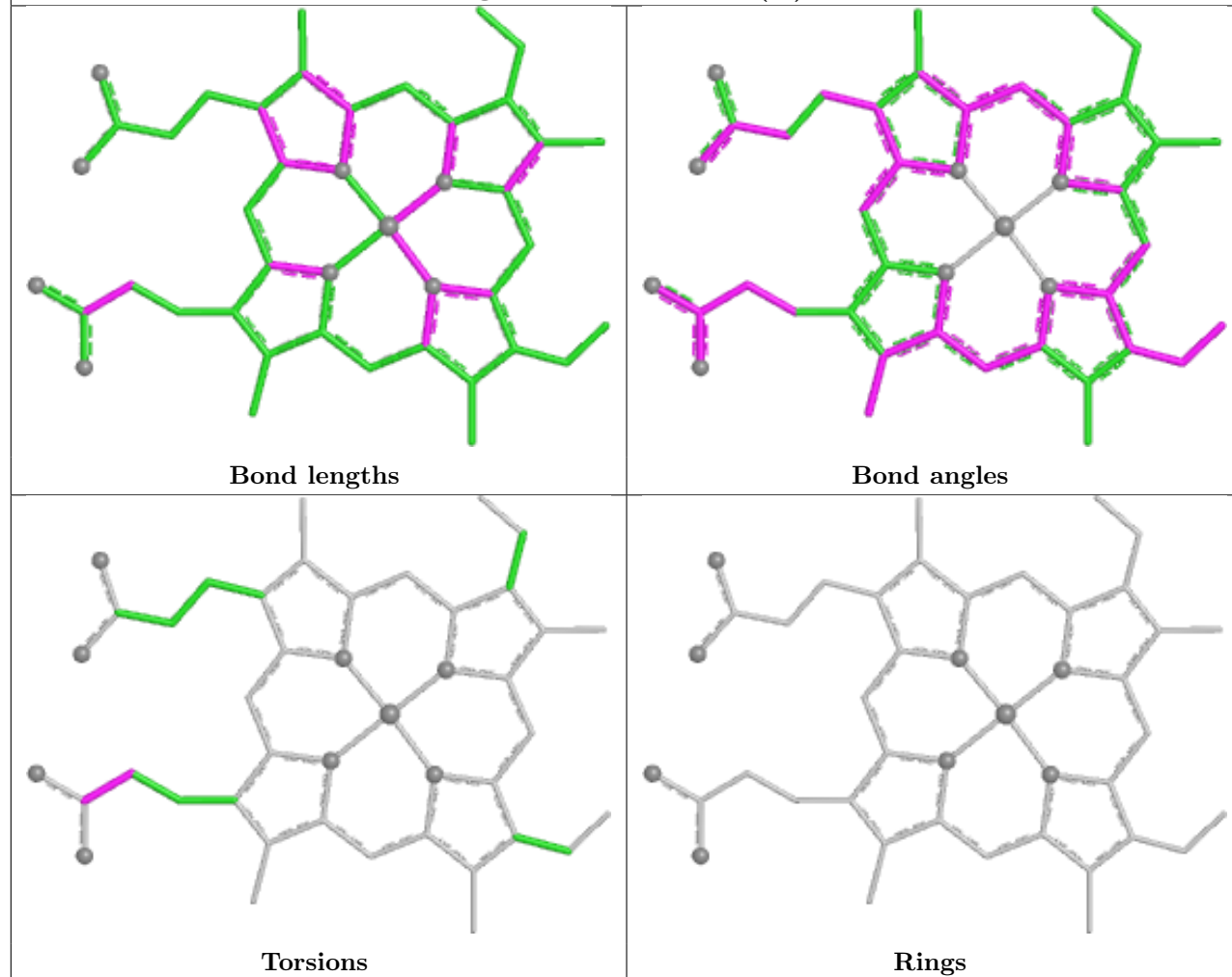
Ligand HEM A 904 (A)

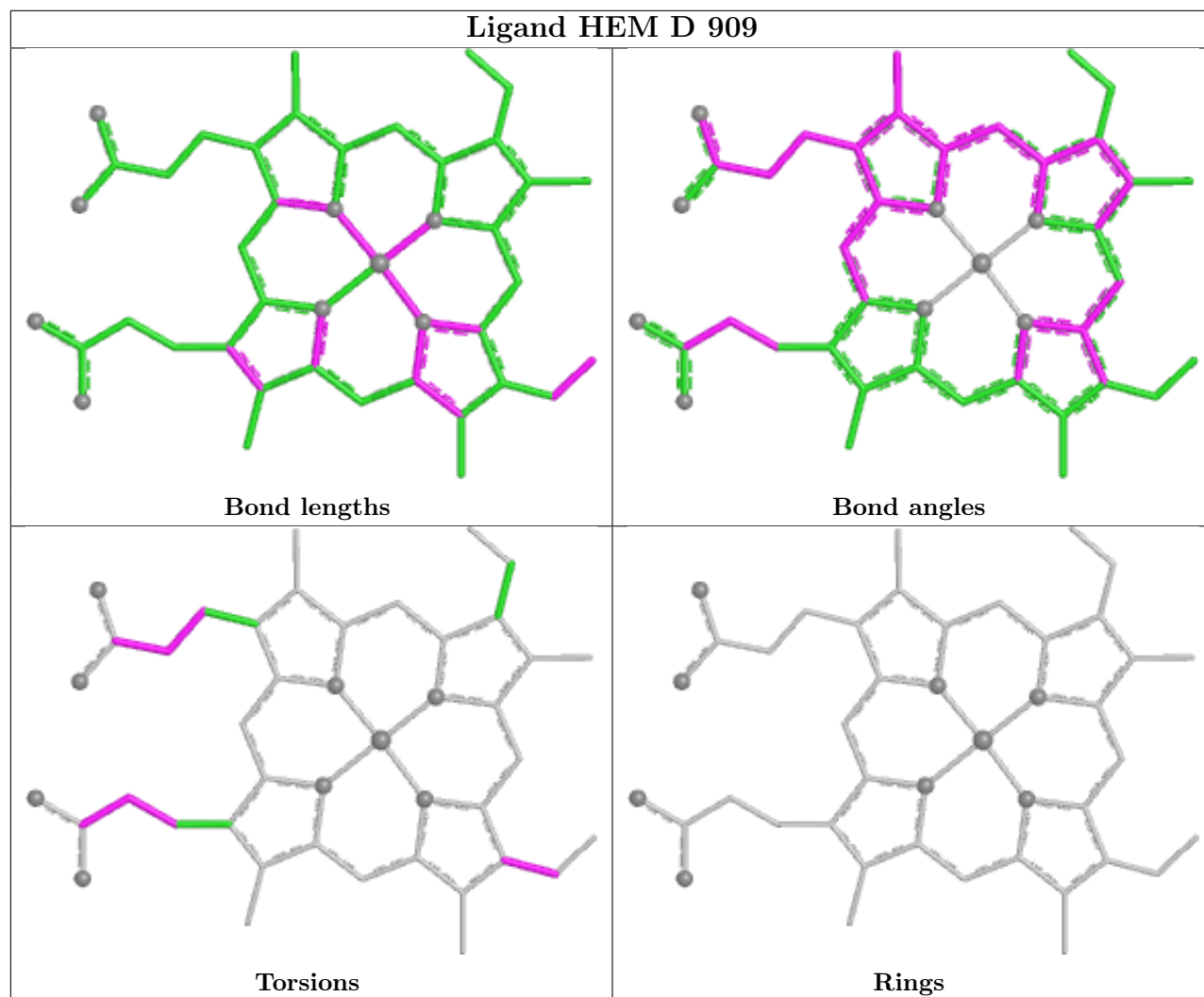


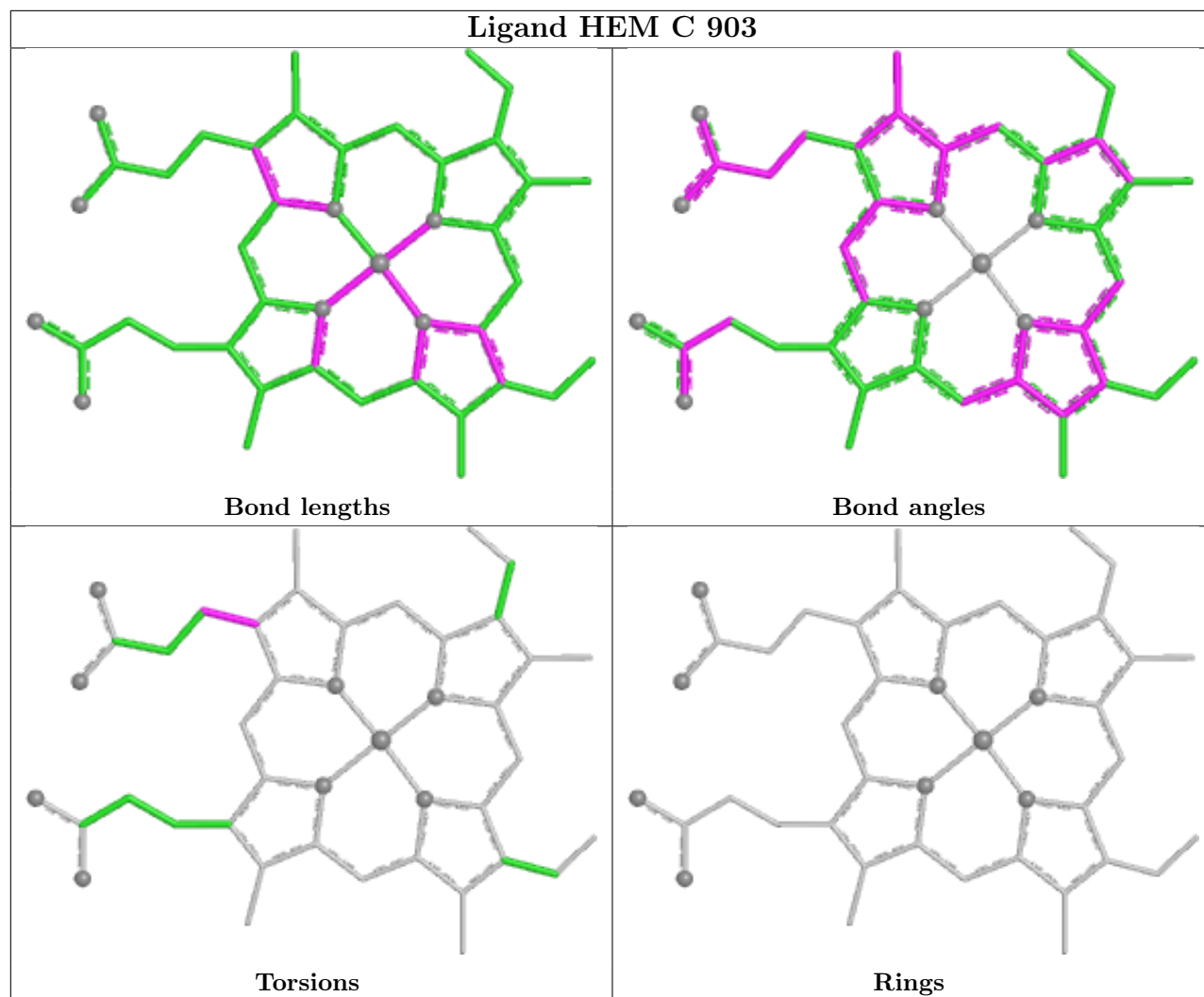


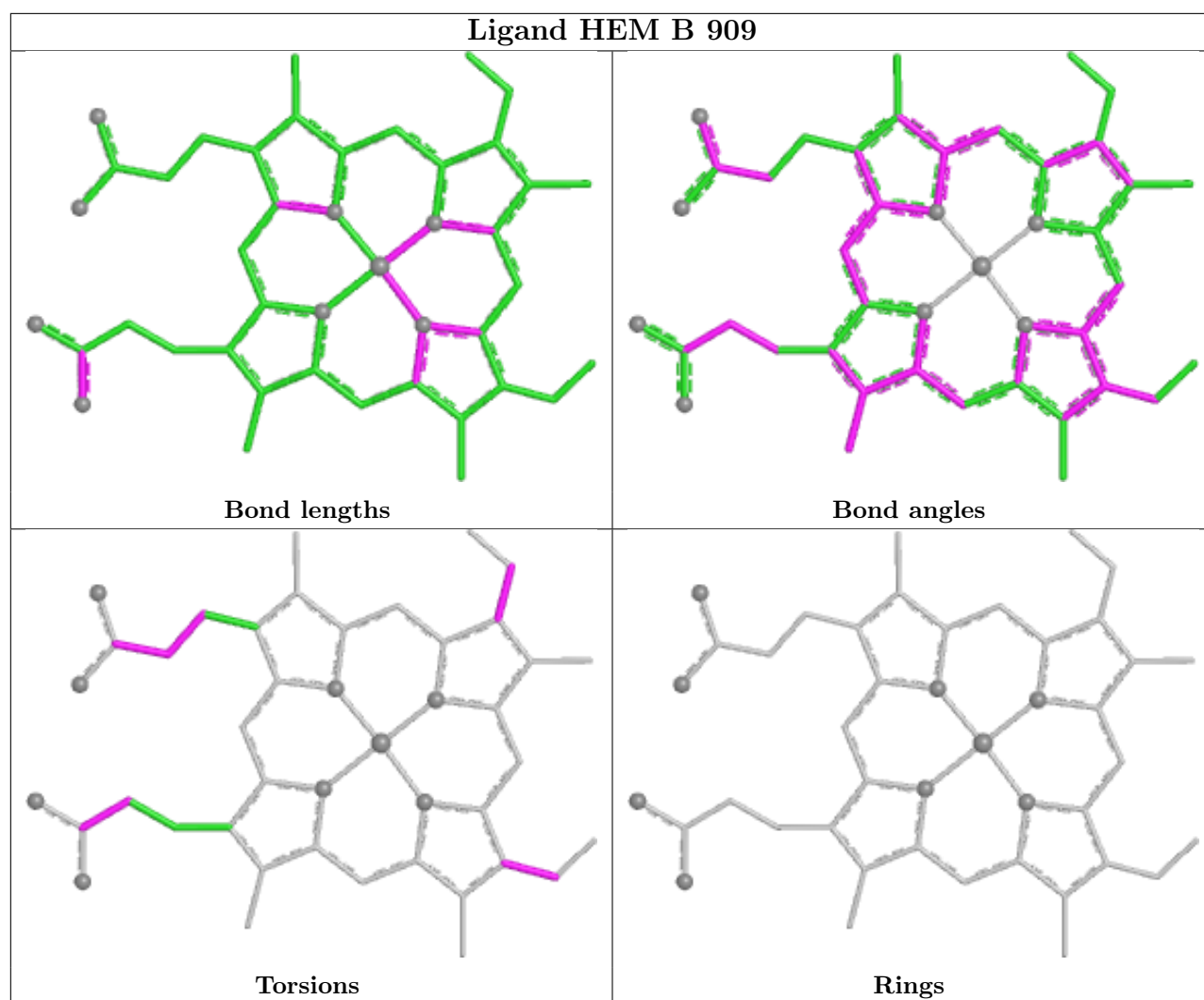


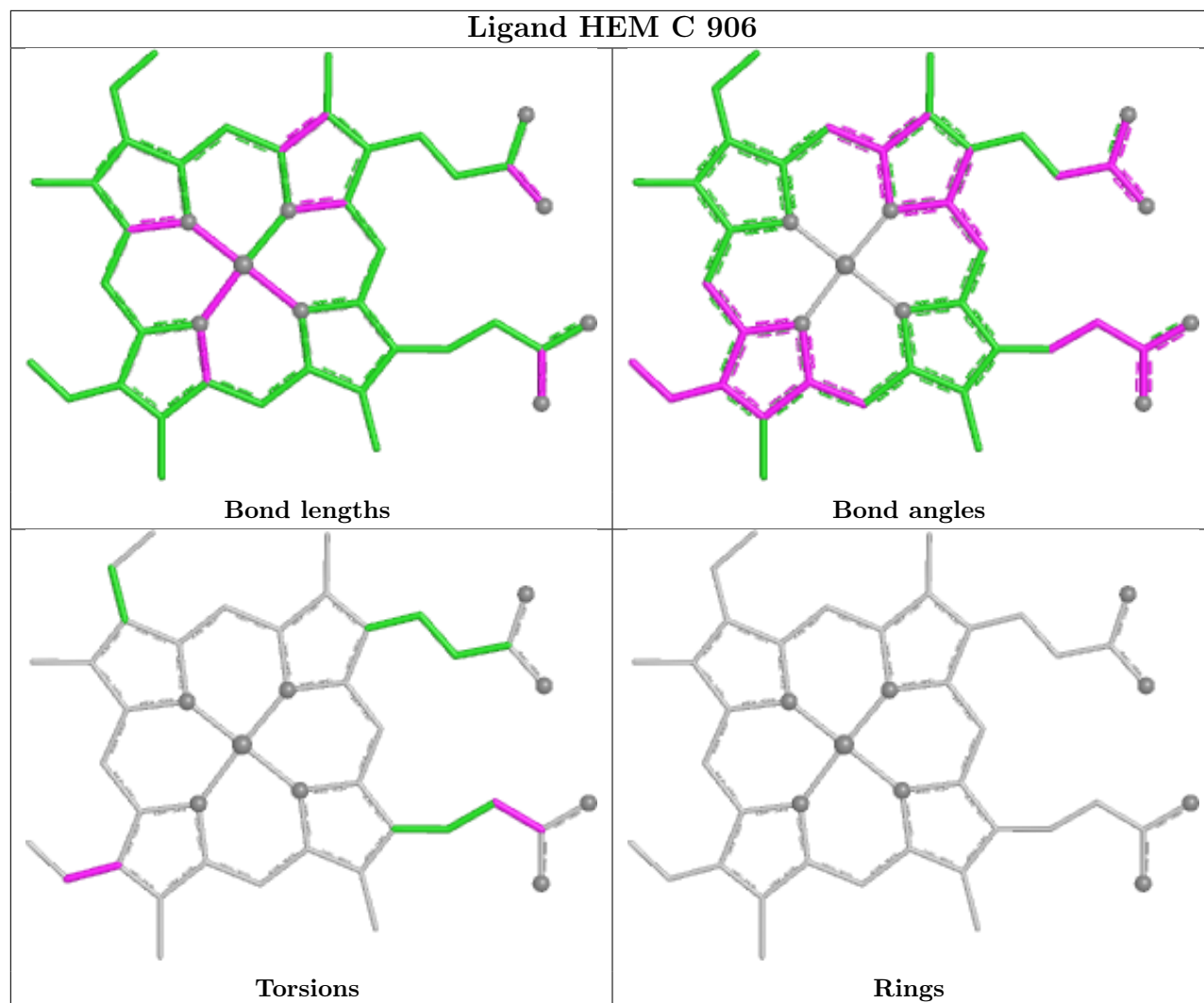
Ligand HEM A 904 (B)

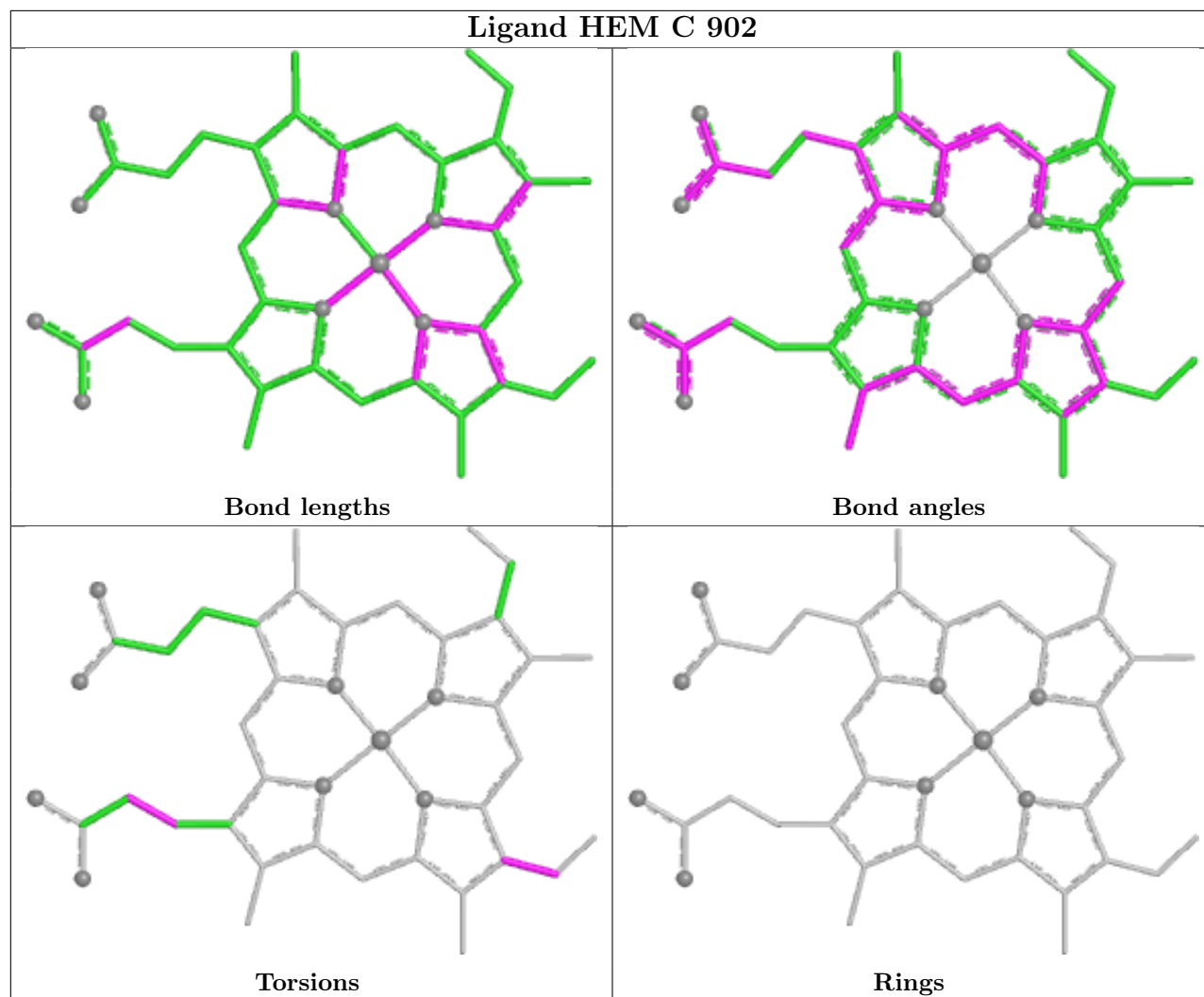


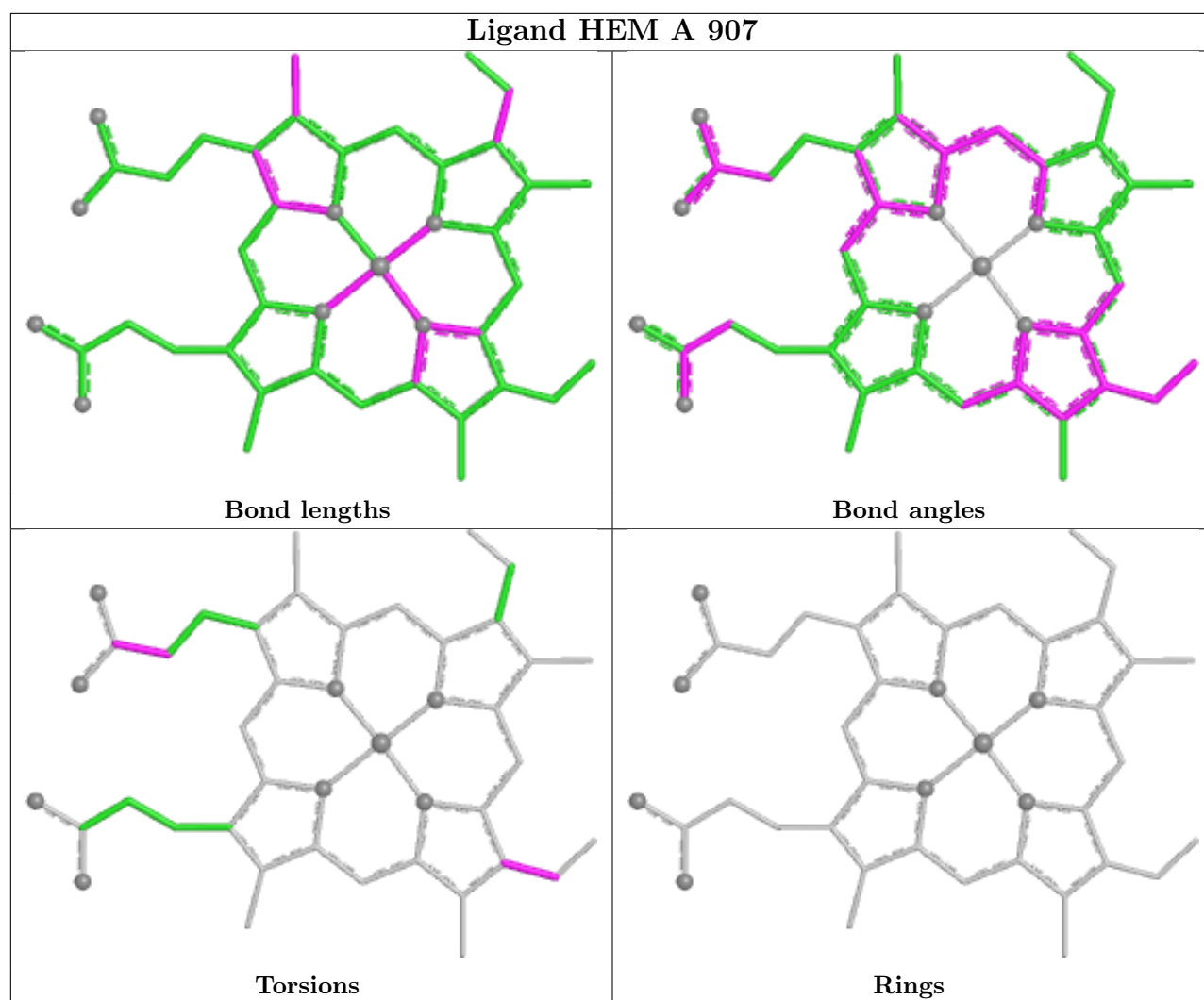




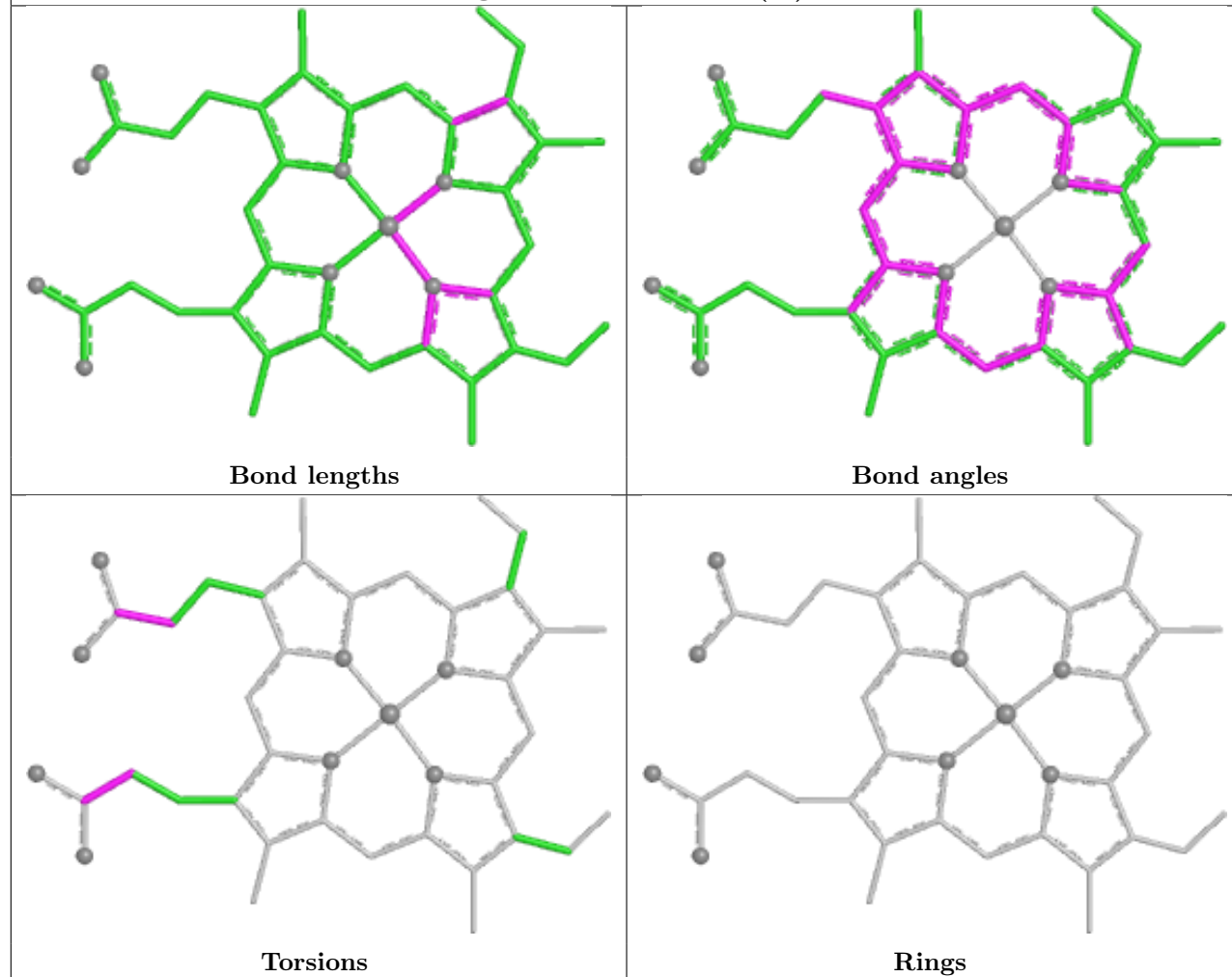


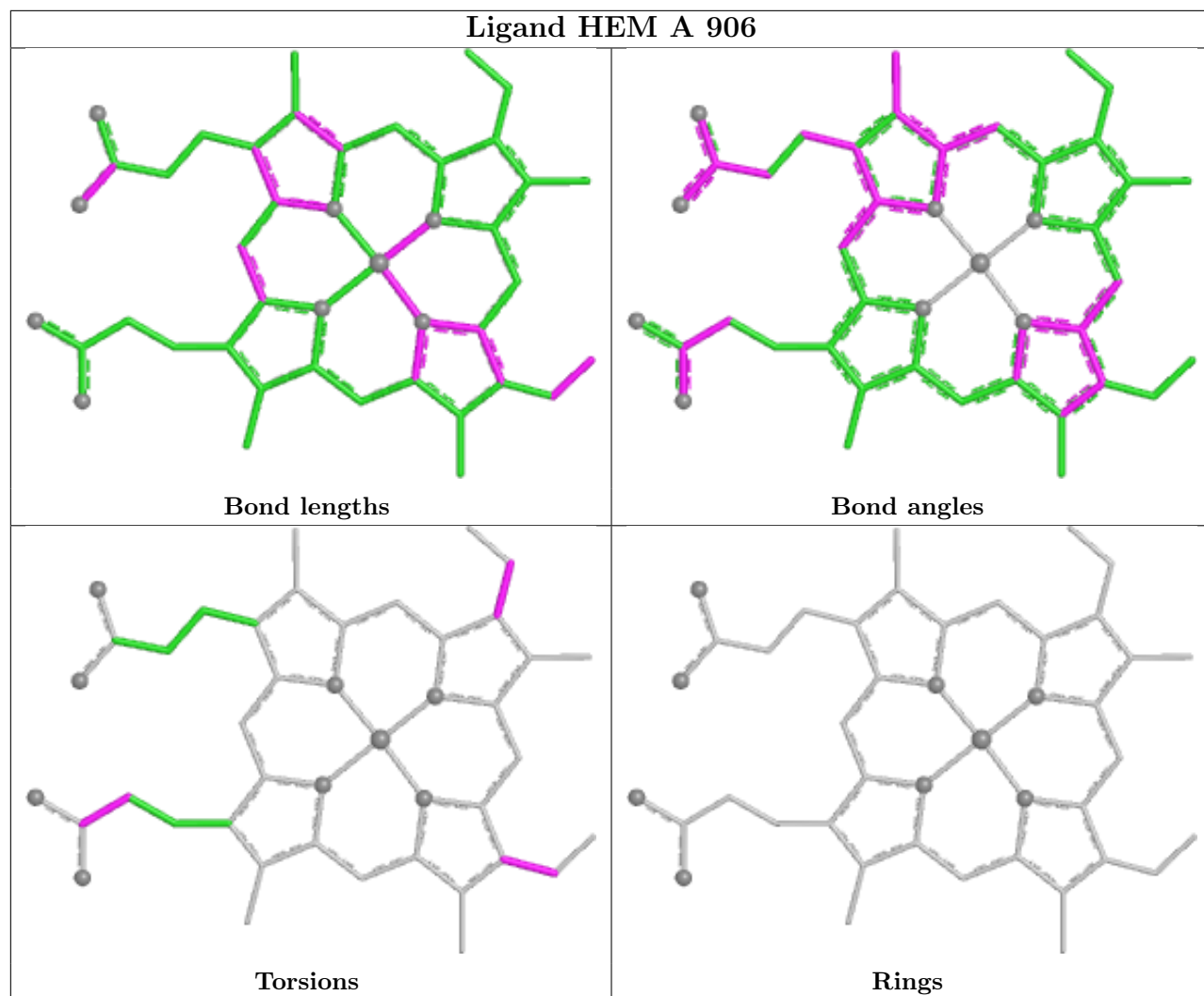




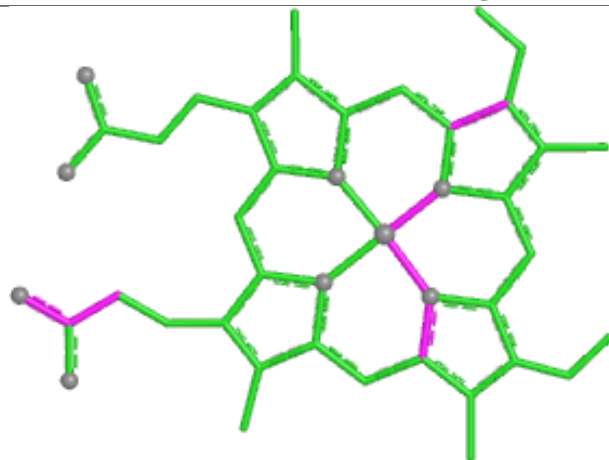


Ligand HEM D 904 (A)

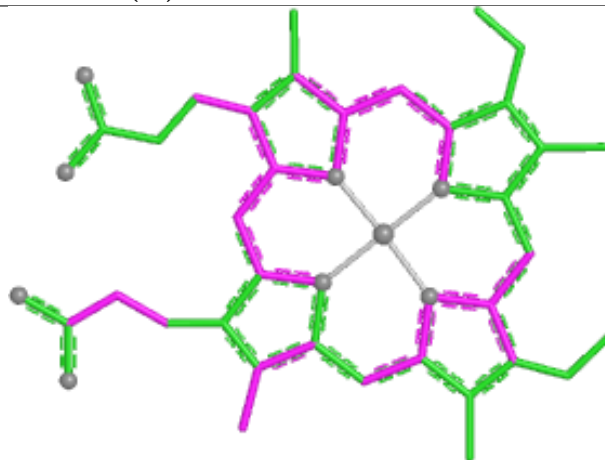




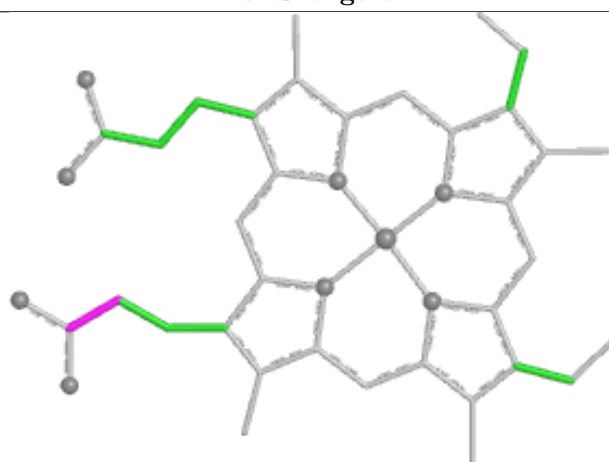
Ligand HEM D 904 (B)



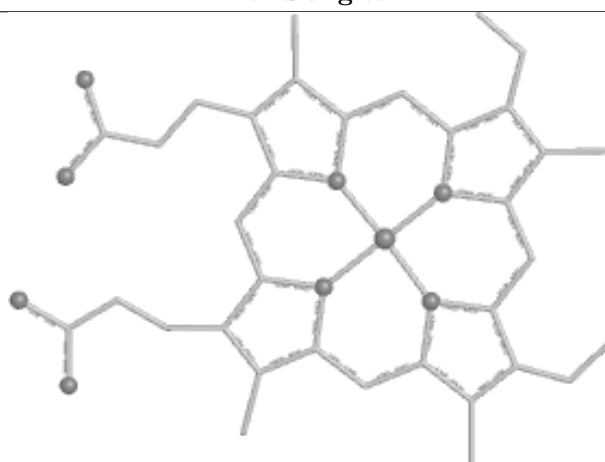
Bond lengths



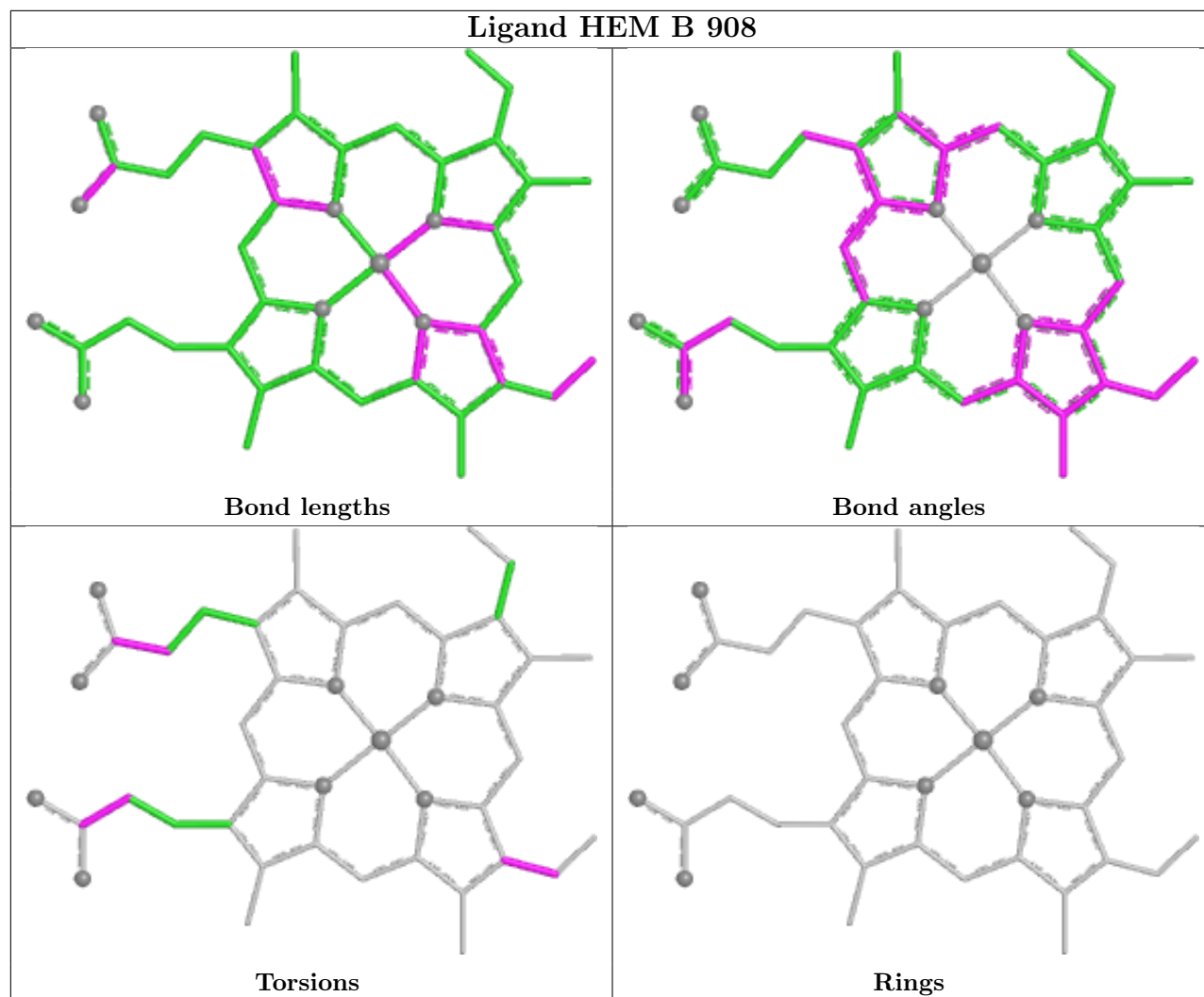
Bond angles



Torsions



Rings



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	660/732 (90%)	-0.52	3 (0%) 87 88	11, 26, 43, 82	3 (0%)
1	B	660/732 (90%)	-0.57	1 (0%) 91 92	11, 24, 43, 67	3 (0%)
1	C	659/732 (90%)	-0.45	2 (0%) 90 91	13, 27, 46, 71	3 (0%)
1	D	660/732 (90%)	-0.66	3 (0%) 87 88	8, 21, 40, 76	2 (0%)
All	All	2639/2928 (90%)	-0.55	9 (0%) 90 91	8, 25, 44, 82	11 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	VAL	2.8
1	B	30	GLY	2.4
1	D	379	LEU	2.4
1	C	437	ILE	2.2
1	D	629	VAL	2.2
1	D	689	SER	2.1
1	C	435	LYS	2.1
1	A	690	LEU	2.1
1	A	630	LYS	2.0

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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DTN	A	901	6/6	0.84	0.16	25,33,40,42	6
2	DTN	C	901	6/6	0.89	0.11	56,57,64,67	6
2	DTN	B	901	6/6	0.90	0.13	27,36,37,40	6
2	DTN	D	901	6/6	0.90	0.14	33,38,51,51	6
2	DTN	A	911	6/6	0.93	0.09	23,28,36,37	6
5	SO3	D	911	4/4	0.93	0.09	40,48,50,62	0
3	HEM	A	909	43/43	0.97	0.07	19,23,45,72	0
3	HEM	B	907	43/43	0.97	0.06	15,16,29,54	0
3	HEM	B	909	43/43	0.97	0.06	17,20,40,71	0
3	HEM	C	902	43/43	0.97	0.06	15,19,22,25	0
3	HEM	C	903	43/43	0.97	0.06	18,21,26,29	0
3	HEM	C	904[A]	43/43	0.97	0.06	14,17,19,21	43
3	HEM	C	904[B]	43/43	0.97	0.06	15,17,19,21	43
3	HEM	C	907	43/43	0.97	0.06	16,18,29,45	0
3	HEM	C	909	43/43	0.97	0.06	20,23,41,61	0
4	CU	C	910	1/1	0.97	0.04	17,17,17,17	1
3	HEM	A	903	43/43	0.97	0.06	16,19,22,24	0
3	HEM	B	906	43/43	0.98	0.05	13,16,25,34	0
3	HEM	A	904[A]	43/43	0.98	0.05	14,17,18,20	43
3	HEM	B	908	43/43	0.98	0.05	14,17,21,22	0
3	HEM	A	904[B]	43/43	0.98	0.05	12,18,19,20	43
3	HEM	A	906	43/43	0.98	0.05	13,16,24,31	0
3	HEM	A	907	43/43	0.98	0.06	14,16,25,47	0
3	HEM	A	908	43/43	0.98	0.04	15,17,20,23	0
3	HEM	A	902	43/43	0.98	0.06	17,19,24,28	0
3	HEM	C	905	43/43	0.98	0.05	16,18,20,21	0
3	HEM	C	906	43/43	0.98	0.05	15,18,24,34	0
3	HEM	B	902	43/43	0.98	0.05	16,18,22,25	0
3	HEM	C	908	43/43	0.98	0.05	17,19,24,26	0
3	HEM	B	903	43/43	0.98	0.05	15,18,20,22	0
3	HEM	D	902	43/43	0.98	0.04	12,13,19,22	0
3	HEM	D	903	43/43	0.98	0.04	11,13,14,15	0
3	HEM	D	904[A]	43/43	0.98	0.05	10,11,13,15	43
3	HEM	D	904[B]	43/43	0.98	0.05	9,12,14,15	43
3	HEM	D	906	43/43	0.98	0.05	9,12,17,30	0
3	HEM	D	907	43/43	0.98	0.06	12,14,23,54	0
3	HEM	D	908	43/43	0.98	0.04	12,14,21,22	0

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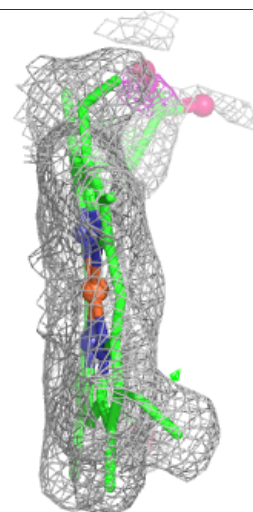
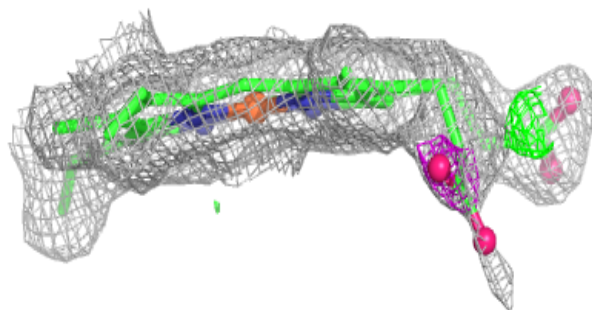
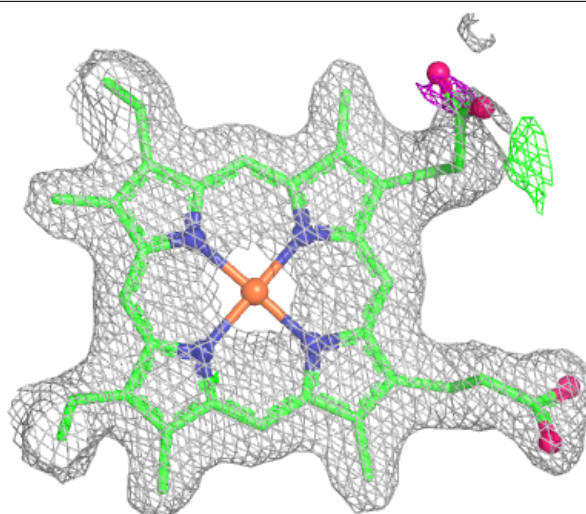
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	D	909	43/43	0.98	0.07	14,19,54,66	0
3	HEM	B	904[A]	43/43	0.98	0.05	15,16,18,20	43
5	SO3	A	912	4/4	0.98	0.07	21,22,25,35	0
5	SO3	C	911	4/4	0.98	0.07	23,25,30,38	0
3	HEM	B	904[B]	43/43	0.98	0.05	11,16,19,21	43
5	SO3	D	912	4/4	0.98	0.06	15,17,21,24	0
3	HEM	D	905	43/43	0.99	0.04	10,11,13,14	0
5	SO3	B	911	4/4	0.99	0.07	23,23,31,34	0
3	HEM	B	905	43/43	0.99	0.04	14,15,18,18	0
4	CU	A	910	1/1	0.99	0.04	15,15,15,15	1
3	HEM	A	905	43/43	0.99	0.04	13,17,19,21	0
4	CU	D	910	1/1	1.00	0.01	9,9,9,9	1
4	CU	B	910	1/1	1.00	0.04	11,11,11,11	1

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.

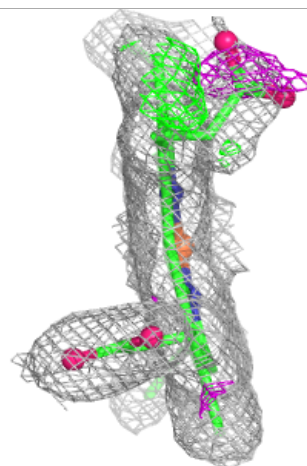
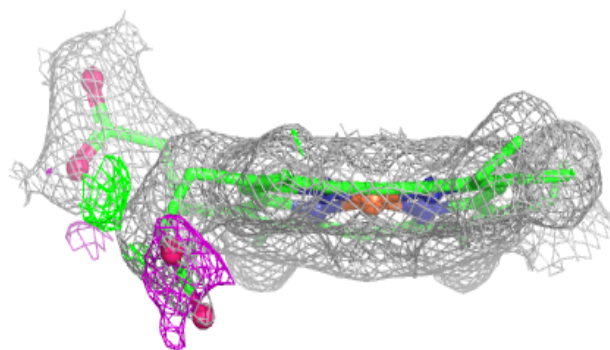
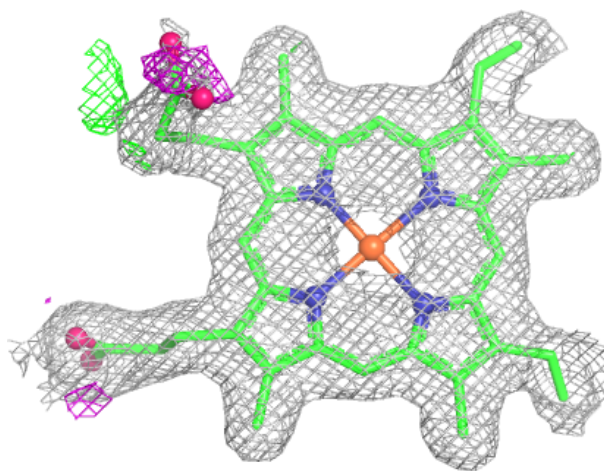
Electron density around HEM A 909:

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



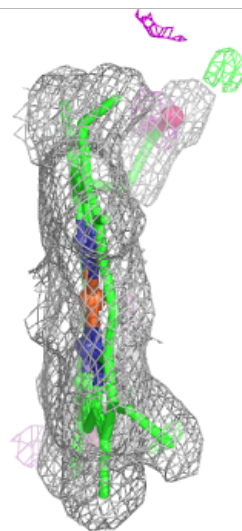
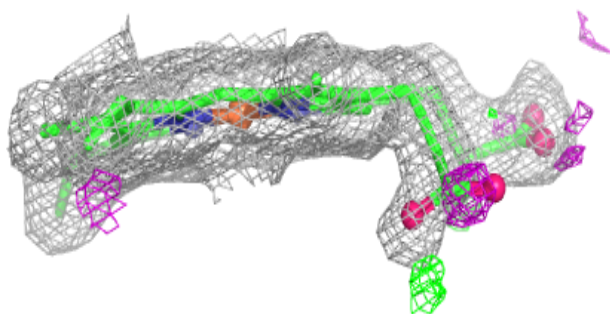
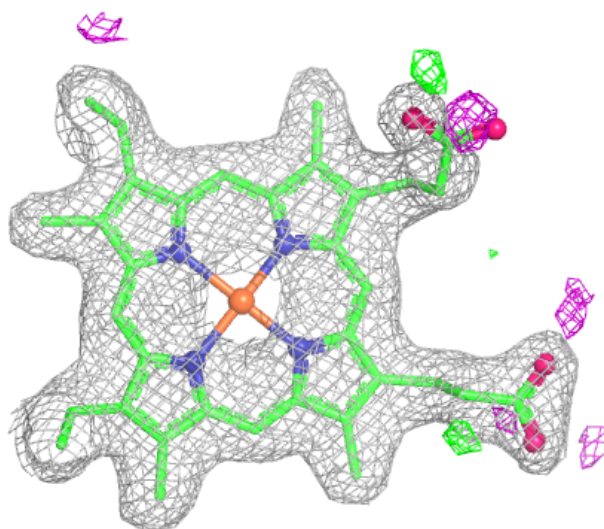
Electron density around HEM B 907:

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



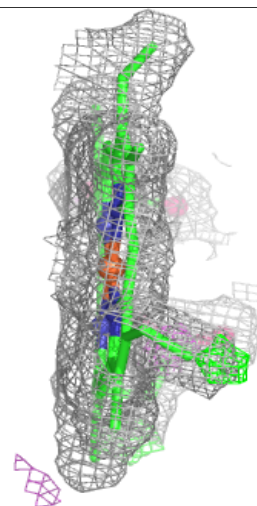
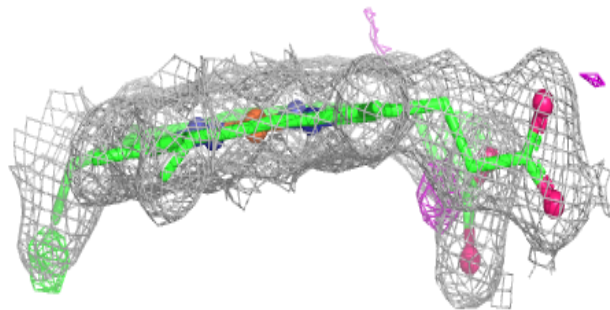
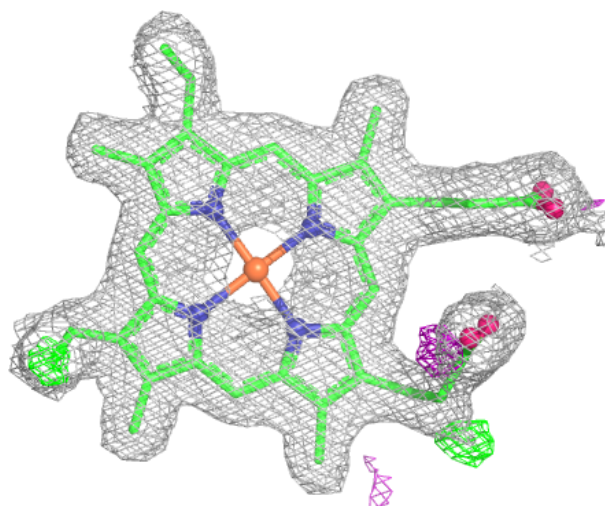
Electron density around HEM B 909:

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



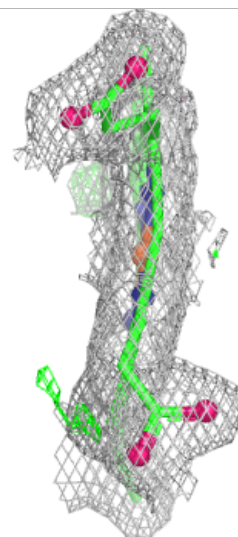
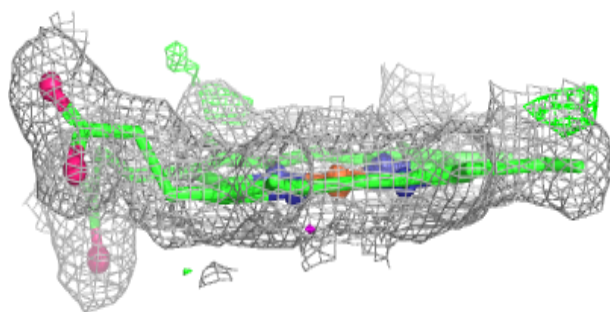
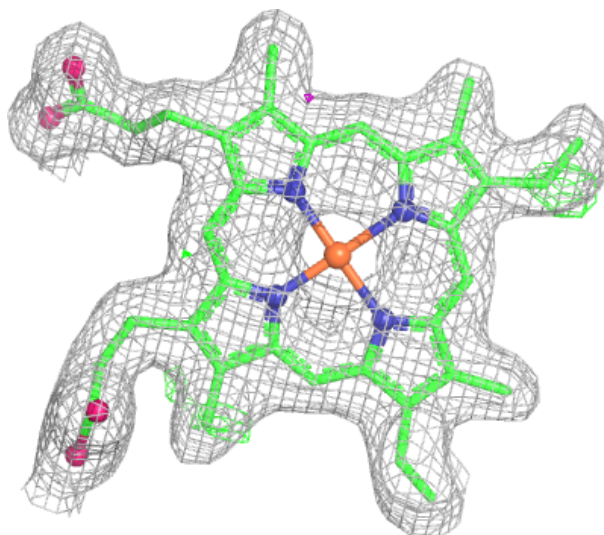
Electron density around HEM C 902:

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



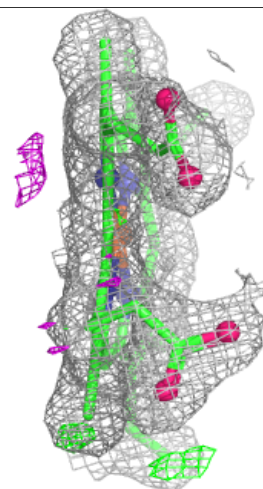
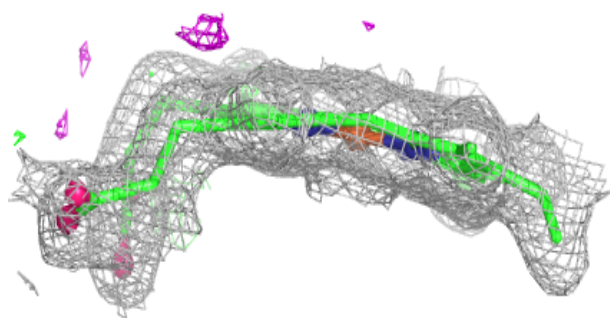
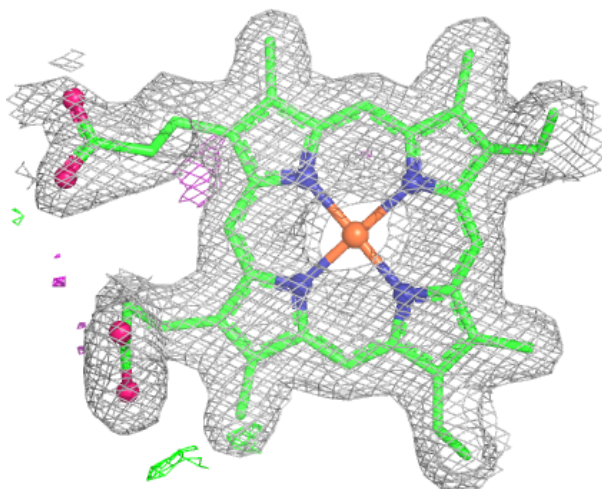
Electron density around HEM C 903:

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



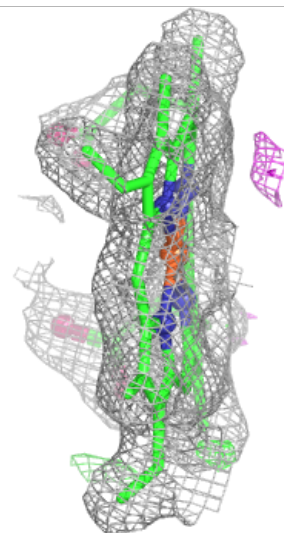
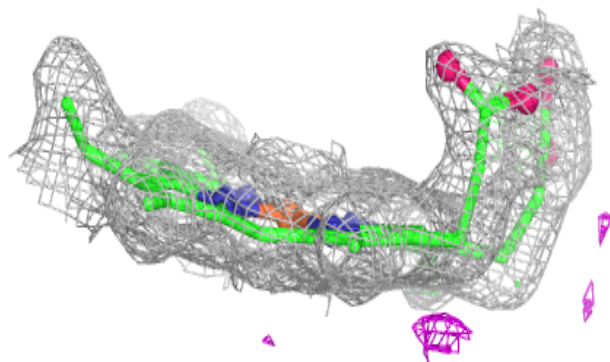
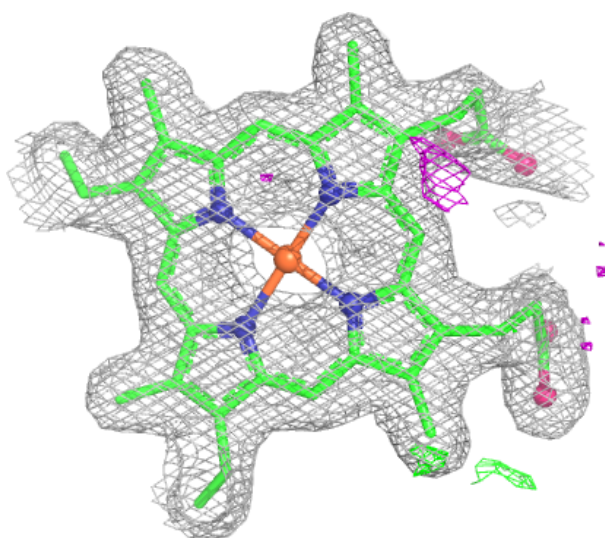
Electron density around HEM C 904 (A):

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



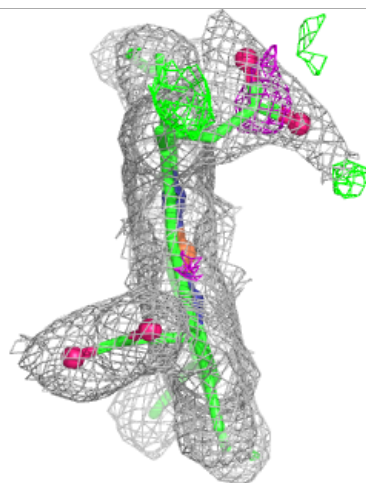
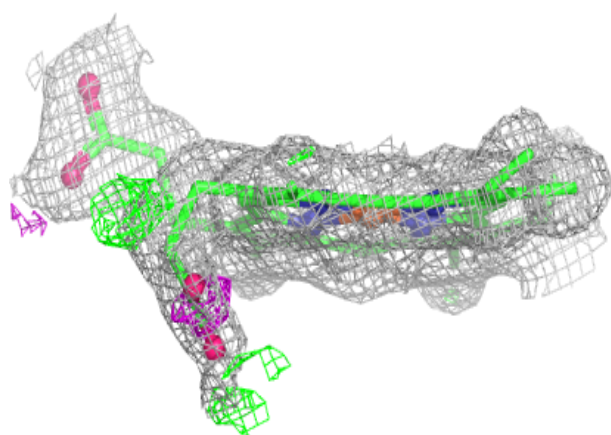
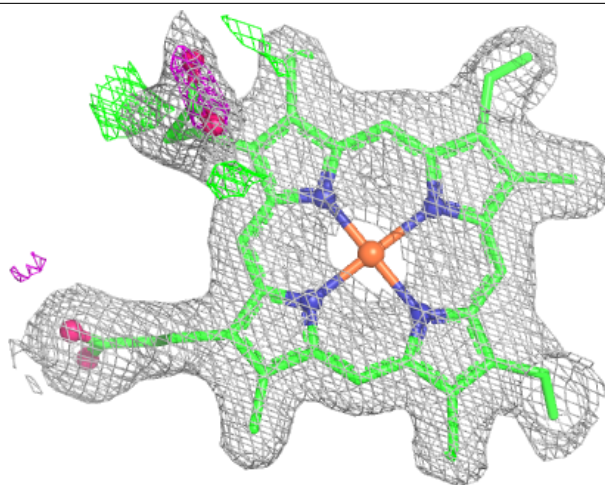
Electron density around HEM C 904 (B):

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



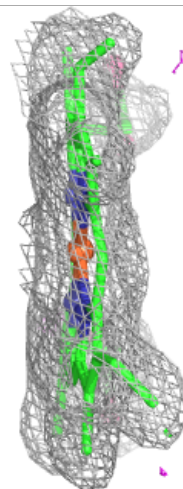
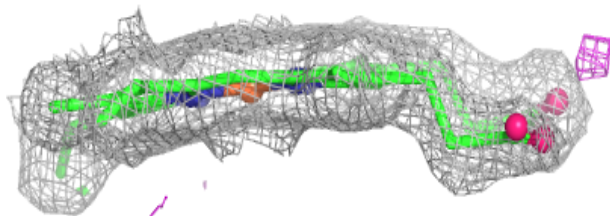
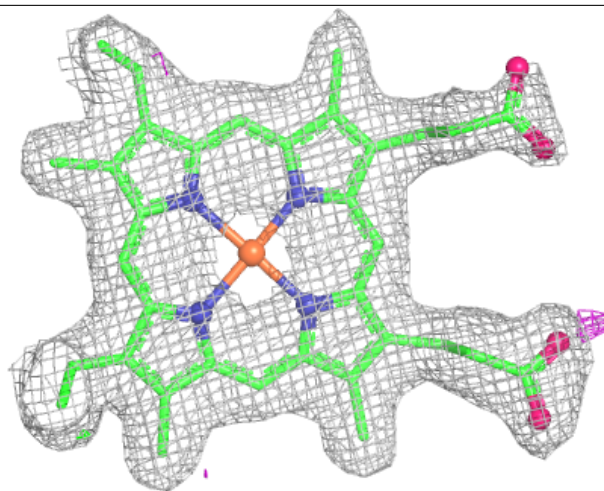
Electron density around HEM C 907:

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



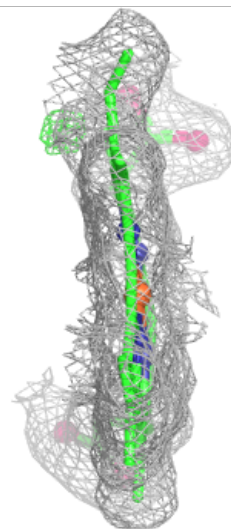
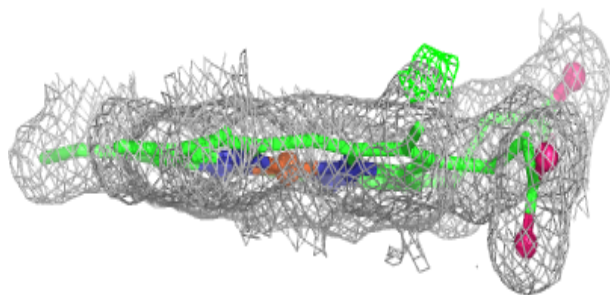
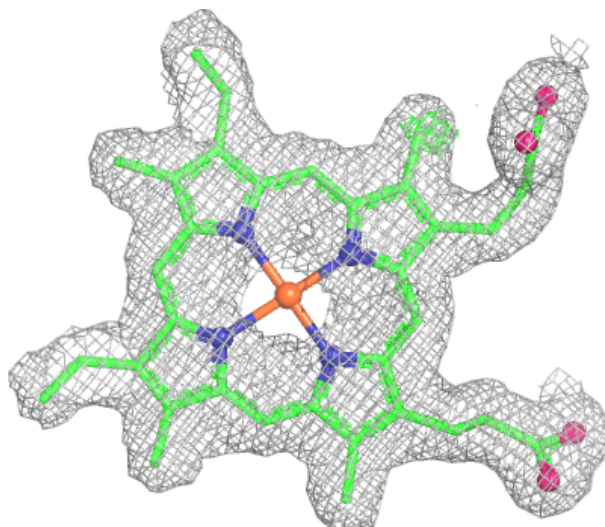
Electron density around HEM C 909:

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



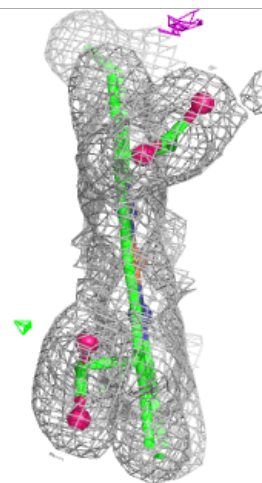
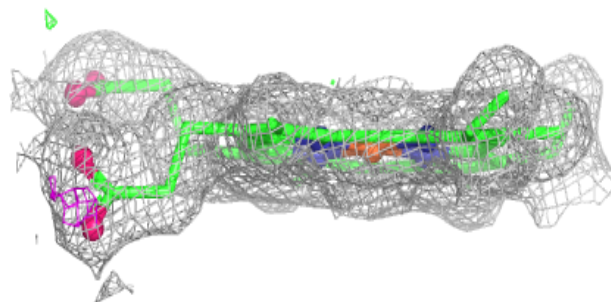
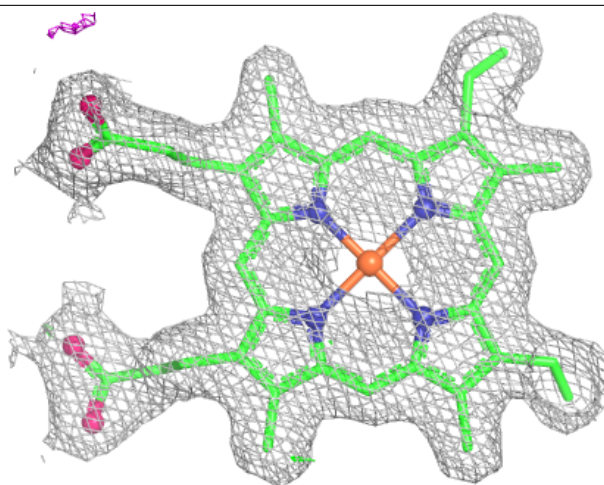
Electron density around HEM A 903:

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



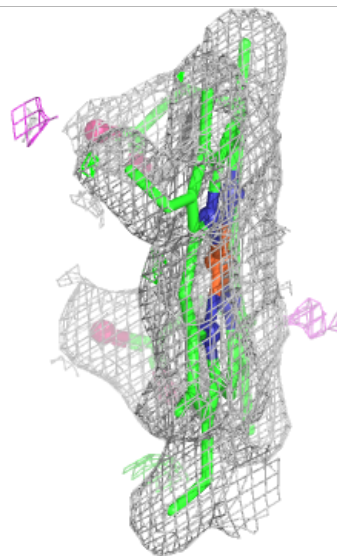
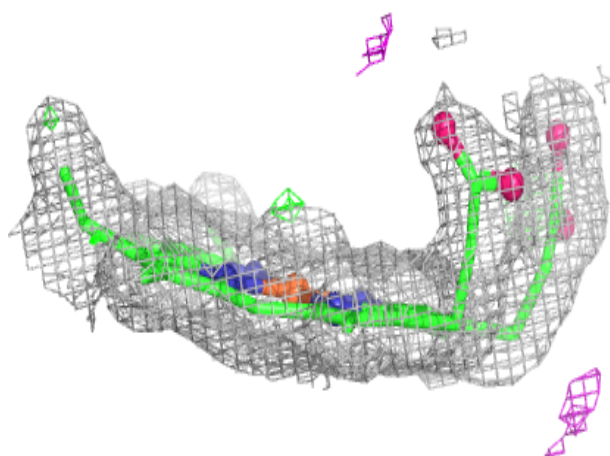
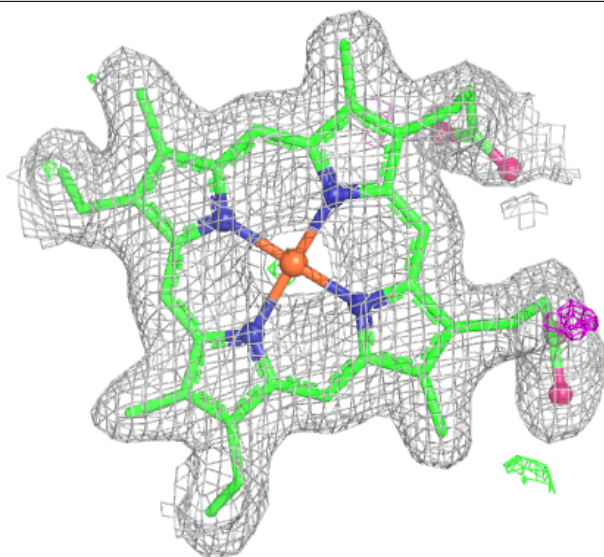
Electron density around HEM B 906:

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



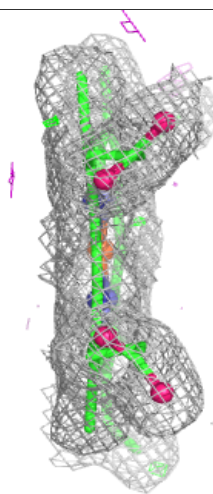
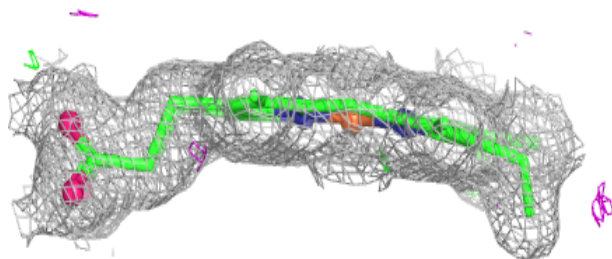
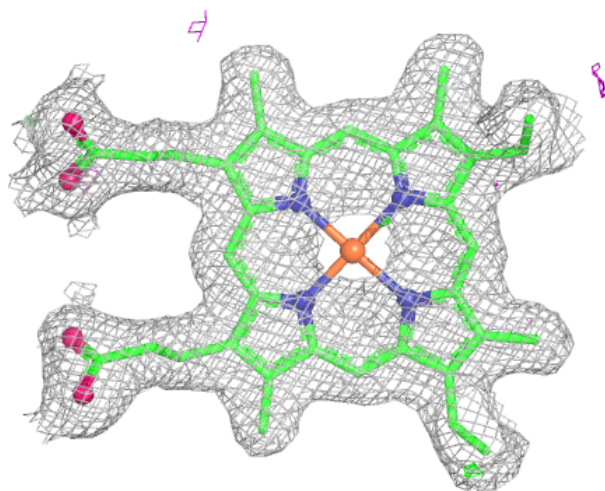
Electron density around HEM A 904 (A):

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



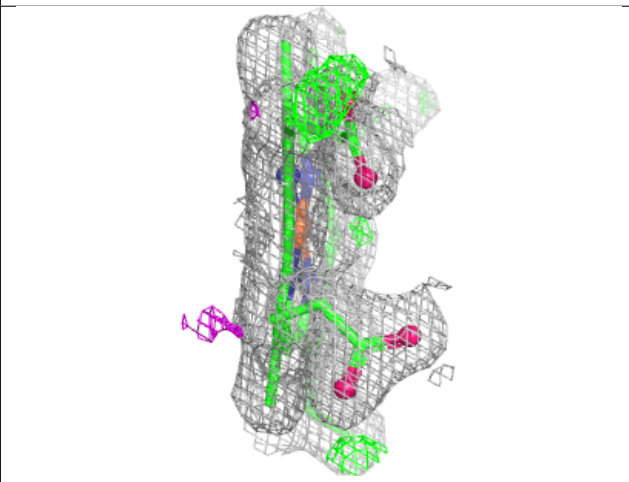
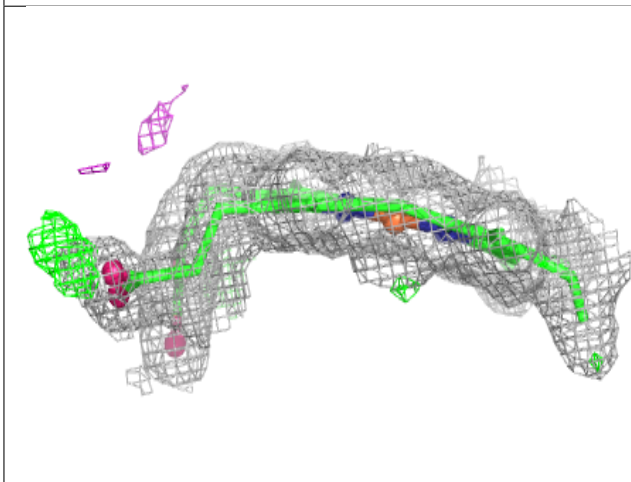
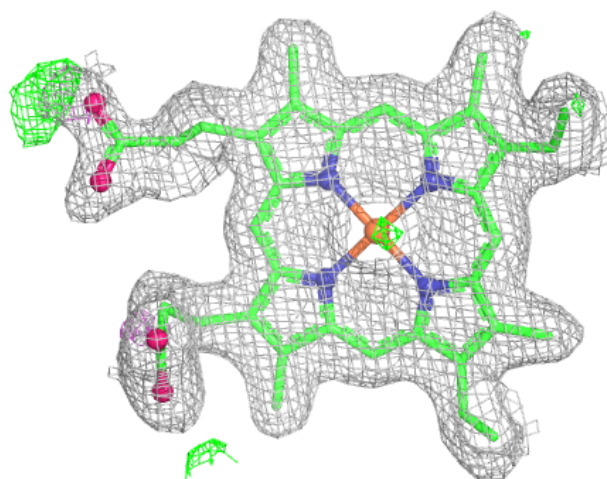
Electron density around HEM B 908:

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



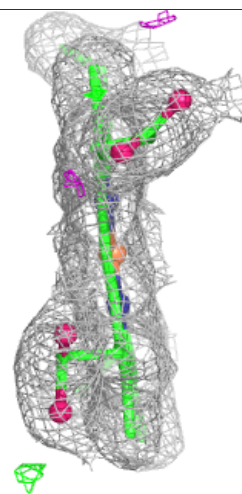
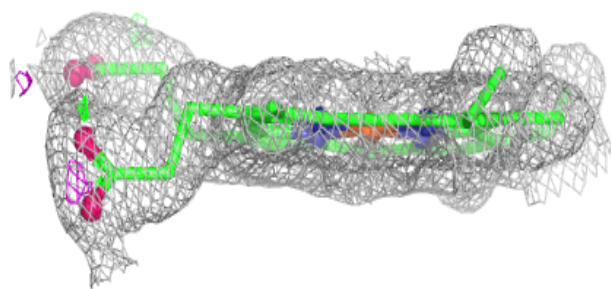
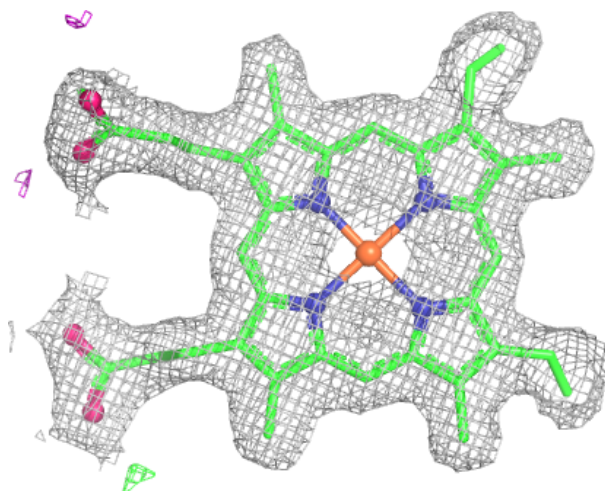
Electron density around HEM A 904 (B):

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



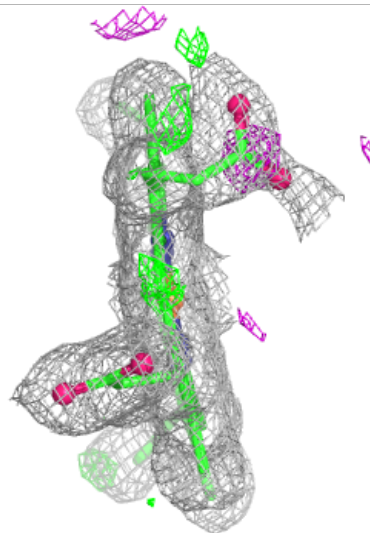
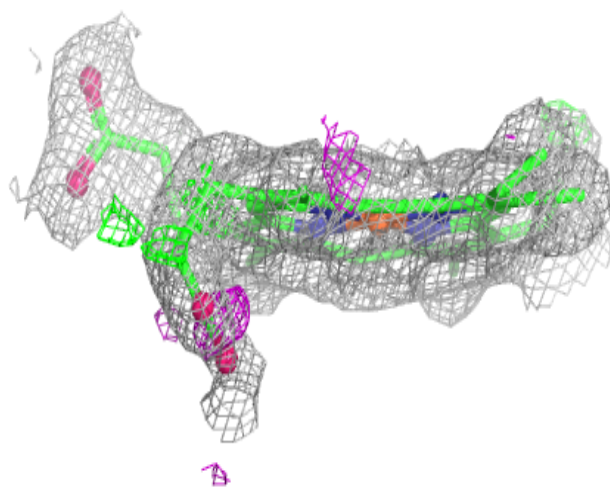
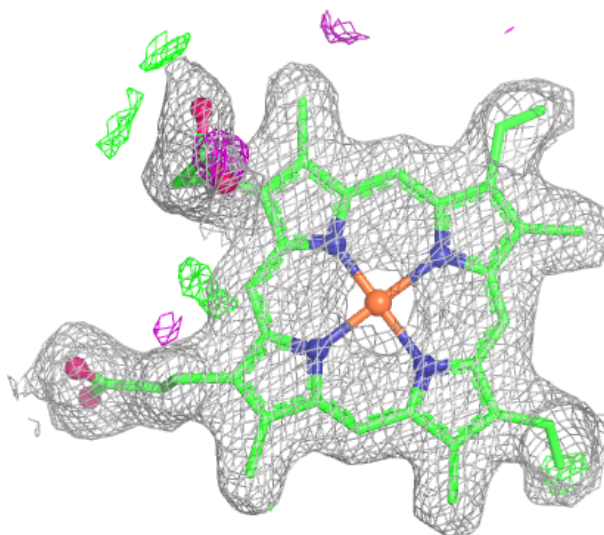
Electron density around HEM A 906:

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



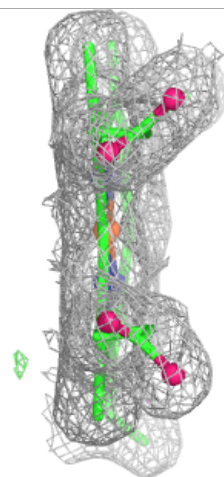
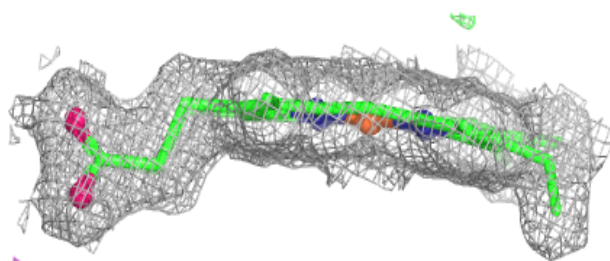
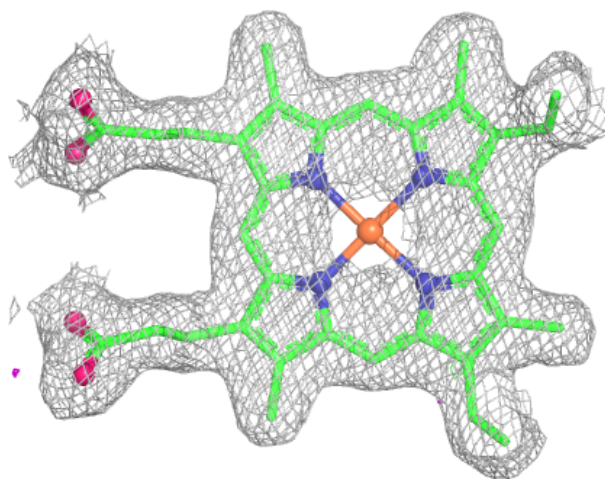
Electron density around HEM A 907:

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



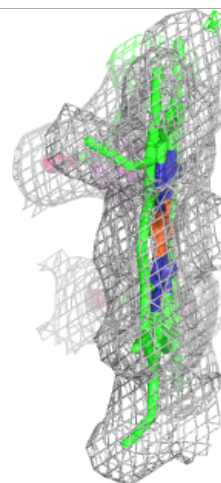
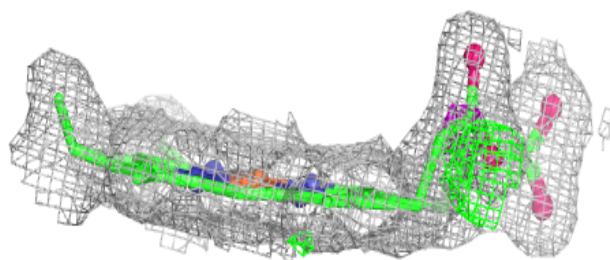
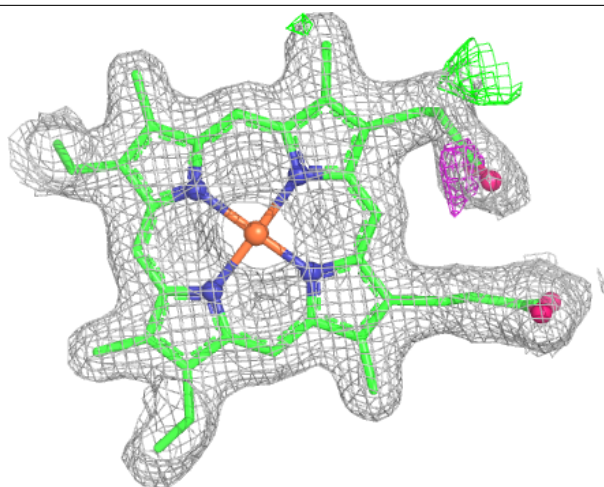
Electron density around HEM A 908:

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



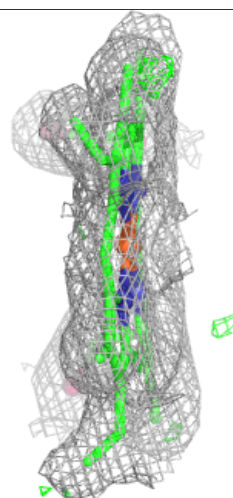
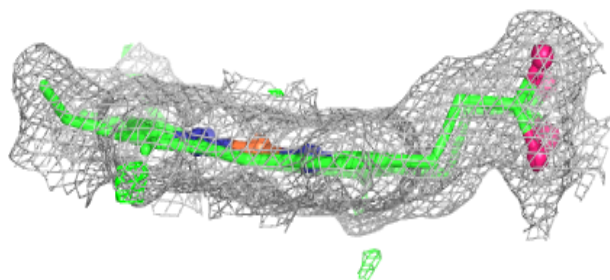
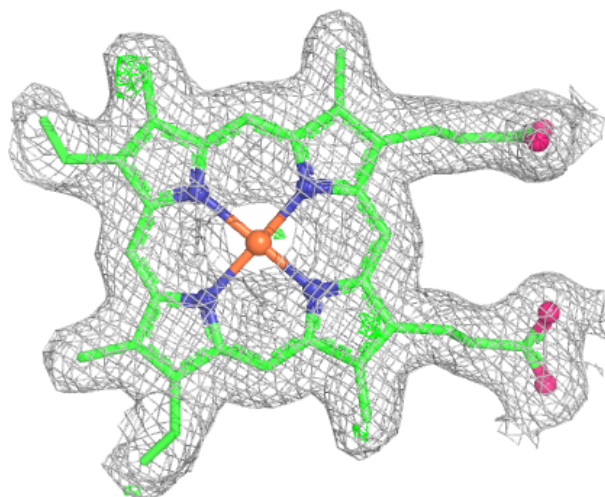
Electron density around HEM A 902:

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



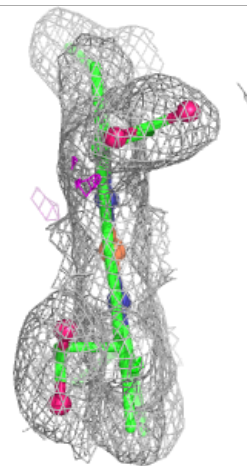
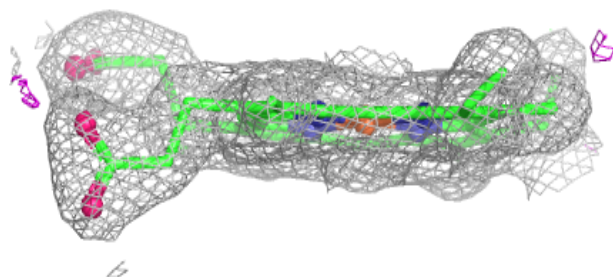
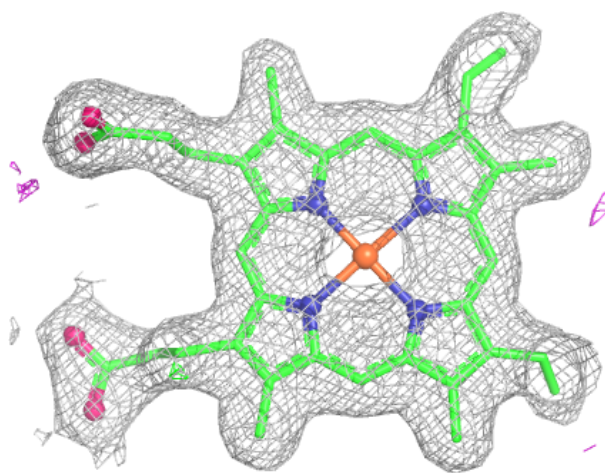
Electron density around HEM C 905:

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



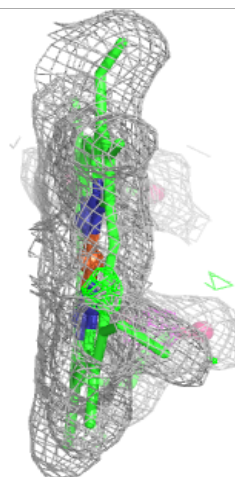
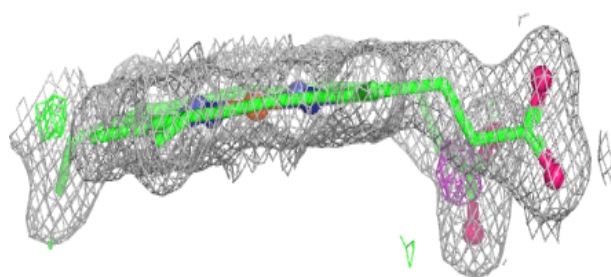
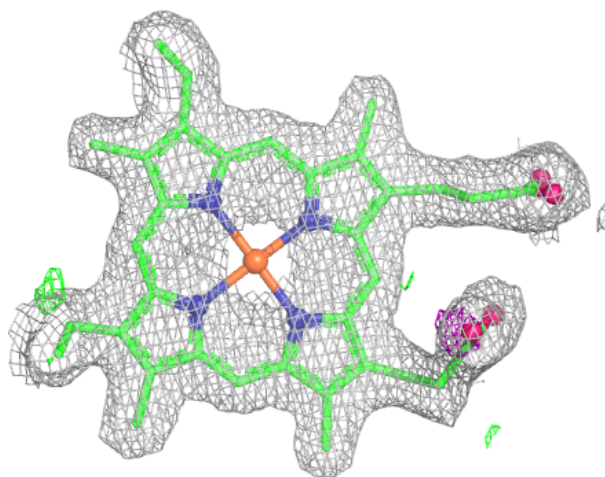
Electron density around HEM C 906:

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



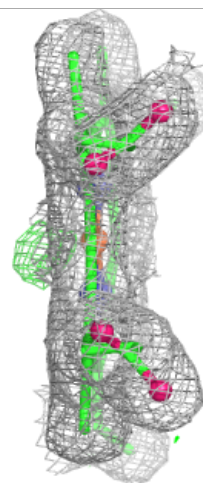
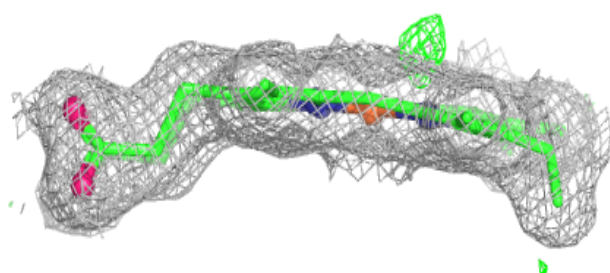
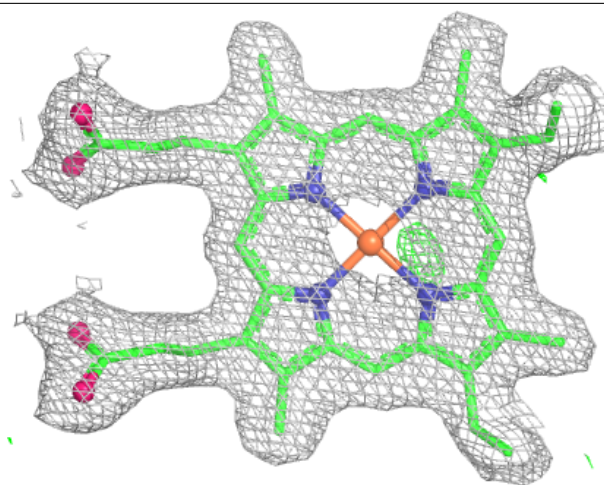
Electron density around HEM B 902:

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



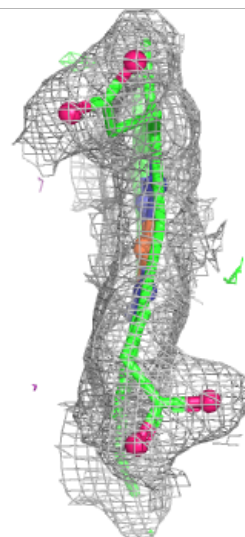
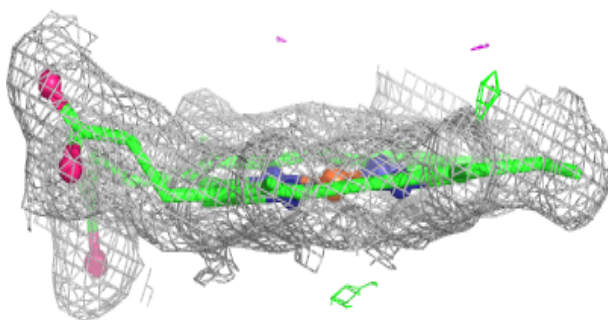
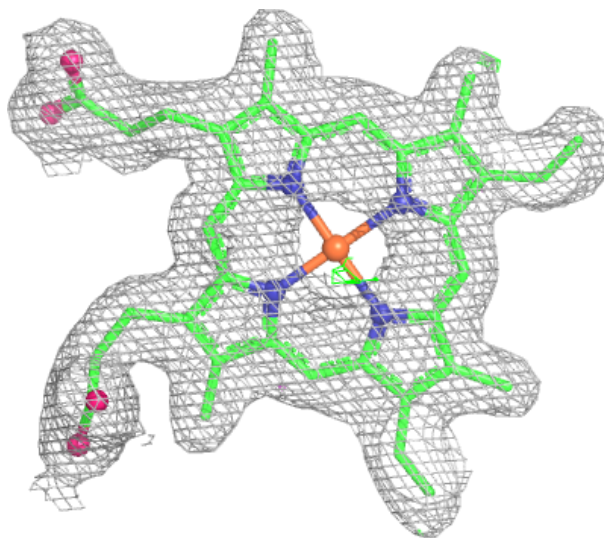
Electron density around HEM C 908:

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



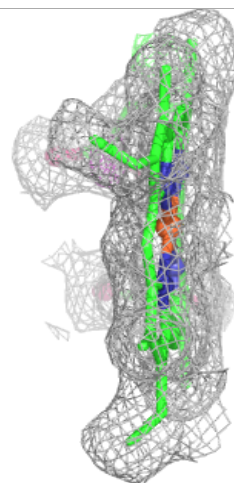
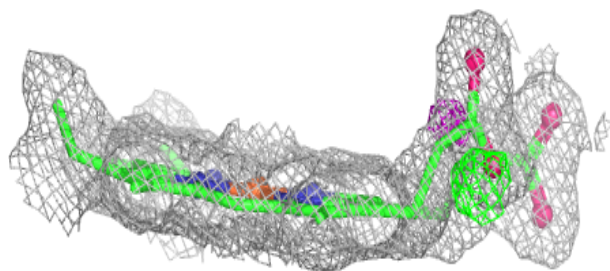
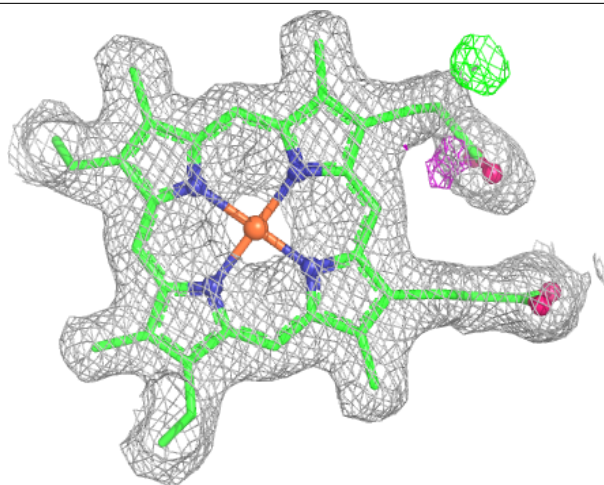
Electron density around HEM B 903:

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



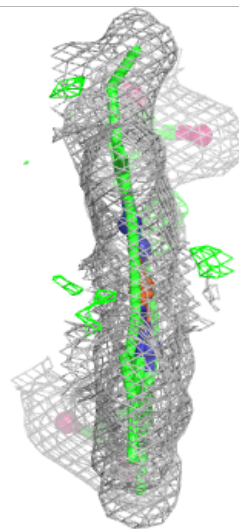
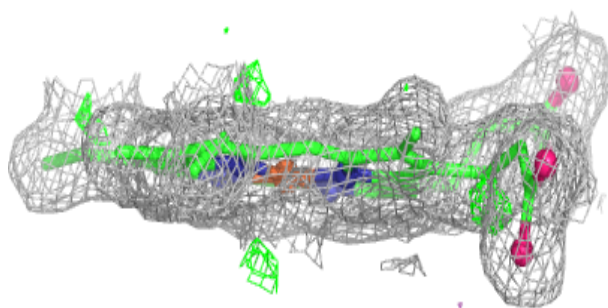
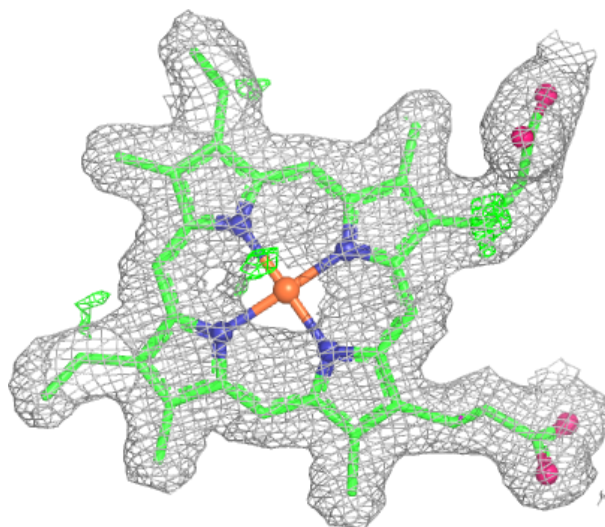
Electron density around HEM D 902:

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



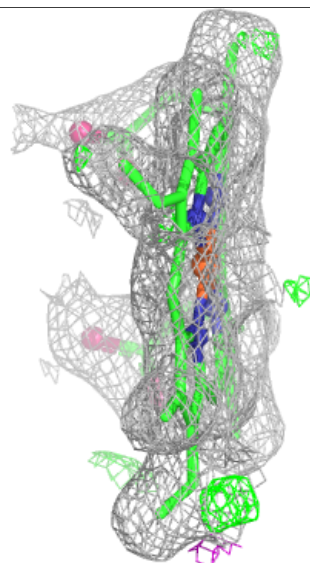
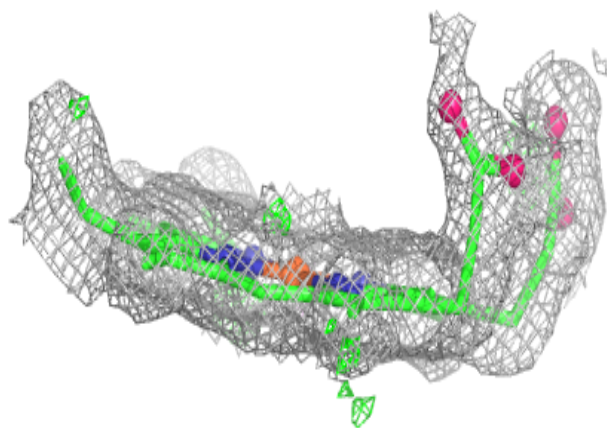
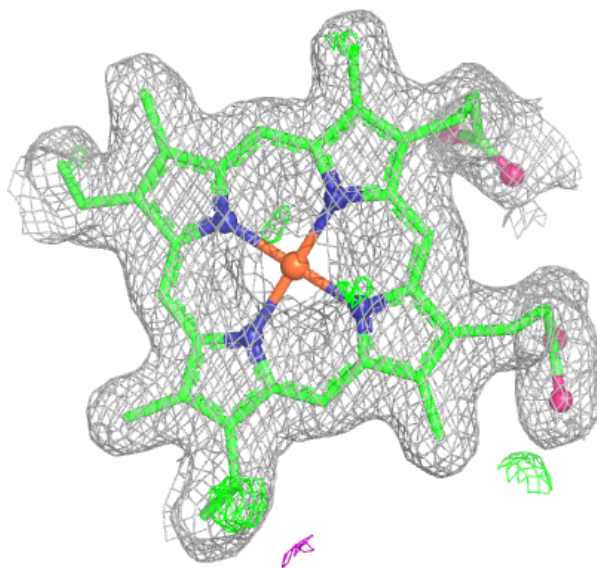
Electron density around HEM D 903:

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



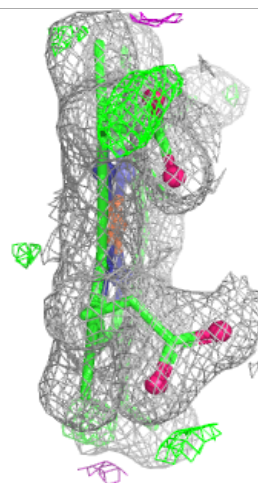
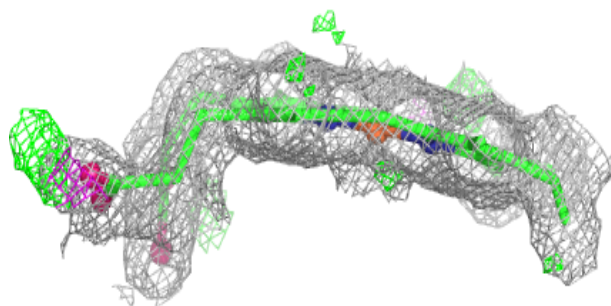
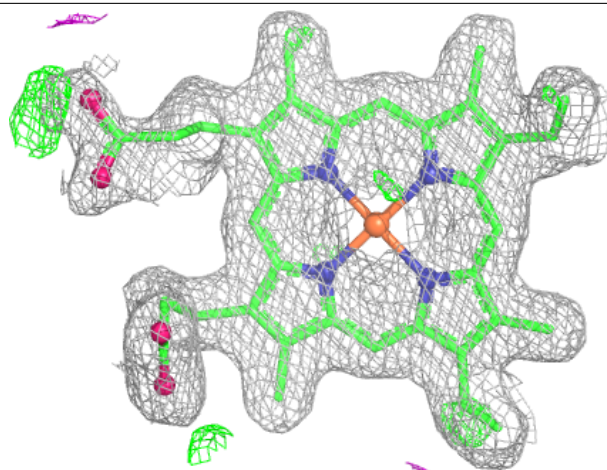
Electron density around HEM D 904 (A):

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



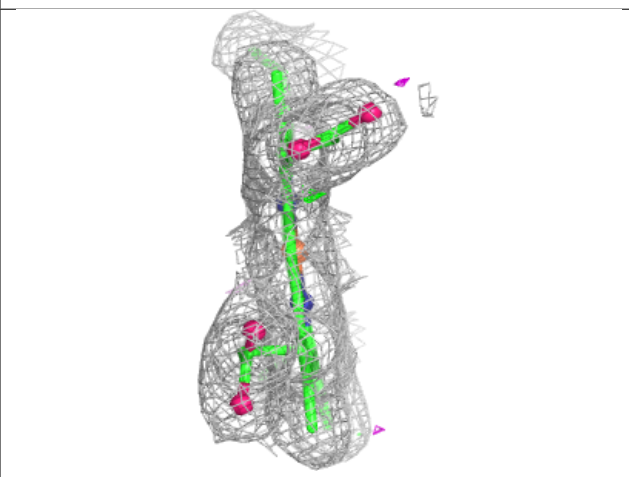
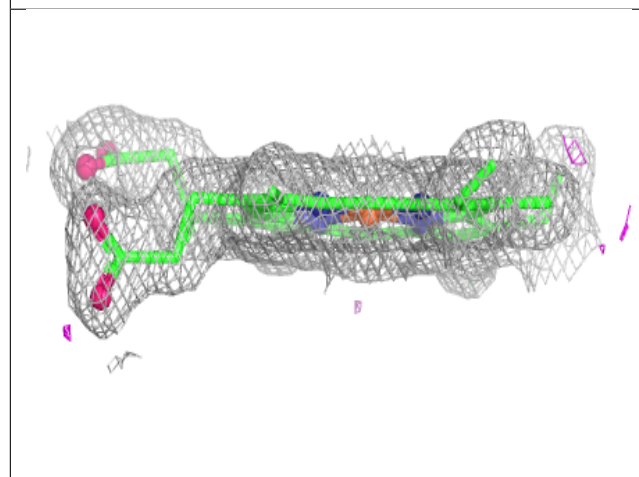
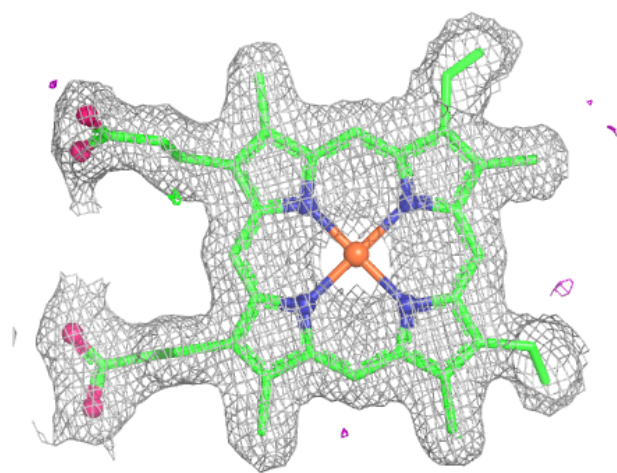
Electron density around HEM D 904 (B):

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



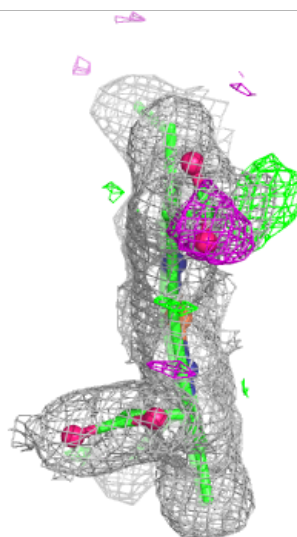
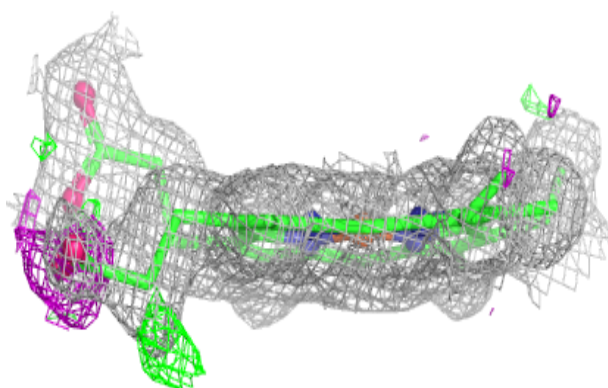
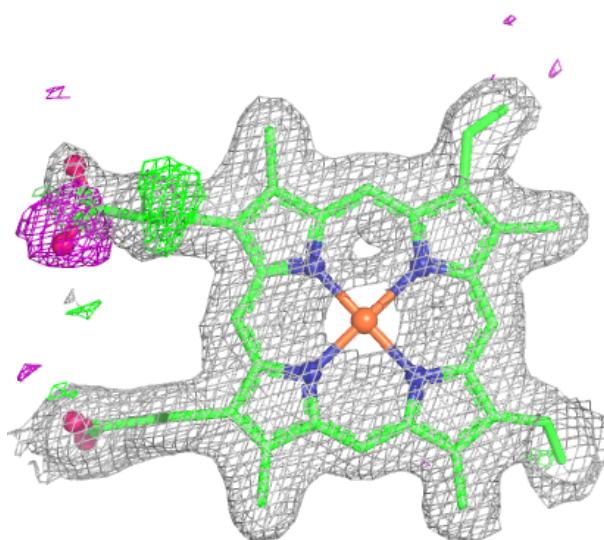
Electron density around HEM D 906:

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



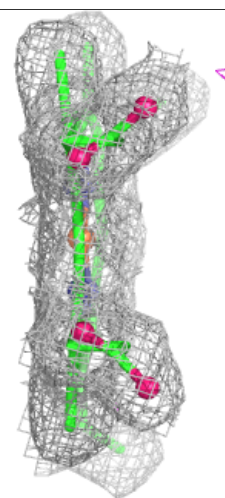
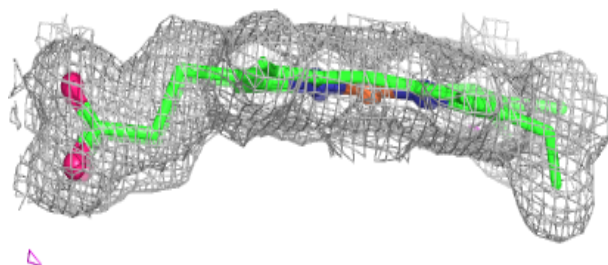
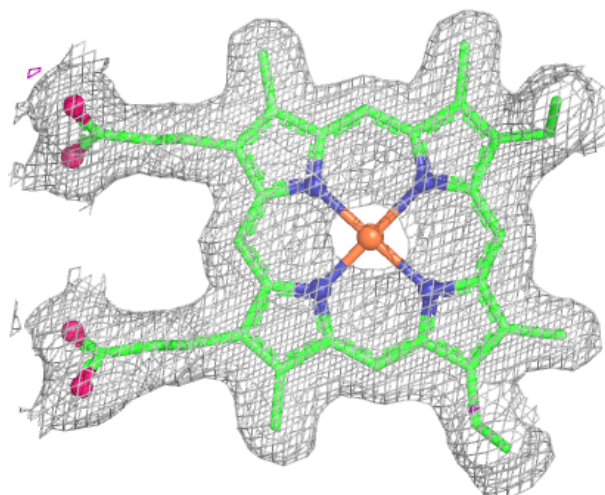
Electron density around HEM D 907:

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



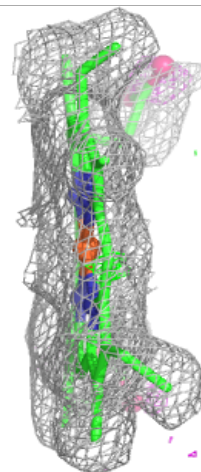
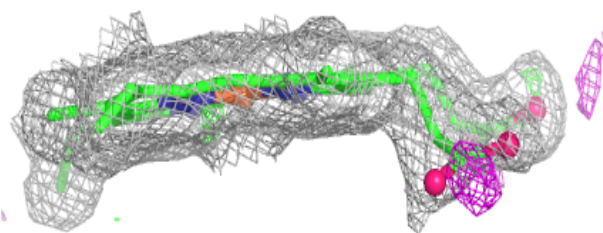
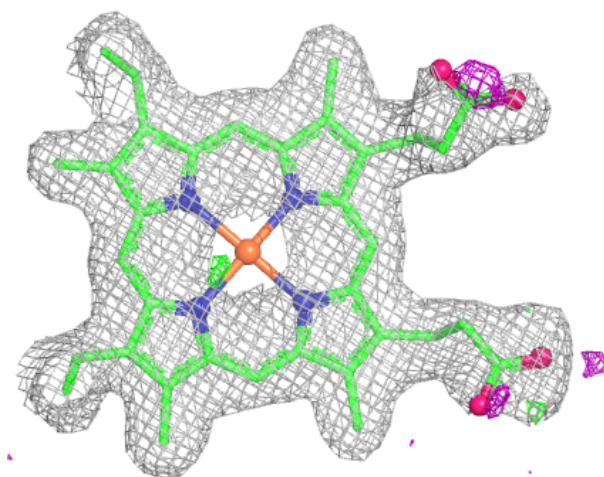
Electron density around HEM D 908:

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



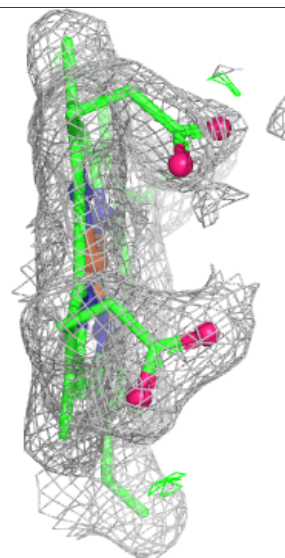
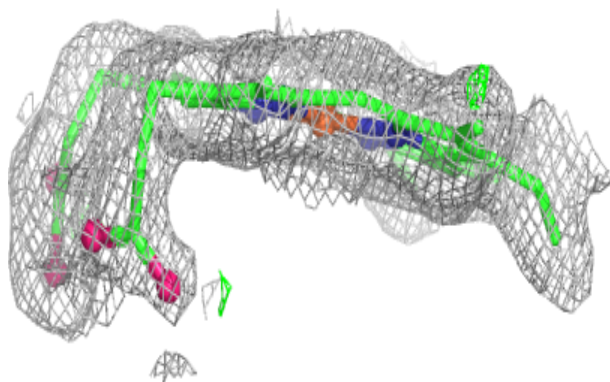
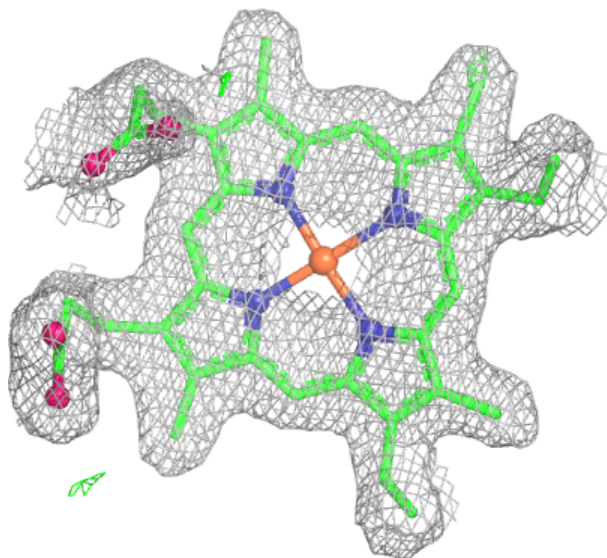
Electron density around HEM D 909:

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



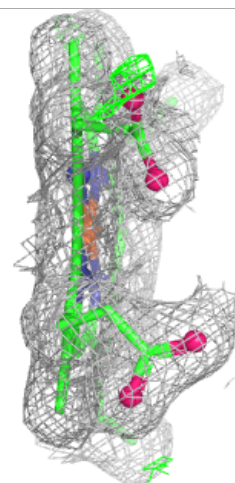
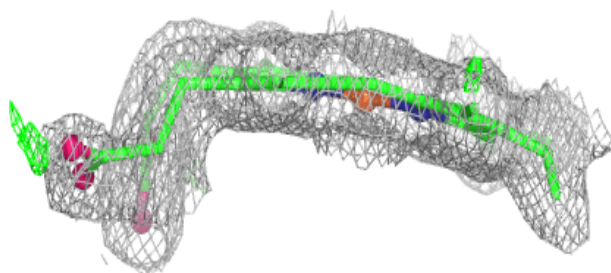
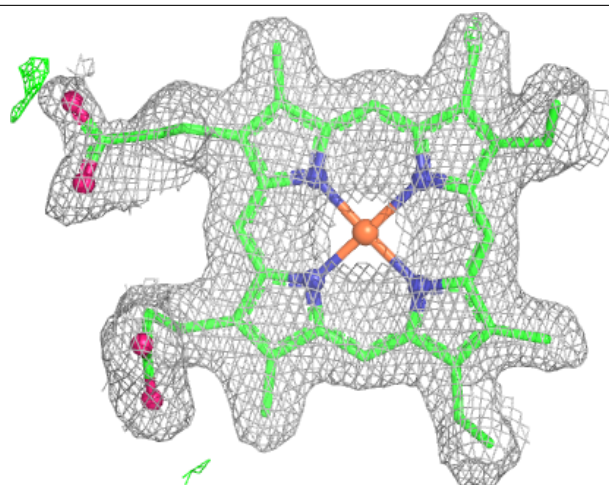
Electron density around HEM B 904 (A):

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



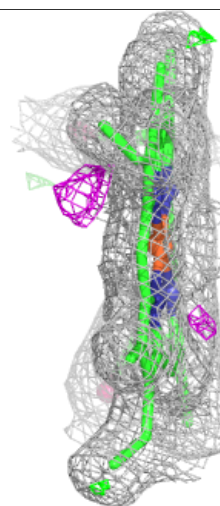
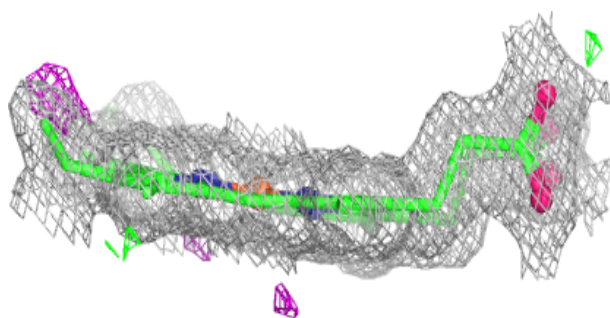
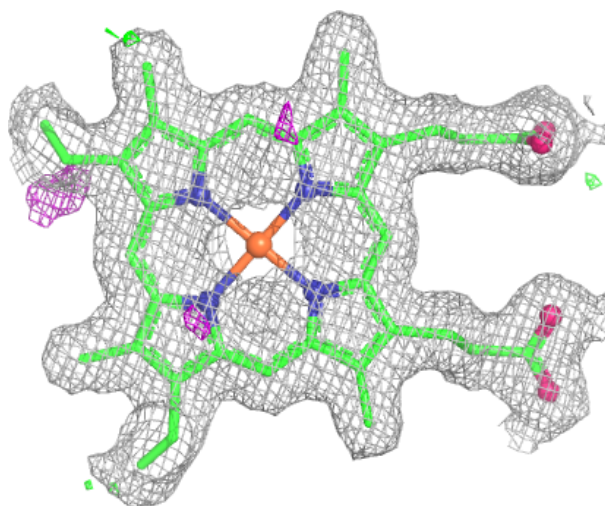
Electron density around HEM B 904 (B):

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



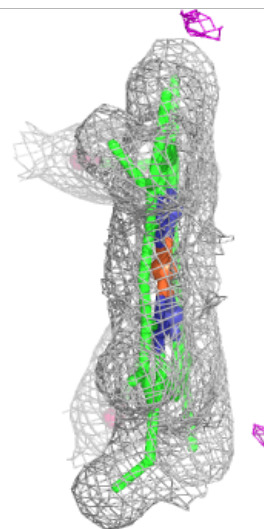
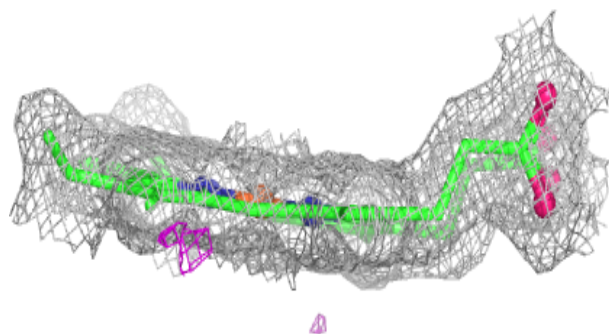
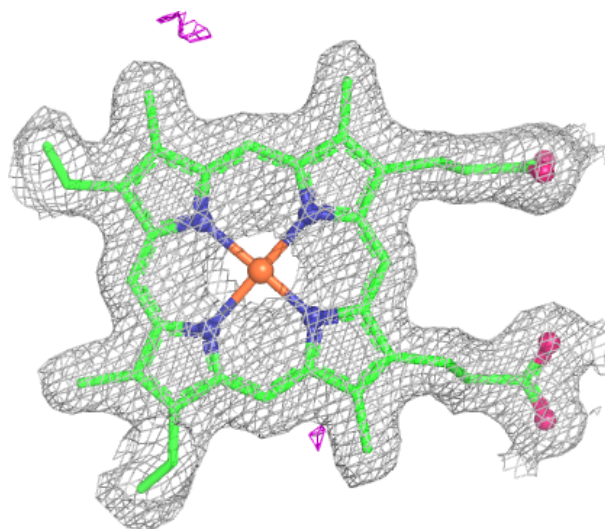
Electron density around HEM D 905:

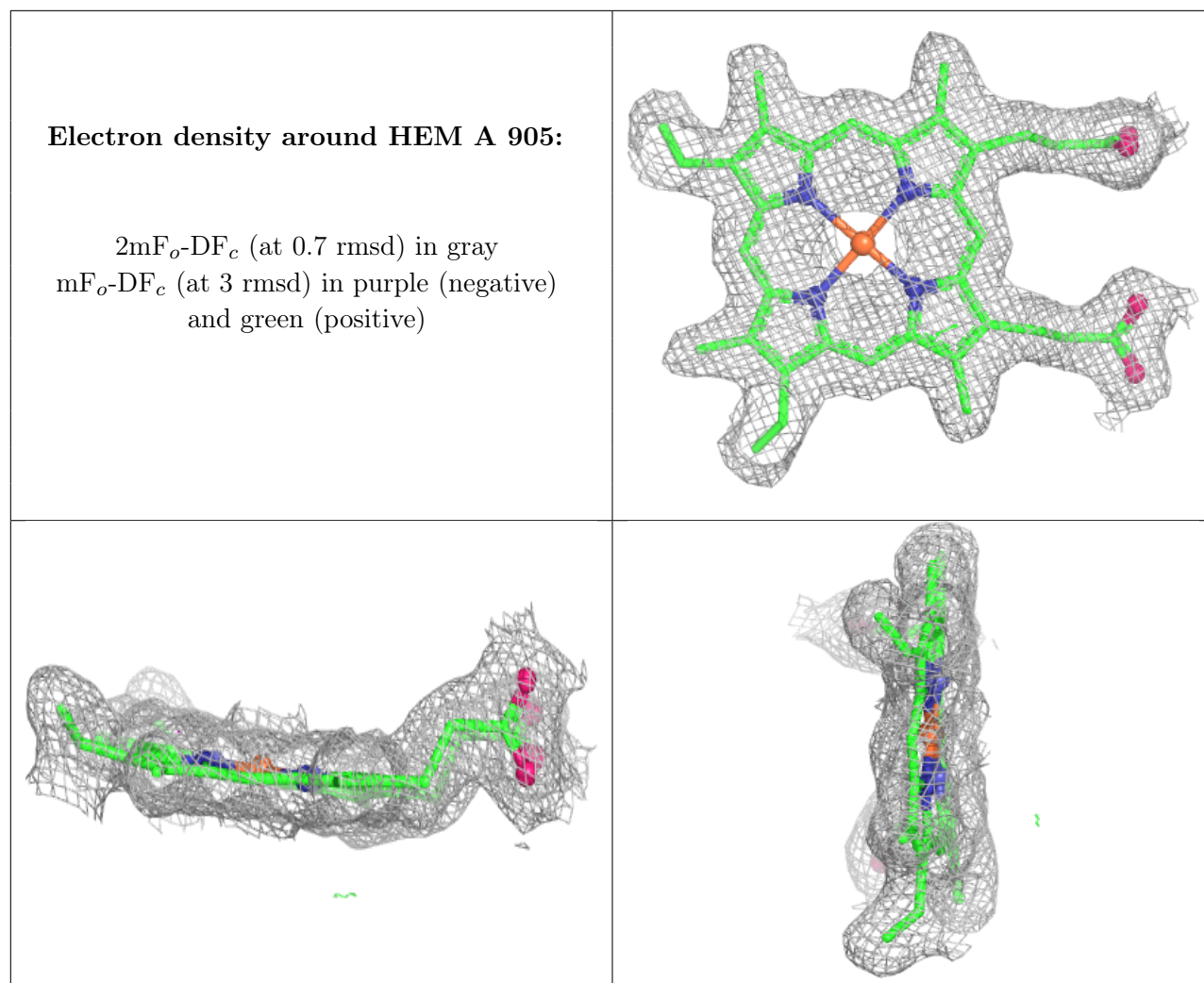
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 905:

$2mF_o-DF_c$ (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.