



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:49 AM UTC

PDB ID : 19HC / pdb_000019hc
Title : NINE-HAEM CYTOCHROME C FROM DESULFOVIBRIO DESULFURICANS ATCC 27774
Authors : Matias, P.M.; Coelho, R.; Pereira, I.A.C.; Coelho, A.V.; Thompson, A.W.; Sieker, L.; Gall, J.L.; Carrondo, M.A.
Deposited on : 1998-12-01
Resolution : 1.80 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

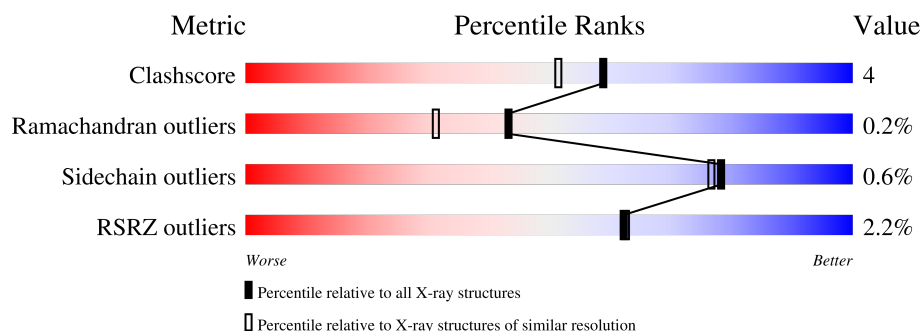
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	292	90% 10%
1	B	292	3% 89% 11%

2 Entry composition [i](#)

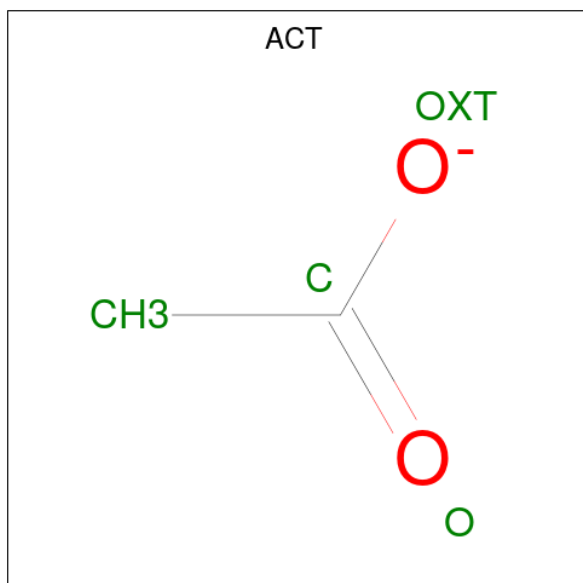
There are 4 unique types of molecules in this entry. The entry contains 6098 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (NINE-HAEM CYTOCHROME C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	17	7	0
			2206	1356	389	433	28			
1	B	292	Total	C	N	O	S	38	7	0
			2213	1359	391	435	28			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



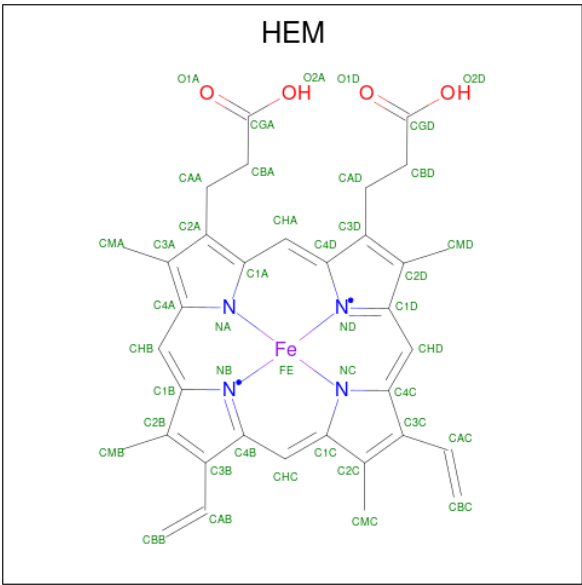
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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

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



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

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

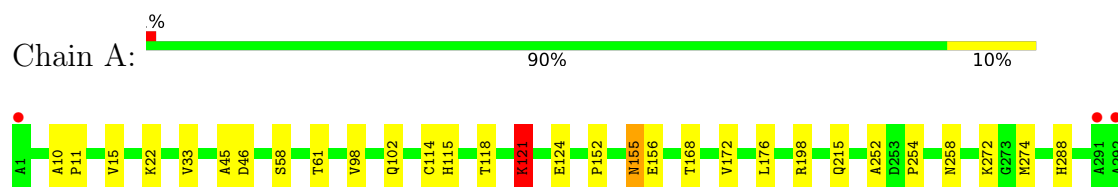
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	475	Total 475	O 475	0	0
4	B	410	Total 410	O 410	0	0

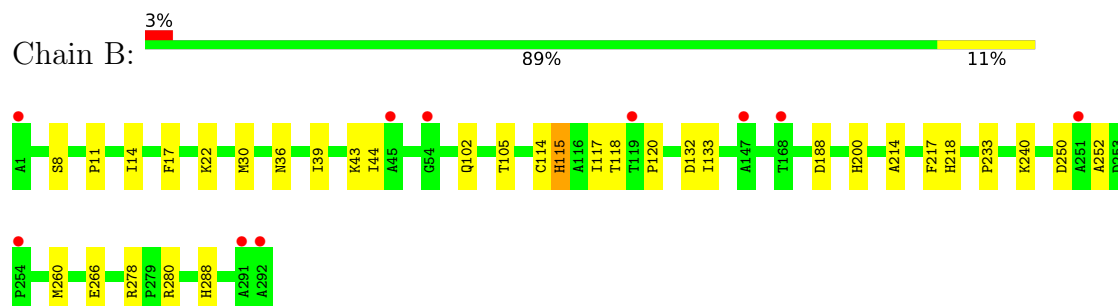
3 Residue-property plots [i](#)

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

- Molecule 1: PROTEIN (NINE-HAEM CYTOCHROME C)



- Molecule 1: PROTEIN (NINE-HAEM CYTOCHROME C)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.38Å 106.07Å 80.62Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	24.00 – 1.80 24.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (24.00-1.80) 99.2 (24.00-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.09 (at 1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.169 , (Not available) 0.160 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6098	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/2272	1.41	5/3088 (0.2%)
1	B	0.55	0/2278	1.35	8/3098 (0.3%)
All	All	0.57	0/4550	1.38	13/6186 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	PHE	O-C-N	8.40	128.49	121.35
1	B	44	ILE	CA-C-N	6.48	128.86	120.44
1	B	44	ILE	C-N-CA	6.48	128.86	120.44
1	B	133	ILE	N-CA-C	6.36	118.60	109.51
1	B	217	PHE	CA-CB-CG	-6.01	107.78	113.80
1	B	115	HIS	CA-CB-CG	-5.56	108.24	113.80
1	A	258	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	121	LYS	CA-C-N	-5.30	115.68	122.79
1	A	121	LYS	C-N-CA	-5.30	115.68	122.79
1	B	132	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	198	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	115	HIS	CA-CB-CG	-5.02	108.78	113.80
1	B	36	ASN	OD1-CG-ND2	5.01	127.61	122.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2206	0	2140	22	0
1	B	2213	0	2131	22	0
2	A	12	0	9	0	0
2	B	8	0	6	1	0
3	A	387	0	270	2	0
3	B	387	0	270	8	0
4	A	475	0	0	7	0
4	B	410	0	0	2	0
All	All	6098	0	4826	44	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 4.

All (44) 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:A:15:VAL:H	1:A:155:ASN:HD21	1.23	0.84
1:A:58[A]:SER:OG	1:A:61:THR:HG23	1.88	0.73
1:B:43:LYS:HG3	3:B:303:HEM:HBD2	1.72	0.71
1:B:278:ARG:NH1	1:B:280:ARG:HE	1.89	0.69
1:B:260:MET:HE3	2:B:294:ACT:H3	1.81	0.61
1:A:46:ASP:HB3	4:A:570:HOH:O	2.01	0.60
1:A:172[A]:VAL:CG2	1:A:176:LEU:HD12	2.32	0.59
1:B:250:ASP:HB3	4:B:316:HOH:O	2.02	0.59
1:A:121:LYS:HE2	4:A:482:HOH:O	2.05	0.57
1:A:15:VAL:H	1:A:155:ASN:ND2	1.97	0.57
1:A:274:MET:HE1	4:A:726:HOH:O	2.06	0.55
1:B:114:CYS:O	1:B:118[A]:THR:HG23	2.06	0.55
1:B:278:ARG:CZ	1:B:280:ARG:HE	2.19	0.54
1:B:30:MET:HG3	3:B:305:HEM:C4A	2.43	0.53
3:B:306:HEM:HBC1	3:B:308:HEM:HMC3	1.92	0.52
4:A:617:HOH:O	1:B:22:LYS:HE3	2.09	0.52
1:A:22:LYS:HG3	4:A:498:HOH:O	2.09	0.52
1:B:117[A]:ILE:HD12	1:B:266:GLU:HG3	1.94	0.50
1:B:250:ASP:OD2	1:B:252:ALA:HB3	2.14	0.48
1:A:124:GLU:HG2	1:B:233:PRO:HA	1.97	0.47
1:B:240:LYS:HD2	4:B:423:HOH:O	2.14	0.47
1:A:168:THR:HG23	1:A:215:GLN:HB3	1.96	0.46
1:B:118[A]:THR:O	1:B:120[A]:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:N	1:A:155:ASN:HD21	2.02	0.44
1:A:172[A]:VAL:HG23	1:A:176:LEU:HD12	1.99	0.44
1:A:98:VAL:O	1:A:102[B]:GLN:HG2	2.18	0.44
1:A:114:CYS:O	1:A:118:THR:HG23	2.18	0.44
1:A:152:PRO:O	1:A:156:GLU:HG3	2.18	0.44
1:B:11:PRO:HD2	1:B:14:ILE:HD11	2.00	0.44
1:B:200:HIS:CD2	3:B:308:HEM:NC	2.86	0.43
1:B:120[B]:PRO:HA	3:B:304:HEM:O1D	2.18	0.43
1:A:45:ALA:HA	4:A:708:HOH:O	2.18	0.43
1:A:252:ALA:C	1:A:254:PRO:HD3	2.44	0.43
1:A:288:HIS:CD2	3:A:309:HEM:ND	2.88	0.42
1:B:8:SER:HB3	3:B:301:HEM:HBB2	2.02	0.41
1:A:10:ALA:HB1	1:A:11:PRO:HD2	2.02	0.41
1:B:117[A]:ILE:HD12	1:B:266:GLU:CG	2.50	0.41
1:B:102:GLN:NE2	3:B:304:HEM:O2A	2.49	0.41
1:B:105:THR:HB	1:B:115:HIS:CG	2.56	0.41
1:B:214:ALA:HB1	1:B:218:HIS:CE1	2.56	0.41
1:A:33:VAL:HG21	3:A:305:HEM:C2D	2.56	0.40
1:A:272:LYS:HD3	4:A:769:HOH:O	2.19	0.40
1:A:168:THR:CG2	1:A:215:GLN:HB3	2.51	0.40
1:B:288:HIS:CD2	3:B:309:HEM:ND	2.90	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	297/292 (102%)	292 (98%)	5 (2%)	0	100	100
1	B	297/292 (102%)	293 (99%)	3 (1%)	1 (0%)	36	25
All	All	594/584 (102%)	585 (98%)	8 (1%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/238 (103%)	243 (99%)	2 (1%)	73	70
1	B	245/238 (103%)	244 (100%)	1 (0%)	84	83
All	All	490/476 (103%)	487 (99%)	3 (1%)	78	77

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	155	ASN
1	B	39	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	155	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	B	302	1	50,50,50	1.19	3 (6%)	67,82,82	1.25	8 (11%)
3	HEM	B	309	1	50,50,50	1.23	5 (10%)	67,82,82	1.10	4 (5%)
2	ACT	B	294	-	3,3,3	0.93	0	3,3,3	0.88	0
3	HEM	B	306	1	50,50,50	1.27	5 (10%)	67,82,82	1.10	5 (7%)
3	HEM	B	305	1	50,50,50	1.28	7 (14%)	67,82,82	1.10	7 (10%)
3	HEM	A	305	1	50,50,50	1.22	3 (6%)	67,82,82	0.96	5 (7%)
3	HEM	A	307	1	50,50,50	1.29	5 (10%)	67,82,82	1.05	5 (7%)
3	HEM	A	302	1	50,50,50	1.28	6 (12%)	67,82,82	0.96	4 (5%)
3	HEM	B	303	1	50,50,50	1.30	7 (14%)	67,82,82	1.10	4 (5%)
3	HEM	A	309	1	50,50,50	1.25	7 (14%)	67,82,82	1.22	7 (10%)
3	HEM	A	301	1	50,50,50	1.35	6 (12%)	67,82,82	1.17	8 (11%)
2	ACT	A	293	-	3,3,3	0.95	0	3,3,3	0.85	0
3	HEM	B	308	1	50,50,50	1.23	6 (12%)	67,82,82	1.25	4 (5%)
3	HEM	B	304	1	50,50,50	1.28	5 (10%)	67,82,82	1.01	4 (5%)
3	HEM	B	307	1	50,50,50	1.27	5 (10%)	67,82,82	1.06	5 (7%)
2	ACT	A	294	-	3,3,3	0.99	0	3,3,3	0.76	0
3	HEM	A	304	1	50,50,50	1.23	4 (8%)	67,82,82	1.15	8 (11%)
3	HEM	A	306	1	50,50,50	1.24	4 (8%)	67,82,82	1.12	5 (7%)
3	HEM	A	308	1	50,50,50	1.27	7 (14%)	67,82,82	1.20	9 (13%)
3	HEM	B	301	1	50,50,50	1.31	6 (12%)	67,82,82	1.26	7 (10%)
2	ACT	B	293	-	3,3,3	0.93	0	3,3,3	0.82	0
3	HEM	A	303	1	50,50,50	1.31	4 (8%)	67,82,82	1.17	7 (10%)
2	ACT	A	295	-	3,3,3	0.95	0	3,3,3	1.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	306	1	-	3/14/54/54	-
3	HEM	B	305	1	-	8/14/54/54	-
3	HEM	B	309	1	-	5/14/54/54	-
3	HEM	A	304	1	-	8/14/54/54	-
3	HEM	A	305	1	-	7/14/54/54	-
3	HEM	A	307	1	-	8/14/54/54	-
3	HEM	A	306	1	-	5/14/54/54	-
3	HEM	A	302	1	-	5/14/54/54	-
3	HEM	B	303	1	-	5/14/54/54	-
3	HEM	A	308	1	-	6/14/54/54	-
3	HEM	B	301	1	-	8/14/54/54	-
3	HEM	B	308	1	-	6/14/54/54	-
3	HEM	B	302	1	-	6/14/54/54	-
3	HEM	B	304	1	-	8/14/54/54	-
3	HEM	A	309	1	-	5/14/54/54	-
3	HEM	A	301	1	-	6/14/54/54	-
3	HEM	A	303	1	-	5/14/54/54	-
3	HEM	B	307	1	-	5/14/54/54	-

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	HEM	CAC-C3C	3.60	1.57	1.47
3	A	303	HEM	CAC-C3C	3.36	1.56	1.47
3	A	303	HEM	CAB-C3B	3.34	1.56	1.47
3	A	301	HEM	CAC-C3C	3.31	1.56	1.47
3	A	309	HEM	CAB-C3B	3.27	1.56	1.47
3	B	302	HEM	CAB-C3B	3.22	1.56	1.47
3	B	303	HEM	CAB-C3B	3.18	1.55	1.47
3	B	301	HEM	CAC-C3C	3.17	1.55	1.47
3	B	305	HEM	CAB-C3B	3.12	1.55	1.47
3	B	305	HEM	CAC-C3C	3.12	1.55	1.47
3	A	307	HEM	CAB-C3B	3.09	1.55	1.47
3	B	304	HEM	CAB-C3B	3.08	1.55	1.47
3	A	308	HEM	CAC-C3C	3.06	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	303	HEM	CAC-C3C	3.05	1.55	1.47
3	B	306	HEM	CAB-C3B	3.04	1.55	1.47
3	A	304	HEM	CAC-C3C	2.99	1.55	1.47
3	B	308	HEM	CAB-C3B	2.98	1.55	1.47
3	B	307	HEM	CAC-C3C	2.97	1.55	1.47
3	B	309	HEM	CAB-C3B	2.94	1.55	1.47
3	B	304	HEM	CAC-C3C	2.92	1.55	1.47
3	B	302	HEM	CAC-C3C	2.90	1.55	1.47
3	A	306	HEM	CAB-C3B	2.88	1.55	1.47
3	A	302	HEM	CAB-C3B	2.88	1.55	1.47
3	B	301	HEM	CAB-C3B	2.86	1.55	1.47
3	A	307	HEM	CAC-C3C	2.85	1.55	1.47
3	A	306	HEM	CMB-C2B	2.84	1.56	1.50
3	A	301	HEM	CMA-C3A	2.81	1.56	1.50
3	B	306	HEM	CAC-C3C	2.81	1.54	1.47
3	A	305	HEM	CAB-C3B	2.80	1.54	1.47
3	A	301	HEM	CMD-C2D	2.75	1.56	1.50
3	A	304	HEM	CAB-C3B	2.69	1.54	1.47
3	A	308	HEM	CAB-C3B	2.68	1.54	1.47
3	B	308	HEM	CAC-C3C	2.67	1.54	1.47
3	B	304	HEM	CMC-C2C	2.67	1.56	1.50
3	B	307	HEM	CMB-C2B	2.67	1.56	1.50
3	A	301	HEM	CAB-C3B	2.67	1.54	1.47
3	A	307	HEM	CMA-C3A	2.67	1.56	1.50
3	B	309	HEM	CAC-C3C	2.63	1.54	1.47
3	A	306	HEM	CAC-C3C	2.62	1.54	1.47
3	B	306	HEM	CMA-C3A	2.61	1.56	1.50
3	B	303	HEM	CMD-C2D	2.60	1.56	1.50
3	B	309	HEM	CMD-C2D	2.57	1.56	1.50
3	B	307	HEM	CAB-C3B	2.55	1.54	1.47
3	A	305	HEM	CAC-C3C	2.55	1.54	1.47
3	A	303	HEM	CMB-C2B	2.53	1.56	1.50
3	B	301	HEM	CMD-C2D	2.51	1.55	1.50
3	A	305	HEM	CMB-C2B	2.51	1.55	1.50
3	B	305	HEM	CMC-C2C	2.50	1.55	1.50
3	B	307	HEM	CMC-C2C	2.50	1.55	1.50
3	A	307	HEM	CMB-C2B	2.49	1.55	1.50
3	A	302	HEM	CMB-C2B	2.44	1.55	1.50
3	B	304	HEM	CMB-C2B	2.43	1.55	1.50
3	A	309	HEM	CAC-C3C	2.42	1.53	1.47
3	B	303	HEM	CMB-C2B	2.38	1.55	1.50
3	B	306	HEM	CMB-C2B	2.37	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	HEM	CMC-C2C	2.36	1.55	1.50
3	A	308	HEM	CMA-C3A	2.36	1.55	1.50
3	B	301	HEM	CMB-C2B	2.35	1.55	1.50
3	A	304	HEM	C2A-C3A	-2.35	1.32	1.38
3	B	301	HEM	CMC-C2C	2.34	1.55	1.50
3	B	307	HEM	CMD-C2D	2.34	1.55	1.50
3	B	305	HEM	CMA-C3A	2.33	1.55	1.50
3	A	308	HEM	CMC-C2C	2.31	1.55	1.50
3	B	301	HEM	CMA-C3A	2.27	1.55	1.50
3	B	308	HEM	C2A-C3A	-2.25	1.33	1.38
3	A	309	HEM	CMB-C2B	2.25	1.55	1.50
3	A	307	HEM	CMD-C2D	2.23	1.55	1.50
3	A	304	HEM	CMB-C2B	2.23	1.55	1.50
3	A	302	HEM	CMD-C2D	2.23	1.55	1.50
3	A	301	HEM	C2A-C3A	-2.21	1.33	1.38
3	A	308	HEM	CMD-C2D	2.20	1.55	1.50
3	B	308	HEM	CMB-C2B	2.19	1.55	1.50
3	B	303	HEM	CMA-C3A	2.19	1.55	1.50
3	B	308	HEM	CMA-C3A	2.18	1.55	1.50
3	A	308	HEM	C2A-C3A	-2.18	1.33	1.38
3	B	305	HEM	CMB-C2B	2.17	1.55	1.50
3	B	309	HEM	CMC-C2C	2.15	1.55	1.50
3	A	301	HEM	CMB-C2B	2.14	1.55	1.50
3	A	309	HEM	CMC-C2C	2.13	1.55	1.50
3	B	303	HEM	CMC-C2C	2.13	1.55	1.50
3	B	306	HEM	CAA-C2A	2.11	1.56	1.51
3	A	303	HEM	CMC-C2C	2.11	1.55	1.50
3	B	304	HEM	CMA-C3A	2.11	1.55	1.50
3	A	308	HEM	CMB-C2B	2.11	1.55	1.50
3	B	305	HEM	C3B-C2B	-2.10	1.32	1.37
3	B	302	HEM	CMB-C2B	2.08	1.55	1.50
3	B	305	HEM	C2A-C3A	-2.07	1.33	1.38
3	A	306	HEM	CMC-C2C	2.07	1.55	1.50
3	A	309	HEM	CMA-C3A	2.07	1.55	1.50
3	B	308	HEM	CMC-C2C	2.07	1.55	1.50
3	B	303	HEM	CAA-C2A	2.06	1.56	1.51
3	B	309	HEM	CMB-C2B	2.04	1.55	1.50
3	A	302	HEM	CMA-C3A	2.03	1.54	1.50
3	A	309	HEM	C2A-C3A	-2.03	1.33	1.38
3	A	309	HEM	C3B-C2B	-2.03	1.33	1.37

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	HEM	CMC-C2C-C1C	-3.98	117.72	124.73
3	B	309	HEM	CAD-C3D-C4D	-3.78	118.11	124.70
3	B	308	HEM	CMC-C2C-C1C	-3.65	118.29	124.73
3	B	301	HEM	C3B-C2B-C1B	3.64	109.14	106.41
3	B	308	HEM	CMA-C3A-C4A	-3.62	119.91	125.42
3	A	309	HEM	CHB-C1B-NB	3.59	128.81	124.37
3	A	306	HEM	CMB-C2B-C1B	-3.54	119.50	125.03
3	B	306	HEM	C3B-C2B-C1B	3.10	108.74	106.41
3	A	309	HEM	CAD-C3D-C4D	-3.09	119.31	124.70
3	A	303	HEM	O1A-CGA-CBA	-2.97	113.67	123.09
3	B	306	HEM	CMB-C2B-C1B	-2.97	120.39	125.03
3	A	304	HEM	CBC-CAC-C3C	-2.94	112.85	127.53
3	B	308	HEM	CMA-C3A-C2A	2.92	131.81	125.62
3	A	306	HEM	CBC-CAC-C3C	-2.90	113.02	127.53
3	A	307	HEM	CMB-C2B-C1B	-2.88	120.54	125.03
3	A	308	HEM	C3B-C4B-NB	2.85	111.51	109.47
3	A	303	HEM	C3B-C2B-C1B	2.82	108.53	106.41
3	A	304	HEM	CMA-C3A-C4A	-2.81	121.14	125.42
3	B	302	HEM	CHD-C1D-ND	2.79	127.43	124.42
3	A	309	HEM	CBC-CAC-C3C	-2.78	113.62	127.53
3	B	305	HEM	CBB-CAB-C3B	-2.77	113.68	127.53
3	B	302	HEM	C4C-CHD-C1D	-2.73	120.22	126.02
3	A	301	HEM	O1A-CGA-CBA	-2.71	114.51	123.09
3	A	308	HEM	C3B-C2B-C1B	2.70	108.44	106.41
3	A	306	HEM	C3B-C2B-C1B	2.70	108.44	106.41
3	A	304	HEM	CBB-CAB-C3B	-2.67	114.18	127.53
3	B	304	HEM	O1D-CGD-CBD	-2.65	114.70	123.09
3	A	309	HEM	CBB-CAB-C3B	-2.61	114.48	127.53
3	A	308	HEM	O1D-CGD-CBD	-2.60	114.85	123.09
3	A	301	HEM	CAD-C3D-C4D	-2.55	120.25	124.70
3	B	303	HEM	CMC-C2C-C3C	2.54	134.56	128.43
3	A	308	HEM	CMC-C2C-C1C	-2.51	120.30	124.73
3	B	302	HEM	CBB-CAB-C3B	-2.50	115.02	127.53
3	A	307	HEM	CBB-CAB-C3B	-2.47	115.17	127.53
3	A	305	HEM	C1C-CHC-C4B	-2.46	120.79	126.02
3	B	301	HEM	CMB-C2B-C1B	-2.46	121.19	125.03
3	B	309	HEM	CBB-CAB-C3B	-2.43	115.36	127.53
3	B	305	HEM	CMB-C2B-C1B	-2.43	121.24	125.03
3	A	303	HEM	CMC-C2C-C1C	-2.41	120.48	124.73
3	B	304	HEM	O2D-CGD-O1D	2.41	129.53	123.33
3	B	301	HEM	CHA-C4D-ND	2.41	127.35	124.37
3	A	303	HEM	CHD-C1D-ND	2.41	127.01	124.42
3	A	301	HEM	CBC-CAC-C3C	-2.40	115.53	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	HEM	CAA-C2A-C3A	2.38	132.41	127.07
3	B	309	HEM	C3B-C2B-C1B	2.38	108.20	106.41
3	A	301	HEM	C1C-CHC-C4B	-2.38	120.96	126.02
3	B	301	HEM	C1A-CHA-C4D	-2.38	120.65	126.25
3	B	304	HEM	CMB-C2B-C1B	-2.38	121.32	125.03
3	B	302	HEM	O1D-CGD-CBD	-2.36	115.60	123.09
3	B	305	HEM	CHC-C4B-NB	2.35	126.96	124.42
3	B	302	HEM	CBC-CAC-C3C	-2.35	115.80	127.53
3	A	302	HEM	CMD-C2D-C1D	-2.34	121.38	125.03
3	B	307	HEM	O1D-CGD-CBD	-2.33	115.69	123.09
3	A	305	HEM	CBB-CAB-C3B	-2.32	115.94	127.53
3	A	303	HEM	C3B-C4B-NB	2.32	111.13	109.47
3	A	307	HEM	C3B-C2B-C1B	2.31	108.15	106.41
3	B	305	HEM	C3B-C2B-C1B	2.30	108.14	106.41
3	A	301	HEM	CAD-C3D-C2D	2.30	132.18	127.87
3	A	309	HEM	CMB-C2B-C1B	-2.30	121.45	125.03
3	B	305	HEM	CBC-CAC-C3C	-2.28	116.12	127.53
3	B	302	HEM	CHC-C4B-NB	-2.28	121.97	124.42
3	B	307	HEM	CHD-C1D-ND	-2.28	121.97	124.42
3	A	304	HEM	C1A-CHA-C4D	-2.28	120.89	126.25
3	A	306	HEM	CBB-CAB-C3B	-2.27	116.16	127.53
3	B	305	HEM	CMA-C3A-C4A	-2.27	121.96	125.42
3	A	302	HEM	CMC-C2C-C1C	-2.27	120.74	124.73
3	B	307	HEM	CBC-CAC-C3C	-2.26	116.25	127.53
3	A	308	HEM	C4A-CHB-C1B	-2.26	120.94	126.25
3	A	303	HEM	CBB-CAB-C3B	-2.26	116.26	127.53
3	B	301	HEM	CAA-C2A-C1A	-2.24	120.57	124.94
3	A	308	HEM	O2D-CGD-O1D	2.23	129.06	123.33
3	A	302	HEM	C3B-C2B-C1B	2.21	108.07	106.41
3	A	305	HEM	CMC-C2C-C1C	-2.21	120.83	124.73
3	B	303	HEM	CMD-C2D-C1D	-2.20	121.60	125.03
3	B	305	HEM	CMA-C3A-C2A	2.20	130.28	125.62
3	B	309	HEM	CAA-C2A-C1A	-2.18	120.68	124.94
3	B	306	HEM	CBC-CAC-C3C	-2.18	116.64	127.53
3	A	301	HEM	O1D-CGD-CBD	-2.17	116.20	123.09
3	A	309	HEM	C4A-CHB-C1B	-2.17	121.14	126.25
3	A	304	HEM	CHA-C1A-NA	2.17	127.80	123.86
3	A	304	HEM	CMA-C3A-C2A	2.17	130.23	125.62
3	A	307	HEM	CBD-CAD-C3D	2.17	118.53	112.53
3	A	301	HEM	CHA-C4D-ND	2.17	127.05	124.37
3	A	302	HEM	CBC-CAC-C3C	-2.17	116.70	127.53
3	B	304	HEM	CBC-CAC-C3C	-2.15	116.76	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	HEM	CAA-C2A-C1A	-2.15	120.74	124.94
3	B	307	HEM	O1A-CGA-CBA	-2.13	116.34	123.09
3	A	305	HEM	CBA-CAA-C2A	2.12	118.39	112.53
3	B	308	HEM	CBC-CAC-C3C	-2.12	116.95	127.53
3	A	308	HEM	C4B-C3B-C2B	-2.10	105.35	107.28
3	A	303	HEM	CHD-C4C-NC	-2.10	122.17	124.45
3	B	301	HEM	CAA-C2A-C3A	2.09	131.75	127.07
3	A	306	HEM	O1A-CGA-CBA	-2.08	116.49	123.09
3	B	301	HEM	CMC-C2C-C3C	-2.08	123.40	128.43
3	B	306	HEM	CBB-CAB-C3B	-2.06	117.22	127.53
3	B	302	HEM	C3B-C4B-NB	-2.05	108.00	109.47
3	B	306	HEM	O2A-CGA-O1A	2.04	128.59	123.33
3	A	309	HEM	CHC-C4B-NB	2.04	126.61	124.42
3	A	301	HEM	CMA-C3A-C2A	2.03	129.94	125.62
3	B	307	HEM	O2D-CGD-O1D	2.03	128.55	123.33
3	A	308	HEM	CAD-C3D-C4D	-2.03	121.17	124.70
3	A	305	HEM	CMB-C2B-C1B	-2.02	121.87	125.03
3	A	308	HEM	CAA-C2A-C1A	-2.02	121.00	124.94
3	B	303	HEM	CAA-C2A-C1A	-2.02	121.00	124.94
3	B	302	HEM	O1A-CGA-CBA	-2.02	116.69	123.09
3	A	307	HEM	O1A-CGA-CBA	-2.01	116.72	123.09

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	HEM	C4B-C3B-CAB-CBB
3	A	301	HEM	C2C-C3C-CAC-CBC
3	A	304	HEM	C2C-C3C-CAC-CBC
3	A	309	HEM	C2B-C3B-CAB-CBB
3	A	309	HEM	C4B-C3B-CAB-CBB
3	B	301	HEM	C2B-C3B-CAB-CBB
3	B	305	HEM	C2C-C3C-CAC-CBC
3	B	307	HEM	C2B-C3B-CAB-CBB
3	A	308	HEM	C2A-CAA-CBA-CGA
3	B	308	HEM	C2A-CAA-CBA-CGA
3	A	302	HEM	C2B-C3B-CAB-CBB
3	A	309	HEM	C2C-C3C-CAC-CBC
3	B	304	HEM	C2C-C3C-CAC-CBC
3	B	309	HEM	C2B-C3B-CAB-CBB
3	A	302	HEM	C4B-C3B-CAB-CBB
3	A	307	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
3	B	301	HEM	C4B-C3B-CAB-CBB
3	B	302	HEM	C4B-C3B-CAB-CBB
3	B	302	HEM	C4C-C3C-CAC-CBC
3	B	306	HEM	C4B-C3B-CAB-CBB
3	B	307	HEM	C4B-C3B-CAB-CBB
3	A	301	HEM	C2B-C3B-CAB-CBB
3	A	304	HEM	C2B-C3B-CAB-CBB
3	A	305	HEM	C2C-C3C-CAC-CBC
3	A	307	HEM	C2B-C3B-CAB-CBB
3	A	307	HEM	C2C-C3C-CAC-CBC
3	B	302	HEM	C2C-C3C-CAC-CBC
3	B	306	HEM	C2B-C3B-CAB-CBB
3	B	307	HEM	C2C-C3C-CAC-CBC
3	B	309	HEM	C2C-C3C-CAC-CBC
3	B	301	HEM	C4C-C3C-CAC-CBC
3	B	305	HEM	C4B-C3B-CAB-CBB
3	B	309	HEM	C4B-C3B-CAB-CBB
3	B	302	HEM	C4D-C3D-CAD-CBD
3	B	304	HEM	C2B-C3B-CAB-CBB
3	A	302	HEM	C4C-C3C-CAC-CBC
3	A	303	HEM	C4B-C3B-CAB-CBB
3	A	304	HEM	C4B-C3B-CAB-CBB
3	A	304	HEM	C4C-C3C-CAC-CBC
3	A	306	HEM	C4B-C3B-CAB-CBB
3	B	304	HEM	C4B-C3B-CAB-CBB
3	B	304	HEM	C4C-C3C-CAC-CBC
3	B	303	HEM	C2A-CAA-CBA-CGA
3	A	307	HEM	CAD-CBD-CGD-O1D
3	B	303	HEM	CAA-CBA-CGA-O1A
3	B	308	HEM	CAD-CBD-CGD-O2D
3	A	305	HEM	CAD-CBD-CGD-O1D
3	A	307	HEM	CAA-CBA-CGA-O1A
3	B	307	HEM	CAA-CBA-CGA-O1A
3	B	308	HEM	CAA-CBA-CGA-O2A
3	B	305	HEM	CAD-CBD-CGD-O1D
3	B	308	HEM	CAD-CBD-CGD-O1D
3	B	305	HEM	CAA-CBA-CGA-O1A
3	A	307	HEM	CAA-CBA-CGA-O2A
3	B	305	HEM	CAD-CBD-CGD-O2D
3	A	301	HEM	CAD-CBD-CGD-O1D
3	B	303	HEM	CAA-CBA-CGA-O2A
3	A	304	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	A	307	HEM	CAD-CBD-CGD-O2D
3	A	308	HEM	CAD-CBD-CGD-O1D
3	A	306	HEM	CAA-CBA-CGA-O2A
3	B	304	HEM	CAD-CBD-CGD-O1D
3	A	303	HEM	C2A-CAA-CBA-CGA
3	A	302	HEM	CAD-CBD-CGD-O2D
3	A	301	HEM	CAD-CBD-CGD-O2D
3	B	302	HEM	CAD-CBD-CGD-O2D
3	A	304	HEM	CAD-CBD-CGD-O1D
3	B	305	HEM	CAA-CBA-CGA-O2A
3	B	308	HEM	CAA-CBA-CGA-O1A
3	A	305	HEM	CAD-CBD-CGD-O2D
3	A	308	HEM	CAD-CBD-CGD-O2D
3	B	307	HEM	CAA-CBA-CGA-O2A
3	A	303	HEM	CAA-CBA-CGA-O1A
3	A	305	HEM	CAA-CBA-CGA-O2A
3	B	304	HEM	CAA-CBA-CGA-O2A
3	A	304	HEM	CAD-CBD-CGD-O2D
3	B	304	HEM	CAD-CBD-CGD-O2D
3	A	306	HEM	C2C-C3C-CAC-CBC
3	B	301	HEM	C2C-C3C-CAC-CBC
3	B	303	HEM	C2B-C3B-CAB-CBB
3	A	303	HEM	CAA-CBA-CGA-O2A
3	A	302	HEM	CAD-CBD-CGD-O1D
3	B	302	HEM	CAD-CBD-CGD-O1D
3	A	306	HEM	CAA-CBA-CGA-O1A
3	A	304	HEM	CAA-CBA-CGA-O1A
3	A	301	HEM	C4C-C3C-CAC-CBC
3	A	305	HEM	C4B-C3B-CAB-CBB
3	A	305	HEM	C4C-C3C-CAC-CBC
3	A	306	HEM	C4C-C3C-CAC-CBC
3	A	307	HEM	C4C-C3C-CAC-CBC
3	A	308	HEM	C4B-C3B-CAB-CBB
3	B	303	HEM	C4B-C3B-CAB-CBB
3	B	305	HEM	C4C-C3C-CAC-CBC
3	B	306	HEM	C4C-C3C-CAC-CBC
3	B	308	HEM	C4B-C3B-CAB-CBB
3	A	305	HEM	CAA-CBA-CGA-O1A
3	A	308	HEM	CAA-CBA-CGA-O1A
3	A	308	HEM	CAA-CBA-CGA-O2A
3	B	304	HEM	CAA-CBA-CGA-O1A
3	B	301	HEM	CAD-CBD-CGD-O1D

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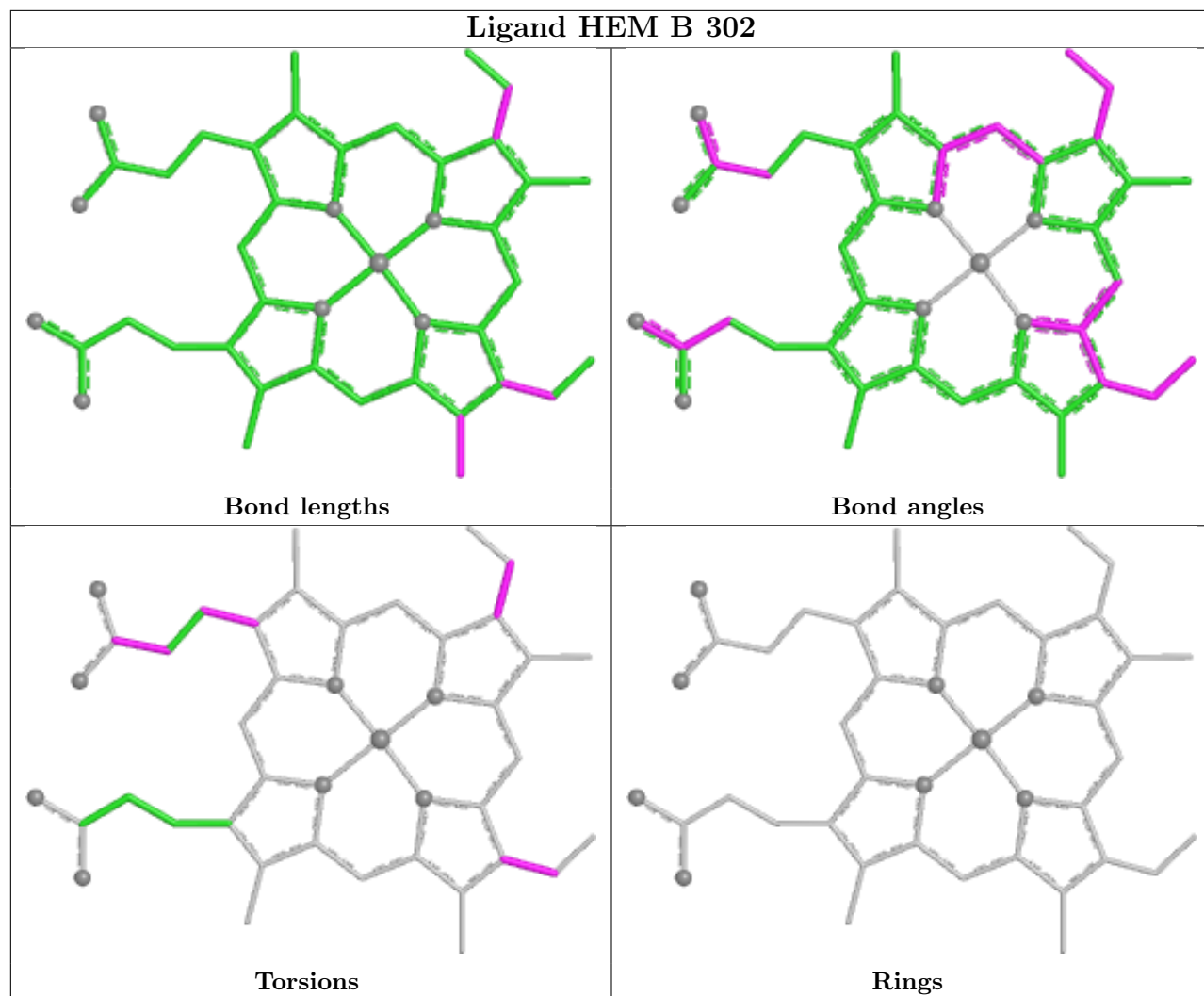
Mol	Chain	Res	Type	Atoms
3	B	301	HEM	CAD-CBD-CGD-O2D
3	B	301	HEM	CAA-CBA-CGA-O2A
3	B	301	HEM	CAA-CBA-CGA-O1A
3	A	309	HEM	CAD-CBD-CGD-O2D
3	A	303	HEM	C2B-C3B-CAB-CBB
3	B	305	HEM	C2B-C3B-CAB-CBB
3	B	309	HEM	CAD-CBD-CGD-O2D
3	B	309	HEM	CAD-CBD-CGD-O1D
3	A	309	HEM	CAD-CBD-CGD-O1D

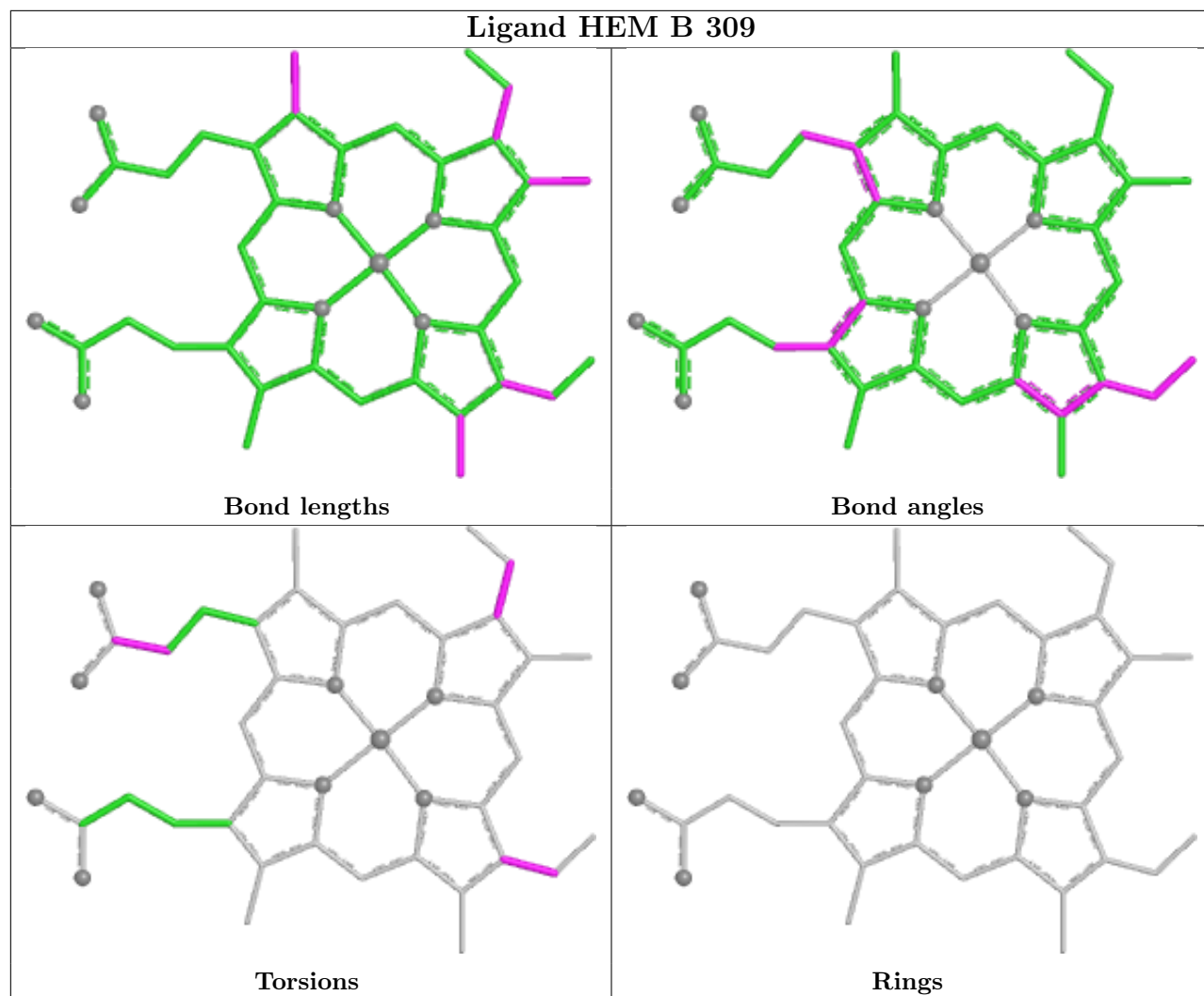
There are no ring outliers.

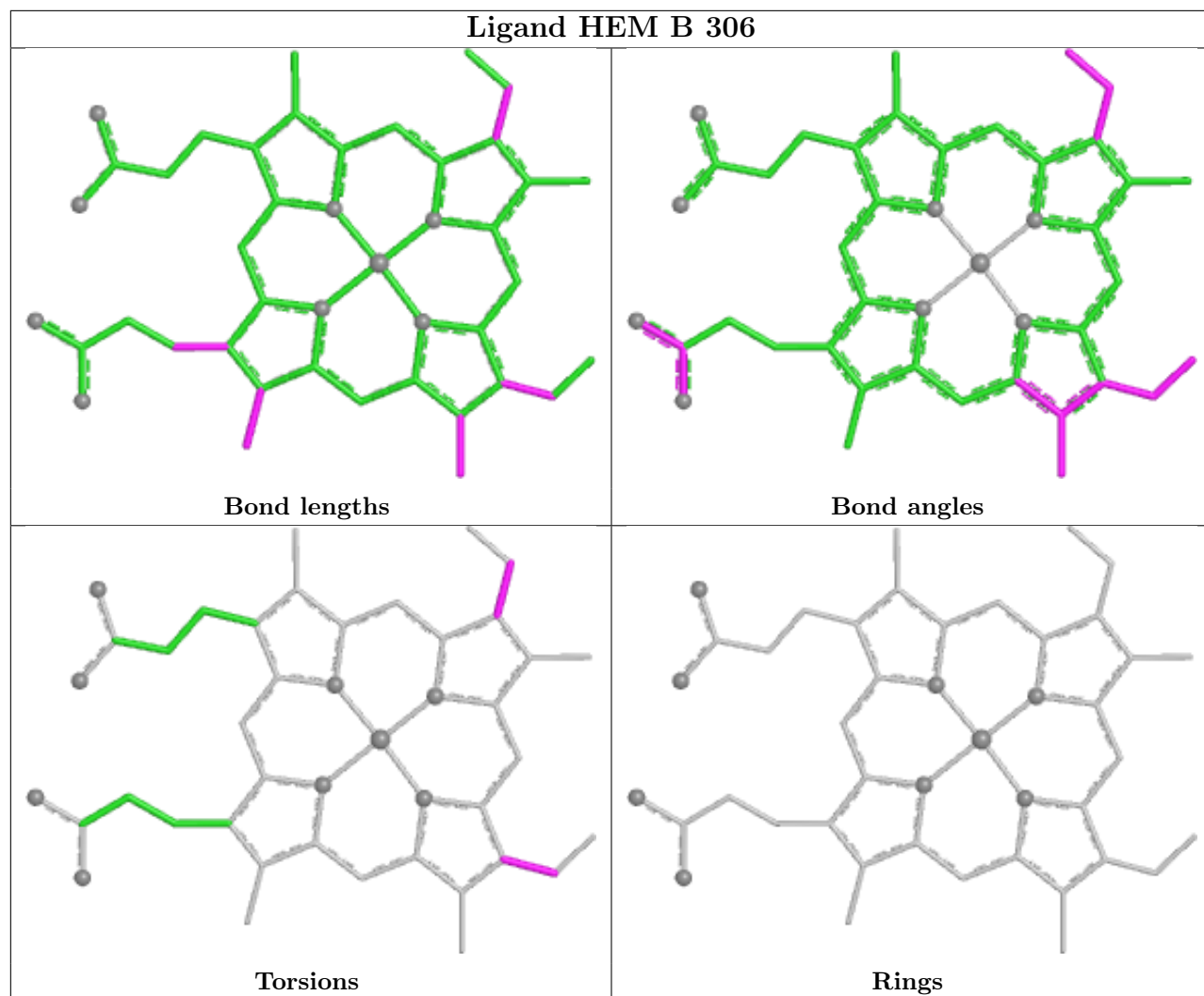
10 monomers are involved in 11 short contacts:

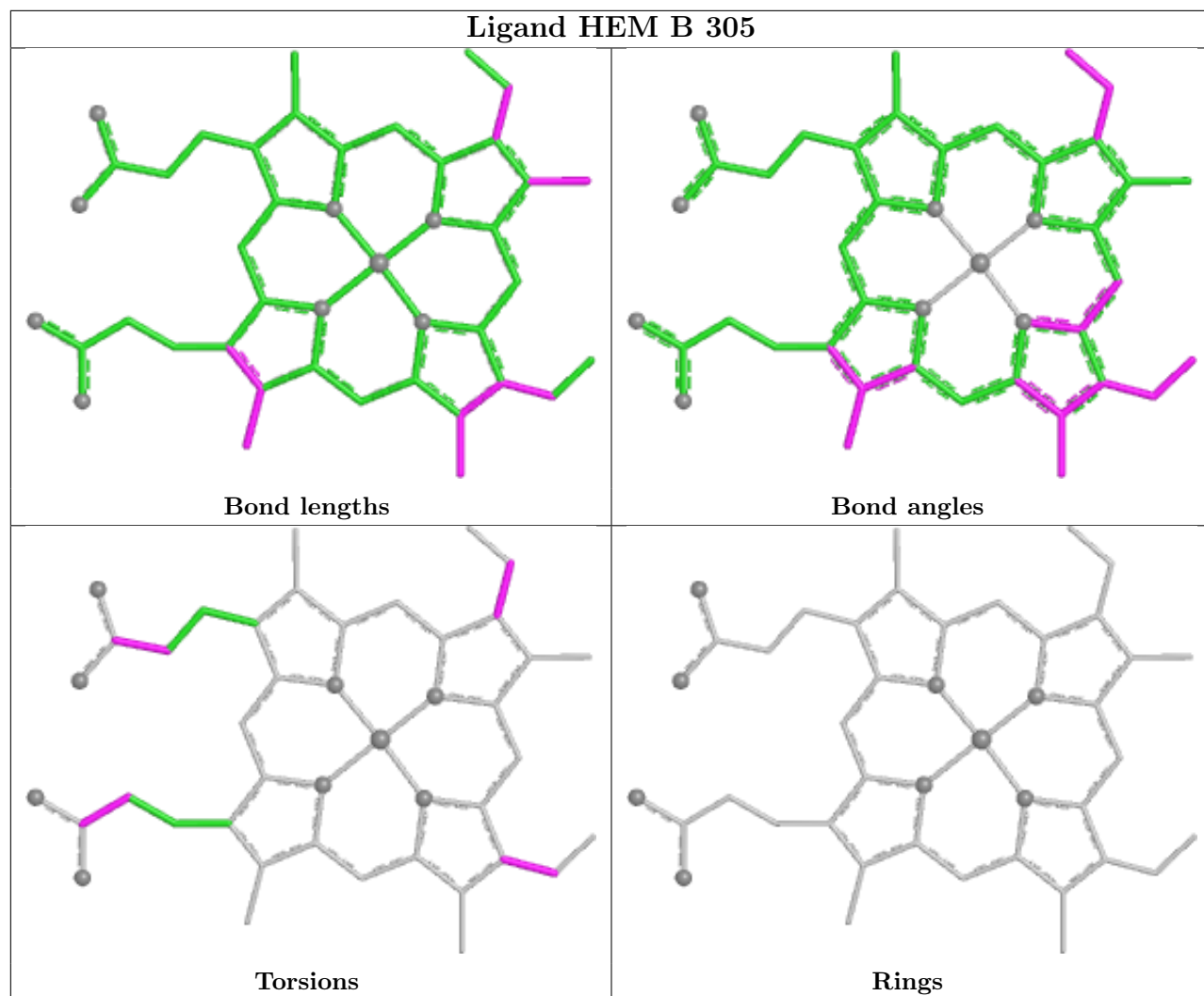
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	309	HEM	1	0
2	B	294	ACT	1	0
3	B	306	HEM	1	0
3	B	305	HEM	1	0
3	A	305	HEM	1	0
3	B	303	HEM	1	0
3	A	309	HEM	1	0
3	B	308	HEM	2	0
3	B	304	HEM	2	0
3	B	301	HEM	1	0

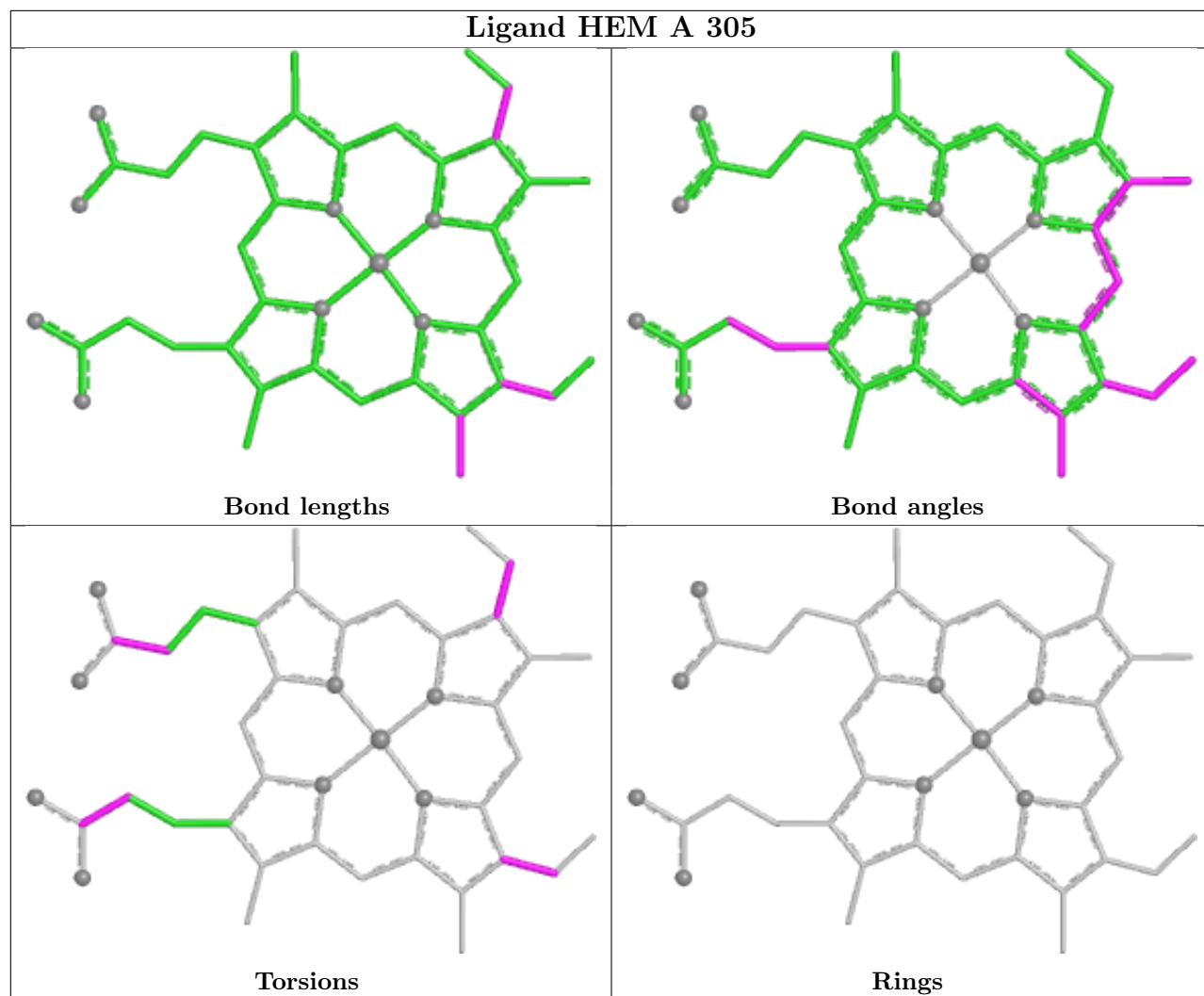
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

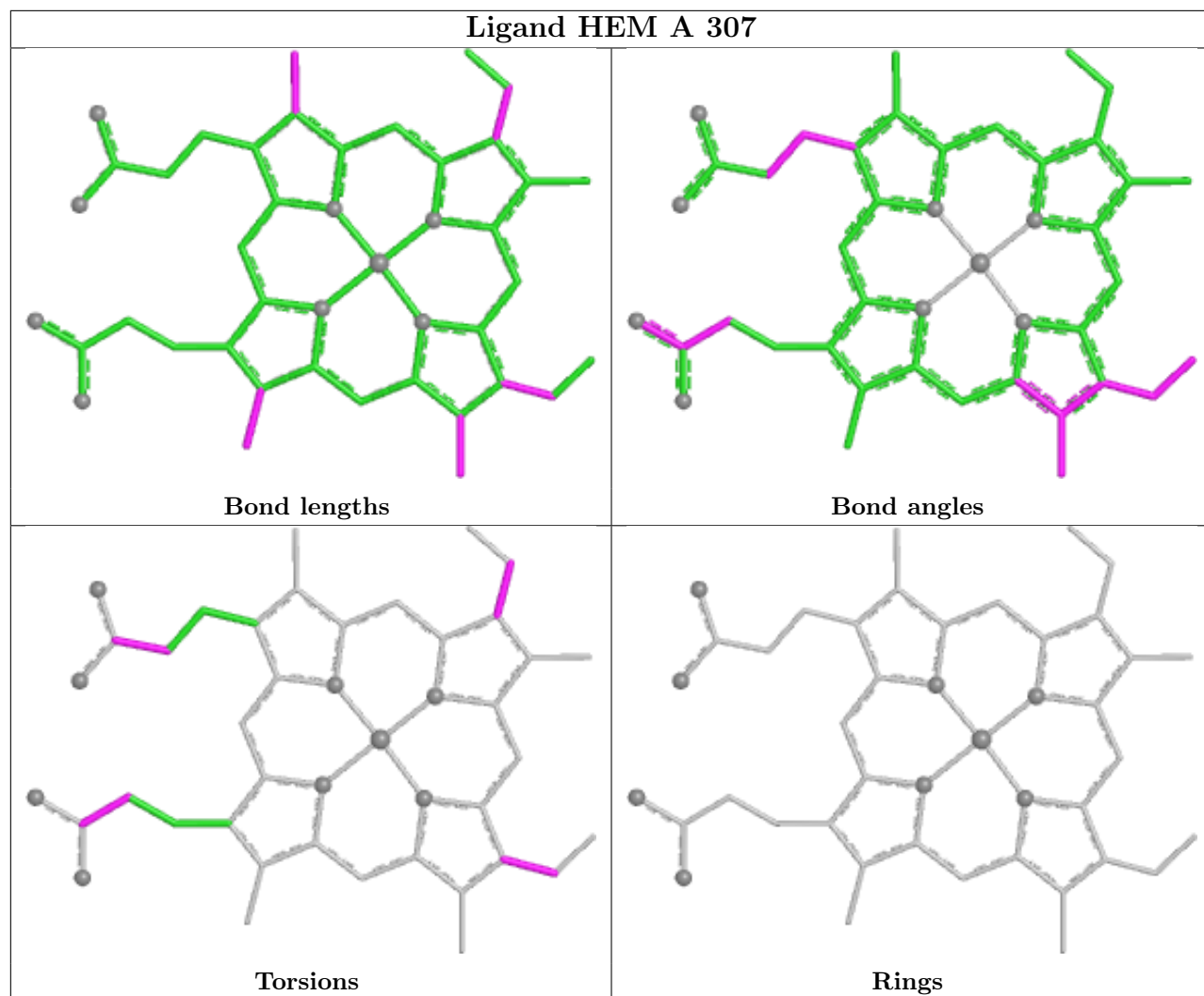


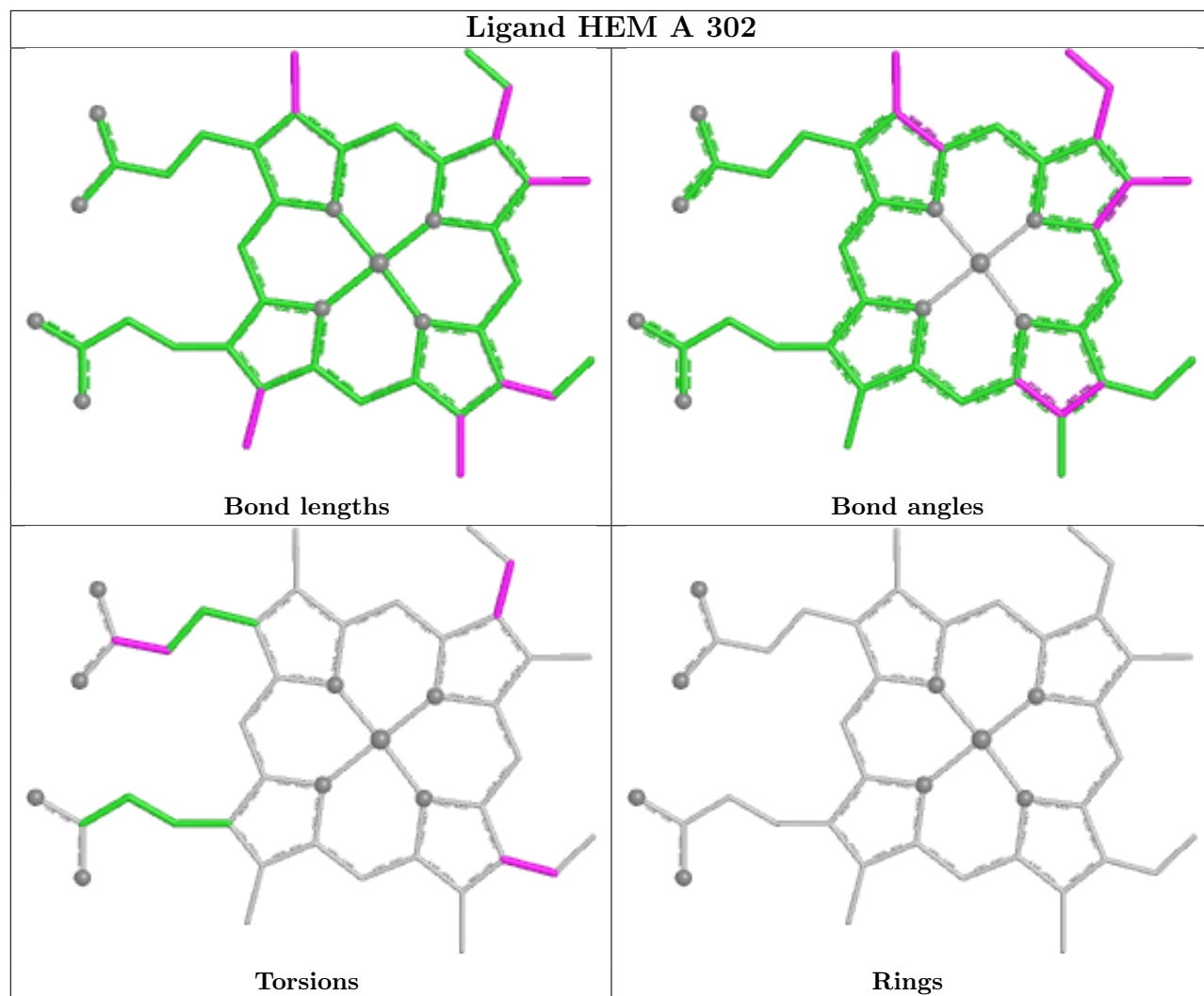


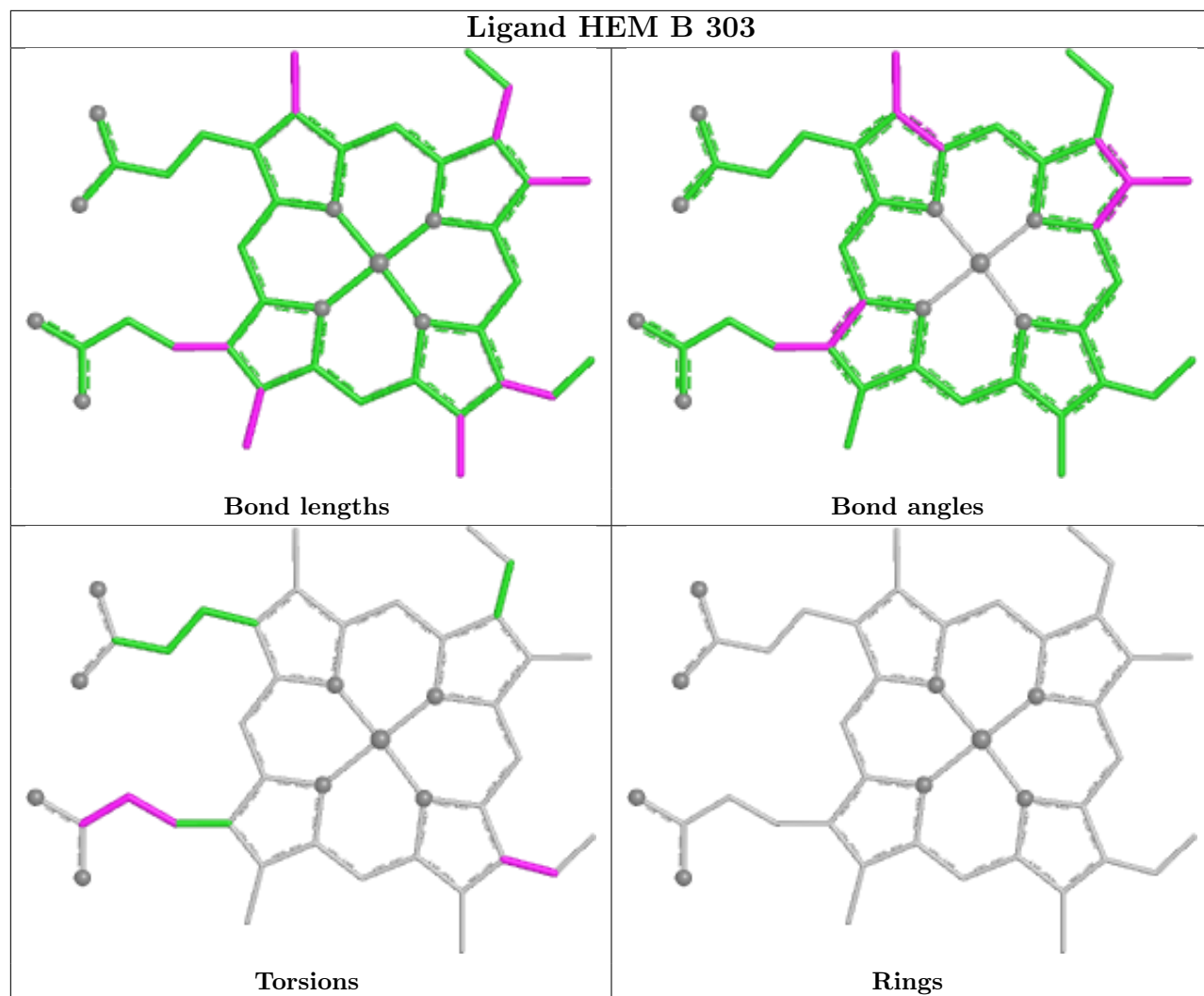


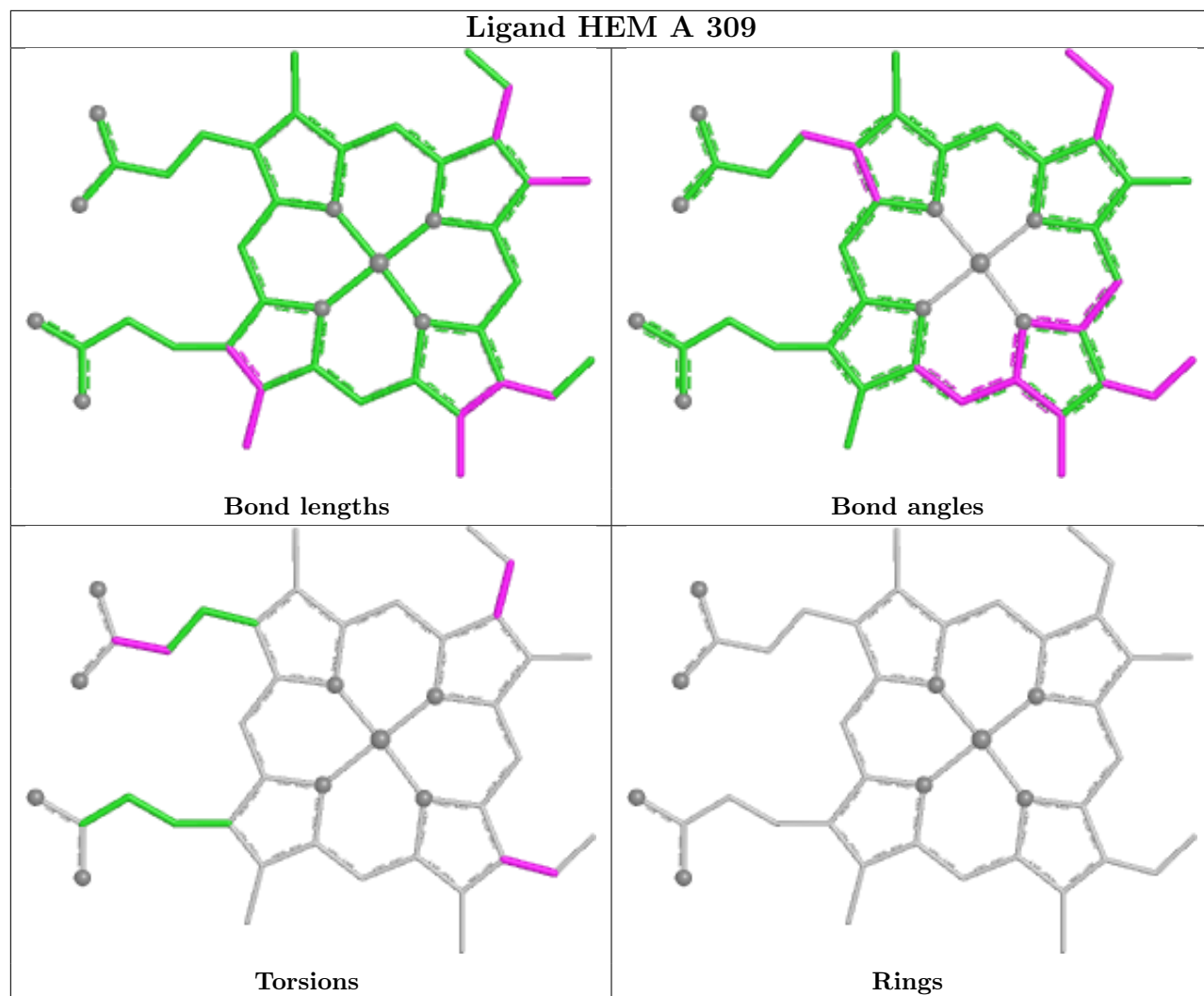


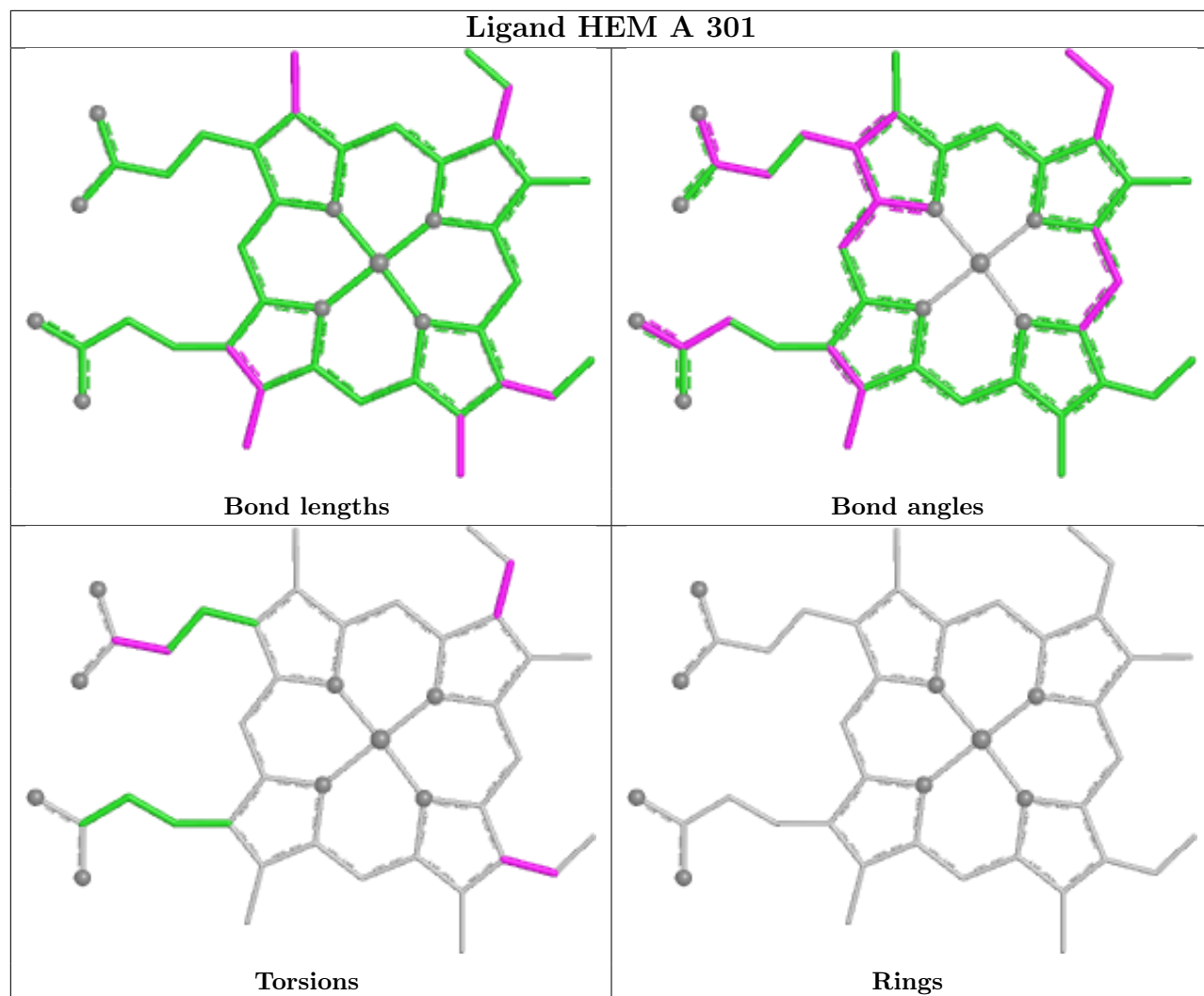


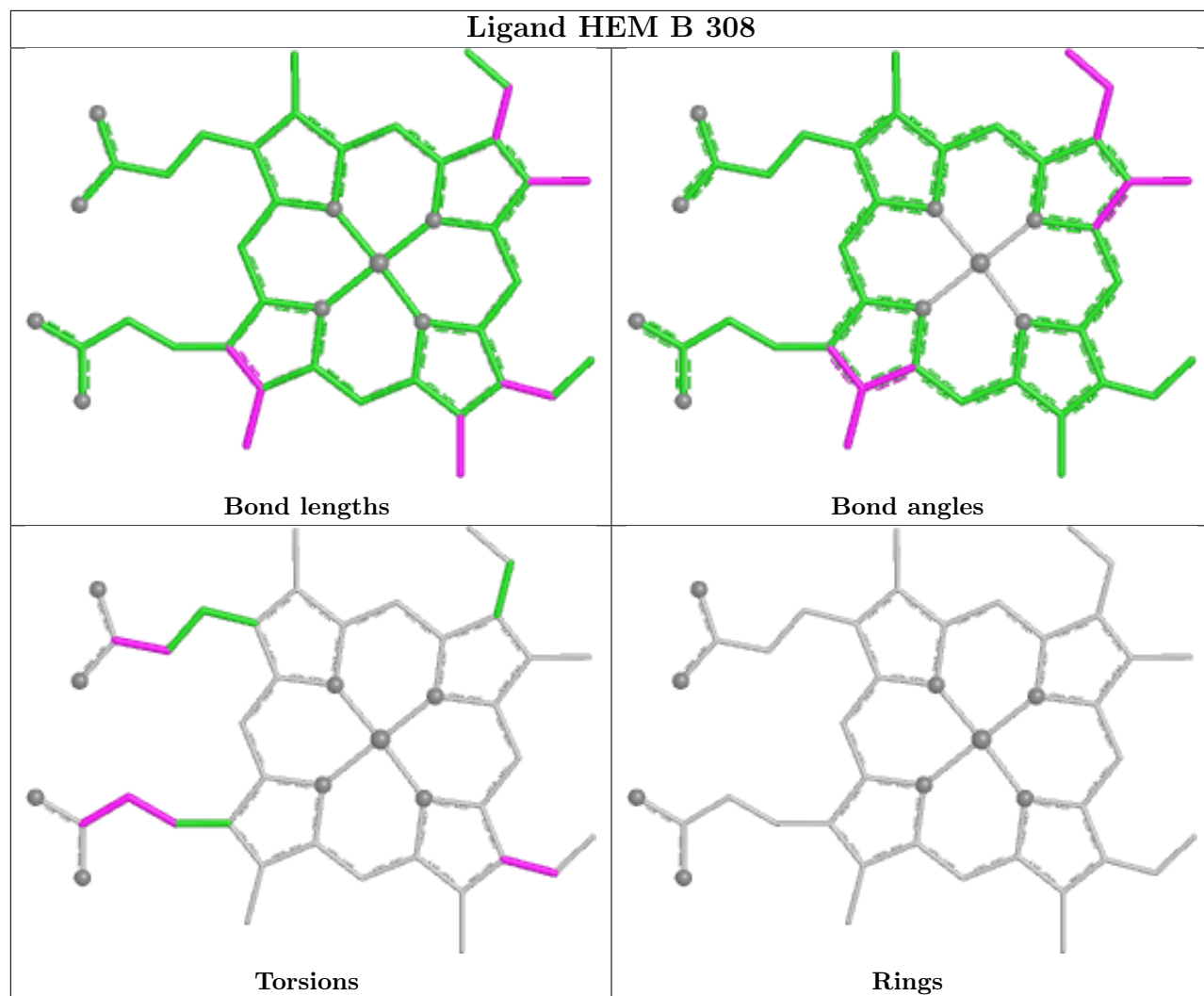


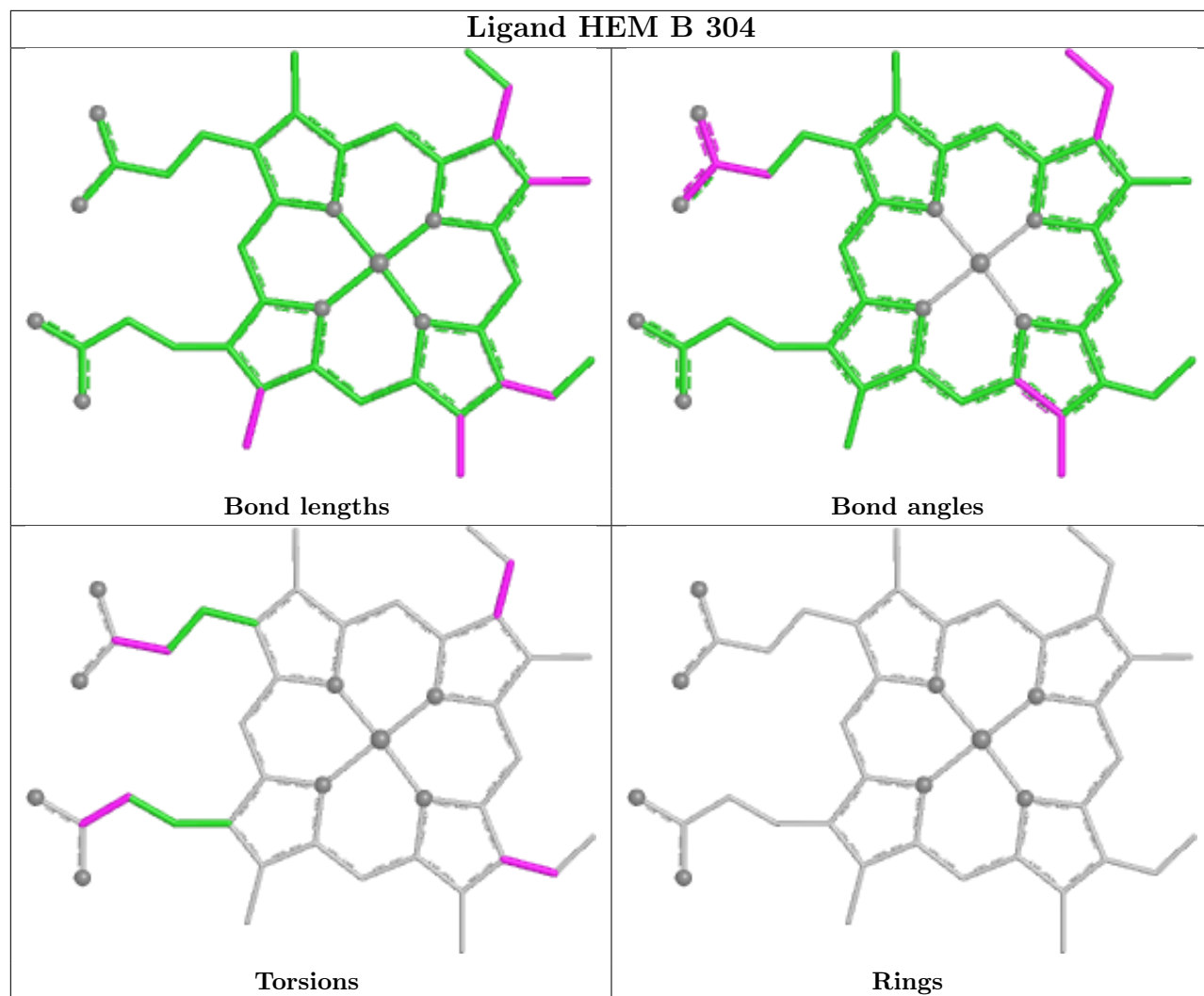


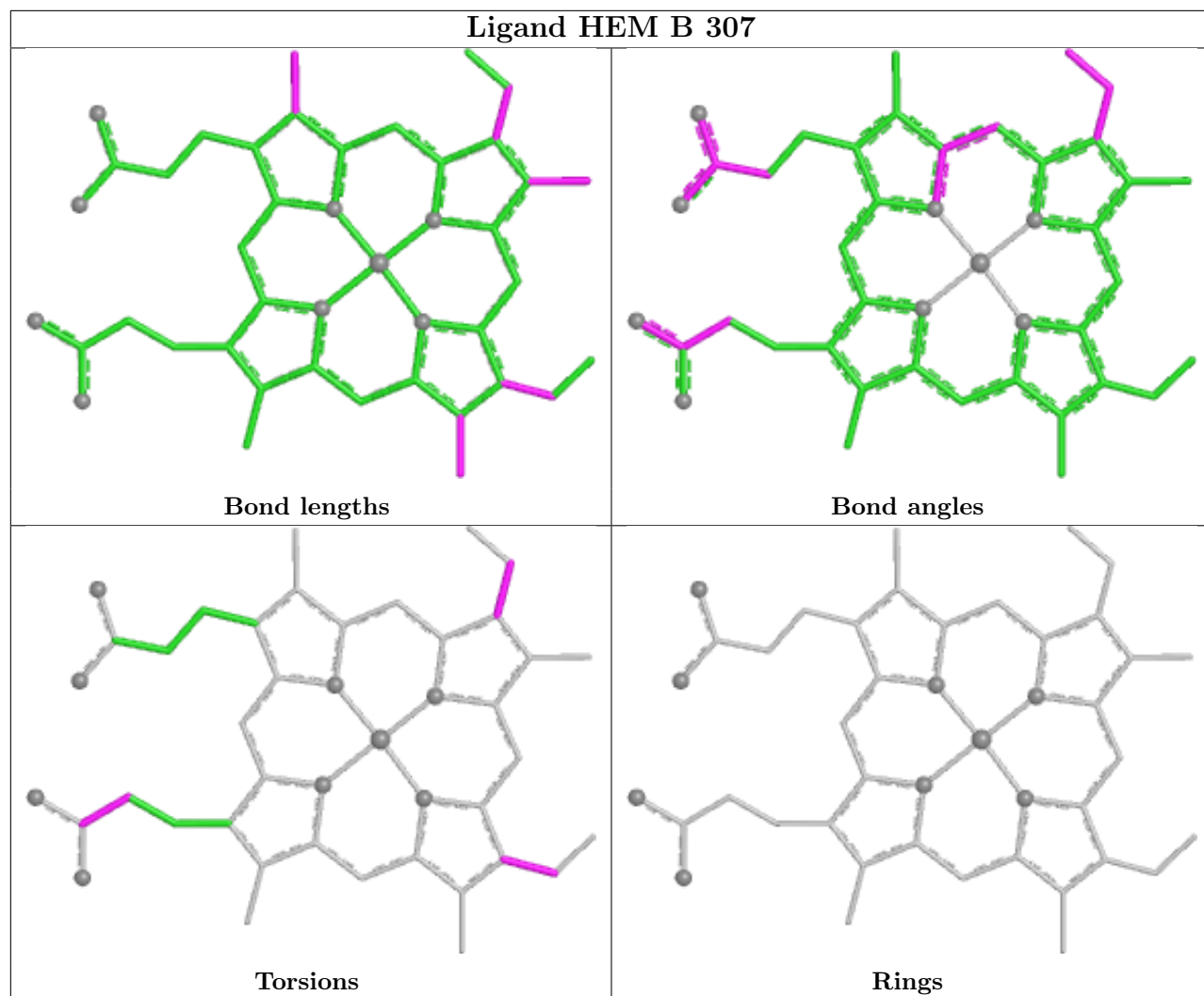


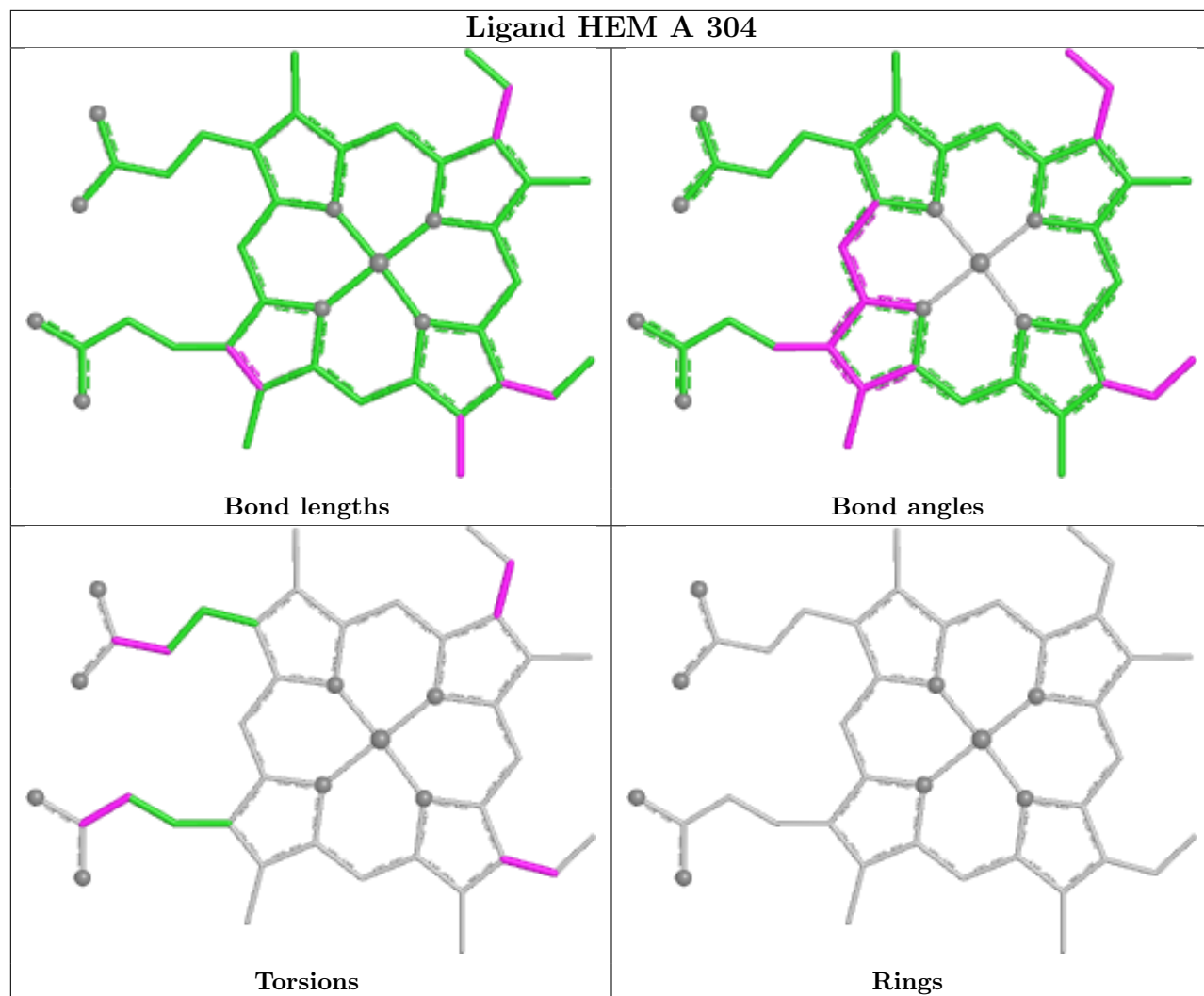


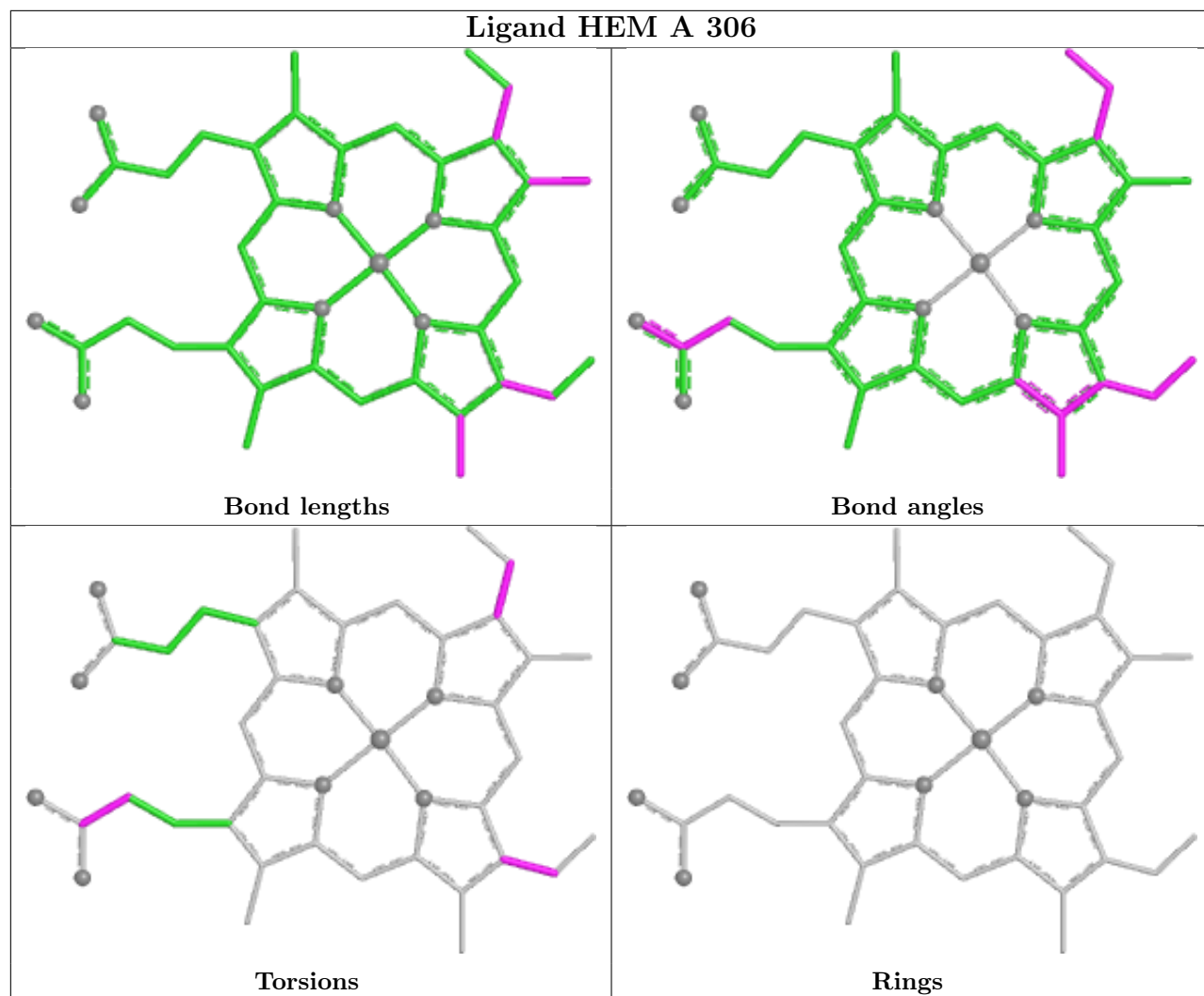


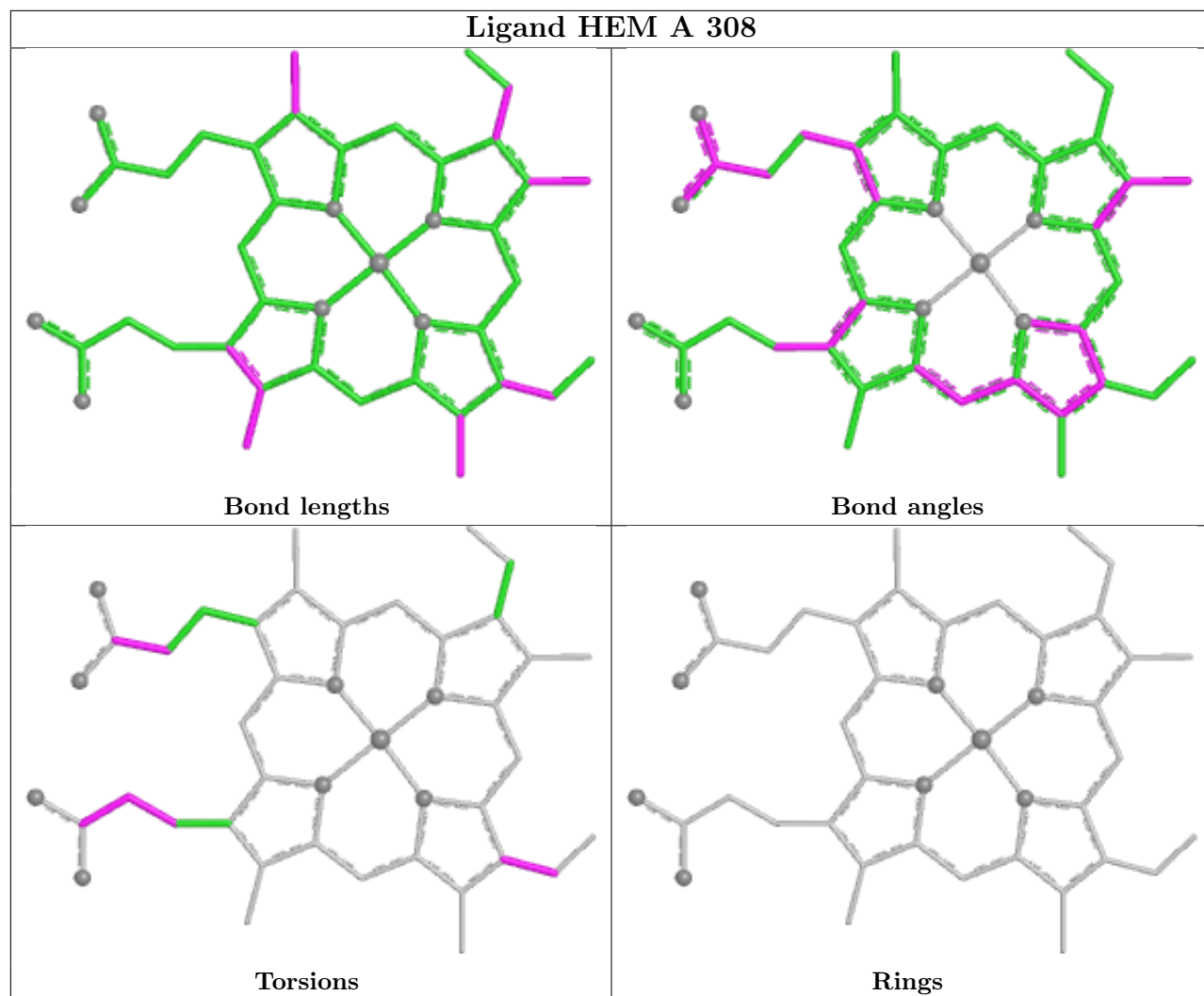


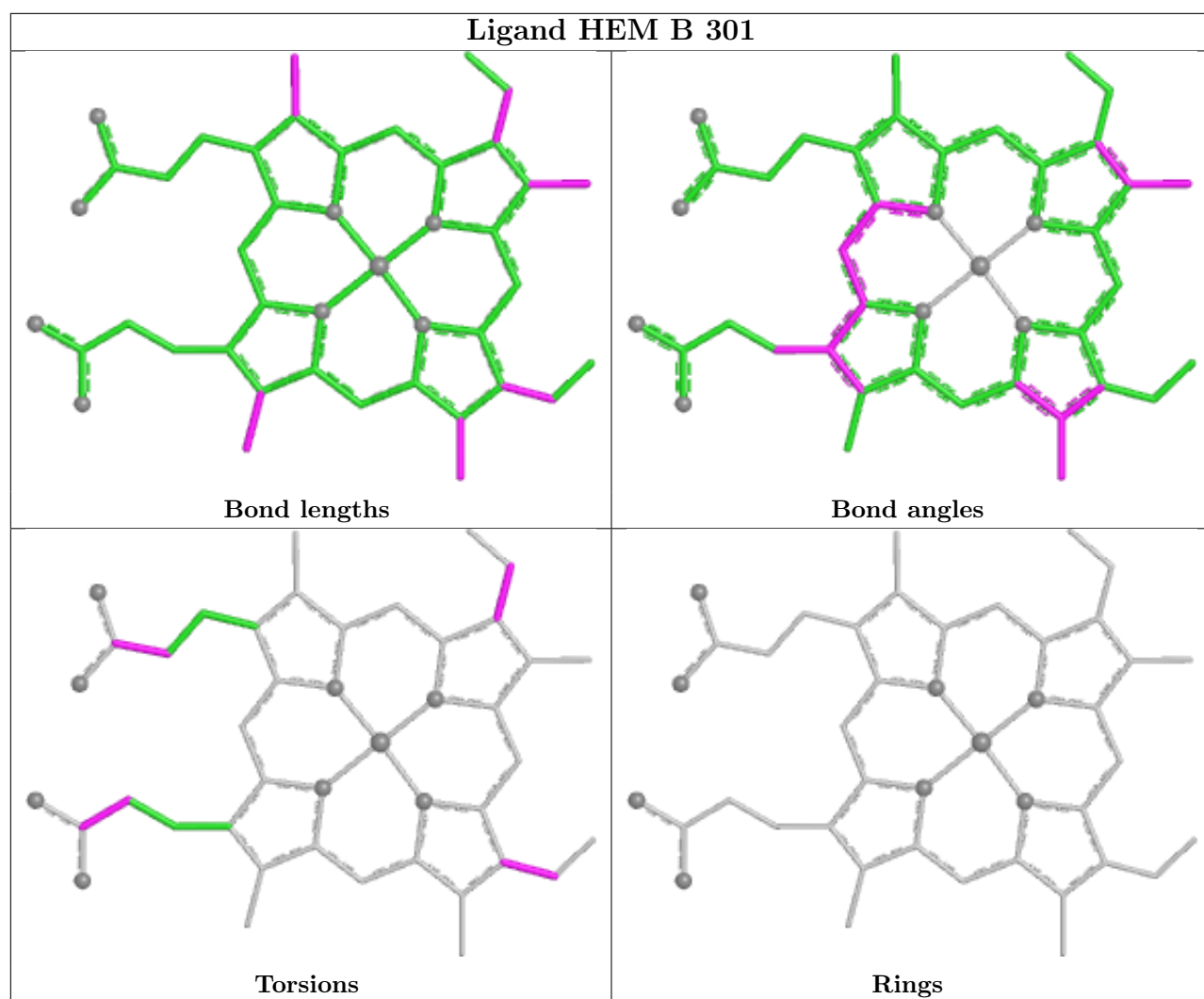


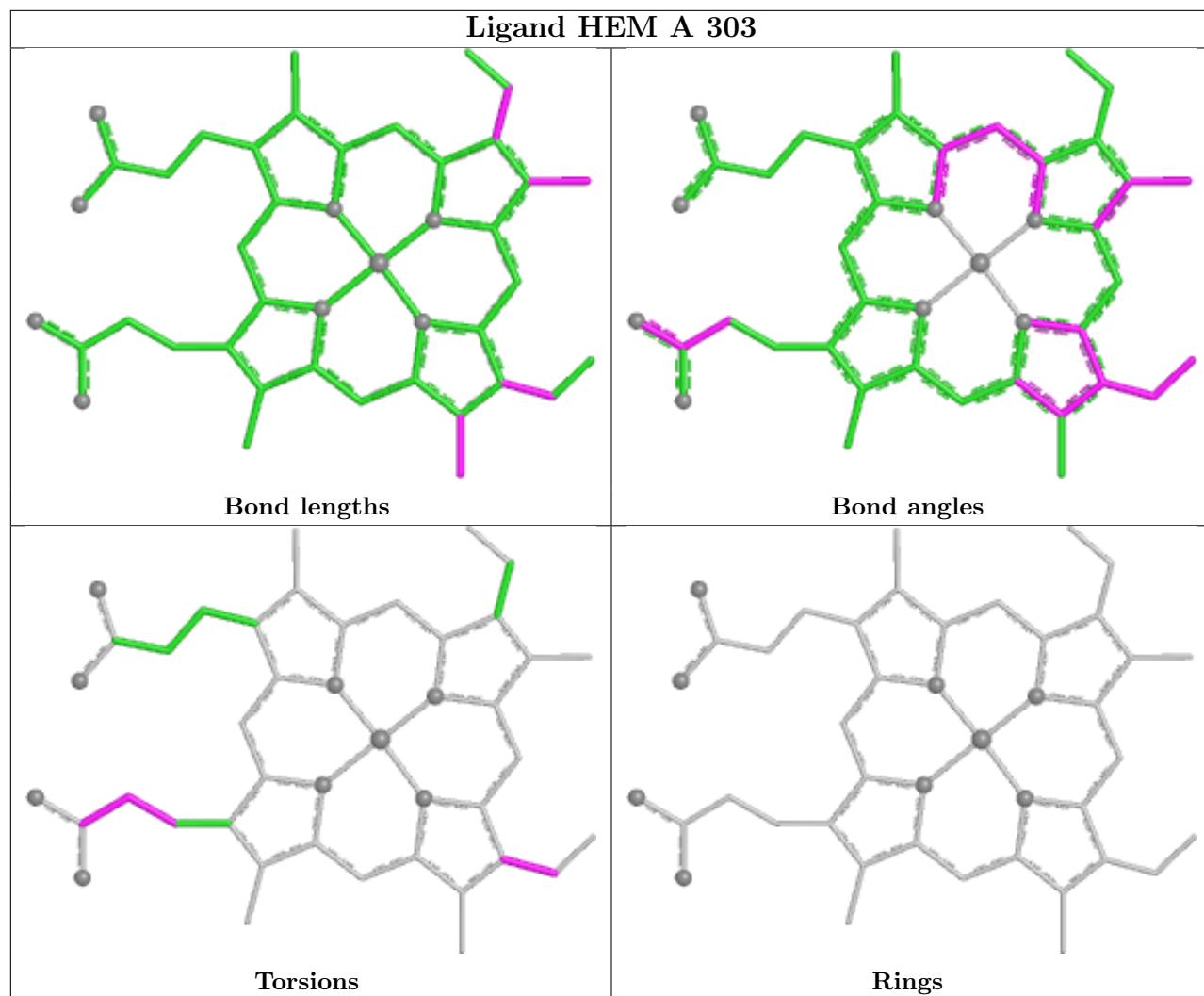












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	292/292 (100%)	-0.24	3 (1%) 79 80	7, 17, 31, 48	14 (4%)
1	B	292/292 (100%)	-0.02	10 (3%) 48 48	8, 20, 35, 58	22 (7%)
All	All	584/584 (100%)	-0.13	13 (2%) 62 62	7, 19, 32, 58	36 (6%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	5.2
1	B	292	ALA	4.9
1	B	291	ALA	3.5
1	B	119[A]	THR	2.9
1	B	54	GLY	2.9
1	B	45	ALA	2.7
1	A	292	ALA	2.5
1	B	147	ALA	2.3
1	B	168	THR	2.3
1	B	251	ALA	2.1
1	A	291	ALA	2.0
1	B	1	ALA	2.0
1	B	254	PRO	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 ⓘ

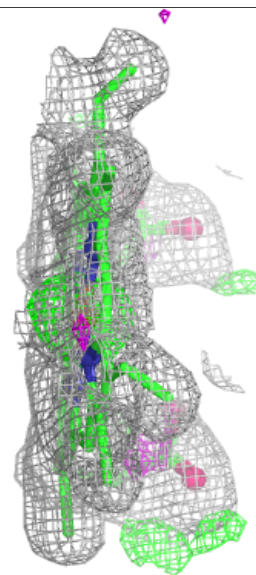
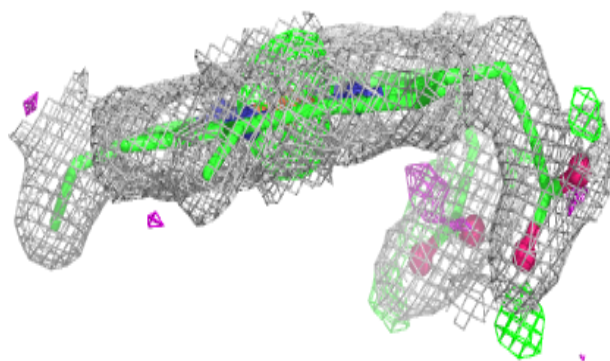
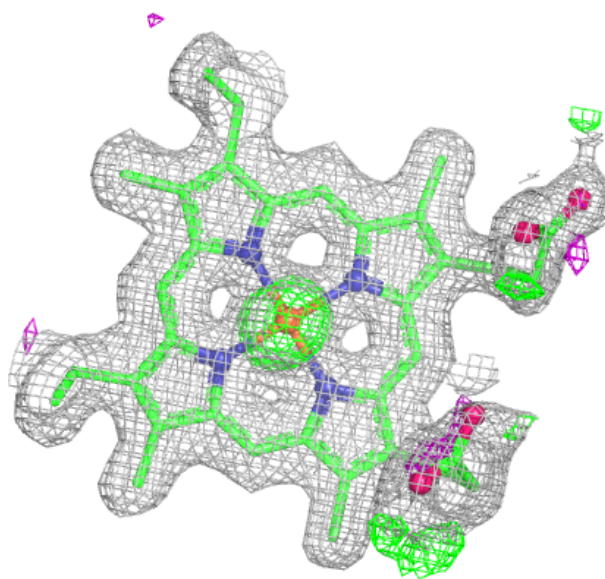
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	B	294	4/4	0.74	0.28	34,46,48,49	0
2	ACT	A	294	4/4	0.84	0.14	29,32,34,36	0
2	ACT	A	295	4/4	0.85	0.17	23,27,37,45	0
2	ACT	B	293	4/4	0.89	0.11	30,30,38,47	0
2	ACT	A	293	4/4	0.92	0.09	16,17,24,30	0
3	HEM	B	308	43/43	0.95	0.09	11,18,33,51	0
3	HEM	A	302	43/43	0.96	0.08	10,16,25,35	0
3	HEM	A	303	43/43	0.96	0.06	6,11,20,25	0
3	HEM	A	305	43/43	0.96	0.06	9,12,14,17	0
3	HEM	A	306	43/43	0.96	0.07	7,11,21,26	0
3	HEM	A	308	43/43	0.96	0.08	8,12,31,45	0
3	HEM	A	309	43/43	0.96	0.07	8,13,17,19	0
3	HEM	B	301	43/43	0.96	0.09	12,19,29,59	0
3	HEM	B	302	43/43	0.96	0.08	12,17,29,36	2
3	HEM	B	303	43/43	0.96	0.07	11,15,27,42	0
3	HEM	B	304	43/43	0.96	0.07	11,15,20,21	0
3	HEM	B	305	43/43	0.96	0.06	10,12,16,17	0
3	HEM	B	306	43/43	0.96	0.07	11,15,29,33	0
3	HEM	B	307	43/43	0.96	0.07	10,17,26,44	0
3	HEM	A	301	43/43	0.96	0.07	9,12,22,27	0
3	HEM	B	309	43/43	0.96	0.07	13,17,21,24	0
3	HEM	A	307	43/43	0.97	0.07	6,11,21,39	0
3	HEM	A	304	43/43	0.97	0.06	6,11,15,18	0

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

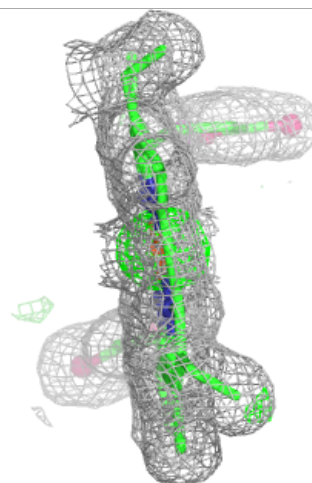
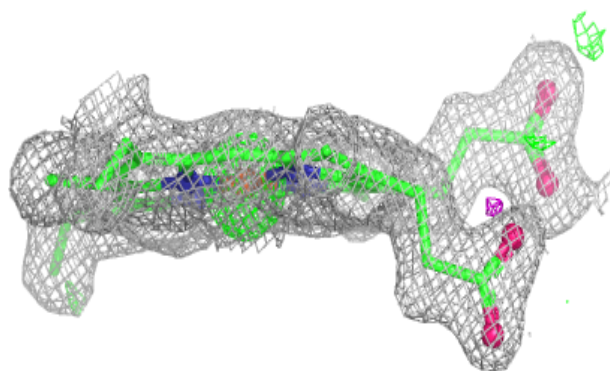
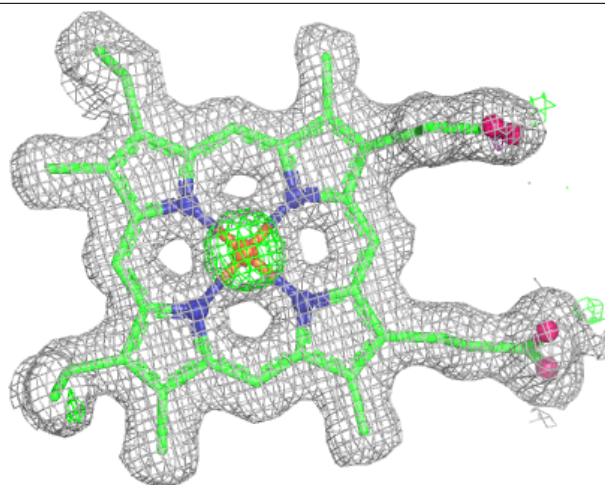
Electron density around HEM B 308:

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



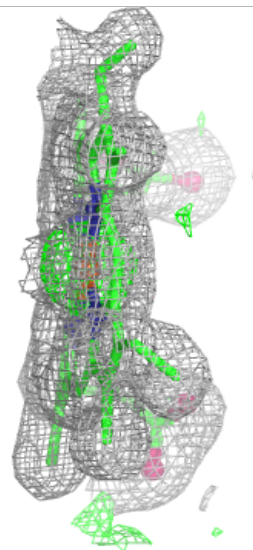
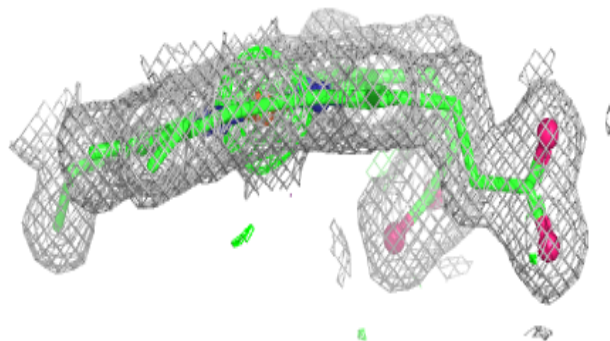
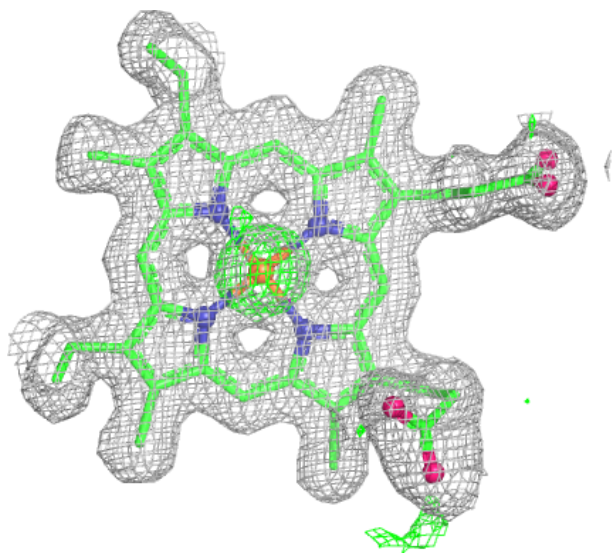
Electron density around HEM A 302:

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



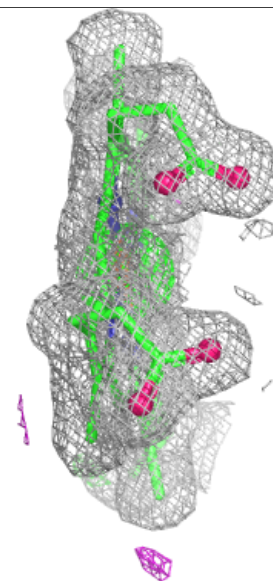
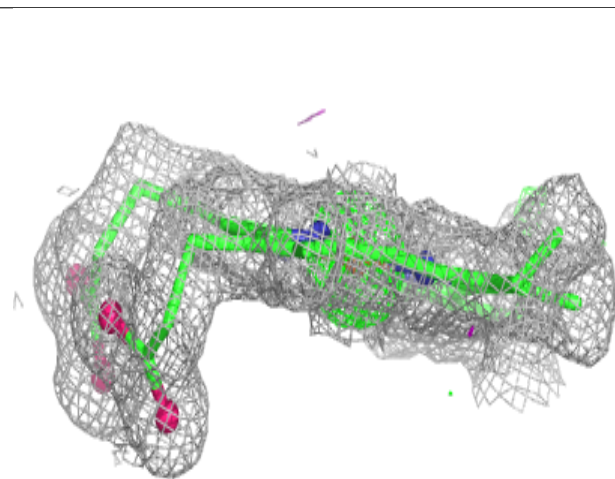
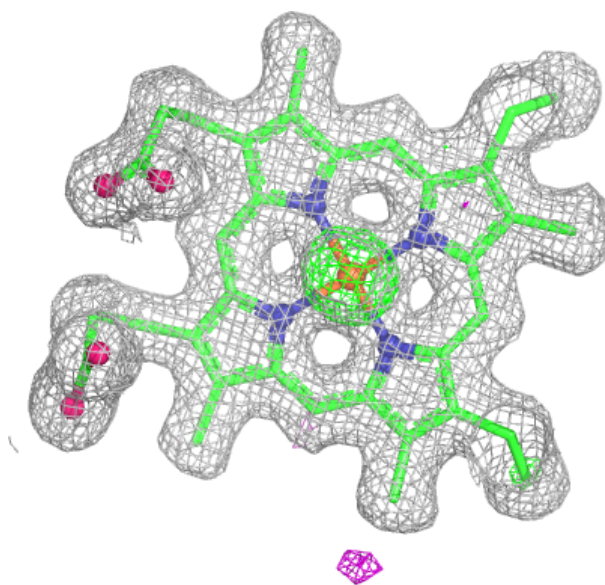
Electron density around HEM A 303:

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



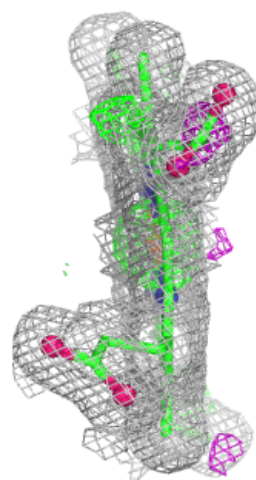
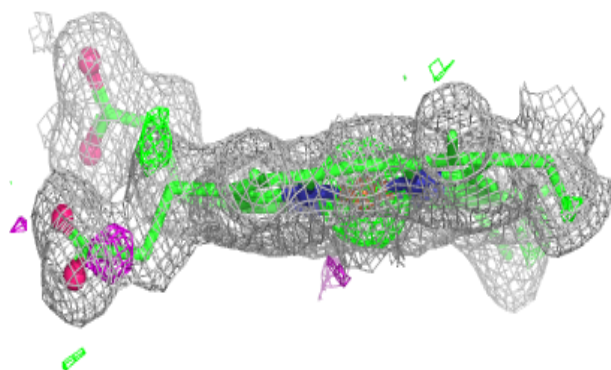
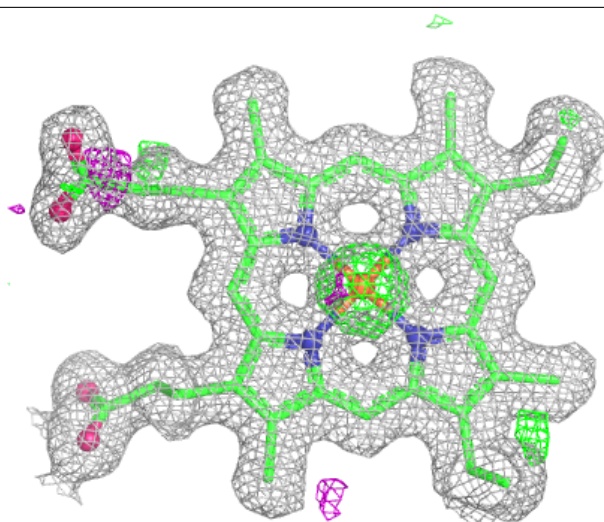
Electron density around HEM A 305:

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



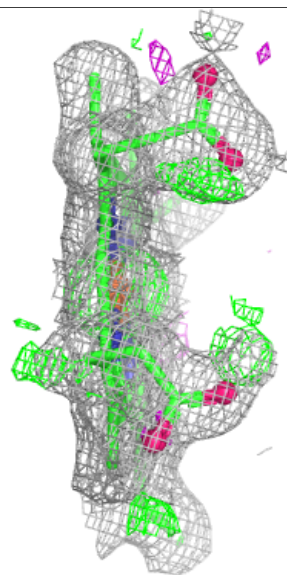
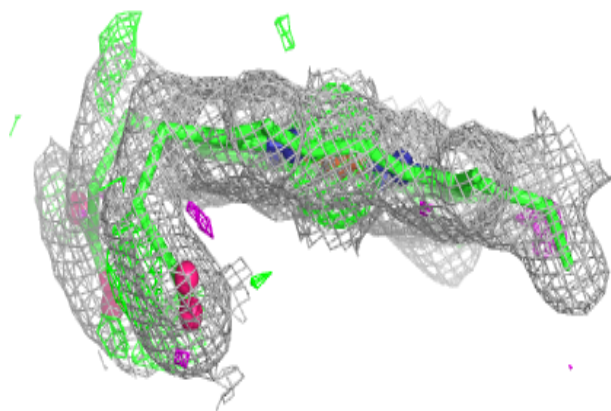
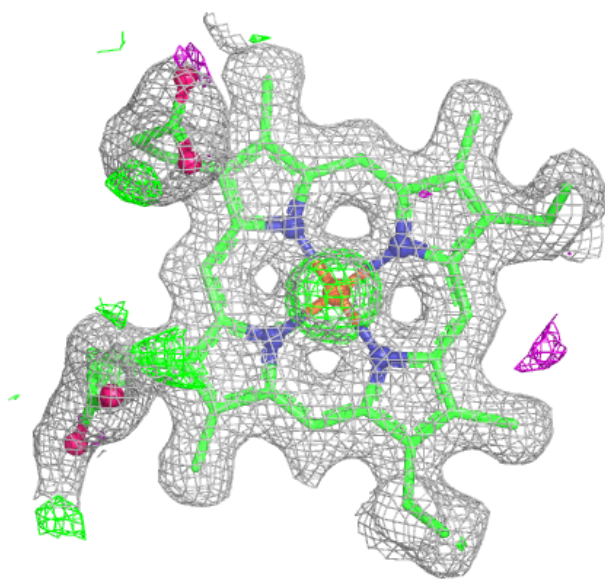
Electron density around HEM A 306:

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and green (positive)



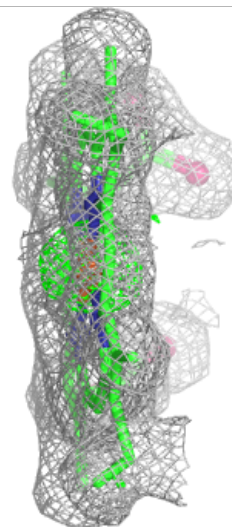
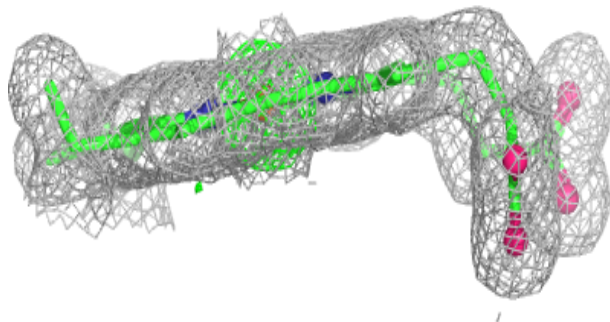
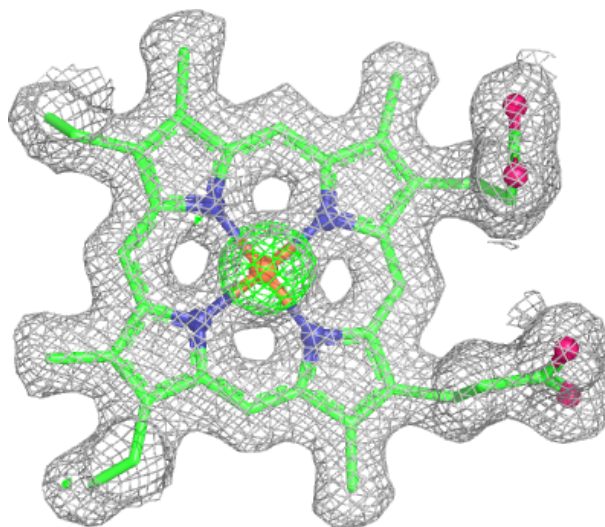
Electron density around HEM A 308:

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



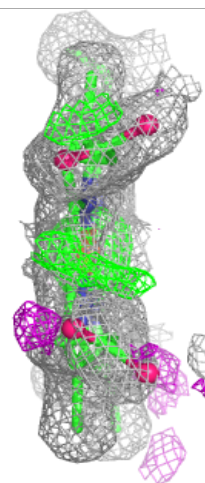
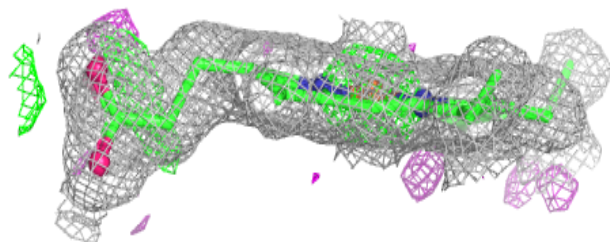
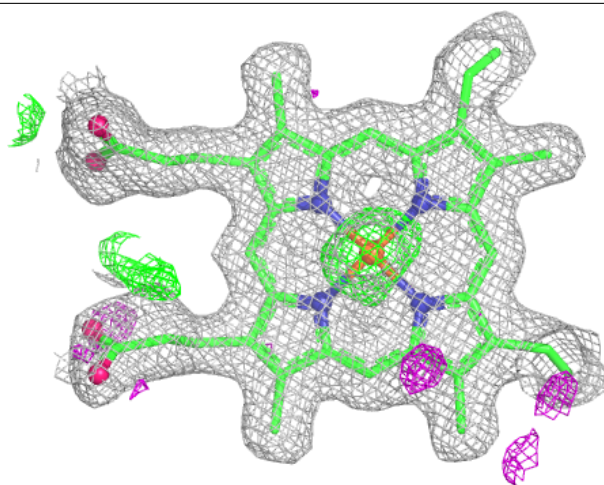
Electron density around HEM A 309:

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



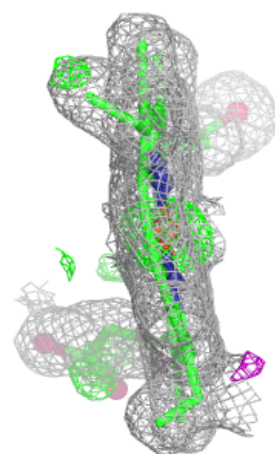
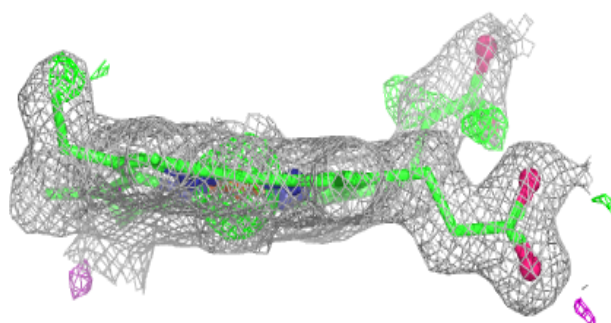
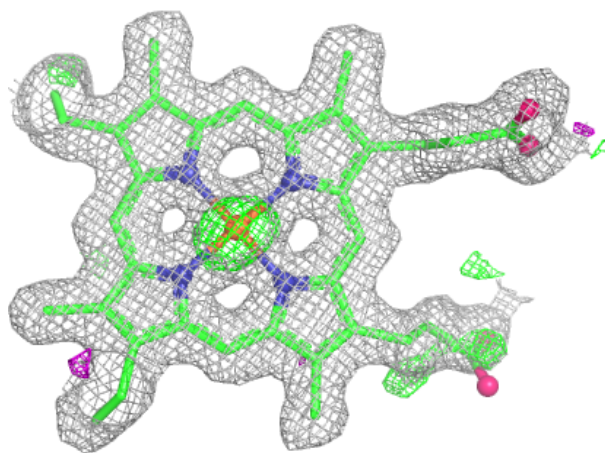
Electron density around HEM B 301:

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



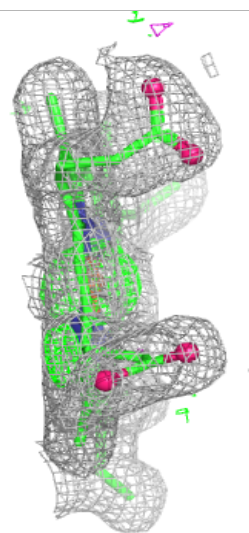
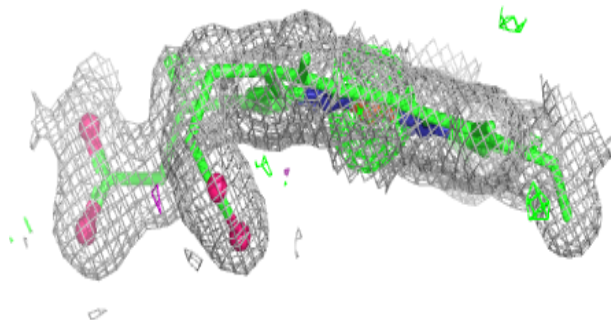
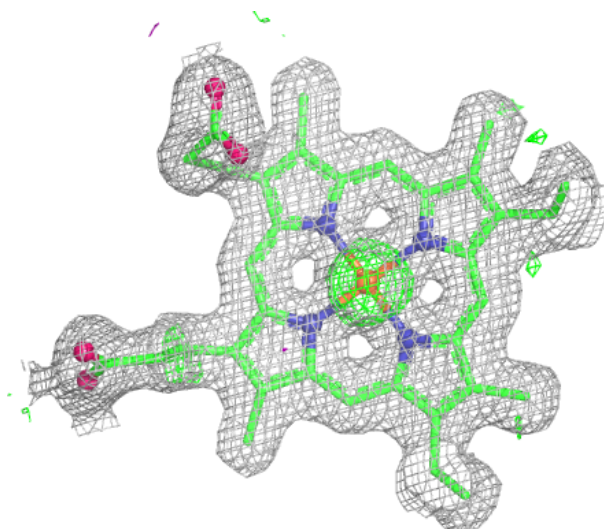
Electron density around HEM B 302:

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



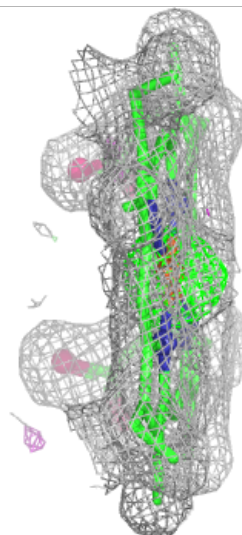
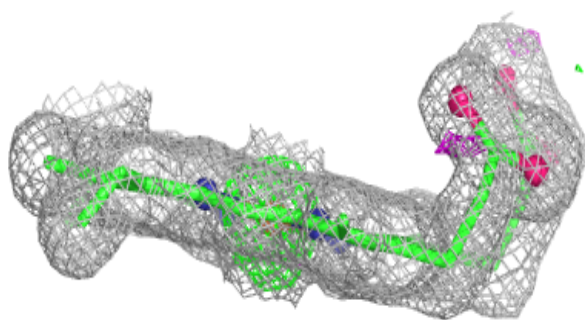
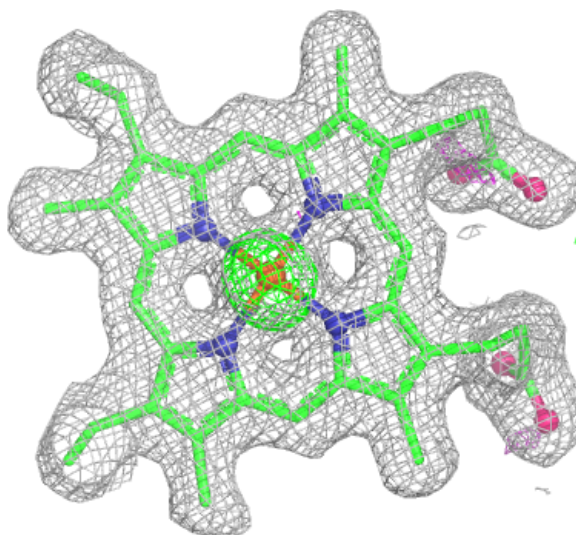
Electron density around HEM B 303:

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



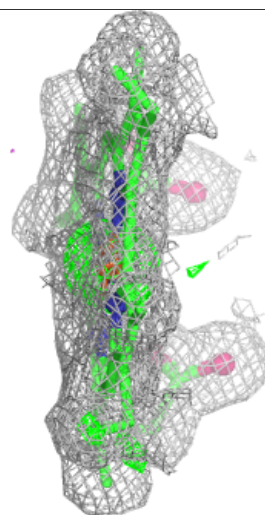
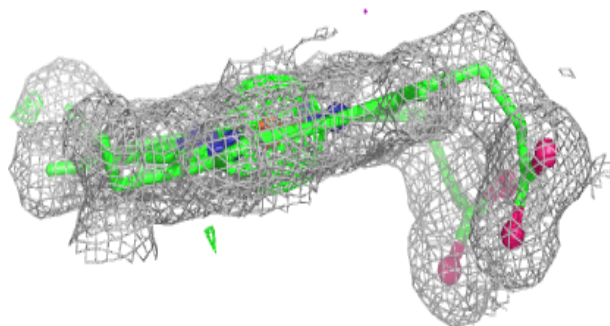
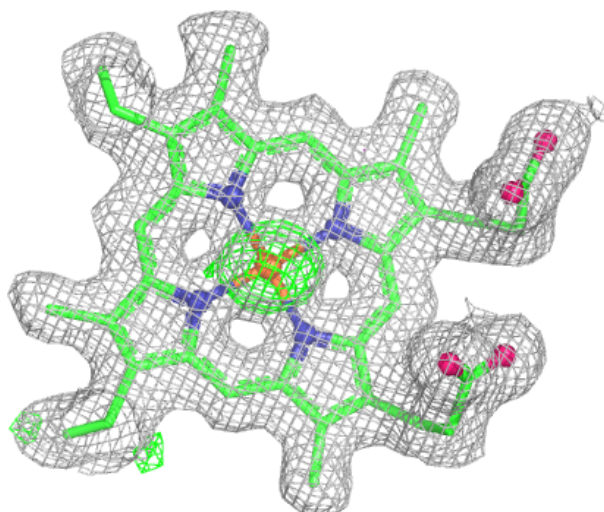
Electron density around HEM B 304:

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



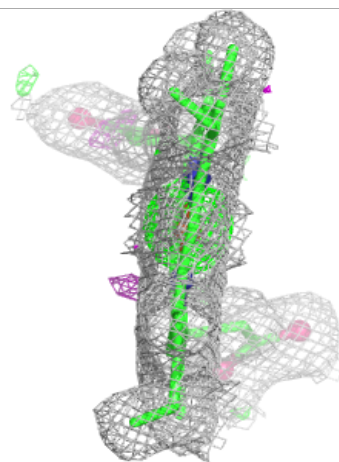
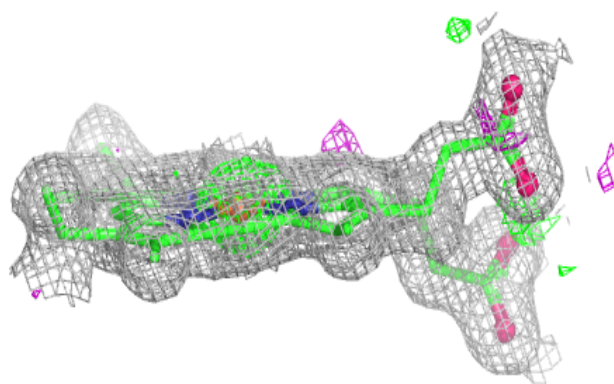
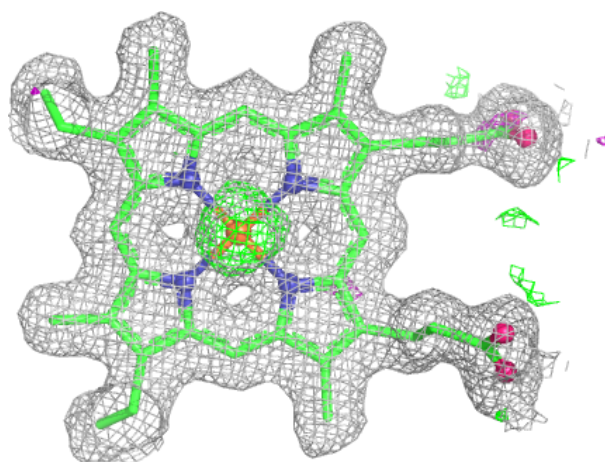
Electron density around HEM B 305:

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



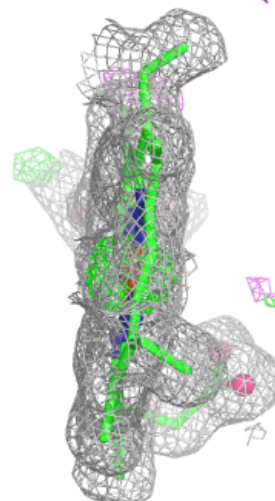
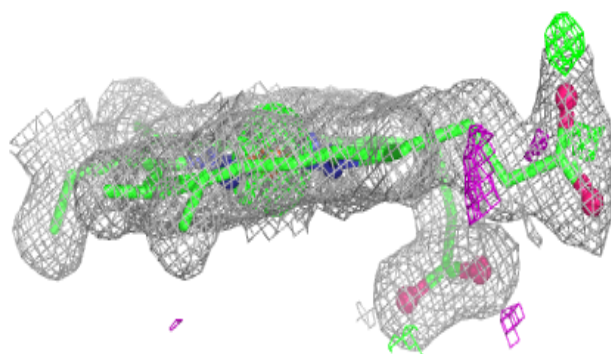
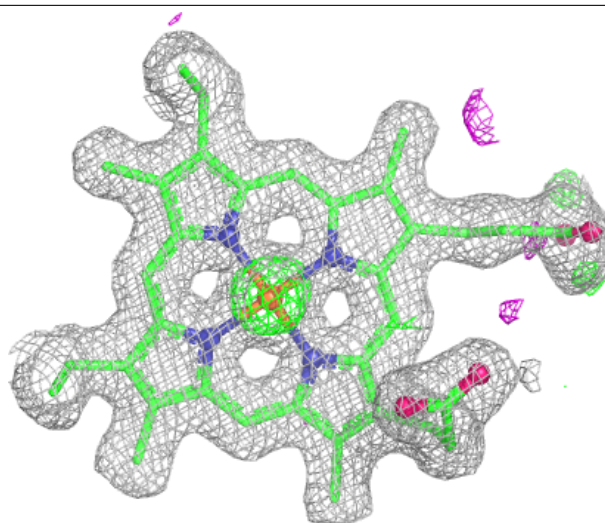
Electron density around HEM B 306:

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



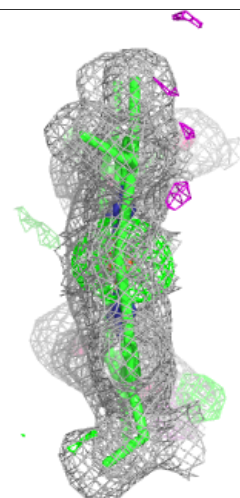
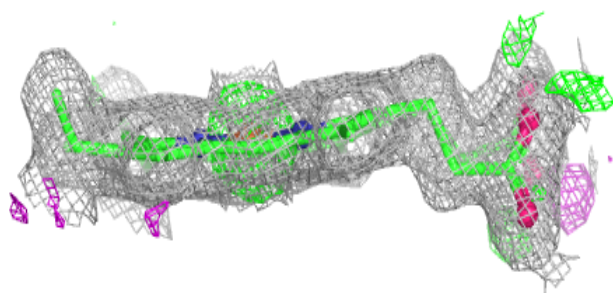
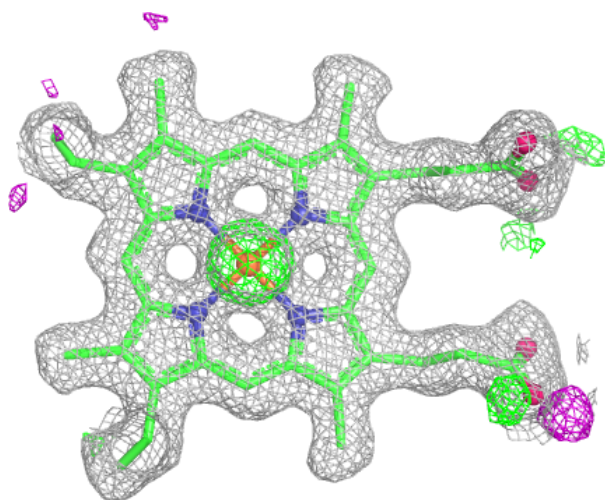
Electron density around HEM B 307:

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



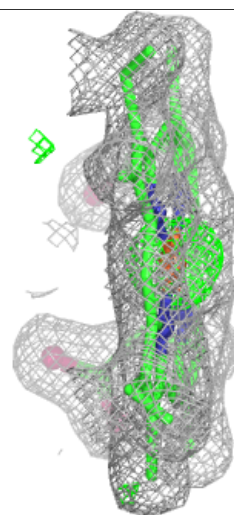
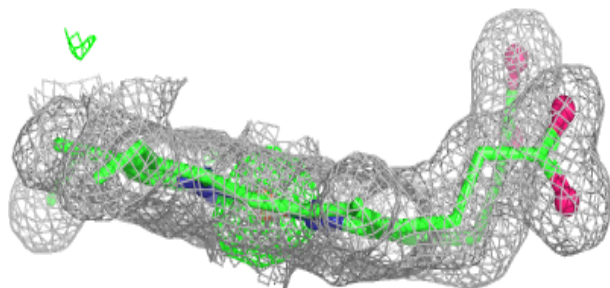
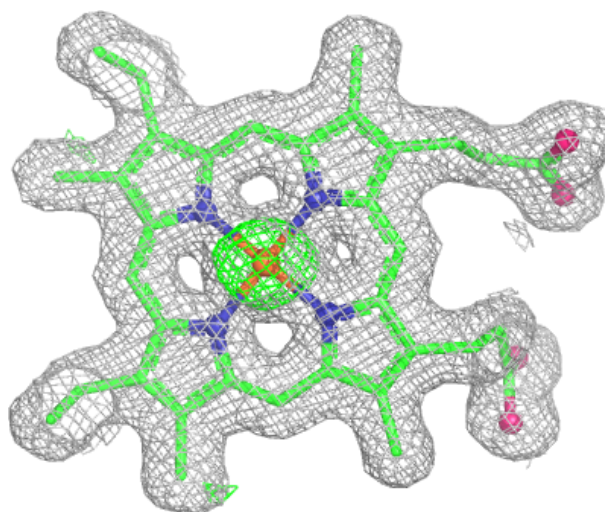
Electron density around HEM A 301:

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



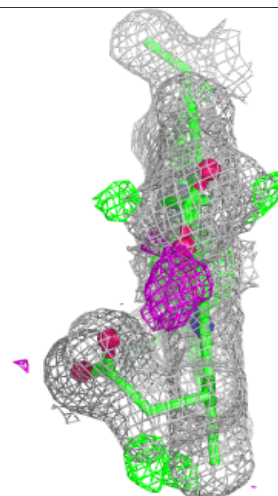
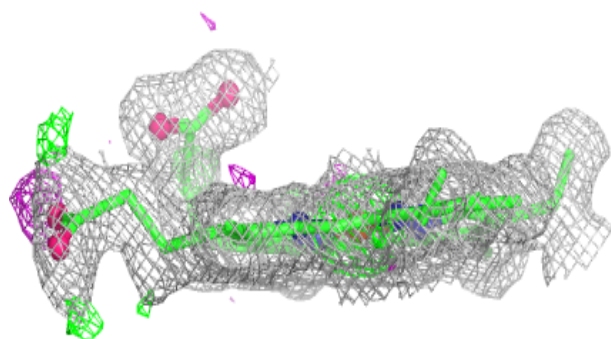
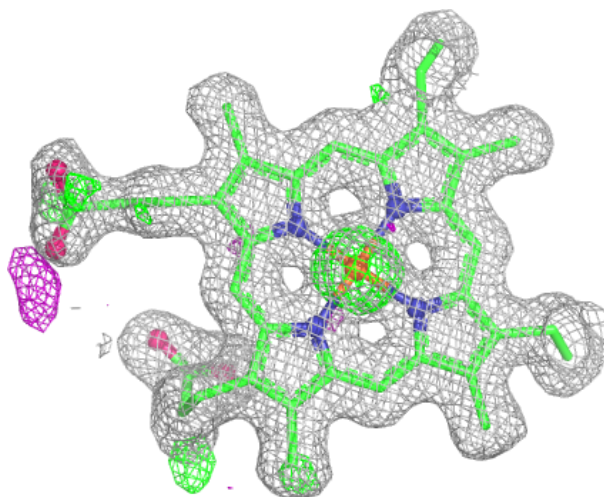
Electron density around HEM B 309:

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



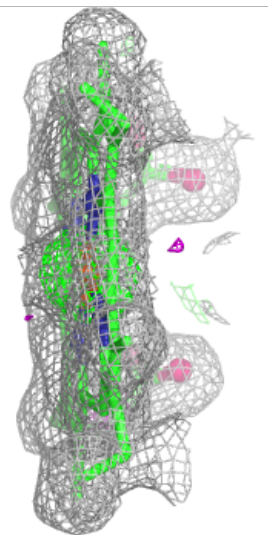
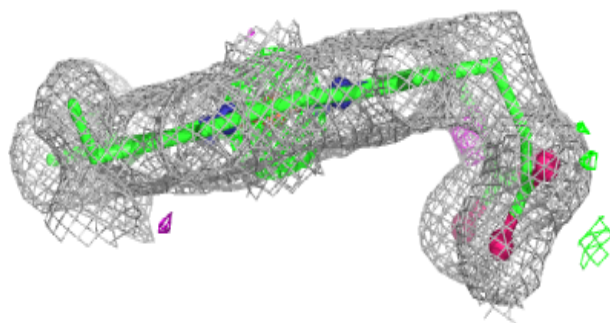
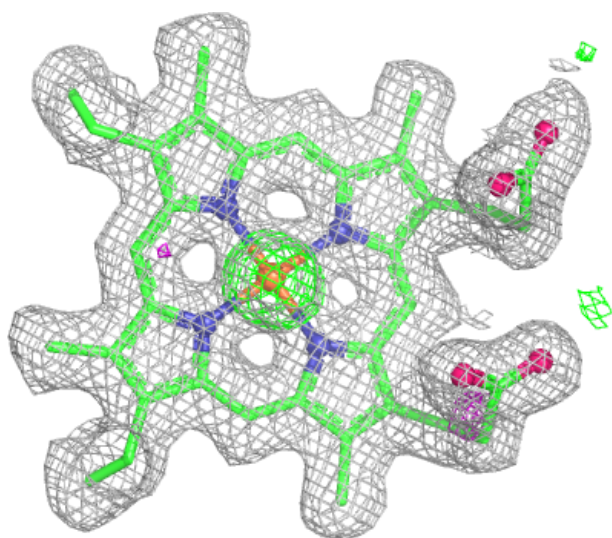
Electron density around HEM A 307:

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



Electron density around HEM A 304:

$2mF_o-DF_c$ (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.