



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 01:05 am BST

PDB ID : 19HC
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

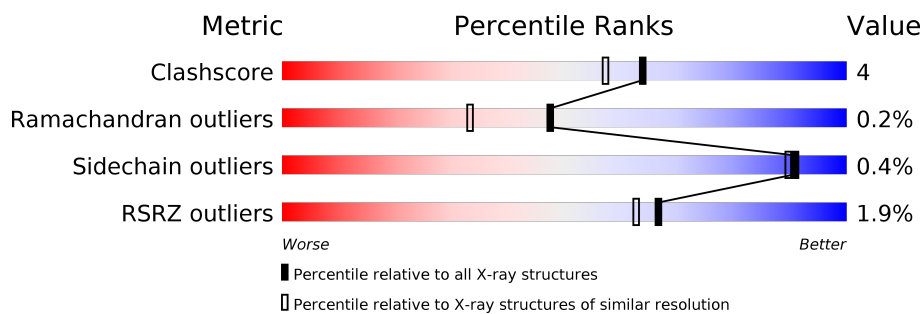
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 on 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	
1	B	292	

2 Entry composition [i](#)

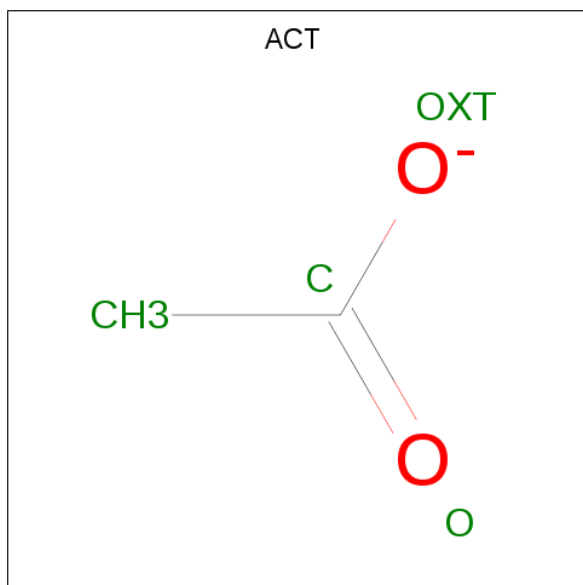
There are 4 unique types of molecules in this entry. The entry contains 6098 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



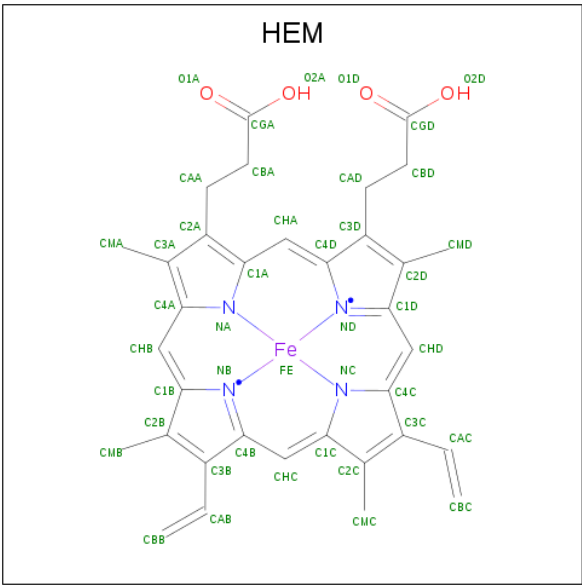
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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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

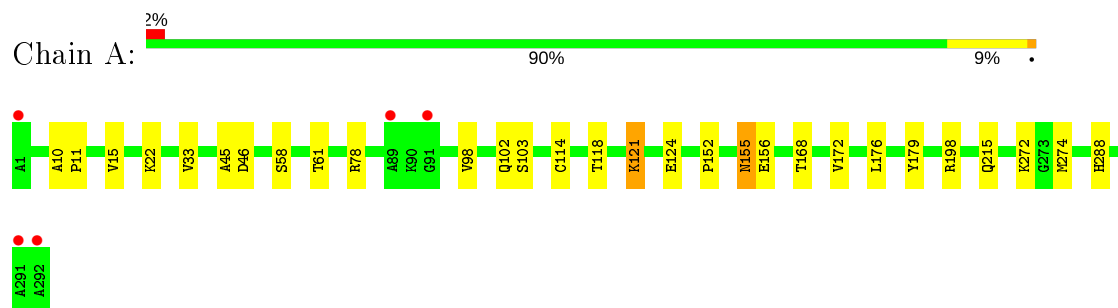
- Molecule 4 is water.

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

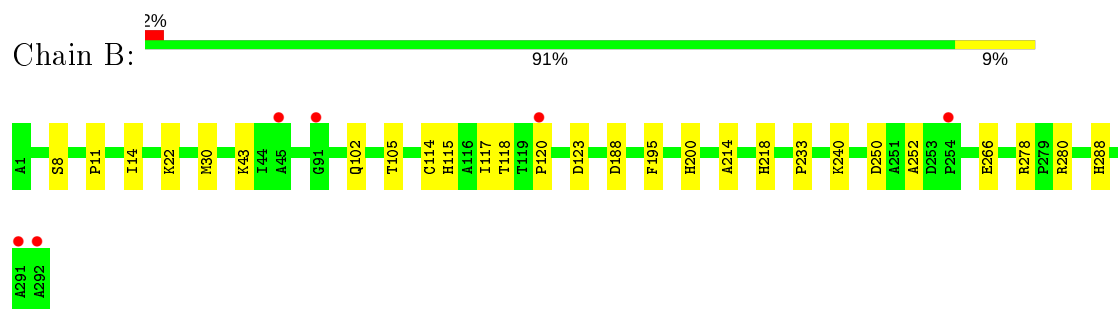
3 Residue-property plots

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

- Molecule 1: 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	60.38 Å 106.07 Å 80.62 Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	24.00 – 1.80 24.17 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (24.00-1.80) 99.1 (24.17-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.09 (at 1.80 Å)	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)	0.36 , 70.5	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: HEM, ACT

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	0.44	0/2272	1.09	3/3088 (0.1%)
1	B	0.40	0/2278	1.03	3/3098 (0.1%)
All	All	0.42	0/4550	1.06	6/6186 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	A	198	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	A	179	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	B	195	PHE	CB-CG-CD2	-6.92	115.95	120.80
1	B	195	PHE	CB-CG-CD1	6.53	125.37	120.80
1	B	123	ASP	CB-CG-OD1	5.13	122.92	118.30

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	21	0
2	A	12	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	6	0	0
3	A	387	0	270	2	0
3	B	387	0	270	7	0
4	A	475	0	0	8	0
4	B	410	0	0	2	0
All	All	6098	0	4826	42	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 (42) 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: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: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
1:A:274:MET:HE1	4:A:726:HOH:O	2.09	0.53
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
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: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:A:98:VAL:O	1:A:102[B]:GLN:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103[B]:SER:CB	4:A:510:HOH:O	2.67	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:105:THR:HB	1:B:115:HIS:CG	2.56	0.41
1:B:102:GLN:NE2	3:B:304:HEM:O2A	2.49	0.41
1:B:214:ALA:HB1	1:B:218:HIS:CE1	2.56	0.41
1:A:272:LYS:HD3	4:A:769:HOH:O	2.19	0.40
1:A:33:VAL:HG21	3:A:305:HEM:C2D	2.56	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/292 (102%)	292 (98%)	5 (2%)	0	100	100
1	B	297/292 (102%)	293 (99%)	3 (1%)	1 (0%)	41	27
All	All	594/584 (102%)	585 (98%)	8 (1%)	1 (0%)	47	33

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%)	81	78
1	B	245/238 (103%)	245 (100%)	0	100	100
All	All	490/476 (103%)	488 (100%)	2 (0%)	91	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	155	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 carbohydrates 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
2	ACT	A	295	-	1,3,3	3.23	1 (100%)	0,3,3	0.00	-
3	HEM	B	306	1	27,50,50	2.01	6 (22%)	17,82,82	2.02	6 (35%)
2	ACT	B	294	-	1,3,3	3.03	1 (100%)	0,3,3	0.00	-
2	ACT	B	293	-	1,3,3	2.94	1 (100%)	0,3,3	0.00	-
2	ACT	A	294	-	1,3,3	2.86	1 (100%)	0,3,3	0.00	-
3	HEM	B	308	1	27,50,50	1.99	7 (25%)	17,82,82	2.63	8 (47%)
3	HEM	B	304	1	27,50,50	2.09	6 (22%)	17,82,82	1.43	4 (23%)
3	HEM	B	303	1	27,50,50	2.07	6 (22%)	17,82,82	2.18	5 (29%)
3	HEM	A	301	1	27,50,50	2.07	7 (25%)	17,82,82	2.03	8 (47%)
3	HEM	B	302	1	27,50,50	1.94	5 (18%)	17,82,82	2.00	6 (35%)
3	HEM	B	301	1	27,50,50	1.95	5 (18%)	17,82,82	1.89	6 (35%)
3	HEM	A	303	1	27,50,50	2.15	5 (18%)	17,82,82	1.68	3 (17%)
3	HEM	B	305	1	27,50,50	1.98	5 (18%)	17,82,82	1.95	7 (41%)
3	HEM	A	304	1	27,50,50	1.85	4 (14%)	17,82,82	1.96	5 (29%)
3	HEM	B	307	1	27,50,50	1.93	6 (22%)	17,82,82	1.37	2 (11%)
3	HEM	A	305	1	27,50,50	1.95	5 (18%)	17,82,82	1.89	6 (35%)
3	HEM	A	307	1	27,50,50	2.07	6 (22%)	17,82,82	1.39	2 (11%)
3	HEM	A	302	1	27,50,50	1.95	4 (14%)	17,82,82	1.65	3 (17%)
3	HEM	A	306	1	27,50,50	1.96	6 (22%)	17,82,82	1.42	3 (17%)
3	HEM	A	308	1	27,50,50	1.91	6 (22%)	17,82,82	1.59	3 (17%)
2	ACT	A	293	-	1,3,3	3.26	1 (100%)	0,3,3	0.00	-
3	HEM	B	309	1	27,50,50	2.00	5 (18%)	17,82,82	1.48	3 (17%)
3	HEM	A	309	1	27,50,50	2.01	6 (22%)	17,82,82	1.48	3 (17%)

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	301	1	-	0/6/54/54	-
3	HEM	B	307	1	-	0/6/54/54	-
3	HEM	B	308	1	-	0/6/54/54	-
3	HEM	A	305	1	-	0/6/54/54	-
3	HEM	A	307	1	-	0/6/54/54	-
3	HEM	A	302	1	-	0/6/54/54	-
3	HEM	B	302	1	-	1/6/54/54	-
3	HEM	A	306	1	-	0/6/54/54	-
3	HEM	B	306	1	-	0/6/54/54	-
3	HEM	A	308	1	-	0/6/54/54	-
3	HEM	B	304	1	-	0/6/54/54	-
3	HEM	B	301	1	-	0/6/54/54	-
3	HEM	A	303	1	-	0/6/54/54	-
3	HEM	B	305	1	-	0/6/54/54	-
3	HEM	B	309	1	-	0/6/54/54	-
3	HEM	A	309	1	-	0/6/54/54	-
3	HEM	A	304	1	-	0/6/54/54	-
3	HEM	B	303	1	-	0/6/54/54	-

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	305	HEM	C3B-C2B	-5.38	1.32	1.40
3	A	309	HEM	C3B-C2B	-5.28	1.33	1.40
3	B	309	HEM	C3B-C2B	-5.16	1.33	1.40
3	A	303	HEM	C3B-C2B	-5.11	1.33	1.40
3	B	304	HEM	C3B-C2B	-5.09	1.33	1.40
3	A	305	HEM	C3B-C2B	-5.07	1.33	1.40
3	B	308	HEM	C3C-C2C	-4.99	1.33	1.40
3	B	301	HEM	C3B-C2B	-4.89	1.33	1.40
3	A	303	HEM	C3C-C2C	-4.87	1.33	1.40
3	A	307	HEM	C3B-C2B	-4.82	1.33	1.40
3	A	307	HEM	C3C-C2C	-4.68	1.33	1.40
3	A	306	HEM	C3B-C2B	-4.63	1.33	1.40
3	B	303	HEM	C3C-C2C	-4.61	1.34	1.40
3	A	302	HEM	C3B-C2B	-4.60	1.34	1.40
3	A	304	HEM	C3B-C2B	-4.56	1.34	1.40
3	B	306	HEM	C3B-C2B	-4.56	1.34	1.40
3	A	301	HEM	C3C-C2C	-4.54	1.34	1.40
3	B	309	HEM	C3C-C2C	-4.53	1.34	1.40
3	A	302	HEM	C3C-CAC	4.49	1.57	1.47
3	B	302	HEM	C3C-C2C	-4.35	1.34	1.40
3	B	304	HEM	C3C-C2C	-4.33	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	306	HEM	C3C-C2C	-4.32	1.34	1.40
3	B	303	HEM	C3B-C2B	-4.19	1.34	1.40
3	A	303	HEM	C3C-CAC	4.17	1.56	1.47
3	B	306	HEM	C3C-C2C	-4.14	1.34	1.40
3	A	303	HEM	C3B-CAB	4.11	1.56	1.47
3	A	301	HEM	C3C-CAC	4.10	1.56	1.47
3	A	304	HEM	C3C-C2C	-4.05	1.34	1.40
3	A	301	HEM	C3B-C2B	-4.01	1.34	1.40
3	A	309	HEM	C3B-CAB	4.01	1.56	1.47
3	B	302	HEM	C3B-C2B	-3.97	1.34	1.40
3	A	305	HEM	C3C-C2C	-3.97	1.34	1.40
3	B	302	HEM	C3B-CAB	3.94	1.56	1.47
3	B	301	HEM	C3C-CAC	3.92	1.55	1.47
3	B	307	HEM	C3B-C2B	-3.92	1.34	1.40
3	B	308	HEM	C3B-C2B	-3.91	1.34	1.40
3	B	303	HEM	C3B-CAB	3.89	1.55	1.47
3	B	305	HEM	C3C-CAC	3.86	1.55	1.47
3	A	308	HEM	C3C-C2C	-3.85	1.35	1.40
3	B	307	HEM	C3C-C2C	-3.85	1.35	1.40
3	B	305	HEM	C3B-CAB	3.82	1.55	1.47
3	A	307	HEM	C3B-CAB	3.78	1.55	1.47
3	A	308	HEM	C3C-CAC	3.78	1.55	1.47
3	B	303	HEM	C3C-CAC	3.76	1.55	1.47
3	B	304	HEM	C3B-CAB	3.76	1.55	1.47
3	A	309	HEM	C3C-C2C	-3.72	1.35	1.40
3	B	306	HEM	C3B-CAB	3.71	1.55	1.47
3	A	304	HEM	C3C-CAC	3.69	1.55	1.47
3	A	308	HEM	C3B-C2B	-3.68	1.35	1.40
3	B	307	HEM	C3C-CAC	3.66	1.55	1.47
3	B	308	HEM	C3B-CAB	3.63	1.55	1.47
3	B	304	HEM	C3C-CAC	3.59	1.55	1.47
3	B	309	HEM	C3B-CAB	3.58	1.55	1.47
3	B	302	HEM	C3C-CAC	3.57	1.55	1.47
3	A	306	HEM	C3B-CAB	3.50	1.55	1.47
3	A	307	HEM	C3C-CAC	3.50	1.55	1.47
3	A	302	HEM	C3B-CAB	3.50	1.55	1.47
3	B	301	HEM	C3B-CAB	3.48	1.55	1.47
3	B	306	HEM	C3C-CAC	3.45	1.54	1.47
3	B	301	HEM	C3C-C2C	-3.44	1.35	1.40
3	A	302	HEM	C3C-C2C	-3.41	1.35	1.40
3	A	305	HEM	C3B-CAB	3.40	1.54	1.47
3	B	305	HEM	C3C-C2C	-3.30	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	308	HEM	C3C-CAC	3.28	1.54	1.47
2	A	293	ACT	CH3-C	3.26	1.52	1.48
3	A	304	HEM	C3B-CAB	3.25	1.54	1.47
3	A	308	HEM	C3B-CAB	3.24	1.54	1.47
2	A	295	ACT	CH3-C	3.23	1.52	1.48
3	B	306	HEM	CAA-C2A	3.22	1.56	1.52
3	A	301	HEM	C3B-CAB	3.22	1.54	1.47
3	B	309	HEM	C3C-CAC	3.21	1.54	1.47
3	A	306	HEM	C3C-CAC	3.21	1.54	1.47
3	B	303	HEM	CAA-C2A	3.14	1.56	1.52
3	A	305	HEM	C3C-CAC	3.11	1.54	1.47
3	B	307	HEM	C3B-CAB	3.07	1.54	1.47
2	B	294	ACT	CH3-C	3.03	1.52	1.48
3	A	309	HEM	C3C-CAC	2.95	1.53	1.47
2	B	293	ACT	CH3-C	2.94	1.52	1.48
3	A	301	HEM	CAA-C2A	2.91	1.56	1.52
2	A	294	ACT	CH3-C	2.86	1.52	1.48
3	B	304	HEM	CAA-C2A	2.81	1.56	1.52
3	A	306	HEM	CAA-C2A	2.72	1.56	1.52
3	B	302	HEM	CAA-C2A	2.69	1.56	1.52
3	A	309	HEM	CAA-C2A	2.63	1.55	1.52
3	A	303	HEM	CAA-C2A	2.58	1.55	1.52
3	B	307	HEM	C1D-ND	2.47	1.41	1.36
3	A	309	HEM	C1A-NA	2.42	1.41	1.36
3	B	307	HEM	CAA-C2A	2.40	1.55	1.52
3	A	308	HEM	CAD-C3D	2.36	1.56	1.52
3	A	301	HEM	CMA-C3A	2.35	1.56	1.51
3	B	308	HEM	CAD-C3D	2.30	1.56	1.52
3	A	301	HEM	CMD-C2D	2.29	1.56	1.51
3	A	307	HEM	CAA-C2A	2.27	1.55	1.52
3	A	305	HEM	CAD-C3D	2.23	1.56	1.52
3	A	307	HEM	CMA-C3A	2.21	1.56	1.51
3	B	306	HEM	CMA-C3A	2.15	1.56	1.51
3	B	303	HEM	CMD-C2D	2.15	1.56	1.51
3	B	305	HEM	CAA-C2A	2.12	1.55	1.52
3	B	309	HEM	CMD-C2D	2.11	1.56	1.51
3	A	306	HEM	CMB-C2B	2.11	1.56	1.51
3	B	308	HEM	C4B-NB	2.08	1.40	1.36
3	B	308	HEM	CAA-C2A	2.06	1.55	1.52
3	B	301	HEM	CMD-C2D	2.06	1.55	1.51
3	B	304	HEM	C4B-NB	2.05	1.40	1.36
3	A	308	HEM	C4A-NA	2.03	1.40	1.36

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	308	HEM	CMA-C3A-C4A	-5.57	119.91	128.46
3	B	303	HEM	CMC-C2C-C3C	5.28	134.56	124.68
3	A	304	HEM	CMA-C3A-C4A	-4.77	121.14	128.46
3	A	302	HEM	CMD-C2D-C1D	-4.61	121.38	128.46
3	B	308	HEM	CMC-C2C-C3C	4.56	133.22	124.68
3	B	303	HEM	CMD-C2D-C1D	-4.47	121.60	128.46
3	B	305	HEM	CMA-C3A-C4A	-4.23	121.96	128.46
3	B	308	HEM	CMD-C2D-C1D	-4.17	122.05	128.46
3	B	302	HEM	CMD-C2D-C1D	-4.17	122.06	128.46
3	B	301	HEM	CMD-C2D-C1D	-3.95	122.39	128.46
3	A	301	HEM	CMD-C2D-C1D	-3.95	122.40	128.46
3	B	308	HEM	CMA-C3A-C2A	3.64	131.81	124.94
3	A	308	HEM	CMA-C3A-C4A	-3.59	122.95	128.46
3	A	303	HEM	CMC-C2C-C3C	3.58	131.37	124.68
3	A	305	HEM	CMA-C3A-C4A	-3.51	123.07	128.46
3	A	305	HEM	CMD-C2D-C1D	-3.39	123.25	128.46
3	B	306	HEM	CMD-C2D-C1D	-3.38	123.28	128.46
3	B	303	HEM	CMA-C3A-C4A	-3.37	123.29	128.46
3	A	303	HEM	CMA-C3A-C4A	-3.33	123.34	128.46
3	B	302	HEM	CMD-C2D-C3D	3.33	131.22	124.94
3	B	306	HEM	CMB-C2B-C3B	3.31	130.86	124.68
3	B	306	HEM	CMA-C3A-C4A	-3.29	123.41	128.46
3	A	307	HEM	CBD-CAD-C3D	3.29	118.53	112.48
3	B	308	HEM	CAD-CBD-CGD	3.27	118.16	112.67
3	A	304	HEM	CMD-C2D-C1D	-3.24	123.48	128.46
3	A	308	HEM	CMC-C2C-C3C	3.23	130.72	124.68
3	A	305	HEM	CBA-CAA-C2A	3.20	118.39	112.49
3	B	304	HEM	CMB-C2B-C3B	3.19	130.65	124.68
3	B	306	HEM	CMC-C2C-C3C	3.18	130.63	124.68
3	B	305	HEM	CMB-C2B-C3B	3.17	130.62	124.68
3	A	301	HEM	CMA-C3A-C4A	-3.17	123.60	128.46
3	B	301	HEM	CMA-C3A-C4A	-3.12	123.66	128.46
3	A	305	HEM	CMC-C2C-C3C	3.05	130.38	124.68
3	A	309	HEM	CMB-C2B-C3B	3.01	130.31	124.68
3	A	307	HEM	CMB-C2B-C3B	2.96	130.22	124.68
3	B	306	HEM	CAA-CBA-CGA	2.92	117.57	112.67
3	A	306	HEM	CMB-C2B-C3B	2.91	130.12	124.68
3	A	302	HEM	CMA-C3A-C4A	-2.91	124.00	128.46
3	B	308	HEM	CAA-CBA-CGA	2.90	117.54	112.67
3	B	305	HEM	CMA-C3A-C2A	2.83	130.28	124.94
3	A	304	HEM	CMA-C3A-C2A	2.80	130.23	124.94
3	B	304	HEM	CMA-C3A-C4A	-2.78	124.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	HEM	CMC-C2C-C3C	2.71	129.75	124.68
3	B	307	HEM	CMA-C3A-C4A	-2.70	124.32	128.46
3	B	302	HEM	CMA-C3A-C4A	-2.68	124.35	128.46
3	B	302	HEM	CMB-C2B-C3B	2.68	129.68	124.68
3	B	301	HEM	CBD-CAD-C3D	2.67	117.40	112.48
3	A	306	HEM	CMD-C2D-C1D	-2.67	124.36	128.46
3	A	301	HEM	CMA-C3A-C2A	2.65	129.94	124.94
3	B	305	HEM	CMD-C2D-C1D	-2.65	124.39	128.46
3	A	303	HEM	CMD-C2D-C1D	-2.64	124.40	128.46
3	A	309	HEM	CMA-C3A-C4A	-2.59	124.49	128.46
3	B	302	HEM	CAD-CBD-CGD	2.55	116.95	112.67
3	B	309	HEM	CAA-CBA-CGA	2.51	116.89	112.67
3	B	301	HEM	CMB-C2B-C3B	2.50	129.35	124.68
3	B	303	HEM	CAA-CBA-CGA	2.48	116.84	112.67
3	B	308	HEM	CBD-CAD-C3D	2.47	117.03	112.48
3	B	305	HEM	CBA-CAA-C2A	2.47	117.04	112.49
3	B	305	HEM	CAA-CBA-CGA	2.44	116.76	112.67
3	A	309	HEM	CMD-C2D-C1D	-2.41	124.76	128.46
3	B	306	HEM	CMD-C2D-C3D	2.40	129.47	124.94
3	A	306	HEM	CMC-C2C-C3C	2.39	129.15	124.68
3	B	307	HEM	CMD-C2D-C1D	-2.37	124.82	128.46
3	A	301	HEM	CMD-C2D-C3D	2.35	129.37	124.94
3	A	301	HEM	CAA-CBA-CGA	2.32	116.56	112.67
3	A	305	HEM	CMD-C2D-C3D	2.31	129.30	124.94
3	A	302	HEM	CBD-CAD-C3D	2.24	116.60	112.48
3	A	301	HEM	CBD-CAD-C3D	2.21	116.55	112.48
3	A	304	HEM	CMB-C2B-C3B	2.18	128.76	124.68
3	A	308	HEM	CMD-C2D-C1D	-2.15	125.15	128.46
3	A	305	HEM	CMB-C2B-C3B	2.13	128.66	124.68
3	B	305	HEM	CBD-CAD-C3D	2.12	116.39	112.48
3	B	301	HEM	CAD-CBD-CGD	2.11	116.22	112.67
3	B	301	HEM	CAA-CBA-CGA	2.11	116.21	112.67
3	A	301	HEM	CMB-C2B-C3B	2.09	128.60	124.68
3	B	309	HEM	CMD-C2D-C1D	-2.08	125.27	128.46
3	B	304	HEM	CMD-C2D-C1D	-2.08	125.27	128.46
3	B	309	HEM	CMB-C2B-C3B	2.07	128.54	124.68
3	B	304	HEM	CMA-C3A-C2A	2.06	128.83	124.94
3	B	302	HEM	CBD-CAD-C3D	2.04	116.23	112.48
3	B	303	HEM	CBD-CAD-C3D	2.03	116.22	112.48
3	B	308	HEM	CMB-C2B-C3B	2.02	128.47	124.68
3	A	301	HEM	CBA-CAA-C2A	-2.01	108.78	112.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

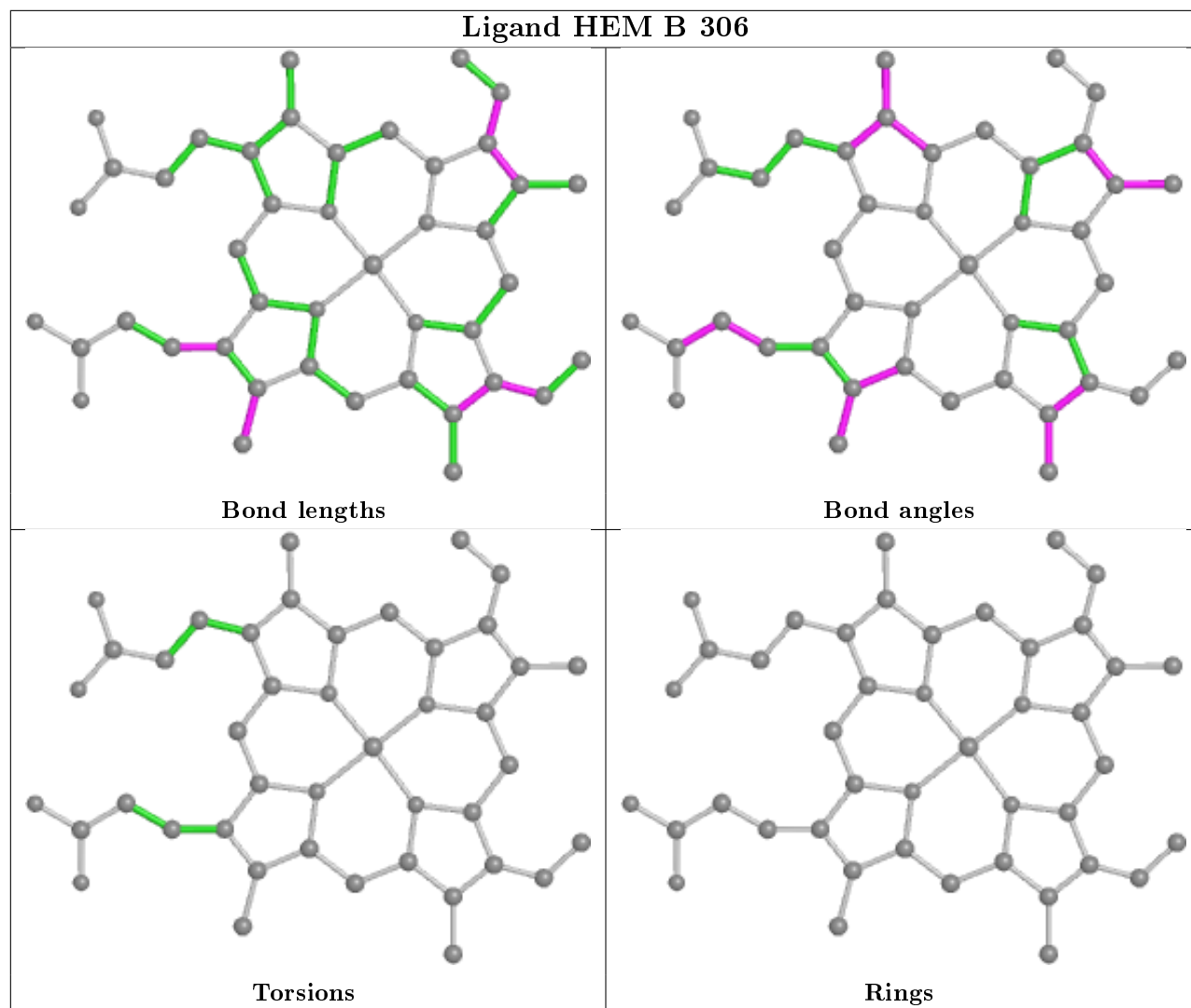
Mol	Chain	Res	Type	Atoms
3	B	302	HEM	C4D-C3D-CAD-CBD

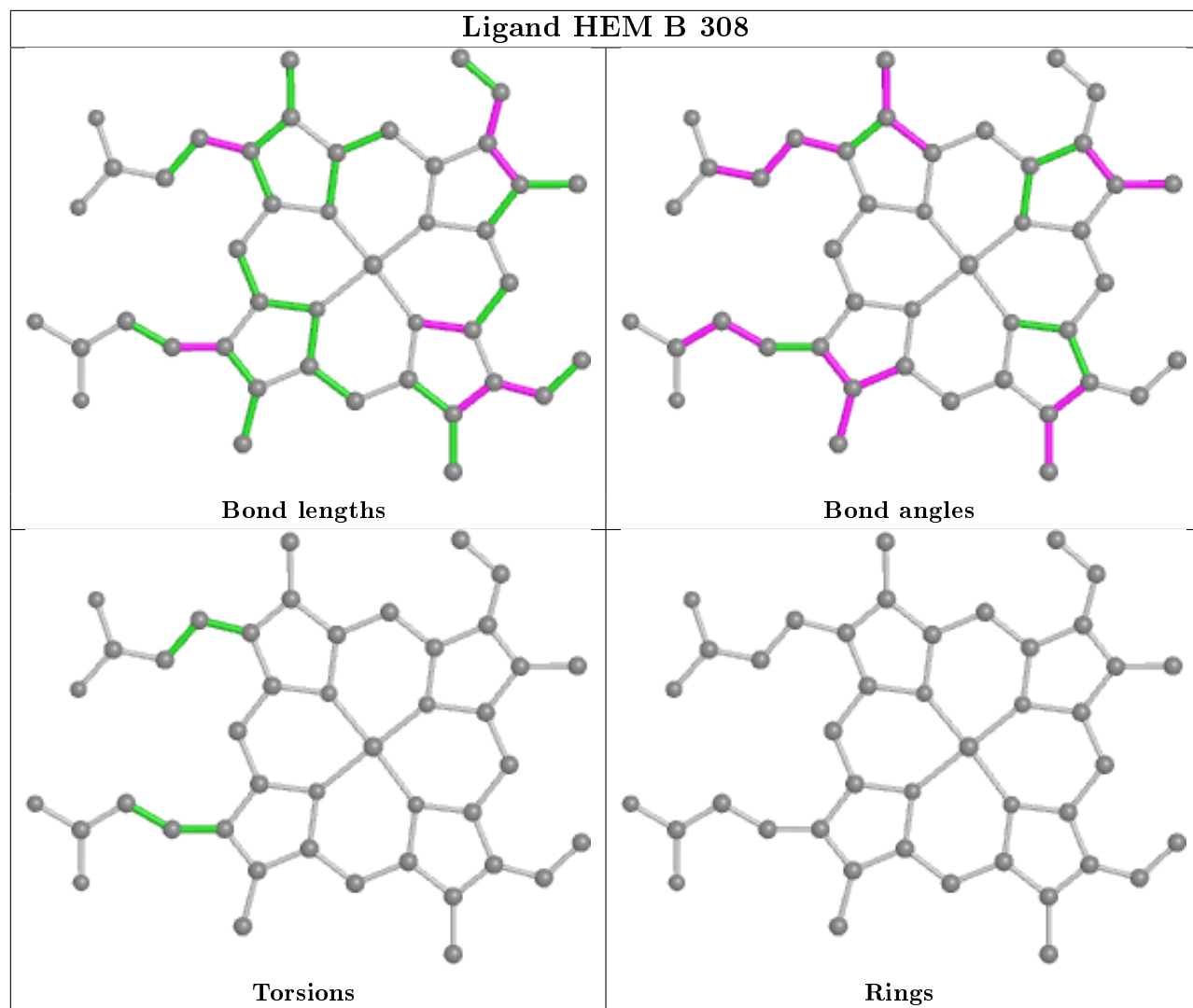
There are no ring outliers.

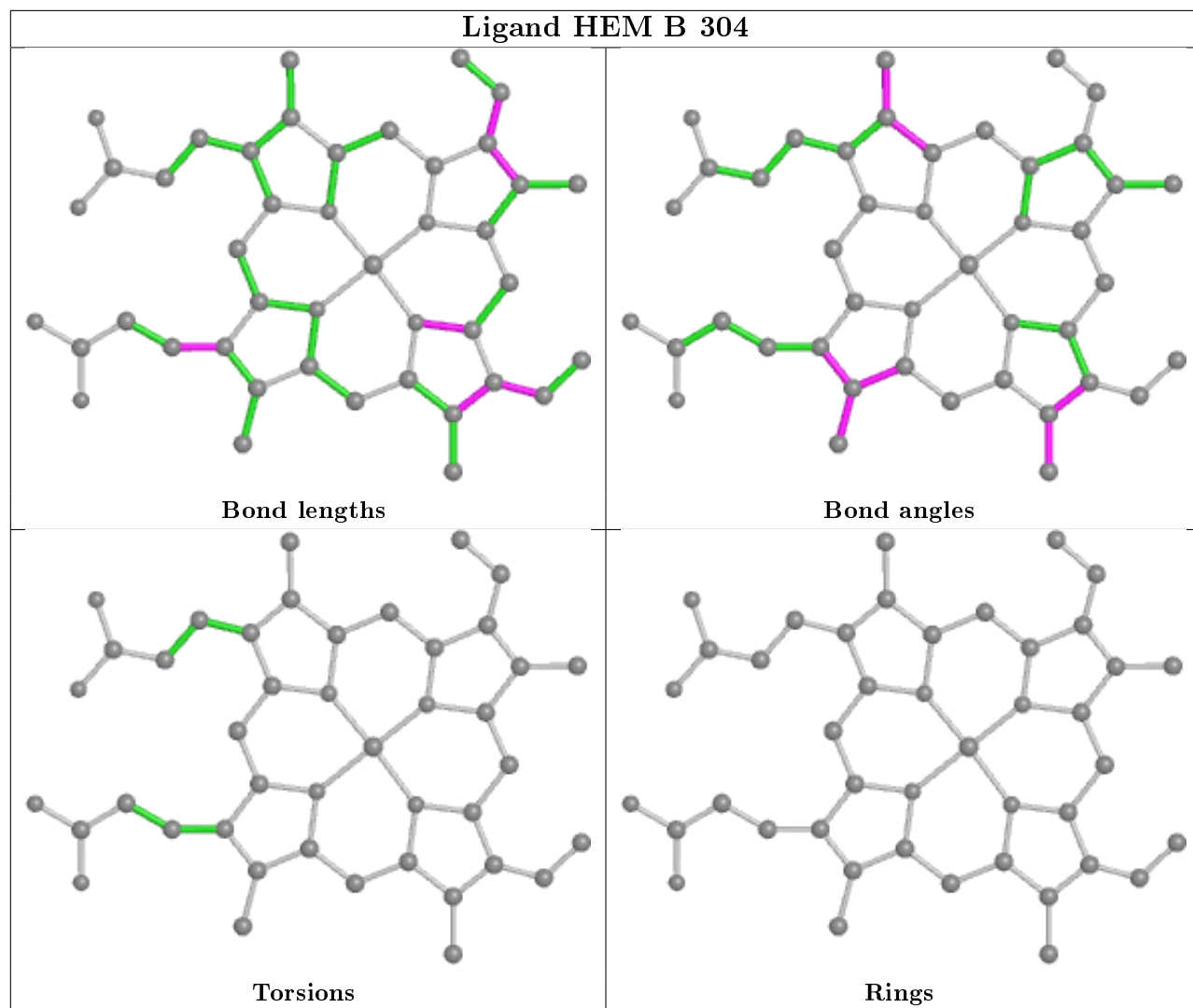
8 monomers are involved in 9 short contacts:

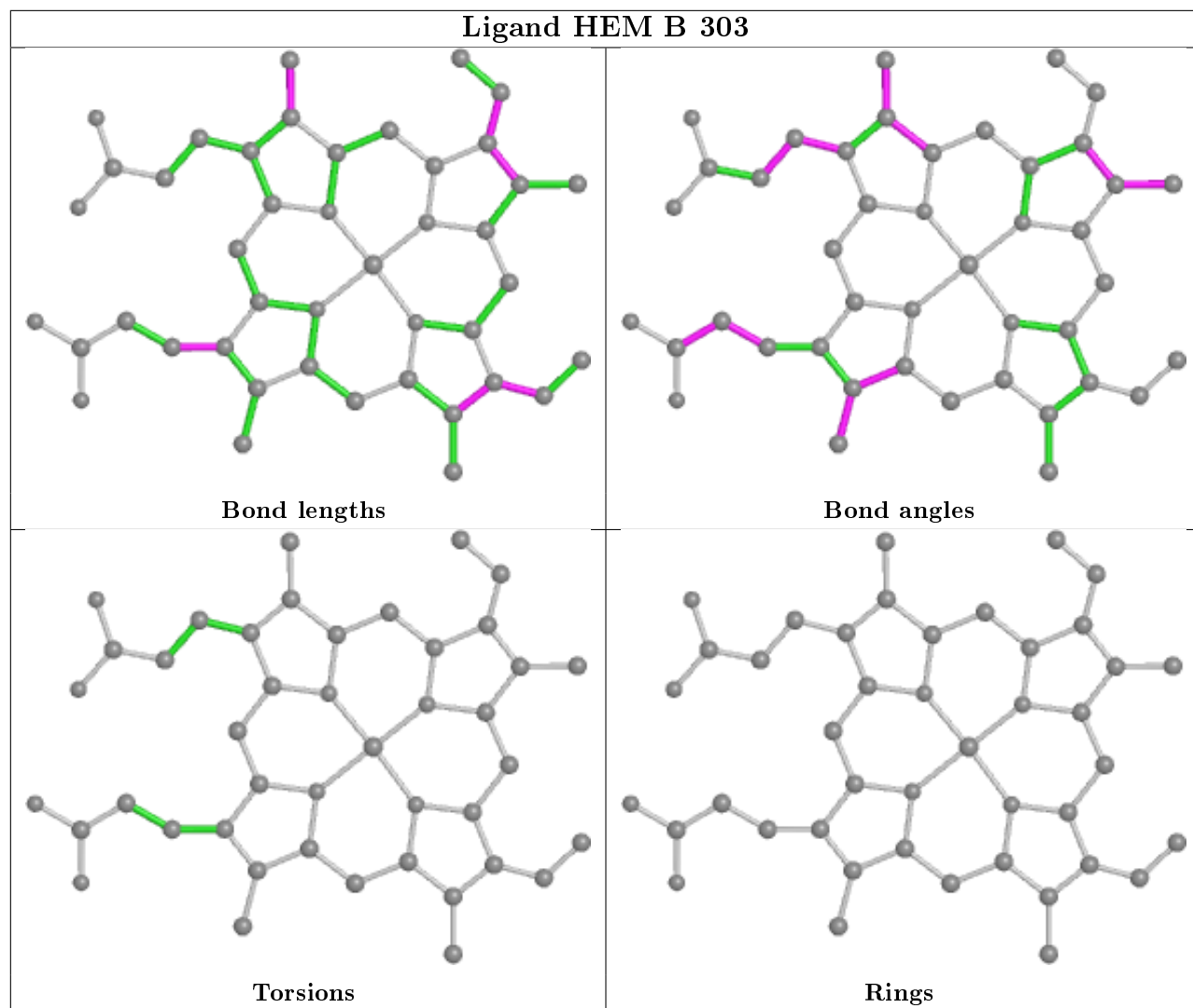
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	308	HEM	1	0
3	B	304	HEM	2	0
3	B	303	HEM	1	0
3	B	301	HEM	1	0
3	B	305	HEM	1	0
3	A	305	HEM	1	0
3	B	309	HEM	1	0
3	A	309	HEM	1	0

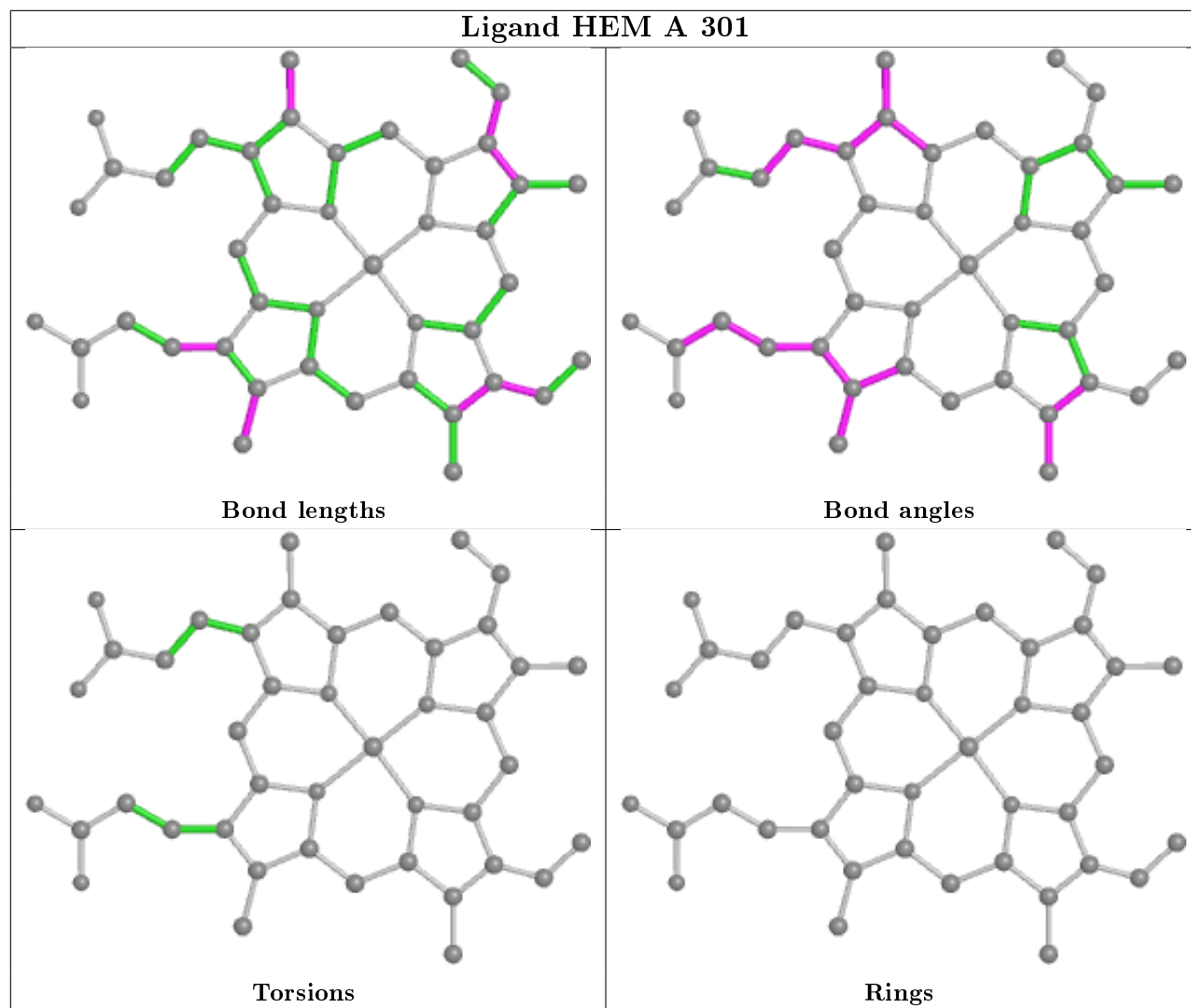
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

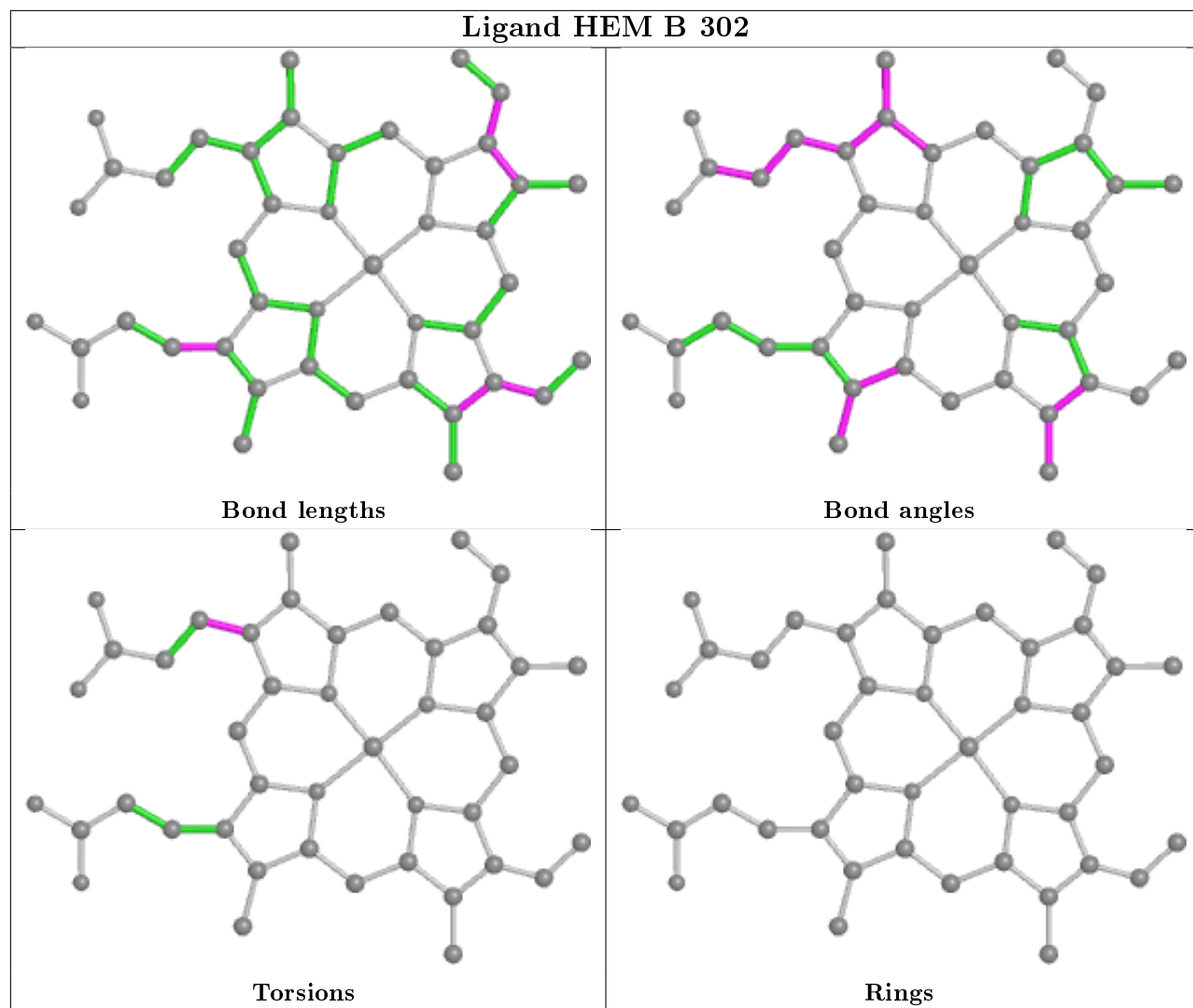


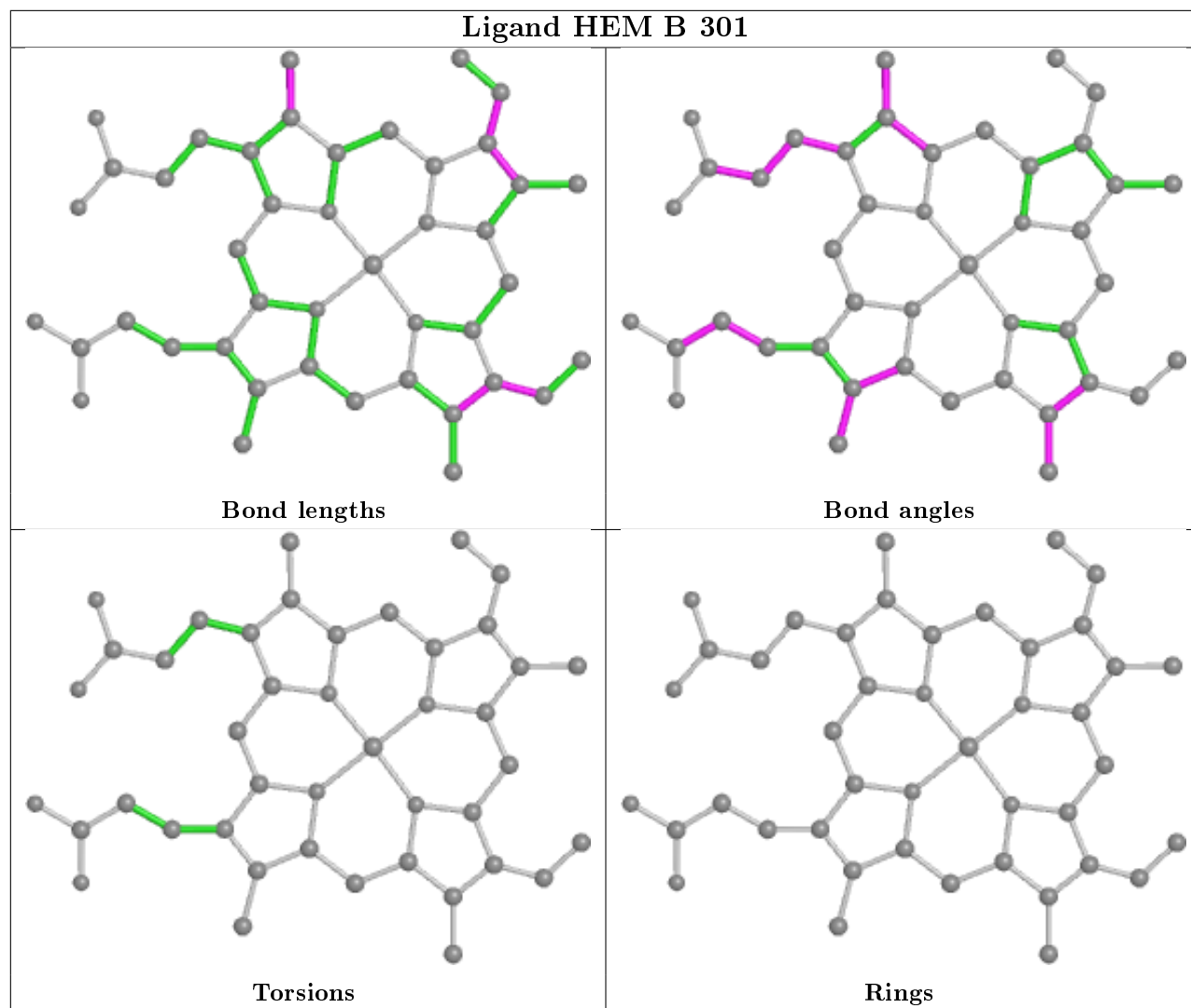


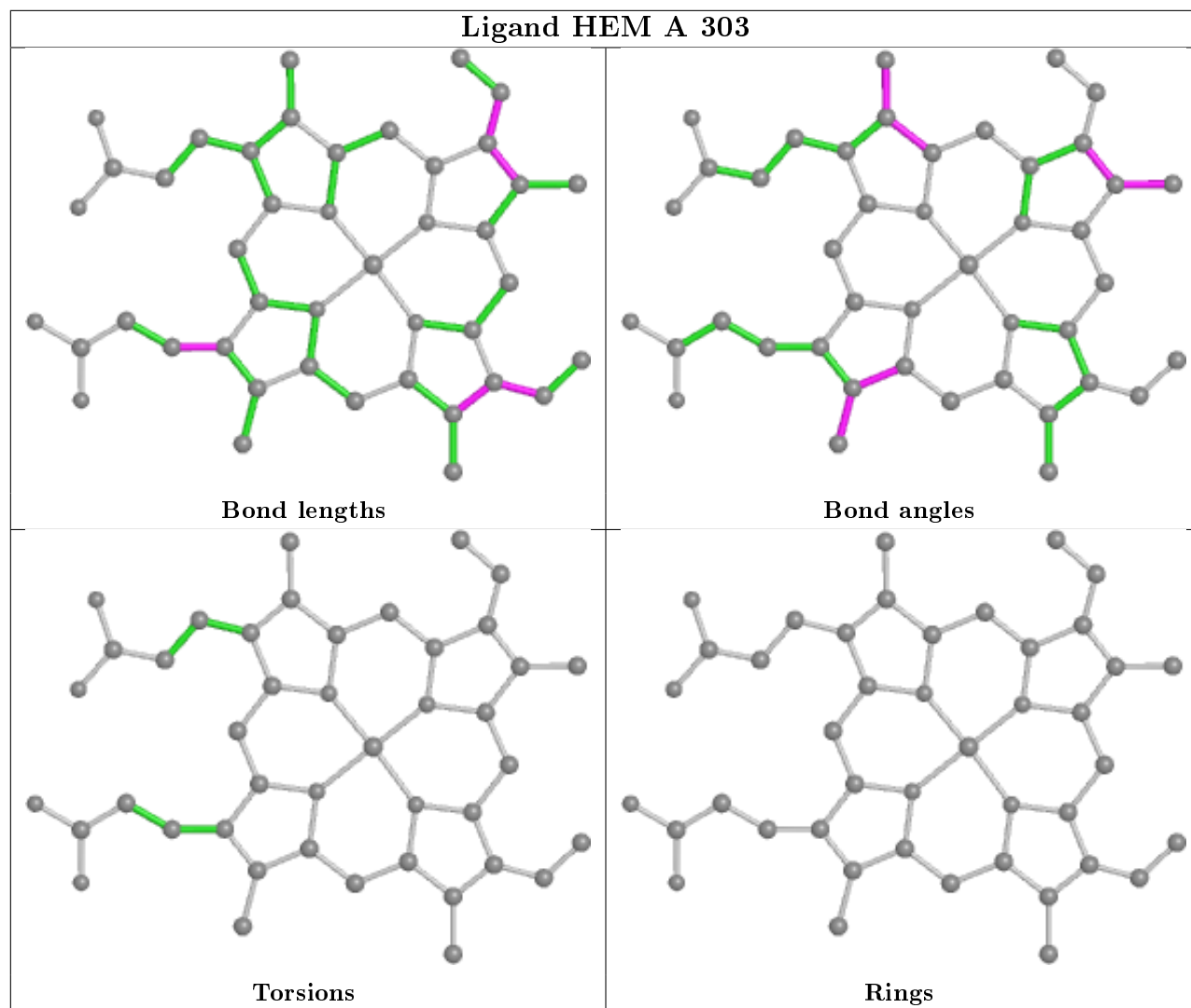


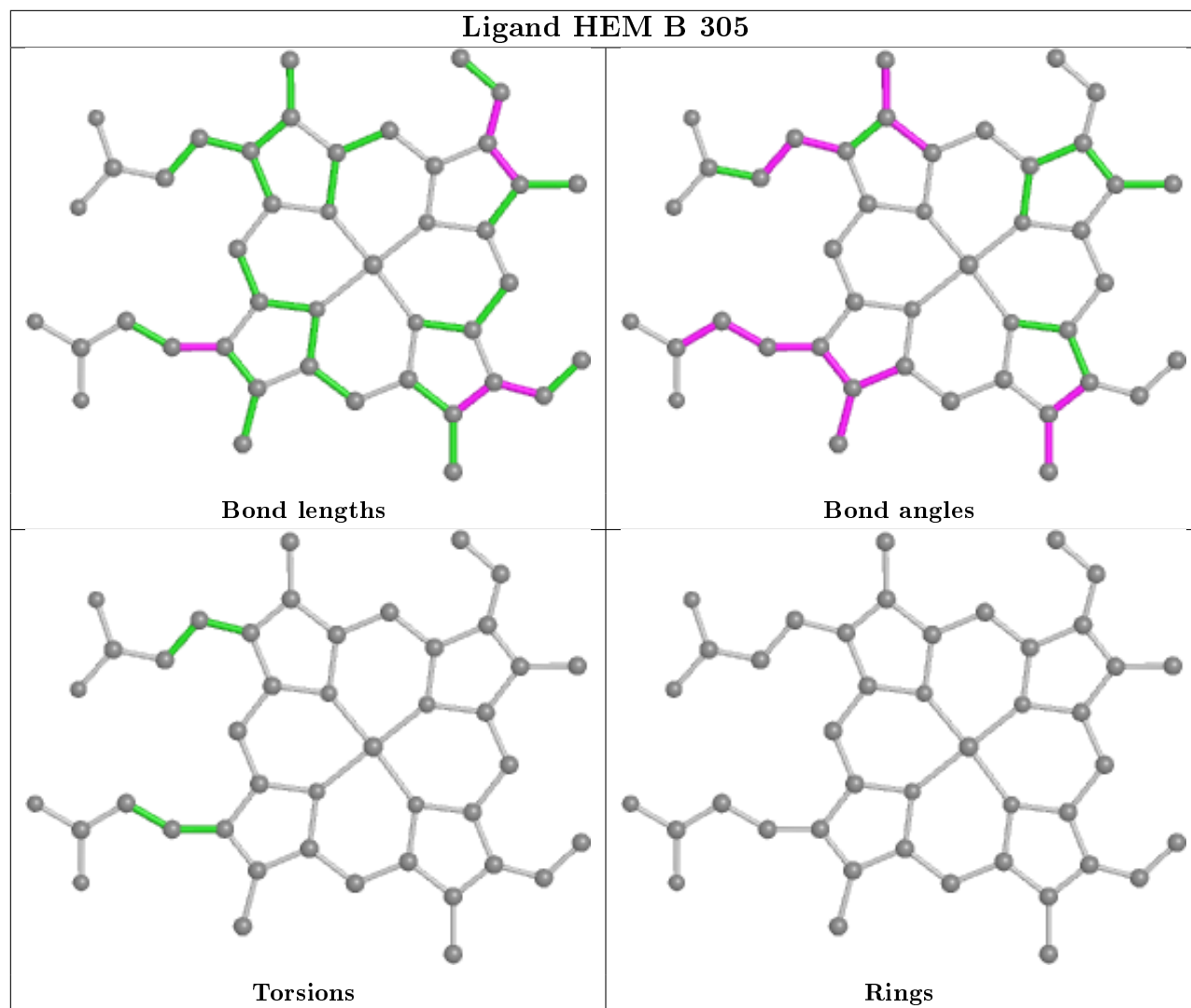


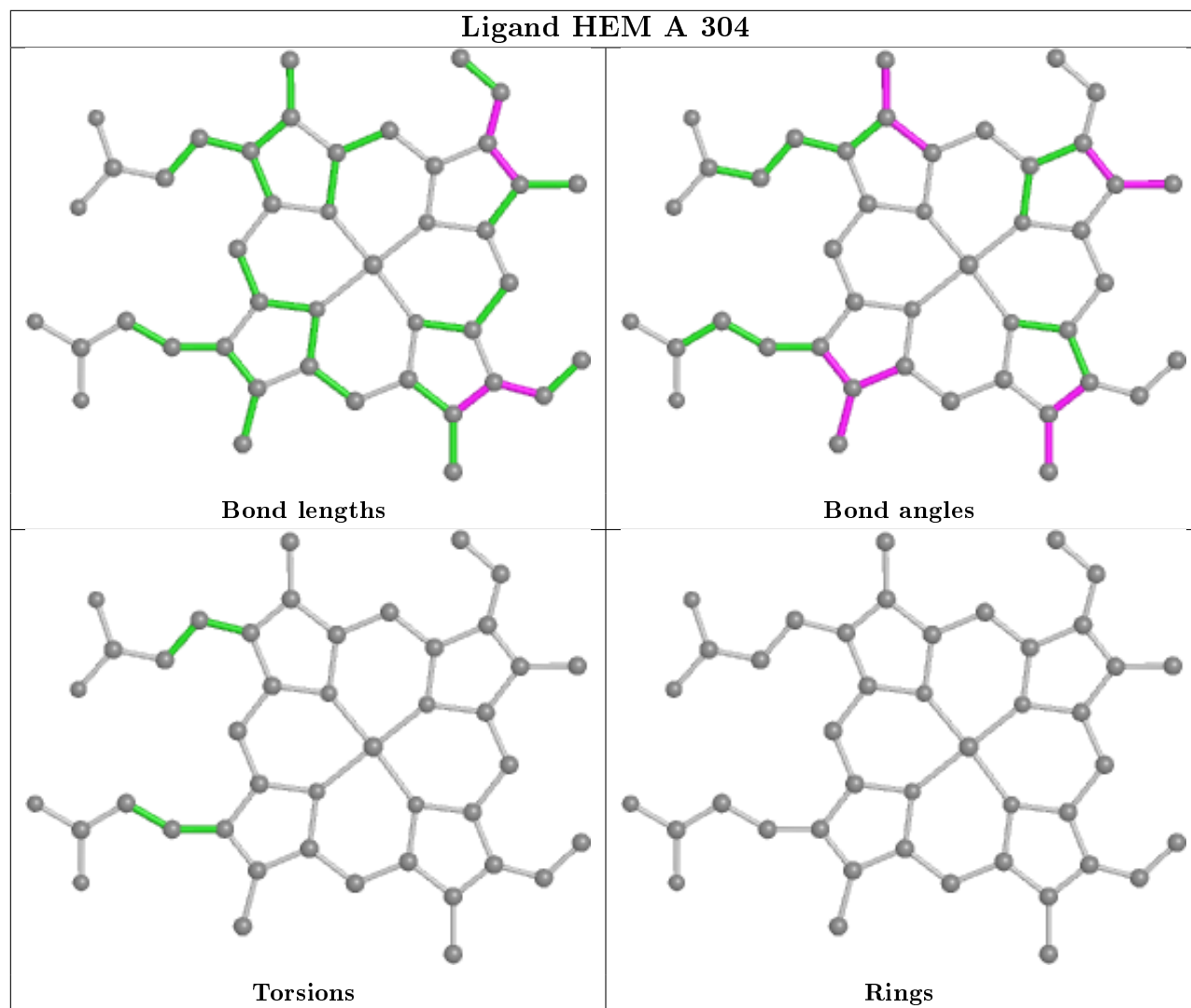


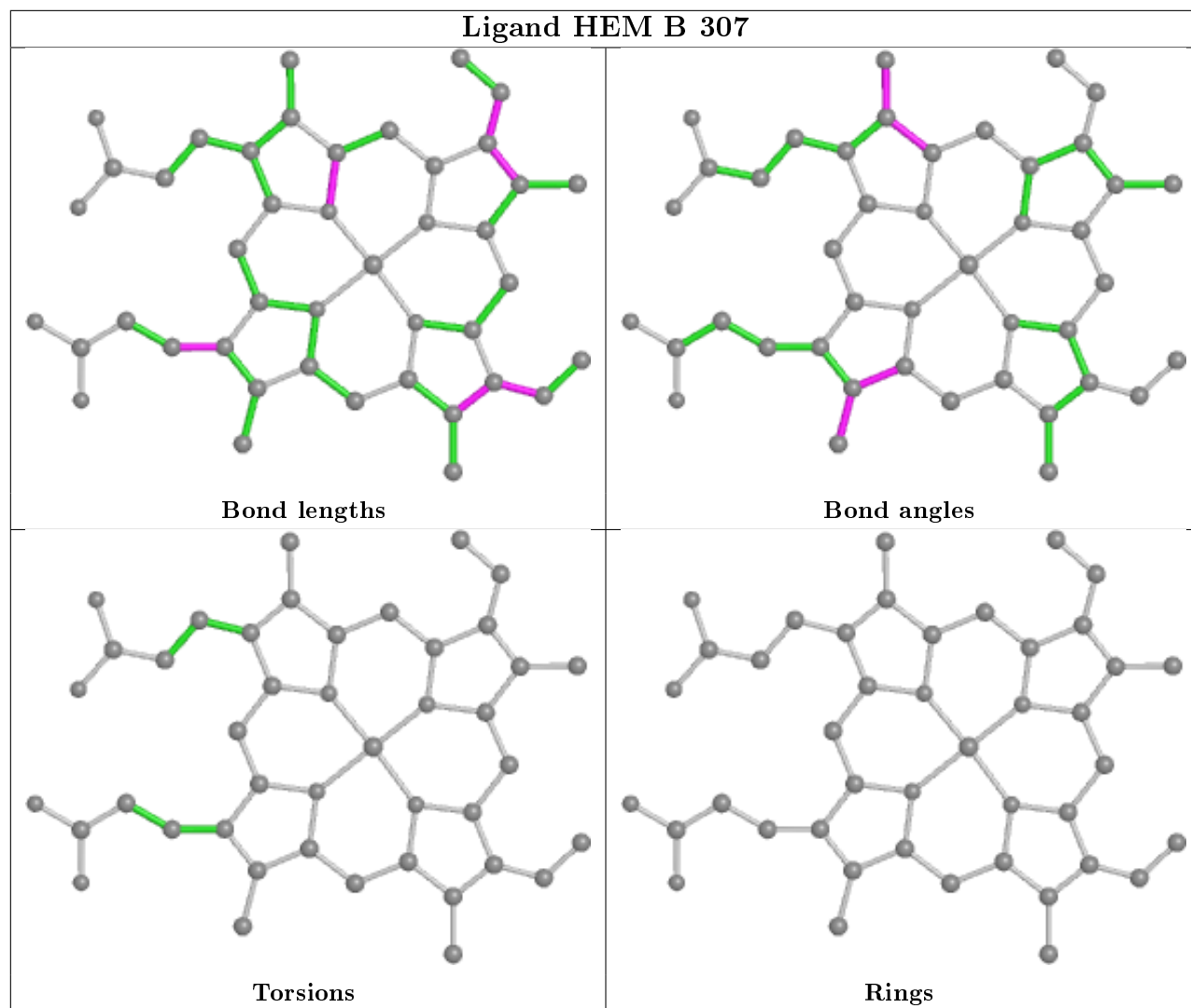


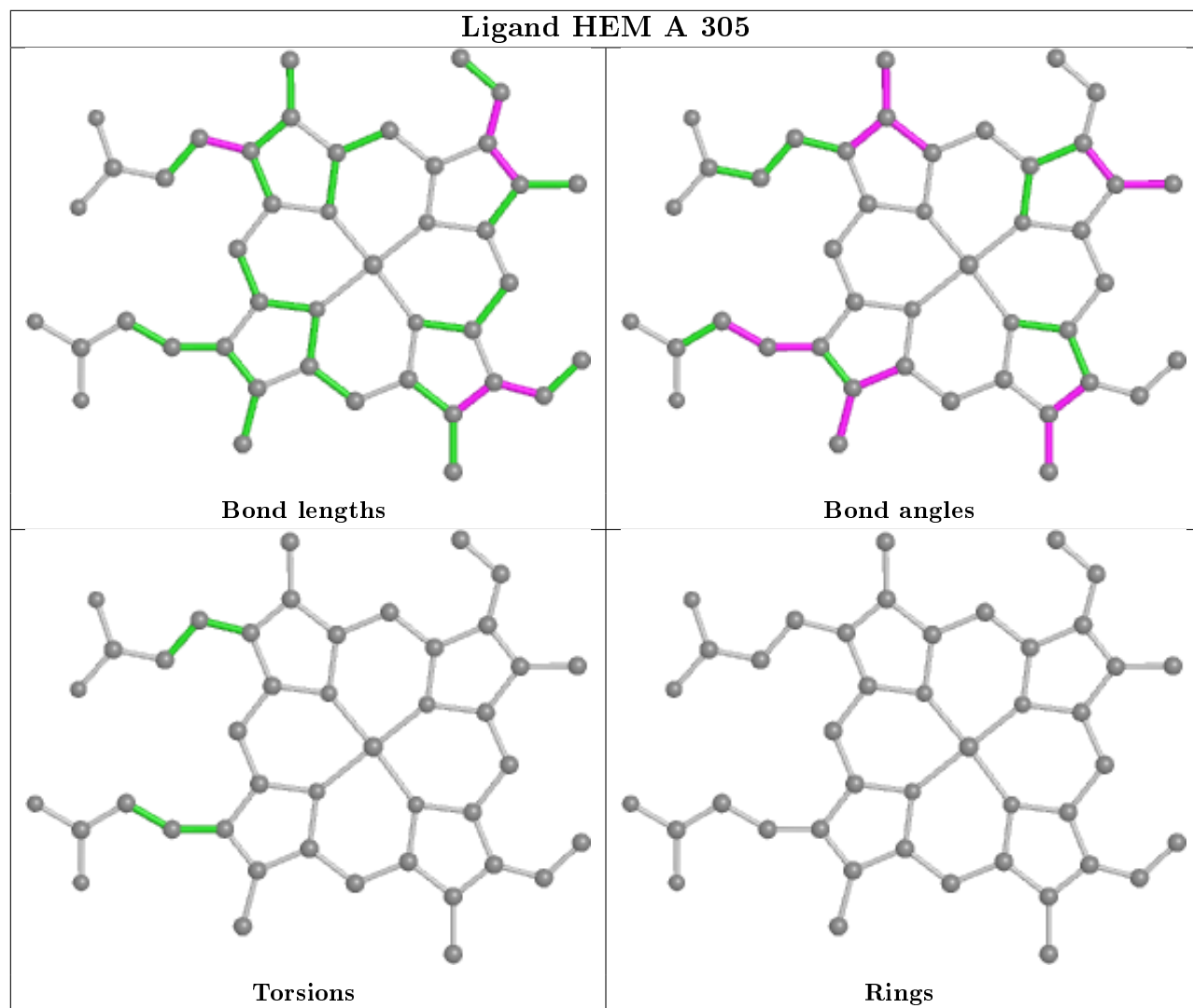


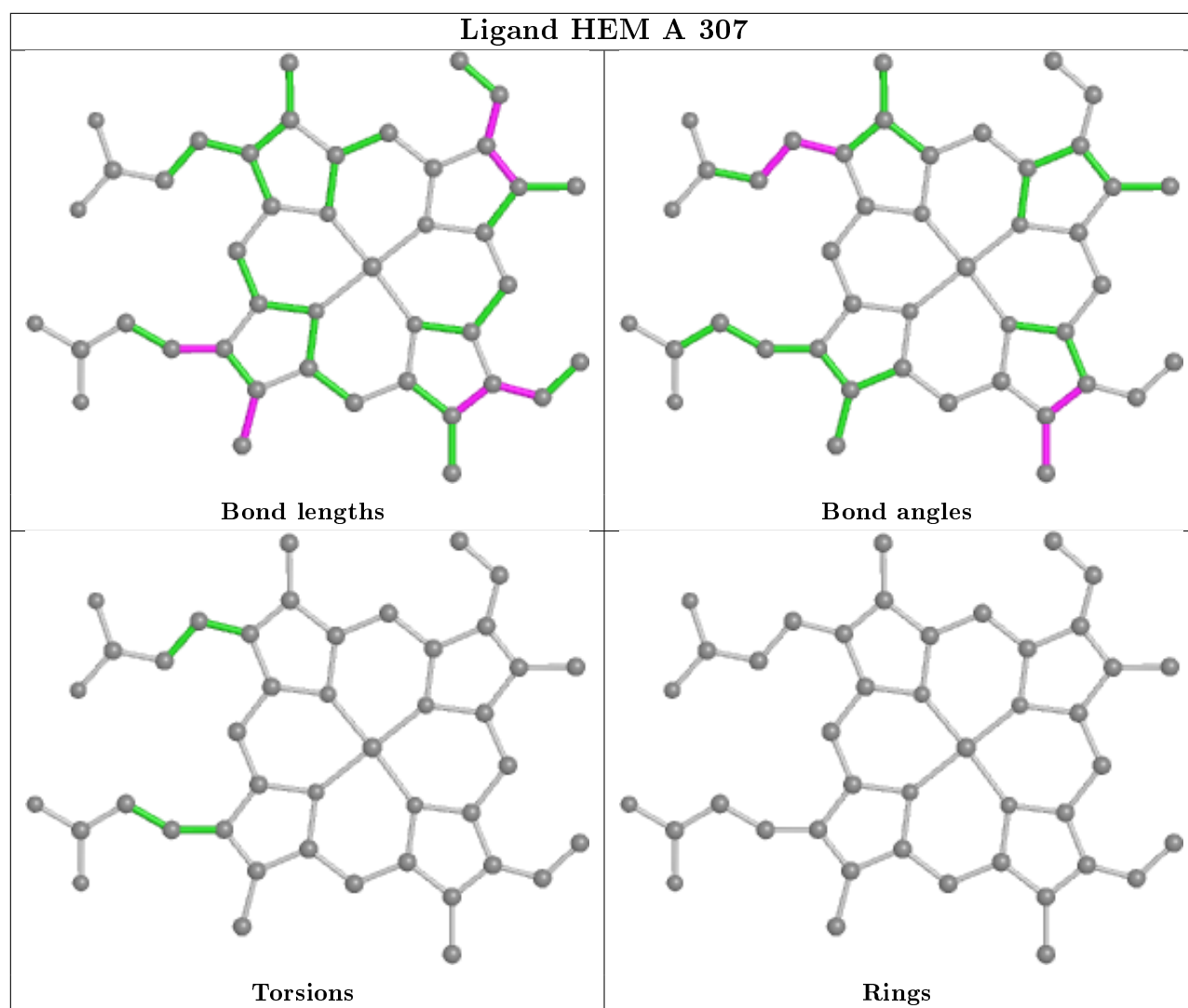


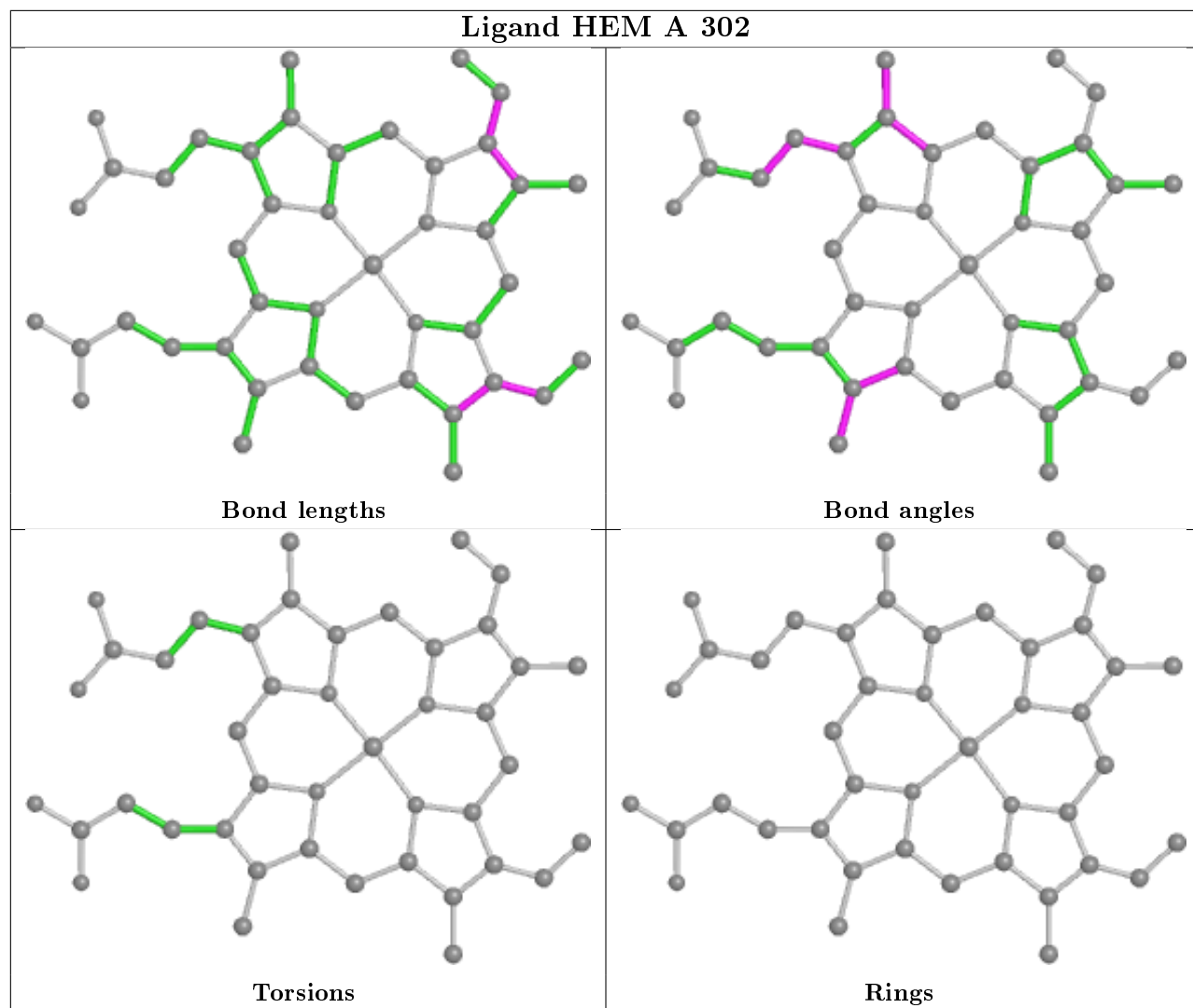


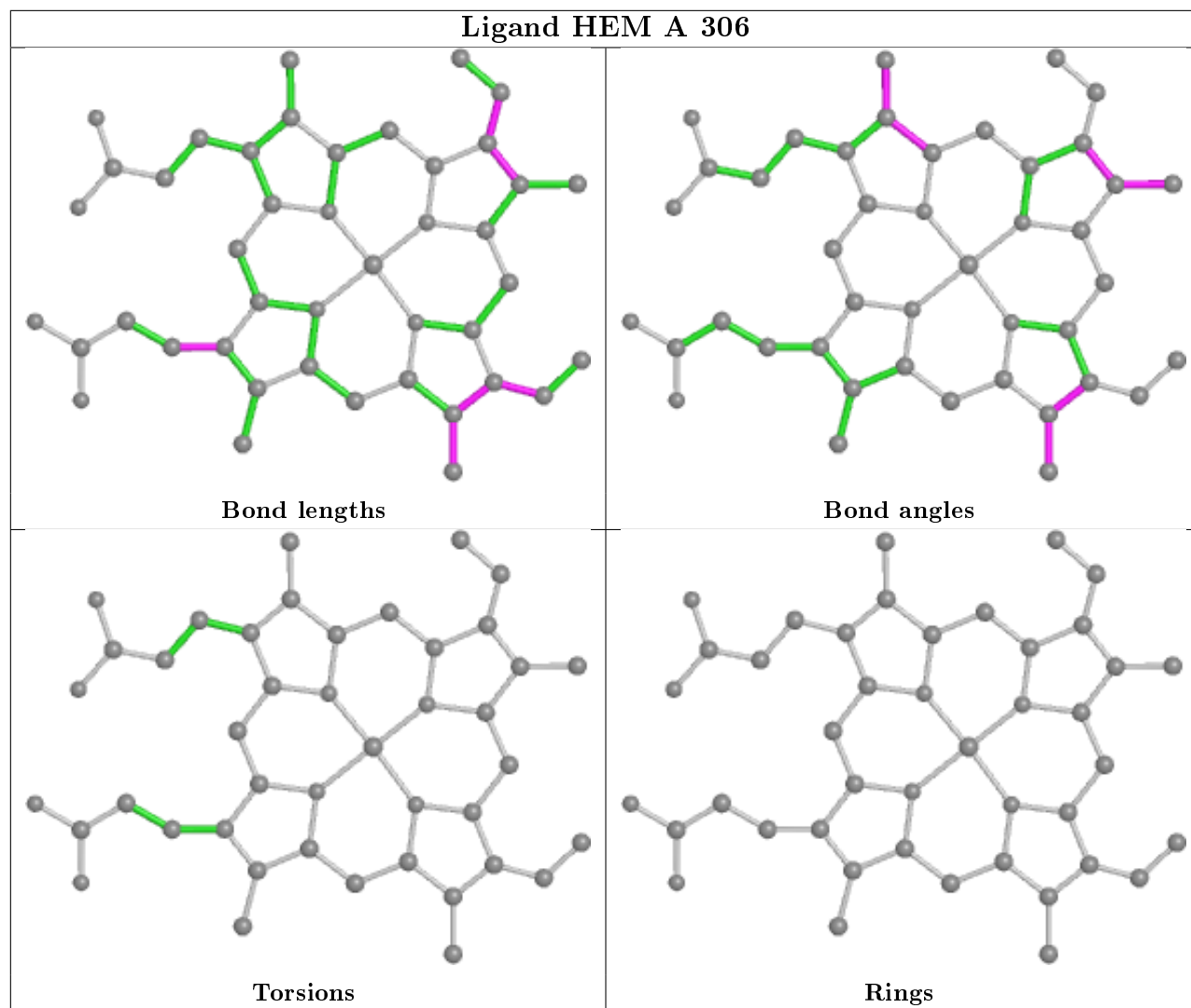


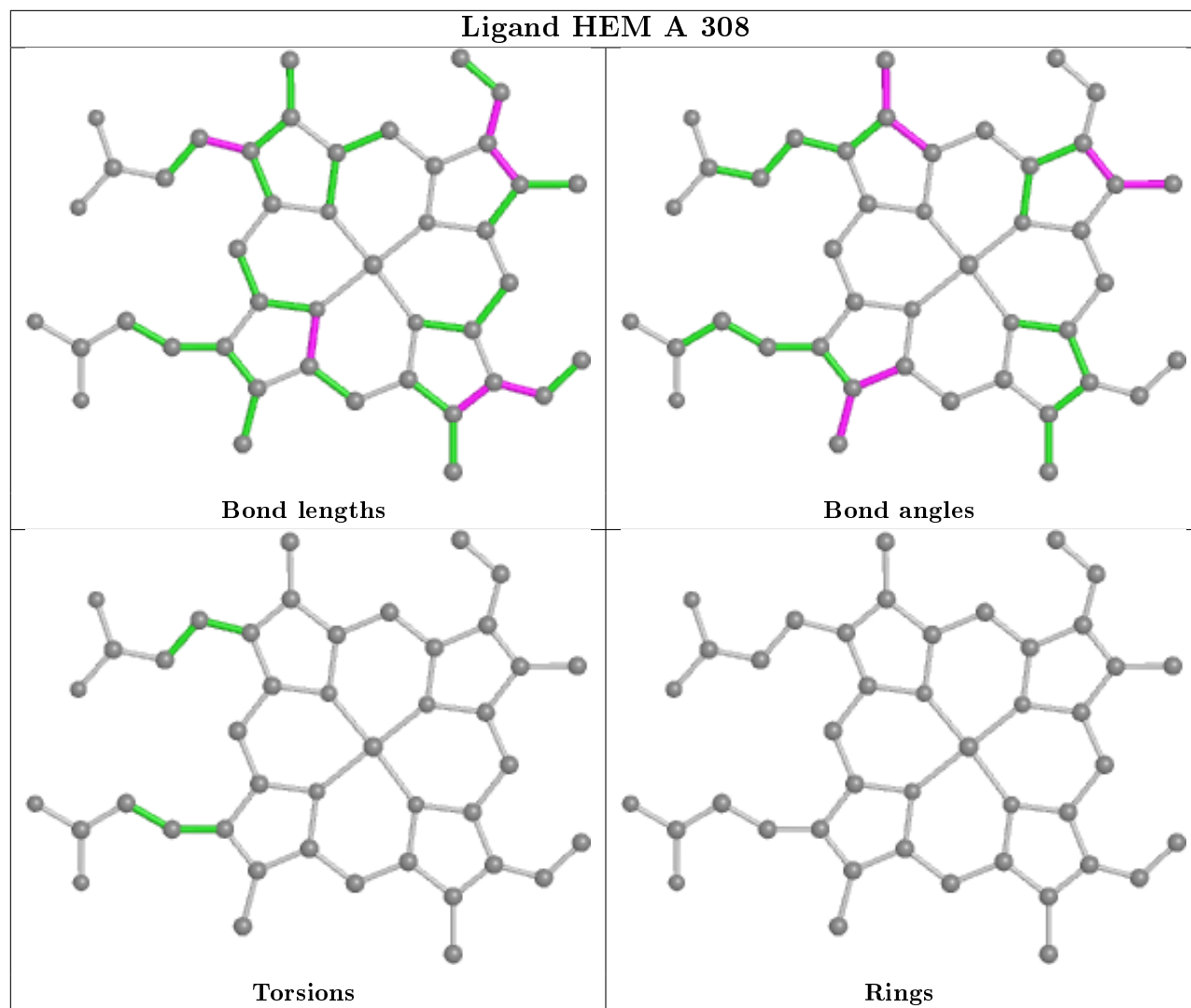


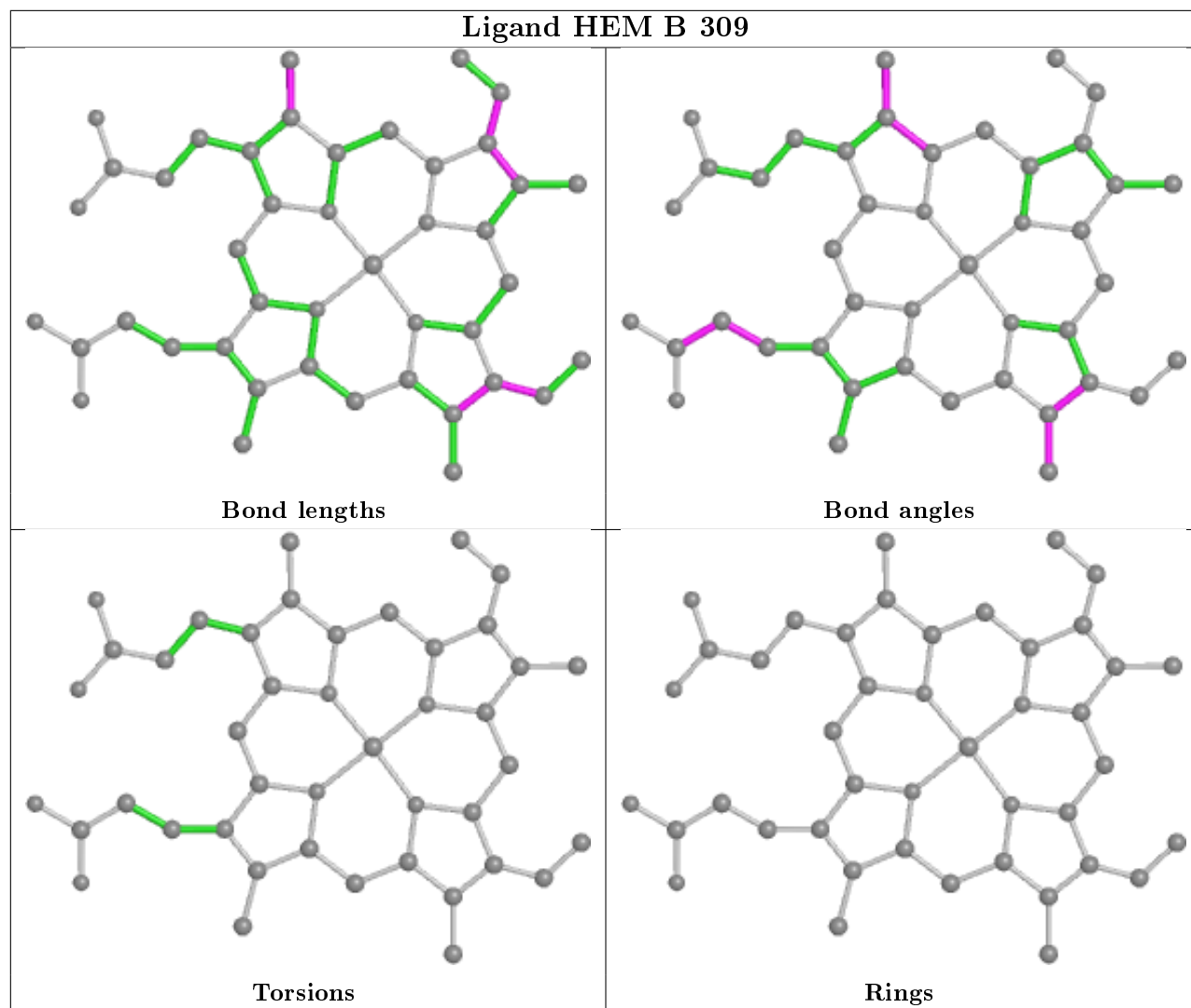


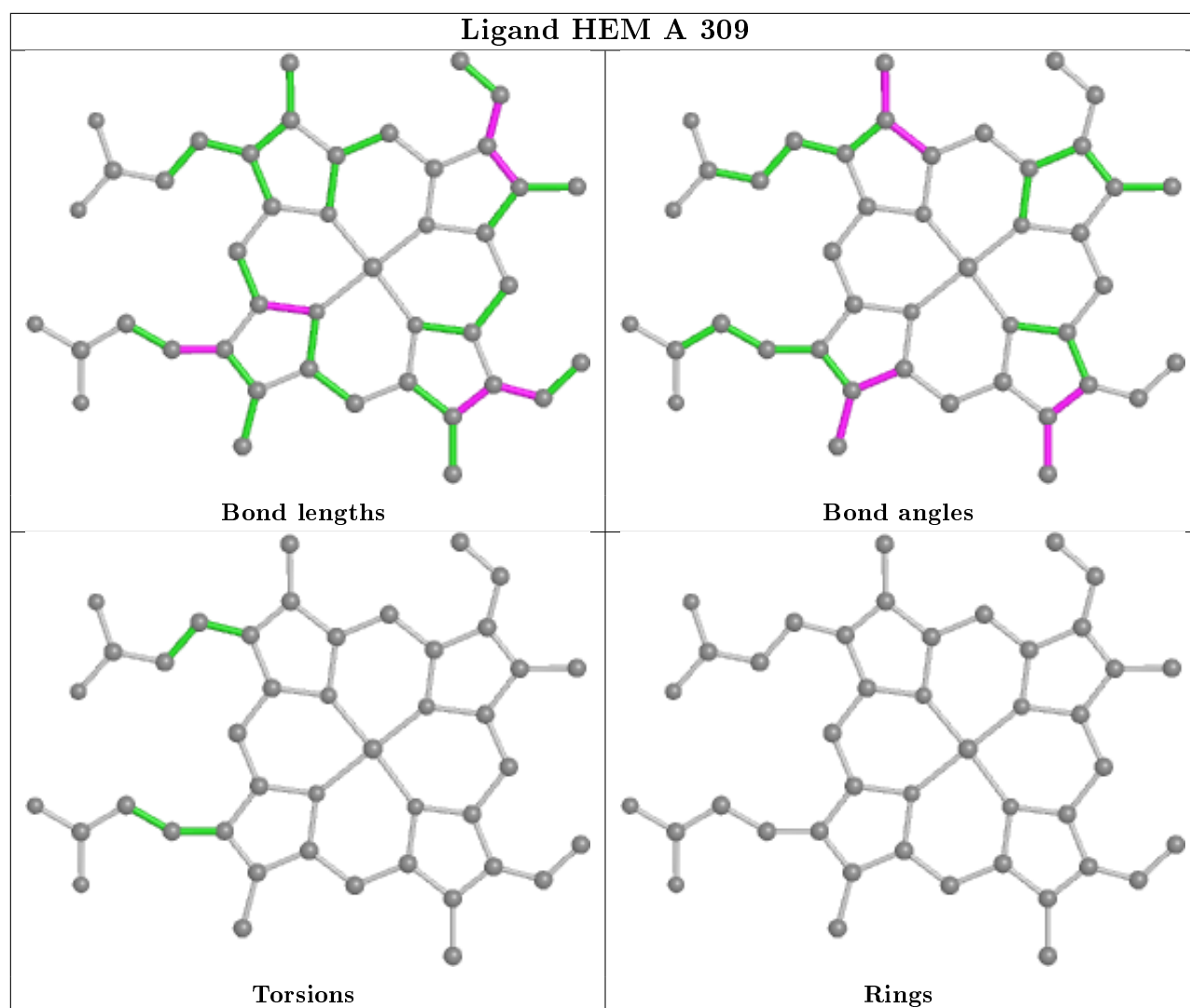












5.7 Other polymers [i](#)

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%)	-0.43	5 (1%) 70 66	10, 17, 31, 50	7 (2%)
1	B	292/292 (100%)	-0.27	6 (2%) 63 59	12, 21, 35, 58	16 (5%)
All	All	584/584 (100%)	-0.35	11 (1%) 66 63	10, 19, 32, 58	23 (3%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	ALA	5.1
1	A	1	ALA	3.9
1	A	292	ALA	3.7
1	A	89	ALA	3.2
1	B	291	ALA	2.8
1	A	291	ALA	2.5
1	B	45	ALA	2.5
1	B	254	PRO	2.4
1	A	91	GLY	2.4
1	B	91	GLY	2.3
1	B	120[A]	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

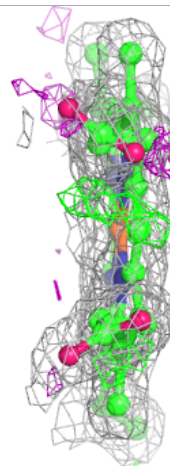
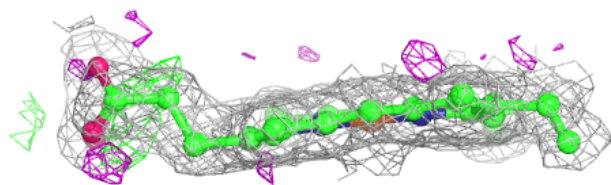
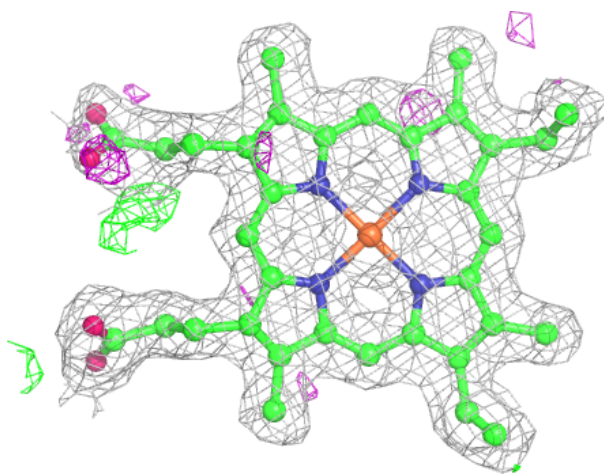
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.24	34,46,48,49	0
2	ACT	A	294	4/4	0.85	0.15	29,32,34,36	0
2	ACT	B	293	4/4	0.94	0.11	30,30,38,47	0
2	ACT	A	295	4/4	0.94	0.12	23,27,37,45	0
2	ACT	A	293	4/4	0.95	0.08	16,17,24,30	0
3	HEM	B	301	43/43	0.96	0.10	12,19,29,59	0
3	HEM	B	308	43/43	0.96	0.11	11,18,33,51	0
3	HEM	A	302	43/43	0.97	0.10	10,16,25,35	0
3	HEM	B	307	43/43	0.97	0.09	10,17,26,44	0
3	HEM	B	302	43/43	0.98	0.08	12,17,29,36	2
3	HEM	B	306	43/43	0.98	0.13	11,15,29,33	0
3	HEM	A	303	43/43	0.98	0.10	6,11,20,25	0
3	HEM	B	305	43/43	0.98	0.09	10,12,16,17	0
3	HEM	B	304	43/43	0.98	0.09	11,15,20,21	0
3	HEM	A	305	43/43	0.98	0.09	9,12,14,17	0
3	HEM	A	307	43/43	0.98	0.09	6,11,21,39	0
3	HEM	B	303	43/43	0.98	0.11	11,15,27,42	0
3	HEM	A	306	43/43	0.98	0.11	7,11,21,26	0
3	HEM	A	308	43/43	0.98	0.09	8,12,31,45	0
3	HEM	A	301	43/43	0.98	0.08	9,12,22,27	0
3	HEM	B	309	43/43	0.98	0.08	13,17,21,24	0
3	HEM	A	309	43/43	0.98	0.07	8,13,17,19	0
3	HEM	A	304	43/43	0.99	0.09	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.

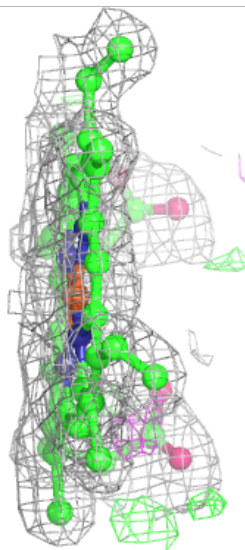
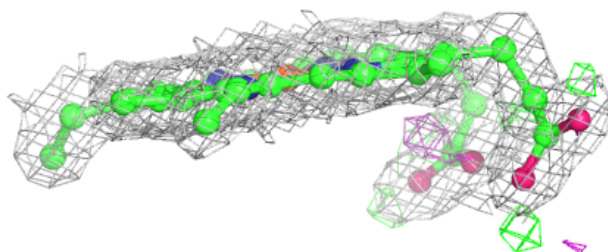
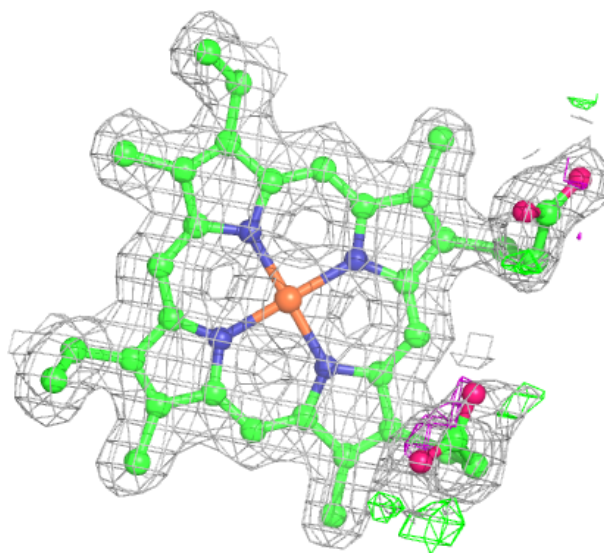
Electron density around HEM B 301:

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



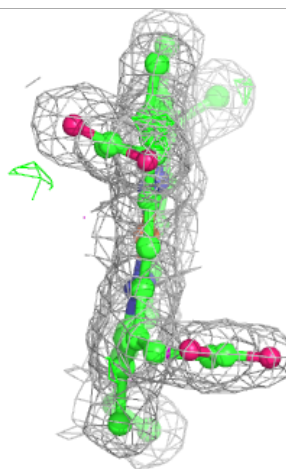
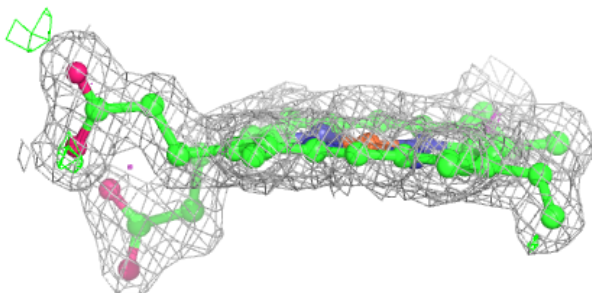
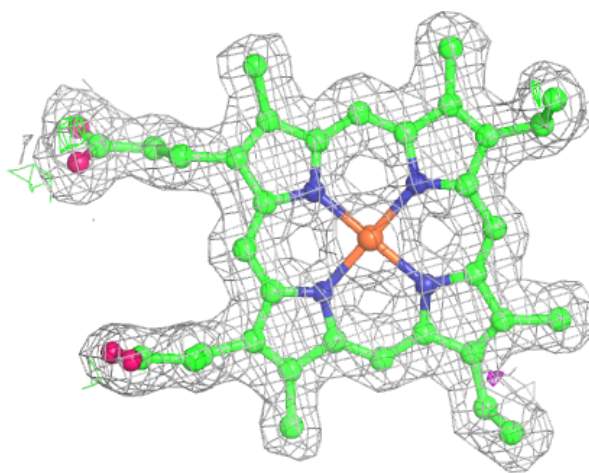
Electron density around HEM B 308:

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



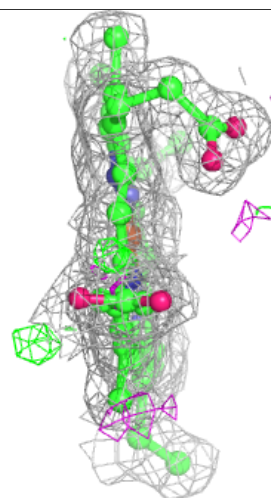
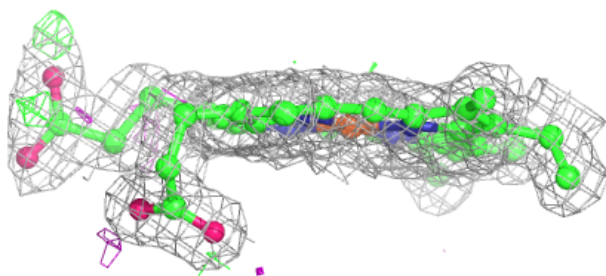
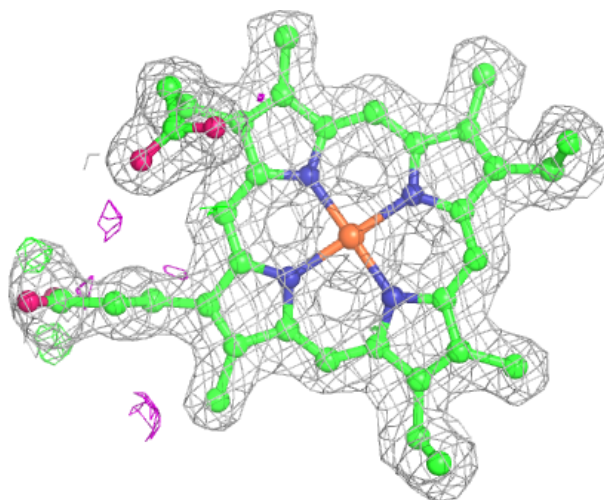
Electron density around HEM A 302:

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



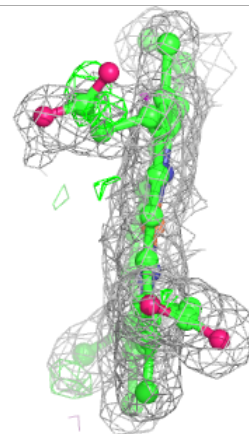
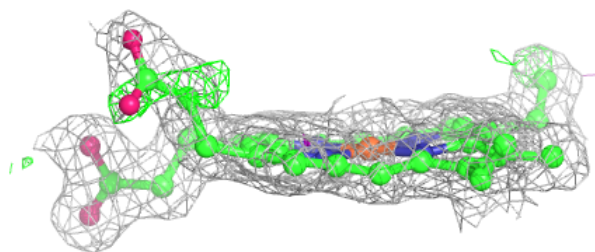
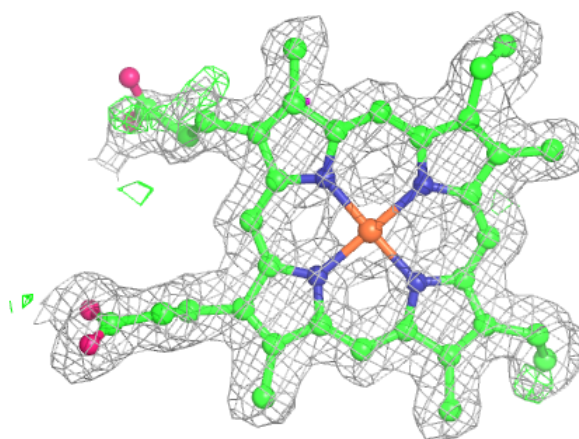
Electron density around HEM B 307:

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



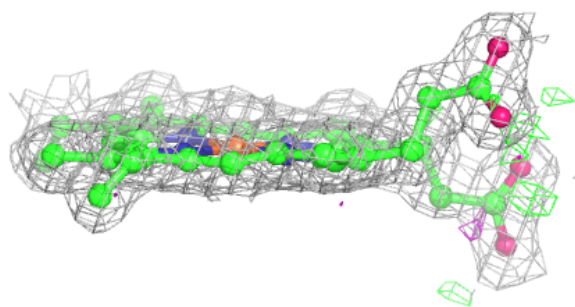
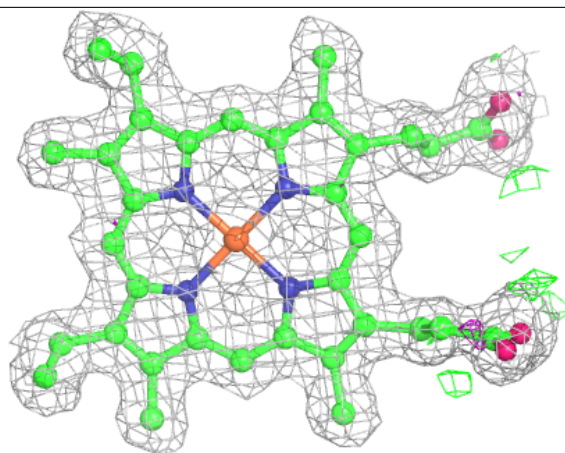
Electron density around HEM B 302:

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



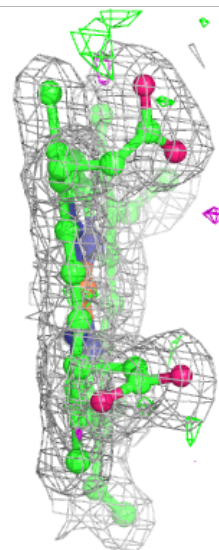
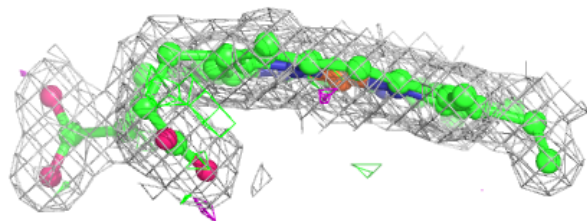
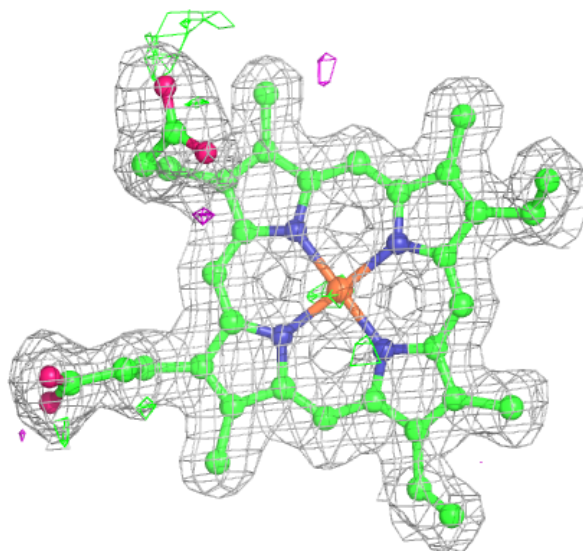
Electron density around HEM B 306:

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



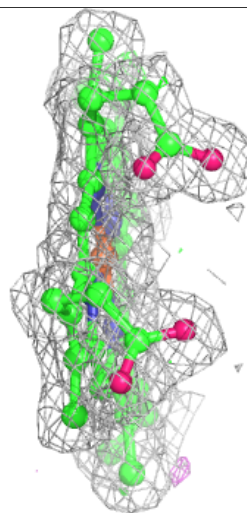
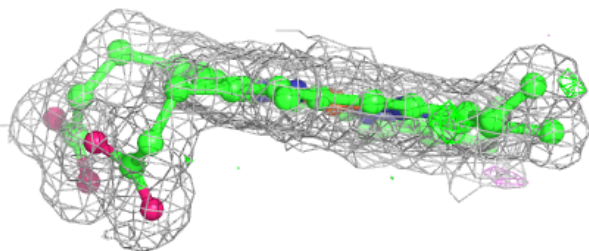
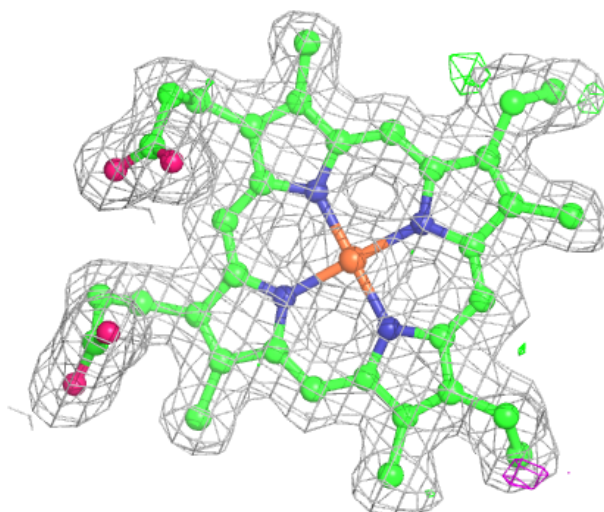
Electron density around HEM A 303:

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



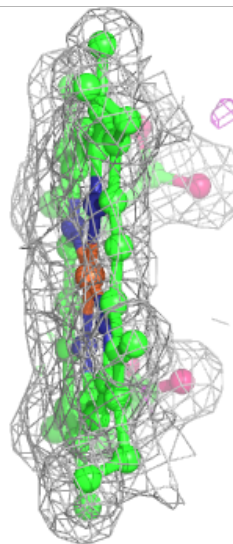
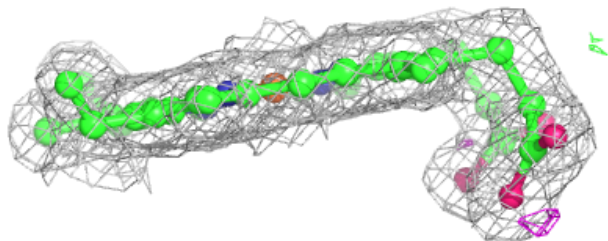
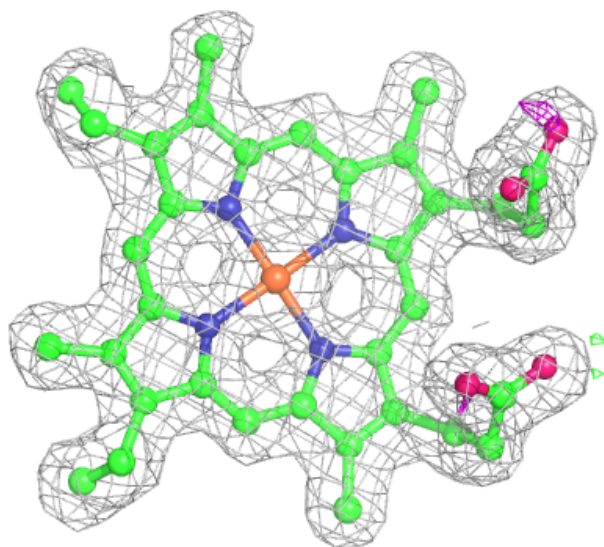
Electron density around HEM B 305:

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



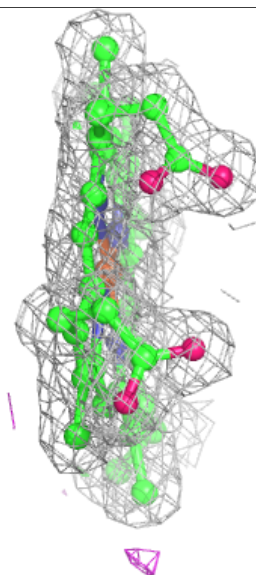
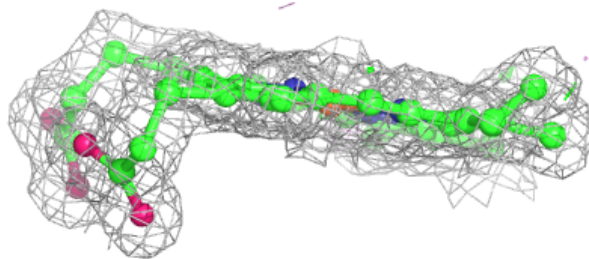
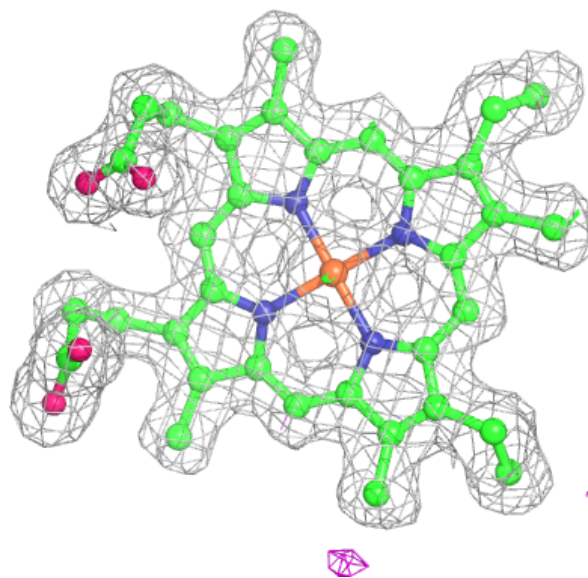
Electron density around HEM B 304:

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



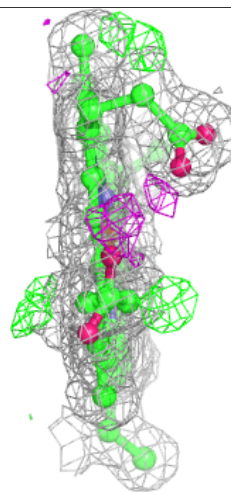
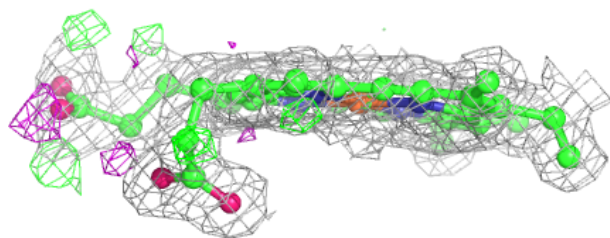
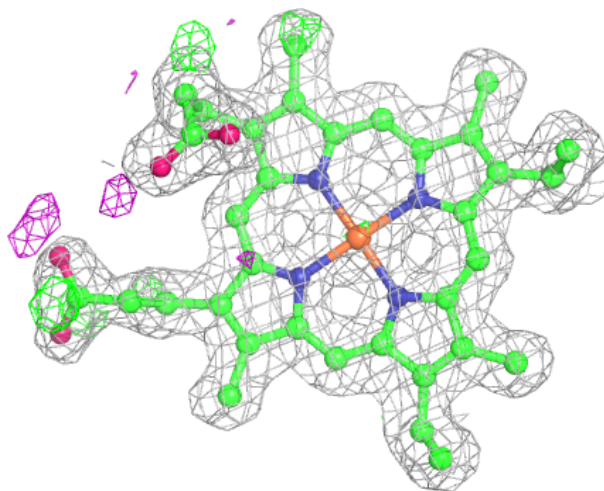
Electron density around HEM A 305:

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



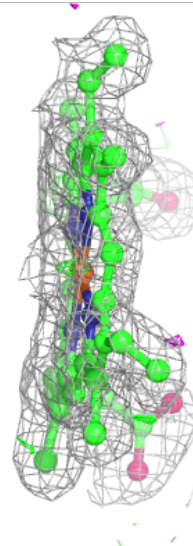
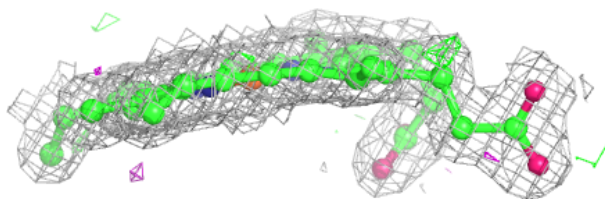
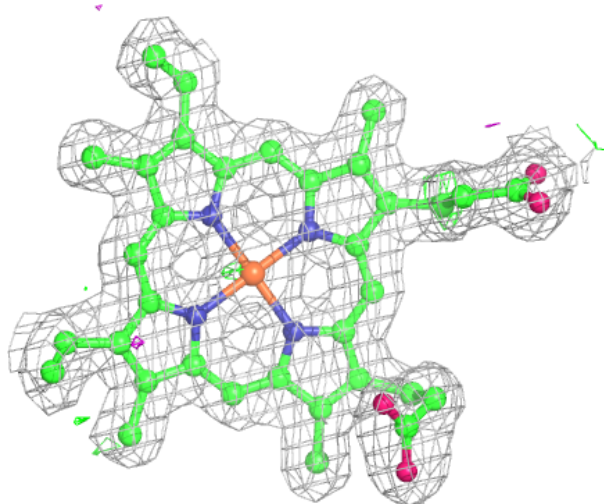
Electron density around HEM A 307:

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



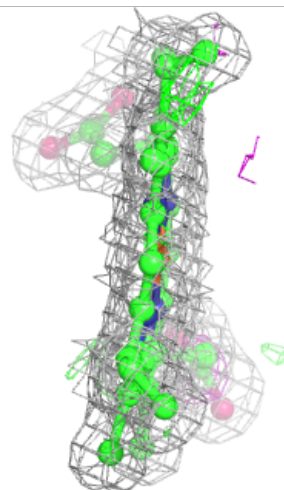
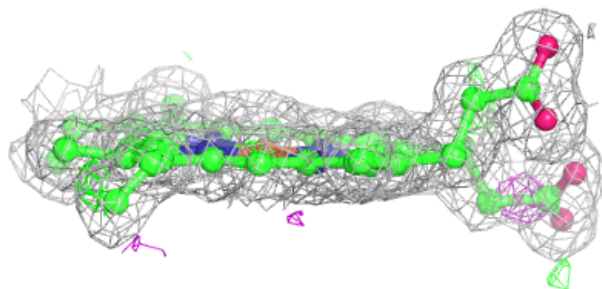
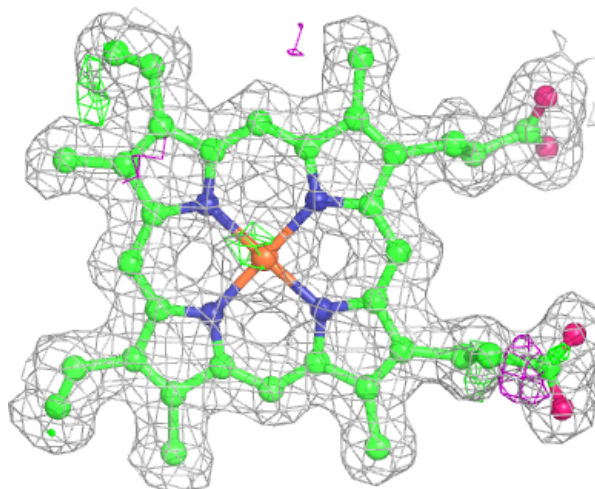
Electron density around HEM B 303:

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



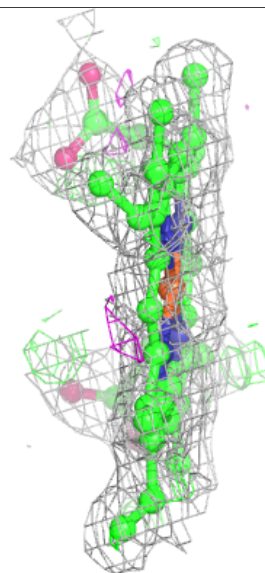
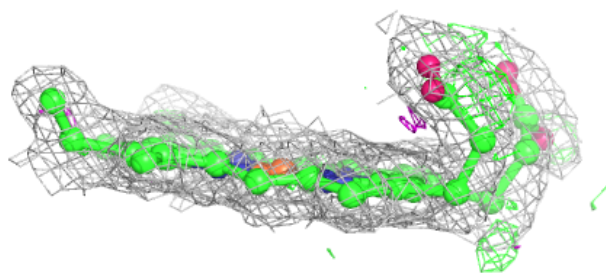
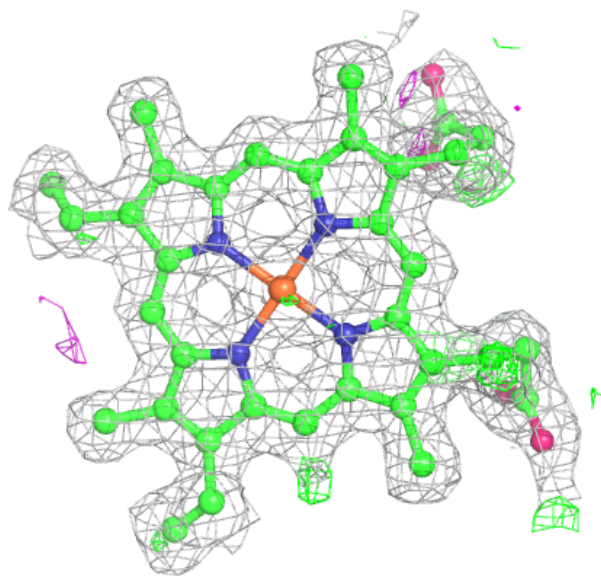
Electron density around HEM A 306:

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



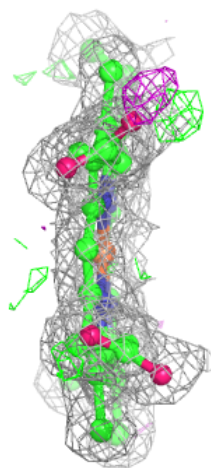
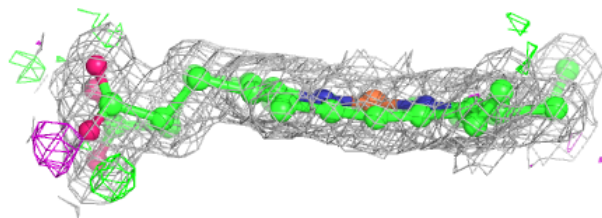
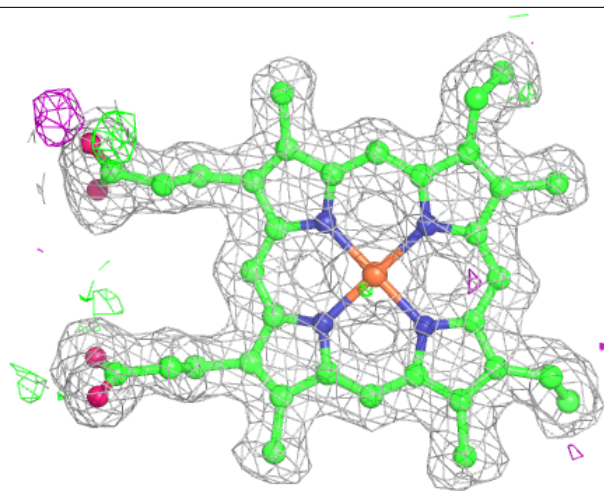
Electron density around HEM A 308:

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



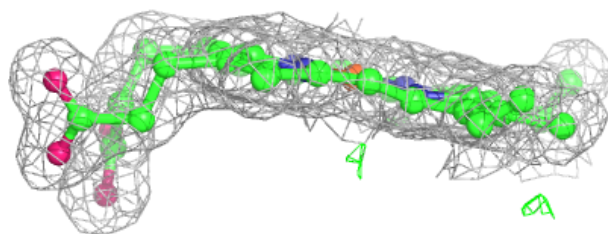
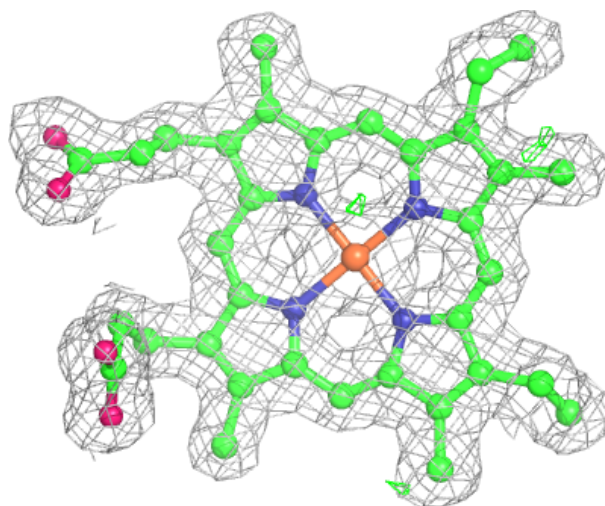
Electron density around HEM A 301:

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



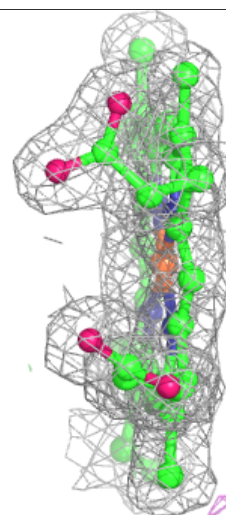
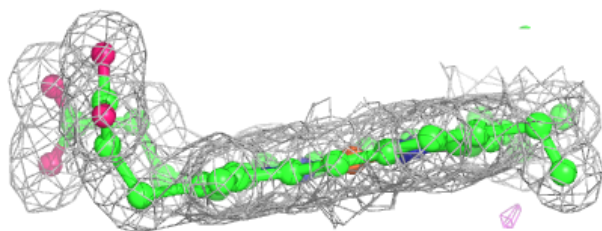
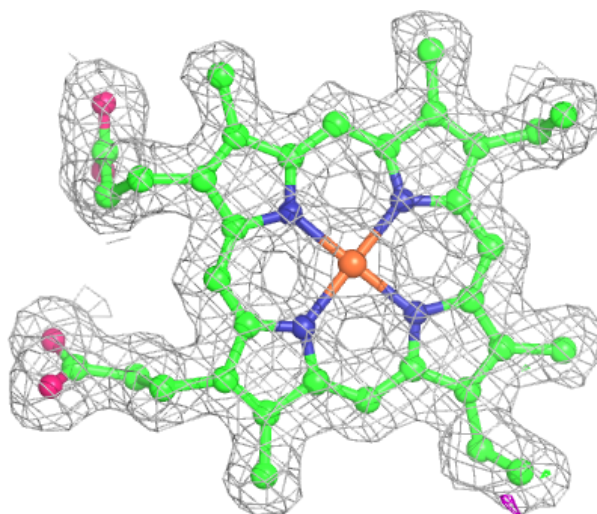
Electron density around HEM B 309:

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



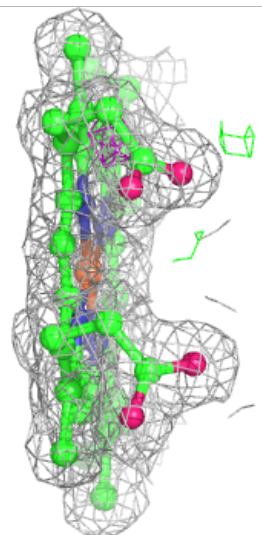
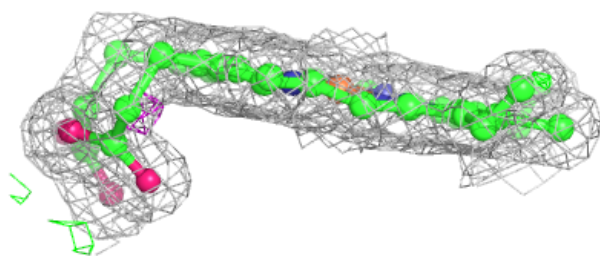
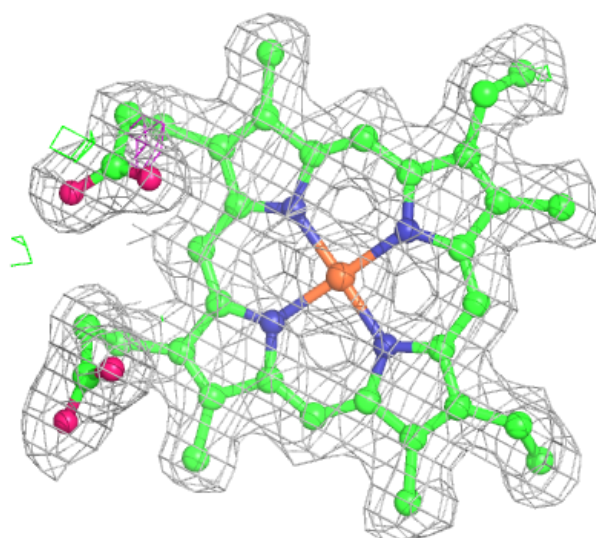
Electron density around HEM A 309:

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



Electron density around HEM A 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.