



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:15 PM UTC

PDB ID : 2Y3Q / pdb_00002y3q
Title : 1.55Å structure of apo bacterioferritin from E. coli
Authors : Hough, M.A.; Antonyuk, S.V.
Deposited on : 2010-12-22
Resolution : 1.55 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

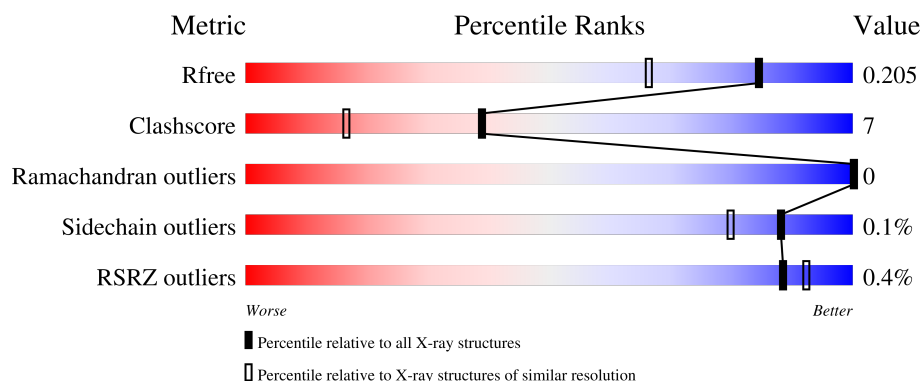
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	158	% 84% 16%
1	B	158	86% 14%
1	C	158	% 86% 14%
1	D	158	% 87% 12% .
1	E	158	89% 11% .

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Mol	Chain	Length	Quality of chain
1	F	158	% 87% 12% .
1	G	158	89% 11% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20288 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 BACTERIOFERRITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	15	1
			1394	879	231	277	7			
1	B	158	Total	C	N	O	S	0	17	1
			1403	887	234	275	7			
1	C	158	Total	C	N	O	S	0	15	1
			1383	876	229	271	7			
1	D	158	Total	C	N	O	S	0	13	1
			1371	868	230	266	7			
1	E	158	Total	C	N	O	S	0	14	1
			1381	874	229	271	7			
1	F	158	Total	C	N	O	S	0	16	1
			1400	883	236	274	7			
1	G	158	Total	C	N	O	S	0	16	1
			1393	881	233	272	7			
1	H	158	Total	C	N	O	S	0	13	1
			1379	868	232	272	7			
1	I	158	Total	C	N	O	S	0	16	1
			1388	877	232	272	7			
1	J	158	Total	C	N	O	S	0	12	1
			1365	863	227	268	7			
1	K	158	Total	C	N	O	S	0	14	1
			1373	868	228	270	7			
1	L	158	Total	C	N	O	S	0	11	1
			1361	860	228	266	7			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	B	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	C	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	D	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	G	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	H	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	I	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	J	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	K	1	Total 45	C 36	Fe 1	N 4	O 4	0	1
2	L	1	Total 45	C 36	Fe 1	N 4	O 4	0	1

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



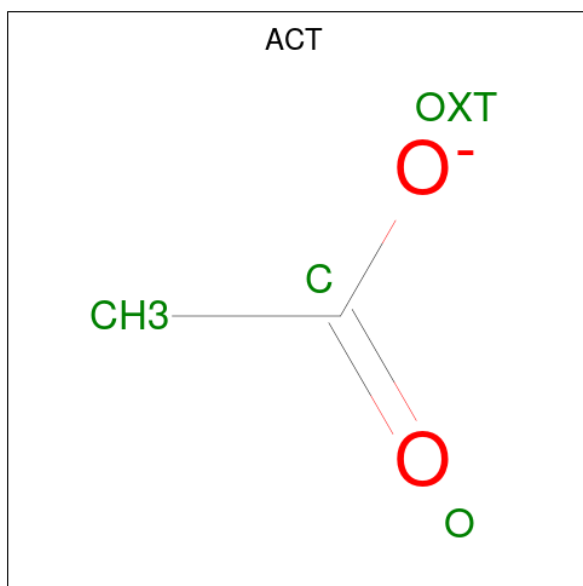
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



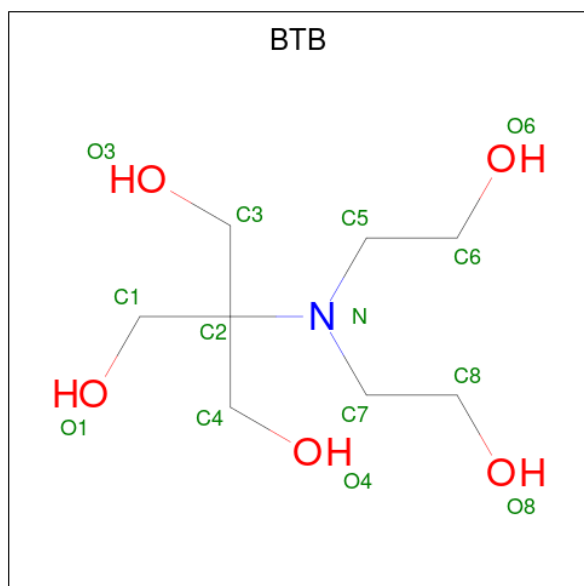
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			8	4	1	3		
5	I	1	Total	C	N	O	0	0
			8	4	1	3		
5	K	1	Total	C	N	O	0	0
			8	4	1	3		
5	L	1	Total	C	N	O	0	0
			8	4	1	3		

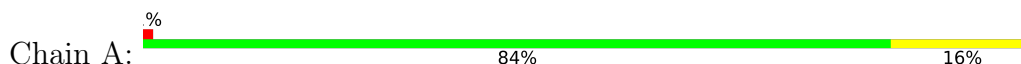
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	254	Total 256	O 256	0	2
6	B	235	Total 236	O 236	0	1
6	C	249	Total 251	O 251	0	2
6	D	247	Total 247	O 247	0	0
6	E	256	Total 257	O 257	0	1
6	F	243	Total 243	O 243	0	0
6	G	250	Total 250	O 250	0	0
6	H	245	Total 245	O 245	0	0
6	I	257	Total 257	O 257	0	0
6	J	254	Total 254	O 254	0	0
6	K	255	Total 255	O 255	0	0
6	L	233	Total 233	O 233	0	0

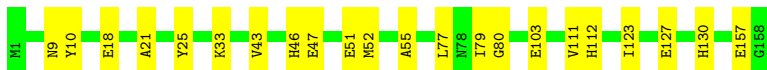
3 Residue-property plots [i](#)

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.

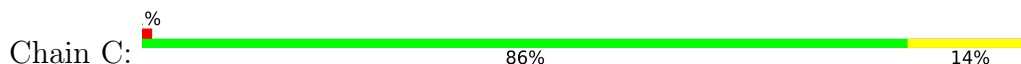
- Molecule 1: BACTERIOFERRITIN



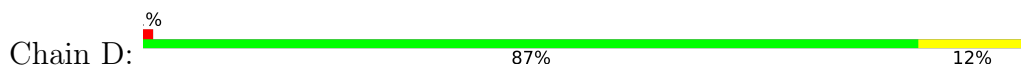
- Molecule 1: BACTERIOFERRITIN



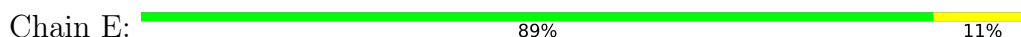
- Molecule 1: BACTERIOFERRITIN



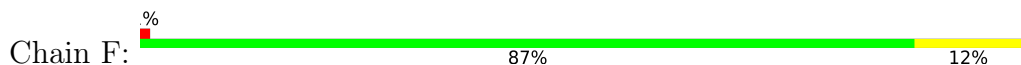
- Molecule 1: BACTERIOFERRITIN

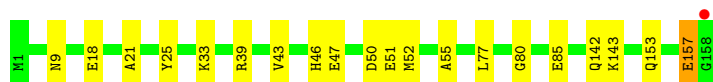


- Molecule 1: BACTERIOFERRITIN

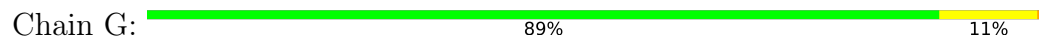


- Molecule 1: BACTERIOFERRITIN

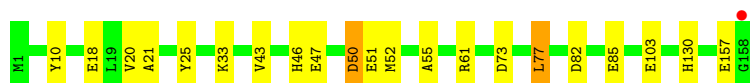
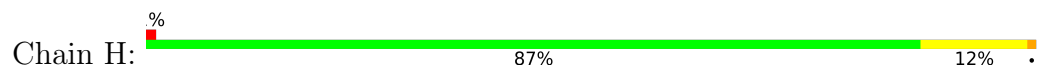




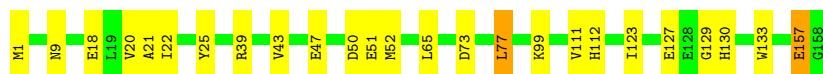
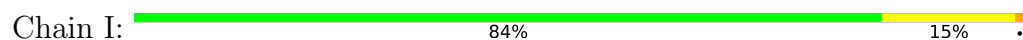
• Molecule 1: BACTERIOFERRITIN



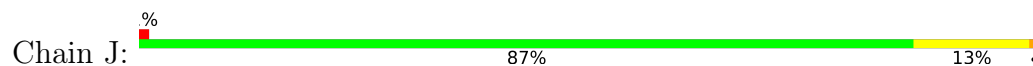
• Molecule 1: BACTERIOFERRITIN



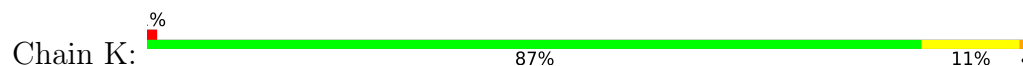
• Molecule 1: BACTERIOFERRITIN



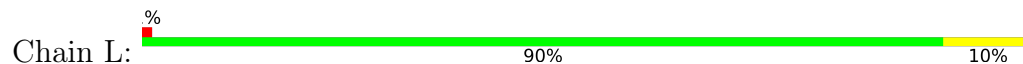
• Molecule 1: BACTERIOFERRITIN



• Molecule 1: BACTERIOFERRITIN



• Molecule 1: BACTERIOFERRITIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	208.00Å 208.00Å 142.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.23 – 1.55 43.23 – 1.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.23-1.55) 98.4 (43.23-1.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.55Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.165 , 0.200 0.174 , 0.205	Depositor DCC
R_{free} test set	21922 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20288	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3450e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, BTB, ACT, SO4

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	0.83	1/1448 (0.1%)	0.93	3/1949 (0.2%)
1	B	0.82	1/1464 (0.1%)	0.97	6/1970 (0.3%)
1	C	0.83	1/1444 (0.1%)	0.96	2/1944 (0.1%)
1	D	0.83	1/1427 (0.1%)	0.95	2/1921 (0.1%)
1	E	0.83	1/1441 (0.1%)	0.97	2/1938 (0.1%)
1	F	0.83	1/1456 (0.1%)	0.92	4/1958 (0.2%)
1	G	0.80	1/1448 (0.1%)	0.97	2/1949 (0.1%)
1	H	0.82	1/1422 (0.1%)	0.97	6/1915 (0.3%)
1	I	0.82	1/1449 (0.1%)	0.97	2/1952 (0.1%)
1	J	0.83	1/1418 (0.1%)	0.96	5/1908 (0.3%)
1	K	0.81	1/1436 (0.1%)	0.98	4/1934 (0.2%)
1	L	0.85	1/1409 (0.1%)	0.95	0/1896
All	All	0.83	12/17262 (0.1%)	0.96	38/23234 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	157	GLU	C-N	-8.11	1.22	1.33
1	F	157	GLU	C-N	-7.91	1.22	1.33
1	B	157	GLU	C-N	-7.90	1.22	1.33
1	L	157	GLU	C-N	-7.26	1.23	1.33
1	J	157	GLU	C-N	-7.25	1.23	1.33
1	K	157	GLU	C-N	-7.21	1.23	1.33
1	E	157	GLU	C-N	-7.13	1.23	1.33
1	C	157	GLU	C-N	-7.12	1.23	1.33
1	D	157	GLU	C-N	-7.06	1.23	1.33
1	A	157	GLU	C-N	-6.86	1.23	1.33
1	H	157	GLU	C-N	-6.37	1.24	1.33
1	G	157	GLU	C-N	-5.83	1.25	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77	LEU	CA-C-N	-6.00	114.31	122.95
1	D	77	LEU	C-N-CA	-6.00	114.31	122.95
1	I	77	LEU	CA-C-N	-5.88	114.48	122.95
1	I	77	LEU	C-N-CA	-5.88	114.48	122.95
1	J	77	LEU	CA-C-N	-5.87	114.19	123.23
1	J	77	LEU	C-N-CA	-5.87	114.19	123.23
1	H	77	LEU	CA-C-N	-5.84	114.23	123.23
1	H	77	LEU	C-N-CA	-5.84	114.23	123.23
1	E	77	LEU	CA-C-N	-5.84	114.24	123.23
1	E	77	LEU	C-N-CA	-5.84	114.24	123.23
1	K	80	GLY	CA-C-N	-5.82	113.08	121.98
1	K	80	GLY	C-N-CA	-5.82	113.08	121.98
1	F	77	LEU	CA-C-N	-5.77	114.35	123.23
1	F	77	LEU	C-N-CA	-5.77	114.35	123.23
1	A	80	GLY	CA-C-N	-5.72	113.23	121.98
1	A	80	GLY	C-N-CA	-5.72	113.23	121.98
1	G	80	GLY	CA-C-N	-5.68	113.29	121.98
1	G	80	GLY	C-N-CA	-5.68	113.29	121.98
1	B	80	GLY	CA-C-N	-5.65	113.34	121.98
1	B	80	GLY	C-N-CA	-5.65	113.34	121.98
1	K	77	LEU	CA-C-N	-5.64	114.55	123.23
1	K	77	LEU	C-N-CA	-5.64	114.55	123.23
1	C	77	LEU	CA-C-N	-5.57	114.66	123.23
1	C	77	LEU	C-N-CA	-5.57	114.66	123.23
1	A	79	ILE	N-CA-C	5.50	115.69	110.53
1	H	50[A]	ASP	CA-C-N	-5.46	112.02	120.31
1	H	50[A]	ASP	C-N-CA	-5.46	112.02	120.31
1	H	50[B]	ASP	CA-C-N	-5.46	112.02	120.31
1	H	50[B]	ASP	C-N-CA	-5.46	112.02	120.31
1	J	109	ASP	O-C-N	5.37	127.60	122.07
1	B	79	ILE	CA-C-N	-5.35	114.31	122.06
1	B	79	ILE	C-N-CA	-5.35	114.31	122.06
1	F	80	GLY	CA-C-N	-5.14	114.11	121.98
1	F	80	GLY	C-N-CA	-5.14	114.11	121.98
1	B	77	LEU	CA-C-N	-5.13	115.33	123.23
1	B	77	LEU	C-N-CA	-5.13	115.33	123.23
1	J	49	ILE	CA-C-N	-5.05	113.51	120.28
1	J	49	ILE	C-N-CA	-5.05	113.51	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1394	0	1357	19	0
1	B	1403	0	1374	22	0
1	C	1383	0	1353	16	0
1	D	1371	0	1342	19	0
1	E	1381	0	1363	16	0
1	F	1400	0	1376	17	0
1	G	1393	0	1363	19	0
1	H	1379	0	1332	22	0
1	I	1388	0	1359	31	0
1	J	1365	0	1336	16	0
1	K	1373	0	1345	17	0
1	L	1361	0	1338	13	1
2	A	45	0	6	1	0
2	B	45	0	6	0	0
2	C	45	0	6	0	0
2	D	45	0	6	0	0
2	E	43	0	30	0	0
2	F	45	0	6	2	0
2	G	45	0	6	0	0
2	H	45	0	6	2	0
2	I	45	0	6	0	0
2	J	45	0	6	1	0
2	K	45	0	6	0	0
2	L	45	0	6	0	0
3	A	5	0	0	1	0
3	B	15	0	0	1	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	1	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	10	0	0	1	0
3	I	10	0	0	0	0
3	J	5	0	0	1	0
3	K	5	0	0	1	0
3	L	5	0	0	1	0
4	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	3	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
4	E	4	0	3	0	0
4	F	4	0	3	0	0
4	G	4	0	3	0	0
4	H	4	0	3	0	0
4	I	4	0	3	0	0
4	J	4	0	3	0	0
4	K	4	0	3	0	0
4	L	4	0	3	0	0
5	D	8	0	9	3	0
5	I	8	0	9	1	0
5	K	8	0	9	0	0
5	L	8	0	9	3	0
6	A	256	0	0	5	1
6	B	236	0	0	12	0
6	C	251	0	0	3	0
6	D	247	0	0	8	0
6	E	257	0	0	5	0
6	F	243	0	0	6	2
6	G	250	0	0	10	1
6	H	245	0	0	6	0
6	I	257	0	0	8	0
6	J	254	0	0	6	0
6	K	255	0	0	8	1
6	L	233	0	0	4	2
All	All	20288	0	16406	232	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (232) 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:C:33[A]:LYS:NZ	6:C:2077:HOH:O	1.71	1.17
3:H:1160:SO4:O4	6:H:2244:HOH:O	1.61	1.16
1:B:33[B]:LYS:NZ	6:B:2063:HOH:O	1.80	1.13
1:A:33[B]:LYS:NZ	6:A:2077:HOH:O	1.87	1.07
1:L:33[B]:LYS:NZ	6:L:2063:HOH:O	1.86	1.07
1:J:33:LYS:NZ	6:J:2077:HOH:O	1.89	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9[A]:ASN:ND2	6:F:2018:HOH:O	1.88	1.04
1:G:33[B]:LYS:NZ	6:G:2078:HOH:O	1.93	1.01
1:A:9[A]:ASN:ND2	6:A:2024:HOH:O	1.94	1.00
1:B:103[B]:GLU:CD	6:B:2165:HOH:O	2.02	0.99
1:G:112[B]:HIS:CD2	6:G:2200:HOH:O	2.15	0.98
1:I:9[A]:ASN:OD1	6:I:2020:HOH:O	1.81	0.98
1:H:33[A]:LYS:NZ	6:H:2071:HOH:O	1.97	0.97
3:K:1159:SO4:O2	6:K:2251:HOH:O	1.82	0.97
1:G:112[B]:HIS:HD2	6:G:2200:HOH:O	1.45	0.95
1:J:9[A]:ASN:ND2	6:J:2024:HOH:O	2.01	0.92
1:I:22[A]:ILE:HD11	1:I:52:MET:N	1.84	0.92
1:K:18:GLU:OE1	1:K:51[B]:GLU:OE1	1.89	0.91
1:B:103[B]:GLU:OE1	6:B:2165:HOH:O	1.88	0.91
1:A:18:GLU:OE1	1:A:51[B]:GLU:OE1	1.89	0.90
1:E:18:GLU:OE1	1:E:51[B]:GLU:OE1	1.90	0.90
1:G:50[B]:ASP:OD1	6:G:2112:HOH:O	1.89	0.89
1:D:9[A]:ASN:OD1	6:D:2027:HOH:O	1.90	0.88
1:F:18:GLU:OE1	1:F:51[B]:GLU:OE1	1.93	0.87
3:B:1161:SO4:O3	6:B:2234:HOH:O	1.92	0.87
1:I:112[A]:HIS:HD2	6:I:2196:HOH:O	1.58	0.86
1:H:50[B]:ASP:OD1	6:H:2111:HOH:O	1.92	0.86
1:B:9[B]:ASN:OD1	6:B:2017:HOH:O	1.94	0.85
3:E:1160:SO4:O2	6:E:2253:HOH:O	1.95	0.83
1:I:18:GLU:OE1	1:I:51[B]:GLU:OE1	1.96	0.83
1:A:50[A]:ASP:OD1	6:A:2111:HOH:O	1.97	0.82
1:I:112[A]:HIS:CD2	6:I:2196:HOH:O	2.30	0.82
1:D:47[A]:GLU:OE1	1:D:130:HIS:CD2	2.33	0.81
1:I:22[A]:ILE:HD12	1:I:52:MET:HG3	1.62	0.81
1:I:50[B]:ASP:OD1	6:I:2106:HOH:O	1.97	0.81
1:I:22[A]:ILE:CD1	1:I:52:MET:N	2.43	0.80
1:H:18:GLU:OE1	1:H:51[B]:GLU:OE1	2.00	0.78
1:B:9[B]:ASN:ND2	6:B:2016:HOH:O	1.92	0.78
1:I:22[A]:ILE:HD12	1:I:52:MET:CG	2.14	0.77
1:B:18:GLU:OE1	1:B:51[B]:GLU:OE1	2.03	0.77
1:B:9[B]:ASN:ND2	6:B:2020:HOH:O	2.17	0.76
1:H:50[A]:ASP:OD1	6:H:2112:HOH:O	2.03	0.76
1:I:99:LYS:HE3	6:I:2175:HOH:O	1.85	0.76
1:K:50[A]:ASP:OD1	6:K:2108:HOH:O	2.03	0.76
1:C:18:GLU:OE1	1:C:51[B]:GLU:OE1	2.05	0.75
1:J:39[A]:ARG:HD3	1:J:153:GLN:OE1	1.86	0.75
1:L:50[B]:ASP:OD1	6:L:2089:HOH:O	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50[B]:ASP:OD1	6:E:2110:HOH:O	2.05	0.74
1:E:76:LYS:HE2	1:E:77:LEU:O	1.88	0.74
1:K:9[A]:ASN:OD1	6:K:2026:HOH:O	2.06	0.74
1:L:18:GLU:OE1	1:L:51[B]:GLU:OE1	2.05	0.73
1:B:103[B]:GLU:OE2	6:B:2165:HOH:O	2.04	0.73
1:J:18:GLU:OE1	1:J:51[B]:GLU:OE1	2.07	0.72
1:I:22[A]:ILE:HD13	1:I:51[A]:GLU:HB2	1.72	0.71
1:D:39[B]:ARG:NH2	1:D:157:GLU:OE1	2.22	0.71
1:J:50[A]:ASP:OD1	6:J:2110:HOH:O	2.10	0.70
1:C:46[B]:HIS:CD2	6:C:2101:HOH:O	2.44	0.70
1:F:50[B]:ASP:OD1	6:F:2099:HOH:O	2.08	0.69
1:D:18:GLU:OE1	1:D:51[B]:GLU:OE1	2.13	0.67
1:I:50[A]:ASP:OD1	6:I:2105:HOH:O	2.12	0.67
1:K:73[A]:ASP:O	6:K:2141:HOH:O	2.12	0.67
1:D:46[A]:HIS:NE2	6:D:2106:HOH:O	2.03	0.66
1:J:39[B]:ARG:CZ	6:J:2091:HOH:O	2.45	0.65
1:D:21:ALA:HB1	1:D:25[B]:TYR:CE2	2.30	0.65
1:D:39[B]:ARG:NE	1:D:157:GLU:OE1	2.30	0.64
1:D:47[A]:GLU:OE1	1:D:130:HIS:NE2	2.31	0.63
1:G:33[B]:LYS:HD3	6:G:2030:HOH:O	1.98	0.63
5:D:1161:BTB:C4	6:D:2246:HOH:O	2.45	0.63
1:D:9[B]:ASN:ND2	6:D:2028:HOH:O	2.30	0.63
1:H:61:ARG:HH11	5:L:1161:BTB:H31	1.63	0.62
6:E:2125:HOH:O	1:F:33[A]:LYS:HE3	1.99	0.61
1:F:55:ALA:HB3	2:F:200[A]:HEM:CBC	2.32	0.60
1:K:43:VAL:O	1:K:47[A]:GLU:HG2	2.03	0.58
1:I:18:GLU:O	1:I:22[A]:ILE:HG12	2.03	0.58
1:C:82[A]:ASP:OD1	1:C:85[A]:GLU:HG3	2.04	0.58
1:G:39:ARG:NH2	1:G:157:GLU:OE1	2.36	0.57
1:B:51[B]:GLU:OE2	1:B:130:HIS:CE1	2.57	0.57
1:F:55:ALA:HB3	2:F:200[A]:HEM:HBC2	1.86	0.56
1:H:61:ARG:HH11	5:L:1161:BTB:C3	2.19	0.56
1:J:55:ALA:HB3	2:J:200[A]:HEM:CBC	2.35	0.56
1:C:10:TYR:OH	1:C:103[C]:GLU:HG2	2.06	0.56
1:G:112[B]:HIS:CD2	6:G:2202:HOH:O	2.59	0.56
1:L:47[A]:GLU:OE1	1:L:130:HIS:CD2	2.59	0.55
1:F:142[A]:GLN:HG2	6:F:2219:HOH:O	2.05	0.55
1:D:33[B]:LYS:HG3	6:D:2085:HOH:O	2.05	0.55
1:E:10:TYR:OH	1:E:103[B]:GLU:HG2	2.05	0.55
1:H:73[A]:ASP:O	6:H:2146:HOH:O	2.17	0.55
1:H:46[A]:HIS:HD2	6:H:2102:HOH:O	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:OD2	1:A:156[A]:GLU:OE2	2.26	0.54
1:J:50[A]:ASP:CG	6:J:2110:HOH:O	2.51	0.54
1:H:61:ARG:NH1	5:L:1161:BTB:H31	2.23	0.54
1:D:20:VAL:HG13	1:D:77:LEU:HD23	1.89	0.53
5:D:1161:BTB:H41	6:D:2246:HOH:O	2.06	0.53
1:L:51[B]:GLU:OE2	1:L:130:HIS:CE1	2.61	0.53
1:H:55:ALA:HB3	2:H:200[A]:HEM:HBC2	1.91	0.52
1:A:43:VAL:O	1:A:47[A]:GLU:HG2	2.10	0.52
1:H:43:VAL:O	1:H:47[A]:GLU:HG2	2.09	0.52
1:G:143:LYS:HE2	6:G:2111:HOH:O	2.10	0.52
1:B:10:TYR:OH	1:B:103[A]:GLU:HG2	2.09	0.52
1:K:20:VAL:HG13	1:K:77:LEU:HD23	1.92	0.52
1:G:33[A]:LYS:HG3	6:G:2077:HOH:O	2.11	0.51
1:D:39[B]:ARG:CZ	1:D:157:GLU:OE1	2.58	0.51
1:G:39:ARG:NE	1:G:157:GLU:OE1	2.41	0.51
1:C:43:VAL:O	1:C:47[A]:GLU:HG2	2.10	0.51
1:K:99:LYS:HE3	6:K:2176:HOH:O	2.10	0.51
1:K:50[B]:ASP:OD1	6:K:2109:HOH:O	2.18	0.51
1:I:22[A]:ILE:CD1	1:I:51[A]:GLU:HB2	2.41	0.50
1:J:142:GLN:CD	1:J:142:GLN:C	2.80	0.50
1:H:82:ASP:OD1	1:H:85[B]:GLU:HG3	2.11	0.50
1:K:39[B]:ARG:NE	1:K:157:GLU:OE1	2.41	0.50
1:B:51[B]:GLU:OE2	1:B:130:HIS:HE1	1.94	0.50
1:H:82:ASP:CG	1:H:85[B]:GLU:HG3	2.37	0.50
1:L:43:VAL:O	1:L:47[A]:GLU:HG2	2.12	0.49
1:I:73[A]:ASP:O	6:I:2142:HOH:O	2.19	0.49
1:D:43:VAL:O	1:D:47[A]:GLU:HG2	2.13	0.49
1:H:55:ALA:HB3	2:H:200[A]:HEM:CB	2.42	0.49
1:I:129:GLY:HA2	5:I:1162:BTB:H12	1.95	0.49
1:A:144:MET:HE1	1:J:154:ILE:HD13	1.94	0.48
1:B:9[B]:ASN:CG	6:B:2016:HOH:O	2.47	0.48
1:B:43:VAL:O	1:B:47[A]:GLU:HG2	2.13	0.48
1:G:142[B]:GLN:HG2	6:G:2229:HOH:O	2.13	0.48
1:E:20:VAL:HG13	1:E:77:LEU:HD23	1.95	0.48
1:E:43:VAL:O	1:E:47[A]:GLU:HG2	2.13	0.48
1:F:43:VAL:O	1:F:47[A]:GLU:HG2	2.14	0.48
1:L:46[A]:HIS:CE1	6:L:2085:HOH:O	2.66	0.48
1:L:21:ALA:HB1	1:L:25[B]:TYR:CE2	2.49	0.48
1:B:21:ALA:HB1	1:B:25[B]:TYR:CE2	2.49	0.48
1:E:82[A]:ASP:OD2	1:E:85[A]:GLU:CD	2.57	0.48
1:I:73[A]:ASP:OD2	6:I:2136:HOH:O	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:ALA:HB1	1:K:25[B]:TYR:CE2	2.49	0.48
1:L:51[B]:GLU:OE2	1:L:130:HIS:HE1	1.97	0.48
1:A:155:ARG:NH2	1:D:39[B]:ARG:HD2	2.29	0.47
1:I:22[A]:ILE:HD11	1:I:52:MET:CA	2.45	0.47
1:C:39:ARG:HD3	1:C:153:GLN:OE1	2.15	0.47
1:I:20:VAL:HG13	1:I:77:LEU:HD23	1.97	0.47
1:I:21:ALA:HB1	1:I:25[B]:TYR:CE2	2.50	0.47
1:H:51[B]:GLU:OE2	1:H:130:HIS:CE1	2.68	0.46
1:L:20:VAL:HG13	1:L:77:LEU:HD23	1.96	0.46
1:C:33[A]:LYS:HG3	6:C:2074:HOH:O	2.16	0.46
1:J:43:VAL:O	1:J:47[A]:GLU:HG2	2.16	0.46
1:C:111:VAL:O	1:C:112[B]:HIS:HB2	2.15	0.46
1:H:82:ASP:OD2	1:H:85[B]:GLU:HG3	2.15	0.46
1:J:39[B]:ARG:HD3	1:J:153:GLN:OE1	2.15	0.46
1:K:39[B]:ARG:NH2	1:K:157:GLU:OE1	2.47	0.46
1:K:46:HIS:CD2	6:K:2101:HOH:O	2.68	0.46
1:F:21:ALA:HB1	1:F:25[B]:TYR:CE2	2.51	0.45
1:G:43:VAL:HG11	1:G:133:TRP:CE2	2.50	0.45
3:L:1159:SO4:O4	6:L:2229:HOH:O	2.21	0.45
1:E:51[B]:GLU:OE2	1:E:130:HIS:HE1	1.98	0.45
1:F:46[B]:HIS:CD2	6:F:2095:HOH:O	2.69	0.45
1:A:43:VAL:HG11	1:A:133:TRP:CE2	2.52	0.45
1:A:147:GLN:HG3	3:A:1159:SO4:O3	2.17	0.45
1:G:43:VAL:O	1:G:47[A]:GLU:HG2	2.17	0.45
1:J:21:ALA:HB1	1:J:25[B]:TYR:CE2	2.52	0.45
1:I:1:MET:O	1:I:65:LEU:HA	2.17	0.45
1:I:39[B]:ARG:NE	1:I:157:GLU:OE1	2.45	0.45
1:C:53:LYS:CE	6:D:2241:HOH:O	2.64	0.44
1:C:21:ALA:HB1	1:C:25[B]:TYR:CE2	2.53	0.44
1:G:20:VAL:HG13	1:G:77:LEU:HD23	1.98	0.44
1:G:21:ALA:HB1	1:G:25[B]:TYR:CE2	2.51	0.44
1:G:33[B]:LYS:CD	6:G:2030:HOH:O	2.61	0.44
1:J:46[B]:HIS:CE1	6:J:2100:HOH:O	2.70	0.44
1:A:123:ILE:O	1:A:127[A]:GLU:HG2	2.18	0.44
1:K:109:ASP:OD1	6:K:2189:HOH:O	2.21	0.44
2:A:200[A]:HEM:CBC	1:B:55:ALA:HB3	2.48	0.43
1:E:51[B]:GLU:OE2	1:E:130:HIS:CE1	2.70	0.43
1:A:20:VAL:HG13	1:A:77:LEU:HD23	1.99	0.43
1:I:111:VAL:O	1:I:112[B]:HIS:HB2	2.19	0.43
1:B:33[B]:LYS:HG3	6:B:2064:HOH:O	2.19	0.43
1:C:155:ARG:NH2	1:F:39[B]:ARG:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51[B]:GLU:OE2	1:C:130:HIS:CE1	2.72	0.43
1:A:21:ALA:HB1	1:A:25[B]:TYR:CE2	2.55	0.42
1:E:76:LYS:HA	1:E:76:LYS:HD2	1.90	0.42
1:B:123:ILE:O	1:B:127[B]:GLU:HG2	2.19	0.42
1:D:43:VAL:HG11	1:D:133:TRP:CE2	2.54	0.42
1:H:51[B]:GLU:OE2	1:H:130:HIS:HE1	2.03	0.42
1:J:147:GLN:HG3	3:J:1159:SO4:O1	2.19	0.42
1:D:29:ALA:HB2	1:D:44[B]:GLU:HB3	2.00	0.42
1:A:33[B]:LYS:HG3	6:A:2093:HOH:O	2.20	0.42
5:D:1161:BTB:H42	6:D:2246:HOH:O	2.17	0.42
1:E:21:ALA:HB1	1:E:25[B]:TYR:CE2	2.54	0.42
1:F:39[B]:ARG:NE	1:F:157:GLU:OE1	2.45	0.42
1:G:123:ILE:O	1:G:127:GLU:HG2	2.20	0.42
1:A:130:HIS:HD2	6:A:2107:HOH:O	2.03	0.42
1:E:112:HIS:HD2	6:E:2198:HOH:O	2.02	0.42
1:H:21:ALA:HB1	1:H:25[C]:TYR:CE2	2.55	0.42
1:B:47[A]:GLU:OE2	6:B:2098:HOH:O	2.22	0.41
1:B:111:VAL:O	1:B:112[B]:HIS:HB2	2.20	0.41
1:D:123:ILE:O	1:D:127:GLU:HG2	2.21	0.41
1:I:43:VAL:O	1:I:47[A]:GLU:HG2	2.20	0.41
1:A:47[A]:GLU:OE1	1:A:130:HIS:CD2	2.73	0.41
1:K:32:PHE:CD2	1:K:40:LEU:HB3	2.56	0.41
1:B:46[A]:HIS:CE1	6:B:2094:HOH:O	2.73	0.41
1:F:39[A]:ARG:HD3	1:F:153:GLN:OE1	2.20	0.41
1:F:85[B]:GLU:HG3	6:F:2149:HOH:O	2.20	0.41
1:F:143[A]:LYS:HE2	6:F:2224:HOH:O	2.20	0.41
1:H:20:VAL:HG13	1:H:77:LEU:HD23	2.01	0.41
1:J:144:MET:HE2	1:J:144:MET:HB3	1.94	0.41
1:H:10:TYR:OH	1:H:103[B]:GLU:HG2	2.22	0.40
1:E:85[A]:GLU:HG3	6:E:2162:HOH:O	2.19	0.40
1:I:51[B]:GLU:OE2	1:I:130:HIS:CE1	2.74	0.40
1:D:144:MET:HE2	1:D:144:MET:HB3	1.93	0.40
1:I:43:VAL:HG11	1:I:133:TRP:CE2	2.57	0.40
1:I:22[A]:ILE:HD12	1:I:52:MET:HG2	1.99	0.40
1:I:123:ILE:O	1:I:127[A]:GLU:HG2	2.20	0.40
1:L:43:VAL:HG11	1:L:133:TRP:CE2	2.56	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:2230:HOH:O	6:L:2075:HOH:O[8_665]	1.52	0.68
1:L:6:LYS:CE	6:F:2007:HOH:O[5_555]	1.96	0.24
6:F:2185:HOH:O	6:L:2170:HOH:O[5_545]	2.14	0.06
6:A:2190:HOH:O	6:K:2193:HOH:O[6_565]	2.16	0.04

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	172/158 (109%)	170 (99%)	2 (1%)	0	100	100
1	B	173/158 (110%)	169 (98%)	4 (2%)	0	100	100
1	C	171/158 (108%)	168 (98%)	3 (2%)	0	100	100
1	D	169/158 (107%)	166 (98%)	3 (2%)	0	100	100
1	E	170/158 (108%)	168 (99%)	2 (1%)	0	100	100
1	F	173/158 (110%)	172 (99%)	1 (1%)	0	100	100
1	G	172/158 (109%)	167 (97%)	5 (3%)	0	100	100
1	H	169/158 (107%)	166 (98%)	3 (2%)	0	100	100
1	I	172/158 (109%)	170 (99%)	2 (1%)	0	100	100
1	J	168/158 (106%)	166 (99%)	2 (1%)	0	100	100
1	K	170/158 (108%)	168 (99%)	2 (1%)	0	100	100
1	L	167/158 (106%)	166 (99%)	1 (1%)	0	100	100
All	All	2046/1896 (108%)	2016 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	153/139 (110%)	153 (100%)	0	100	100
1	B	154/139 (111%)	154 (100%)	0	100	100
1	C	151/139 (109%)	151 (100%)	0	100	100
1	D	149/139 (107%)	149 (100%)	0	100	100
1	E	152/139 (109%)	152 (100%)	0	100	100
1	F	154/139 (111%)	154 (100%)	0	100	100
1	G	152/139 (109%)	152 (100%)	0	100	100
1	H	149/139 (107%)	149 (100%)	0	100	100
1	I	153/139 (110%)	153 (100%)	0	100	100
1	J	150/139 (108%)	148 (99%)	2 (1%)	61	36
1	K	151/139 (109%)	151 (100%)	0	100	100
1	L	149/139 (107%)	149 (100%)	0	100	100
All	All	1817/1668 (109%)	1815 (100%)	2 (0%)	88	80

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

Mol	Chain	Res	Type
1	J	50[A]	ASP
1	J	50[B]	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	153	GLN
1	D	17	ASN
1	D	100	ASN
1	E	9	ASN
1	E	34	ASN
1	I	142	GLN
1	K	46	HIS
1	L	112	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

58 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	SO4	G	1159	-	4,4,4	0.40	0	6,6,6	0.75	0
3	SO4	K	1159	-	4,4,4	0.41	0	6,6,6	1.00	0
3	SO4	J	1159	-	4,4,4	0.26	0	6,6,6	0.68	0
5	BTB	I	1162	-	7,7,13	0.82	0	9,9,16	1.22	0
5	BTB	K	1161	-	7,7,13	0.85	0	9,9,16	1.42	1 (11%)
2	HEM	C	200[A]	-	50,50,50	1.63	7 (14%)	67,82,82	1.32	8 (11%)
3	SO4	D	1159	-	4,4,4	0.24	0	6,6,6	0.39	0
2	HEM	C	200[B]	-	50,50,50	1.64	7 (14%)	67,82,82	1.32	8 (11%)
4	ACT	C	1161	-	3,3,3	0.88	0	3,3,3	1.43	0
2	HEM	B	200[B]	-	50,50,50	1.89	8 (16%)	67,82,82	1.46	8 (11%)
2	HEM	J	200[B]	-	50,50,50	1.62	7 (14%)	67,82,82	1.24	7 (10%)
2	HEM	L	200[B]	-	50,50,50	1.71	8 (16%)	67,82,82	1.21	3 (4%)
2	HEM	B	200[A]	-	50,50,50	1.89	8 (16%)	67,82,82	1.41	7 (10%)
2	HEM	J	200[A]	-	50,50,50	1.62	7 (14%)	67,82,82	1.24	7 (10%)
2	HEM	L	200[A]	-	50,50,50	1.71	8 (16%)	67,82,82	1.21	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	E	1161	-	3,3,3	0.83	0	3,3,3	1.29	0
5	BTB	L	1161	-	7,7,13	0.71	0	9,9,16	0.68	0
3	SO4	H	1160	-	4,4,4	0.35	0	6,6,6	0.82	0
2	HEM	D	200[B]	-	50,50,50	2.01	7 (14%)	67,82,82	1.45	8 (11%)
3	SO4	I	1161	-	4,4,4	0.30	0	6,6,6	0.48	0
2	HEM	D	200[A]	-	50,50,50	2.01	7 (14%)	67,82,82	1.47	8 (11%)
4	ACT	I	1160	-	3,3,3	0.88	0	3,3,3	1.25	0
2	HEM	I	200[B]	-	50,50,50	1.80	8 (16%)	67,82,82	1.33	6 (8%)
3	SO4	C	1159	-	4,4,4	0.14	0	6,6,6	0.98	0
2	HEM	F	200[B]	-	50,50,50	1.82	7 (14%)	67,82,82	1.27	6 (8%)
2	HEM	I	200[A]	-	50,50,50	1.80	8 (16%)	67,82,82	1.33	6 (8%)
3	SO4	L	1159	-	4,4,4	0.17	0	6,6,6	0.51	0
2	HEM	F	200[A]	-	50,50,50	1.83	7 (14%)	67,82,82	1.28	6 (8%)
4	ACT	G	1160	-	3,3,3	0.87	0	3,3,3	1.68	1 (33%)
4	ACT	H	1161	-	3,3,3	0.71	0	3,3,3	1.48	0
5	BTB	D	1161	-	7,7,13	0.75	0	9,9,16	1.11	0
3	SO4	C	1158	-	4,4,4	0.33	0	6,6,6	0.35	0
2	HEM	G	200[B]	-	50,50,50	1.90	8 (16%)	67,82,82	1.34	6 (8%)
4	ACT	F	1160	-	3,3,3	0.83	0	3,3,3	1.47	0
2	HEM	G	200[A]	-	50,50,50	1.90	8 (16%)	67,82,82	1.35	6 (8%)
2	HEM	A	200[B]	-	50,50,50	1.64	7 (14%)	67,82,82	1.25	5 (7%)
3	SO4	B	1161	-	4,4,4	0.34	0	6,6,6	0.99	0
2	HEM	H	200[A]	-	50,50,50	1.68	10 (20%)	67,82,82	1.31	8 (11%)
2	HEM	A	200[A]	-	50,50,50	1.65	7 (14%)	67,82,82	1.25	5 (7%)
2	HEM	H	200[B]	-	50,50,50	1.68	10 (20%)	67,82,82	1.34	8 (11%)
3	SO4	B	1159	-	4,4,4	0.17	0	6,6,6	0.32	0
3	SO4	I	1159	-	4,4,4	0.35	0	6,6,6	0.80	0
3	SO4	C	1160	-	4,4,4	0.22	0	6,6,6	0.25	0
4	ACT	J	1160	-	3,3,3	0.63	0	3,3,3	1.34	0
2	HEM	K	200[A]	-	50,50,50	1.77	8 (16%)	67,82,82	1.33	6 (8%)
4	ACT	L	1160	-	3,3,3	0.90	0	3,3,3	1.20	0
4	ACT	B	1162	-	3,3,3	0.71	0	3,3,3	1.27	0
3	SO4	B	1160	-	4,4,4	0.31	0	6,6,6	0.36	0
2	HEM	K	200[B]	-	50,50,50	1.76	8 (16%)	67,82,82	1.32	6 (8%)
4	ACT	A	1160	-	3,3,3	0.83	0	3,3,3	1.71	1 (33%)
4	ACT	D	1160	-	3,3,3	0.93	0	3,3,3	1.39	1 (33%)
3	SO4	E	1159	-	4,4,4	0.34	0	6,6,6	0.38	0
3	SO4	E	1160	-	4,4,4	0.29	0	6,6,6	0.65	0
2	HEM	E	200	1	50,50,50	1.72	7 (14%)	67,82,82	1.41	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	1159	-	4,4,4	0.28	0	6,6,6	1.07	1 (16%)
4	ACT	K	1160	-	3,3,3	0.81	0	3,3,3	1.55	1 (33%)
3	SO4	H	1159	-	4,4,4	0.48	0	6,6,6	0.24	0
3	SO4	A	1159	-	4,4,4	0.46	0	6,6,6	0.81	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
5	BTB	I	1162	-	-	7/9/9/21	-
5	BTB	K	1161	-	-	6/9/9/21	-
2	HEM	C	200[A]	-	-	4/14/54/54	-
2	HEM	C	200[B]	-	-	4/14/54/54	-
2	HEM	B	200[B]	-	-	4/14/54/54	-
2	HEM	J	200[B]	-	-	4/14/54/54	-
2	HEM	L	200[B]	-	-	4/14/54/54	-
2	HEM	B	200[A]	-	-	6/14/54/54	-
2	HEM	J	200[A]	-	-	6/14/54/54	-
2	HEM	L	200[A]	-	-	4/14/54/54	-
5	BTB	L	1161	-	-	1/9/9/21	-
2	HEM	D	200[B]	-	-	4/14/54/54	-
2	HEM	D	200[A]	-	-	6/14/54/54	-
2	HEM	I	200[B]	-	-	4/14/54/54	-
2	HEM	F	200[B]	-	-	4/14/54/54	-
2	HEM	I	200[A]	-	-	6/14/54/54	-
5	BTB	D	1161	-	-	6/9/9/21	-
2	HEM	F	200[A]	-	-	6/14/54/54	-
2	HEM	G	200[B]	-	-	6/14/54/54	-
2	HEM	G	200[A]	-	-	6/14/54/54	-
2	HEM	A	200[B]	-	-	4/14/54/54	-
2	HEM	H	200[A]	-	-	6/14/54/54	-
2	HEM	A	200[A]	-	-	6/14/54/54	-
2	HEM	H	200[B]	-	-	4/14/54/54	-
2	HEM	K	200[A]	-	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	K	200[B]	-	-	6/14/54/54	-
2	HEM	E	200	1	-	5/14/54/54	-

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	200[A]	HEM	C3D-C2D	8.04	1.54	1.36
2	D	200[B]	HEM	C3D-C2D	8.04	1.54	1.36
2	B	200[A]	HEM	C3D-C2D	7.99	1.54	1.36
2	B	200[B]	HEM	C3D-C2D	7.99	1.54	1.36
2	G	200[A]	HEM	C3D-C2D	7.71	1.53	1.36
2	G	200[B]	HEM	C3D-C2D	7.71	1.53	1.36
2	F	200[A]	HEM	C3D-C2D	7.65	1.53	1.36
2	F	200[B]	HEM	C3D-C2D	7.65	1.53	1.36
2	E	200	HEM	C3D-C2D	7.58	1.53	1.36
2	I	200[A]	HEM	C3D-C2D	7.50	1.52	1.36
2	I	200[B]	HEM	C3D-C2D	7.50	1.52	1.36
2	J	200[A]	HEM	C3D-C2D	7.45	1.52	1.36
2	J	200[B]	HEM	C3D-C2D	7.45	1.52	1.36
2	C	200[A]	HEM	C3D-C2D	7.39	1.52	1.36
2	C	200[B]	HEM	C3D-C2D	7.39	1.52	1.36
2	L	200[A]	HEM	C3D-C2D	7.21	1.52	1.36
2	L	200[B]	HEM	C3D-C2D	7.21	1.52	1.36
2	K	200[A]	HEM	C3D-C2D	7.16	1.52	1.36
2	K	200[B]	HEM	C3D-C2D	7.16	1.52	1.36
2	A	200[A]	HEM	C3D-C2D	7.13	1.52	1.36
2	A	200[B]	HEM	C3D-C2D	7.13	1.52	1.36
2	D	200[A]	HEM	FE-NA	6.99	2.18	1.95
2	D	200[B]	HEM	FE-NA	6.99	2.18	1.95
2	H	200[A]	HEM	C3D-C2D	6.79	1.51	1.36
2	H	200[B]	HEM	C3D-C2D	6.79	1.51	1.36
2	F	200[A]	HEM	FE-ND	6.20	2.14	1.94
2	F	200[B]	HEM	FE-ND	6.20	2.14	1.94
2	G	200[A]	HEM	FE-NC	5.73	2.14	1.95
2	G	200[B]	HEM	FE-NC	5.73	2.14	1.95
2	I	200[A]	HEM	FE-NB	5.30	2.11	1.94
2	I	200[B]	HEM	FE-NB	5.30	2.11	1.94
2	G	200[A]	HEM	FE-NB	5.29	2.11	1.94
2	G	200[B]	HEM	FE-NB	5.29	2.11	1.94
2	D	200[A]	HEM	FE-NB	5.28	2.11	1.94
2	D	200[B]	HEM	FE-NB	5.28	2.11	1.94
2	B	200[A]	HEM	FE-ND	4.98	2.10	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200[B]	HEM	FE-ND	4.98	2.10	1.94
2	E	200	HEM	FE-NB	4.59	2.09	1.94
2	B	200[A]	HEM	FE-NB	4.55	2.08	1.94
2	B	200[B]	HEM	FE-NB	4.55	2.08	1.94
2	A	200[A]	HEM	FE-NC	4.11	2.08	1.95
2	A	200[B]	HEM	FE-NC	4.11	2.08	1.95
2	F	200[A]	HEM	FE-NA	3.62	2.07	1.95
2	F	200[B]	HEM	FE-NA	3.62	2.07	1.95
2	L	200[A]	HEM	FE-NB	3.54	2.05	1.94
2	L	200[B]	HEM	FE-NB	3.54	2.05	1.94
2	K	200[A]	HEM	FE-NB	3.50	2.05	1.94
2	K	200[B]	HEM	FE-NB	3.50	2.05	1.94
2	E	200	HEM	FE-NC	3.36	2.06	1.95
2	I	200[A]	HEM	FE-NA	3.35	2.06	1.95
2	I	200[B]	HEM	FE-NA	3.35	2.06	1.95
2	K	200[A]	HEM	FE-NC	3.19	2.05	1.95
2	K	200[B]	HEM	FE-NC	3.19	2.05	1.95
2	B	200[B]	HEM	CAC-C3C	3.17	1.55	1.47
2	B	200[A]	HEM	CAC-C3C	3.13	1.55	1.47
2	I	200[A]	HEM	FE-NC	3.06	2.05	1.95
2	I	200[B]	HEM	FE-NC	3.06	2.05	1.95
2	G	200[B]	HEM	CAC-C3C	3.05	1.55	1.47
2	C	200[A]	HEM	FE-NB	3.03	2.04	1.94
2	C	200[B]	HEM	FE-NB	3.03	2.04	1.94
2	H	200[A]	HEM	FE-NC	3.02	2.05	1.95
2	H	200[B]	HEM	FE-NC	3.02	2.05	1.95
2	K	200[A]	HEM	CAC-C3C	2.98	1.55	1.47
2	J	200[A]	HEM	FE-NB	2.98	2.04	1.94
2	J	200[B]	HEM	FE-NB	2.98	2.04	1.94
2	F	200[A]	HEM	CAC-C3C	2.95	1.55	1.47
2	L	200[A]	HEM	FE-NA	2.93	2.04	1.95
2	L	200[B]	HEM	FE-NA	2.93	2.04	1.95
2	K	200[B]	HEM	CAC-C3C	2.90	1.55	1.47
2	D	200[A]	HEM	CAC-C3C	2.89	1.55	1.47
2	H	200[A]	HEM	FE-ND	2.88	2.03	1.94
2	H	200[B]	HEM	FE-ND	2.88	2.03	1.94
2	I	200[A]	HEM	CAC-C3C	2.88	1.55	1.47
2	L	200[A]	HEM	CMA-C3A	2.86	1.56	1.50
2	L	200[B]	HEM	CMA-C3A	2.86	1.56	1.50
2	I	200[B]	HEM	CAC-C3C	2.85	1.55	1.47
2	G	200[A]	HEM	CAC-C3C	2.83	1.54	1.47
2	B	200[A]	HEM	FE-NC	2.82	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200[B]	HEM	FE-NC	2.82	2.04	1.95
2	B	200[A]	HEM	FE-NA	2.81	2.04	1.95
2	B	200[B]	HEM	FE-NA	2.81	2.04	1.95
2	K	200[A]	HEM	FE-NA	2.80	2.04	1.95
2	K	200[B]	HEM	FE-NA	2.80	2.04	1.95
2	D	200[B]	HEM	CAC-C3C	2.78	1.54	1.47
2	F	200[B]	HEM	CAC-C3C	2.75	1.54	1.47
2	I	200[A]	HEM	CAB-C3B	2.72	1.54	1.47
2	I	200[B]	HEM	CAB-C3B	2.72	1.54	1.47
2	E	200	HEM	FE-ND	2.71	2.03	1.94
2	L	200[B]	HEM	CAC-C3C	2.69	1.54	1.47
2	C	200[B]	HEM	CAC-C3C	2.64	1.54	1.47
2	L	200[A]	HEM	CAB-C3B	2.64	1.54	1.47
2	L	200[B]	HEM	CAB-C3B	2.64	1.54	1.47
2	B	200[A]	HEM	CAB-C3B	2.62	1.54	1.47
2	B	200[B]	HEM	CAB-C3B	2.62	1.54	1.47
2	K	200[A]	HEM	CAB-C3B	2.62	1.54	1.47
2	K	200[B]	HEM	CAB-C3B	2.62	1.54	1.47
2	A	200[A]	HEM	CAC-C3C	2.60	1.54	1.47
2	E	200	HEM	CAC-C3C	2.60	1.54	1.47
2	J	200[A]	HEM	CMA-C3A	2.56	1.56	1.50
2	J	200[B]	HEM	CMA-C3A	2.56	1.56	1.50
2	L	200[A]	HEM	FE-NC	2.54	2.03	1.95
2	L	200[B]	HEM	FE-NC	2.54	2.03	1.95
2	K	200[A]	HEM	C2A-C3A	-2.53	1.32	1.38
2	K	200[B]	HEM	C2A-C3A	-2.53	1.32	1.38
2	H	200[A]	HEM	CAC-C3C	2.52	1.54	1.47
2	G	200[A]	HEM	CAB-C3B	2.51	1.54	1.47
2	G	200[B]	HEM	CAB-C3B	2.51	1.54	1.47
2	H	200[A]	HEM	FE-NB	2.51	2.02	1.94
2	H	200[B]	HEM	FE-NB	2.51	2.02	1.94
2	L	200[A]	HEM	CAC-C3C	2.50	1.54	1.47
2	I	200[A]	HEM	C2A-C3A	-2.50	1.32	1.38
2	I	200[B]	HEM	C2A-C3A	-2.50	1.32	1.38
2	A	200[B]	HEM	CAC-C3C	2.49	1.54	1.47
2	H	200[A]	HEM	C2A-C3A	-2.49	1.32	1.38
2	H	200[B]	HEM	C2A-C3A	-2.49	1.32	1.38
2	H	200[B]	HEM	CAC-C3C	2.47	1.54	1.47
2	J	200[B]	HEM	CAC-C3C	2.39	1.53	1.47
2	J	200[A]	HEM	CAC-C3C	2.39	1.53	1.47
2	D	200[A]	HEM	CAB-C3B	2.38	1.53	1.47
2	D	200[B]	HEM	CAB-C3B	2.38	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	200[A]	HEM	FE-ND	2.37	2.02	1.94
2	L	200[B]	HEM	FE-ND	2.37	2.02	1.94
2	E	200	HEM	CAB-C3B	2.34	1.53	1.47
2	H	200[A]	HEM	FE-NA	2.33	2.02	1.95
2	H	200[B]	HEM	FE-NA	2.33	2.02	1.95
2	G	200[A]	HEM	C2A-C3A	-2.32	1.32	1.38
2	G	200[B]	HEM	C2A-C3A	-2.32	1.32	1.38
2	B	200[A]	HEM	C2A-C3A	-2.32	1.32	1.38
2	B	200[B]	HEM	C2A-C3A	-2.32	1.32	1.38
2	J	200[A]	HEM	CAB-C3B	2.29	1.53	1.47
2	J	200[B]	HEM	CAB-C3B	2.29	1.53	1.47
2	F	200[A]	HEM	C2A-C3A	-2.27	1.33	1.38
2	F	200[B]	HEM	C2A-C3A	-2.27	1.33	1.38
2	C	200[A]	HEM	CAC-C3C	2.24	1.53	1.47
2	K	200[A]	HEM	FE-ND	2.22	2.01	1.94
2	K	200[B]	HEM	FE-ND	2.22	2.01	1.94
2	J	200[A]	HEM	FE-ND	2.20	2.01	1.94
2	J	200[B]	HEM	FE-ND	2.20	2.01	1.94
2	F	200[A]	HEM	CAB-C3B	2.20	1.53	1.47
2	F	200[B]	HEM	CAB-C3B	2.20	1.53	1.47
2	H	200[A]	HEM	CAB-C3B	2.19	1.53	1.47
2	H	200[B]	HEM	CAB-C3B	2.19	1.53	1.47
2	J	200[A]	HEM	C2A-C3A	-2.18	1.33	1.38
2	J	200[B]	HEM	C2A-C3A	-2.18	1.33	1.38
2	A	200[A]	HEM	CAB-C3B	2.17	1.53	1.47
2	A	200[B]	HEM	CAB-C3B	2.17	1.53	1.47
2	G	200[A]	HEM	FE-ND	2.16	2.01	1.94
2	G	200[B]	HEM	FE-ND	2.16	2.01	1.94
2	A	200[A]	HEM	FE-NB	2.16	2.01	1.94
2	A	200[B]	HEM	FE-NB	2.16	2.01	1.94
2	C	200[A]	HEM	C2A-C3A	-2.14	1.33	1.38
2	C	200[B]	HEM	C2A-C3A	-2.14	1.33	1.38
2	F	200[A]	HEM	CMB-C2B	2.14	1.55	1.50
2	F	200[B]	HEM	CMB-C2B	2.14	1.55	1.50
2	D	200[A]	HEM	CMD-C2D	2.13	1.55	1.50
2	D	200[B]	HEM	CMD-C2D	2.13	1.55	1.50
2	A	200[A]	HEM	C2A-C3A	-2.13	1.33	1.38
2	A	200[B]	HEM	C2A-C3A	-2.13	1.33	1.38
2	I	200[A]	HEM	CMC-C2C	2.13	1.55	1.50
2	I	200[B]	HEM	CMC-C2C	2.13	1.55	1.50
2	C	200[A]	HEM	CAB-C3B	2.13	1.53	1.47
2	C	200[B]	HEM	CAB-C3B	2.13	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	200[A]	HEM	CMA-C3A	2.12	1.55	1.50
2	C	200[B]	HEM	CMA-C3A	2.12	1.55	1.50
2	H	200[A]	HEM	C3B-C2B	-2.08	1.32	1.37
2	H	200[B]	HEM	C3B-C2B	-2.08	1.32	1.37
2	A	200[A]	HEM	CMD-C2D	2.08	1.55	1.50
2	A	200[B]	HEM	CMD-C2D	2.08	1.55	1.50
2	H	200[A]	HEM	CMD-C2D	2.07	1.55	1.50
2	H	200[B]	HEM	CMD-C2D	2.07	1.55	1.50
2	D	200[A]	HEM	C2A-C3A	-2.06	1.33	1.38
2	D	200[B]	HEM	C2A-C3A	-2.06	1.33	1.38
2	C	200[A]	HEM	C1B-NB	-2.04	1.36	1.40
2	C	200[B]	HEM	C1B-NB	-2.04	1.36	1.40
2	G	200[A]	HEM	CMA-C3A	2.01	1.54	1.50
2	G	200[B]	HEM	CMA-C3A	2.01	1.54	1.50
2	E	200	HEM	C2A-C3A	-2.01	1.33	1.38

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	200[A]	HEM	C4D-ND-C1D	5.86	112.15	105.21
2	D	200[B]	HEM	C4D-ND-C1D	5.86	112.15	105.21
2	B	200[A]	HEM	C4D-ND-C1D	5.67	111.92	105.21
2	B	200[B]	HEM	C4D-ND-C1D	5.67	111.92	105.21
2	G	200[A]	HEM	C4D-ND-C1D	5.67	111.92	105.21
2	G	200[B]	HEM	C4D-ND-C1D	5.67	111.92	105.21
2	I	200[A]	HEM	C4D-ND-C1D	5.62	111.86	105.21
2	I	200[B]	HEM	C4D-ND-C1D	5.62	111.86	105.21
2	E	200	HEM	C4D-ND-C1D	5.48	111.70	105.21
2	H	200[A]	HEM	C4D-ND-C1D	5.13	111.28	105.21
2	H	200[B]	HEM	C4D-ND-C1D	5.13	111.28	105.21
2	K	200[A]	HEM	C4D-ND-C1D	5.12	111.27	105.21
2	K	200[B]	HEM	C4D-ND-C1D	5.12	111.27	105.21
2	F	200[A]	HEM	C4D-ND-C1D	4.56	110.61	105.21
2	F	200[B]	HEM	C4D-ND-C1D	4.56	110.61	105.21
2	L	200[A]	HEM	C4D-ND-C1D	4.47	110.50	105.21
2	L	200[B]	HEM	C4D-ND-C1D	4.47	110.50	105.21
2	J	200[A]	HEM	C4D-ND-C1D	4.38	110.40	105.21
2	J	200[B]	HEM	C4D-ND-C1D	4.38	110.40	105.21
2	A	200[A]	HEM	C4D-ND-C1D	4.01	109.95	105.21
2	A	200[B]	HEM	C4D-ND-C1D	4.01	109.95	105.21
2	C	200[A]	HEM	C4D-ND-C1D	3.83	109.74	105.21
2	C	200[B]	HEM	C4D-ND-C1D	3.83	109.74	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	200[A]	HEM	CHD-C4C-NC	3.46	128.22	124.45
2	C	200[B]	HEM	CHD-C4C-NC	3.46	128.22	124.45
2	E	200	HEM	CHD-C1D-ND	3.14	127.80	124.42
2	L	200[A]	HEM	CHC-C4B-NB	3.13	127.79	124.42
2	L	200[B]	HEM	CHC-C4B-NB	3.13	127.79	124.42
2	B	200[A]	HEM	C3B-C4B-NB	-3.10	107.24	109.47
2	B	200[B]	HEM	C3B-C4B-NB	-3.10	107.24	109.47
2	K	200[A]	HEM	CHC-C1C-NC	3.09	127.82	124.45
2	K	200[B]	HEM	CHC-C1C-NC	3.09	127.82	124.45
2	B	200[A]	HEM	CBA-CAA-C2A	-3.01	104.20	112.53
2	B	200[B]	HEM	CBA-CAA-C2A	-3.01	104.20	112.53
2	H	200[A]	HEM	CHB-C1B-NB	3.01	128.09	124.37
2	H	200[B]	HEM	CHB-C1B-NB	3.01	128.09	124.37
2	E	200	HEM	CHC-C1C-NC	2.95	127.66	124.45
2	B	200[A]	HEM	C1B-NB-C4B	2.92	108.66	105.21
2	B	200[B]	HEM	C1B-NB-C4B	2.92	108.66	105.21
2	J	200[A]	HEM	CHB-C1B-NB	2.91	127.97	124.37
2	J	200[B]	HEM	CHB-C1B-NB	2.91	127.97	124.37
2	A	200[A]	HEM	CHD-C1D-ND	2.89	127.53	124.42
2	A	200[B]	HEM	CHD-C1D-ND	2.89	127.53	124.42
2	D	200[A]	HEM	CHB-C1B-NB	2.87	127.92	124.37
2	D	200[B]	HEM	CHB-C1B-NB	2.87	127.92	124.37
2	H	200[A]	HEM	CHD-C1D-ND	2.86	127.50	124.42
2	H	200[B]	HEM	CHD-C1D-ND	2.86	127.50	124.42
2	I	200[A]	HEM	CBA-CAA-C2A	-2.84	104.67	112.53
2	I	200[B]	HEM	CBA-CAA-C2A	-2.84	104.67	112.53
2	K	200[A]	HEM	CMD-C2D-C1D	2.84	129.48	125.03
2	K	200[B]	HEM	CMD-C2D-C1D	2.84	129.48	125.03
2	B	200[A]	HEM	CHC-C1C-NC	2.84	127.54	124.45
2	B	200[B]	HEM	CHC-C1C-NC	2.84	127.54	124.45
2	D	200[A]	HEM	CHA-C4D-ND	2.84	127.88	124.37
2	D	200[B]	HEM	CHA-C4D-ND	2.84	127.88	124.37
2	G	200[A]	HEM	C2A-C1A-NA	-2.82	107.02	110.15
2	G	200[B]	HEM	C2A-C1A-NA	-2.82	107.02	110.15
2	K	200[A]	HEM	CHA-C4D-ND	2.78	127.81	124.37
2	K	200[B]	HEM	CHA-C4D-ND	2.78	127.81	124.37
2	A	200[A]	HEM	CBA-CAA-C2A	-2.78	104.85	112.53
2	A	200[B]	HEM	CBA-CAA-C2A	-2.78	104.85	112.53
2	B	200[A]	HEM	C3C-C2C-C1C	2.76	109.65	107.05
2	B	200[B]	HEM	C3C-C2C-C1C	2.76	109.65	107.05
2	D	200[A]	HEM	C3B-C4B-NB	-2.74	107.50	109.47
2	D	200[B]	HEM	C3B-C4B-NB	-2.74	107.50	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	200[A]	HEM	CBA-CAA-C2A	-2.71	105.04	112.53
2	D	200[B]	HEM	CBA-CAA-C2A	-2.71	105.04	112.53
2	C	200[A]	HEM	CBA-CAA-C2A	-2.69	105.10	112.53
2	C	200[B]	HEM	CBA-CAA-C2A	-2.69	105.10	112.53
2	G	200[A]	HEM	CBA-CAA-C2A	-2.68	105.11	112.53
2	G	200[B]	HEM	CBA-CAA-C2A	-2.68	105.11	112.53
2	J	200[A]	HEM	C3B-C2B-C1B	2.66	108.41	106.41
2	J	200[B]	HEM	C3B-C2B-C1B	2.66	108.41	106.41
2	C	200[A]	HEM	CBD-CAD-C3D	-2.65	105.22	112.53
2	C	200[B]	HEM	CBD-CAD-C3D	-2.65	105.22	112.53
2	H	200[A]	HEM	C3B-C2B-C1B	2.63	108.39	106.41
2	H	200[B]	HEM	C3B-C2B-C1B	2.63	108.39	106.41
2	H	200[A]	HEM	CBA-CAA-C2A	-2.62	105.30	112.53
2	H	200[B]	HEM	CBA-CAA-C2A	-2.62	105.30	112.53
2	I	200[A]	HEM	CHA-C4D-ND	2.56	127.53	124.37
2	I	200[B]	HEM	CHA-C4D-ND	2.56	127.53	124.37
2	K	200[A]	HEM	C3B-C2B-C1B	2.50	108.29	106.41
2	K	200[B]	HEM	C3B-C2B-C1B	2.50	108.29	106.41
2	H	200[A]	HEM	C4C-C3C-C2C	2.48	108.97	106.81
2	H	200[B]	HEM	C4C-C3C-C2C	2.48	108.97	106.81
2	L	200[A]	HEM	CBA-CAA-C2A	-2.47	105.69	112.53
2	L	200[B]	HEM	CBA-CAA-C2A	-2.47	105.69	112.53
2	C	200[A]	HEM	CHC-C4B-NB	2.46	127.07	124.42
2	C	200[B]	HEM	CHC-C4B-NB	2.46	127.07	124.42
2	B	200[B]	HEM	CAC-C3C-C4C	2.45	130.66	124.82
2	K	200[A]	HEM	CAD-C3D-C4D	2.43	128.94	124.70
2	K	200[B]	HEM	CAD-C3D-C4D	2.43	128.94	124.70
2	C	200[A]	HEM	CHB-C1B-NB	2.43	127.37	124.37
2	C	200[B]	HEM	CHB-C1B-NB	2.43	127.37	124.37
2	I	200[A]	HEM	CHD-C1D-ND	2.40	127.01	124.42
2	I	200[B]	HEM	CHD-C1D-ND	2.40	127.01	124.42
2	F	200[A]	HEM	C3B-C4B-NB	-2.33	107.80	109.47
2	F	200[B]	HEM	C3B-C4B-NB	-2.33	107.80	109.47
4	A	1160	ACT	OXT-C-CH3	2.32	124.80	115.05
2	E	200	HEM	CBD-CAD-C3D	-2.32	106.11	112.53
2	F	200[A]	HEM	CBA-CAA-C2A	-2.29	106.19	112.53
2	F	200[B]	HEM	CBA-CAA-C2A	-2.29	106.19	112.53
2	F	200[A]	HEM	CHD-C1D-ND	2.29	126.89	124.42
2	F	200[B]	HEM	CHD-C1D-ND	2.29	126.89	124.42
2	A	200[A]	HEM	CHB-C1B-NB	2.26	127.17	124.37
2	A	200[B]	HEM	CHB-C1B-NB	2.26	127.17	124.37
2	G	200[A]	HEM	CHD-C1D-ND	2.26	126.86	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	200[B]	HEM	CHD-C1D-ND	2.26	126.86	124.42
2	E	200	HEM	CHB-C1B-NB	2.25	127.15	124.37
2	F	200[A]	HEM	C1B-NB-C4B	2.25	107.87	105.21
2	F	200[B]	HEM	C1B-NB-C4B	2.25	107.87	105.21
2	J	200[A]	HEM	CBD-CAD-C3D	-2.24	106.34	112.53
2	J	200[B]	HEM	CBD-CAD-C3D	-2.24	106.34	112.53
2	G	200[A]	HEM	C3B-C2B-C1B	2.24	108.09	106.41
2	G	200[B]	HEM	C3B-C2B-C1B	2.24	108.09	106.41
2	D	200[A]	HEM	C4C-NC-C1C	2.23	109.46	105.82
2	D	200[B]	HEM	C4C-NC-C1C	2.23	109.46	105.82
2	J	200[A]	HEM	CBA-CAA-C2A	-2.23	106.38	112.53
2	J	200[B]	HEM	CBA-CAA-C2A	-2.23	106.38	112.53
4	G	1160	ACT	OXT-C-CH3	2.22	124.36	115.05
3	F	1159	SO4	O4-S-O1	-2.22	97.97	109.56
2	H	200[A]	HEM	CHD-C4C-NC	2.22	126.87	124.45
2	H	200[B]	HEM	CHD-C4C-NC	2.22	126.87	124.45
2	D	200[A]	HEM	C1B-NB-C4B	2.19	107.81	105.21
2	D	200[B]	HEM	C1B-NB-C4B	2.19	107.81	105.21
2	J	200[A]	HEM	CHD-C4C-NC	2.19	126.84	124.45
2	J	200[B]	HEM	CHD-C4C-NC	2.19	126.84	124.45
2	D	200[A]	HEM	CHD-C1D-ND	2.19	126.78	124.42
2	D	200[B]	HEM	CHD-C1D-ND	2.19	126.78	124.42
2	I	200[A]	HEM	C2A-C1A-NA	-2.12	107.80	110.15
2	I	200[B]	HEM	C2A-C1A-NA	-2.12	107.80	110.15
2	E	200	HEM	CBA-CAA-C2A	-2.11	106.69	112.53
2	G	200[A]	HEM	CBD-CAD-C3D	-2.11	106.70	112.53
2	G	200[B]	HEM	CBD-CAD-C3D	-2.11	106.70	112.53
2	I	200[A]	HEM	CHB-C1B-NB	2.10	126.97	124.37
2	I	200[B]	HEM	CHB-C1B-NB	2.10	126.97	124.37
5	K	1161	BTB	O4-C4-C2	-2.10	105.03	110.88
2	C	200[A]	HEM	C4C-C3C-C2C	2.08	108.62	106.81
2	C	200[B]	HEM	C4C-C3C-C2C	2.08	108.62	106.81
2	J	200[A]	HEM	C4C-C3C-C2C	2.07	108.61	106.81
2	J	200[B]	HEM	C4C-C3C-C2C	2.07	108.61	106.81
2	B	200[A]	HEM	CHD-C1D-ND	2.06	126.64	124.42
2	B	200[B]	HEM	CHD-C1D-ND	2.06	126.64	124.42
2	F	200[A]	HEM	C1D-C2D-C3D	-2.06	104.81	106.98
2	F	200[B]	HEM	C1D-C2D-C3D	-2.06	104.81	106.98
2	E	200	HEM	CBB-CAB-C3B	-2.06	117.24	127.53
2	H	200[A]	HEM	CBD-CAD-C3D	-2.03	106.92	112.53
2	H	200[B]	HEM	CBD-CAD-C3D	-2.03	106.92	112.53
2	C	200[A]	HEM	C3B-C4B-NB	-2.03	108.01	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	200[B]	HEM	C3B-C4B-NB	-2.03	108.01	109.47
2	A	200[A]	HEM	CAD-C3D-C4D	2.02	128.22	124.70
2	A	200[B]	HEM	CAD-C3D-C4D	2.02	128.22	124.70
4	K	1160	ACT	OXT-C-O	-2.02	114.53	122.03
2	E	200	HEM	CHB-C4A-NA	2.01	127.50	123.86
2	E	200	HEM	O1A-CGA-CBA	-2.00	116.73	123.09
4	D	1160	ACT	OXT-C-O	-2.00	114.60	122.03

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	200[A]	HEM	C2C-C3C-CAC-CBC
2	H	200[A]	HEM	C2C-C3C-CAC-CBC
2	H	200[A]	HEM	C4C-C3C-CAC-CBC
2	J	200[A]	HEM	C2C-C3C-CAC-CBC
5	D	1161	BTB	O1-C1-C2-N
5	D	1161	BTB	C1-C2-C3-O3
5	D	1161	BTB	N-C2-C3-O3
5	I	1162	BTB	C1-C2-C3-O3
5	I	1162	BTB	C4-C2-C3-O3
5	I	1162	BTB	N-C2-C3-O3
5	K	1161	BTB	C1-C2-C3-O3
5	K	1161	BTB	N-C2-C3-O3
5	D	1161	BTB	O1-C1-C2-C4
5	K	1161	BTB	O1-C1-C2-C4
2	B	200[A]	HEM	C2C-C3C-CAC-CBC
5	D	1161	BTB	C4-C2-C3-O3
5	K	1161	BTB	O1-C1-C2-N
5	K	1161	BTB	C4-C2-C3-O3
2	A	200[A]	HEM	C2C-C3C-CAC-CBC
2	D	200[A]	HEM	C2B-C3B-CAB-CBB
2	D	200[A]	HEM	C2C-C3C-CAC-CBC
2	D	200[B]	HEM	C2B-C3B-CAB-CBB
2	I	200[A]	HEM	C2C-C3C-CAC-CBC
2	K	200[A]	HEM	C2B-C3B-CAB-CBB
2	K	200[B]	HEM	C2B-C3B-CAB-CBB
2	A	200[A]	HEM	C4C-C3C-CAC-CBC
2	B	200[A]	HEM	C4C-C3C-CAC-CBC
2	D	200[A]	HEM	C4C-C3C-CAC-CBC
2	F	200[A]	HEM	C4C-C3C-CAC-CBC
2	I	200[A]	HEM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	J	200[A]	HEM	C4C-C3C-CAC-CBC
5	I	1162	BTB	O1-C1-C2-C3
5	I	1162	BTB	C1-C2-C4-O4
2	J	200[A]	HEM	CAA-CBA-CGA-O1A
2	J	200[B]	HEM	CAA-CBA-CGA-O1A
2	E	200	HEM	CAD-CBD-CGD-O1D
2	E	200	HEM	CAD-CBD-CGD-O2D
2	A	200[A]	HEM	CAD-CBD-CGD-O1D
2	A	200[B]	HEM	CAD-CBD-CGD-O1D
2	L	200[A]	HEM	CAA-CBA-CGA-O2A
2	L	200[B]	HEM	CAA-CBA-CGA-O2A
2	G	200[A]	HEM	CAA-CBA-CGA-O2A
2	G	200[B]	HEM	CAA-CBA-CGA-O2A
2	H	200[A]	HEM	CAA-CBA-CGA-O1A
2	H	200[B]	HEM	CAA-CBA-CGA-O1A
2	D	200[A]	HEM	CAA-CBA-CGA-O1A
2	D	200[B]	HEM	CAA-CBA-CGA-O1A
2	G	200[A]	HEM	CAA-CBA-CGA-O1A
2	G	200[B]	HEM	CAA-CBA-CGA-O1A
2	H	200[A]	HEM	CAD-CBD-CGD-O2D
2	H	200[B]	HEM	CAD-CBD-CGD-O2D
2	J	200[A]	HEM	CAA-CBA-CGA-O2A
2	J	200[B]	HEM	CAA-CBA-CGA-O2A
2	K	200[A]	HEM	CAD-CBD-CGD-O1D
2	K	200[B]	HEM	CAD-CBD-CGD-O1D
2	C	200[A]	HEM	CAD-CBD-CGD-O2D
2	C	200[B]	HEM	CAD-CBD-CGD-O2D
2	H	200[A]	HEM	CAA-CBA-CGA-O2A
2	H	200[B]	HEM	CAA-CBA-CGA-O2A
2	I	200[A]	HEM	CAA-CBA-CGA-O2A
2	I	200[B]	HEM	CAA-CBA-CGA-O2A
2	A	200[A]	HEM	CAA-CBA-CGA-O2A
2	A	200[B]	HEM	CAA-CBA-CGA-O2A
2	D	200[A]	HEM	CAA-CBA-CGA-O2A
2	D	200[B]	HEM	CAA-CBA-CGA-O2A
2	C	200[A]	HEM	CAD-CBD-CGD-O1D
2	C	200[B]	HEM	CAD-CBD-CGD-O1D
2	H	200[A]	HEM	CAD-CBD-CGD-O1D
2	H	200[B]	HEM	CAD-CBD-CGD-O1D
2	I	200[A]	HEM	CAA-CBA-CGA-O1A
2	I	200[B]	HEM	CAA-CBA-CGA-O1A
2	A	200[A]	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	A	200[B]	HEM	CAD-CBD-CGD-O2D
2	A	200[A]	HEM	CAA-CBA-CGA-O1A
2	A	200[B]	HEM	CAA-CBA-CGA-O1A
2	B	200[A]	HEM	CAA-CBA-CGA-O2A
2	B	200[B]	HEM	CAA-CBA-CGA-O2A
2	G	200[A]	HEM	CAD-CBD-CGD-O1D
2	G	200[A]	HEM	CAD-CBD-CGD-O2D
2	G	200[B]	HEM	CAD-CBD-CGD-O1D
2	G	200[B]	HEM	CAD-CBD-CGD-O2D
2	L	200[A]	HEM	CAA-CBA-CGA-O1A
2	L	200[B]	HEM	CAA-CBA-CGA-O1A
2	E	200	HEM	CAA-CBA-CGA-O2A
2	I	200[A]	HEM	CAD-CBD-CGD-O1D
2	I	200[A]	HEM	CAD-CBD-CGD-O2D
2	I	200[B]	HEM	CAD-CBD-CGD-O1D
2	I	200[B]	HEM	CAD-CBD-CGD-O2D
2	B	200[A]	HEM	CAD-CBD-CGD-O1D
2	B	200[B]	HEM	CAD-CBD-CGD-O1D
2	K	200[A]	HEM	CAD-CBD-CGD-O2D
2	K	200[B]	HEM	CAD-CBD-CGD-O2D
2	B	200[A]	HEM	CAD-CBD-CGD-O2D
2	B	200[B]	HEM	CAD-CBD-CGD-O2D
2	L	200[A]	HEM	CAD-CBD-CGD-O2D
2	L	200[B]	HEM	CAD-CBD-CGD-O2D
2	E	200	HEM	CAA-CBA-CGA-O1A
2	L	200[A]	HEM	CAD-CBD-CGD-O1D
2	L	200[B]	HEM	CAD-CBD-CGD-O1D
2	G	200[A]	HEM	C2B-C3B-CAB-CBB
2	G	200[B]	HEM	C2B-C3B-CAB-CBB
2	J	200[A]	HEM	CAD-CBD-CGD-O2D
2	J	200[B]	HEM	CAD-CBD-CGD-O2D
2	F	200[A]	HEM	CAD-CBD-CGD-O2D
2	F	200[B]	HEM	CAD-CBD-CGD-O2D
2	F	200[A]	HEM	CAA-CBA-CGA-O2A
2	F	200[B]	HEM	CAA-CBA-CGA-O2A
5	D	1161	BTB	O1-C1-C2-C3
5	K	1161	BTB	O1-C1-C2-C3
5	L	1161	BTB	C3-C2-C4-O4
2	F	200[A]	HEM	CAD-CBD-CGD-O1D
2	F	200[B]	HEM	CAD-CBD-CGD-O1D
2	J	200[A]	HEM	CAD-CBD-CGD-O1D
2	J	200[B]	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	D	200[A]	HEM	C4B-C3B-CAB-CBB
2	D	200[B]	HEM	C4B-C3B-CAB-CBB
2	G	200[A]	HEM	C4B-C3B-CAB-CBB
2	G	200[B]	HEM	C4B-C3B-CAB-CBB
2	K	200[A]	HEM	C4B-C3B-CAB-CBB
2	K	200[B]	HEM	C4B-C3B-CAB-CBB
2	B	200[A]	HEM	CAA-CBA-CGA-O1A
2	B	200[B]	HEM	CAA-CBA-CGA-O1A
2	F	200[A]	HEM	CAA-CBA-CGA-O1A
2	F	200[B]	HEM	CAA-CBA-CGA-O1A
2	C	200[A]	HEM	CAA-CBA-CGA-O2A
2	C	200[B]	HEM	CAA-CBA-CGA-O2A
2	C	200[A]	HEM	CAA-CBA-CGA-O1A
2	C	200[B]	HEM	CAA-CBA-CGA-O1A
5	I	1162	BTB	O1-C1-C2-C4
5	I	1162	BTB	O1-C1-C2-N
2	K	200[A]	HEM	CAA-CBA-CGA-O2A
2	K	200[B]	HEM	CAA-CBA-CGA-O2A
2	E	200	HEM	C2C-C3C-CAC-CBC
2	K	200[A]	HEM	CAA-CBA-CGA-O1A
2	K	200[B]	HEM	CAA-CBA-CGA-O1A

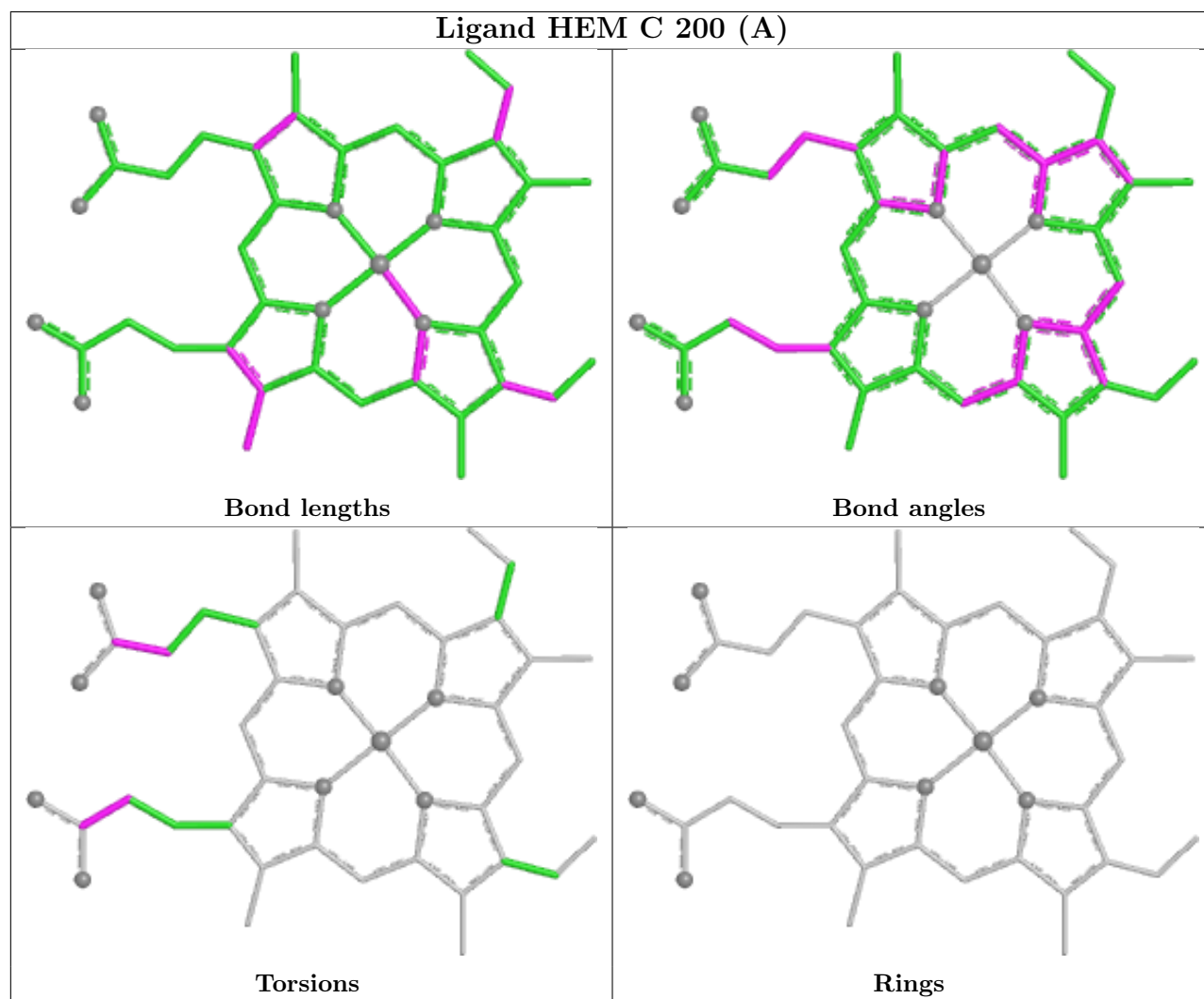
There are no ring outliers.

14 monomers are involved in 20 short contacts:

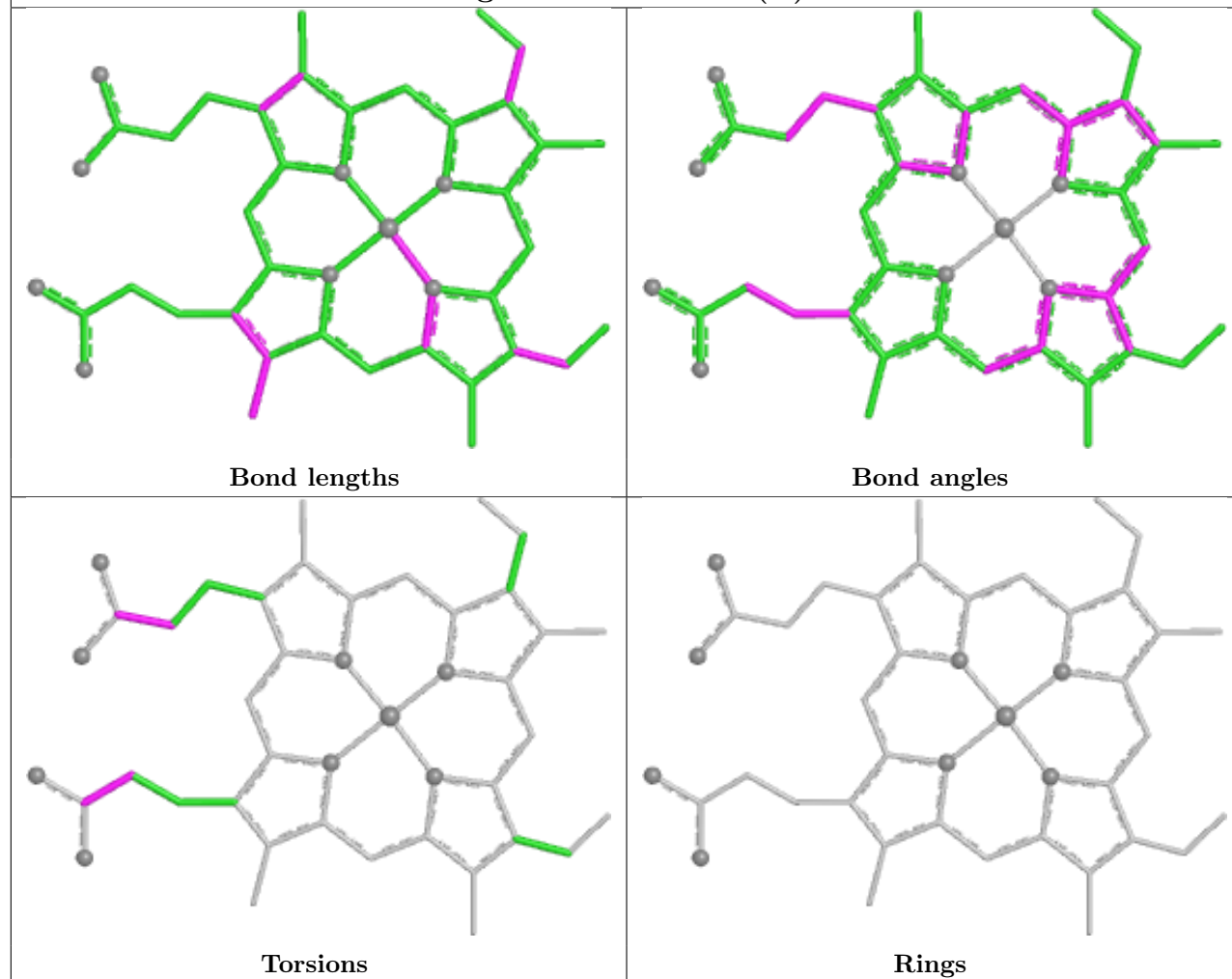
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1159	SO4	1	0
3	J	1159	SO4	1	0
5	I	1162	BTB	1	0
2	J	200[A]	HEM	1	0
5	L	1161	BTB	3	0
3	H	1160	SO4	1	0
3	L	1159	SO4	1	0
2	F	200[A]	HEM	2	0
5	D	1161	BTB	3	0
3	B	1161	SO4	1	0
2	H	200[A]	HEM	2	0
2	A	200[A]	HEM	1	0
3	E	1160	SO4	1	0
3	A	1159	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

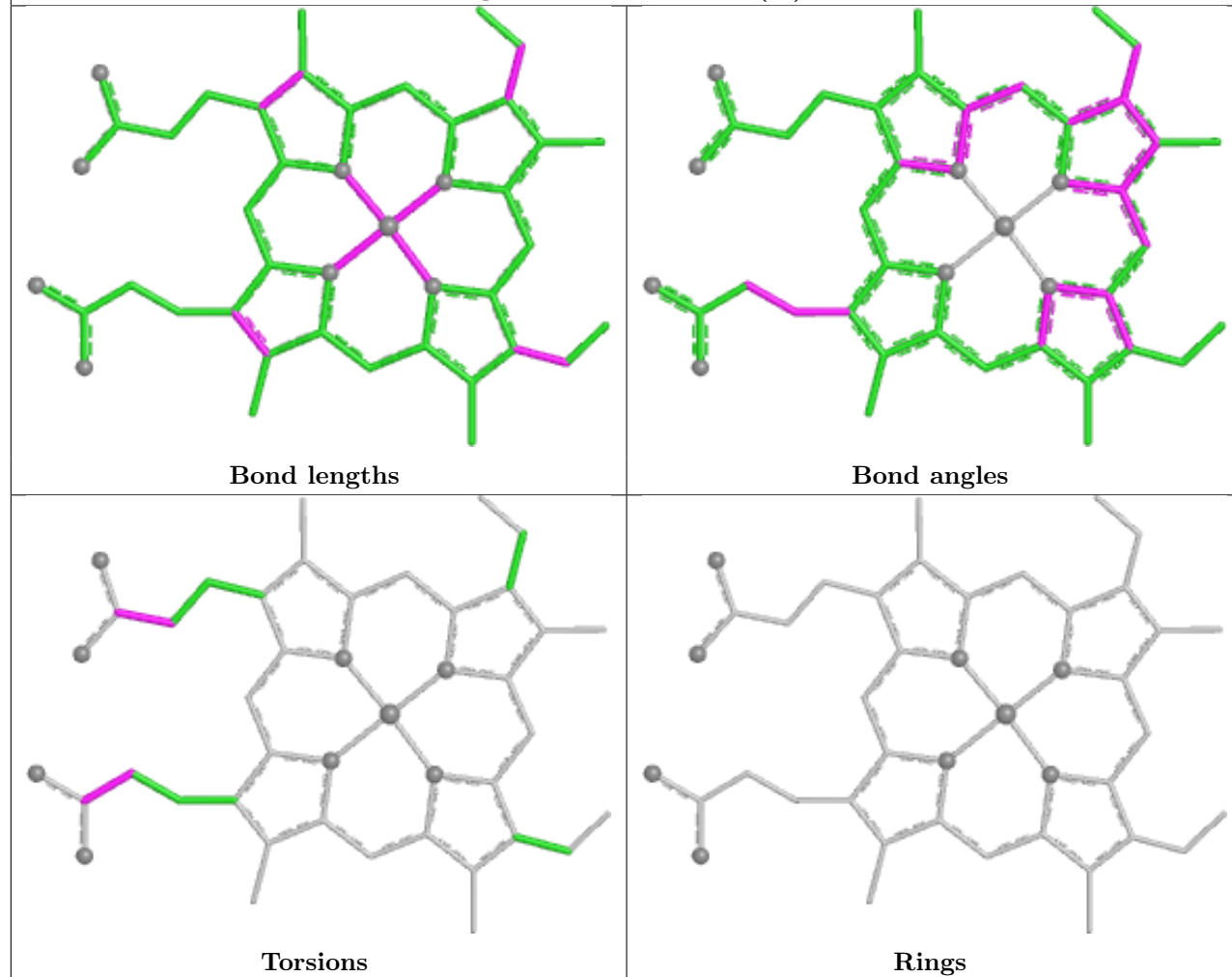
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



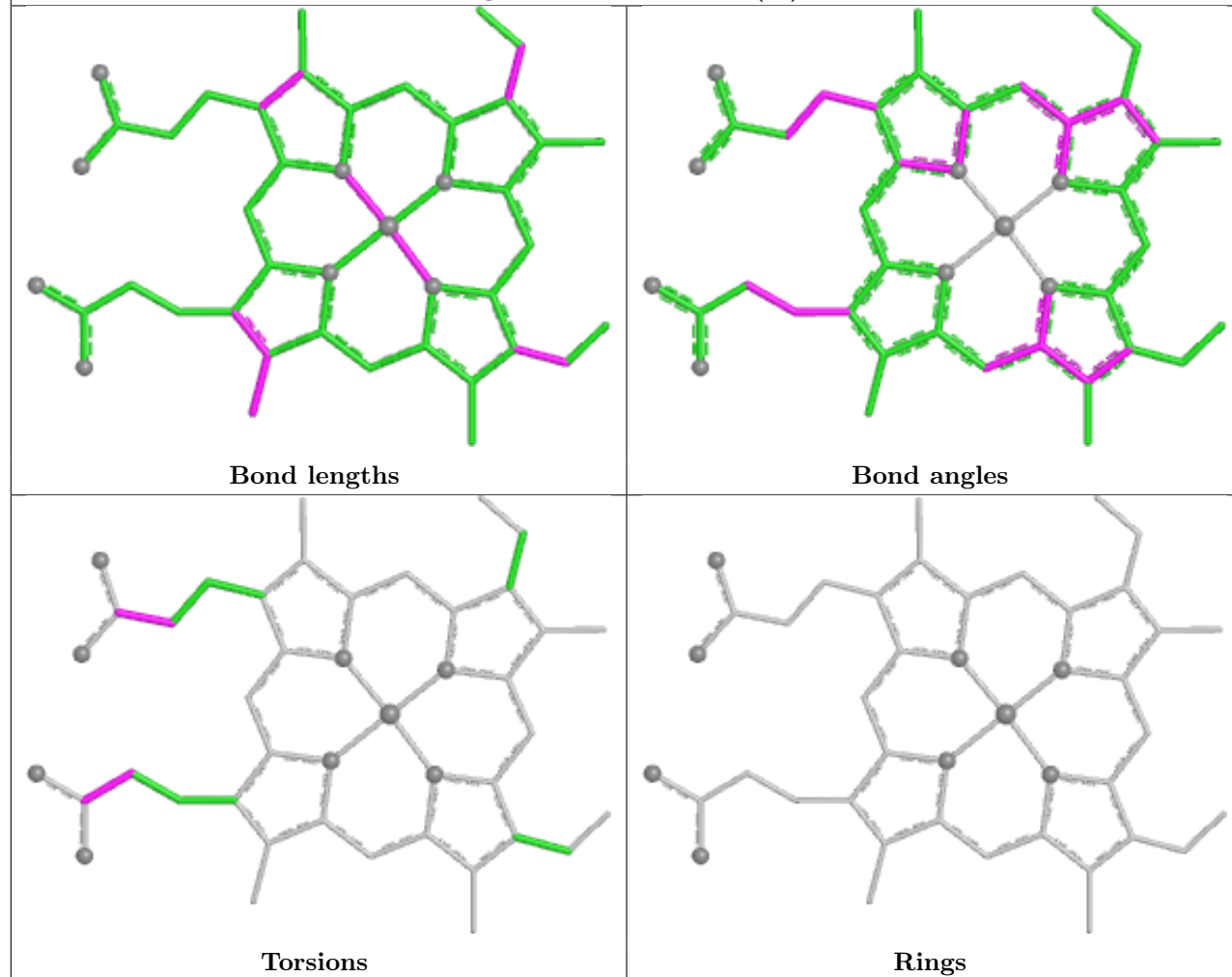
Ligand HEM C 200 (B)



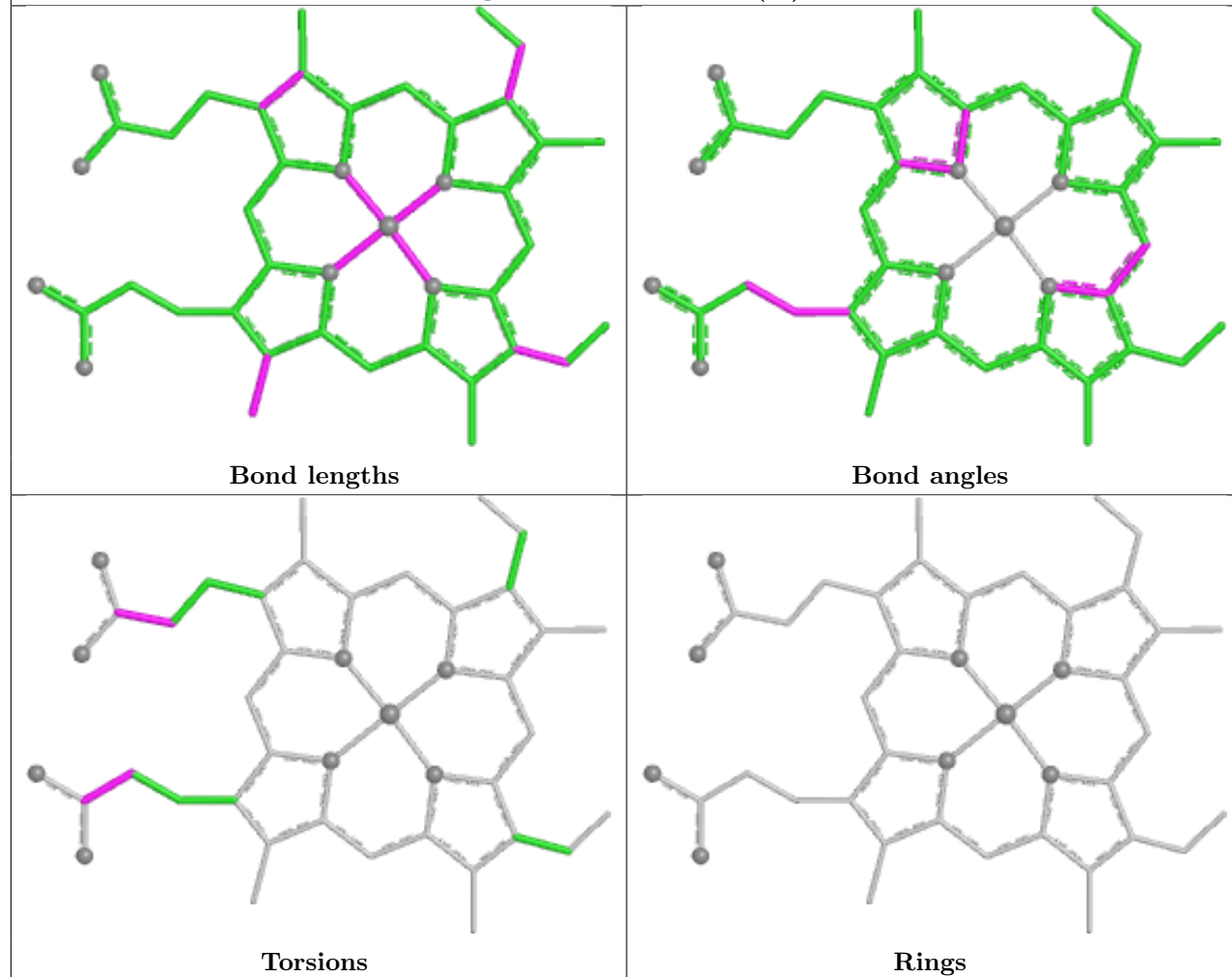
Ligand HEM B 200 (B)



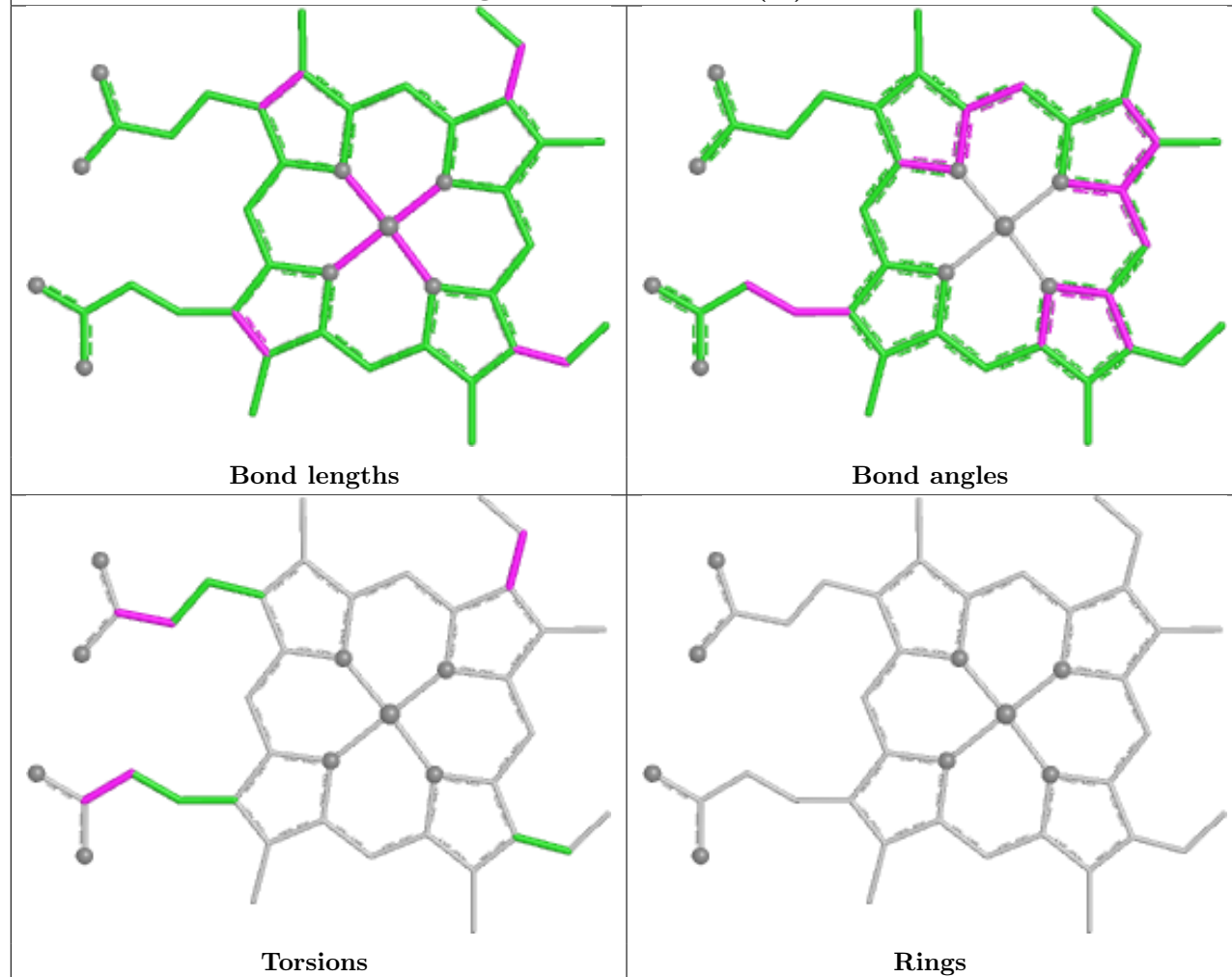
Ligand HEM J 200 (B)



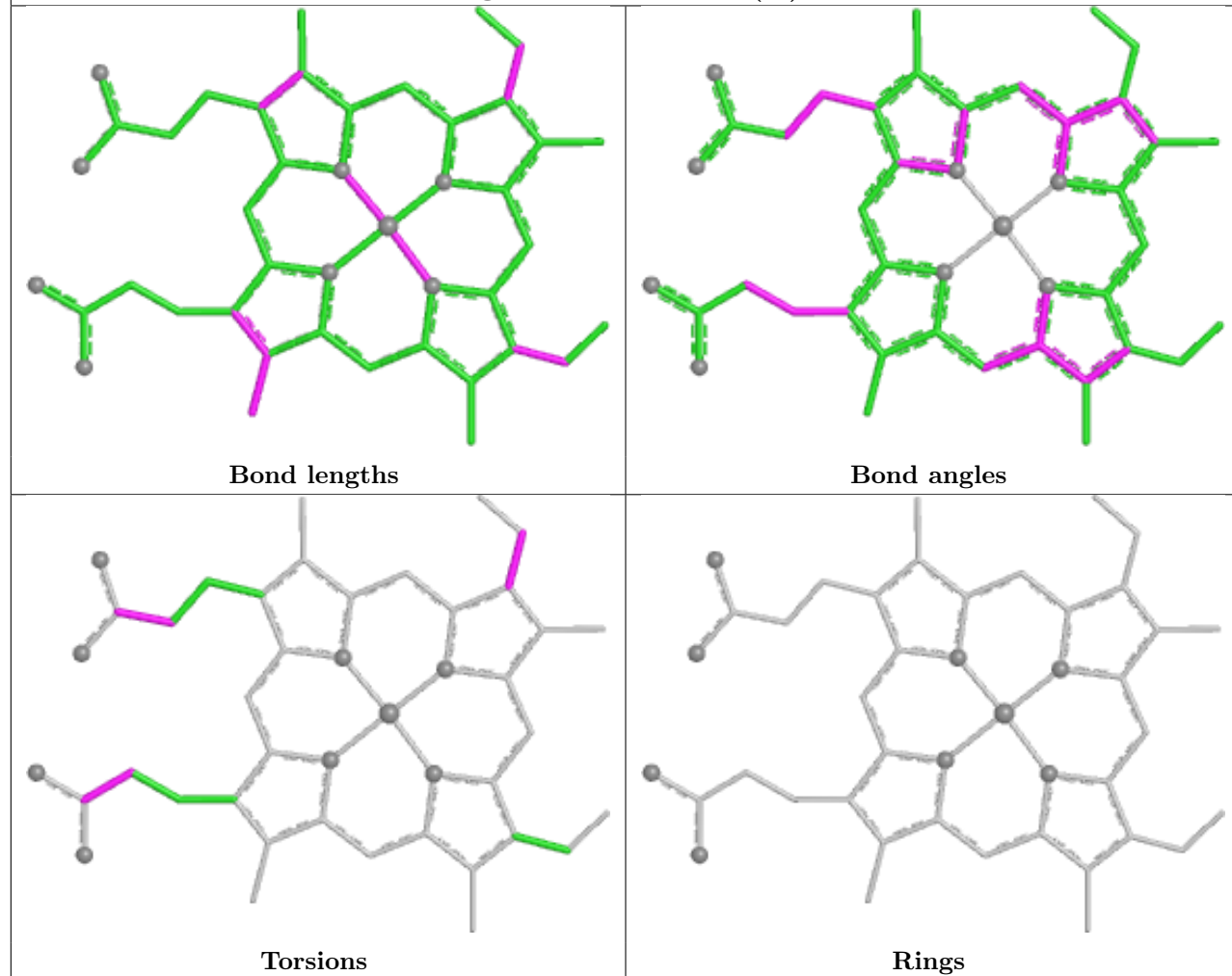
Ligand HEM L 200 (B)



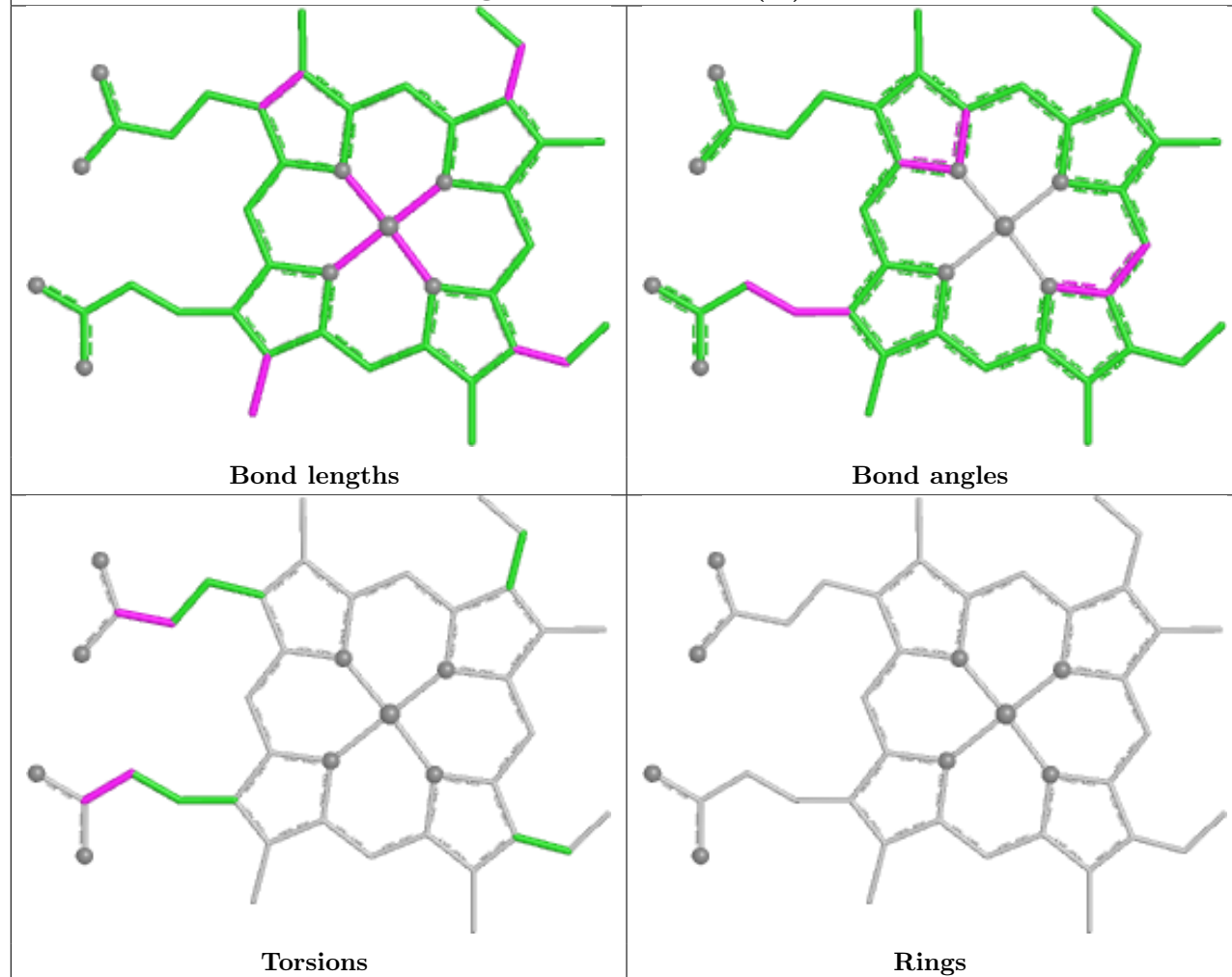
Ligand HEM B 200 (A)



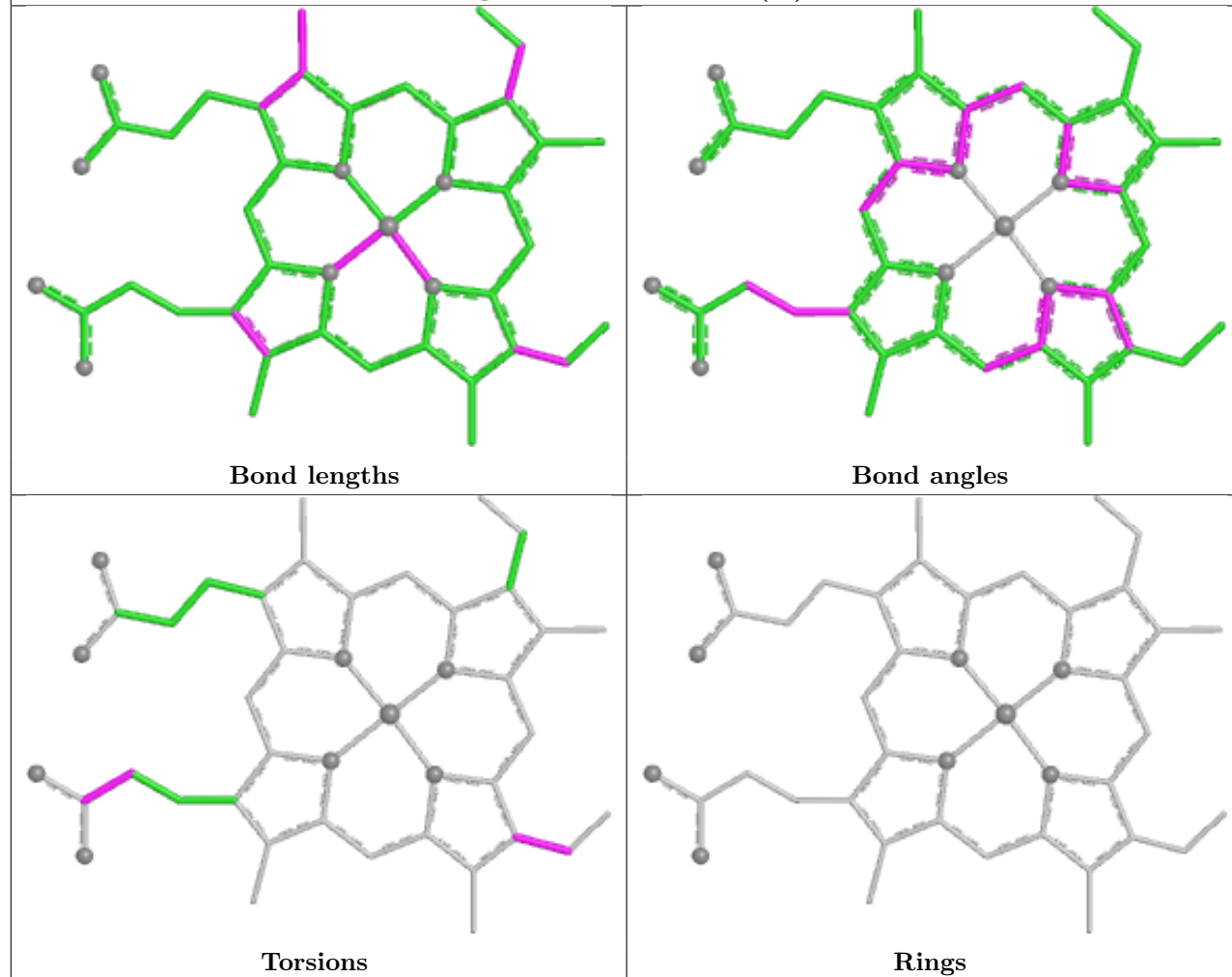
Ligand HEM J 200 (A)



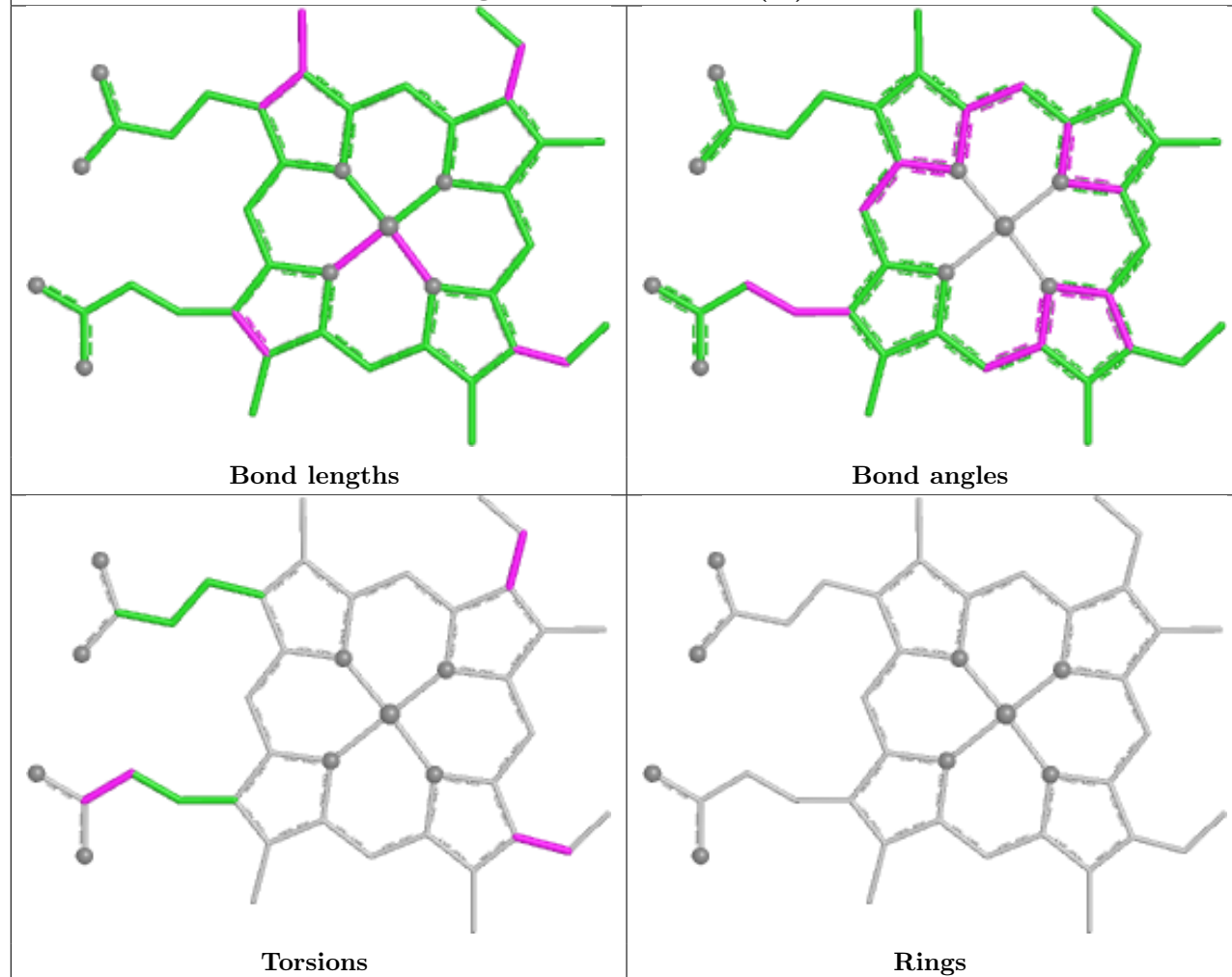
Ligand HEM L 200 (A)



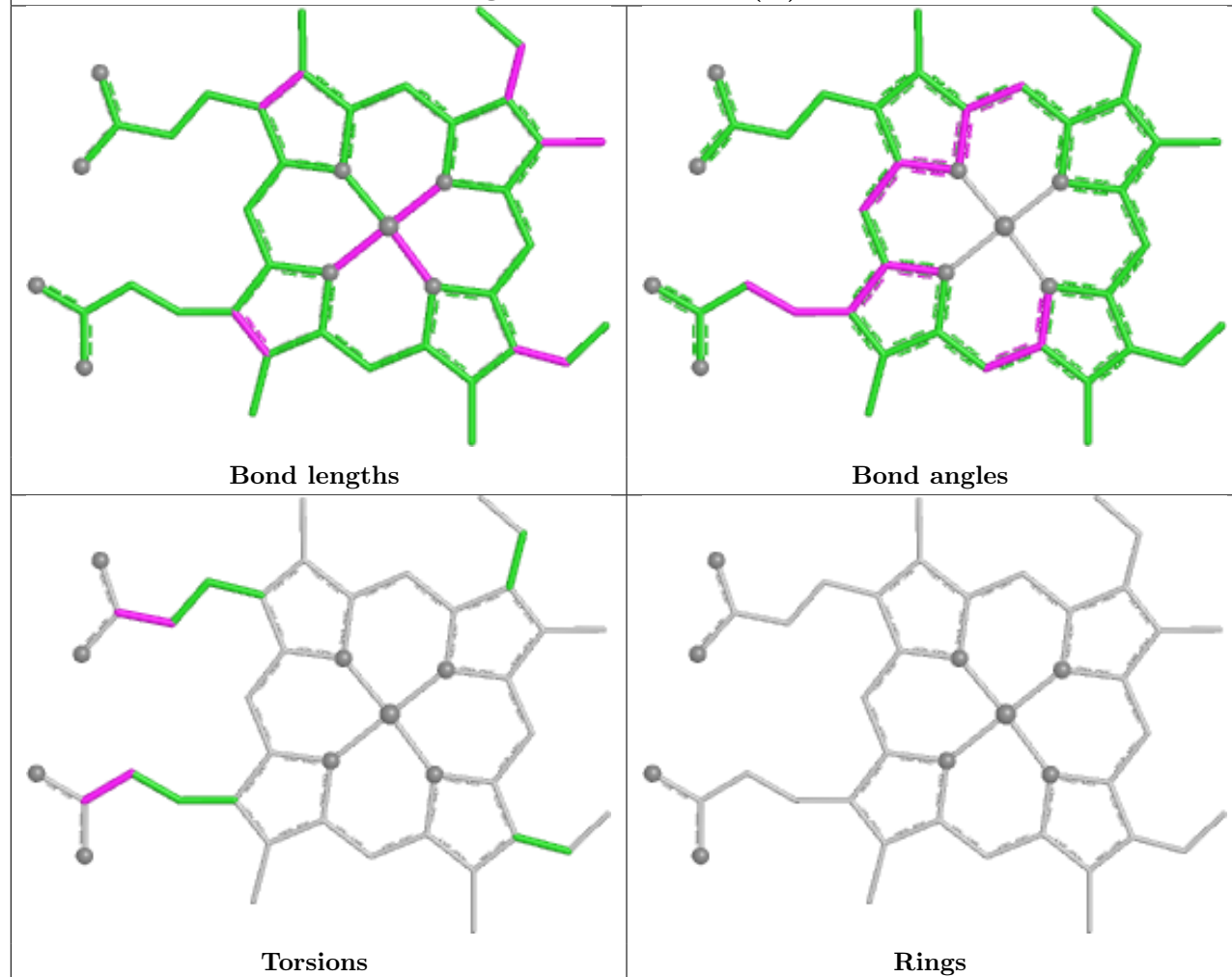
Ligand HEM D 200 (B)



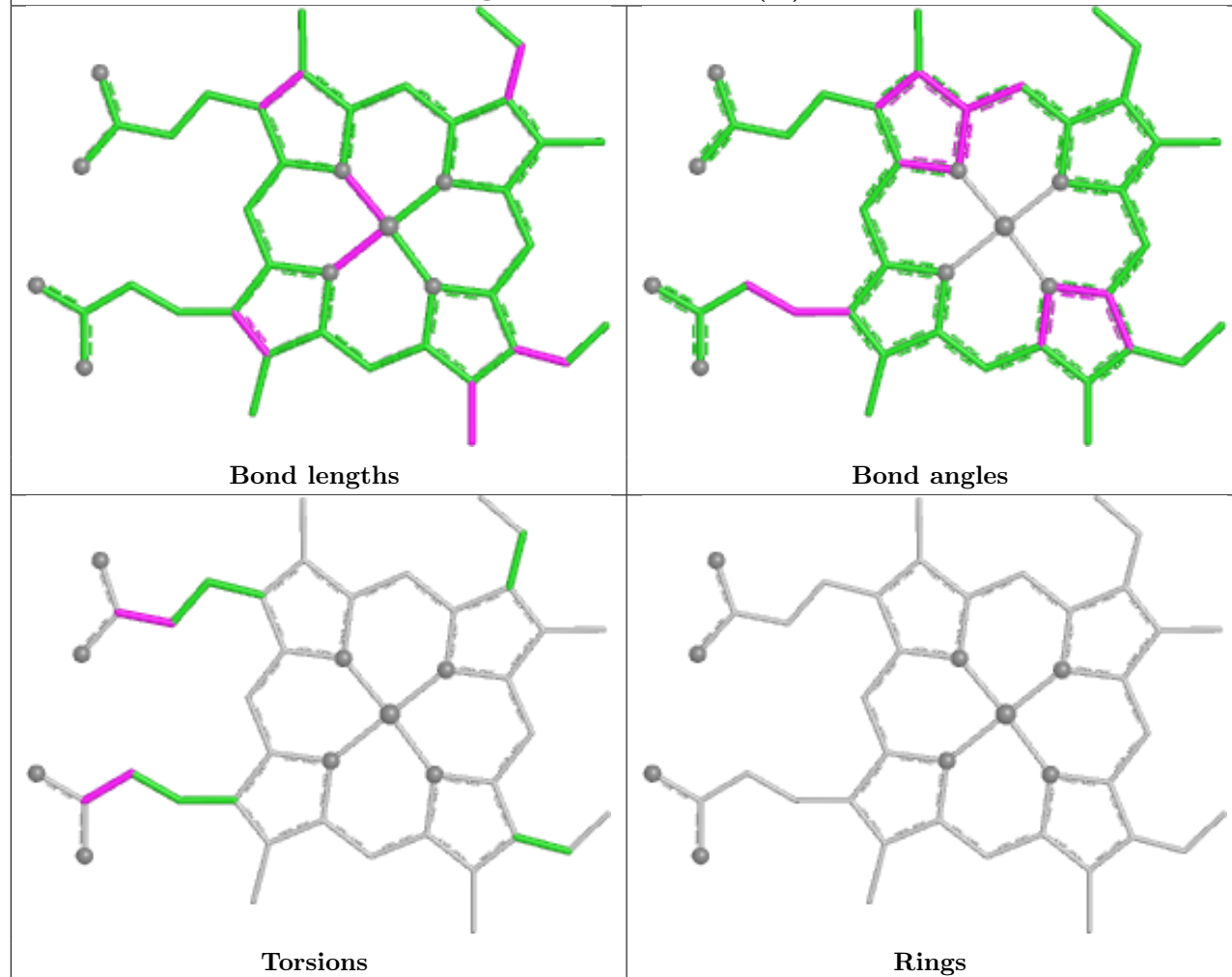
Ligand HEM D 200 (A)



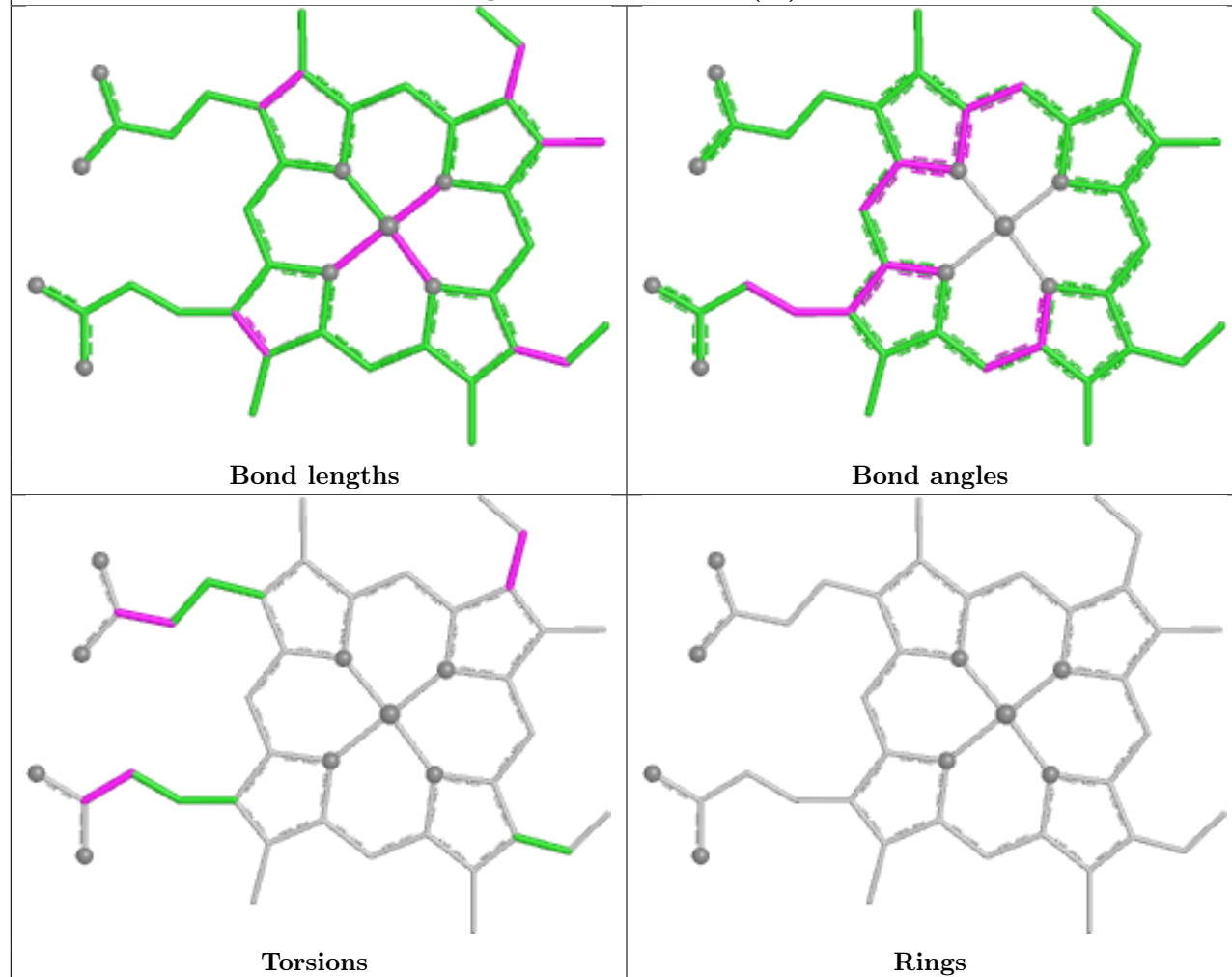
Ligand HEM I 200 (B)



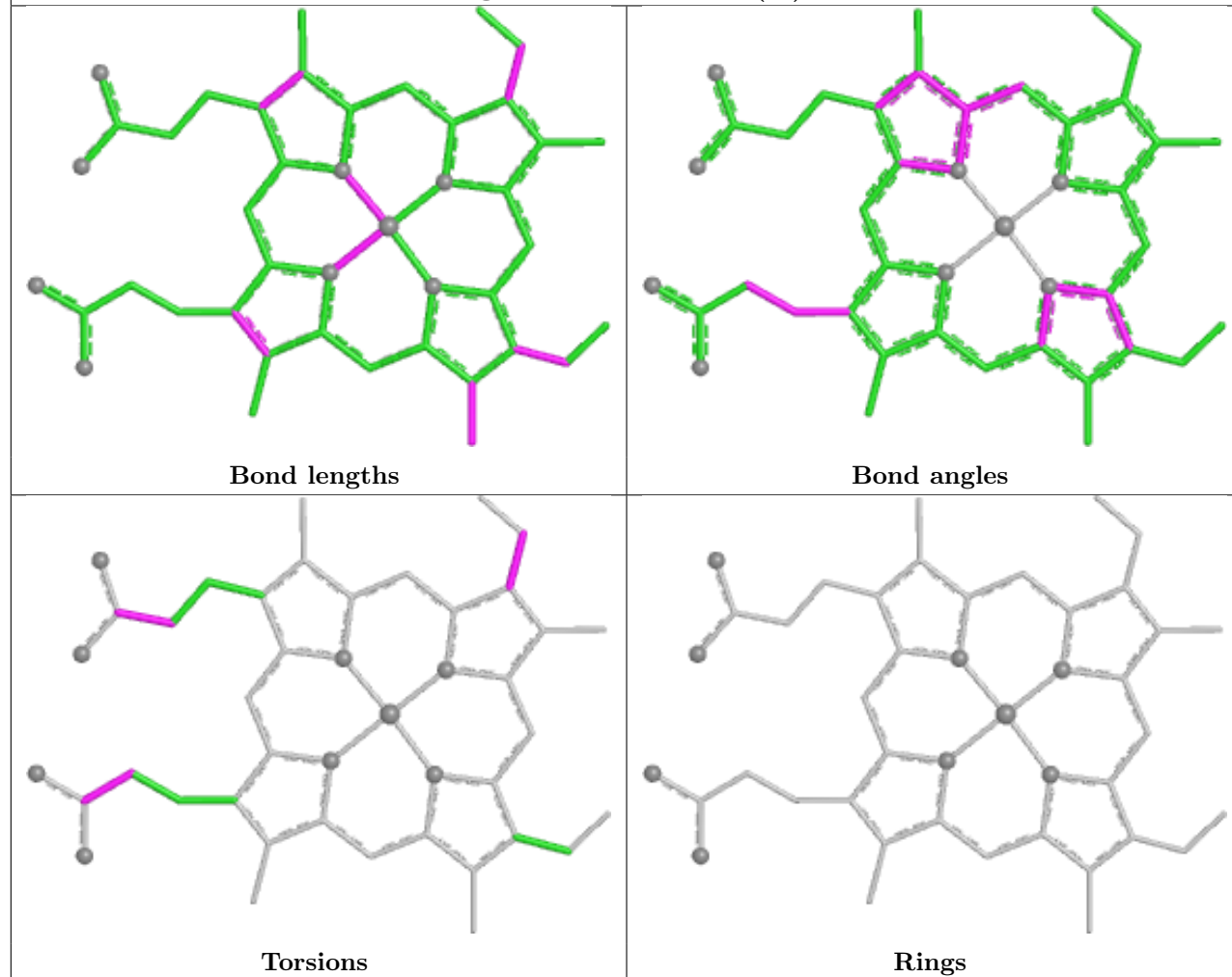
Ligand HEM F 200 (B)



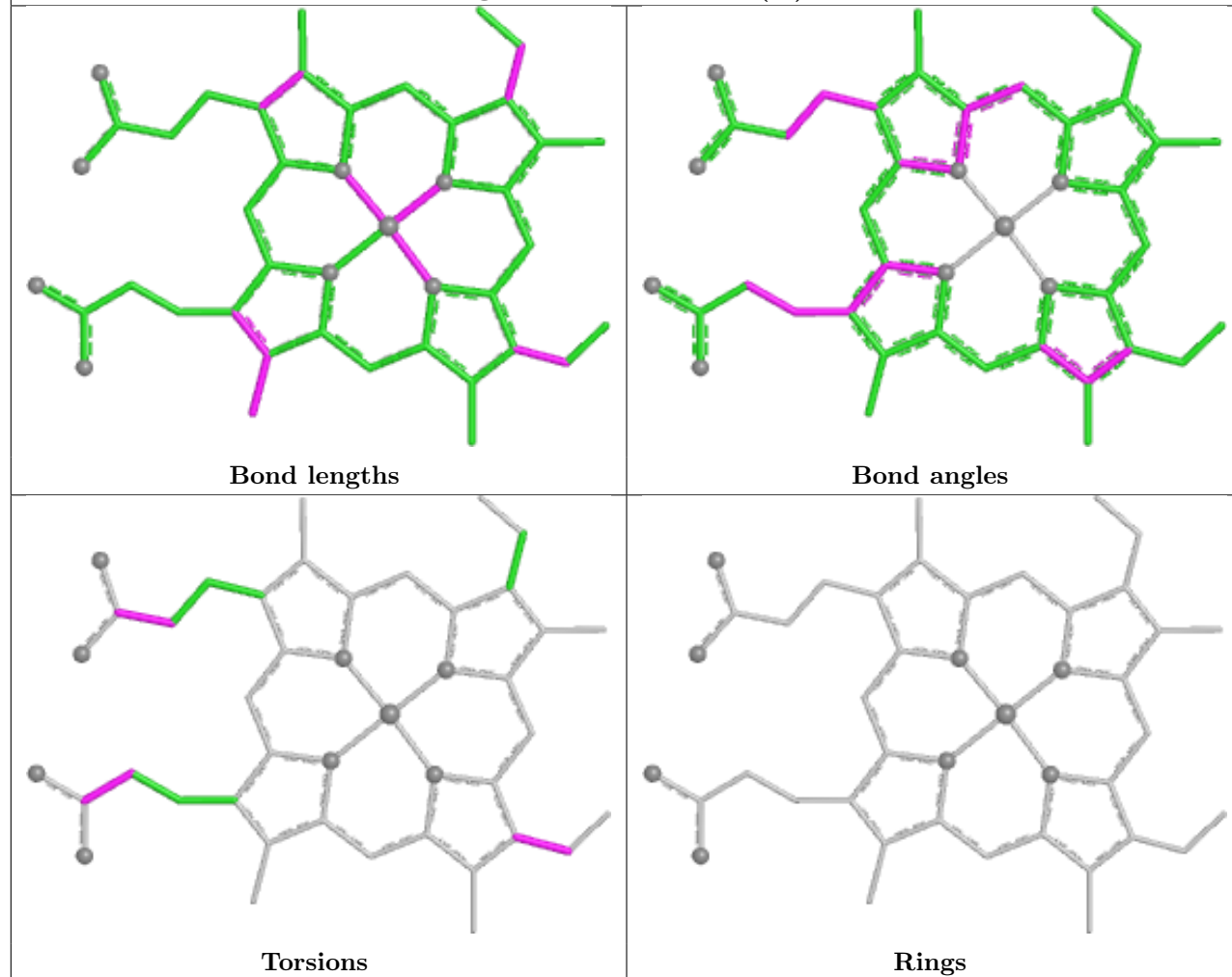
Ligand HEM I 200 (A)



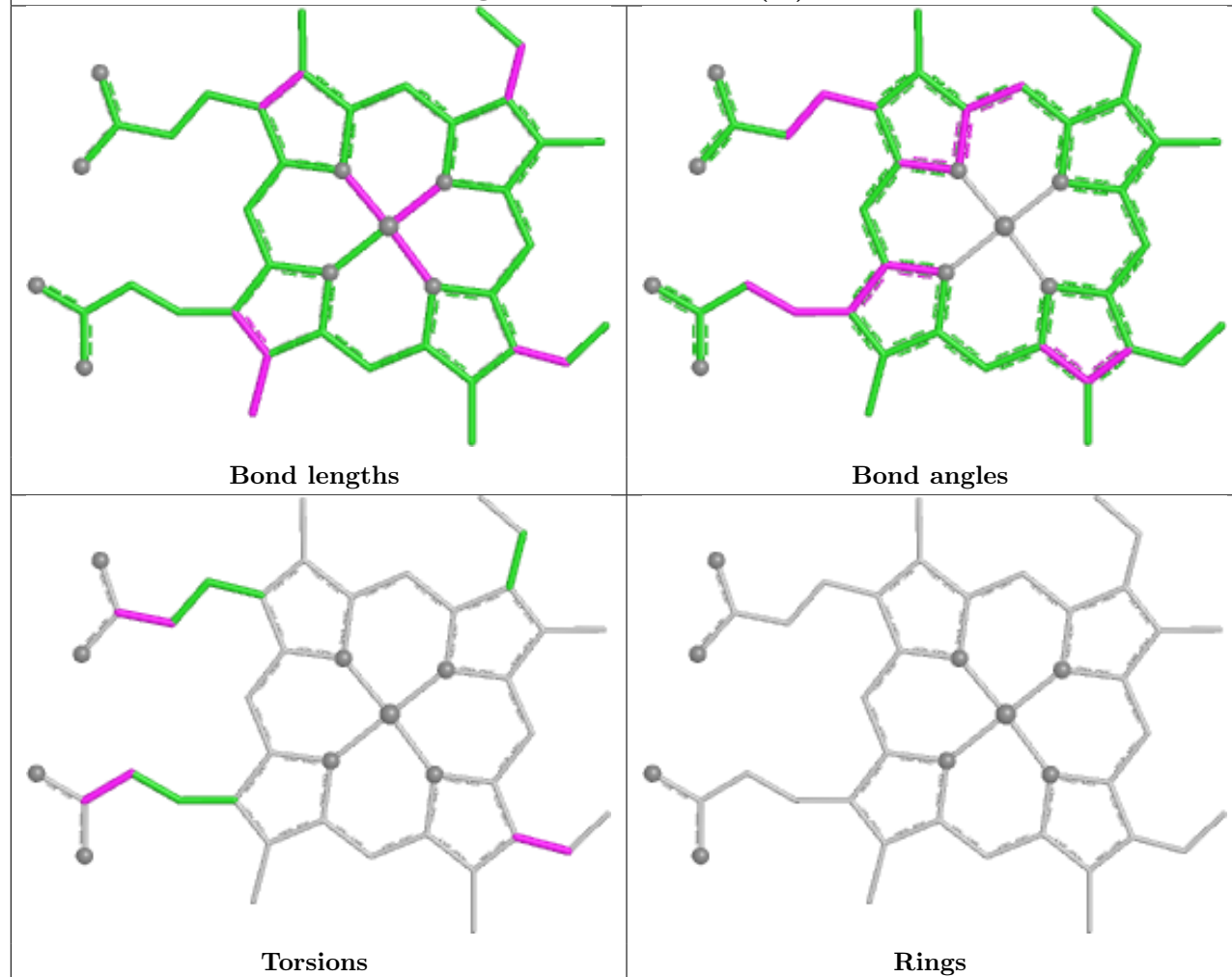
Ligand HEM F 200 (A)



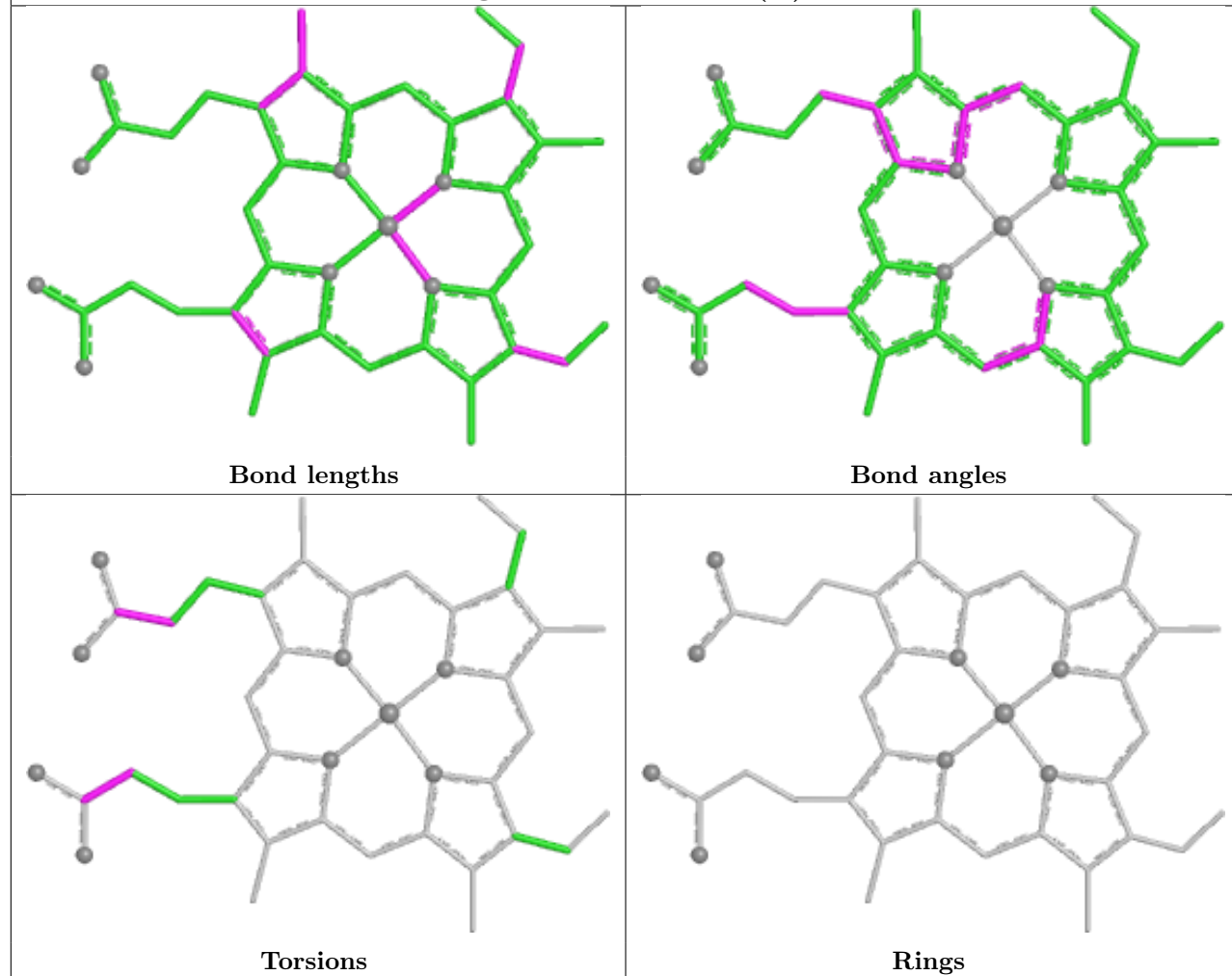
Ligand HEM G 200 (B)



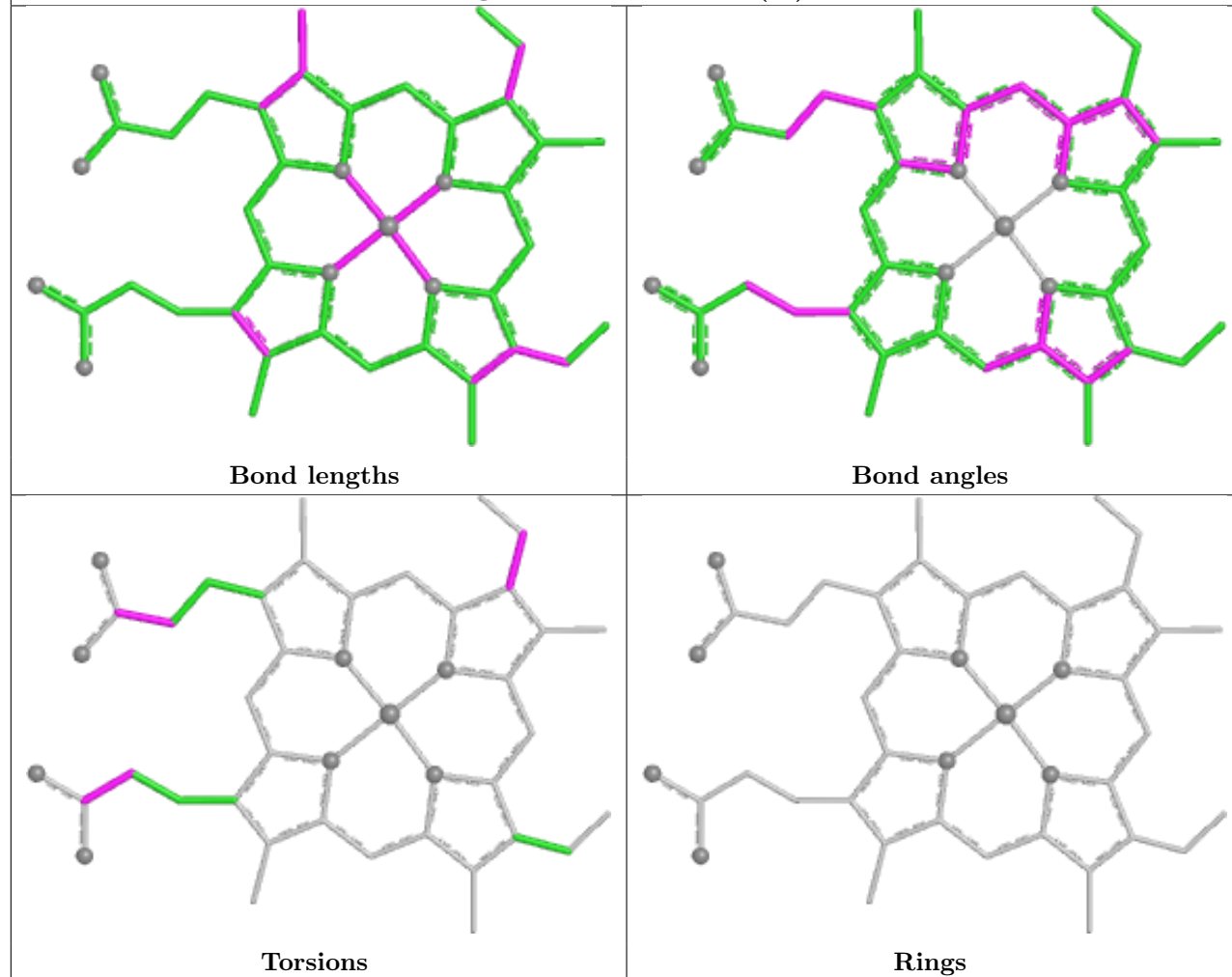
Ligand HEM G 200 (A)



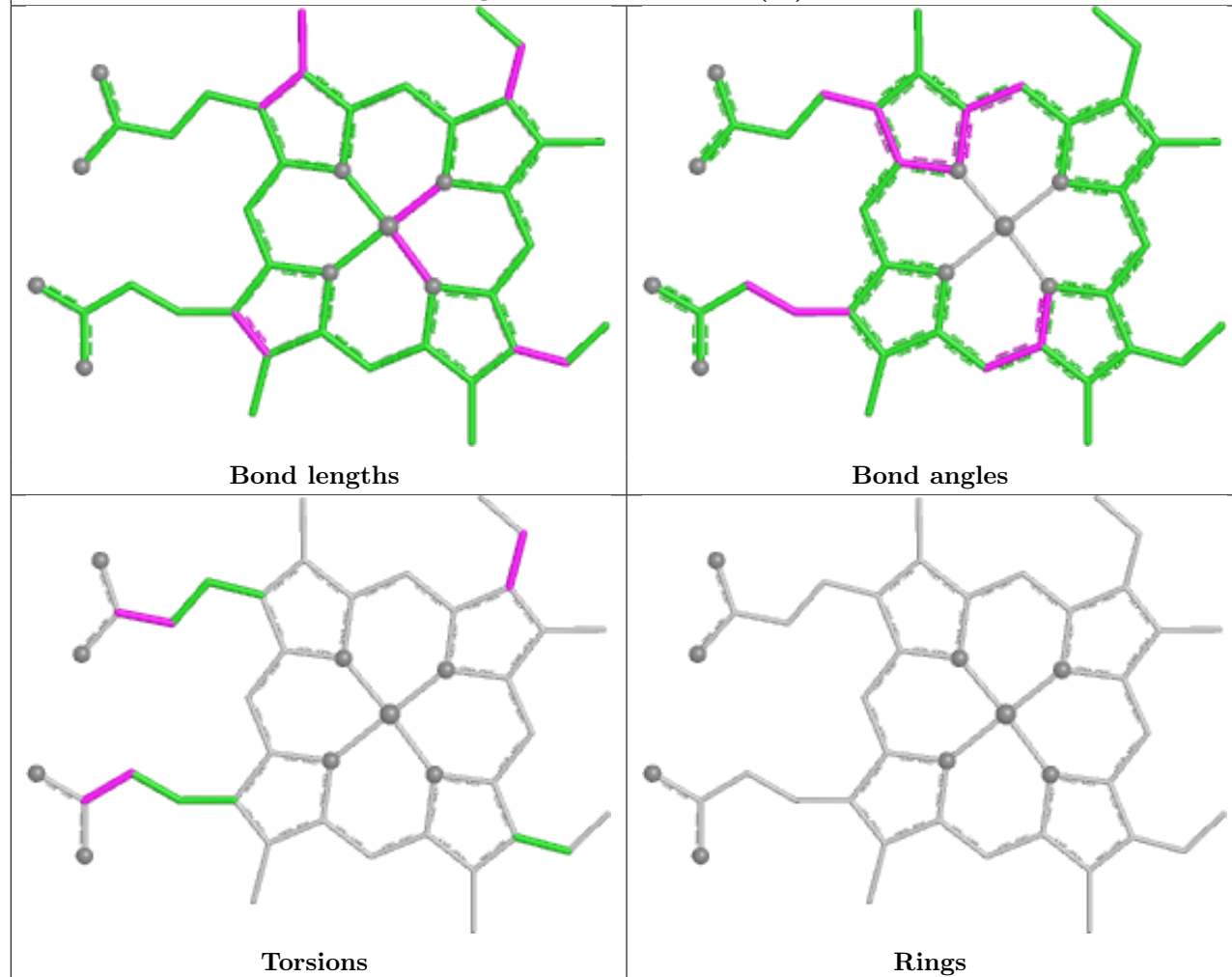
Ligand HEM A 200 (B)



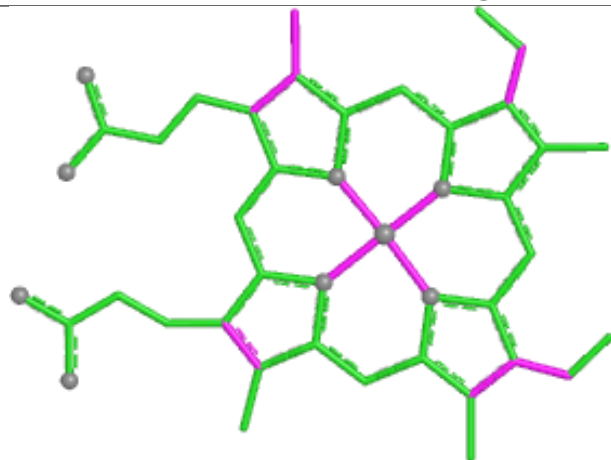
Ligand HEM H 200 (A)



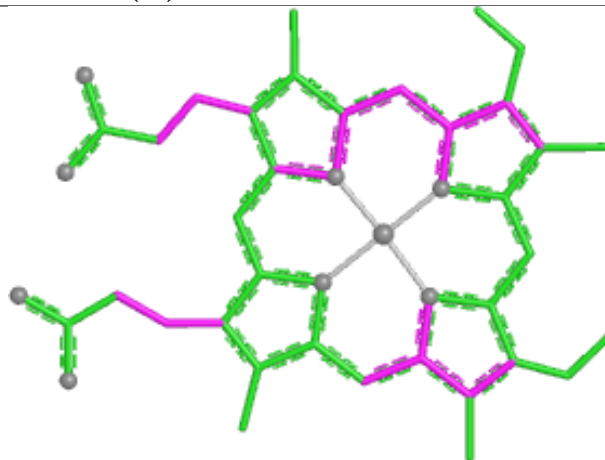
Ligand HEM A 200 (A)



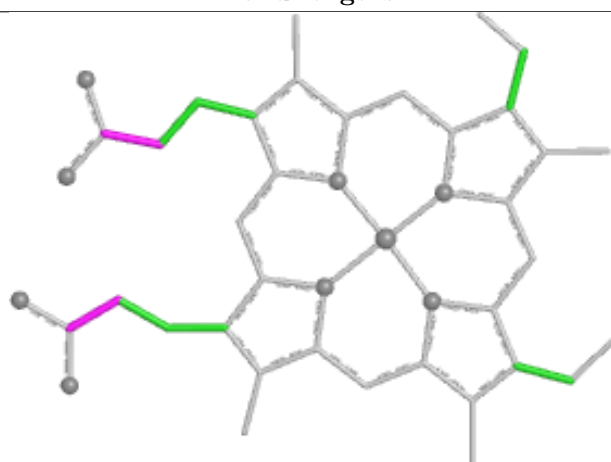
Ligand HEM H 200 (B)



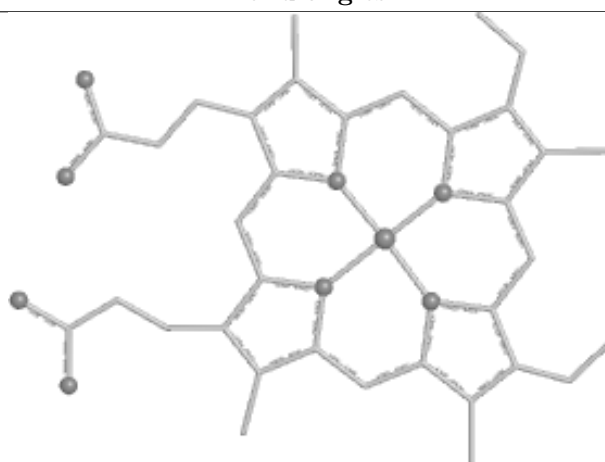
Bond lengths



Bond angles

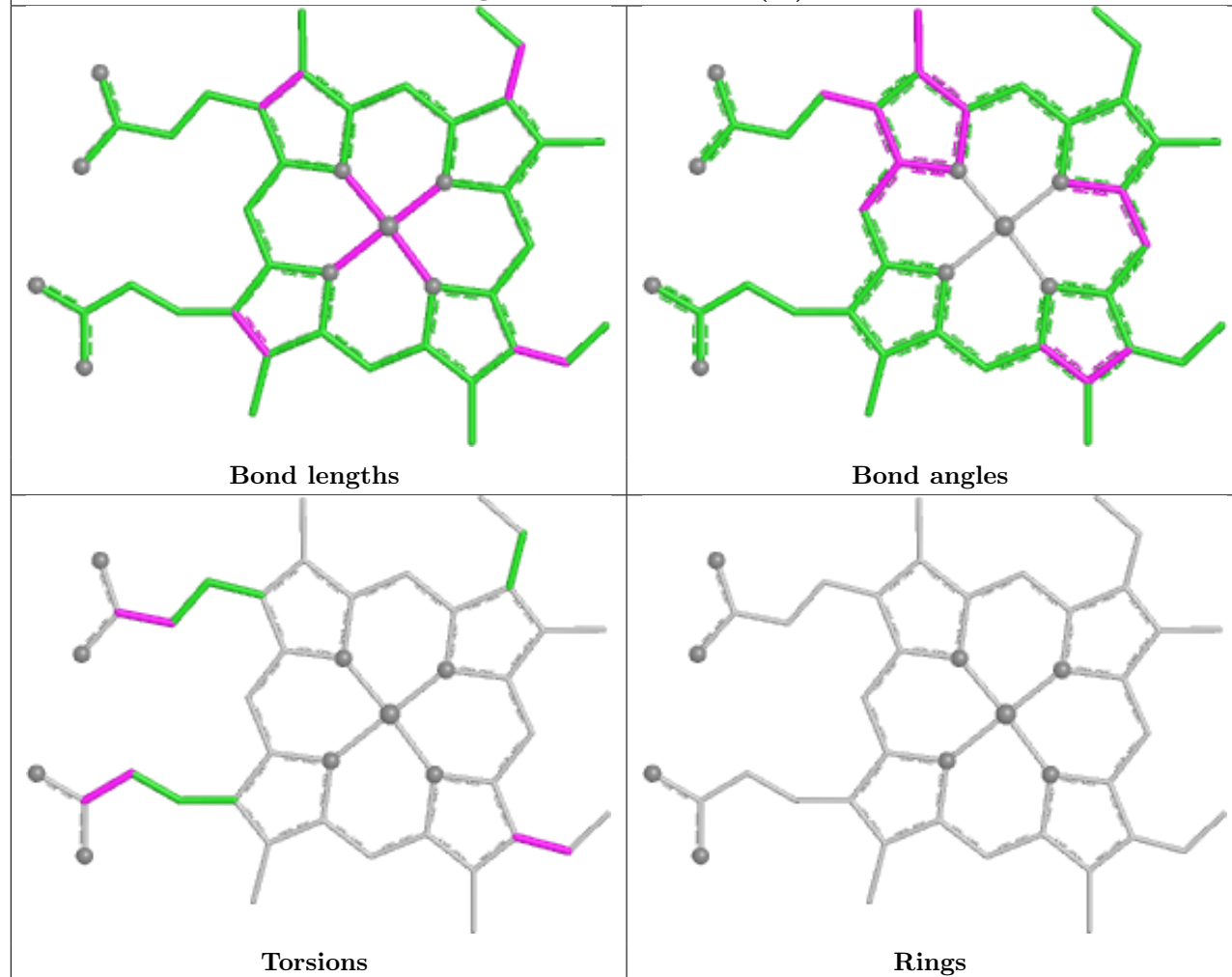


Torsions

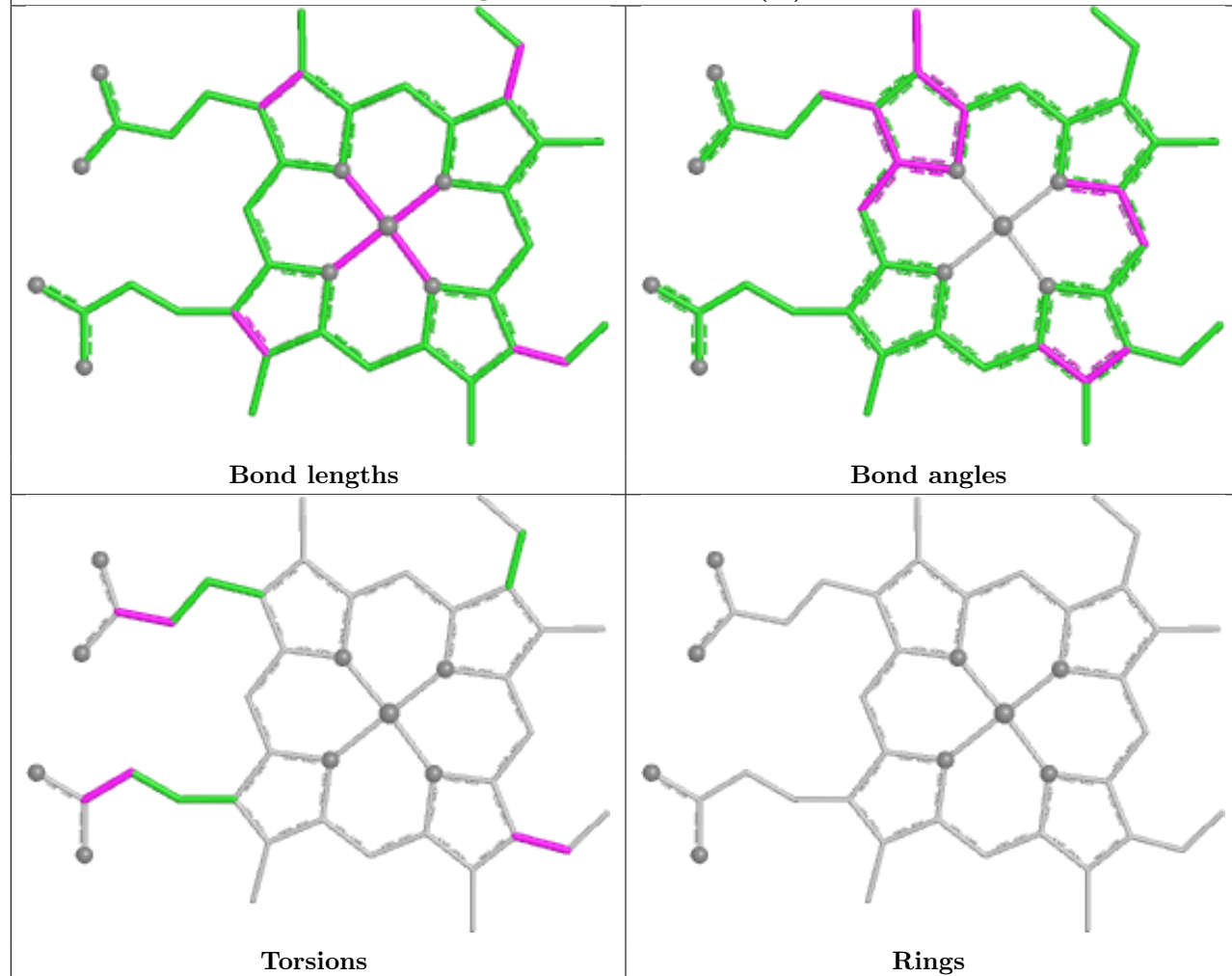


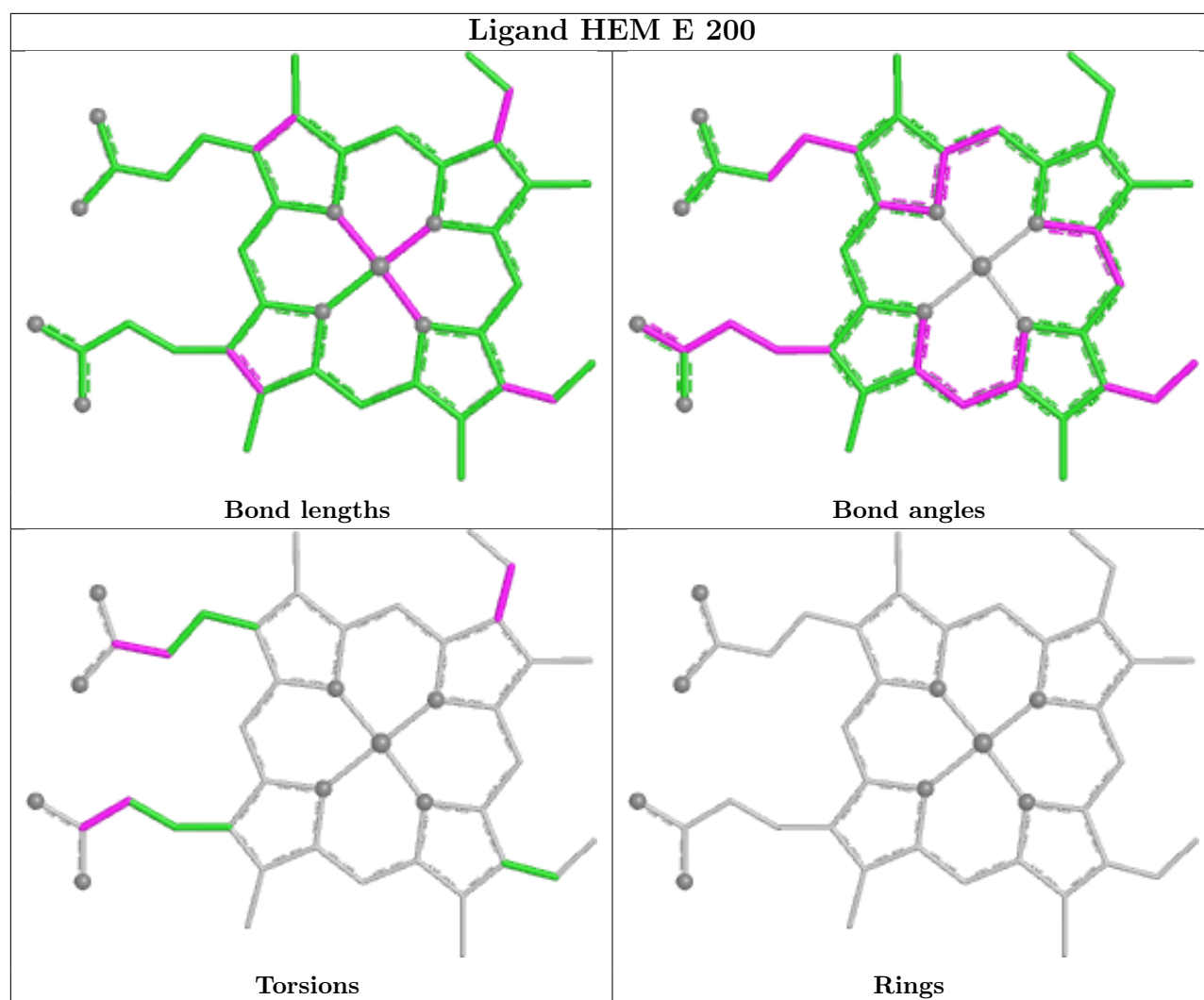
Rings

Ligand HEM K 200 (A)



Ligand HEM K 200 (B)





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

6.1 Protein, DNA and RNA chains

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	158/158 (100%)	-0.52	1 (0%) 85 89	3, 9, 14, 27	18 (11%)
1	B	158/158 (100%)	-0.56	0 100 100	4, 8, 14, 27	19 (12%)
1	C	158/158 (100%)	-0.51	1 (0%) 85 89	4, 8, 13, 29	17 (10%)
1	D	158/158 (100%)	-0.54	1 (0%) 85 89	4, 9, 14, 29	16 (10%)
1	E	158/158 (100%)	-0.57	0 100 100	4, 8, 14, 27	18 (11%)
1	F	158/158 (100%)	-0.53	1 (0%) 85 89	3, 8, 14, 27	17 (10%)
1	G	158/158 (100%)	-0.54	0 100 100	3, 8, 15, 30	19 (12%)
1	H	158/158 (100%)	-0.53	1 (0%) 85 89	3, 9, 14, 29	13 (8%)
1	I	158/158 (100%)	-0.55	0 100 100	4, 8, 14, 25	18 (11%)
1	J	158/158 (100%)	-0.51	1 (0%) 85 89	4, 9, 14, 28	14 (8%)
1	K	158/158 (100%)	-0.52	1 (0%) 85 89	4, 9, 14, 30	16 (10%)
1	L	158/158 (100%)	-0.51	1 (0%) 85 89	3, 9, 15, 28	16 (10%)
All	All	1896/1896 (100%)	-0.53	8 (0%) 88 92	3, 8, 14, 30	201 (10%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	GLY	4.8
1	C	158	GLY	4.2
1	D	158	GLY	3.2
1	K	158	GLY	2.9
1	F	158	GLY	2.7
1	H	158	GLY	2.5
1	J	158	GLY	2.1
1	L	158	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BTB	I	1162	8/14	0.79	0.17	30,32,34,35	1
5	BTB	L	1161	8/14	0.80	0.18	30,32,32,32	0
5	BTB	K	1161	8/14	0.87	0.15	20,31,32,32	0
4	ACT	D	1160	4/4	0.88	0.13	19,21,22,22	0
5	BTB	D	1161	8/14	0.89	0.13	24,32,32,34	0
4	ACT	L	1160	4/4	0.90	0.12	18,21,21,21	0
4	ACT	K	1160	4/4	0.91	0.12	18,19,20,20	0
3	SO4	K	1159	5/5	0.92	0.19	16,16,18,20	5
4	ACT	A	1160	4/4	0.92	0.11	17,20,20,21	0
3	SO4	A	1159	5/5	0.92	0.14	25,26,27,29	5
4	ACT	F	1160	4/4	0.92	0.11	18,22,22,23	0
3	SO4	F	1159	5/5	0.92	0.17	15,16,19,20	5
3	SO4	E	1160	5/5	0.93	0.13	21,22,25,26	5
3	SO4	B	1161	5/5	0.93	0.18	15,15,19,20	5
3	SO4	G	1159	5/5	0.93	0.15	18,19,22,23	5
3	SO4	H	1160	5/5	0.93	0.17	15,15,19,20	5
3	SO4	I	1159	5/5	0.93	0.15	19,19,23,24	5
3	SO4	J	1159	5/5	0.93	0.12	24,25,29,30	5
3	SO4	C	1159	5/5	0.93	0.13	19,20,23,23	5
3	SO4	D	1159	5/5	0.93	0.21	17,18,20,20	5
4	ACT	J	1160	4/4	0.94	0.10	16,19,19,21	0
3	SO4	L	1159	5/5	0.95	0.10	23,25,28,30	5
3	SO4	I	1161	5/5	0.95	0.09	11,13,16,17	5
4	ACT	C	1161	4/4	0.95	0.08	17,19,19,20	0
2	HEM	D	200[B]	43/43	0.95	0.12	16,18,20,23	43
2	HEM	D	200[A]	43/43	0.95	0.12	16,18,20,23	43
4	ACT	G	1160	4/4	0.95	0.08	19,21,21,22	0

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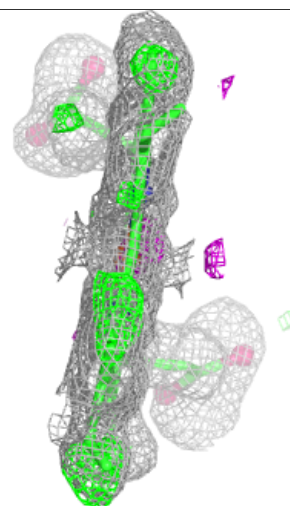
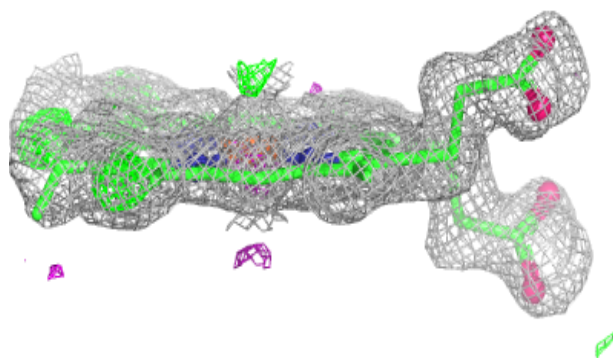
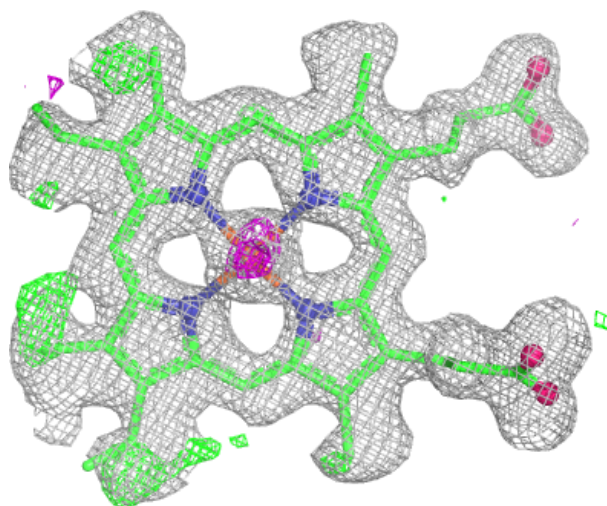
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	I	1160	4/4	0.95	0.10	15,17,18,18	0
2	HEM	G	200[A]	43/43	0.96	0.09	10,15,18,21	43
4	ACT	E	1161	4/4	0.96	0.07	17,18,19,19	0
2	HEM	G	200[B]	43/43	0.96	0.09	10,15,18,19	43
2	HEM	I	200[A]	43/43	0.96	0.10	10,13,18,19	43
4	ACT	H	1161	4/4	0.96	0.07	16,17,17,18	0
2	HEM	I	200[B]	43/43	0.96	0.10	10,13,17,19	43
2	HEM	L	200[A]	43/43	0.96	0.08	8,12,18,20	43
2	HEM	L	200[B]	43/43	0.96	0.08	8,11,18,20	43
2	HEM	B	200[A]	43/43	0.96	0.10	8,13,17,18	43
3	SO4	B	1159	5/5	0.96	0.08	14,15,18,20	5
2	HEM	B	200[B]	43/43	0.96	0.10	8,13,17,17	43
2	HEM	F	200[A]	43/43	0.96	0.09	7,10,17,18	43
2	HEM	F	200[B]	43/43	0.96	0.09	7,10,17,18	43
4	ACT	B	1162	4/4	0.97	0.07	17,19,20,20	0
3	SO4	C	1160	5/5	0.97	0.07	12,15,16,18	5
2	HEM	E	200	43/43	0.97	0.08	5,7,11,14	43
2	HEM	K	200[A]	43/43	0.97	0.07	7,10,15,18	43
2	HEM	K	200[B]	43/43	0.97	0.07	7,10,15,18	43
2	HEM	H	200[B]	43/43	0.98	0.07	2,6,12,13	43
2	HEM	C	200[B]	43/43	0.98	0.07	2,5,12,14	43
2	HEM	A	200[A]	43/43	0.98	0.07	3,7,13,15	43
2	HEM	J	200[A]	43/43	0.98	0.08	4,8,14,17	43
2	HEM	J	200[B]	43/43	0.98	0.08	4,8,14,15	43
2	HEM	A	200[B]	43/43	0.98	0.07	3,7,13,14	43
2	HEM	C	200[A]	43/43	0.98	0.07	2,5,12,14	43
2	HEM	H	200[A]	43/43	0.98	0.07	2,6,12,13	43
3	SO4	E	1159	5/5	0.99	0.04	10,10,11,13	0
3	SO4	H	1159	5/5	0.99	0.04	10,10,11,13	0
3	SO4	C	1158	5/5	0.99	0.03	10,10,11,12	0
3	SO4	B	1160	5/5	0.99	0.04	10,10,12,13	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.

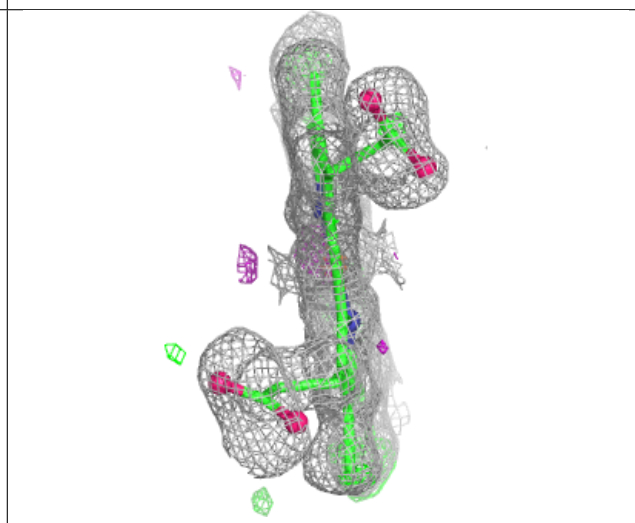
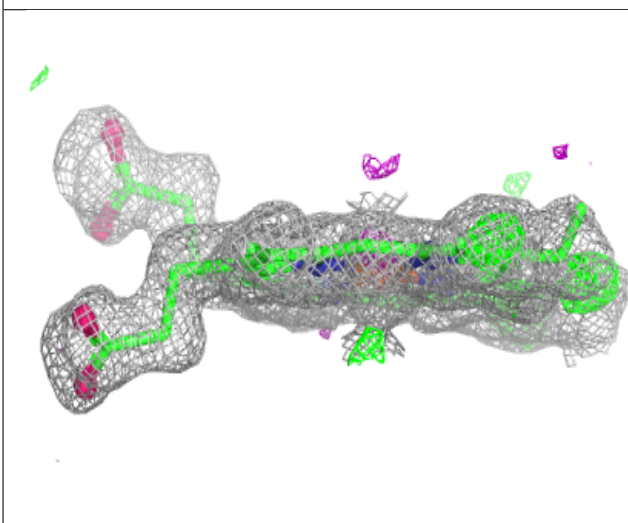
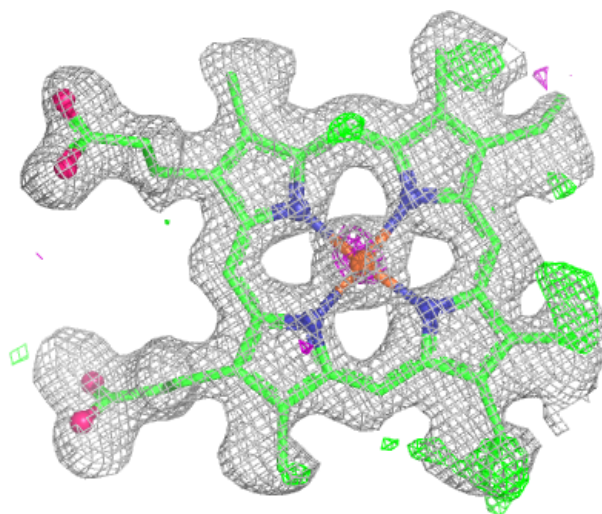
Electron density around HEM D 200 (B):

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



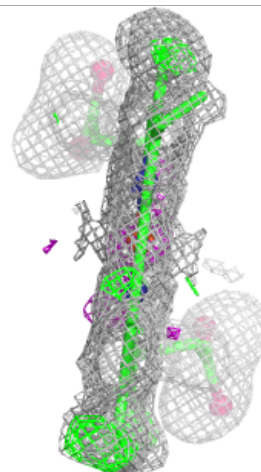
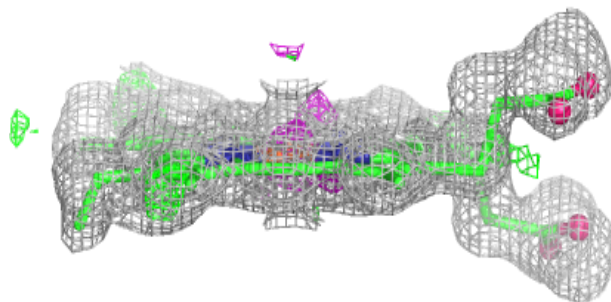
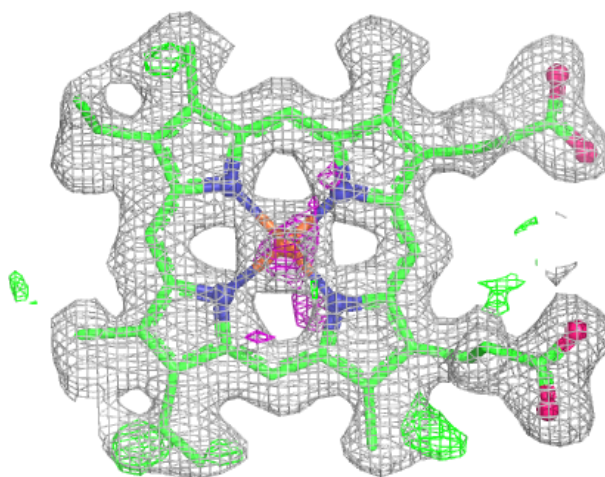
Electron density around HEM D 200 (A):

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



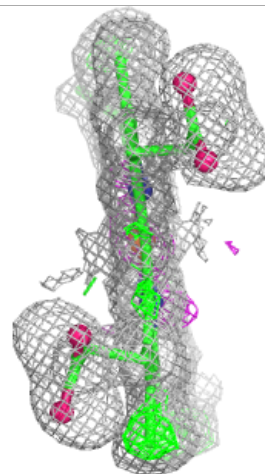
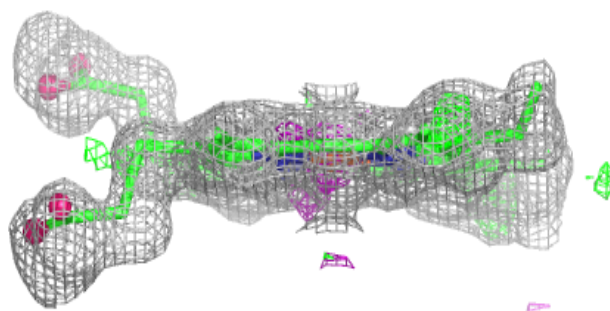
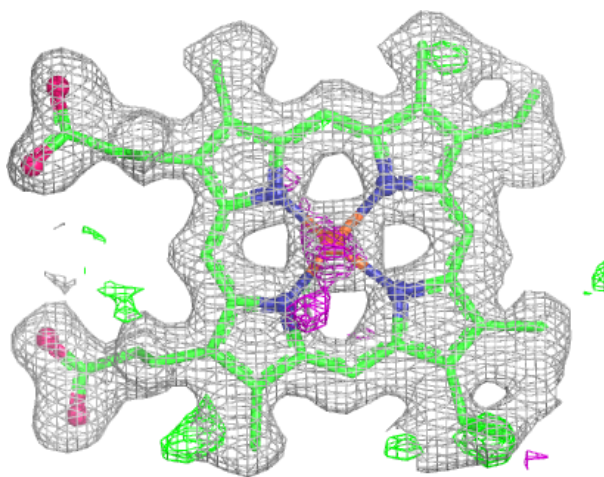
Electron density around HEM G 200 (A):

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



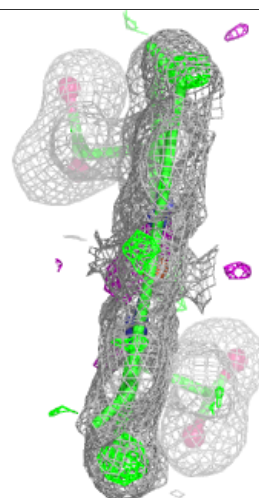
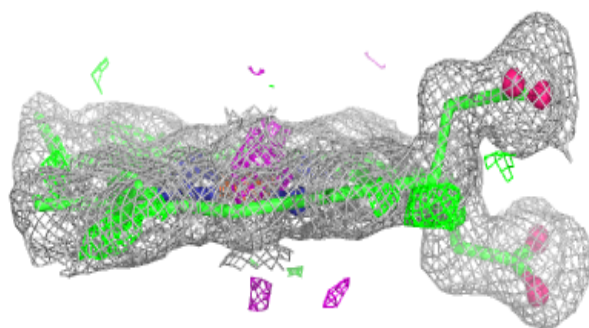
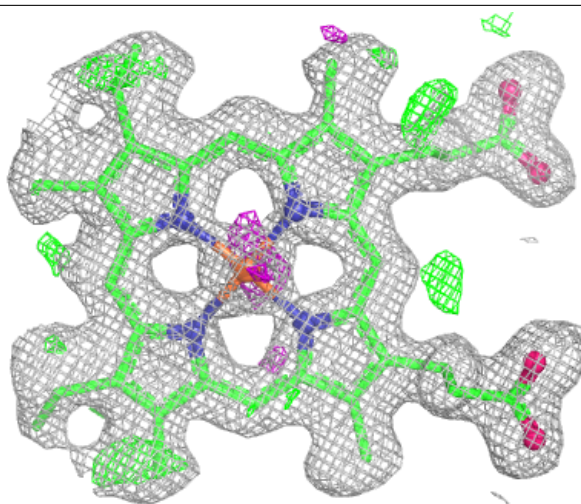
Electron density around HEM G 200 (B):

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



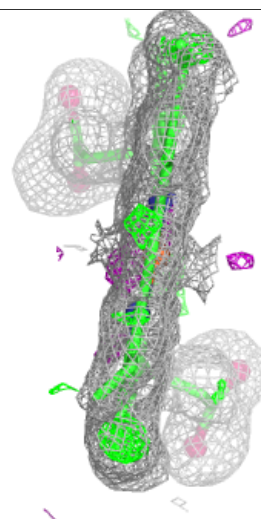
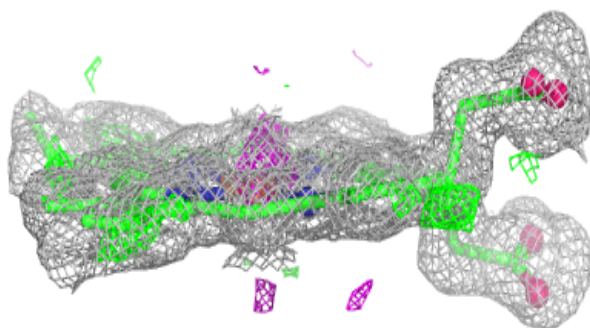
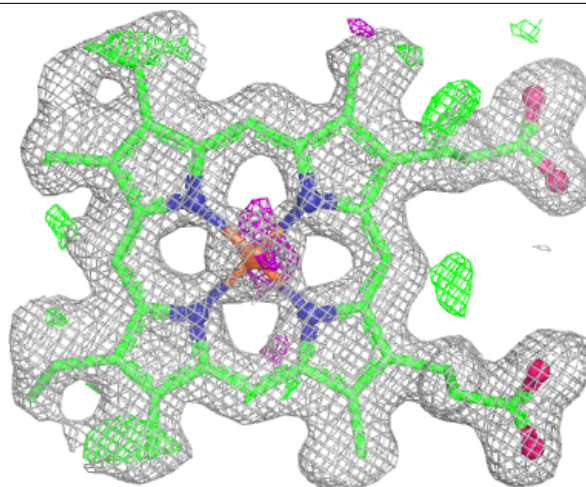
Electron density around HEM I 200 (A):

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



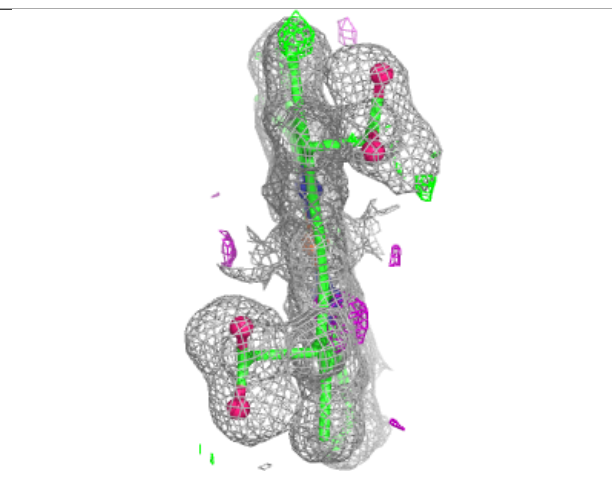
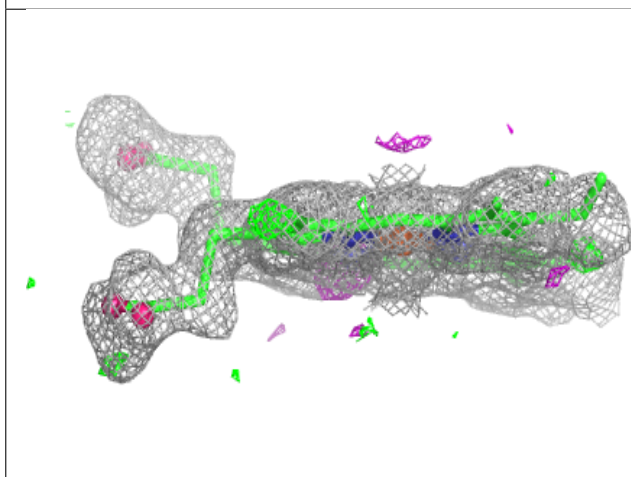
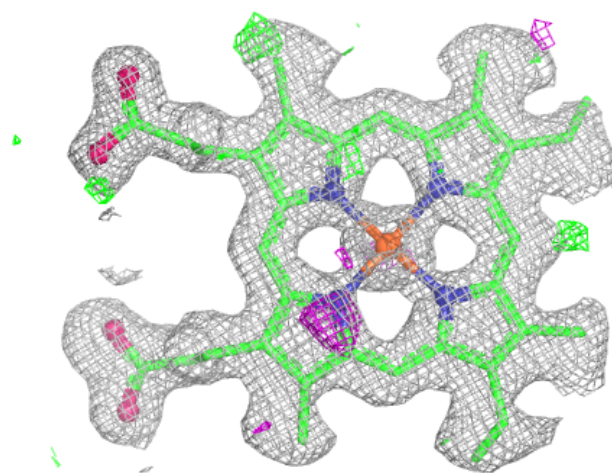
Electron density around HEM I 200 (B):

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and green (positive)



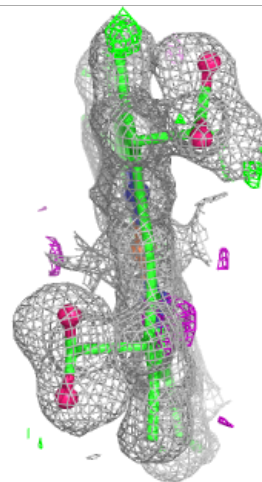
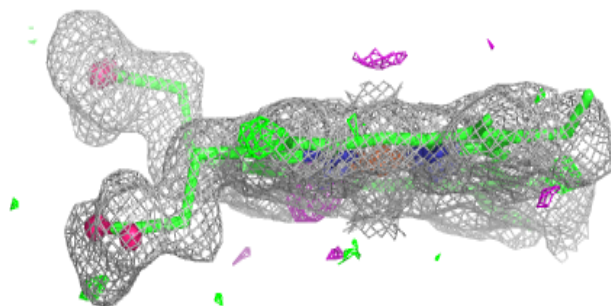
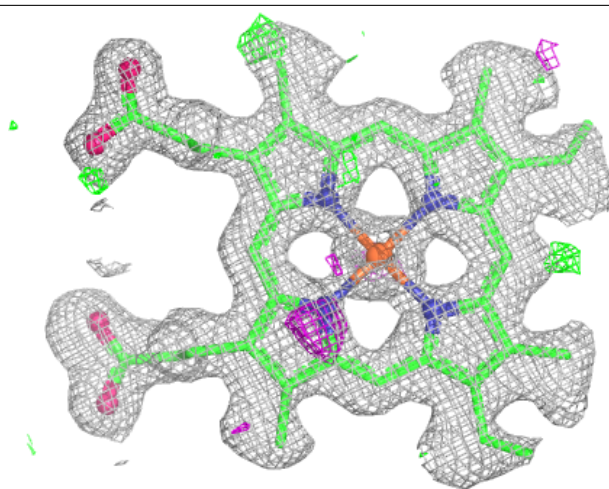
Electron density around HEM L 200 (A):

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



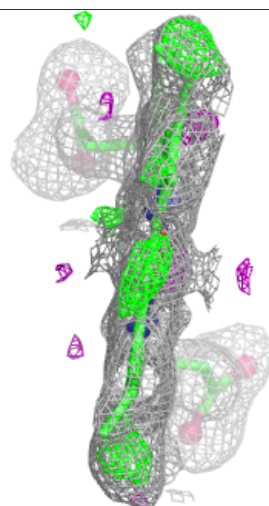
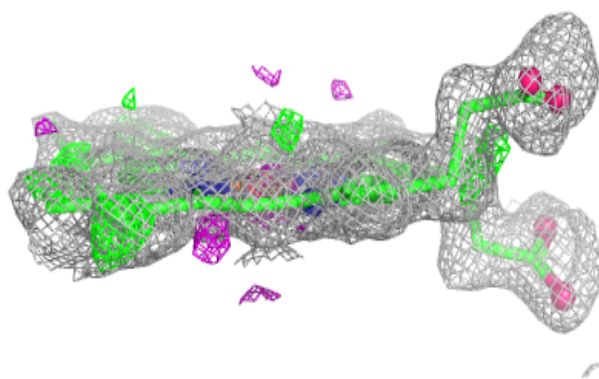
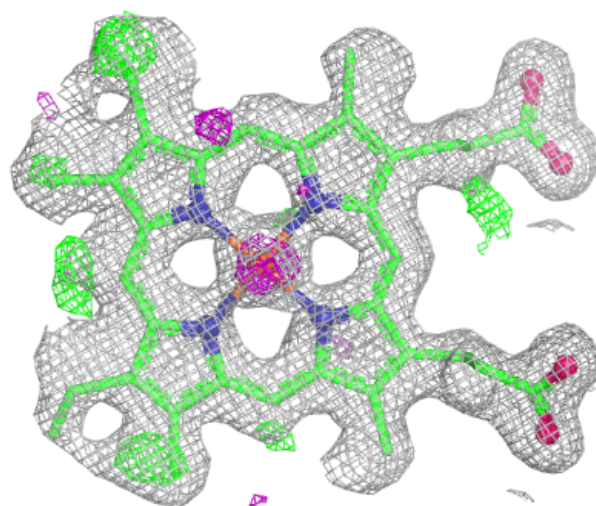
Electron density around HEM L 200 (B):

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



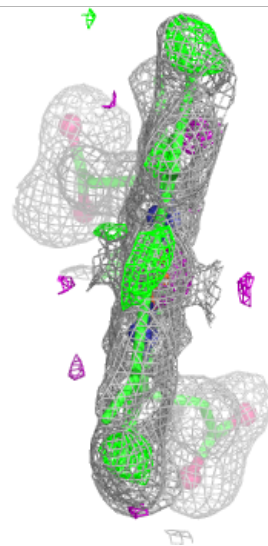
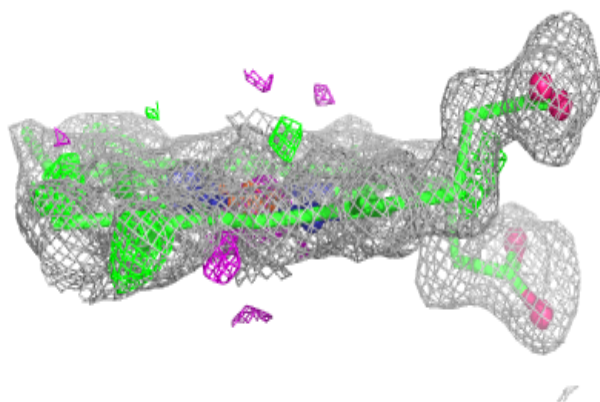
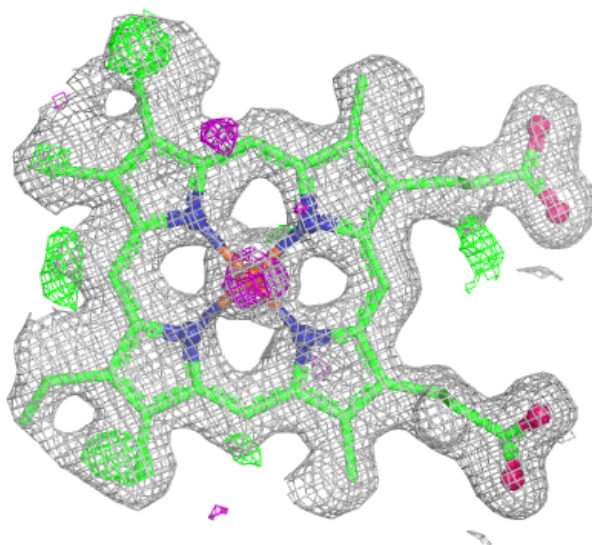
Electron density around HEM B 200 (A):

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



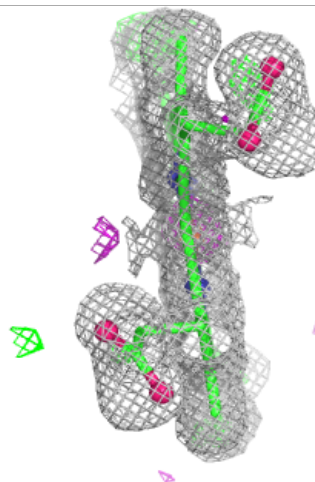
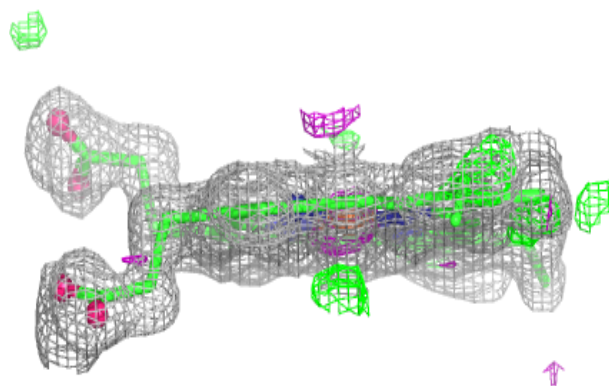
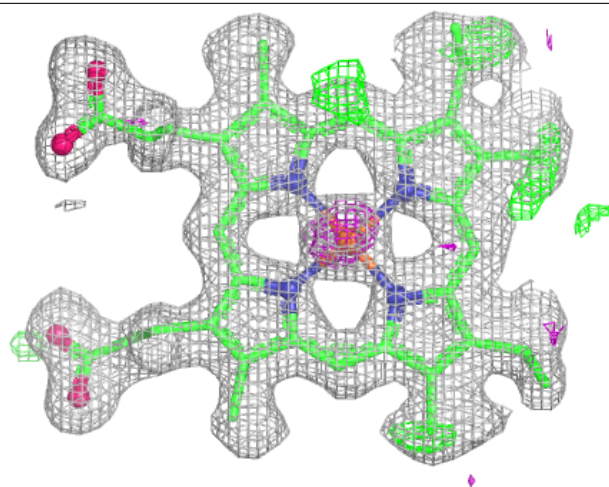
Electron density around HEM B 200 (B):

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



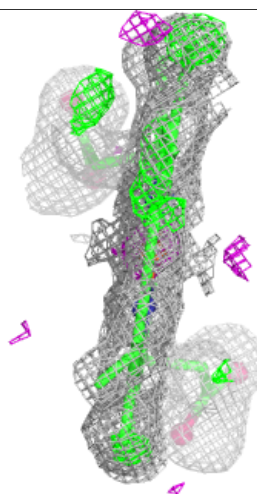
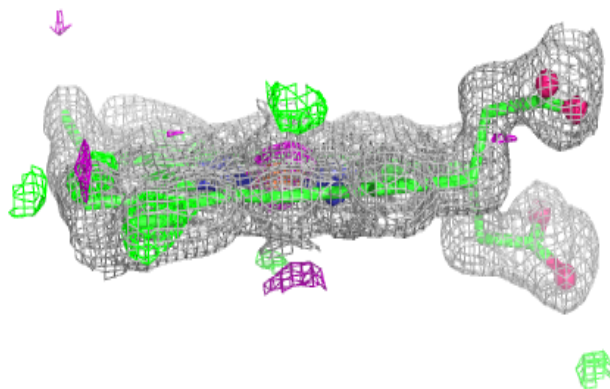
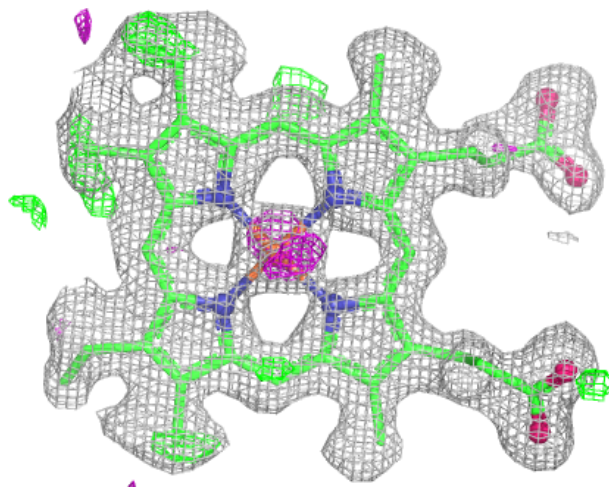
Electron density around HEM F 200 (A):

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and green (positive)



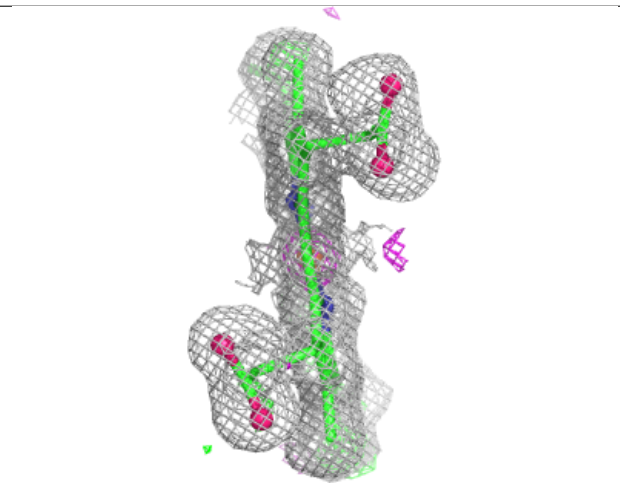
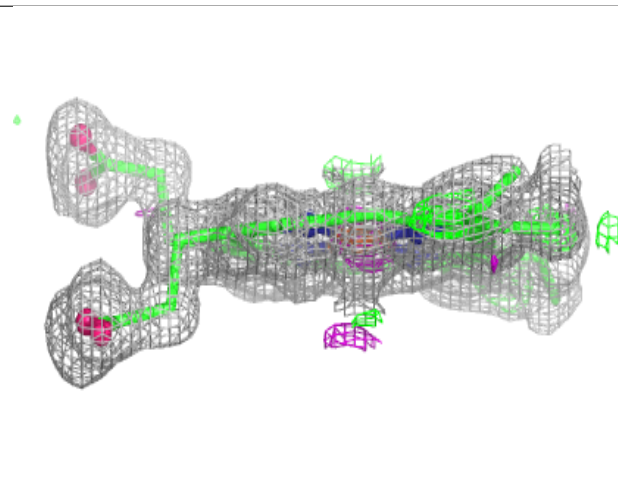
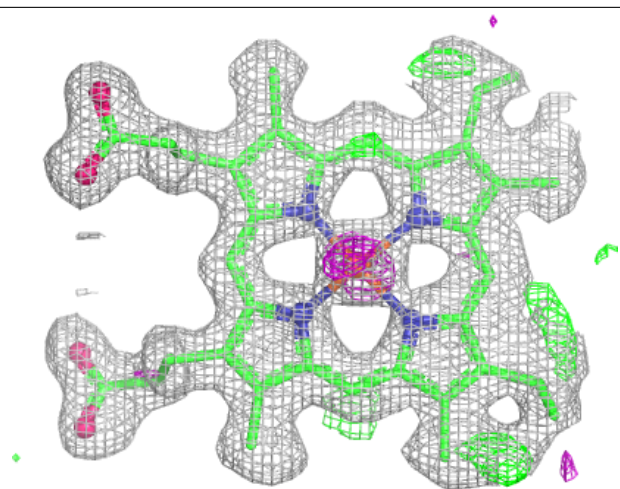
Electron density around HEM F 200 (B):

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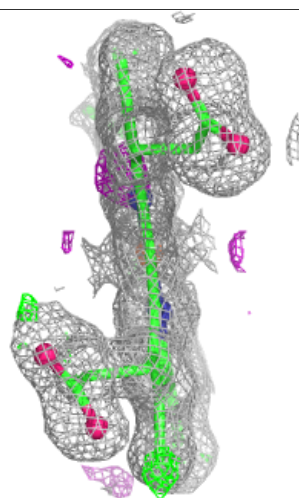
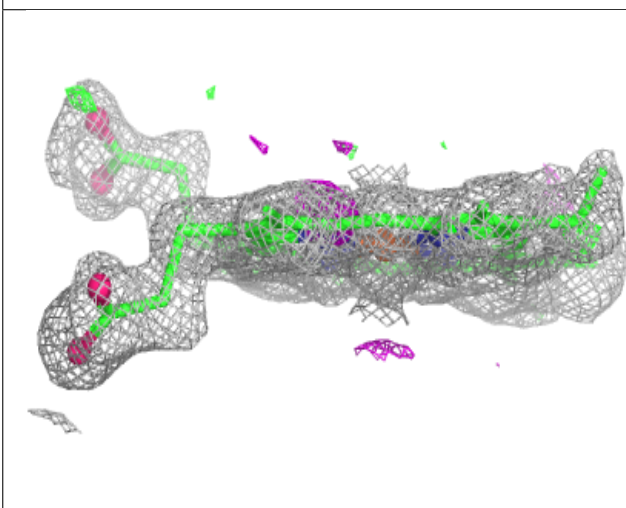
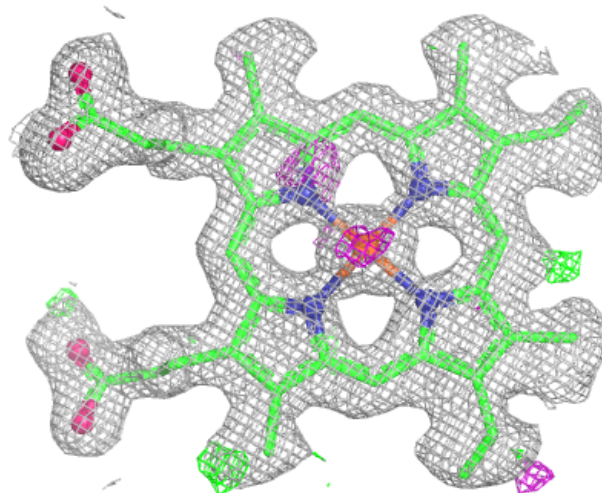
Electron density around HEM E 200:

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and green (positive)



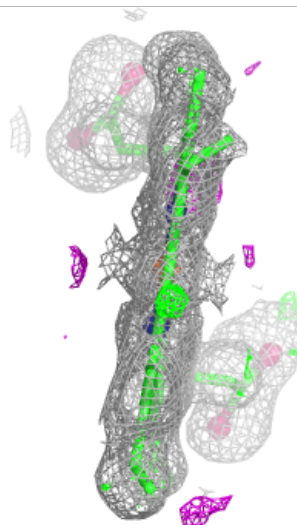
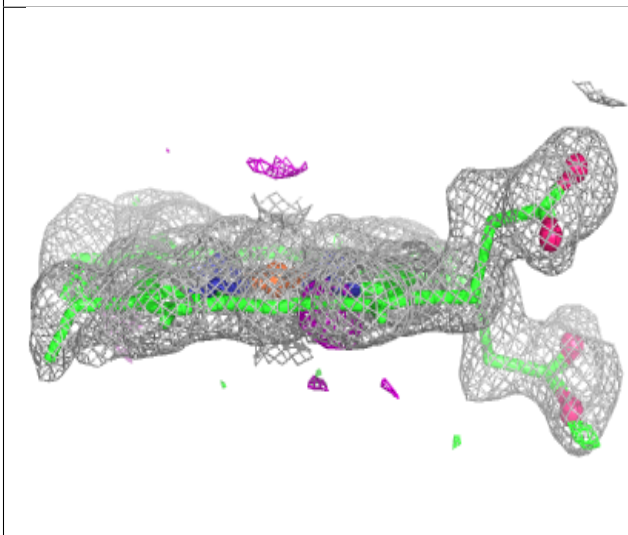
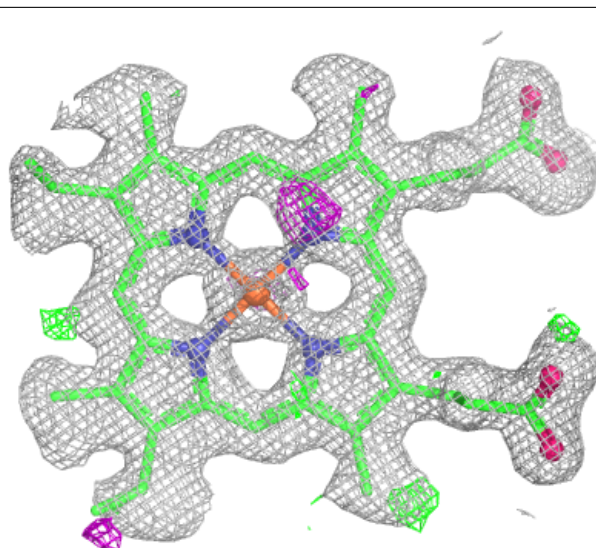
Electron density around HEM K 200 (A):

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and green (positive)



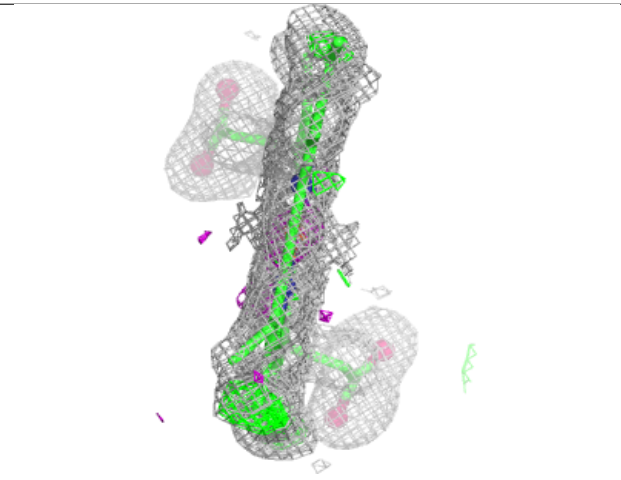
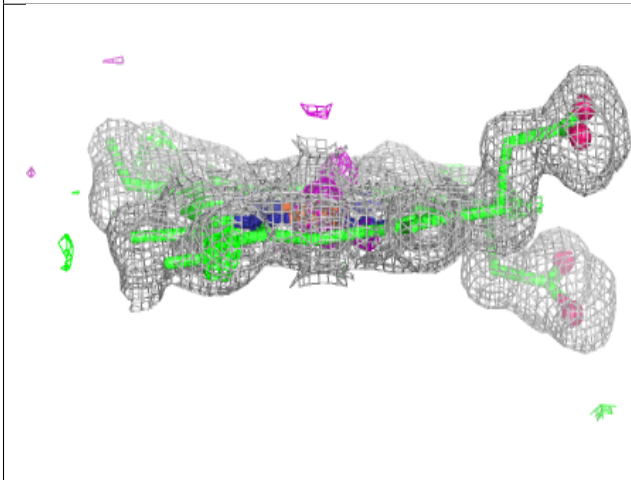
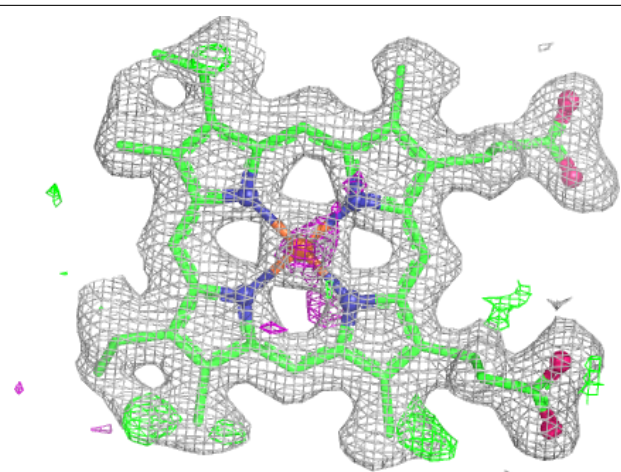
Electron density around HEM K 200 (B):

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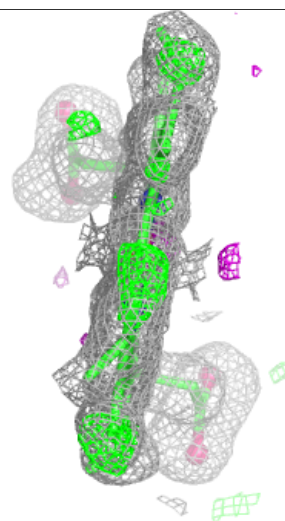
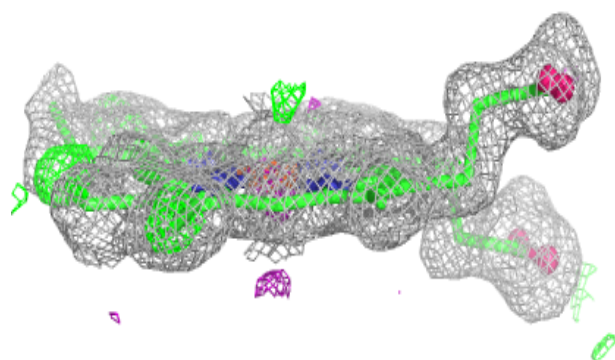
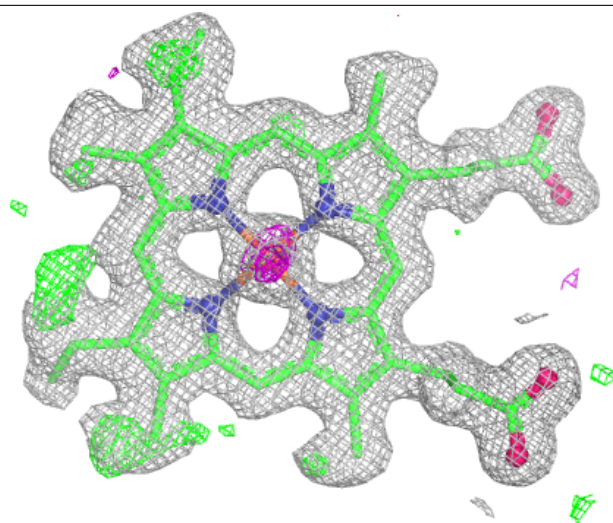
Electron density around HEM H 200 (B):

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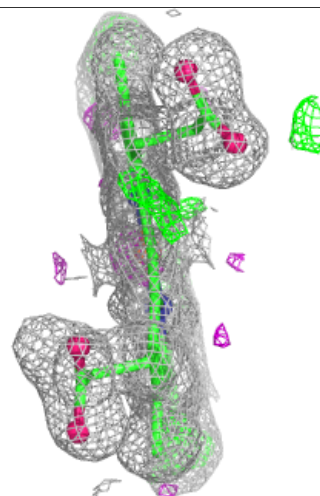
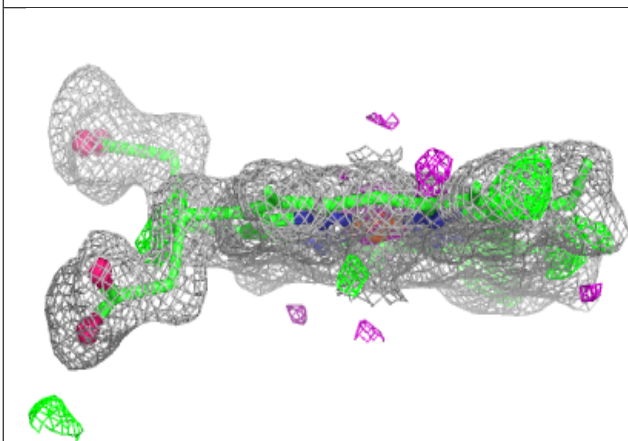
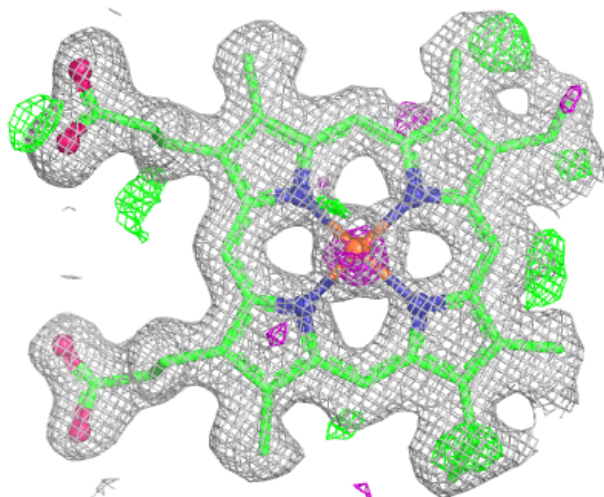
Electron density around HEM C 200 (B):

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and green (positive)



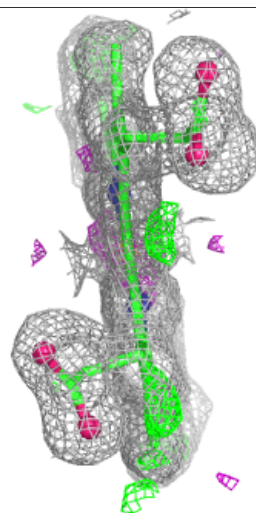
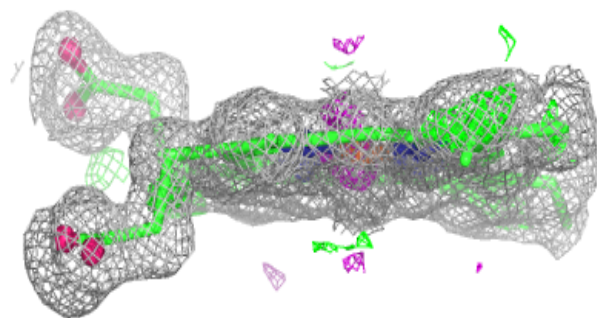
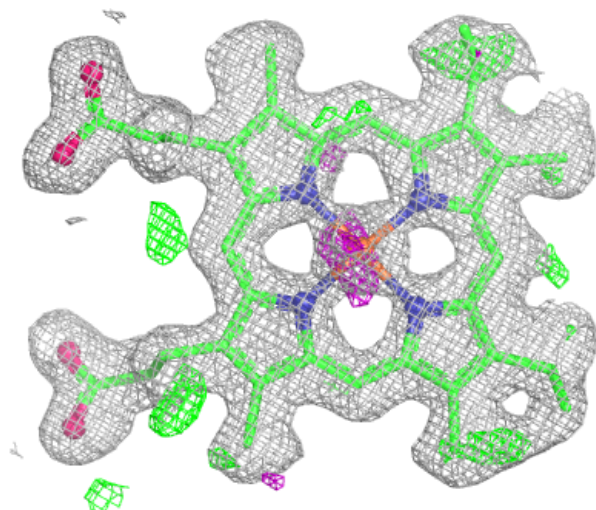
Electron density around HEM A 200 (A):

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



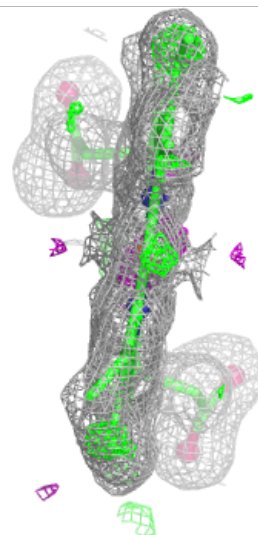
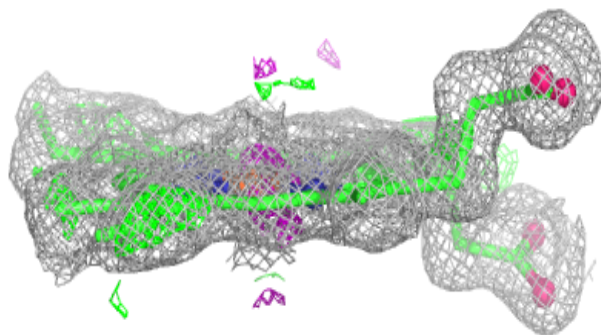
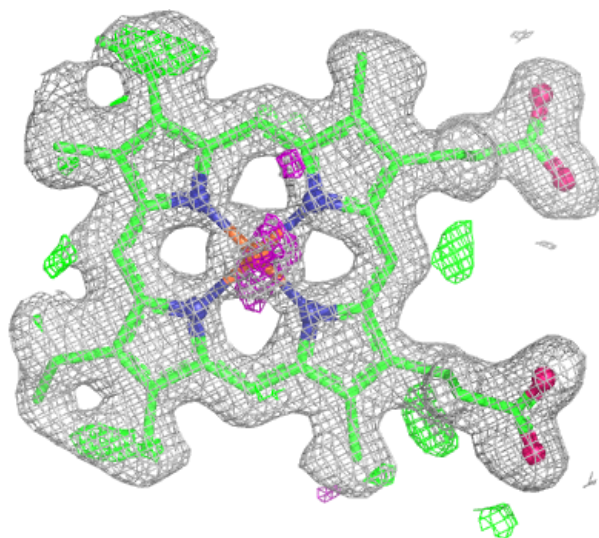
Electron density around HEM J 200 (A):

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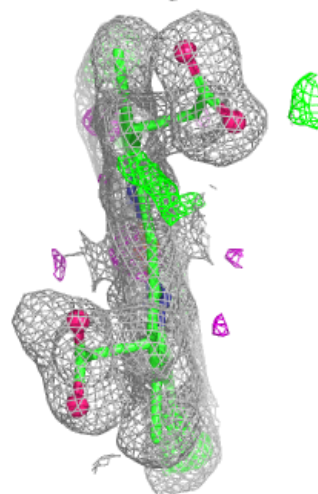
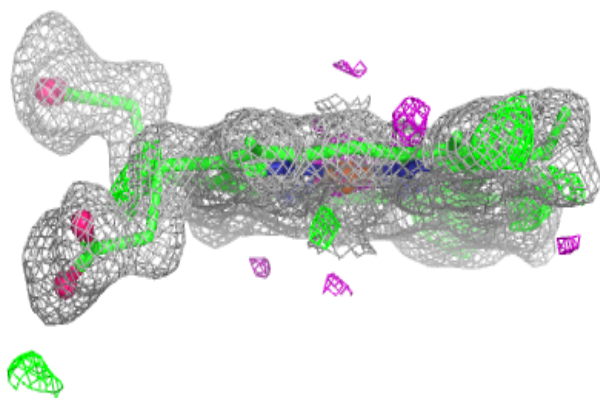
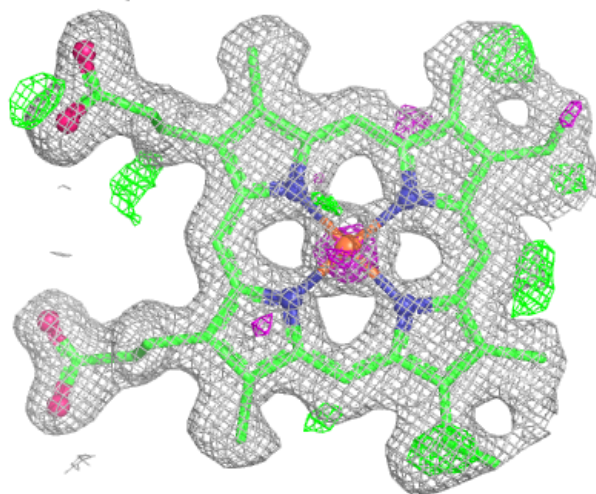
Electron density around HEM J 200 (B):

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



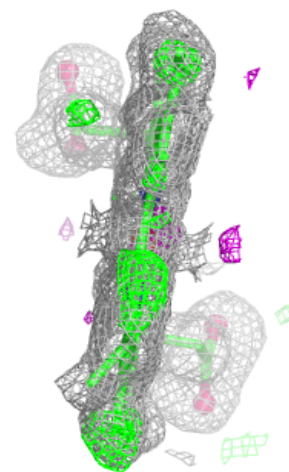
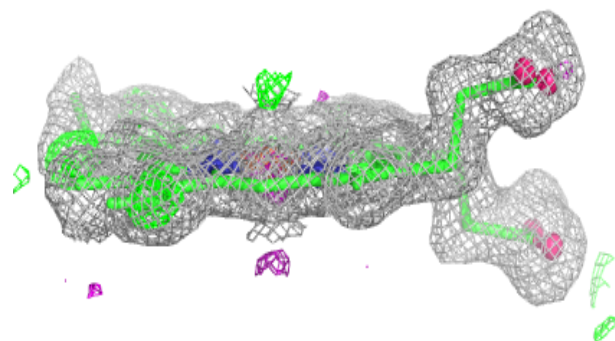
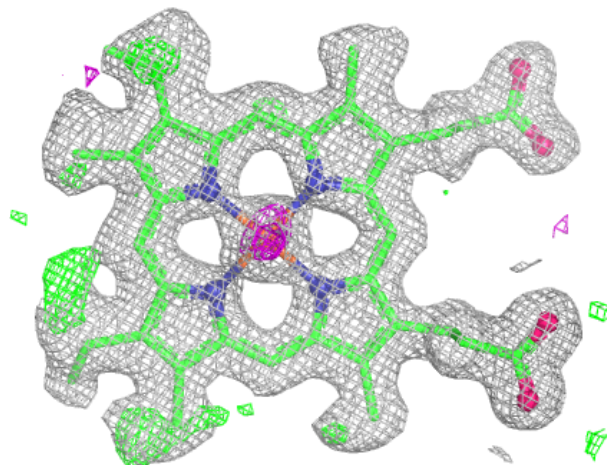
Electron density around HEM A 200 (B):

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



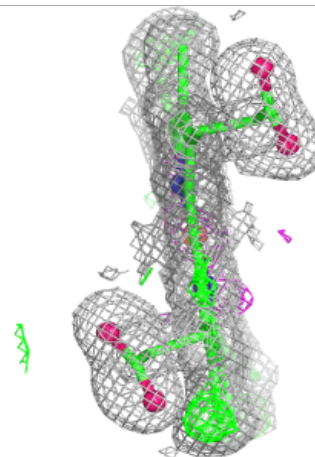
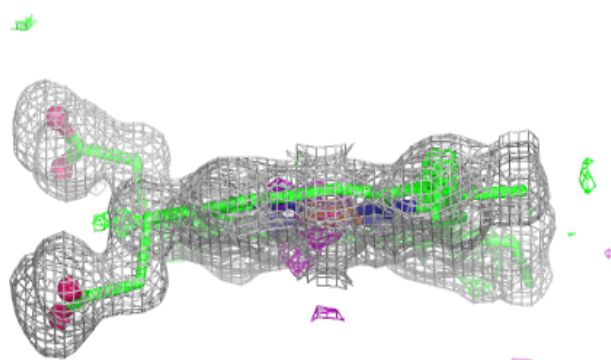
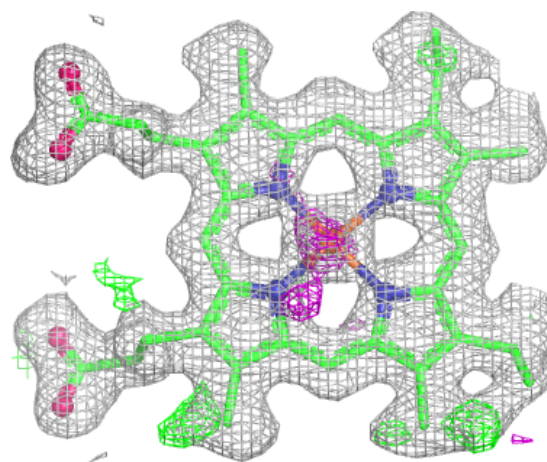
Electron density around HEM C 200 (A):

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



Electron density around HEM H 200 (A):

$2mF_o-DF_c$ (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.