



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:01 PM UTC

PDB ID : 4TOB / pdb_00004tob
Title : 1.95Å resolution structure of BfrB (Q151L) from *Pseudomonas aeruginosa*
Authors : Lovell, S.; Battaile, K.P.; Yao, H.; Kumar, R.; Eshelman, K.; Rivera, M.
Deposited on : 2014-06-05
Resolution : 1.95 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

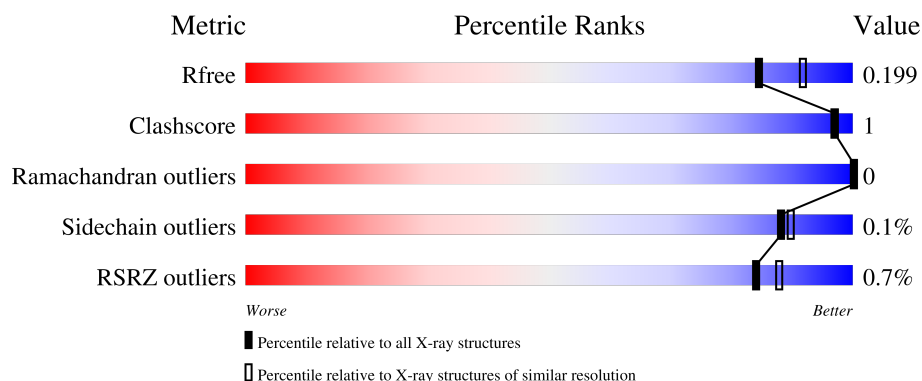
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

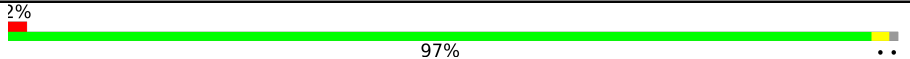
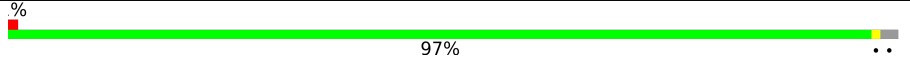
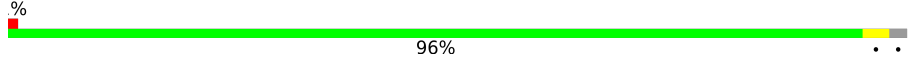
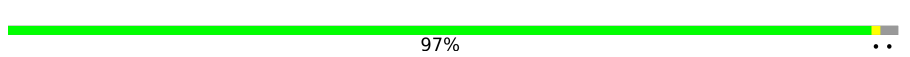
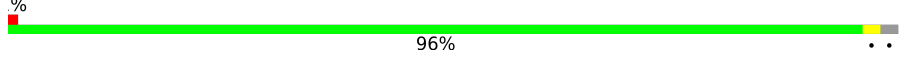
The reported resolution of this entry is 1.95 Å.

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.



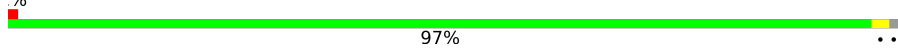
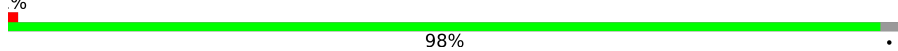
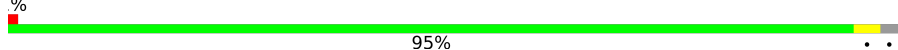
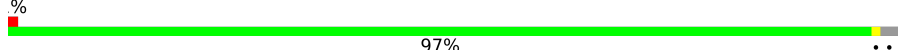
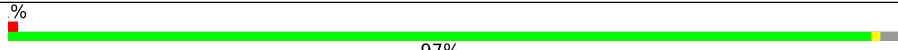
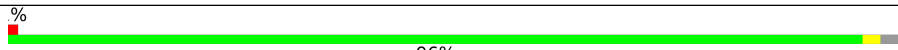
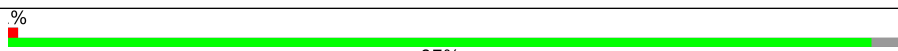
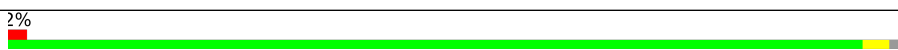
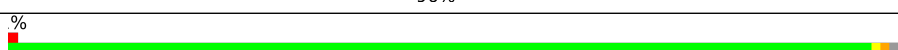
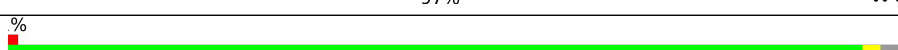
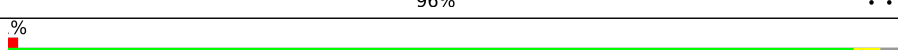
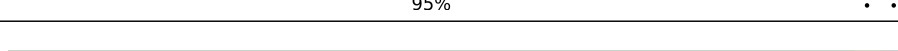
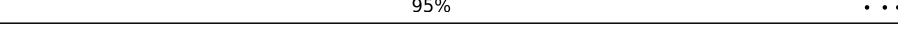
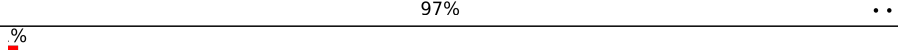
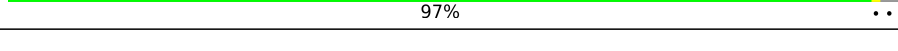
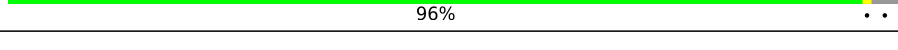
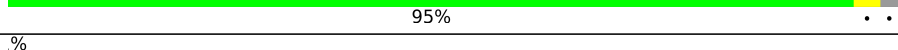
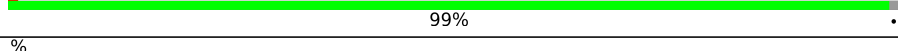
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	 2% 97% ..
1	B	158	 % 97% ..
1	C	158	 % 96% ..
1	D	158	 % 97% ..
1	E	158	 % 96% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	158	%  97% ..
1	G	158	%  98% .
1	H	158	%  95% ..
1	I	158	%  97% ..
1	J	158	%  97% ..
1	K	158	%  97% ..
1	L	158	%  96% ..
1	M	158	%  97% .
1	N	158	2%  96% ..
1	O	158	%  97% ...
1	P	158	%  96% ..
1	Q	158	%  95% ..
1	R	158	 95% ...
1	S	158	 97% ..
1	T	158	%  97% ..
1	U	158	 96% ..
1	V	158	 95% ..
1	W	158	%  99% .
1	X	158	%  98% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34054 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	156	Total	C	N	O	S	0	0	0
			1266	802	214	243	7			
1	B	155	Total	C	N	O	S	0	0	0
			1264	800	216	242	6			
1	C	155	Total	C	N	O	S	0	0	0
			1253	795	212	240	6			
1	D	155	Total	C	N	O	S	0	0	0
			1257	798	214	239	6			
1	E	155	Total	C	N	O	S	0	0	0
			1259	799	213	241	6			
1	F	156	Total	C	N	O	S	0	0	0
			1264	801	214	243	6			
1	G	155	Total	C	N	O	S	0	0	0
			1265	802	215	242	6			
1	H	155	Total	C	N	O	S	0	0	0
			1263	801	214	242	6			
1	I	155	Total	C	N	O	S	0	0	0
			1260	799	214	241	6			
1	J	155	Total	C	N	O	S	0	0	0
			1260	798	214	242	6			
1	K	155	Total	C	N	O	S	0	0	0
			1264	802	216	240	6			
1	L	154	Total	C	N	O	S	0	0	0
			1260	799	214	241	6			
1	M	154	Total	C	N	O	S	0	0	0
			1253	796	212	239	6			
1	N	156	Total	C	N	O	S	0	0	0
			1267	804	214	243	6			
1	O	155	Total	C	N	O	S	0	0	0
			1263	801	214	242	6			
1	P	155	Total	C	N	O	S	0	0	0
			1259	798	213	242	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	154	Total	C	N	O	S	0	0	0
			1259	799	213	241	6			
1	R	155	Total	C	N	O	S	0	0	0
			1261	800	214	241	6			
1	S	155	Total	C	N	O	S	0	0	0
			1258	798	213	241	6			
1	T	155	Total	C	N	O	S	0	0	0
			1259	797	214	242	6			
1	U	154	Total	C	N	O	S	0	0	0
			1255	796	214	239	6			
1	V	155	Total	C	N	O	S	0	0	0
			1251	795	213	237	6			
1	W	156	Total	C	N	O	S	0	0	0
			1272	806	217	243	6			
1	X	155	Total	C	N	O	S	0	0	0
			1260	800	214	240	6			

There are 24 discrepancies between the modelled and reference sequences:

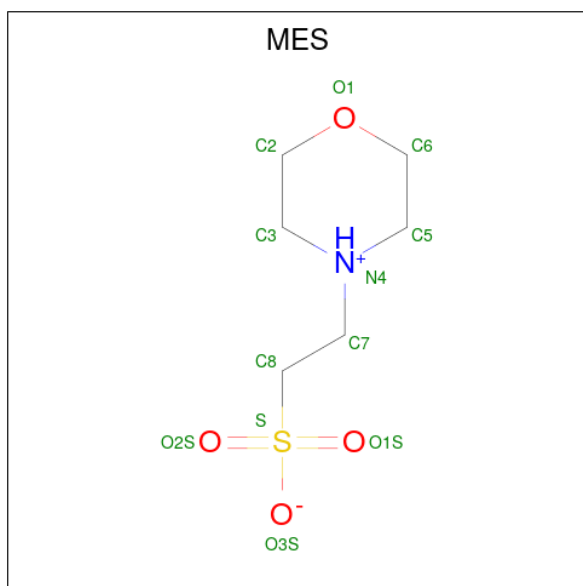
Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LEU	GLN	engineered mutation	UNP Q9HY79
B	151	LEU	GLN	engineered mutation	UNP Q9HY79
C	151	LEU	GLN	engineered mutation	UNP Q9HY79
D	151	LEU	GLN	engineered mutation	UNP Q9HY79
E	151	LEU	GLN	engineered mutation	UNP Q9HY79
F	151	LEU	GLN	engineered mutation	UNP Q9HY79
G	151	LEU	GLN	engineered mutation	UNP Q9HY79
H	151	LEU	GLN	engineered mutation	UNP Q9HY79
I	151	LEU	GLN	engineered mutation	UNP Q9HY79
J	151	LEU	GLN	engineered mutation	UNP Q9HY79
K	151	LEU	GLN	engineered mutation	UNP Q9HY79
L	151	LEU	GLN	engineered mutation	UNP Q9HY79
M	151	LEU	GLN	engineered mutation	UNP Q9HY79
N	151	LEU	GLN	engineered mutation	UNP Q9HY79
O	151	LEU	GLN	engineered mutation	UNP Q9HY79
P	151	LEU	GLN	engineered mutation	UNP Q9HY79
Q	151	LEU	GLN	engineered mutation	UNP Q9HY79
R	151	LEU	GLN	engineered mutation	UNP Q9HY79
S	151	LEU	GLN	engineered mutation	UNP Q9HY79
T	151	LEU	GLN	engineered mutation	UNP Q9HY79
U	151	LEU	GLN	engineered mutation	UNP Q9HY79
V	151	LEU	GLN	engineered mutation	UNP Q9HY79
W	151	LEU	GLN	engineered mutation	UNP Q9HY79

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	151	LEU	GLN	engineered mutation	UNP Q9HY79

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



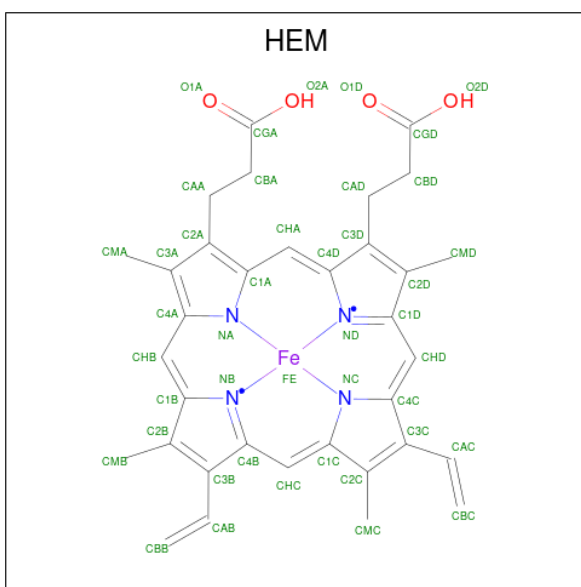
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	L	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	N	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	O	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	P	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	Q	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	R	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	S	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	T	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	U	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	V	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	W	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	X	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	O	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	T	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	X	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	119	Total O 119 119	0	0
4	B	136	Total O 136 136	0	0
4	C	141	Total O 141 141	0	0
4	D	134	Total O 134 134	0	0
4	E	94	Total O 94 94	0	0
4	F	119	Total O 119 119	0	0
4	G	141	Total O 141 141	0	0
4	H	146	Total O 146 146	0	0
4	I	117	Total O 117 117	0	0
4	J	130	Total O 130 130	0	0
4	K	130	Total O 130 130	0	0
4	L	129	Total O 129 129	0	0
4	M	110	Total O 110 110	0	0
4	N	130	Total O 130 130	0	0
4	O	132	Total O 132 132	0	0
4	P	123	Total O 123 123	0	0
4	Q	125	Total O 125 125	0	0
4	R	118	Total O 118 118	0	0
4	S	120	Total O 120 120	0	0
4	T	116	Total O 116 116	0	0
4	U	104	Total O 104 104	0	0
4	V	111	Total O 111 111	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	135	Total 135	O 135	0	0
4	X	138	Total 138	O 138	0	0

3 Residue-property plots

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

- Molecule 1: Bacterioferritin



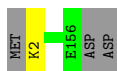
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



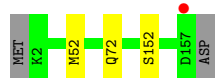
- Molecule 1: Bacterioferritin



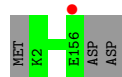
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



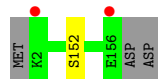
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



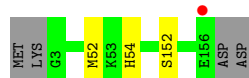
- Molecule 1: Bacterioferritin



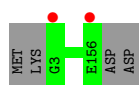
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



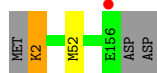
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



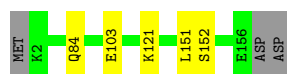
- Molecule 1: Bacterioferritin



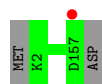
- Molecule 1: Bacterioferritin



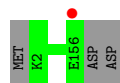
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.67Å 203.15Å 207.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 1.95 49.34 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.34-1.95) 100.0 (49.34-1.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1450)	Depositor
R, R_{free}	0.156 , 0.188 0.171 , 0.199	Depositor DCC
R_{free} test set	19331 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34054	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/1287	0.51	0/1737
1	B	0.44	0/1285	0.52	0/1733
1	C	0.42	0/1274	0.51	0/1721
1	D	0.44	0/1278	0.51	0/1724
1	E	0.42	0/1280	0.54	0/1727
1	F	0.45	0/1285	0.50	0/1735
1	G	0.45	0/1286	0.52	0/1734
1	H	0.46	0/1284	0.54	0/1732
1	I	0.44	0/1281	0.51	0/1728
1	J	0.43	0/1281	0.48	0/1729
1	K	0.41	0/1285	0.49	0/1732
1	L	0.41	0/1281	0.51	0/1727
1	M	0.41	0/1274	0.51	0/1719
1	N	0.44	0/1288	0.52	0/1738
1	O	0.44	0/1284	0.52	0/1732
1	P	0.41	0/1280	0.49	0/1728
1	Q	0.40	0/1280	0.49	0/1726
1	R	0.41	0/1282	0.48	0/1729
1	S	0.39	0/1279	0.49	0/1726
1	T	0.40	0/1280	0.50	0/1728
1	U	0.42	0/1276	0.49	0/1721
1	V	0.41	0/1272	0.49	0/1717
1	W	0.43	0/1293	0.51	0/1743
1	X	0.45	0/1281	0.53	0/1728
All	All	0.43	0/30756	0.51	0/41494

There are no bond length outliers.

There are no bond angle outliers.

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	1266	0	1226	3	0
1	B	1264	0	1235	2	0
1	C	1253	0	1205	3	0
1	D	1257	0	1224	1	0
1	E	1259	0	1221	3	0
1	F	1264	0	1218	3	0
1	G	1265	0	1234	0	0
1	H	1263	0	1227	4	0
1	I	1260	0	1226	1	0
1	J	1260	0	1221	1	0
1	K	1264	0	1239	1	0
1	L	1260	0	1232	3	0
1	M	1253	0	1216	0	0
1	N	1267	0	1227	5	0
1	O	1263	0	1227	2	0
1	P	1259	0	1216	3	0
1	Q	1259	0	1227	4	0
1	R	1261	0	1228	5	0
1	S	1258	0	1219	2	0
1	T	1259	0	1219	2	0
1	U	1255	0	1226	2	0
1	V	1251	0	1213	5	0
1	W	1272	0	1243	0	0
1	X	1260	0	1225	0	0
2	A	12	0	13	0	0
2	B	12	0	13	0	0
2	C	12	0	13	0	0
2	D	12	0	13	0	0
2	E	12	0	13	0	0
2	F	12	0	13	0	0
2	G	12	0	13	0	0
2	H	12	0	13	0	0
2	I	12	0	13	0	0
2	J	12	0	13	0	0
2	K	12	0	13	0	0
2	L	12	0	13	0	0
2	M	12	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	12	0	13	0	0
2	O	12	0	13	0	0
2	P	12	0	13	0	0
2	Q	12	0	13	0	0
2	R	12	0	13	0	0
2	S	12	0	13	0	0
2	T	12	0	13	0	0
2	U	12	0	13	0	0
2	V	12	0	13	0	0
2	W	12	0	13	0	0
2	X	12	0	13	0	0
3	B	43	0	30	0	0
3	C	43	0	30	2	0
3	F	43	0	30	2	0
3	H	43	0	30	1	0
3	J	43	0	30	1	0
3	K	43	0	30	3	0
3	N	43	0	30	1	0
3	O	43	0	30	2	0
3	Q	43	0	30	4	0
3	T	43	0	30	0	0
3	V	43	0	30	0	0
3	X	43	0	30	1	0
4	A	119	0	0	1	0
4	B	136	0	0	1	0
4	C	141	0	0	0	0
4	D	134	0	0	1	0
4	E	94	0	0	0	0
4	F	119	0	0	0	0
4	G	141	0	0	0	0
4	H	146	0	0	1	1
4	I	117	0	0	1	0
4	J	130	0	0	0	0
4	K	130	0	0	0	0
4	L	129	0	0	1	0
4	M	110	0	0	0	0
4	N	130	0	0	4	1
4	O	132	0	0	0	0
4	P	123	0	0	3	0
4	Q	125	0	0	1	0
4	R	118	0	0	3	0
4	S	120	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	116	0	0	1	0
4	U	104	0	0	0	0
4	V	111	0	0	2	0
4	W	135	0	0	0	0
4	X	138	0	0	0	0
All	All	34054	0	30066	52	1

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 1.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:201:HEM:HHC	3:Q:201:HEM:HBB2	1.71	0.73
3:F:201:HEM:HBB2	3:F:201:HEM:HHC	1.74	0.70
1:E:77:LEU:H	1:F:72:GLN:HE22	1.41	0.67
1:Q:72:GLN:HE22	1:R:77:LEU:H	1.45	0.65
1:S:84:GLN:NE2	4:S:392:HOH:O	2.31	0.62
1:Q:84:GLN:NE2	4:Q:348:HOH:O	2.32	0.62
1:A:84:GLN:NE2	4:A:334:HOH:O	2.33	0.61
4:R:353:HOH:O	1:V:121:LYS:CG	2.52	0.57
1:R:2:LYS:N	4:R:352:HOH:O	2.38	0.56
1:P:94:GLU:OE2	4:P:342:HOH:O	2.18	0.53
1:H:54:HIS:HD2	4:H:446:HOH:O	1.93	0.52
1:V:84:GLN:NE2	4:V:336:HOH:O	2.42	0.52
1:R:118:ASP:HB2	4:R:353:HOH:O	2.10	0.51
1:I:84:GLN:NE2	4:I:328:HOH:O	2.45	0.49
1:P:2:LYS:N	4:P:409:HOH:O	2.45	0.49
3:O:201:HEM:HMC2	3:O:201:HEM:HBC2	1.94	0.49
1:D:2:LYS:N	4:D:346:HOH:O	2.47	0.48
4:N:430:HOH:O	1:O:2:LYS:HD2	2.15	0.47
1:N:84:GLN:NE2	4:N:361:HOH:O	2.47	0.47
1:V:103:GLU:CG	4:V:408:HOH:O	2.63	0.46
3:C:201:HEM:HMC2	3:C:201:HEM:HBC2	1.97	0.46
1:T:2:LYS:N	4:T:327:HOH:O	2.48	0.46
3:X:201:HEM:HMC1	3:X:201:HEM:HBC2	1.98	0.45
1:O:52:MET:HB3	3:O:201:HEM:CHD	2.47	0.45
1:E:152:SER:OG	1:V:151:LEU:CD1	2.65	0.44
1:K:52:MET:HB3	3:K:201:HEM:CHD	2.48	0.44
1:B:84:GLN:NE2	4:B:354:HOH:O	2.50	0.44
1:Q:151:LEU:CD1	1:V:152:SER:OG	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:110:GLN:CG	4:N:302:HOH:O	2.67	0.43
1:F:152:SER:OG	1:H:151:LEU:CD1	2.67	0.43
1:A:1:MET:HE1	1:H:102:ARG:HH21	1.84	0.43
1:N:81:GLU:HG2	1:N:85:GLU:OE2	2.19	0.43
1:P:84:GLN:NE2	4:P:325:HOH:O	2.52	0.42
3:K:201:HEM:HMC2	3:K:201:HEM:HBC2	2.01	0.42
1:B:151:LEU:CD1	1:H:152:SER:OG	2.68	0.42
1:C:52:MET:HB3	3:C:201:HEM:CHD	2.50	0.42
3:Q:201:HEM:HBC2	3:Q:201:HEM:HMC2	2.01	0.42
1:C:151:LEU:CD1	1:U:152:SER:OG	2.68	0.42
1:F:52:MET:HB3	3:F:201:HEM:CHB	2.50	0.42
1:A:151:LEU:CD1	1:L:152:SER:OG	2.68	0.42
1:Q:52:MET:HB3	3:Q:201:HEM:CHD	2.50	0.41
1:R:152:SER:OG	1:T:151:LEU:CD1	2.68	0.41
3:K:201:HEM:CHB	1:L:52:MET:HB3	2.50	0.41
1:E:151:LEU:CD1	1:J:152:SER:OG	2.69	0.41
3:J:201:HEM:HMC2	3:J:201:HEM:HBC2	2.02	0.41
1:N:52:MET:HB3	3:N:201:HEM:CHB	2.51	0.41
1:S:152:SER:OG	1:U:151:LEU:CD1	2.69	0.41
1:C:38:LYS:HB3	1:C:156:GLU:HG3	2.04	0.40
1:N:110:GLN:HG3	4:N:302:HOH:O	2.21	0.40
3:H:201:HEM:HMC2	3:H:201:HEM:HBC2	2.03	0.40
1:L:54:HIS:HD2	4:L:429:HOH:O	2.04	0.40
3:Q:201:HEM:CHB	1:R:52:MET:HB3	2.51	0.40

All (1) 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)
4:H:311:HOH:O	4:N:302:HOH:O[3_455]	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	154/158 (98%)	154 (100%)	0	0	100	100
1	B	153/158 (97%)	153 (100%)	0	0	100	100
1	C	153/158 (97%)	153 (100%)	0	0	100	100
1	D	153/158 (97%)	153 (100%)	0	0	100	100
1	E	153/158 (97%)	153 (100%)	0	0	100	100
1	F	154/158 (98%)	154 (100%)	0	0	100	100
1	G	153/158 (97%)	153 (100%)	0	0	100	100
1	H	153/158 (97%)	153 (100%)	0	0	100	100
1	I	153/158 (97%)	153 (100%)	0	0	100	100
1	J	153/158 (97%)	153 (100%)	0	0	100	100
1	K	153/158 (97%)	153 (100%)	0	0	100	100
1	L	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	M	152/158 (96%)	152 (100%)	0	0	100	100
1	N	154/158 (98%)	154 (100%)	0	0	100	100
1	O	153/158 (97%)	153 (100%)	0	0	100	100
1	P	153/158 (97%)	153 (100%)	0	0	100	100
1	Q	152/158 (96%)	152 (100%)	0	0	100	100
1	R	153/158 (97%)	153 (100%)	0	0	100	100
1	S	153/158 (97%)	153 (100%)	0	0	100	100
1	T	153/158 (97%)	153 (100%)	0	0	100	100
1	U	152/158 (96%)	152 (100%)	0	0	100	100
1	V	153/158 (97%)	153 (100%)	0	0	100	100
1	W	154/158 (98%)	154 (100%)	0	0	100	100
1	X	153/158 (97%)	153 (100%)	0	0	100	100
All	All	3672/3792 (97%)	3671 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/144 (94%)	135 (100%)	0	100	100
1	B	137/144 (95%)	137 (100%)	0	100	100
1	C	132/144 (92%)	132 (100%)	0	100	100
1	D	134/144 (93%)	134 (100%)	0	100	100
1	E	134/144 (93%)	134 (100%)	0	100	100
1	F	134/144 (93%)	134 (100%)	0	100	100
1	G	136/144 (94%)	136 (100%)	0	100	100
1	H	135/144 (94%)	134 (99%)	1 (1%)	76	76
1	I	135/144 (94%)	135 (100%)	0	100	100
1	J	135/144 (94%)	135 (100%)	0	100	100
1	K	136/144 (94%)	136 (100%)	0	100	100
1	L	136/144 (94%)	136 (100%)	0	100	100
1	M	133/144 (92%)	133 (100%)	0	100	100
1	N	134/144 (93%)	134 (100%)	0	100	100
1	O	135/144 (94%)	134 (99%)	1 (1%)	76	76
1	P	134/144 (93%)	134 (100%)	0	100	100
1	Q	135/144 (94%)	135 (100%)	0	100	100
1	R	135/144 (94%)	134 (99%)	1 (1%)	76	76
1	S	134/144 (93%)	134 (100%)	0	100	100
1	T	135/144 (94%)	135 (100%)	0	100	100
1	U	135/144 (94%)	135 (100%)	0	100	100
1	V	132/144 (92%)	132 (100%)	0	100	100
1	W	137/144 (95%)	137 (100%)	0	100	100
1	X	134/144 (93%)	134 (100%)	0	100	100
All	All	3232/3456 (94%)	3229 (100%)	3 (0%)	88	90

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

Mol	Chain	Res	Type
1	H	85	GLU
1	O	2	LYS
1	R	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	54	HIS
1	A	84	GLN
1	A	137	GLN
1	A	142	GLN
1	B	33	ASN
1	B	54	HIS
1	B	84	GLN
1	B	137	GLN
1	C	33	ASN
1	C	54	HIS
1	C	88	GLN
1	C	137	GLN
1	C	148	ASN
1	D	33	ASN
1	D	54	HIS
1	D	137	GLN
1	D	142	GLN
1	E	137	GLN
1	E	142	GLN
1	E	148	ASN
1	F	33	ASN
1	F	46	HIS
1	F	54	HIS
1	F	72	GLN
1	F	88	GLN
1	G	33	ASN
1	G	46	HIS
1	G	54	HIS
1	G	112	HIS
1	G	137	GLN
1	H	33	ASN
1	H	54	HIS
1	H	84	GLN
1	H	137	GLN
1	I	33	ASN
1	I	46	HIS
1	I	54	HIS
1	I	84	GLN
1	I	148	ASN
1	J	33	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	46	HIS
1	J	54	HIS
1	J	84	GLN
1	K	33	ASN
1	K	88	GLN
1	L	33	ASN
1	L	54	HIS
1	M	33	ASN
1	M	43	HIS
1	M	88	GLN
1	N	33	ASN
1	N	84	GLN
1	N	88	GLN
1	N	137	GLN
1	O	9	GLN
1	O	33	ASN
1	O	54	HIS
1	O	88	GLN
1	O	92	ASN
1	P	33	ASN
1	P	84	GLN
1	P	142	GLN
1	P	148	ASN
1	Q	33	ASN
1	Q	54	HIS
1	Q	72	GLN
1	Q	84	GLN
1	Q	137	GLN
1	R	33	ASN
1	S	33	ASN
1	S	54	HIS
1	T	33	ASN
1	T	54	HIS
1	T	88	GLN
1	U	10	HIS
1	U	33	ASN
1	U	54	HIS
1	V	33	ASN
1	V	46	HIS
1	V	54	HIS
1	V	84	GLN
1	V	137	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	142	GLN
1	V	148	ASN
1	W	9	GLN
1	W	33	ASN
1	W	84	GLN
1	W	148	ASN
1	X	33	ASN
1	X	54	HIS
1	X	137	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	X	201	1	50,50,50	1.71	9 (18%)	67,82,82	1.44	8 (11%)
2	MES	T	202	-	12,12,12	1.77	1 (8%)	15,16,16	1.37	3 (20%)
2	MES	U	201	-	12,12,12	1.86	1 (8%)	15,16,16	1.41	2 (13%)
3	HEM	F	201	1	50,50,50	1.74	10 (20%)	67,82,82	1.40	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	C	201	1	50,50,50	1.79	8 (16%)	67,82,82	1.48	11 (16%)
2	MES	H	202	-	12,12,12	1.73	1 (8%)	15,16,16	1.34	2 (13%)
3	HEM	B	201	1	50,50,50	1.77	9 (18%)	67,82,82	1.45	9 (13%)
2	MES	P	201	-	12,12,12	1.86	1 (8%)	15,16,16	1.44	3 (20%)
2	MES	C	202	-	12,12,12	1.94	1 (8%)	15,16,16	1.55	5 (33%)
2	MES	E	201	-	12,12,12	1.91	1 (8%)	15,16,16	1.48	4 (26%)
2	MES	G	201	-	12,12,12	1.89	1 (8%)	15,16,16	1.33	2 (13%)
3	HEM	N	201	1	50,50,50	1.69	9 (18%)	67,82,82	1.28	8 (11%)
2	MES	J	202	-	12,12,12	1.95	1 (8%)	15,16,16	1.52	3 (20%)
2	MES	B	202	-	12,12,12	1.99	1 (8%)	15,16,16	1.77	6 (40%)
3	HEM	V	201	1	50,50,50	1.77	10 (20%)	67,82,82	1.40	7 (10%)
2	MES	Q	202	-	12,12,12	1.76	1 (8%)	15,16,16	1.77	3 (20%)
2	MES	O	202	-	12,12,12	1.89	1 (8%)	15,16,16	1.45	2 (13%)
2	MES	A	201	-	12,12,12	1.84	1 (8%)	15,16,16	1.82	2 (13%)
2	MES	N	202	-	12,12,12	1.65	1 (8%)	15,16,16	1.55	4 (26%)
2	MES	V	202	-	12,12,12	2.02	1 (8%)	15,16,16	1.67	4 (26%)
2	MES	X	202	-	12,12,12	1.82	1 (8%)	15,16,16	1.39	2 (13%)
2	MES	W	201	-	12,12,12	1.98	1 (8%)	15,16,16	1.50	4 (26%)
3	HEM	J	201	1	50,50,50	1.78	9 (18%)	67,82,82	1.40	7 (10%)
2	MES	I	201	-	12,12,12	1.88	1 (8%)	15,16,16	1.41	4 (26%)
2	MES	M	201	-	12,12,12	1.86	1 (8%)	15,16,16	1.38	3 (20%)
3	HEM	K	201	1	50,50,50	1.71	9 (18%)	67,82,82	1.30	8 (11%)
2	MES	K	202	-	12,12,12	1.82	1 (8%)	15,16,16	1.66	2 (13%)
2	MES	S	201	-	12,12,12	1.84	1 (8%)	15,16,16	1.60	3 (20%)
2	MES	F	202	-	12,12,12	1.82	1 (8%)	15,16,16	1.65	4 (26%)
3	HEM	H	201	1	50,50,50	1.71	11 (22%)	67,82,82	1.42	10 (14%)
3	HEM	Q	201	1	50,50,50	1.78	8 (16%)	67,82,82	1.43	8 (11%)
3	HEM	O	201	1	50,50,50	1.69	8 (16%)	67,82,82	1.39	8 (11%)
2	MES	D	201	-	12,12,12	1.68	1 (8%)	15,16,16	1.40	3 (20%)
3	HEM	T	201	1	50,50,50	1.80	8 (16%)	67,82,82	1.41	6 (8%)
2	MES	R	201	-	12,12,12	1.83	1 (8%)	15,16,16	1.38	2 (13%)
2	MES	L	201	-	12,12,12	1.80	1 (8%)	15,16,16	1.41	2 (13%)

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	X	201	1	-	4/14/54/54	-
2	MES	T	202	-	-	1/6/14/14	0/1/1/1
2	MES	U	201	-	-	3/6/14/14	0/1/1/1
3	HEM	F	201	1	-	5/14/54/54	-
3	HEM	C	201	1	-	4/14/54/54	-
2	MES	H	202	-	-	1/6/14/14	0/1/1/1
3	HEM	B	201	1	-	4/14/54/54	-
2	MES	P	201	-	-	1/6/14/14	0/1/1/1
2	MES	C	202	-	-	2/6/14/14	0/1/1/1
2	MES	E	201	-	-	1/6/14/14	0/1/1/1
2	MES	G	201	-	-	1/6/14/14	0/1/1/1
3	HEM	N	201	1	-	4/14/54/54	-
2	MES	J	202	-	-	1/6/14/14	0/1/1/1
2	MES	B	202	-	-	1/6/14/14	0/1/1/1
3	HEM	V	201	1	-	4/14/54/54	-
2	MES	Q	202	-	-	1/6/14/14	0/1/1/1
2	MES	O	202	-	-	1/6/14/14	0/1/1/1
2	MES	A	201	-	-	1/6/14/14	0/1/1/1
2	MES	N	202	-	-	1/6/14/14	0/1/1/1
2	MES	V	202	-	-	1/6/14/14	0/1/1/1
2	MES	X	202	-	-	1/6/14/14	0/1/1/1
2	MES	W	201	-	-	1/6/14/14	0/1/1/1
3	HEM	J	201	1	-	4/14/54/54	-
2	MES	I	201	-	-	4/6/14/14	0/1/1/1
2	MES	M	201	-	-	1/6/14/14	0/1/1/1
3	HEM	K	201	1	-	4/14/54/54	-
2	MES	K	202	-	-	1/6/14/14	0/1/1/1
2	MES	S	201	-	-	1/6/14/14	0/1/1/1
2	MES	F	202	-	-	4/6/14/14	0/1/1/1
3	HEM	H	201	1	-	4/14/54/54	-
3	HEM	Q	201	1	-	5/14/54/54	-
3	HEM	O	201	1	-	4/14/54/54	-
2	MES	D	201	-	-	1/6/14/14	0/1/1/1
3	HEM	T	201	1	-	4/14/54/54	-
2	MES	R	201	-	-	1/6/14/14	0/1/1/1
2	MES	L	201	-	-	1/6/14/14	0/1/1/1

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	201	HEM	C3D-C2D	7.45	1.52	1.36
3	T	201	HEM	C3D-C2D	7.41	1.52	1.36
3	K	201	HEM	C3D-C2D	7.22	1.52	1.36
3	V	201	HEM	C3D-C2D	7.22	1.52	1.36
3	N	201	HEM	C3D-C2D	7.16	1.52	1.36
3	J	201	HEM	C3D-C2D	7.14	1.52	1.36
3	B	201	HEM	C3D-C2D	6.98	1.51	1.36
3	C	201	HEM	C3D-C2D	6.92	1.51	1.36
3	X	201	HEM	C3D-C2D	6.84	1.51	1.36
3	O	201	HEM	C3D-C2D	6.81	1.51	1.36
3	F	201	HEM	C3D-C2D	6.72	1.51	1.36
3	H	201	HEM	C3D-C2D	6.53	1.50	1.36
2	V	202	MES	C8-S	-6.40	1.68	1.77
2	B	202	MES	C8-S	-6.21	1.68	1.77
2	W	201	MES	C8-S	-6.13	1.69	1.77
2	C	202	MES	C8-S	-6.10	1.69	1.77
2	J	202	MES	C8-S	-6.07	1.69	1.77
2	E	201	MES	C8-S	-5.98	1.69	1.77
2	G	201	MES	C8-S	-5.93	1.69	1.77
2	S	201	MES	C8-S	-5.85	1.69	1.77
2	U	201	MES	C8-S	-5.85	1.69	1.77
2	M	201	MES	C8-S	-5.78	1.69	1.77
2	R	201	MES	C8-S	-5.78	1.69	1.77
2	O	202	MES	C8-S	-5.75	1.69	1.77
2	A	201	MES	C8-S	-5.72	1.69	1.77
2	F	202	MES	C8-S	-5.70	1.69	1.77
2	K	202	MES	C8-S	-5.70	1.69	1.77
2	P	201	MES	C8-S	-5.67	1.69	1.77
2	I	201	MES	C8-S	-5.66	1.69	1.77
2	X	202	MES	C8-S	-5.55	1.69	1.77
2	T	202	MES	C8-S	-5.54	1.69	1.77
2	Q	202	MES	C8-S	-5.47	1.69	1.77
2	L	201	MES	C8-S	-5.40	1.70	1.77
2	H	202	MES	C8-S	-5.35	1.70	1.77
3	T	201	HEM	FE-ND	5.27	2.11	1.94
2	D	201	MES	C8-S	-5.03	1.70	1.77
3	B	201	HEM	FE-ND	4.98	2.10	1.94
2	N	202	MES	C8-S	-4.75	1.70	1.77
3	C	201	HEM	FE-ND	4.74	2.09	1.94
3	V	201	HEM	FE-ND	4.68	2.09	1.94
3	X	201	HEM	FE-ND	4.59	2.09	1.94
3	H	201	HEM	FE-ND	4.37	2.08	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	201	HEM	FE-ND	4.29	2.08	1.94
3	F	201	HEM	FE-ND	4.22	2.07	1.94
3	C	201	HEM	FE-NA	3.93	2.08	1.95
3	J	201	HEM	FE-ND	3.80	2.06	1.94
3	O	201	HEM	FE-ND	3.75	2.06	1.94
3	O	201	HEM	FE-NB	3.74	2.06	1.94
3	J	201	HEM	FE-NA	3.73	2.07	1.95
3	Q	201	HEM	FE-NA	3.59	2.07	1.95
3	V	201	HEM	FE-NB	3.49	2.05	1.94
3	N	201	HEM	FE-NA	3.37	2.06	1.95
3	C	201	HEM	FE-NB	3.34	2.05	1.94
3	B	201	HEM	FE-NC	3.30	2.06	1.95
3	F	201	HEM	CAB-C3B	3.22	1.56	1.47
3	F	201	HEM	CAC-C3C	3.16	1.55	1.47
3	H	201	HEM	FE-NA	3.15	2.05	1.95
3	J	201	HEM	FE-NB	3.04	2.04	1.94
3	T	201	HEM	CAB-C3B	2.98	1.55	1.47
3	T	201	HEM	FE-NA	2.97	2.04	1.95
3	K	201	HEM	FE-NB	2.94	2.03	1.94
3	T	201	HEM	FE-NC	2.93	2.04	1.95
3	K	201	HEM	CAB-C3B	2.93	1.55	1.47
3	Q	201	HEM	CAB-C3B	2.92	1.55	1.47
3	K	201	HEM	FE-ND	2.90	2.03	1.94
3	X	201	HEM	FE-NB	2.89	2.03	1.94
3	V	201	HEM	CAC-C3C	2.87	1.55	1.47
3	C	201	HEM	CAB-C3B	2.82	1.54	1.47
3	H	201	HEM	FE-NC	2.82	2.04	1.95
3	Q	201	HEM	CAC-C3C	2.81	1.54	1.47
3	X	201	HEM	CAB-C3B	2.80	1.54	1.47
3	H	201	HEM	FE-NB	2.78	2.03	1.94
3	N	201	HEM	FE-ND	2.77	2.03	1.94
3	V	201	HEM	CMC-C2C	2.74	1.56	1.50
3	C	201	HEM	CAC-C3C	2.71	1.54	1.47
3	T	201	HEM	CAC-C3C	2.71	1.54	1.47
3	N	201	HEM	CMC-C2C	2.71	1.56	1.50
3	B	201	HEM	CAB-C3B	2.68	1.54	1.47
3	K	201	HEM	FE-NA	2.68	2.04	1.95
3	J	201	HEM	FE-NC	2.66	2.03	1.95
3	O	201	HEM	FE-NA	2.66	2.03	1.95
3	O	201	HEM	CAB-C3B	2.66	1.54	1.47
3	K	201	HEM	CMC-C2C	2.65	1.56	1.50
3	X	201	HEM	CAC-C3C	2.64	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	201	HEM	FE-NC	2.63	2.03	1.95
3	H	201	HEM	CAB-C3B	2.63	1.54	1.47
3	B	201	HEM	CAC-C3C	2.61	1.54	1.47
3	K	201	HEM	CAC-C3C	2.58	1.54	1.47
3	F	201	HEM	FE-NB	2.58	2.02	1.94
3	J	201	HEM	CAB-C3B	2.58	1.54	1.47
3	O	201	HEM	CAC-C3C	2.58	1.54	1.47
3	F	201	HEM	FE-NA	2.57	2.03	1.95
3	N	201	HEM	FE-NC	2.56	2.03	1.95
3	B	201	HEM	FE-NB	2.56	2.02	1.94
3	F	201	HEM	CMC-C2C	2.51	1.55	1.50
3	X	201	HEM	FE-NA	2.51	2.03	1.95
3	T	201	HEM	FE-NB	2.50	2.02	1.94
3	V	201	HEM	CMB-C2B	2.49	1.55	1.50
3	V	201	HEM	CAB-C3B	2.46	1.54	1.47
3	H	201	HEM	CMB-C2B	2.45	1.55	1.50
3	J	201	HEM	CAC-C3C	2.44	1.53	1.47
3	N	201	HEM	CAC-C3C	2.41	1.53	1.47
3	Q	201	HEM	FE-NC	2.41	2.03	1.95
3	H	201	HEM	CAC-C3C	2.39	1.53	1.47
3	B	201	HEM	CMB-C2B	2.37	1.55	1.50
3	X	201	HEM	FE-NC	2.35	2.02	1.95
3	V	201	HEM	CMA-C3A	2.35	1.55	1.50
3	V	201	HEM	FE-NA	2.34	2.02	1.95
3	N	201	HEM	CMA-C3A	2.32	1.55	1.50
3	J	201	HEM	CMA-C3A	2.30	1.55	1.50
3	K	201	HEM	CMB-C2B	2.29	1.55	1.50
3	B	201	HEM	FE-NA	2.29	2.02	1.95
3	N	201	HEM	CAB-C3B	2.25	1.53	1.47
3	C	201	HEM	FE-NC	2.24	2.02	1.95
3	K	201	HEM	FE-NC	2.23	2.02	1.95
3	X	201	HEM	CMB-C2B	2.19	1.55	1.50
3	J	201	HEM	CMC-C2C	2.19	1.55	1.50
3	Q	201	HEM	CMC-C2C	2.19	1.55	1.50
3	C	201	HEM	CMC-C2C	2.18	1.55	1.50
3	O	201	HEM	CMC-C2C	2.14	1.55	1.50
3	H	201	HEM	O2A-CGA	-2.10	1.23	1.30
3	B	201	HEM	CMC-C2C	2.10	1.55	1.50
3	H	201	HEM	CMA-C3A	2.10	1.55	1.50
3	H	201	HEM	CMC-C2C	2.09	1.55	1.50
3	Q	201	HEM	FE-NB	2.09	2.01	1.94
3	V	201	HEM	FE-NC	2.07	2.02	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	201	HEM	FE-NC	2.05	2.01	1.95
3	N	201	HEM	CMB-C2B	2.04	1.55	1.50
3	F	201	HEM	CMB-C2B	2.04	1.54	1.50
3	X	201	HEM	CMC-C2C	2.04	1.54	1.50
3	F	201	HEM	O2A-CGA	-2.03	1.24	1.30
3	T	201	HEM	CMB-C2B	2.01	1.54	1.50

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	201	HEM	C4D-ND-C1D	6.07	112.40	105.21
3	B	201	HEM	C4D-ND-C1D	5.79	112.06	105.21
3	C	201	HEM	C4D-ND-C1D	5.56	111.79	105.21
2	A	201	MES	O1S-S-C8	5.51	115.06	106.73
3	F	201	HEM	C4D-ND-C1D	5.32	111.50	105.21
3	J	201	HEM	C4D-ND-C1D	5.31	111.50	105.21
3	O	201	HEM	C4D-ND-C1D	5.29	111.47	105.21
3	T	201	HEM	C4D-ND-C1D	5.28	111.47	105.21
3	X	201	HEM	C4D-ND-C1D	5.28	111.46	105.21
3	Q	201	HEM	C4D-ND-C1D	5.19	111.35	105.21
3	H	201	HEM	C4D-ND-C1D	5.12	111.27	105.21
3	K	201	HEM	C4D-ND-C1D	4.67	110.73	105.21
2	F	202	MES	O3S-S-C8	4.53	114.86	106.00
2	Q	202	MES	O1S-S-C8	4.48	113.50	106.73
2	K	202	MES	O1S-S-C8	4.43	113.42	106.73
2	S	201	MES	O1S-S-C8	4.14	112.99	106.73
2	J	202	MES	O1S-S-C8	3.59	112.15	106.73
2	D	201	MES	O3S-S-C8	3.42	112.69	106.00
2	V	202	MES	O1S-S-C8	3.40	111.87	106.73
3	N	201	HEM	C4D-ND-C1D	3.37	109.20	105.21
3	J	201	HEM	CHC-C4B-NB	3.35	128.02	124.42
2	O	202	MES	O3S-S-C8	3.26	112.37	106.00
2	N	202	MES	O2S-S-C8	3.24	111.63	106.73
3	F	201	HEM	C3B-C4B-NB	-3.22	107.15	109.47
2	C	202	MES	O1S-S-C8	3.21	111.58	106.73
3	V	201	HEM	CHC-C4B-NB	3.19	127.86	124.42
2	G	201	MES	C5-N4-C3	3.14	115.60	108.84
3	B	201	HEM	CBD-CAD-C3D	-3.14	103.86	112.53
2	H	202	MES	C5-N4-C3	3.14	115.60	108.84
2	X	202	MES	O1S-S-C8	3.14	111.47	106.73
2	R	201	MES	O3S-S-C8	3.08	112.03	106.00
2	U	201	MES	O1S-S-C8	3.06	111.36	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	201	HEM	CBD-CAD-C3D	-3.04	104.13	112.53
2	L	201	MES	O3S-S-C8	3.03	111.94	106.00
3	X	201	HEM	C2A-C1A-NA	-2.95	106.88	110.15
2	P	201	MES	O1S-S-C8	2.94	111.17	106.73
2	M	201	MES	O3S-S-C8	2.93	111.73	106.00
2	Q	202	MES	O2S-S-O1S	-2.92	104.33	113.82
3	C	201	HEM	C3B-C4B-NB	-2.91	107.38	109.47
3	H	201	HEM	CBD-CAD-C3D	-2.90	104.52	112.53
2	H	202	MES	O1S-S-C8	2.85	111.03	106.73
3	C	201	HEM	CBA-CAA-C2A	-2.84	104.68	112.53
3	H	201	HEM	CBA-CAA-C2A	-2.84	104.68	112.53
3	X	201	HEM	CBD-CAD-C3D	-2.84	104.69	112.53
3	Q	201	HEM	C3B-C4B-NB	-2.83	107.44	109.47
3	N	201	HEM	CHD-C4C-NC	2.77	127.47	124.45
2	K	202	MES	C5-N4-C3	2.77	114.80	108.84
2	E	201	MES	O1S-S-C8	2.73	110.86	106.73
3	T	201	HEM	CBD-CAD-C3D	-2.73	104.98	112.53
3	O	201	HEM	CHD-C4C-NC	2.73	127.42	124.45
2	R	201	MES	C5-N4-C3	2.72	114.71	108.84
3	T	201	HEM	C2A-C1A-NA	-2.70	107.15	110.15
3	B	201	HEM	CHC-C4B-NB	2.70	127.33	124.42
3	B	201	HEM	C3B-C4B-NB	-2.69	107.54	109.47
2	T	202	MES	O3S-S-C8	2.68	111.25	106.00
3	O	201	HEM	CBA-CAA-C2A	-2.68	105.14	112.53
3	Q	201	HEM	CHA-C4D-ND	2.67	127.67	124.37
2	N	202	MES	O1S-S-C8	2.67	110.76	106.73
2	E	201	MES	O3S-S-C8	2.67	111.22	106.00
3	F	201	HEM	CHA-C4D-ND	2.66	127.66	124.37
2	I	201	MES	O3S-S-C8	2.64	111.18	106.00
3	K	201	HEM	CAD-C3D-C4D	2.64	129.29	124.70
3	C	201	HEM	C1B-NB-C4B	2.63	108.32	105.21
3	N	201	HEM	CAC-C3C-C4C	-2.62	118.56	124.82
2	W	201	MES	O1S-S-C8	2.62	110.69	106.73
2	O	202	MES	O1S-S-C8	2.62	110.69	106.73
2	L	201	MES	C5-N4-C3	2.60	114.45	108.84
3	V	201	HEM	C1B-NB-C4B	2.59	108.27	105.21
2	V	202	MES	O2S-S-C8	2.59	110.64	106.73
3	O	201	HEM	CBD-CAD-C3D	-2.56	105.44	112.53
2	B	202	MES	C5-N4-C3	2.56	114.35	108.84
2	B	202	MES	O2S-S-C8	2.56	110.59	106.73
2	X	202	MES	C5-N4-C3	2.55	114.34	108.84
2	A	201	MES	C5-N4-C3	2.55	114.33	108.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	202	MES	O1-C2-C3	2.54	117.25	111.77
3	Q	201	HEM	CHD-C1D-ND	2.51	127.12	124.42
3	Q	201	HEM	CBA-CAA-C2A	-2.50	105.61	112.53
2	P	201	MES	C5-N4-C3	2.49	114.21	108.84
3	N	201	HEM	C2A-C1A-NA	-2.49	107.39	110.15
3	B	201	HEM	C3D-C4D-ND	-2.49	107.44	110.17
3	B	201	HEM	CHA-C4D-ND	2.48	127.43	124.37
3	H	201	HEM	C2A-C1A-NA	-2.46	107.42	110.15
3	T	201	HEM	CHC-C1C-NC	2.46	127.13	124.45
3	V	201	HEM	C3B-C4B-NB	-2.46	107.70	109.47
3	O	201	HEM	CMD-C2D-C1D	2.45	128.87	125.03
2	J	202	MES	C5-N4-C3	2.45	114.13	108.84
2	V	202	MES	C5-N4-C3	2.45	114.13	108.84
3	C	201	HEM	C1D-C2D-C3D	-2.44	104.41	106.98
3	J	201	HEM	CBD-CAD-C3D	-2.43	105.81	112.53
3	F	201	HEM	CAC-C3C-C4C	-2.42	119.04	124.82
3	F	201	HEM	CBD-CAD-C3D	-2.42	105.84	112.53
3	V	201	HEM	CBA-CAA-C2A	-2.39	105.92	112.53
3	X	201	HEM	CHA-C4D-ND	2.38	127.31	124.37
3	J	201	HEM	O2A-CGA-CBA	2.38	121.51	114.00
3	J	201	HEM	C2A-C1A-NA	-2.37	107.52	110.15
3	Q	201	HEM	CBD-CAD-C3D	-2.37	105.98	112.53
3	V	201	HEM	CBD-CAD-C3D	-2.37	105.98	112.53
3	C	201	HEM	CHA-C4D-ND	2.37	127.30	124.37
3	J	201	HEM	CBA-CAA-C2A	-2.37	105.99	112.53
3	F	201	HEM	C1B-NB-C4B	2.36	108.00	105.21
2	G	201	MES	O2S-S-C8	2.35	110.28	106.73
2	I	201	MES	O2S-S-C8	2.34	110.27	106.73
2	T	202	MES	O2S-S-C8	2.33	110.25	106.73
2	C	202	MES	C5-N4-C3	2.33	113.86	108.84
3	C	201	HEM	CBD-CAD-C3D	-2.33	106.09	112.53
3	F	201	HEM	CBA-CAA-C2A	-2.32	106.13	112.53
3	Q	201	HEM	C1B-NB-C4B	2.31	107.94	105.21
2	N	202	MES	C5-N4-C3	2.31	113.81	108.84
3	H	201	HEM	CHA-C4D-ND	2.31	127.22	124.37
3	K	201	HEM	CAC-C3C-C4C	-2.30	119.32	124.82
2	P	201	MES	O3S-S-C8	2.30	110.51	106.00
2	S	201	MES	C5-N4-C3	2.29	113.78	108.84
3	H	201	HEM	CAD-C3D-C4D	2.28	128.68	124.70
2	V	202	MES	O3S-S-C8	2.28	110.47	106.00
2	W	201	MES	O2S-S-C8	2.28	110.18	106.73
2	W	201	MES	C5-N4-C3	2.28	113.75	108.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	202	MES	C5-N4-C3	2.28	113.75	108.84
3	N	201	HEM	CBA-CAA-C2A	-2.28	106.23	112.53
2	D	201	MES	C7-N4-C3	2.28	117.30	111.24
2	M	201	MES	C5-N4-C3	2.27	113.72	108.84
3	K	201	HEM	CHC-C4B-NB	2.26	126.86	124.42
3	V	201	HEM	CHD-C1D-ND	2.26	126.85	124.42
3	T	201	HEM	CHA-C4D-ND	2.26	127.16	124.37
2	C	202	MES	O2S-S-C8	2.26	110.14	106.73
3	C	201	HEM	CMD-C2D-C1D	2.25	128.55	125.03
2	W	201	MES	C7-N4-C3	2.25	117.23	111.24
2	N	202	MES	O2S-S-O1S	-2.24	106.55	113.82
2	E	201	MES	C5-N4-C3	2.23	113.64	108.84
3	N	201	HEM	CMD-C2D-C1D	2.22	128.50	125.03
3	H	201	HEM	CMD-C2D-C1D	2.20	128.47	125.03
3	B	201	HEM	C1D-C2D-C3D	-2.20	104.67	106.98
3	Q	201	HEM	C2A-C1A-NA	-2.19	107.72	110.15
2	S	201	MES	O2S-S-O1S	-2.19	106.69	113.82
2	M	201	MES	O1S-S-C8	2.19	110.04	106.73
2	E	201	MES	C7-N4-C3	2.18	117.06	111.24
3	H	201	HEM	CHC-C4B-NB	2.18	126.77	124.42
3	O	201	HEM	O2A-CGA-CBA	2.18	120.88	114.00
3	N	201	HEM	CHC-C1C-NC	2.16	126.81	124.45
2	I	201	MES	C5-N4-C3	2.16	113.50	108.84
2	D	201	MES	C5-N4-C3	2.16	113.50	108.84
2	F	202	MES	C7-N4-C3	2.16	117.00	111.24
3	K	201	HEM	CBA-CAA-C2A	-2.16	106.56	112.53
2	B	202	MES	O3S-S-C8	2.15	110.21	106.00
3	J	201	HEM	CAC-C3C-C4C	-2.15	119.69	124.82
3	K	201	HEM	C2A-C1A-NA	-2.14	107.78	110.15
3	T	201	HEM	C1D-C2D-C3D	-2.14	104.73	106.98
3	C	201	HEM	CHC-C4B-NB	2.14	126.72	124.42
3	X	201	HEM	CAC-C3C-C4C	-2.12	119.76	124.82
3	C	201	HEM	C2A-C1A-NA	-2.12	107.80	110.15
2	F	202	MES	O3S-S-O2S	-2.10	106.14	111.40
3	X	201	HEM	O2A-CGA-CBA	2.10	120.63	114.00
2	I	201	MES	O1S-S-C8	2.09	109.89	106.73
3	B	201	HEM	CBA-CAA-C2A	-2.09	106.76	112.53
3	K	201	HEM	CHD-C1D-ND	2.09	126.67	124.42
3	O	201	HEM	C3B-C4B-NB	-2.08	107.97	109.47
3	X	201	HEM	CMD-C2D-C1D	2.08	128.29	125.03
3	B	201	HEM	CMD-C2D-C1D	2.08	128.28	125.03
3	H	201	HEM	C1B-NB-C4B	2.08	107.67	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	201	HEM	CHB-C1B-NB	2.07	126.93	124.37
3	F	201	HEM	O1D-CGD-CBD	-2.05	116.58	123.09
3	F	201	HEM	CAB-C3B-C2B	-2.05	121.77	128.43
3	O	201	HEM	C1D-C2D-C3D	-2.03	104.84	106.98
3	H	201	HEM	C1D-C2D-C3D	-2.03	104.84	106.98
3	X	201	HEM	O2D-CGD-CBD	2.03	120.42	114.00
2	C	202	MES	O2S-S-O1S	-2.03	107.23	113.82
2	F	202	MES	C5-N4-C3	2.02	113.20	108.84
2	U	201	MES	O3S-S-C8	2.02	109.95	106.00
2	B	202	MES	C6-C5-N4	-2.01	107.06	110.12
2	B	202	MES	C6-O1-C2	2.01	116.37	109.88
2	C	202	MES	C7-N4-C3	2.01	116.59	111.24
3	C	201	HEM	C3B-C2B-C1B	2.01	107.92	106.41
2	J	202	MES	C7-N4-C3	2.01	116.58	111.24
2	T	202	MES	C5-N4-C3	2.00	113.15	108.84

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	MES	N4-C7-C8-S
2	B	202	MES	N4-C7-C8-S
2	C	202	MES	N4-C7-C8-S
2	D	201	MES	N4-C7-C8-S
2	E	201	MES	N4-C7-C8-S
2	F	202	MES	N4-C7-C8-S
2	G	201	MES	N4-C7-C8-S
2	H	202	MES	N4-C7-C8-S
2	I	201	MES	N4-C7-C8-S
2	I	201	MES	C7-C8-S-O2S
2	J	202	MES	N4-C7-C8-S
2	K	202	MES	N4-C7-C8-S
2	L	201	MES	N4-C7-C8-S
2	M	201	MES	N4-C7-C8-S
2	N	202	MES	N4-C7-C8-S
2	O	202	MES	N4-C7-C8-S
2	P	201	MES	N4-C7-C8-S
2	Q	202	MES	N4-C7-C8-S
2	R	201	MES	N4-C7-C8-S
2	S	201	MES	N4-C7-C8-S
2	T	202	MES	N4-C7-C8-S
2	U	201	MES	N4-C7-C8-S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	U	201	MES	C7-C8-S-O2S
2	V	202	MES	N4-C7-C8-S
2	W	201	MES	N4-C7-C8-S
2	X	202	MES	N4-C7-C8-S
3	F	201	HEM	C4B-C3B-CAB-CBB
2	I	201	MES	C7-C8-S-O3S
2	F	202	MES	C7-C8-S-O1S
2	I	201	MES	C7-C8-S-O1S
3	Q	201	HEM	C4B-C3B-CAB-CBB
2	F	202	MES	C7-C8-S-O3S
2	U	201	MES	C7-C8-S-O3S
3	N	201	HEM	CAA-CBA-CGA-O2A
3	Q	201	HEM	CAA-CBA-CGA-O2A
3	Q	201	HEM	CAA-CBA-CGA-O1A
3	V	201	HEM	CAD-CBD-CGD-O2D
3	C	201	HEM	CAA-CBA-CGA-O2A
3	F	201	HEM	CAD-CBD-CGD-O2D
3	J	201	HEM	CAD-CBD-CGD-O1D
3	K	201	HEM	CAD-CBD-CGD-O1D
3	O	201	HEM	CAD-CBD-CGD-O1D
3	X	201	HEM	CAD-CBD-CGD-O2D
3	H	201	HEM	CAA-CBA-CGA-O1A
3	N	201	HEM	CAD-CBD-CGD-O2D
3	O	201	HEM	CAD-CBD-CGD-O2D
3	C	201	HEM	CAA-CBA-CGA-O1A
3	J	201	HEM	CAA-CBA-CGA-O1A
3	J	201	HEM	CAA-CBA-CGA-O2A
3	H	201	HEM	CAA-CBA-CGA-O2A
3	H	201	HEM	CAD-CBD-CGD-O1D
3	N	201	HEM	CAA-CBA-CGA-O1A
3	X	201	HEM	CAA-CBA-CGA-O1A
3	X	201	HEM	CAD-CBD-CGD-O1D
3	K	201	HEM	CAA-CBA-CGA-O1A
3	B	201	HEM	CAD-CBD-CGD-O2D
3	C	201	HEM	CAD-CBD-CGD-O2D
3	V	201	HEM	CAA-CBA-CGA-O1A
3	J	201	HEM	CAD-CBD-CGD-O2D
3	T	201	HEM	CAA-CBA-CGA-O2A
3	K	201	HEM	CAA-CBA-CGA-O2A
3	T	201	HEM	CAD-CBD-CGD-O2D
3	V	201	HEM	CAA-CBA-CGA-O2A
3	H	201	HEM	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	201	HEM	CAD-CBD-CGD-O2D
3	T	201	HEM	CAA-CBA-CGA-O1A
3	X	201	HEM	CAA-CBA-CGA-O2A
3	N	201	HEM	CAD-CBD-CGD-O1D
3	V	201	HEM	CAD-CBD-CGD-O1D
3	C	201	HEM	CAD-CBD-CGD-O1D
3	F	201	HEM	CAD-CBD-CGD-O1D
3	T	201	HEM	CAD-CBD-CGD-O1D
2	C	202	MES	C7-C8-S-O2S
2	F	202	MES	C7-C8-S-O2S
3	B	201	HEM	CAA-CBA-CGA-O2A
3	B	201	HEM	CAD-CBD-CGD-O1D
3	F	201	HEM	CAA-CBA-CGA-O1A
3	O	201	HEM	CAA-CBA-CGA-O1A
3	Q	201	HEM	CAD-CBD-CGD-O2D
3	B	201	HEM	CAA-CBA-CGA-O1A
3	F	201	HEM	CAA-CBA-CGA-O2A
3	O	201	HEM	CAA-CBA-CGA-O2A
3	Q	201	HEM	CAD-CBD-CGD-O1D

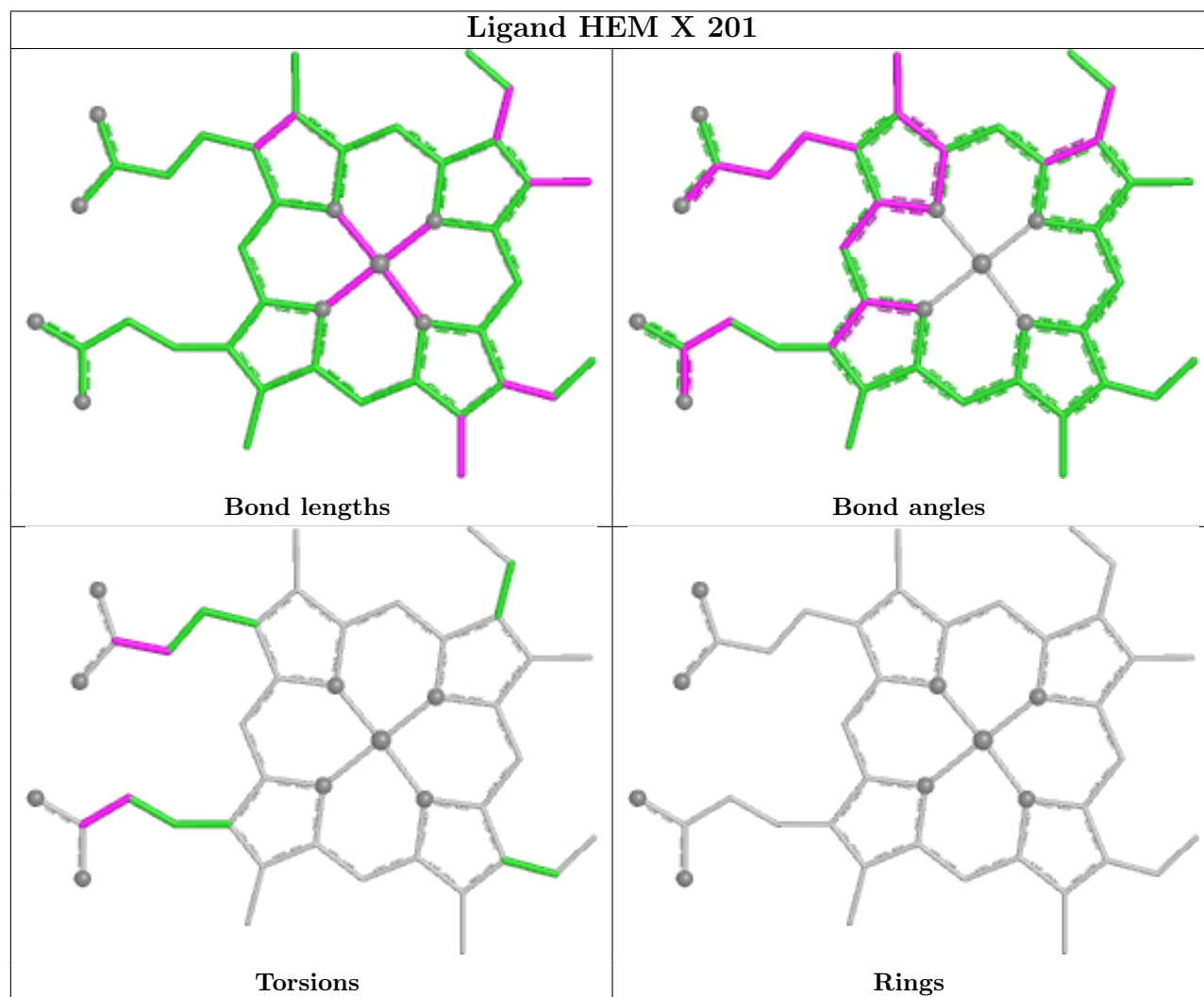
There are no ring outliers.

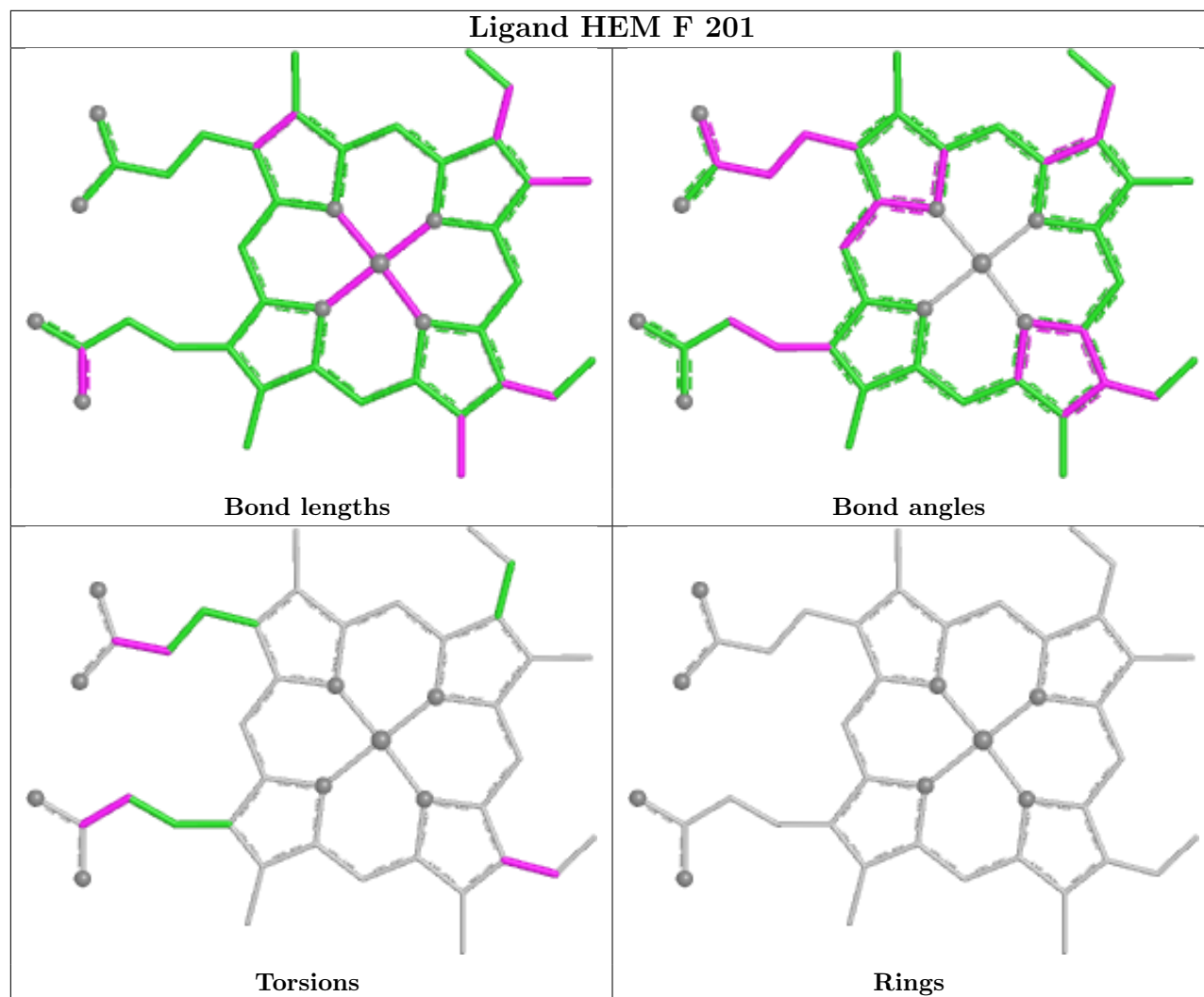
9 monomers are involved in 17 short contacts:

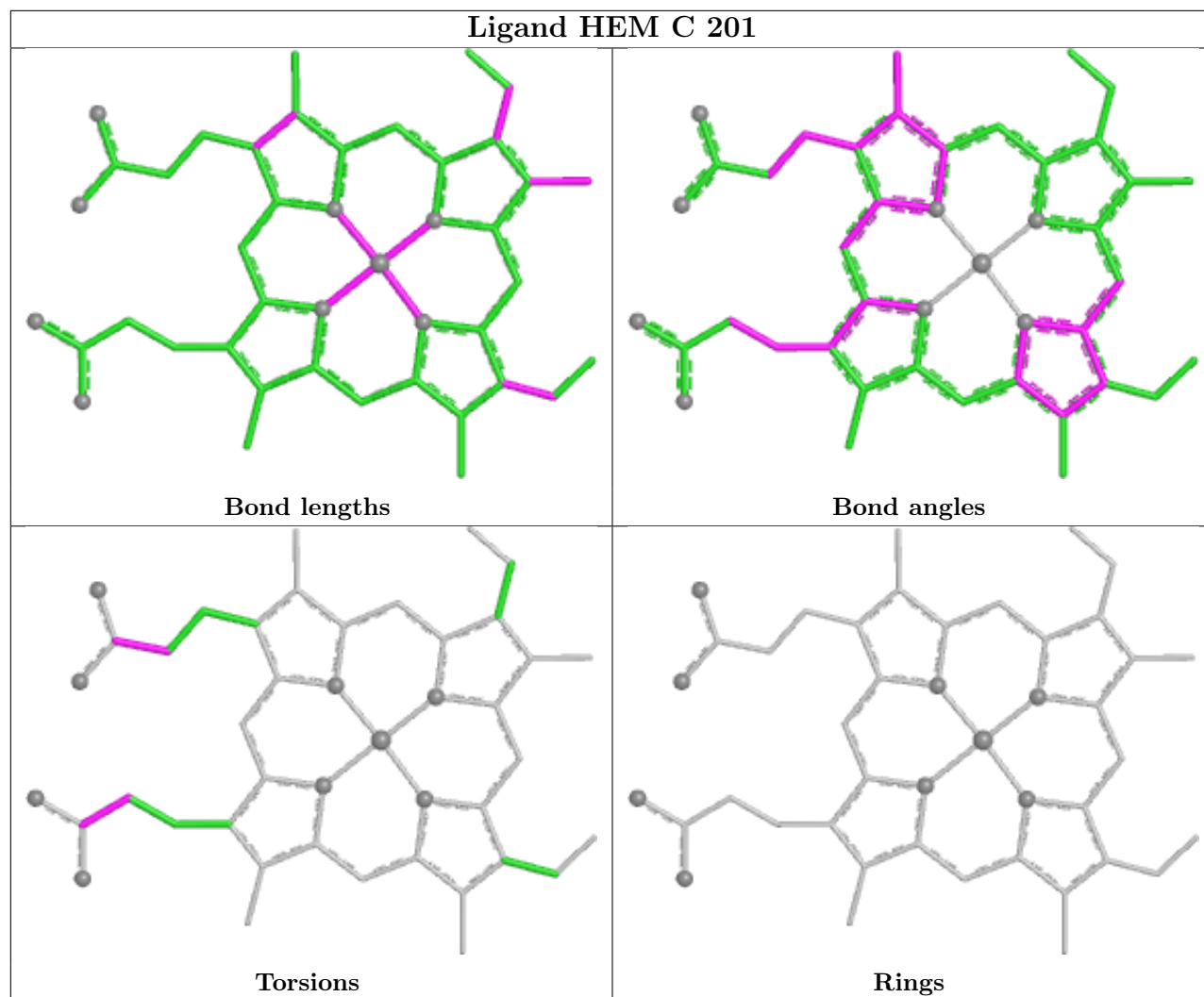
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	201	HEM	1	0
3	F	201	HEM	2	0
3	C	201	HEM	2	0
3	N	201	HEM	1	0
3	J	201	HEM	1	0
3	K	201	HEM	3	0
3	H	201	HEM	1	0
3	Q	201	HEM	4	0
3	O	201	HEM	2	0

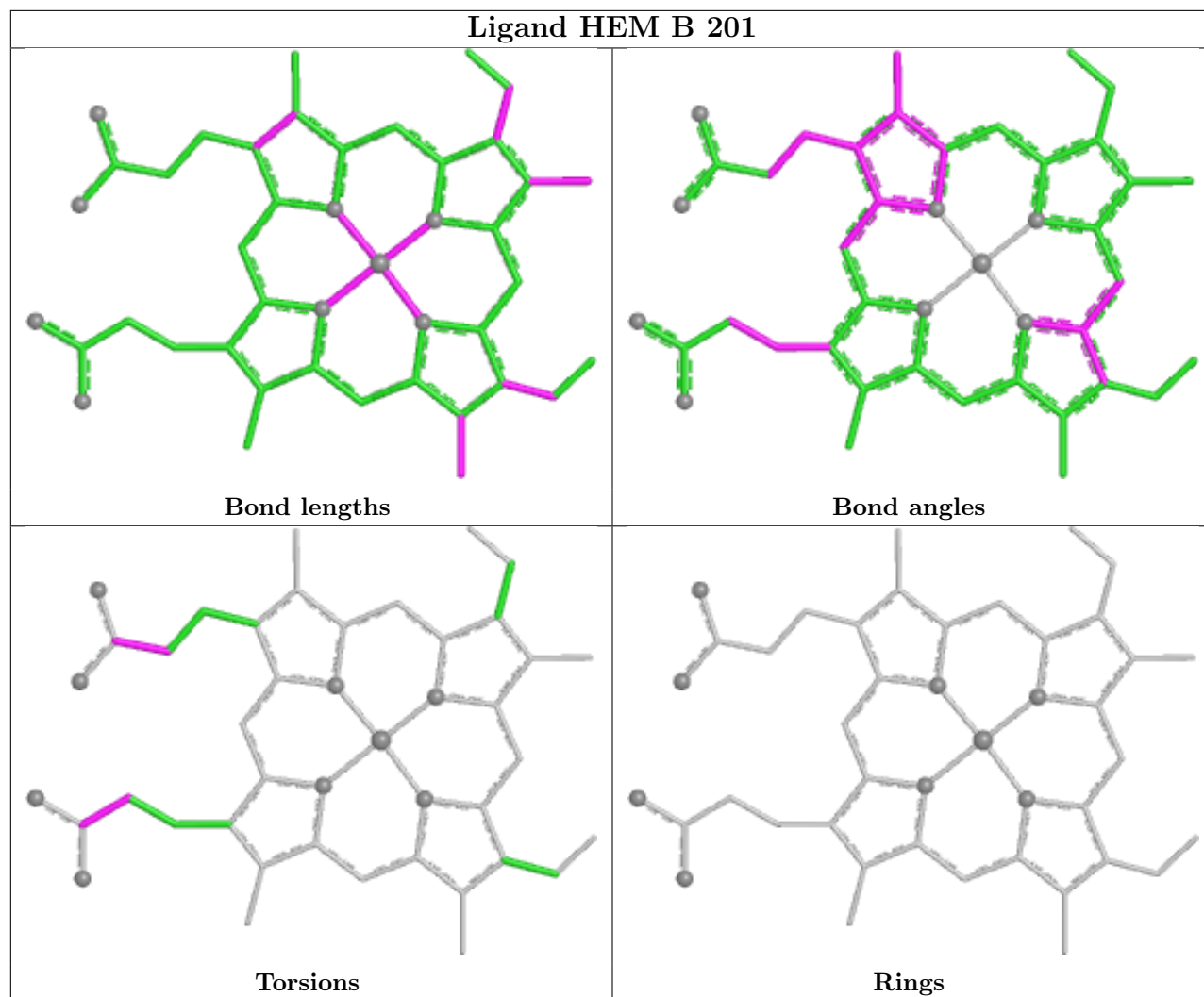
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

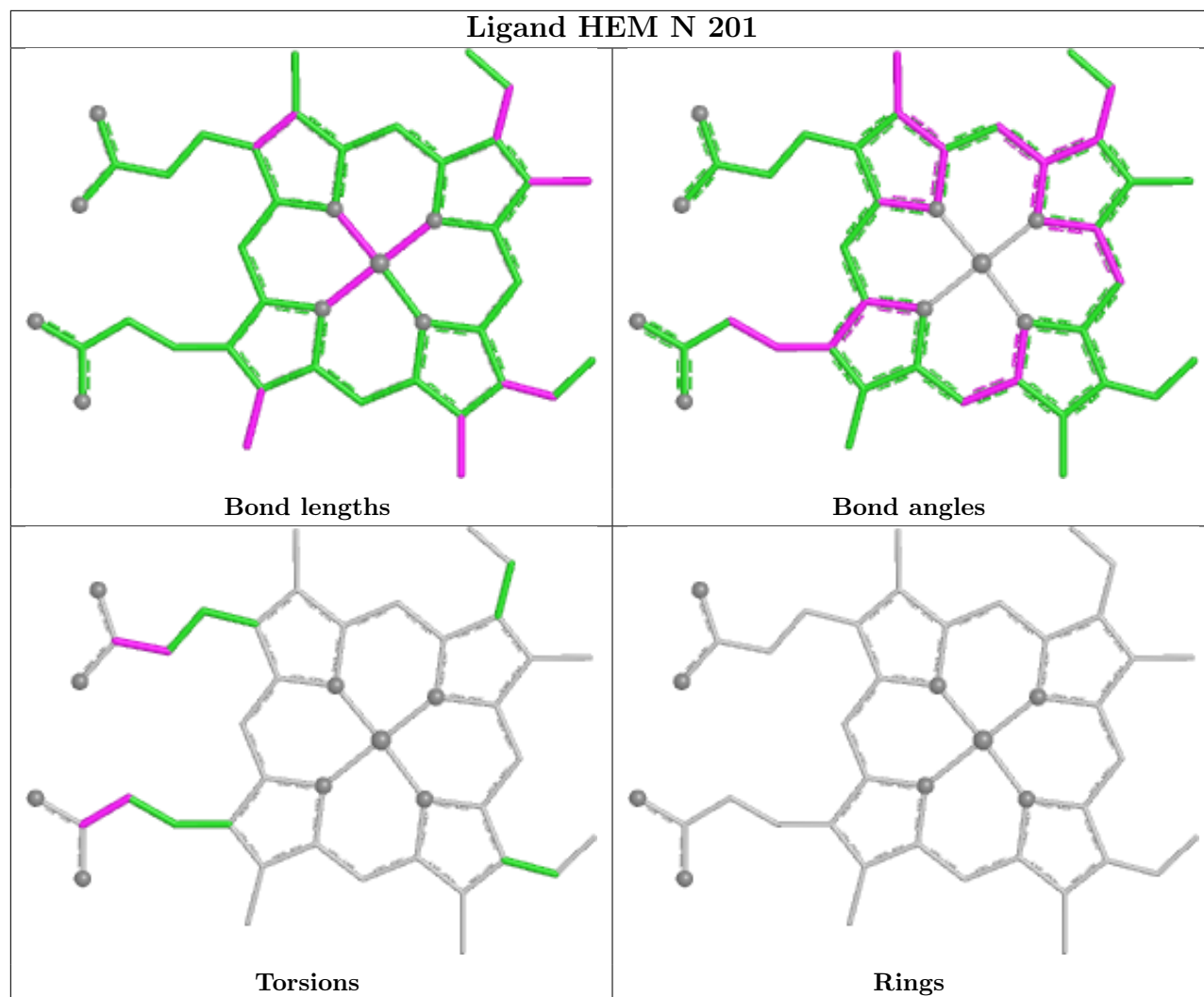
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

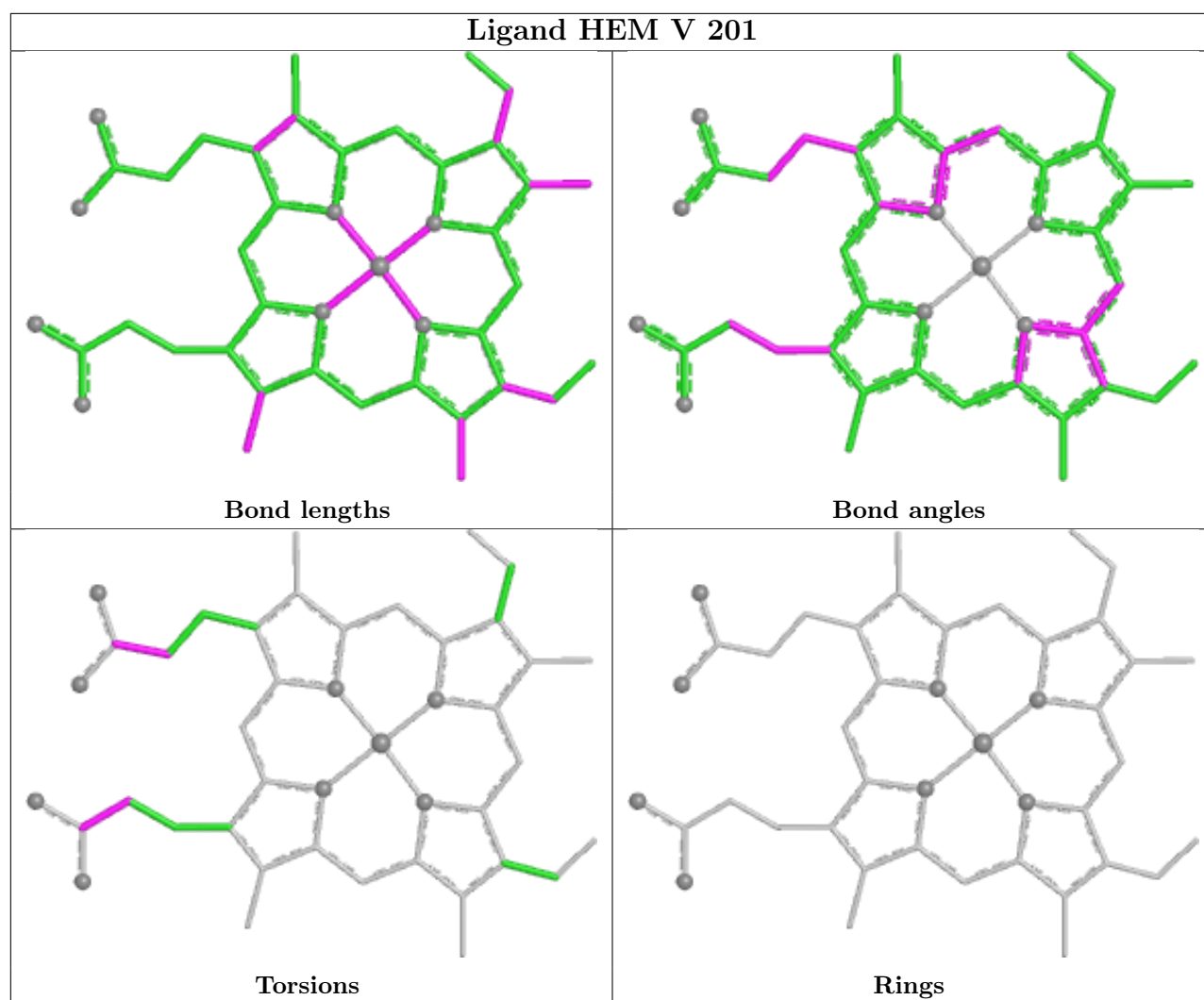




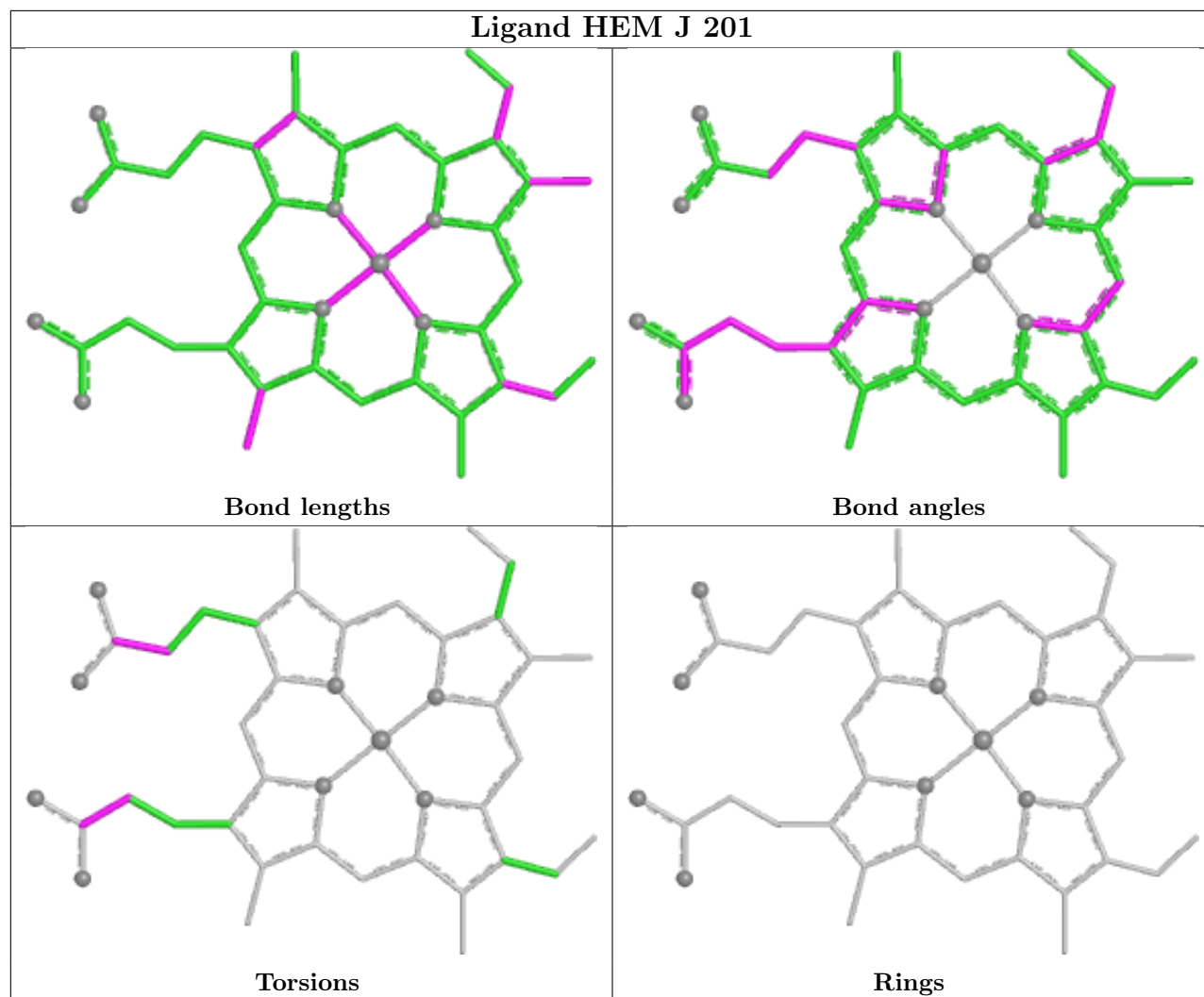


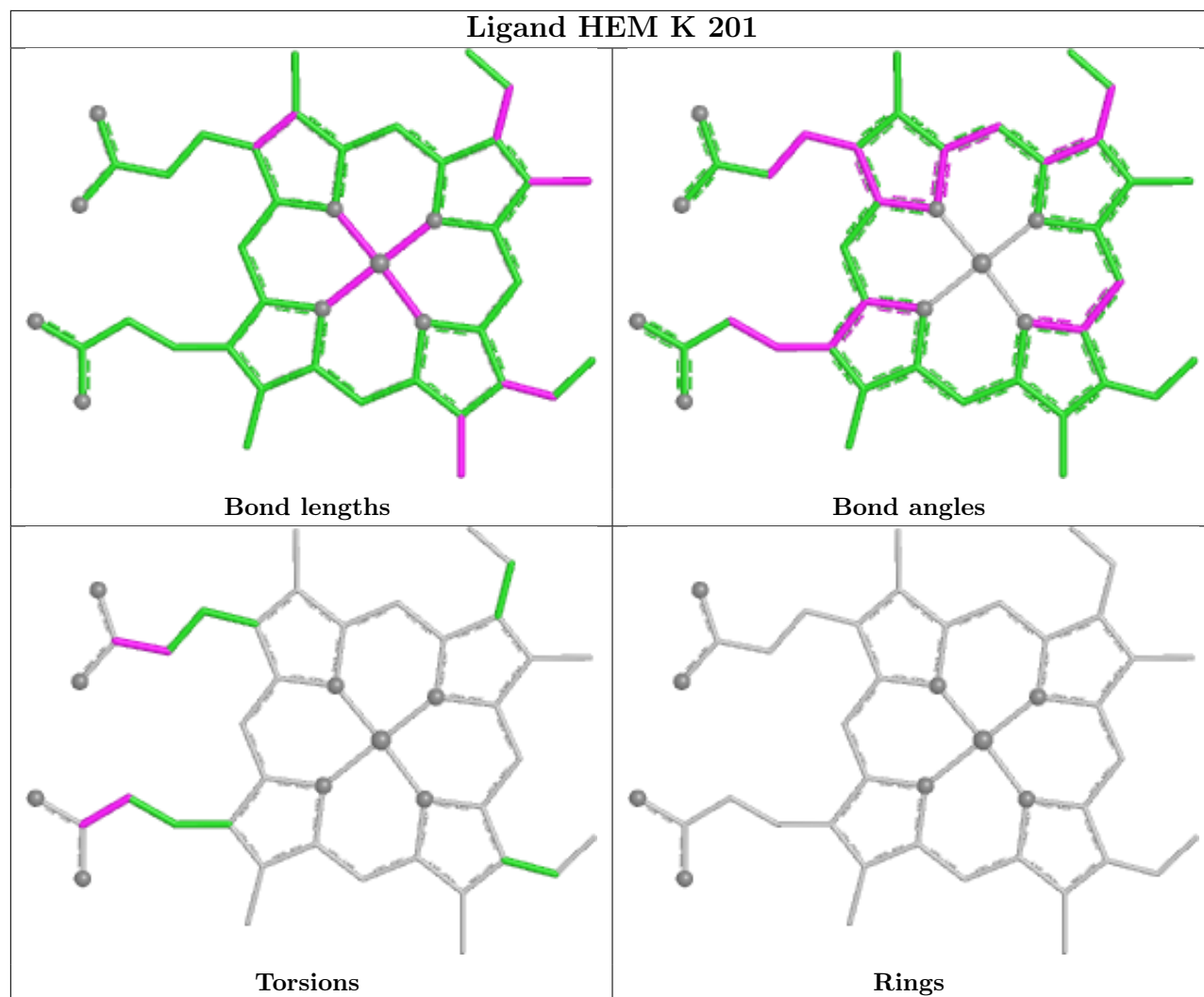


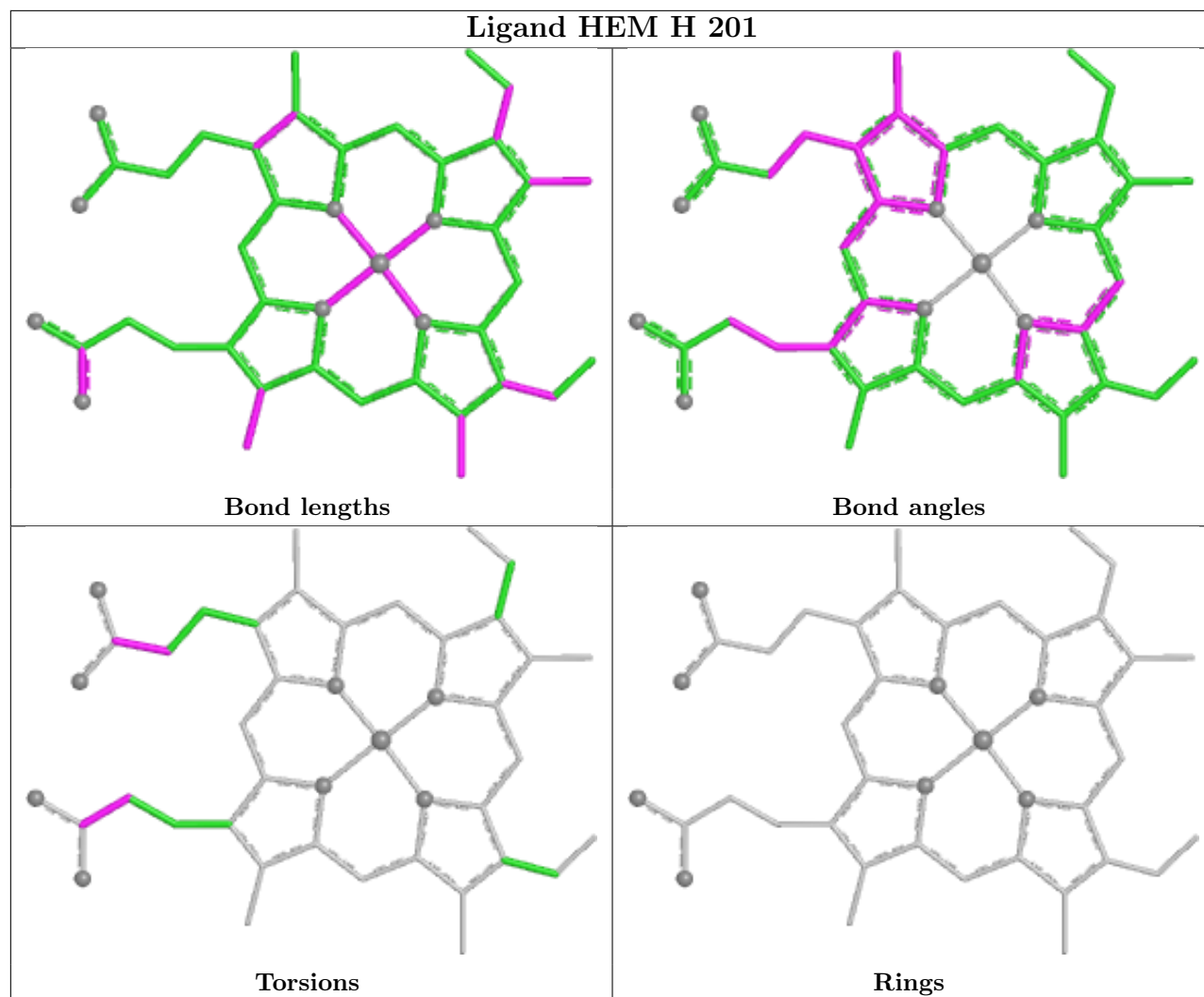


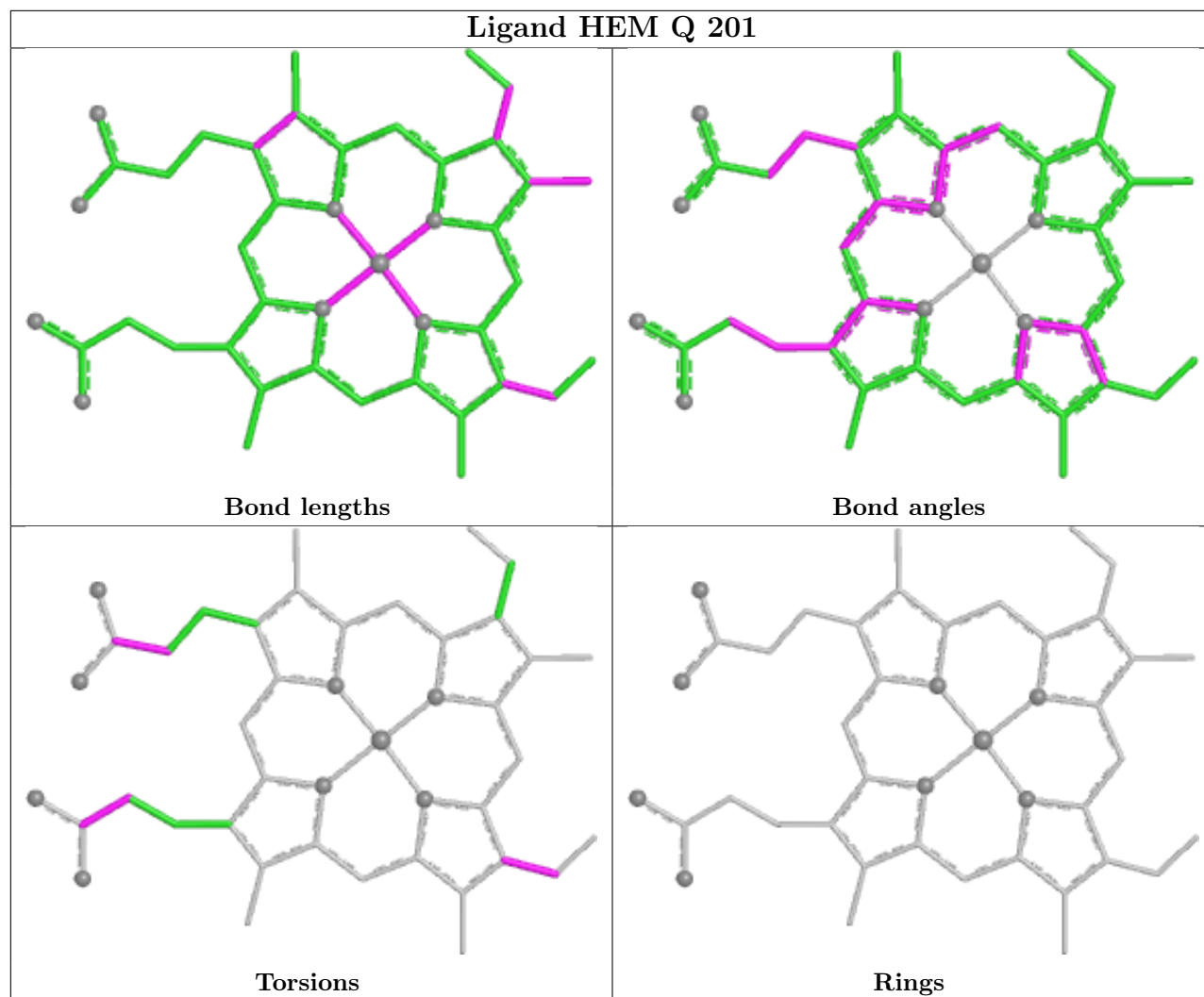


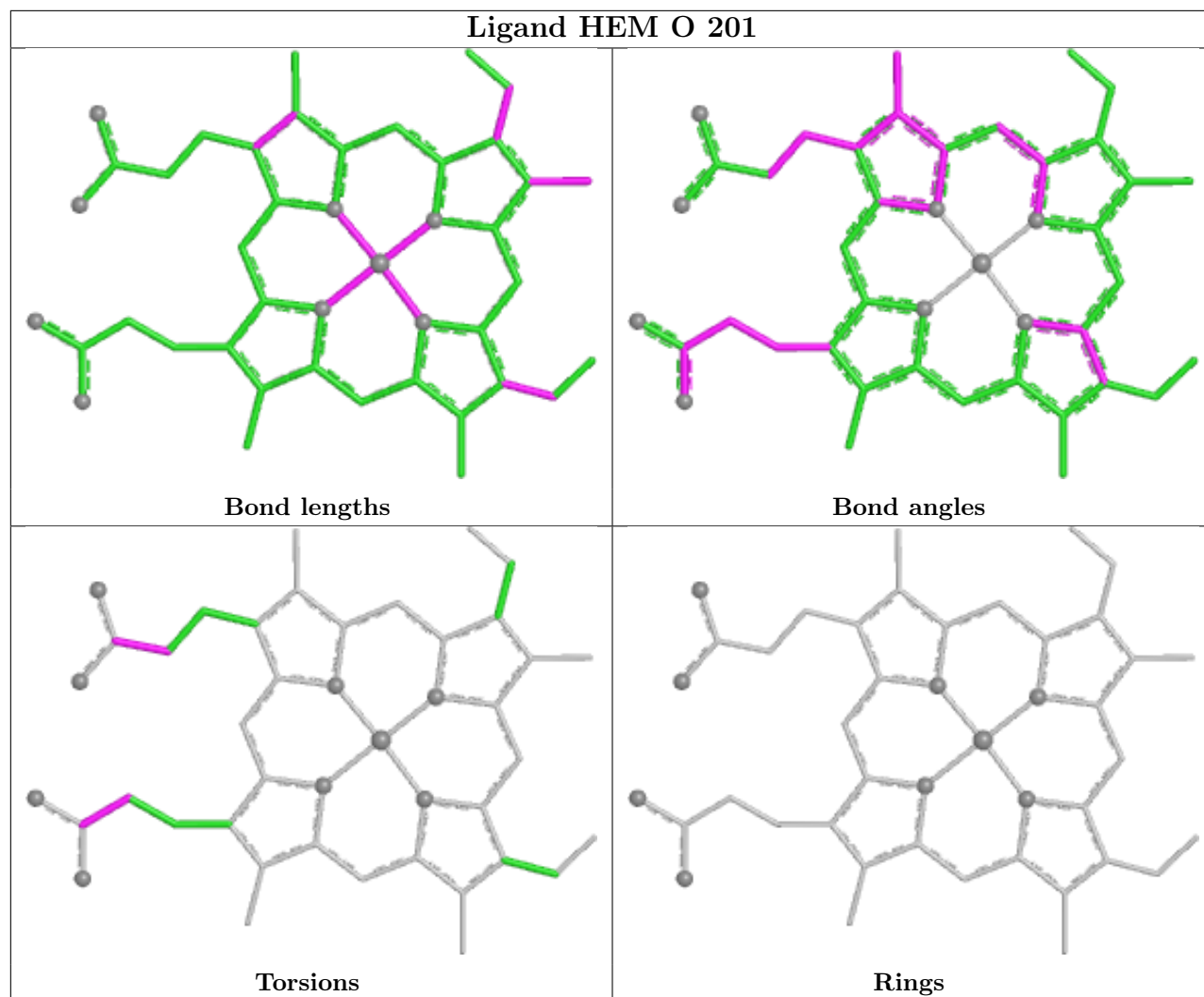
Ligand HEM J 201

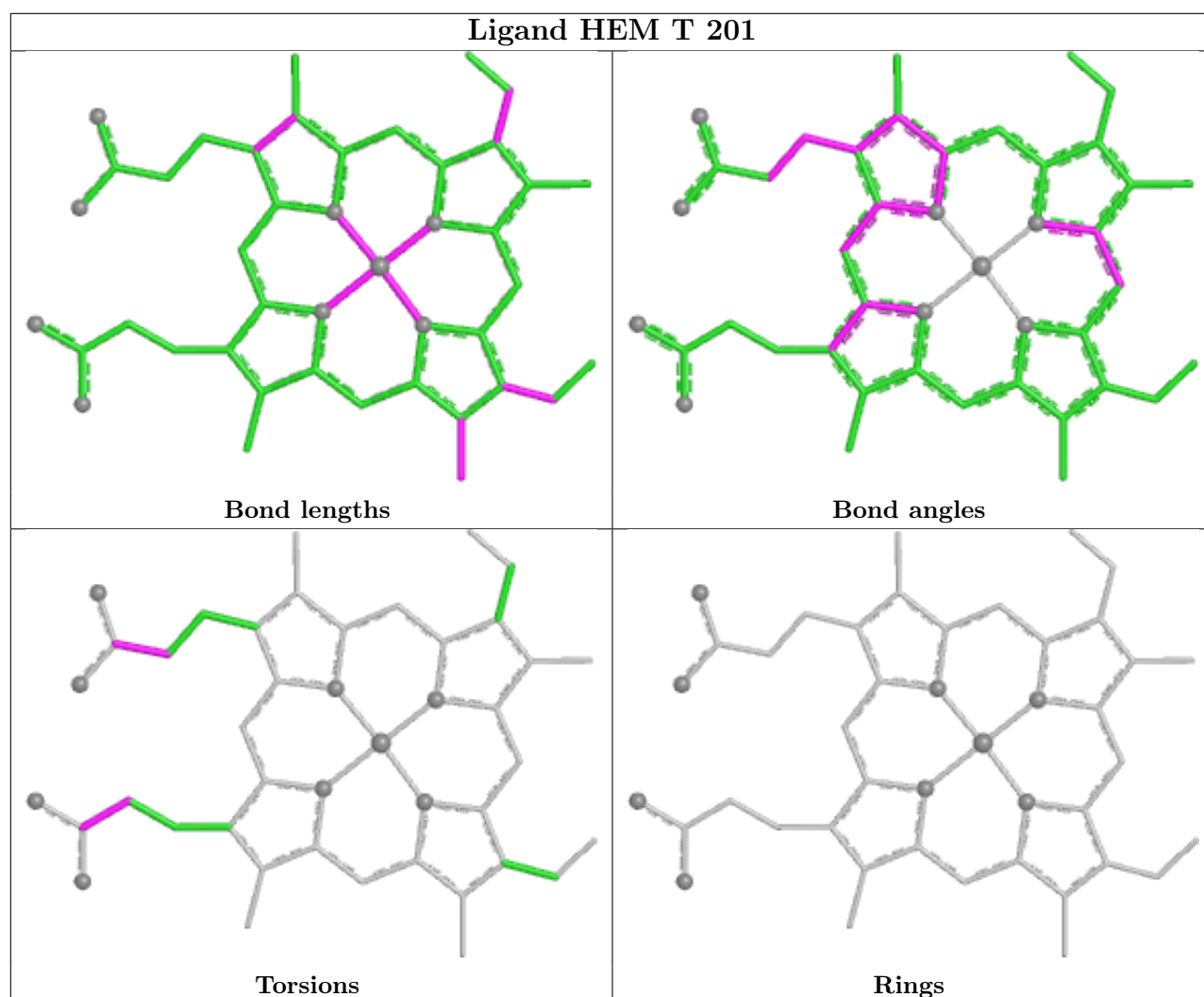












5.7 Other polymers [i](#)

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	156/158 (98%)	-0.30	3 (1%) 66 74	12, 18, 30, 43	0
1	B	155/158 (98%)	-0.37	1 (0%) 85 89	12, 18, 29, 39	0
1	C	155/158 (98%)	-0.35	2 (1%) 75 81	13, 19, 28, 42	0
1	D	155/158 (98%)	-0.39	0 100 100	13, 18, 27, 40	0
1	E	155/158 (98%)	-0.38	1 (0%) 85 89	13, 18, 28, 42	0
1	F	156/158 (98%)	-0.40	1 (0%) 85 89	13, 17, 27, 50	0
1	G	155/158 (98%)	-0.39	1 (0%) 85 89	11, 17, 29, 40	0
1	H	155/158 (98%)	-0.43	1 (0%) 85 89	10, 16, 26, 40	0
1	I	155/158 (98%)	-0.34	1 (0%) 85 89	13, 18, 29, 41	0
1	J	155/158 (98%)	-0.32	2 (1%) 75 81	14, 18, 29, 43	0
1	K	155/158 (98%)	-0.23	1 (0%) 85 89	15, 20, 30, 41	0
1	L	154/158 (97%)	-0.27	1 (0%) 85 89	14, 19, 28, 39	0
1	M	154/158 (97%)	-0.30	2 (1%) 75 81	13, 19, 29, 42	0
1	N	156/158 (98%)	-0.32	3 (1%) 66 74	12, 18, 30, 47	0
1	O	155/158 (98%)	-0.42	1 (0%) 85 89	12, 17, 26, 41	0
1	P	155/158 (98%)	-0.35	1 (0%) 85 89	13, 19, 29, 42	0
1	Q	154/158 (97%)	-0.26	1 (0%) 85 89	15, 19, 31, 43	0
1	R	155/158 (98%)	-0.27	0 100 100	15, 20, 30, 39	0
1	S	155/158 (98%)	-0.21	0 100 100	15, 20, 31, 42	0
1	T	155/158 (98%)	-0.27	1 (0%) 85 89	15, 20, 30, 42	0
1	U	154/158 (97%)	-0.32	0 100 100	14, 19, 31, 40	0
1	V	155/158 (98%)	-0.27	0 100 100	14, 20, 31, 45	0
1	W	156/158 (98%)	-0.40	1 (0%) 85 89	12, 17, 28, 52	0
1	X	155/158 (98%)	-0.40	1 (0%) 85 89	12, 17, 28, 40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3720/3792 (98%)	-0.33	26 (0%) 84 88	10, 19, 30, 52	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	1	MET	6.3
1	W	157	ASP	4.0
1	A	1	MET	3.5
1	F	157	ASP	3.5
1	K	156	GLU	3.2
1	J	156	GLU	2.9
1	A	2	LYS	2.8
1	C	156	GLU	2.6
1	M	156	GLU	2.5
1	J	2	LYS	2.5
1	N	2	LYS	2.5
1	T	2	LYS	2.5
1	B	152	SER	2.4
1	G	156	GLU	2.3
1	N	110	GLN	2.3
1	H	2	LYS	2.3
1	C	152	SER	2.2
1	P	156	GLU	2.2
1	I	2	LYS	2.2
1	X	156	GLU	2.1
1	A	156	GLU	2.1
1	L	156	GLU	2.1
1	O	156	GLU	2.1
1	Q	156	GLU	2.1
1	E	2	LYS	2.0
1	M	3	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

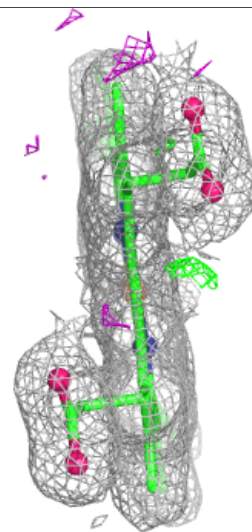
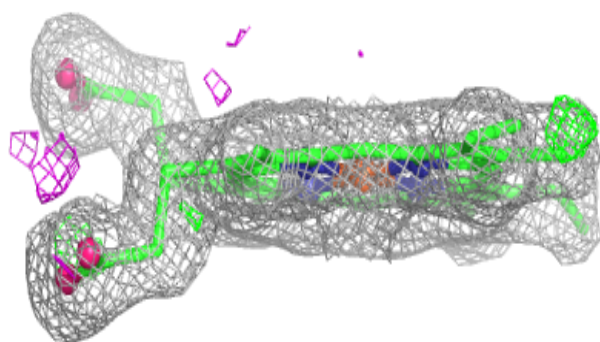
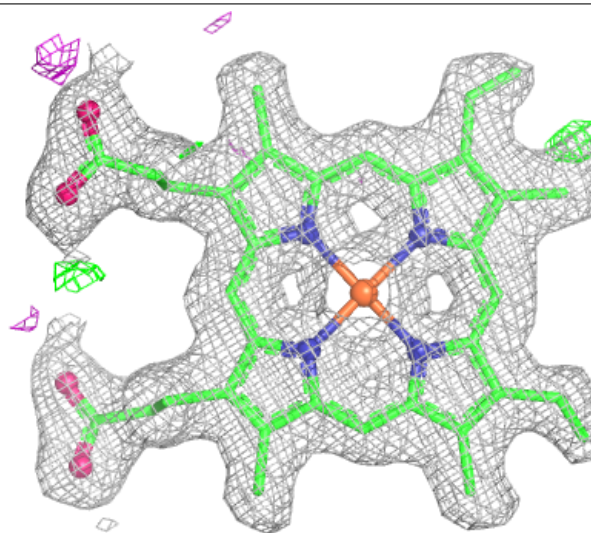
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MES	B	202	12/12	0.82	0.16	32,39,46,47	0
2	MES	C	202	12/12	0.82	0.15	29,37,48,50	0
2	MES	P	201	12/12	0.82	0.15	30,36,41,49	0
2	MES	X	202	12/12	0.83	0.16	31,36,40,48	0
2	MES	V	202	12/12	0.84	0.15	31,37,45,47	0
2	MES	Q	202	12/12	0.84	0.15	31,34,45,46	0
2	MES	J	202	12/12	0.85	0.16	27,35,41,46	0
2	MES	M	201	12/12	0.85	0.15	29,35,39,39	0
2	MES	U	201	12/12	0.86	0.14	27,35,43,46	0
2	MES	I	201	12/12	0.87	0.15	32,35,42,49	0
2	MES	W	201	12/12	0.87	0.15	29,33,42,46	0
2	MES	G	201	12/12	0.87	0.15	29,35,40,42	0
2	MES	F	202	12/12	0.88	0.14	26,34,40,42	0
2	MES	N	202	12/12	0.88	0.14	27,34,42,43	0
2	MES	R	201	12/12	0.88	0.12	27,33,49,50	0
2	MES	T	202	12/12	0.88	0.14	29,35,39,39	0
2	MES	O	202	12/12	0.89	0.13	29,32,37,43	0
2	MES	L	201	12/12	0.90	0.13	27,35,39,41	0
2	MES	A	201	12/12	0.90	0.13	25,31,35,43	0
2	MES	K	202	12/12	0.90	0.14	28,37,41,46	0
2	MES	E	201	12/12	0.91	0.12	27,35,42,47	0
2	MES	S	201	12/12	0.92	0.12	29,36,41,45	0
2	MES	D	201	12/12	0.92	0.13	29,32,36,36	0
2	MES	H	202	12/12	0.93	0.11	22,26,33,34	0
3	HEM	B	201	43/43	0.98	0.06	11,15,25,32	0
3	HEM	C	201	43/43	0.98	0.06	11,15,25,30	0
3	HEM	F	201	43/43	0.98	0.06	10,15,24,33	0
3	HEM	H	201	43/43	0.98	0.06	11,13,22,30	0
3	HEM	J	201	43/43	0.98	0.06	12,16,26,31	0
3	HEM	K	201	43/43	0.98	0.06	14,17,29,35	0
3	HEM	N	201	43/43	0.98	0.06	12,16,26,32	0
3	HEM	O	201	43/43	0.98	0.06	11,15,25,28	0
3	HEM	Q	201	43/43	0.98	0.07	13,18,26,35	0
3	HEM	T	201	43/43	0.98	0.07	14,17,26,33	0
3	HEM	V	201	43/43	0.98	0.06	13,17,25,31	0
3	HEM	X	201	43/43	0.98	0.06	12,15,26,33	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.

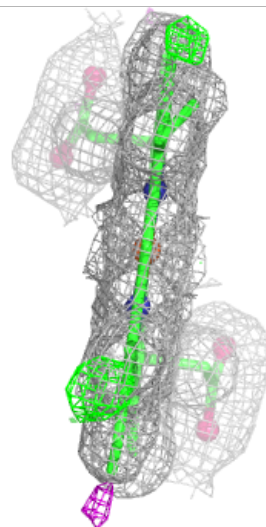
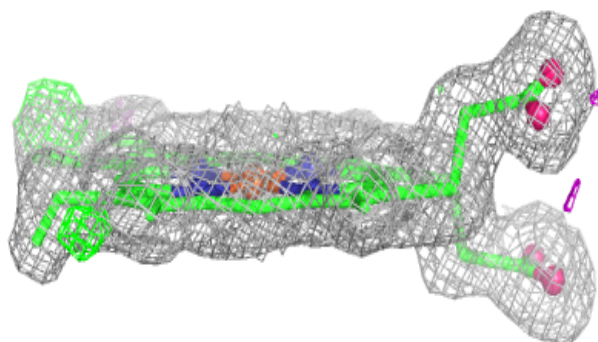
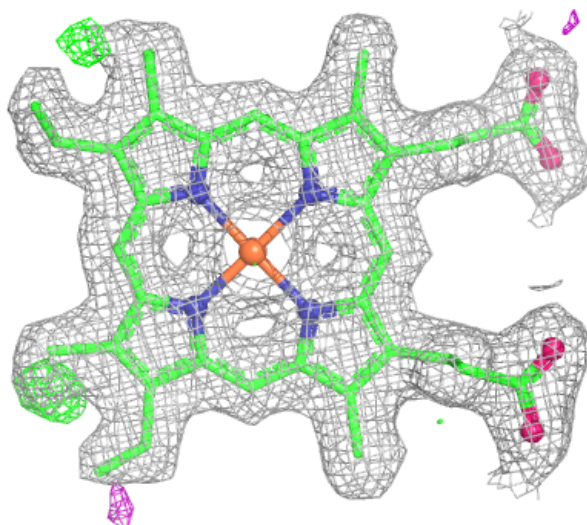
Electron density around HEM B 201:

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



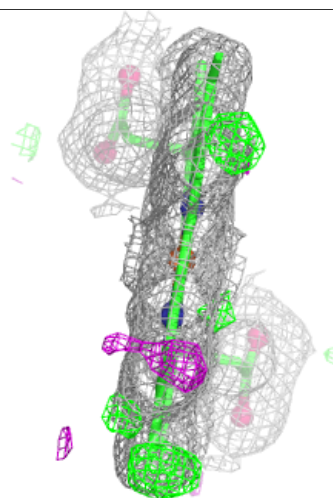
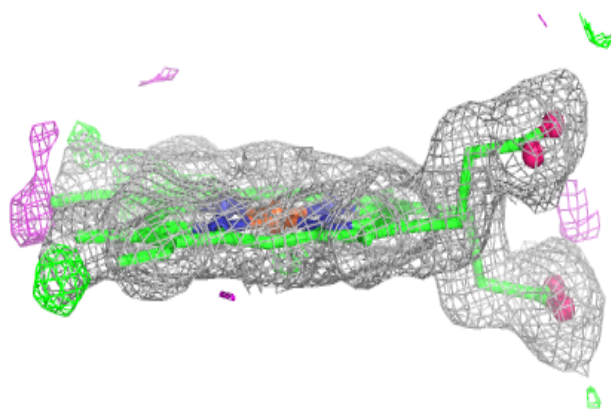
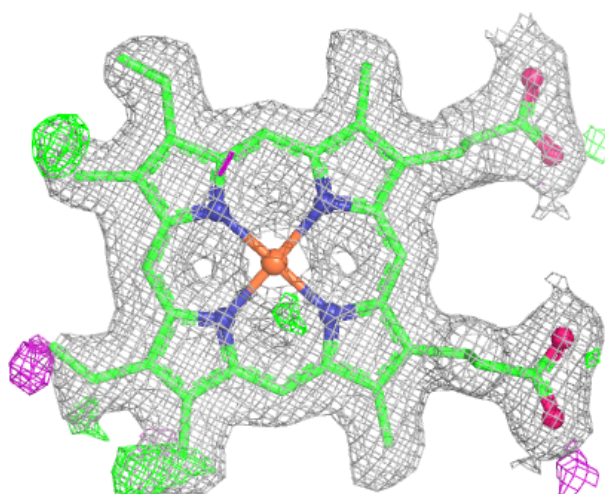
Electron density around HEM C 201:

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



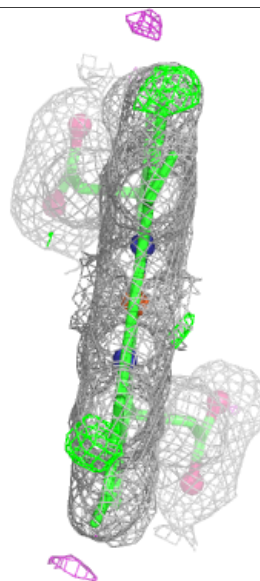
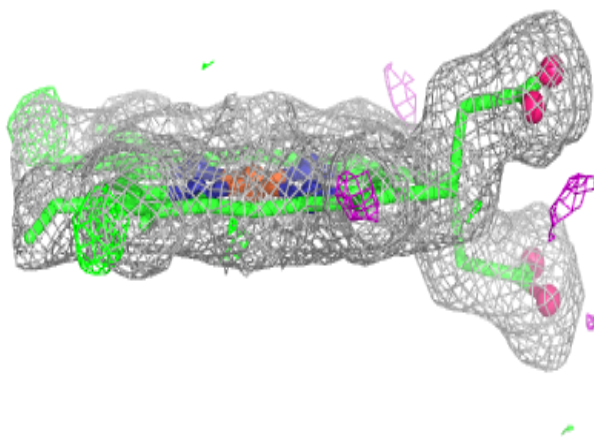
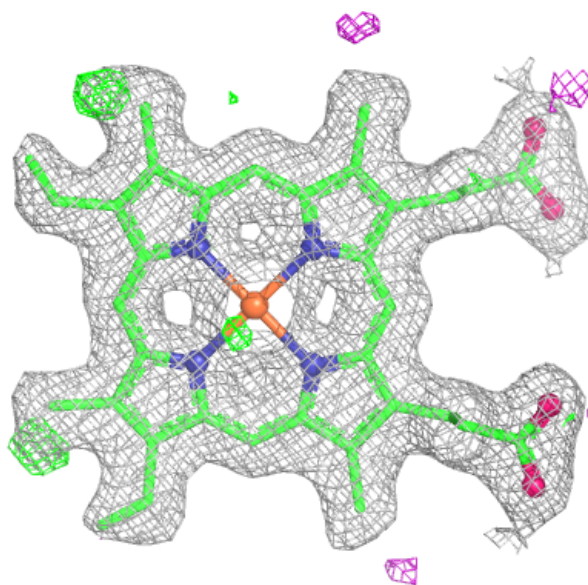
Electron density around HEM F 201:

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



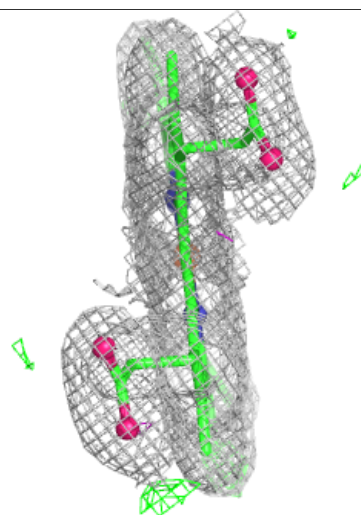
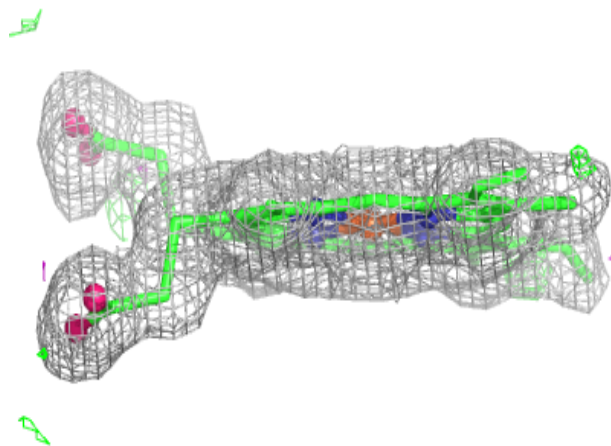
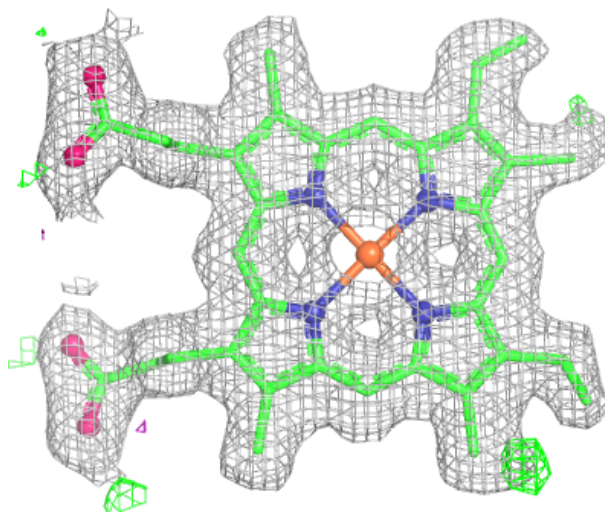
Electron density around HEM H 201:

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



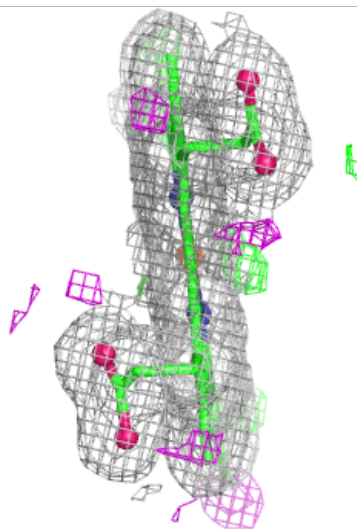
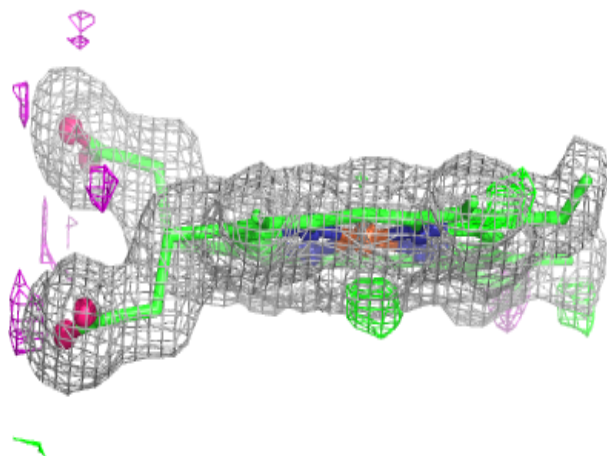
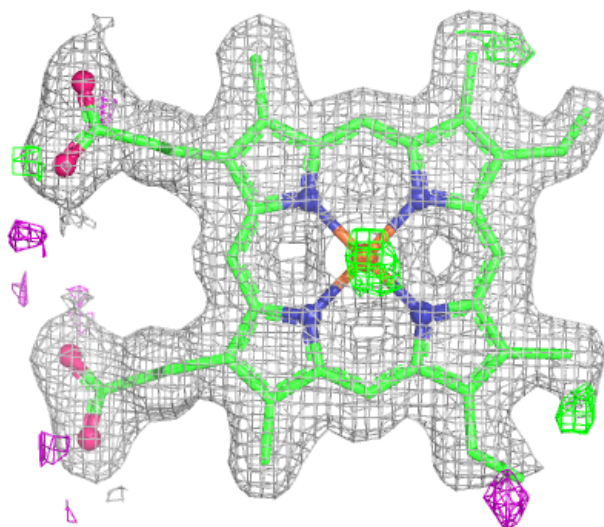
Electron density around HEM J 201:

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



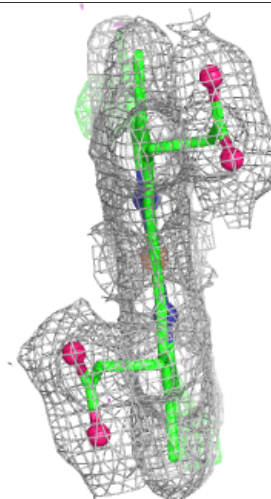
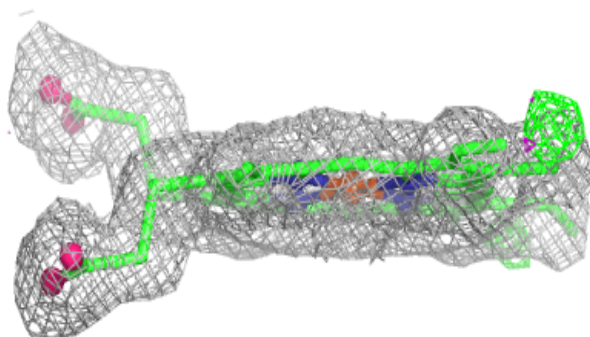
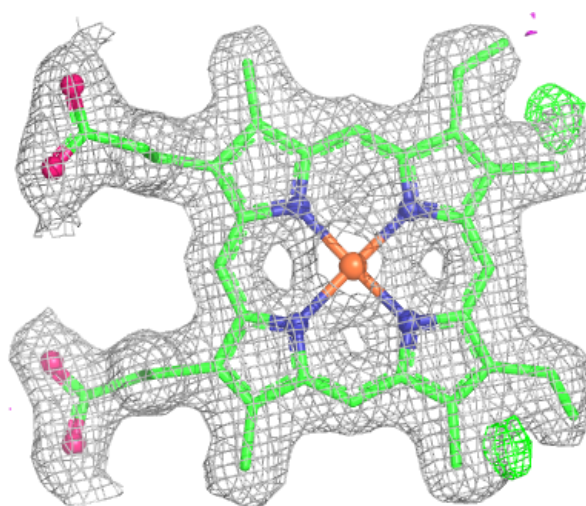
Electron density around HEM K 201:

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



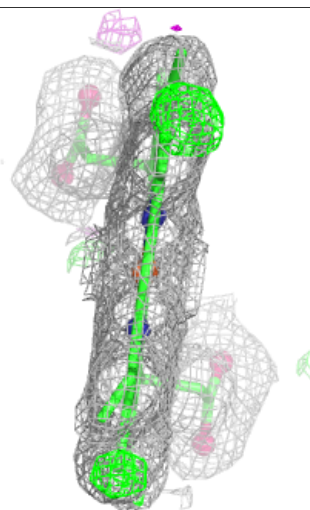
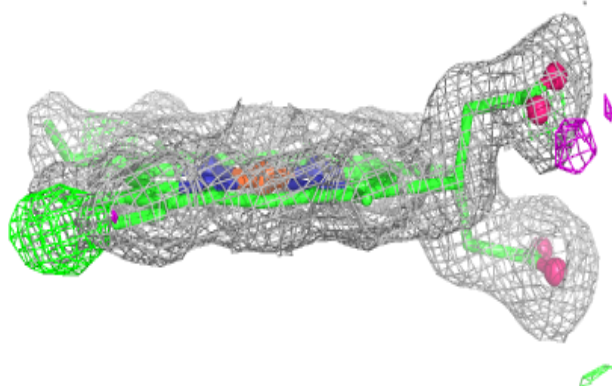
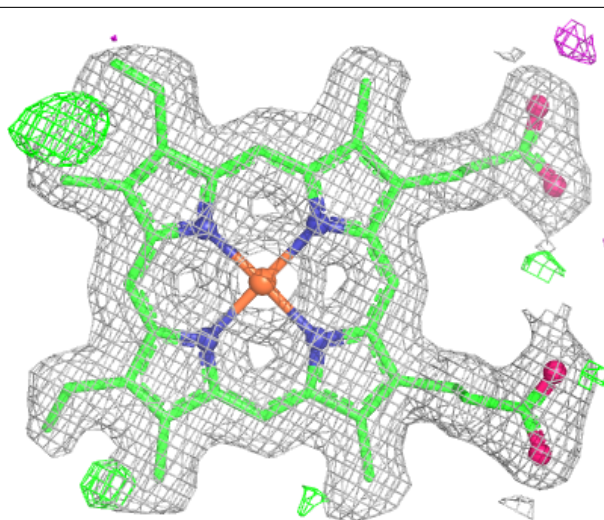
Electron density around HEM N 201:

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



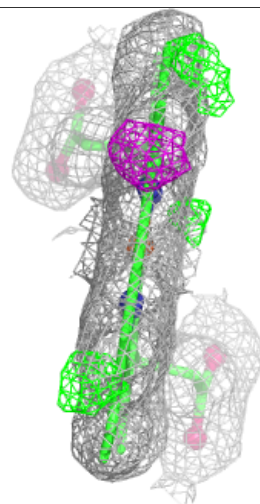
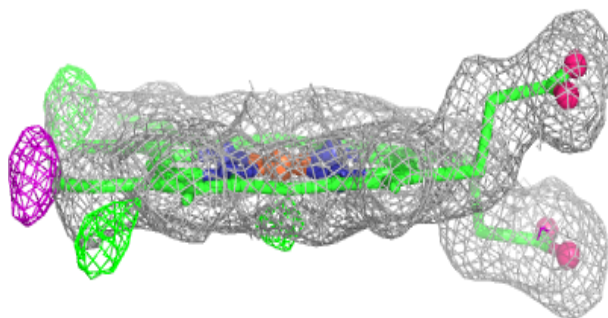
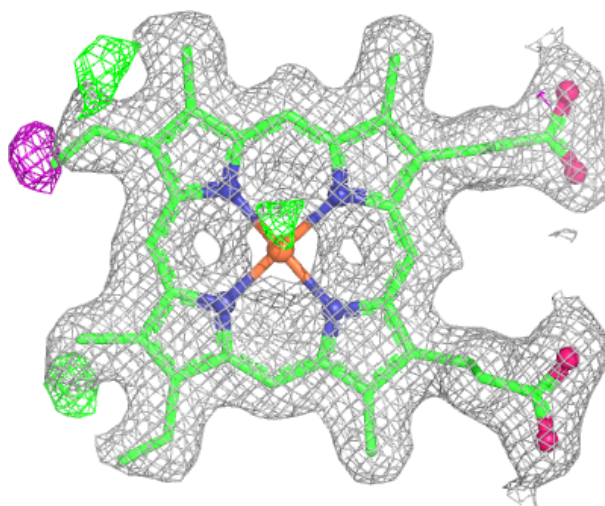
Electron density around HEM O 201:

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



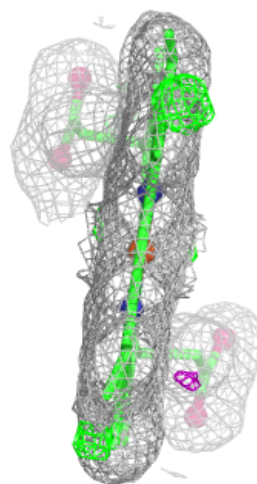
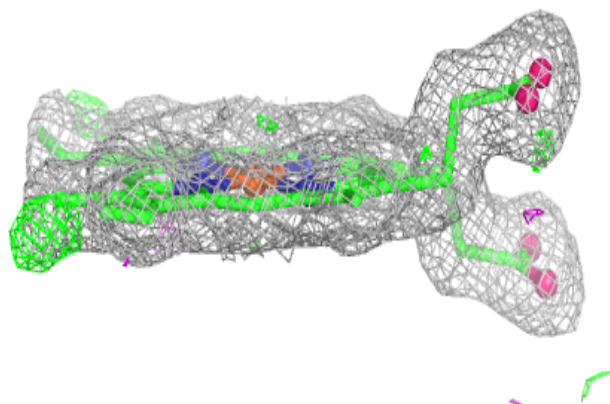
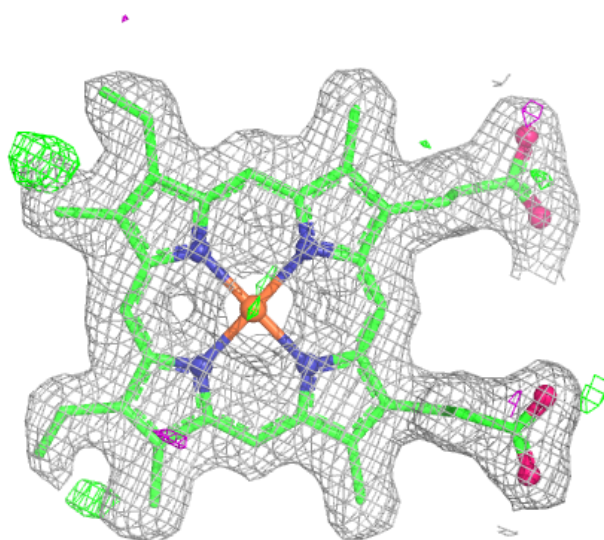
Electron density around HEM Q 201:

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



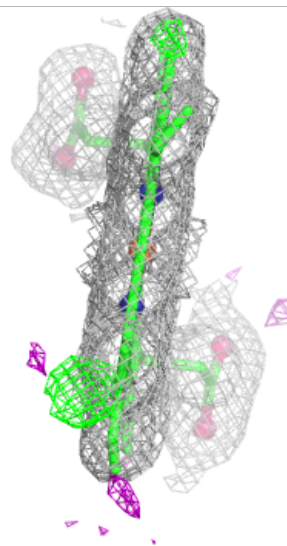
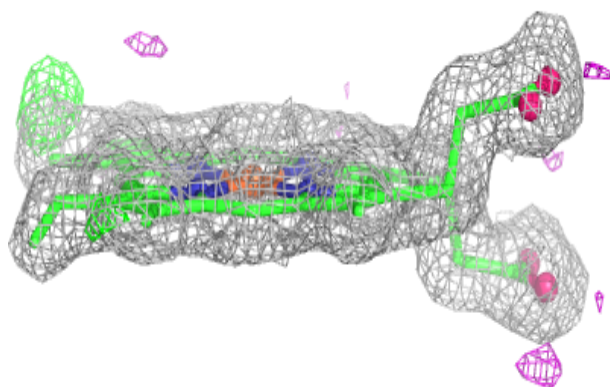
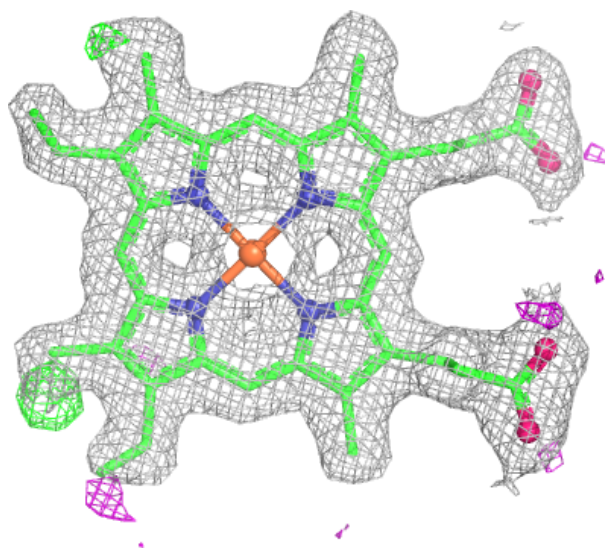
Electron density around HEM T 201:

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



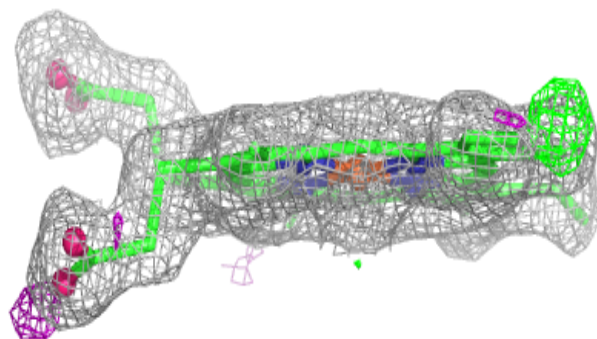
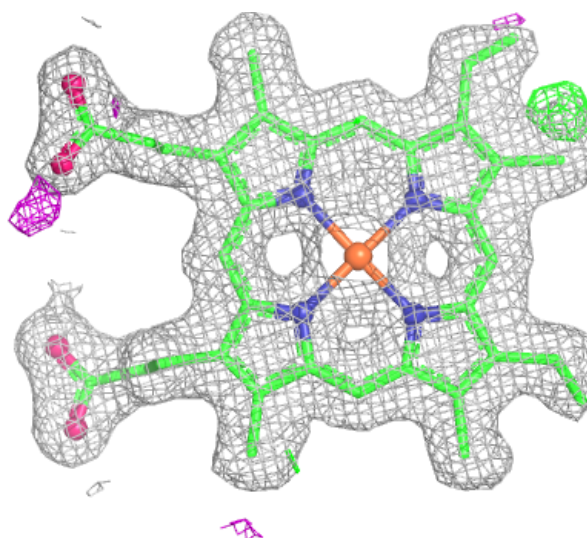
Electron density around HEM V 201:

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



Electron density around HEM X 201:

$2mF_o-DF_c$ (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.