



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:10 pm BST

PDB ID : 4TOC  
Title : 2.25Å resolution structure of Iron Bound 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 : 2.25 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](mailto: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.

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

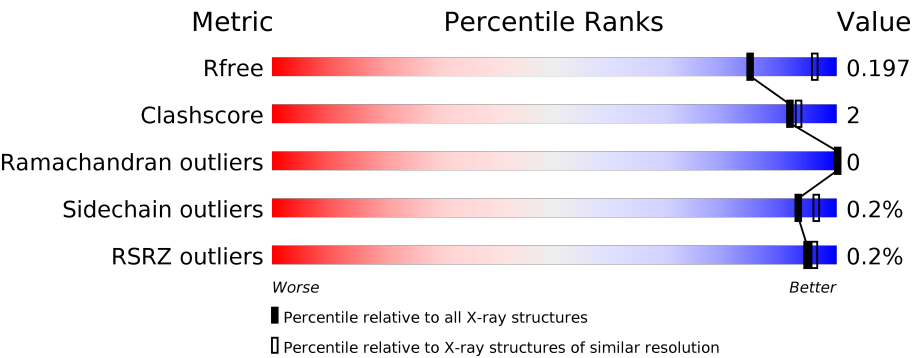
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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.



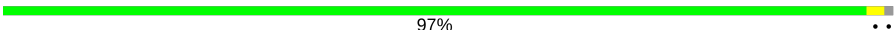
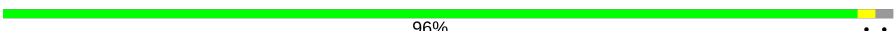

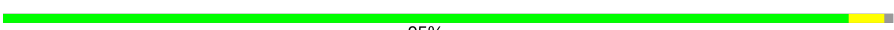








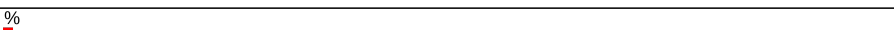

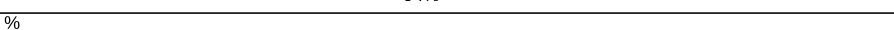
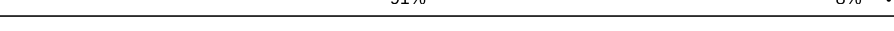
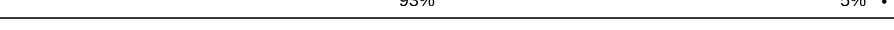
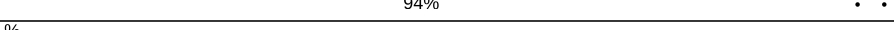
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div><div></div><div>93%</div><div></div></div>
1	B	158	<div><div></div><div>96%</div><div></div></div>
1	C	158	<div><div></div><div>94%</div><div></div></div>
1	D	158	<div><div>%</div><div>95%</div><div></div></div>
1	E	158	<div><div></div><div>94%</div><div></div></div>
1	F	158	<div><div>%</div><div>94%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	158	 97% ..
1	H	158	 96% ..
1	I	158	 91% 8% .
1	J	158	 95% ..
1	K	158	 97% ..
1	L	158	 93% 5% .
1	M	158	 93% . .
1	N	158	 96% ..
1	O	158	 96% ..
1	P	158	 97% ..
1	Q	158	 95% ..
1	R	158	 95% ..
1	S	158	 97% ..
1	T	158	 94% ..
1	U	158	 91% 8% .
1	V	158	 93% 5% .
1	W	158	 94% . .
1	X	158	 97% ..

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33129 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	153	Total	C	N	O	S	0	0	0
			1251	793	212	240	6			
1	B	155	Total	C	N	O	S	0	0	0
			1269	803	218	242	6			
1	C	155	Total	C	N	O	S	0	0	0
			1254	795	213	240	6			
1	D	156	Total	C	N	O	S	0	0	0
			1271	807	217	240	7			
1	E	155	Total	C	N	O	S	0	0	0
			1260	798	214	242	6			
1	F	156	Total	C	N	O	S	0	0	0
			1269	804	215	243	7			
1	G	156	Total	C	N	O	S	0	0	0
			1269	804	216	243	6			
1	H	155	Total	C	N	O	S	0	0	0
			1262	801	215	240	6			
1	I	156	Total	C	N	O	S	0	0	0
			1268	804	215	242	7			
1	J	156	Total	C	N	O	S	0	0	0
			1267	803	216	241	7			
1	K	156	Total	C	N	O	S	0	0	0
			1267	804	217	239	7			
1	L	155	Total	C	N	O	S	0	0	0
			1266	802	216	242	6			
1	M	154	Total	C	N	O	S	0	0	0
			1255	797	213	239	6			
1	N	156	Total	C	N	O	S	0	0	0
			1271	806	215	243	7			
1	O	155	Total	C	N	O	S	0	0	0
			1263	801	214	242	6			
1	P	156	Total	C	N	O	S	0	0	0
			1265	802	214	243	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	156	Total	C	N	O	S	0	0	0
			1274	808	216	243	7			
1	R	155	Total	C	N	O	S	0	0	0
			1259	798	214	241	6			
1	S	156	Total	C	N	O	S	0	0	0
			1265	802	214	242	7			
1	T	156	Total	C	N	O	S	0	0	0
			1270	804	216	243	7			
1	U	156	Total	C	N	O	S	0	0	0
			1267	804	217	239	7			
1	V	155	Total	C	N	O	S	0	0	0
			1246	792	213	235	6			
1	W	155	Total	C	N	O	S	0	0	0
			1263	800	215	242	6			
1	X	156	Total	C	N	O	S	0	0	0
			1272	807	215	243	7			

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

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

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

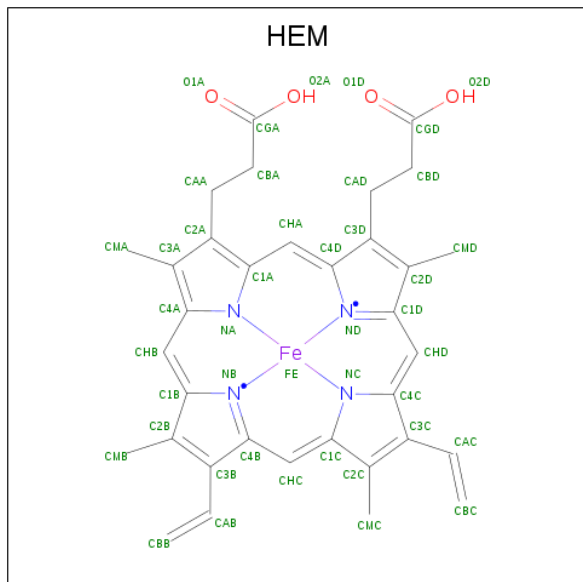
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	4	Total Fe 4 4	0	0
2	K	5	Total Fe 5 5	0	0
2	B	6	Total Fe 6 6	0	0
2	W	5	Total Fe 5 5	0	0
2	N	5	Total Fe 5 5	0	0
2	X	5	Total Fe 5 5	0	0
2	S	3	Total Fe 3 3	0	0
2	J	5	Total Fe 5 5	0	0
2	E	6	Total Fe 6 6	0	0
2	V	7	Total Fe 7 7	0	0
2	A	6	Total Fe 6 6	0	0
2	R	6	Total Fe 6 6	0	0
2	M	5	Total Fe 5 5	0	0
2	D	5	Total Fe 5 5	0	0
2	I	6	Total Fe 6 6	0	0
2	U	4	Total Fe 4 4	0	0
2	L	5	Total Fe 5 5	0	0
2	G	7	Total Fe 7 7	0	0
2	Q	3	Total Fe 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	5	Total	Fe	0	0
			5	5		
2	C	4	Total	Fe	0	0
			4	4		
2	T	5	Total	Fe	0	0
			5	5		
2	O	5	Total	Fe	0	0
			5	5		
2	F	3	Total	Fe	0	0
			3	3		

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



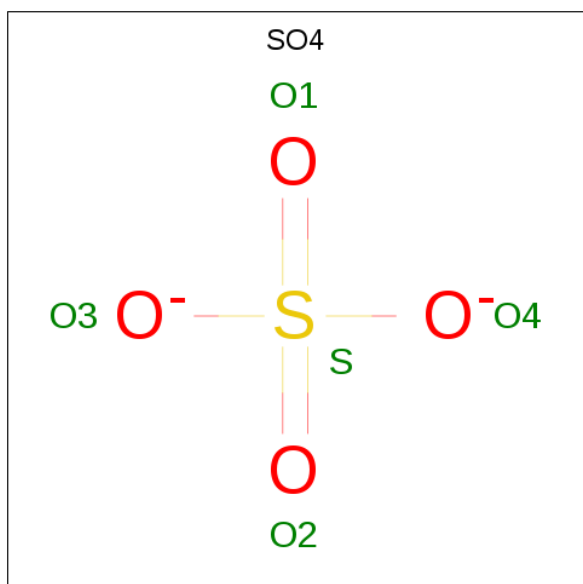
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	T	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	U	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	W	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	N	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	S	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	84	Total	O		0	0
			84	84			
5	B	82	Total	O		0	0
			82	82			
5	C	83	Total	O		0	0
			83	83			
5	D	99	Total	O		0	0
			99	99			
5	E	81	Total	O		0	0
			81	81			
5	F	85	Total	O		0	0
			85	85			
5	G	103	Total	O		0	0
			103	103			
5	H	92	Total	O		0	0
			92	92			
5	I	89	Total	O		0	0
			89	89			
5	J	102	Total	O		0	0
			102	102			
5	K	99	Total	O		0	0
			99	99			
5	L	94	Total	O		0	0
			94	94			
5	M	92	Total	O		0	0
			92	92			
5	N	92	Total	O		0	0
			92	92			
5	O	81	Total	O		0	0
			81	81			
5	P	102	Total	O		0	0
			102	102			

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Q	93	Total 93	O 93	0	0
5	R	80	Total 80	O 80	0	0
5	S	82	Total 82	O 82	0	0
5	T	74	Total 74	O 74	0	0
5	U	75	Total 75	O 75	0	0
5	V	74	Total 74	O 74	0	0
5	W	82	Total 82	O 82	0	0
5	X	90	Total 90	O 90	0	0

### 3 Residue-property plots [i](#)

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

- Molecule 1: Bacterioferritin

Chain A:  93%



- Molecule 1: Bacterioferritin

Chain B:  96%



- Molecule 1: Bacterioferritin

Chain C:  94%



- Molecule 1: Bacterioferritin

Chain D:  95%



- Molecule 1: Bacterioferritin

Chain E:  94%



- Molecule 1: Bacterioferritin

Chain F:  94%



- Molecule 1: Bacterioferritin

Chain G: 97% ..



- Molecule 1: Bacterioferritin

Chain H: 96% ..



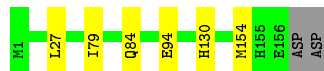
- Molecule 1: Bacterioferritin

Chain I: 91% 8% .



- Molecule 1: Bacterioferritin

Chain J: 95% ..



- Molecule 1: Bacterioferritin

Chain K: 97% ..



- Molecule 1: Bacterioferritin

Chain L: 93% 5% .



- Molecule 1: Bacterioferritin

Chain M: 93% . .



- Molecule 1: Bacterioferritin

Chain N: 96%



- Molecule 1: Bacterioferritin

Chain O: 96%



- Molecule 1: Bacterioferritin

Chain P: 97%



- Molecule 1: Bacterioferritin

Chain Q: 95%



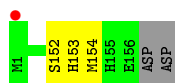
- Molecule 1: Bacterioferritin

Chain R: 95%



- Molecule 1: Bacterioferritin

Chain S: 97%

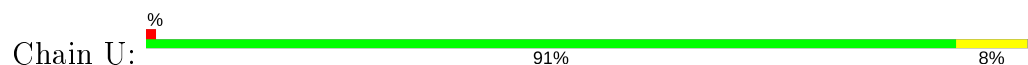


- Molecule 1: Bacterioferritin

Chain T: 94%



- 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, $\alpha$ , $\beta$ , $\gamma$	125.59Å 203.22Å 207.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 2.25 49.35 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.35-2.25) 100.0 (49.35-2.25)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1450)	Depositor
R, $R_{free}$	0.154 , 0.192 0.163 , 0.197	Depositor DCC
$R_{free}$ test set	12586 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	33129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, FE2, 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	0.55	0/1272	0.63	1/1717 (0.1%)
1	B	0.57	0/1290	0.61	0/1738
1	C	0.53	0/1275	0.59	0/1722
1	D	0.56	1/1292 (0.1%)	0.63	0/1740
1	E	0.56	0/1281	0.62	0/1729
1	F	0.60	0/1290	0.64	0/1740
1	G	0.55	0/1290	0.60	0/1740
1	H	0.58	1/1283 (0.1%)	0.62	0/1730
1	I	0.59	1/1289 (0.1%)	0.63	1/1738 (0.1%)
1	J	0.58	0/1288	0.62	0/1737
1	K	0.57	0/1288	0.59	0/1736
1	L	0.55	1/1287 (0.1%)	0.62	1/1735 (0.1%)
1	M	0.58	0/1276	0.62	0/1721
1	N	0.61	1/1292 (0.1%)	0.64	0/1742
1	O	0.55	0/1284	0.59	0/1732
1	P	0.59	0/1286	0.61	0/1736
1	Q	0.51	0/1295	0.62	0/1745
1	R	0.56	0/1280	0.61	0/1727
1	S	0.53	0/1286	0.58	0/1735
1	T	0.54	0/1291	0.59	0/1741
1	U	0.56	0/1288	0.60	0/1736
1	V	0.53	0/1267	0.59	0/1711
1	W	0.55	0/1284	0.59	0/1732
1	X	0.56	0/1293	0.59	0/1743
All	All	0.56	5/30847 (0.0%)	0.61	3/41603 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	147	GLU	CG-CD	6.45	1.61	1.51
1	N	147	GLU	CG-CD	5.89	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	GLU	CG-CD	5.84	1.60	1.51
1	I	85	GLU	CB-CG	-5.60	1.41	1.52
1	L	147	GLU	CG-CD	5.09	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ASP	CB-CG-OD1	5.50	123.25	118.30
1	I	39	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	L	39	ARG	NE-CZ-NH2	-5.11	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1251	0	1216	6	0
1	B	1269	0	1251	2	0
1	C	1254	0	1210	6	0
1	D	1271	0	1254	5	0
1	E	1260	0	1221	5	0
1	F	1269	0	1235	6	0
1	G	1269	0	1234	3	0
1	H	1262	0	1232	2	0
1	I	1268	0	1238	7	0
1	J	1267	0	1238	4	0
1	K	1267	0	1245	3	0
1	L	1266	0	1239	5	0
1	M	1255	0	1223	6	0
1	N	1271	0	1239	2	0
1	O	1263	0	1227	3	0
1	P	1265	0	1220	2	0
1	Q	1274	0	1248	5	0
1	R	1259	0	1224	4	0
1	S	1265	0	1229	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1270	0	1240	5	0
1	U	1267	0	1245	10	0
1	V	1246	0	1207	8	0
1	W	1263	0	1230	5	0
1	X	1272	0	1241	2	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
2	E	6	0	0	0	0
2	F	3	0	0	0	0
2	G	7	0	0	0	0
2	H	5	0	0	0	0
2	I	6	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	4	0	0	0	0
2	Q	3	0	0	0	0
2	R	6	0	0	0	0
2	S	3	0	0	0	0
2	T	5	0	0	0	0
2	U	4	0	0	0	0
2	V	7	0	0	0	0
2	W	5	0	0	0	0
2	X	5	0	0	0	0
3	A	43	0	30	1	0
3	C	43	0	30	1	0
3	E	43	0	30	1	0
3	H	43	0	30	2	0
3	J	43	0	30	3	0
3	K	43	0	30	1	0
3	M	43	0	30	4	0
3	P	43	0	30	3	0
3	Q	43	0	30	2	0
3	T	43	0	30	3	0
3	U	43	0	30	0	0
3	W	43	0	30	1	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	F	5	0	0	0	0
4	M	5	0	0	0	0
4	N	5	0	0	0	0
4	P	5	0	0	0	0
4	S	5	0	0	0	0
5	A	84	0	0	3	0
5	B	82	0	0	0	0
5	C	83	0	0	1	0
5	D	99	0	0	3	0
5	E	81	0	0	1	0
5	F	85	0	0	2	0
5	G	103	0	0	0	0
5	H	92	0	0	0	0
5	I	89	0	0	2	0
5	J	102	0	0	1	0
5	K	99	0	0	0	0
5	L	94	0	0	0	0
5	M	92	0	0	1	0
5	N	92	0	0	0	0
5	O	81	0	0	1	0
5	P	102	0	0	1	0
5	Q	93	0	0	2	0
5	R	80	0	0	0	0
5	S	82	0	0	0	0
5	T	74	0	0	1	0
5	U	75	0	0	0	0
5	V	74	0	0	1	0
5	W	82	0	0	1	0
5	X	90	0	0	0	0
All	All	33129	0	29946	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (99) 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:204:HEM:HHC	3:Q:204:HEM:HBB2	1.70	0.73
1:F:50:ASP:OD2	5:F:364:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:143:LYS:NZ	5:W:362:HOH:O	2.22	0.68
3:E:207:HEM:HHC	3:E:207:HEM:HBB2	1.75	0.68
1:I:103:GLU:OE2	5:I:367:HOH:O	2.12	0.67
1:D:34:ASP:OD1	5:D:364:HOH:O	2.12	0.66
1:L:96:LYS:NZ	1:L:100:ASP:OD2	2.29	0.66
1:C:125:GLU:OE1	5:C:358:HOH:O	2.14	0.65
1:Q:72:GLN:HE22	1:R:77:LEU:H	1.45	0.65
1:P:34:ASP:OD1	5:P:371:HOH:O	2.15	0.63
1:E:77:LEU:H	1:F:72:GLN:HE22	1.46	0.61
1:U:77:LEU:H	1:V:72:GLN:HE22	1.47	0.61
1:E:96:LYS:NZ	5:E:369:HOH:O	2.34	0.60
1:D:147:GLU:OE1	5:D:360:HOH:O	2.18	0.56
1:O:151:LEU:HA	1:O:154:MET:HE2	1.90	0.54
1:Q:84:GLN:NE2	5:Q:340:HOH:O	2.41	0.54
1:F:152:SER:HB3	1:H:151:LEU:CD1	2.39	0.52
1:Q:34:ASP:OD1	5:Q:363:HOH:O	2.19	0.52
3:P:205:HEM:HMC1	3:P:205:HEM:HBC2	1.92	0.51
5:D:353:HOH:O	1:F:147:GLU:HG2	2.10	0.51
3:M:206:HEM:HMB1	3:M:206:HEM:HBB2	1.94	0.49
1:A:151:LEU:HD11	1:L:152:SER:HB3	1.94	0.49
1:C:152:SER:HB3	1:K:151:LEU:CD1	2.43	0.48
1:C:151:LEU:CD1	1:U:152:SER:HB3	2.43	0.48
1:N:151:LEU:CD1	1:T:152:SER:OG	2.61	0.48
1:M:33:ASN:ND2	1:M:41:GLY:HA3	2.29	0.48
1:T:110:GLN:HG3	5:T:340:HOH:O	2.13	0.47
1:O:152:SER:HB3	1:W:151:LEU:CD1	2.44	0.47
3:C:205:HEM:HMC2	3:C:205:HEM:HBC2	1.95	0.47
3:T:206:HEM:HBB2	3:T:206:HEM:HMB1	1.95	0.47
1:S:153:HIS:HE1	1:U:154:MET:HE1	1.79	0.47
1:F:130:HIS:CE1	5:F:350:HOH:O	2.68	0.47
1:A:84:GLN:NE2	5:A:312:HOH:O	2.47	0.46
1:L:20:ILE:HG23	1:L:77:LEU:HD23	1.97	0.46
1:U:77:LEU:H	1:V:72:GLN:NE2	2.13	0.46
3:A:207:HEM:HMC2	3:A:207:HEM:HBC2	1.98	0.46
1:U:76:LYS:HA	1:V:72:GLN:HE22	1.81	0.46
3:J:206:HEM:HBB2	3:J:206:HEM:HMB1	1.97	0.46
3:J:206:HEM:HMC2	3:J:206:HEM:HBC2	1.97	0.45
1:M:34:ASP:OD1	5:M:361:HOH:O	2.21	0.45
1:B:152:SER:HB3	1:D:151:LEU:CD1	2.47	0.45
1:E:152:SER:HB3	1:V:151:LEU:CD1	2.47	0.45
3:M:206:HEM:CMB	3:M:206:HEM:HBB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:81:GLU:HG2	1:T:85:GLU:OE1	2.16	0.45
1:H:52:MET:HB3	3:H:206:HEM:CHD	2.47	0.45
1:A:151:LEU:CD1	1:L:152:SER:HB3	2.47	0.45
1:J:94:GLU:OE2	1:J:130:HIS:ND1	2.49	0.45
1:D:1:MET:N	1:U:135:GLU:OE2	2.50	0.45
1:A:152:SER:OG	1:X:151:LEU:CD1	2.65	0.45
1:L:151:LEU:CD1	1:M:152:SER:HB3	2.47	0.44
1:J:154:MET:HE1	1:Q:153:HIS:HE1	1.82	0.44
3:J:206:HEM:HBB2	3:J:206:HEM:CMB	2.47	0.44
1:M:52:MET:HB3	3:M:206:HEM:CHD	2.47	0.44
1:G:153:HIS:HE1	1:I:154:MET:HE1	1.83	0.44
1:M:151:LEU:CD1	1:X:152:SER:OG	2.66	0.44
1:Q:33:ASN:ND2	1:Q:41:GLY:HA3	2.33	0.44
1:F:33:ASN:ND2	1:F:41:GLY:HA3	2.33	0.44
1:G:152:SER:OG	1:I:151:LEU:CD1	2.65	0.44
1:I:100:ASP:OD1	5:I:367:HOH:O	2.20	0.43
1:O:53:LYS:NZ	5:O:380:HOH:O	2.40	0.43
3:T:206:HEM:HBB2	3:T:206:HEM:CMB	2.48	0.43
1:U:27:LEU:HD23	1:U:79:ILE:HD12	2.00	0.43
1:V:10:HIS:HD2	5:V:339:HOH:O	2.01	0.43
3:W:206:HEM:HBB2	3:W:206:HEM:CMB	2.49	0.43
1:D:123:ILE:O	1:D:127:GLU:HG2	2.19	0.43
1:A:60:GLU:OE1	5:A:374:HOH:O	2.21	0.43
1:R:152:SER:HB3	1:T:151:LEU:CD1	2.48	0.42
1:W:33:ASN:ND2	1:W:41:GLY:HA3	2.33	0.42
3:H:206:HEM:HMB1	3:H:206:HEM:HBB2	2.00	0.42
3:Q:204:HEM:HBC2	3:Q:204:HEM:HMC2	2.00	0.42
1:A:46:HIS:HD2	5:A:377:HOH:O	2.01	0.42
1:I:20:ILE:HD11	1:I:75:GLY:HA3	2.00	0.42
3:P:205:HEM:HBB2	3:P:205:HEM:CMB	2.50	0.42
3:K:206:HEM:HBC2	3:K:206:HEM:HMC2	2.02	0.42
1:C:22:ILE:HD11	1:C:52:MET:HA	2.01	0.42
3:T:206:HEM:HBC2	3:T:206:HEM:HMC1	2.01	0.42
3:P:205:HEM:HBB2	3:P:205:HEM:HMB1	2.00	0.42
1:G:154:MET:HE1	1:W:153:HIS:HE1	1.84	0.42
1:I:33:ASN:ND2	1:I:41:GLY:HA3	2.35	0.42
1:V:123:ILE:O	1:V:127:GLU:HG2	2.20	0.42
1:J:84:GLN:NE2	5:J:322:HOH:O	2.53	0.41
1:M:154:MET:HE2	1:M:154:MET:HB3	1.87	0.41
1:U:33:ASN:ND2	1:U:41:GLY:HA3	2.35	0.41
1:V:25:TYR:CE2	1:V:130:HIS:HE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:123:ILE:O	1:W:127:GLU:HG2	2.20	0.41
1:P:151:LEU:HA	1:P:154:MET:CE	2.51	0.41
1:R:123:ILE:O	1:R:127:GLU:HG2	2.19	0.41
1:R:153:HIS:HE1	1:T:154:MET:HE1	1.84	0.41
1:C:153:HIS:HE1	1:K:154:MET:HE1	1.85	0.41
3:M:206:HEM:HMC1	3:M:206:HEM:HBC2	2.02	0.41
1:S:152:SER:HB3	1:U:151:LEU:CD1	2.51	0.41
1:B:33:ASN:ND2	1:B:41:GLY:HA3	2.36	0.41
1:E:25:TYR:CE2	1:E:130:HIS:HE1	2.39	0.40
1:K:153:HIS:HE1	1:S:154:MET:HE1	1.85	0.40
1:C:151:LEU:HD11	1:U:152:SER:HB3	2.03	0.40
1:E:153:HIS:HE1	1:V:154:MET:HE1	1.86	0.40
1:J:27:LEU:HD23	1:J:79:ILE:HD12	2.04	0.40
1:I:20:ILE:HG23	1:I:77:LEU:HD12	2.03	0.40
1:N:33:ASN:ND2	1:N:41:GLY:HA3	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/158 (96%)	151 (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	154/158 (98%)	154 (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	154/158 (98%)	154 (100%)	0	0	100	100
1	H	153/158 (97%)	153 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	154/158 (98%)	154 (100%)	0	0	100	100
1	J	154/158 (98%)	154 (100%)	0	0	100	100
1	K	154/158 (98%)	154 (100%)	0	0	100	100
1	L	153/158 (97%)	153 (100%)	0	0	100	100
1	M	152/158 (96%)	152 (100%)	0	0	100	100
1	N	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
1	O	153/158 (97%)	153 (100%)	0	0	100	100
1	P	154/158 (98%)	154 (100%)	0	0	100	100
1	Q	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
1	R	153/158 (97%)	153 (100%)	0	0	100	100
1	S	154/158 (98%)	154 (100%)	0	0	100	100
1	T	154/158 (98%)	154 (100%)	0	0	100	100
1	U	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
1	V	153/158 (97%)	153 (100%)	0	0	100	100
1	W	153/158 (97%)	153 (100%)	0	0	100	100
1	X	154/158 (98%)	154 (100%)	0	0	100	100
All	All	3682/3792 (97%)	3679 (100%)	3 (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	139/144 (96%)	139 (100%)	0	100	100
1	C	133/144 (92%)	133 (100%)	0	100	100
1	D	137/144 (95%)	136 (99%)	1 (1%)	84	90
1	E	135/144 (94%)	135 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	136/144 (94%)	136 (100%)	0	100	100
1	G	136/144 (94%)	136 (100%)	0	100	100
1	H	135/144 (94%)	135 (100%)	0	100	100
1	I	136/144 (94%)	135 (99%)	1 (1%)	84	90
1	J	136/144 (94%)	136 (100%)	0	100	100
1	K	136/144 (94%)	136 (100%)	0	100	100
1	L	137/144 (95%)	137 (100%)	0	100	100
1	M	134/144 (93%)	134 (100%)	0	100	100
1	N	136/144 (94%)	136 (100%)	0	100	100
1	O	135/144 (94%)	135 (100%)	0	100	100
1	P	134/144 (93%)	134 (100%)	0	100	100
1	Q	137/144 (95%)	137 (100%)	0	100	100
1	R	135/144 (94%)	135 (100%)	0	100	100
1	S	135/144 (94%)	135 (100%)	0	100	100
1	T	137/144 (95%)	136 (99%)	1 (1%)	84	90
1	U	136/144 (94%)	134 (98%)	2 (2%)	65	75
1	V	131/144 (91%)	131 (100%)	0	100	100
1	W	136/144 (94%)	136 (100%)	0	100	100
1	X	136/144 (94%)	136 (100%)	0	100	100
All	All	3253/3456 (94%)	3248 (100%)	5 (0%)	93	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1	MET
1	I	1	MET
1	T	1	MET
1	U	1	MET
1	U	119	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN

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Mol	Chain	Res	Type
1	A	54	HIS
1	A	84	GLN
1	A	112	HIS
1	A	153	HIS
1	A	155	HIS
1	B	33	ASN
1	B	84	GLN
1	B	112	HIS
1	B	148	ASN
1	B	155	HIS
1	C	33	ASN
1	C	54	HIS
1	C	112	HIS
1	C	148	ASN
1	C	153	HIS
1	C	155	HIS
1	D	33	ASN
1	D	155	HIS
1	E	112	HIS
1	E	153	HIS
1	E	155	HIS
1	F	33	ASN
1	F	72	GLN
1	F	84	GLN
1	G	33	ASN
1	G	54	HIS
1	G	112	HIS
1	G	153	HIS
1	G	155	HIS
1	H	33	ASN
1	H	54	HIS
1	H	153	HIS
1	H	155	HIS
1	I	33	ASN
1	I	54	HIS
1	I	112	HIS
1	J	33	ASN
1	J	54	HIS
1	J	84	GLN
1	J	112	HIS
1	J	148	ASN
1	J	155	HIS

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Mol	Chain	Res	Type
1	K	33	ASN
1	K	153	HIS
1	L	33	ASN
1	L	84	GLN
1	L	112	HIS
1	L	153	HIS
1	M	33	ASN
1	M	54	HIS
1	M	84	GLN
1	M	155	HIS
1	N	33	ASN
1	N	84	GLN
1	N	155	HIS
1	O	9	GLN
1	O	33	ASN
1	O	54	HIS
1	O	112	HIS
1	O	155	HIS
1	P	33	ASN
1	P	84	GLN
1	P	112	HIS
1	P	148	ASN
1	Q	33	ASN
1	Q	72	GLN
1	Q	84	GLN
1	Q	155	HIS
1	R	84	GLN
1	R	148	ASN
1	R	153	HIS
1	S	9	GLN
1	S	33	ASN
1	S	54	HIS
1	S	153	HIS
1	S	155	HIS
1	T	9	GLN
1	T	33	ASN
1	T	84	GLN
1	T	112	HIS
1	T	155	HIS
1	U	33	ASN
1	U	112	HIS
1	U	155	HIS

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Mol	Chain	Res	Type
1	V	9	GLN
1	V	10	HIS
1	V	33	ASN
1	V	54	HIS
1	V	72	GLN
1	V	155	HIS
1	W	33	ASN
1	W	84	GLN
1	W	148	ASN
1	W	155	HIS
1	X	33	ASN
1	X	84	GLN
1	X	112	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 140 ligands modelled in this entry, 120 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	P	206	-	4,4,4	0.16	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEM	P	205	1	27,50,50	1.88	5 (18%)	17,82,82	2.51	7 (41%)
3	HEM	C	205	1	27,50,50	1.94	5 (18%)	17,82,82	2.32	8 (47%)
4	SO4	B	207	2	4,4,4	0.09	0	6,6,6	0.19	0
3	HEM	K	206	1	27,50,50	1.94	6 (22%)	17,82,82	2.31	6 (35%)
4	SO4	N	206	2	4,4,4	0.16	0	6,6,6	0.43	0
3	HEM	Q	204	1	27,50,50	2.08	5 (18%)	17,82,82	1.92	5 (29%)
3	HEM	M	206	1	27,50,50	1.95	5 (18%)	17,82,82	2.40	8 (47%)
3	HEM	H	206	1	27,50,50	1.95	6 (22%)	17,82,82	2.67	7 (41%)
3	HEM	E	207	1	27,50,50	2.07	5 (18%)	17,82,82	2.38	6 (35%)
3	HEM	U	205	1	27,50,50	2.00	6 (22%)	17,82,82	2.04	7 (41%)
4	SO4	F	204	-	4,4,4	0.21	0	6,6,6	0.28	0
3	HEM	A	207	1	27,50,50	1.91	6 (22%)	17,82,82	2.34	8 (47%)
3	HEM	J	206	1	27,50,50	1.87	5 (18%)	17,82,82	2.42	9 (52%)
3	HEM	W	206	1	27,50,50	1.95	5 (18%)	17,82,82	2.05	7 (41%)
3	HEM	T	206	1	27,50,50	1.96	5 (18%)	17,82,82	2.41	7 (41%)
4	SO4	M	207	-	4,4,4	0.22	0	6,6,6	0.14	0
4	SO4	A	208	2	4,4,4	0.20	0	6,6,6	0.42	0
4	SO4	S	204	-	4,4,4	0.22	0	6,6,6	0.20	0
4	SO4	D	206	-	4,4,4	0.20	0	6,6,6	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	K	206	1	-	0/6/54/54	-
3	HEM	C	205	1	-	0/6/54/54	-
3	HEM	P	205	1	-	0/6/54/54	-
3	HEM	Q	204	1	-	0/6/54/54	-
3	HEM	E	207	1	-	0/6/54/54	-
3	HEM	U	205	1	-	0/6/54/54	-
3	HEM	A	207	1	-	0/6/54/54	-
3	HEM	J	206	1	-	0/6/54/54	-
3	HEM	W	206	1	-	0/6/54/54	-
3	HEM	T	206	1	-	0/6/54/54	-
3	HEM	M	206	1	-	0/6/54/54	-
3	HEM	H	206	1	-	0/6/54/54	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	204	HEM	C3B-C2B	-5.90	1.32	1.40
3	E	207	HEM	C3B-C2B	-5.48	1.32	1.40
3	W	206	HEM	C3D-C2D	5.27	1.53	1.37
3	C	205	HEM	C3D-C2D	5.26	1.53	1.37
3	E	207	HEM	C3D-C2D	5.16	1.53	1.37
3	Q	204	HEM	C3D-C2D	4.95	1.52	1.37
3	K	206	HEM	C3D-C2D	4.89	1.52	1.37
3	T	206	HEM	C3D-C2D	4.86	1.52	1.37
3	U	205	HEM	C3D-C2D	4.83	1.52	1.37
3	J	206	HEM	C3D-C2D	4.82	1.51	1.37
3	P	205	HEM	C3D-C2D	4.70	1.51	1.37
3	A	207	HEM	C3D-C2D	4.65	1.51	1.37
3	C	205	HEM	C3B-C2B	-4.63	1.33	1.40
3	M	206	HEM	C3D-C2D	4.55	1.51	1.37
3	U	205	HEM	C3C-C2C	-4.54	1.34	1.40
3	K	206	HEM	C3B-C2B	-4.51	1.34	1.40
3	H	206	HEM	C3D-C2D	4.38	1.50	1.37
3	H	206	HEM	C3C-C2C	-4.37	1.34	1.40
3	M	206	HEM	C3B-C2B	-4.25	1.34	1.40
3	J	206	HEM	C3B-C2B	-4.23	1.34	1.40
3	A	207	HEM	C3B-C2B	-4.20	1.34	1.40
3	M	206	HEM	C3C-C2C	-4.15	1.34	1.40
3	E	207	HEM	C3C-C2C	-4.13	1.34	1.40
3	A	207	HEM	C3C-C2C	-4.02	1.34	1.40
3	P	205	HEM	C3B-C2B	-4.01	1.34	1.40
3	T	206	HEM	C3B-C2B	-4.00	1.34	1.40
3	U	205	HEM	C3B-C2B	-3.99	1.34	1.40
3	J	206	HEM	C3C-C2C	-3.90	1.35	1.40
3	W	206	HEM	C3C-C2C	-3.79	1.35	1.40
3	H	206	HEM	C3B-C2B	-3.73	1.35	1.40
3	P	205	HEM	C3C-C2C	-3.71	1.35	1.40
3	W	206	HEM	C3B-C2B	-3.68	1.35	1.40
3	Q	204	HEM	C3C-C2C	-3.62	1.35	1.40
3	K	206	HEM	C3C-CAC	3.51	1.55	1.47
3	Q	204	HEM	C3C-CAC	3.50	1.55	1.47
3	T	206	HEM	C3C-C2C	-3.44	1.35	1.40
3	E	207	HEM	C3C-CAC	3.42	1.54	1.47
3	C	205	HEM	C3C-C2C	-3.41	1.35	1.40
3	H	206	HEM	C3B-CAB	3.40	1.54	1.47
3	U	205	HEM	C3C-CAC	3.32	1.54	1.47
3	T	206	HEM	C3B-CAB	3.31	1.54	1.47
3	T	206	HEM	C3C-CAC	3.30	1.54	1.47
3	M	206	HEM	C3C-CAC	3.14	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	207	HEM	C3C-CAC	3.04	1.54	1.47
3	W	206	HEM	C3C-CAC	3.01	1.54	1.47
3	P	205	HEM	C3C-CAC	2.99	1.53	1.47
3	C	205	HEM	C3C-CAC	2.95	1.53	1.47
3	K	206	HEM	C3B-CAB	2.87	1.53	1.47
3	H	206	HEM	C3C-CAC	2.83	1.53	1.47
3	U	205	HEM	C3B-CAB	2.74	1.53	1.47
3	P	205	HEM	C3B-CAB	2.68	1.53	1.47
3	W	206	HEM	C3B-CAB	2.61	1.53	1.47
3	J	206	HEM	C3B-CAB	2.56	1.53	1.47
3	Q	204	HEM	C3B-CAB	2.56	1.53	1.47
3	A	207	HEM	C3B-CAB	2.48	1.53	1.47
3	K	206	HEM	C3C-C2C	-2.41	1.37	1.40
3	E	207	HEM	C3B-CAB	2.41	1.52	1.47
3	J	206	HEM	C3C-CAC	2.38	1.52	1.47
3	M	206	HEM	C3B-CAB	2.35	1.52	1.47
3	K	206	HEM	CMC-C2C	2.19	1.56	1.51
3	C	205	HEM	C3B-CAB	2.18	1.52	1.47
3	U	205	HEM	CMB-C2B	2.13	1.56	1.51
3	H	206	HEM	C4B-CHC	-2.04	1.35	1.41
3	A	207	HEM	CMB-C2B	2.01	1.56	1.51

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	206	HEM	CBD-CAD-C3D	-6.99	99.60	112.48
3	K	206	HEM	CBD-CAD-C3D	-5.88	101.65	112.48
3	M	206	HEM	CBD-CAD-C3D	-5.60	102.16	112.48
3	E	207	HEM	CBD-CAD-C3D	-5.23	102.84	112.48
3	A	207	HEM	CBD-CAD-C3D	-4.92	103.41	112.48
3	T	206	HEM	CBA-CAA-C2A	-4.87	103.51	112.49
3	T	206	HEM	CBD-CAD-C3D	-4.85	103.53	112.48
3	P	205	HEM	CBD-CAD-C3D	-4.81	103.61	112.48
3	C	205	HEM	CBD-CAD-C3D	-4.54	104.11	112.48
3	J	206	HEM	CBD-CAD-C3D	-4.22	104.70	112.48
3	U	205	HEM	CBD-CAD-C3D	-4.22	104.71	112.48
3	E	207	HEM	CBA-CAA-C2A	-4.17	104.79	112.49
3	P	205	HEM	CMA-C3A-C4A	-4.15	122.08	128.46
3	H	206	HEM	C1D-C2D-C3D	-4.10	104.14	107.00
3	P	205	HEM	CMC-C2C-C3C	3.85	131.88	124.68
3	J	206	HEM	C1D-C2D-C3D	-3.81	104.35	107.00
3	H	206	HEM	CBA-CAA-C2A	-3.71	105.64	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	207	HEM	CMC-C2C-C3C	3.68	131.56	124.68
3	Q	204	HEM	CBD-CAD-C3D	-3.66	105.73	112.48
3	C	205	HEM	CMC-C2C-C3C	3.53	131.28	124.68
3	W	206	HEM	CBA-CAA-C2A	-3.50	106.02	112.49
3	K	206	HEM	CMC-C2C-C3C	3.49	131.20	124.68
3	P	205	HEM	C1D-C2D-C3D	-3.48	104.58	107.00
3	P	205	HEM	CMB-C2B-C3B	3.39	131.02	124.68
3	M	206	HEM	CBA-CAA-C2A	-3.38	106.26	112.49
3	C	205	HEM	CMA-C3A-C4A	-3.33	123.34	128.46
3	C	205	HEM	CAA-CBA-CGA	-3.30	107.14	112.67
3	E	207	HEM	CMA-C3A-C4A	-3.28	123.43	128.46
3	H	206	HEM	CMC-C2C-C3C	3.27	130.79	124.68
3	M	206	HEM	CMB-C2B-C3B	3.25	130.75	124.68
3	Q	204	HEM	CMC-C2C-C3C	3.22	130.71	124.68
3	U	205	HEM	CBA-CAA-C2A	-3.21	106.56	112.49
3	J	206	HEM	CBA-CAA-C2A	-3.18	106.62	112.49
3	K	206	HEM	C1D-C2D-C3D	-3.17	104.79	107.00
3	W	206	HEM	CMC-C2C-C3C	3.16	130.58	124.68
3	M	206	HEM	C1D-C2D-C3D	-3.13	104.81	107.00
3	U	205	HEM	C1D-C2D-C3D	-3.13	104.81	107.00
3	Q	204	HEM	CBA-CAA-C2A	-3.10	106.78	112.49
3	M	206	HEM	CMC-C2C-C3C	3.08	130.44	124.68
3	W	206	HEM	CMB-C2B-C3B	3.06	130.41	124.68
3	E	207	HEM	CMC-C2C-C3C	3.05	130.38	124.68
3	K	206	HEM	C4C-C3C-C2C	3.04	109.02	106.90
3	E	207	HEM	C1D-C2D-C3D	-3.01	104.90	107.00
3	T	206	HEM	C1D-C2D-C3D	-3.01	104.90	107.00
3	A	207	HEM	CBA-CAA-C2A	-2.89	107.15	112.49
3	U	205	HEM	CMB-C2B-C3B	2.89	130.08	124.68
3	A	207	HEM	C1D-C2D-C3D	-2.89	104.99	107.00
3	Q	204	HEM	CAA-CBA-CGA	-2.88	107.83	112.67
3	P	205	HEM	CBA-CAA-C2A	-2.88	107.18	112.49
3	T	206	HEM	CMC-C2C-C3C	2.87	130.04	124.68
3	W	206	HEM	CBD-CAD-C3D	-2.87	107.20	112.48
3	A	207	HEM	C4C-C3C-C2C	2.87	108.90	106.90
3	M	206	HEM	CMA-C3A-C4A	-2.86	124.07	128.46
3	J	206	HEM	CMB-C2B-C3B	2.86	130.02	124.68
3	T	206	HEM	CMB-C2B-C3B	2.83	129.97	124.68
3	J	206	HEM	CMC-C2C-C3C	2.81	129.94	124.68
3	U	205	HEM	C4C-C3C-C2C	2.78	108.84	106.90
3	A	207	HEM	CMA-C3A-C4A	-2.77	124.20	128.46
3	W	206	HEM	C1D-C2D-C3D	-2.77	105.07	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	206	HEM	CBA-CAA-C2A	-2.75	107.41	112.49
3	A	207	HEM	CAD-CBD-CGD	-2.75	108.06	112.67
3	J	206	HEM	C4C-C3C-C2C	2.74	108.81	106.90
3	J	206	HEM	CMD-C2D-C3D	2.72	130.06	124.94
3	J	206	HEM	CAD-CBD-CGD	-2.60	108.30	112.67
3	T	206	HEM	CAD-CBD-CGD	-2.58	108.34	112.67
3	Q	204	HEM	CAD-CBD-CGD	-2.56	108.37	112.67
3	J	206	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
3	P	205	HEM	CMA-C3A-C2A	2.54	129.73	124.94
3	H	206	HEM	C4C-C3C-C2C	2.54	108.67	106.90
3	E	207	HEM	CMA-C3A-C2A	2.49	129.64	124.94
3	C	205	HEM	CBA-CAA-C2A	-2.46	107.94	112.49
3	W	206	HEM	CMA-C3A-C4A	-2.45	124.69	128.46
3	H	206	HEM	CMB-C2B-C3B	2.42	129.21	124.68
3	C	205	HEM	C1D-C2D-C3D	-2.42	105.31	107.00
3	M	206	HEM	C4C-C3C-C2C	2.40	108.57	106.90
3	C	205	HEM	CMA-C3A-C2A	2.40	129.46	124.94
3	C	205	HEM	CMB-C2B-C3B	2.39	129.14	124.68
3	U	205	HEM	CMC-C2C-C3C	2.36	129.09	124.68
3	T	206	HEM	CMA-C3A-C4A	-2.32	124.90	128.46
3	H	206	HEM	CAD-CBD-CGD	-2.29	108.83	112.67
3	K	206	HEM	CAA-CBA-CGA	-2.19	108.99	112.67
3	W	206	HEM	C4C-C3C-C2C	2.16	108.41	106.90
3	A	207	HEM	CMB-C2B-C3B	2.04	128.49	124.68
3	U	205	HEM	CMA-C3A-C4A	-2.02	125.35	128.46
3	M	206	HEM	CMA-C3A-C2A	2.01	128.73	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	205	HEM	3	0
3	C	205	HEM	1	0
3	K	206	HEM	1	0
3	Q	204	HEM	2	0
3	M	206	HEM	4	0
3	H	206	HEM	2	0
3	E	207	HEM	1	0
3	A	207	HEM	1	0

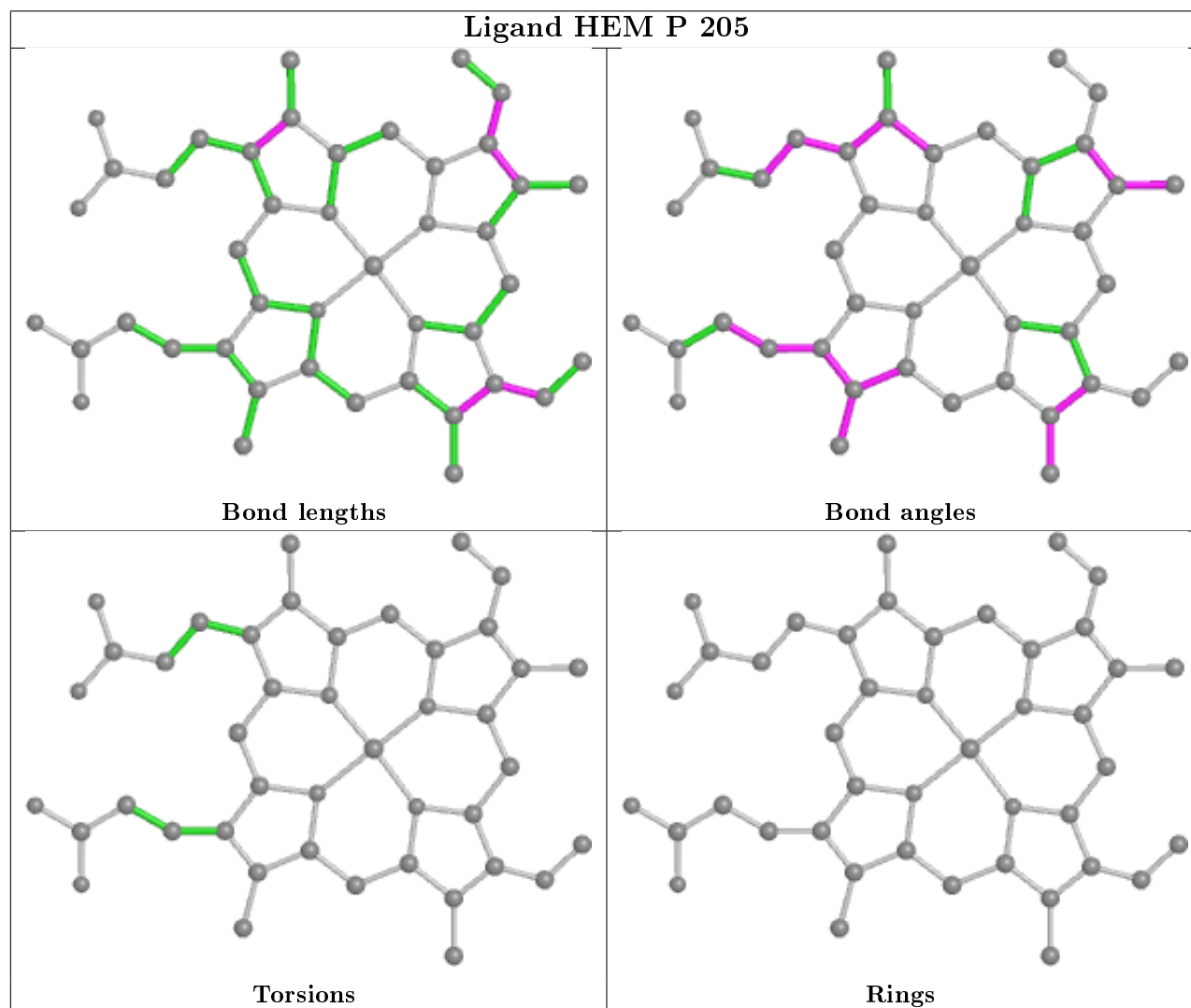
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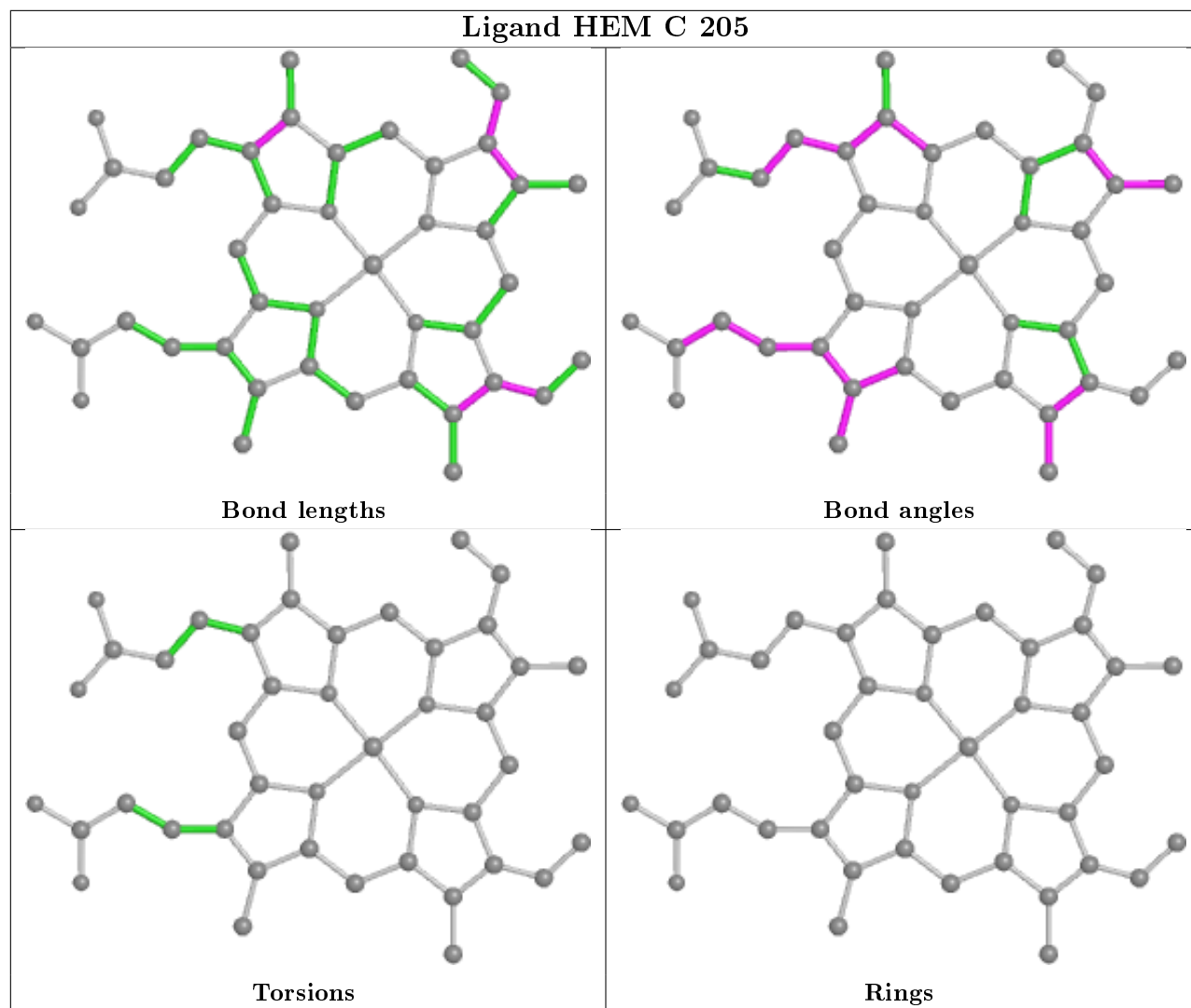


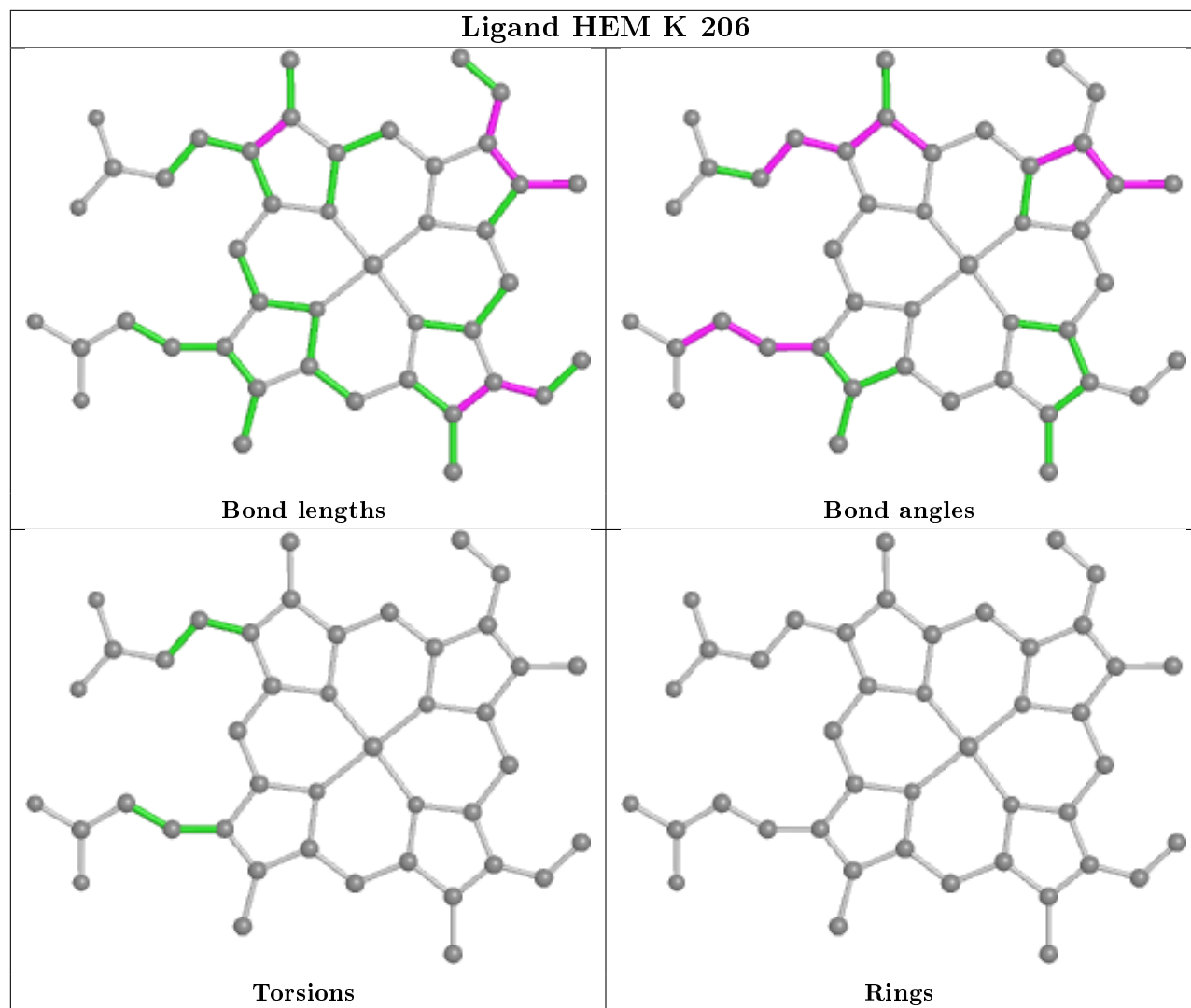
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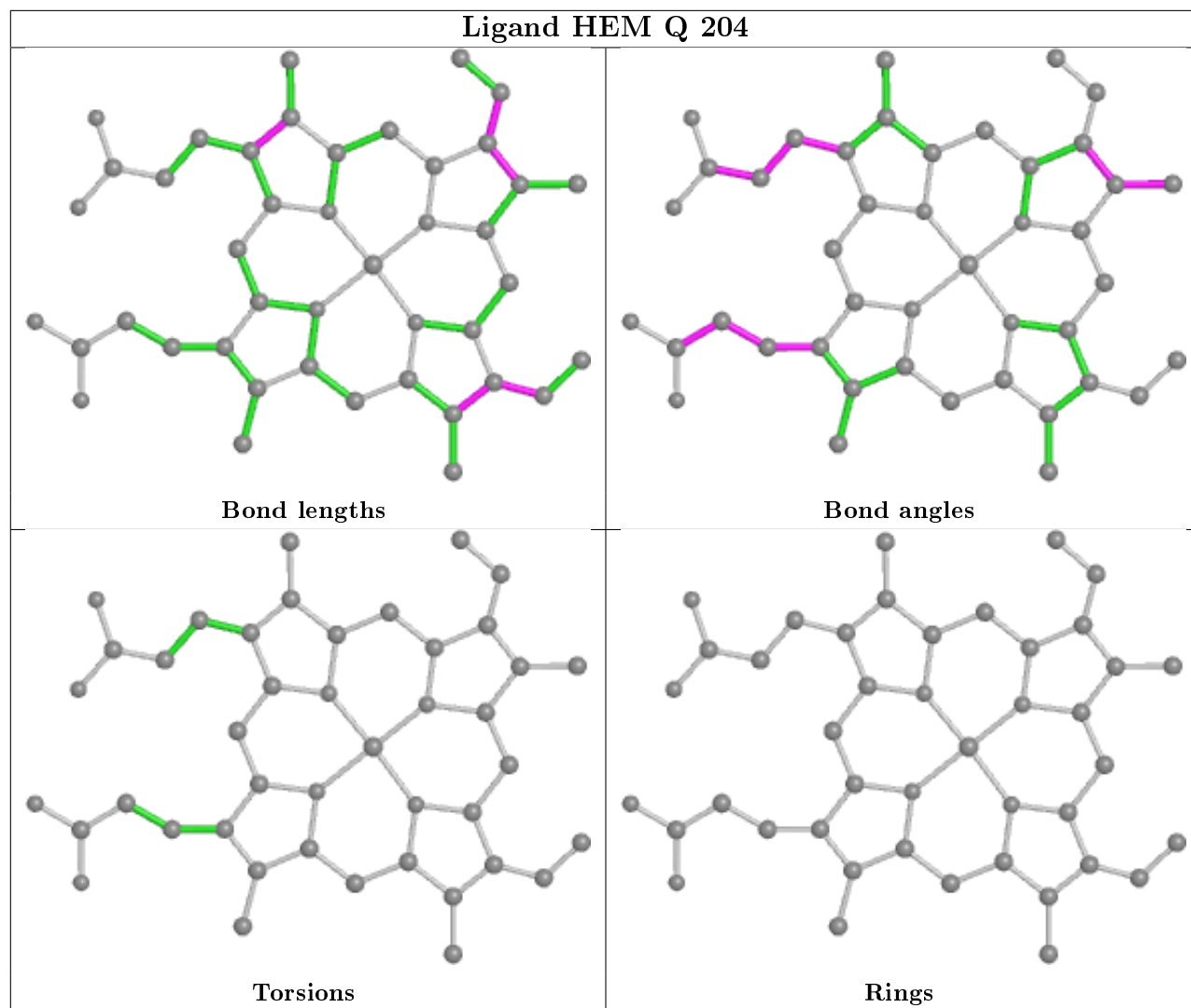
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	206	HEM	3	0
3	W	206	HEM	1	0
3	T	206	HEM	3	0

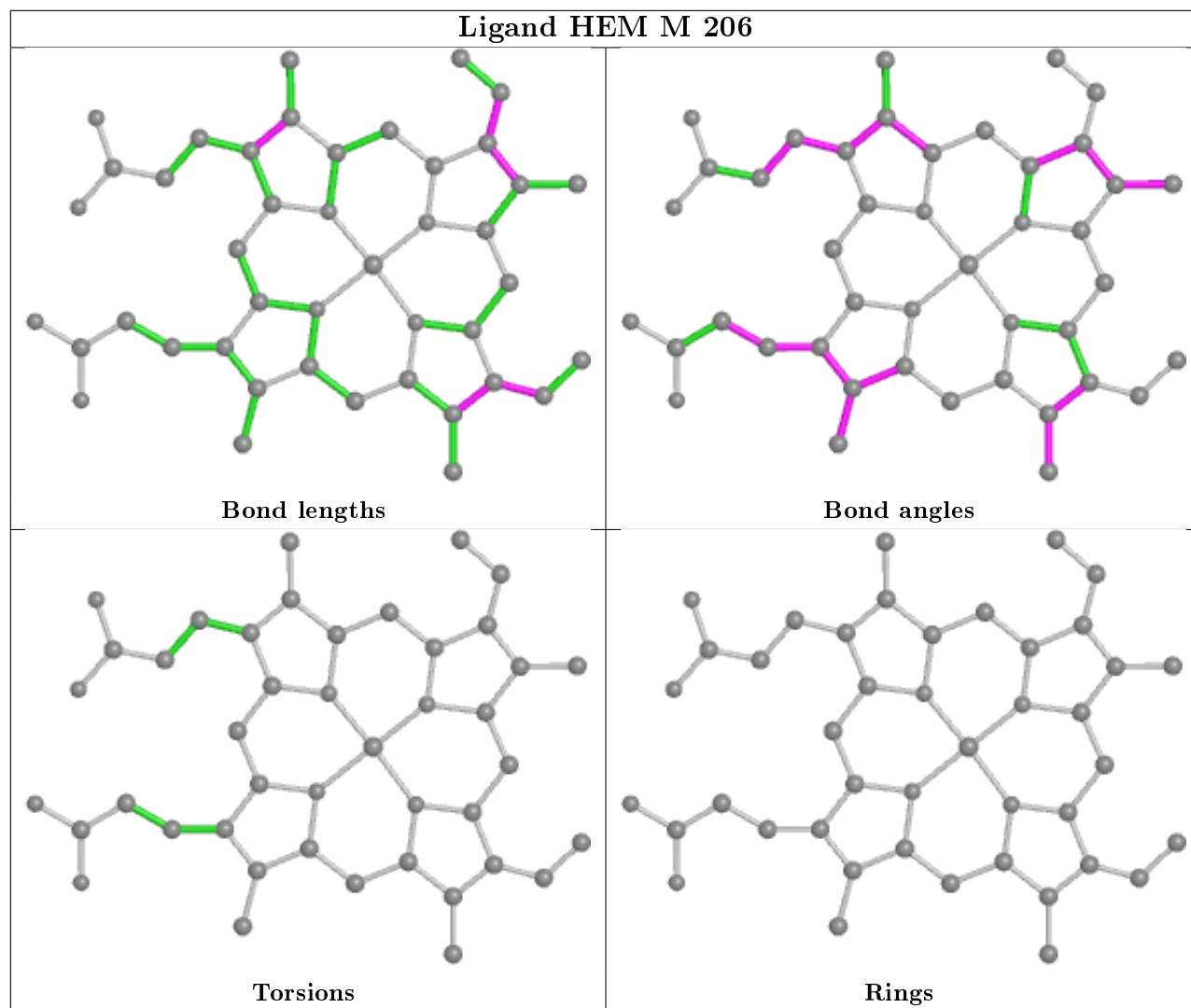
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

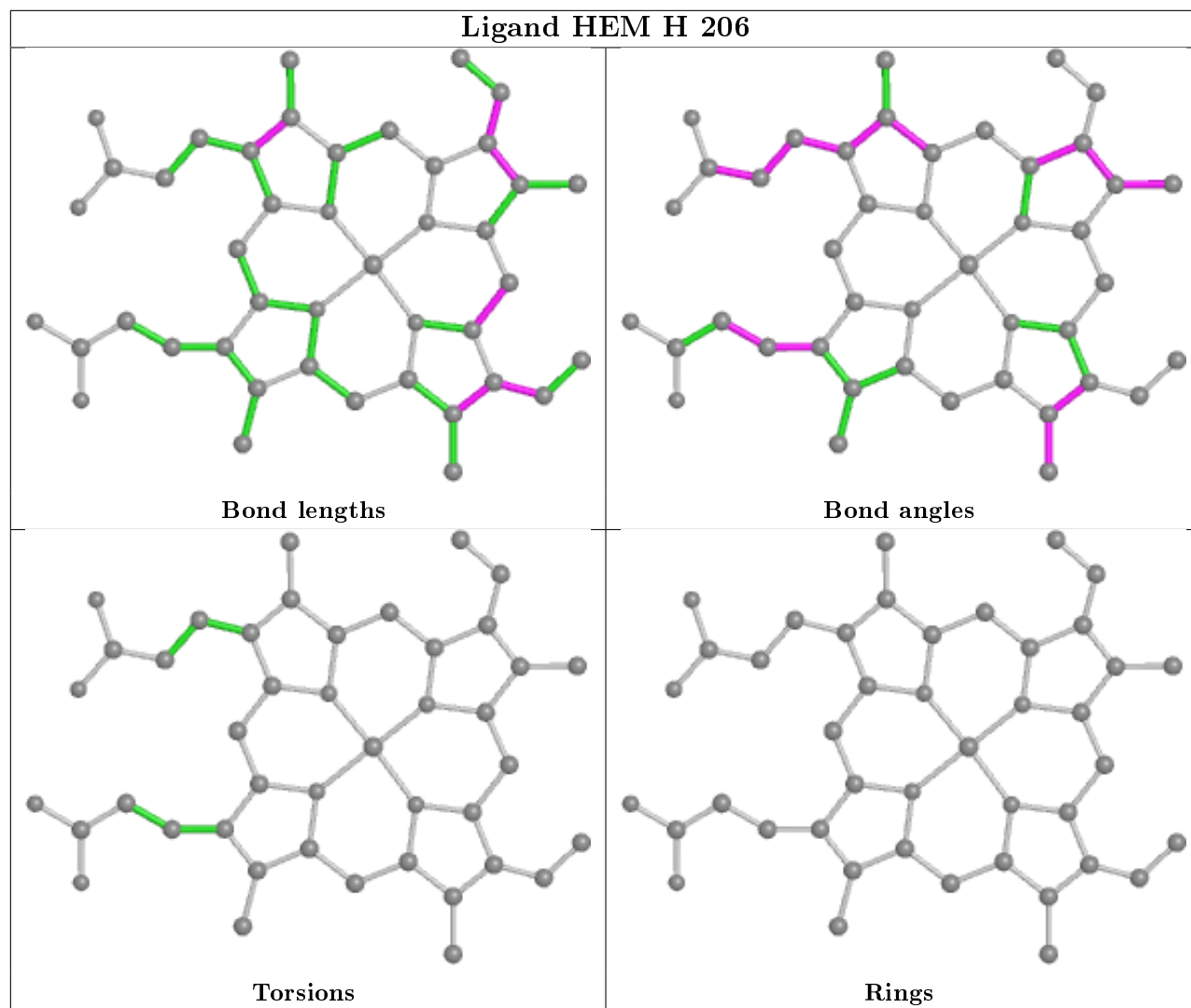


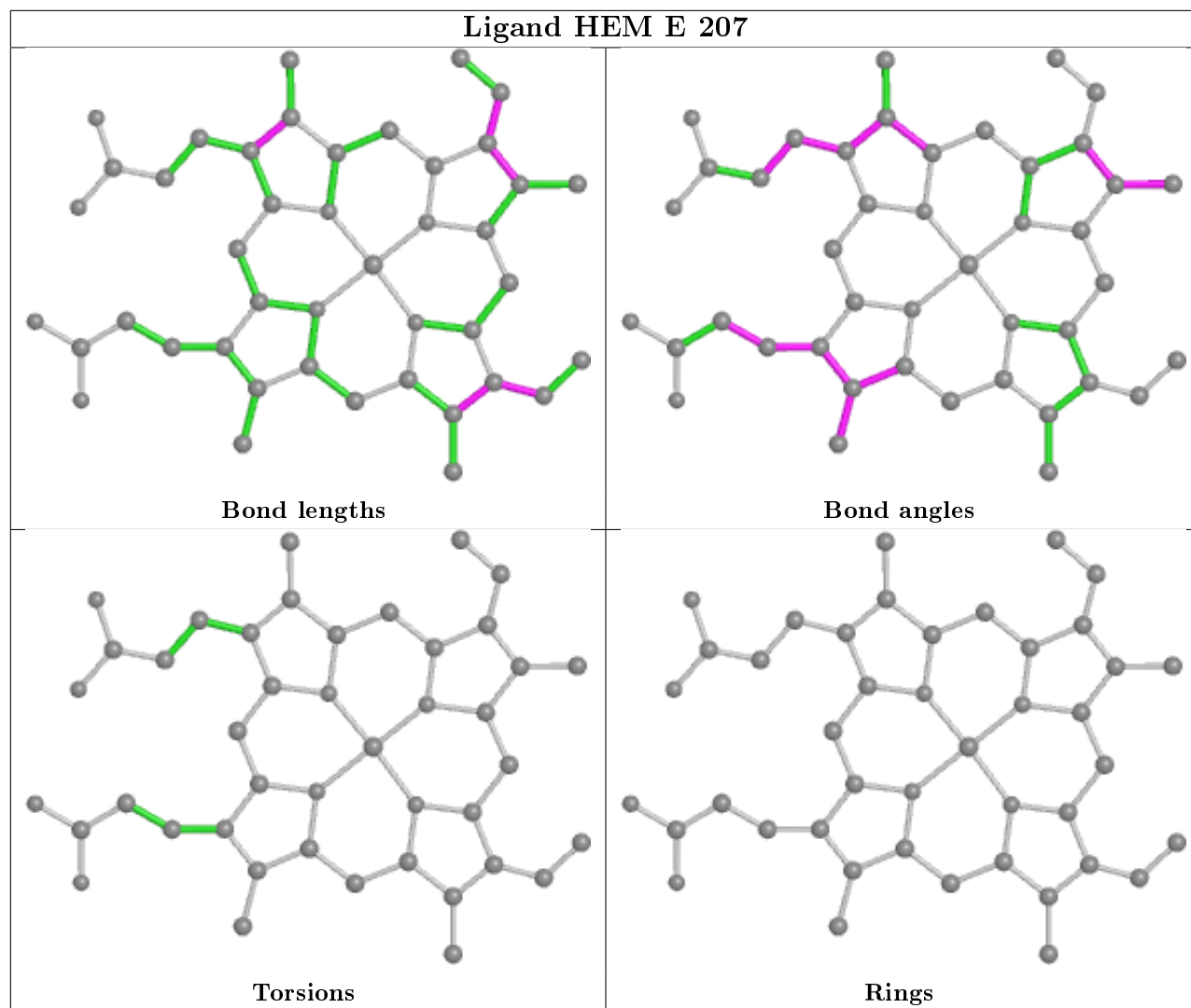


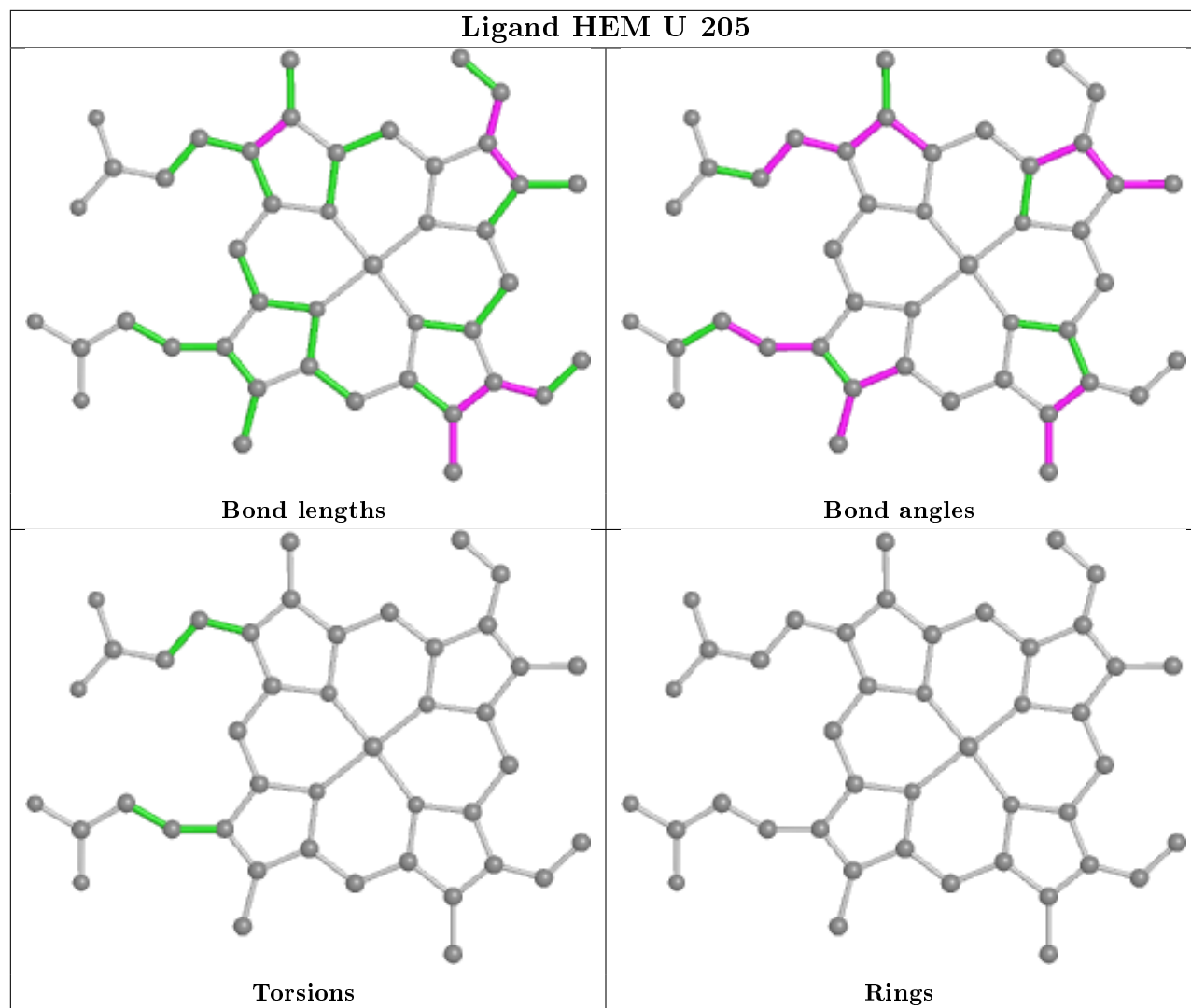




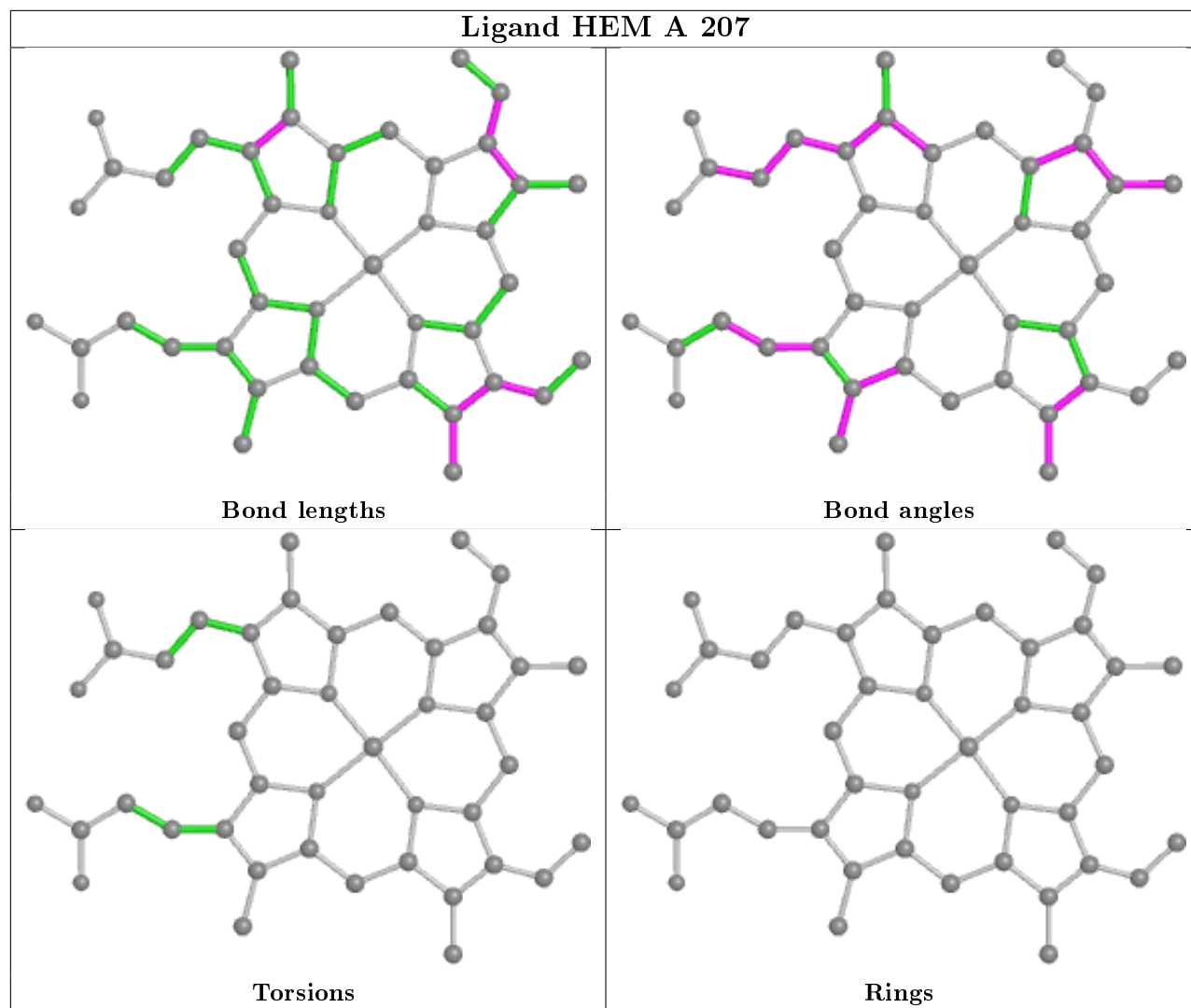


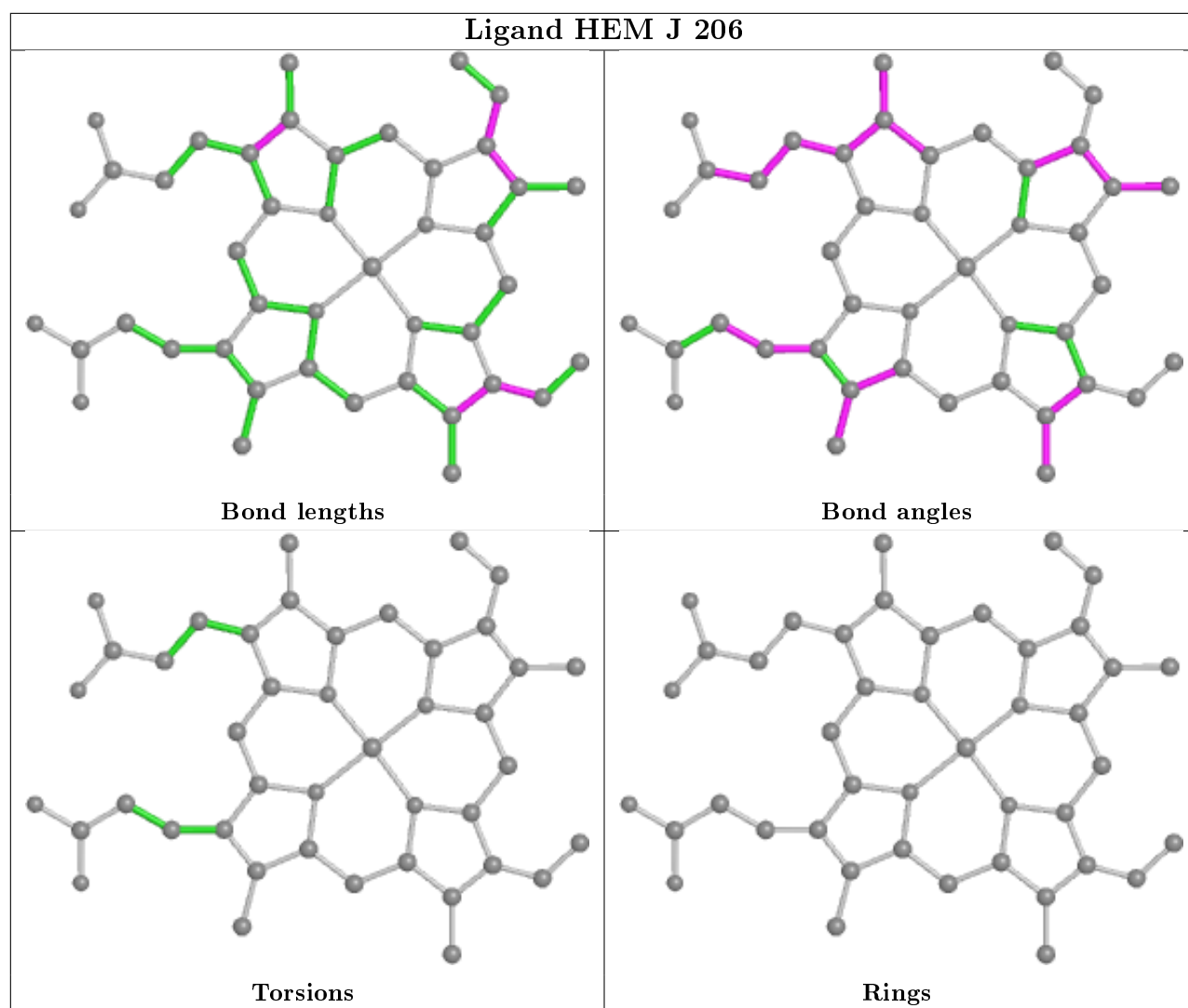


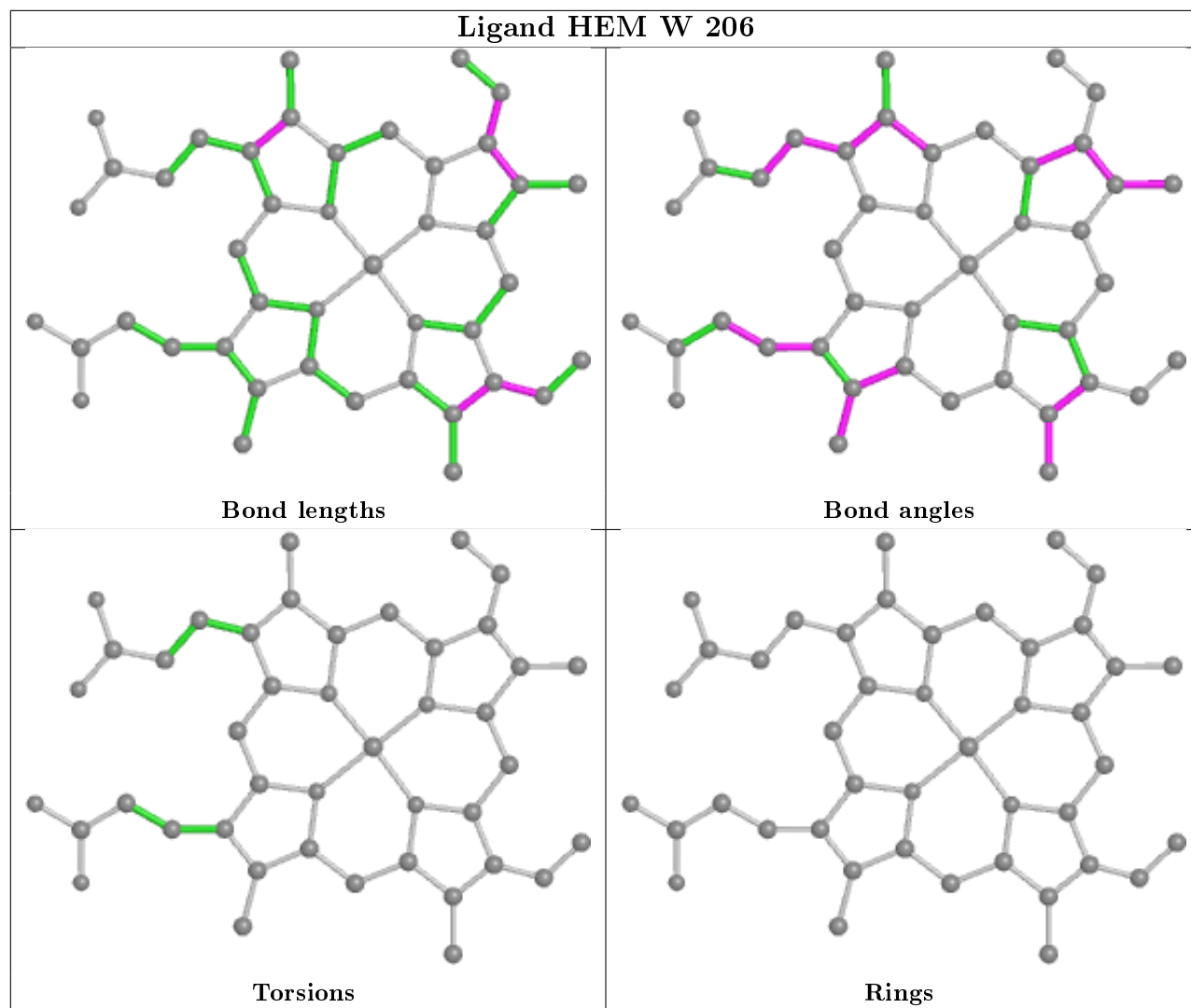


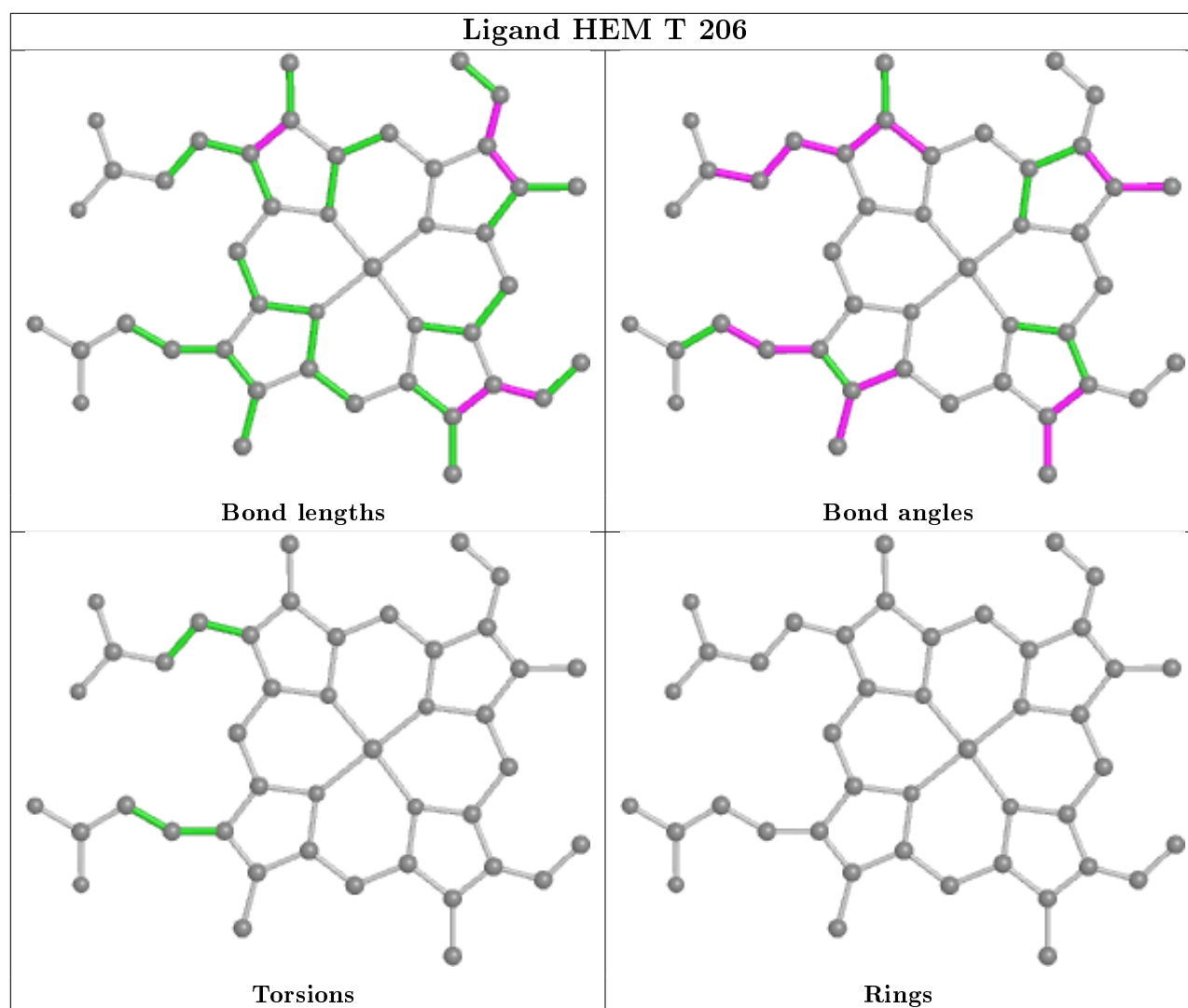












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	153/158 (96%)	-0.63	0 100 100	21, 30, 42, 54	0
1	B	155/158 (98%)	-0.62	0 100 100	21, 30, 45, 56	0
1	C	155/158 (98%)	-0.67	0 100 100	22, 31, 43, 53	0
1	D	156/158 (98%)	-0.63	1 (0%) 89 89	22, 30, 43, 58	0
1	E	155/158 (98%)	-0.62	0 100 100	22, 29, 43, 55	0
1	F	156/158 (98%)	-0.63	1 (0%) 89 89	21, 28, 42, 58	0
1	G	156/158 (98%)	-0.68	0 100 100	21, 30, 42, 70	0
1	H	155/158 (98%)	-0.64	0 100 100	20, 28, 41, 55	0
1	I	156/158 (98%)	-0.69	0 100 100	22, 30, 43, 58	0
1	J	156/158 (98%)	-0.68	0 100 100	23, 30, 42, 56	0
1	K	156/158 (98%)	-0.68	0 100 100	23, 30, 44, 55	0
1	L	155/158 (98%)	-0.68	0 100 100	23, 30, 43, 53	0
1	M	154/158 (97%)	-0.62	0 100 100	22, 30, 42, 56	0
1	N	156/158 (98%)	-0.63	1 (0%) 89 89	22, 29, 42, 69	0
1	O	155/158 (98%)	-0.63	0 100 100	22, 30, 42, 55	0
1	P	156/158 (98%)	-0.61	0 100 100	23, 31, 43, 63	0
1	Q	156/158 (98%)	-0.64	0 100 100	23, 31, 46, 60	0
1	R	155/158 (98%)	-0.65	0 100 100	24, 32, 44, 55	0
1	S	156/158 (98%)	-0.63	1 (0%) 89 89	24, 32, 46, 57	0
1	T	156/158 (98%)	-0.69	1 (0%) 89 89	23, 31, 43, 60	0
1	U	156/158 (98%)	-0.60	1 (0%) 89 89	24, 32, 45, 57	0
1	V	155/158 (98%)	-0.64	0 100 100	25, 32, 44, 58	0
1	W	155/158 (98%)	-0.69	0 100 100	23, 30, 46, 58	0
1	X	156/158 (98%)	-0.68	1 (0%) 89 89	22, 30, 43, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3730/3792 (98%)	-0.65	7 (0%) 95 96	20, 30, 44, 70	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	1	MET	4.3
1	N	1	MET	4.2
1	D	1	MET	3.5
1	S	1	MET	3.0
1	T	1	MET	2.6
1	X	1	MET	2.2
1	F	1	MET	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	FE2	D	205	1/1	0.65	0.13	83,83,83,83	0
2	FE2	X	204	1/1	0.75	0.12	69,69,69,69	0
2	FE2	O	203	1/1	0.77	0.30	73,73,73,73	0
2	FE2	A	206	1/1	0.81	0.22	75,75,75,75	0
2	FE2	P	204	1/1	0.81	0.17	70,70,70,70	0
2	FE2	J	205	1/1	0.81	0.21	75,75,75,75	0
2	FE2	J	201	1/1	0.81	0.18	74,74,74,74	0
2	FE2	U	201	1/1	0.82	0.25	72,72,72,72	0
2	FE2	W	204	1/1	0.83	0.17	70,70,70,70	0
2	FE2	K	201	1/1	0.83	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE2	E	206	1/1	0.84	0.14	72,72,72,72	0
2	FE2	A	201	1/1	0.84	0.33	70,70,70,70	0
2	FE2	B	201	1/1	0.85	0.17	66,66,66,66	0
2	FE2	V	206	1/1	0.85	0.34	74,74,74,74	0
2	FE2	X	202	1/1	0.85	0.36	72,72,72,72	0
2	FE2	V	207	1/1	0.85	0.25	84,84,84,84	0
2	FE2	H	202	1/1	0.85	0.29	67,67,67,67	0
2	FE2	T	205	1/1	0.86	0.19	82,82,82,82	0
2	FE2	U	204	1/1	0.86	0.32	64,64,64,64	0
2	FE2	V	205	1/1	0.86	0.24	70,70,70,70	0
2	FE2	B	203	1/1	0.87	0.31	69,69,69,69	0
2	FE2	B	205	1/1	0.87	0.17	78,78,78,78	0
2	FE2	C	203	1/1	0.87	0.27	62,62,62,62	0
2	FE2	M	202	1/1	0.87	0.28	69,69,69,69	0
2	FE2	R	205	1/1	0.87	0.26	68,68,68,68	0
2	FE2	K	205	1/1	0.88	0.29	65,65,65,65	0
2	FE2	X	205	1/1	0.88	0.20	70,70,70,70	0
2	FE2	L	205	1/1	0.89	0.22	73,73,73,73	0
2	FE2	E	203	1/1	0.90	0.22	63,63,63,63	0
2	FE2	E	205	1/1	0.90	0.34	76,76,76,76	0
2	FE2	I	206	1/1	0.90	0.23	77,77,77,77	0
2	FE2	P	202	1/1	0.90	0.26	69,69,69,69	0
2	FE2	G	204	1/1	0.91	0.30	65,65,65,65	0
2	FE2	R	206	1/1	0.91	0.20	81,81,81,81	0
2	FE2	B	206	1/1	0.91	0.24	76,76,76,76	0
2	FE2	M	201	1/1	0.92	0.16	46,46,46,46	0
2	FE2	N	204	1/1	0.92	0.22	59,59,59,59	0
2	FE2	W	205	1/1	0.92	0.37	75,75,75,75	0
2	FE2	Q	202	1/1	0.92	0.19	43,43,43,43	0
2	FE2	I	204	1/1	0.92	0.32	70,70,70,70	0
2	FE2	A	202	1/1	0.92	0.29	66,66,66,66	0
2	FE2	G	207	1/1	0.92	0.28	77,77,77,77	0
2	FE2	T	202	1/1	0.92	0.22	59,59,59,59	0
2	FE2	J	204	1/1	0.92	0.29	61,61,61,61	0
2	FE2	R	201	1/1	0.93	0.24	68,68,68,68	0
2	FE2	L	201	1/1	0.93	0.23	67,67,67,67	0
2	FE2	L	203	1/1	0.93	0.29	64,64,64,64	0
2	FE2	T	204	1/1	0.93	0.20	71,71,71,71	0
2	FE2	I	202	1/1	0.93	0.19	65,65,65,65	0
3	HEM	J	206	43/43	0.93	0.12	22,26,42,51	0
2	FE2	E	201	1/1	0.93	0.19	65,65,65,65	0
2	FE2	G	203	1/1	0.93	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE2	H	204	1/1	0.93	0.23	67,67,67,67	0
2	FE2	K	202	1/1	0.93	0.17	68,68,68,68	0
2	FE2	M	205	1/1	0.93	0.21	71,71,71,71	0
2	FE2	W	203	1/1	0.93	0.37	70,70,70,70	0
2	FE2	Q	203	1/1	0.93	0.34	68,68,68,68	0
2	FE2	W	201	1/1	0.93	0.16	46,46,46,46	0
2	FE2	M	203	1/1	0.93	0.33	64,64,64,64	0
3	HEM	E	207	43/43	0.94	0.12	20,25,41,41	0
2	FE2	T	201	1/1	0.94	0.19	46,46,46,46	0
3	HEM	Q	204	43/43	0.94	0.13	22,28,43,52	0
2	FE2	S	202	1/1	0.94	0.41	69,69,69,69	0
3	HEM	U	205	43/43	0.94	0.12	23,31,45,49	0
2	FE2	C	201	1/1	0.94	0.17	71,71,71,71	0
2	FE2	A	205	1/1	0.94	0.24	64,64,64,64	0
3	HEM	W	206	43/43	0.94	0.13	21,28,44,51	0
3	HEM	P	205	43/43	0.94	0.12	22,27,42,49	0
3	HEM	K	206	43/43	0.94	0.11	22,28,43,47	0
2	FE2	V	201	1/1	0.94	0.21	61,61,61,61	0
3	HEM	C	205	43/43	0.94	0.12	22,26,44,52	0
2	FE2	D	204	1/1	0.94	0.27	60,60,60,60	0
2	FE2	N	203	1/1	0.94	0.30	65,65,65,65	0
3	HEM	M	206	43/43	0.95	0.12	20,26,45,50	0
2	FE2	P	203	1/1	0.95	0.14	47,47,47,47	0
2	FE2	F	202	1/1	0.95	0.32	65,65,65,65	0
3	HEM	H	206	43/43	0.95	0.11	18,24,42,52	0
2	FE2	L	202	1/1	0.95	0.20	43,43,43,43	0
3	HEM	A	207	43/43	0.95	0.11	19,26,44,50	0
2	FE2	N	201	1/1	0.95	0.13	44,44,44,44	0
3	HEM	T	206	43/43	0.95	0.12	23,27,45,52	0
2	FE2	W	202	1/1	0.95	0.10	48,48,48,48	0
2	FE2	F	201	1/1	0.95	0.22	44,44,44,44	0
2	FE2	V	203	1/1	0.96	0.16	47,47,47,47	0
2	FE2	U	203	1/1	0.96	0.17	45,45,45,45	0
2	FE2	D	202	1/1	0.96	0.26	63,63,63,63	0
2	FE2	I	205	1/1	0.96	0.25	75,75,75,75	0
2	FE2	I	201	1/1	0.96	0.20	44,44,44,44	0
4	SO4	M	207	5/5	0.96	0.08	57,58,62,64	0
2	FE2	N	202	1/1	0.96	0.22	69,69,69,69	0
2	FE2	H	201	1/1	0.96	0.12	56,56,56,56	0
2	FE2	G	201	1/1	0.96	0.27	69,69,69,69	0
2	FE2	H	203	1/1	0.96	0.21	46,46,46,46	0
2	FE2	R	202	1/1	0.96	0.13	68,68,68,68	0

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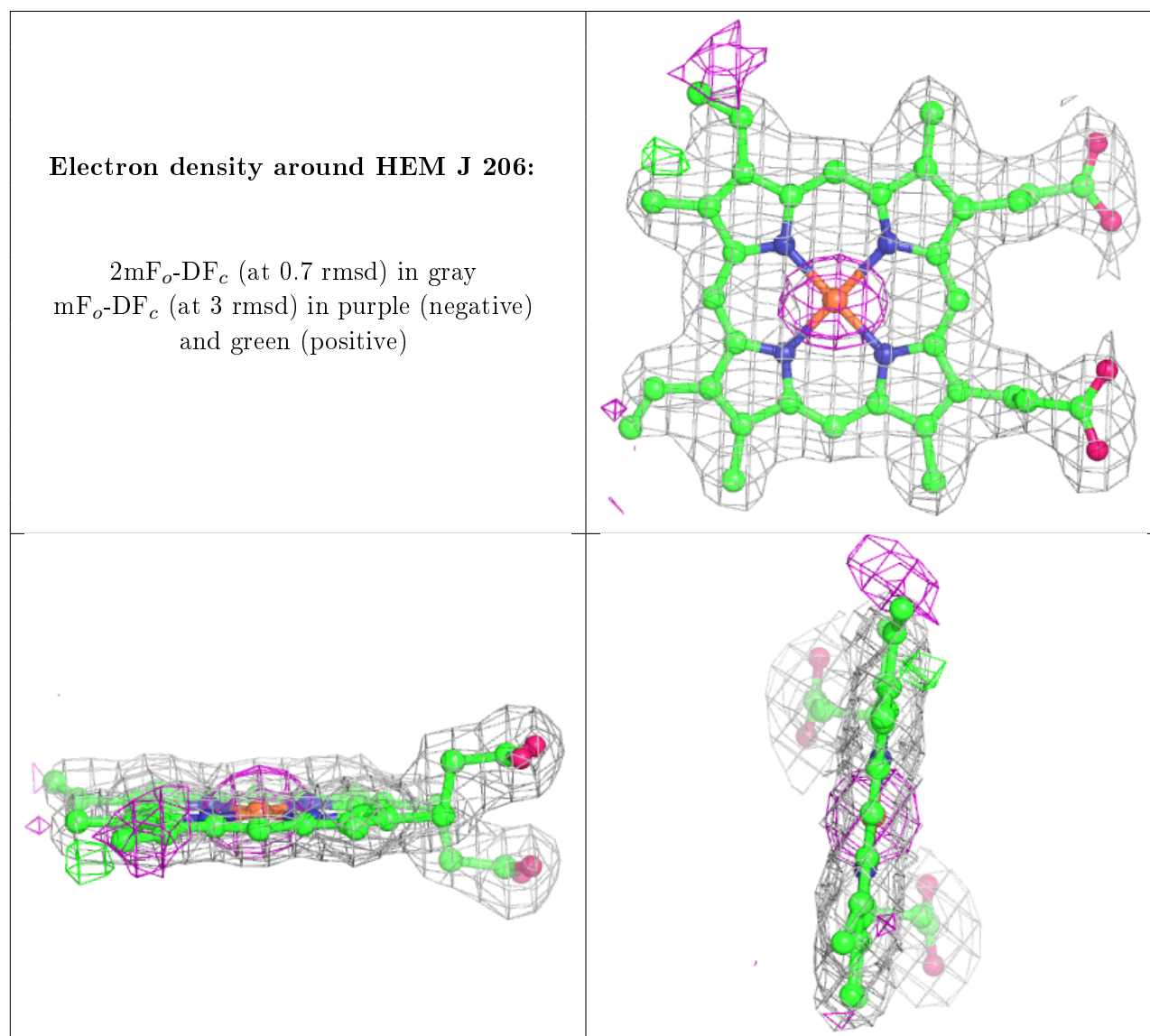
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE2	R	203	1/1	0.96	0.20	45,45,45,45	0
4	SO4	D	206	5/5	0.96	0.09	54,58,59,65	0
4	SO4	F	204	5/5	0.97	0.08	53,55,60,67	0
2	FE2	O	201	1/1	0.97	0.38	69,69,69,69	0
2	FE2	U	202	1/1	0.97	0.19	45,45,45,45	0
2	FE2	G	206	1/1	0.97	0.16	73,73,73,73	0
2	FE2	I	203	1/1	0.97	0.07	32,32,32,32	0
2	FE2	A	203	1/1	0.97	0.16	42,42,42,42	0
4	SO4	B	207	5/5	0.97	0.08	57,59,62,63	0
2	FE2	J	202	1/1	0.97	0.19	45,45,45,45	0
2	FE2	C	202	1/1	0.97	0.17	40,40,40,40	0
4	SO4	S	204	5/5	0.97	0.09	60,62,67,68	0
2	FE2	H	205	1/1	0.97	0.14	41,41,41,41	0
4	SO4	N	206	5/5	0.97	0.07	48,56,58,65	0
2	FE2	P	201	1/1	0.97	0.21	46,46,46,46	0
2	FE2	C	204	1/1	0.97	0.11	44,44,44,44	0
2	FE2	G	202	1/1	0.97	0.17	43,43,43,43	0
2	FE2	O	205	1/1	0.97	0.24	82,82,82,82	0
2	FE2	K	203	1/1	0.97	0.17	47,47,47,47	0
2	FE2	D	203	1/1	0.98	0.10	39,39,39,39	0
2	FE2	S	203	1/1	0.98	0.17	49,49,49,49	0
2	FE2	O	202	1/1	0.98	0.14	41,41,41,41	0
2	FE2	S	201	1/1	0.98	0.20	44,44,44,44	0
2	FE2	E	202	1/1	0.98	0.14	41,41,41,41	0
2	FE2	R	204	1/1	0.98	0.14	53,53,53,53	0
4	SO4	P	206	5/5	0.98	0.07	49,57,60,63	0
2	FE2	M	204	1/1	0.98	0.14	50,50,50,50	0
4	SO4	A	208	5/5	0.98	0.09	52,55,62,62	0
2	FE2	A	204	1/1	0.98	0.12	44,44,44,44	0
2	FE2	T	203	1/1	0.98	0.15	47,47,47,47	0
2	FE2	D	201	1/1	0.98	0.14	44,44,44,44	0
2	FE2	B	202	1/1	0.98	0.19	44,44,44,44	0
2	FE2	X	203	1/1	0.98	0.10	46,46,46,46	0
2	FE2	X	201	1/1	0.98	0.19	44,44,44,44	0
2	FE2	G	205	1/1	0.98	0.11	42,42,42,42	0
2	FE2	O	204	1/1	0.98	0.17	56,56,56,56	0
2	FE2	Q	201	1/1	0.99	0.16	48,48,48,48	0
2	FE2	N	205	1/1	0.99	0.17	55,55,55,55	0
2	FE2	L	204	1/1	0.99	0.10	42,42,42,42	0
2	FE2	J	203	1/1	0.99	0.11	39,39,39,39	0
2	FE2	B	204	1/1	0.99	0.18	48,48,48,48	0
2	FE2	V	202	1/1	0.99	0.31	67,67,67,67	0

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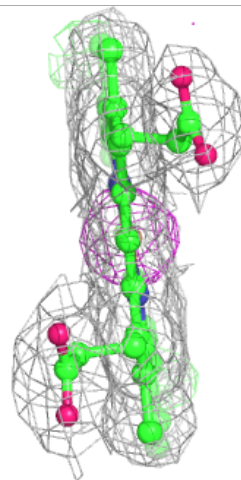
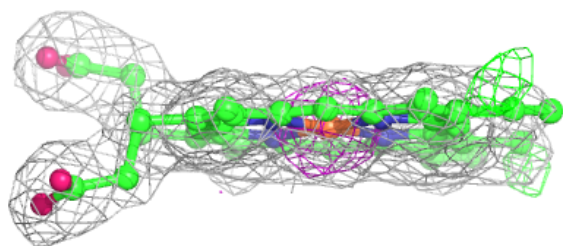
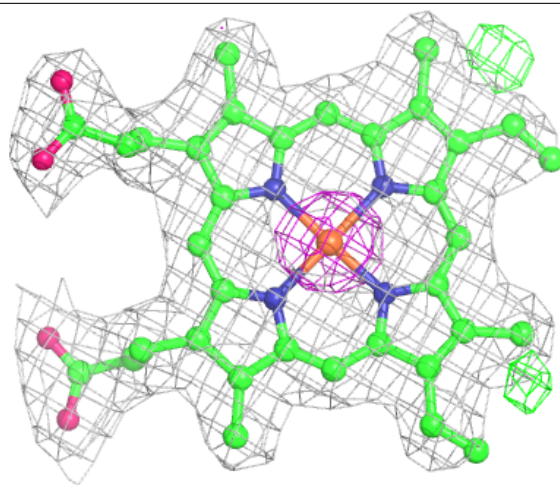
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE2	V	204	1/1	0.99	0.12	47,47,47,47	0
2	FE2	E	204	1/1	0.99	0.12	44,44,44,44	0
2	FE2	K	204	1/1	0.99	0.09	33,33,33,33	0
2	FE2	F	203	1/1	0.99	0.18	40,40,40,40	0

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.



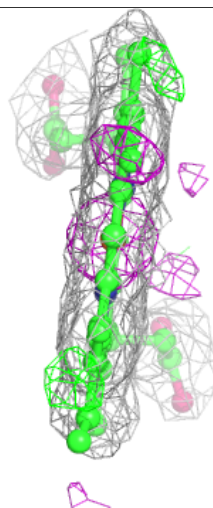
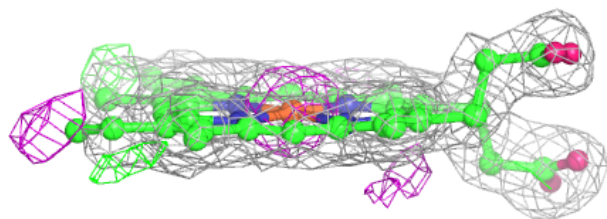
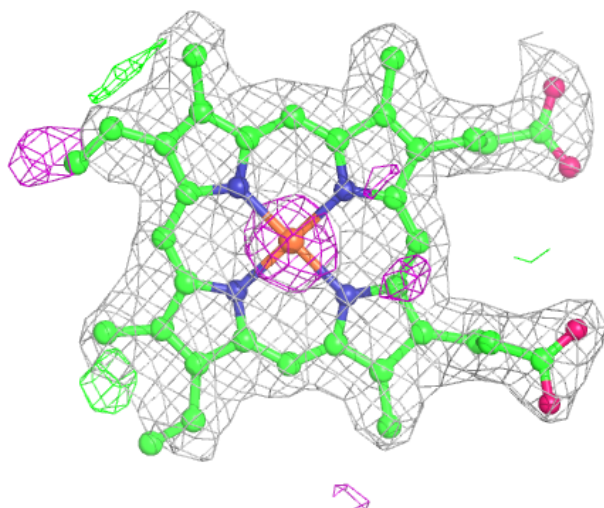
**Electron density around HEM E 207:**

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



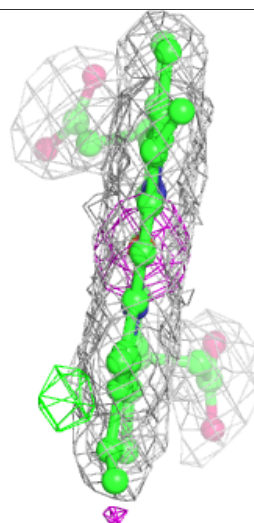
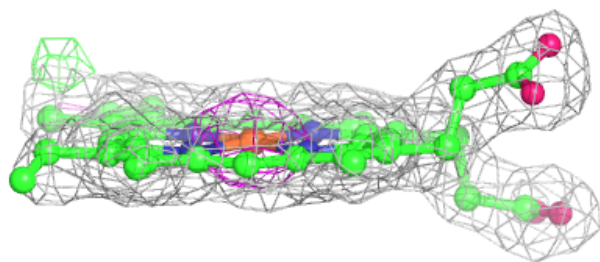
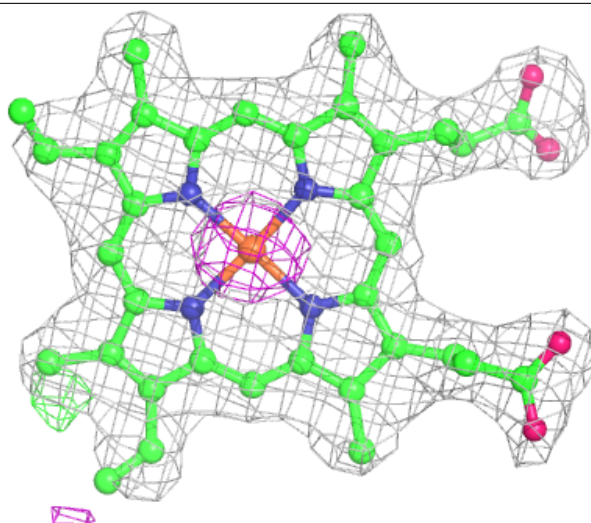
**Electron density around HEM Q 204:**

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



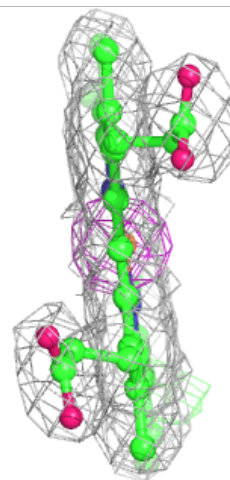
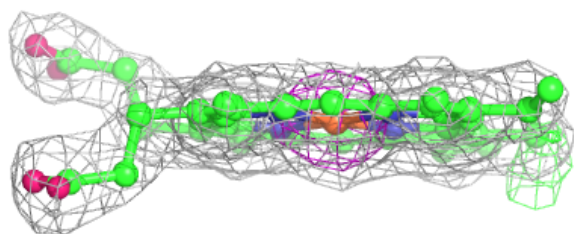
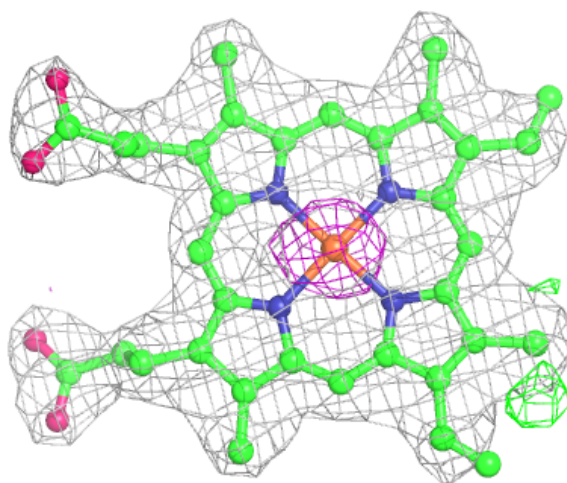
**Electron density around HEM U 205:**

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



**Electron density around HEM W 206:**

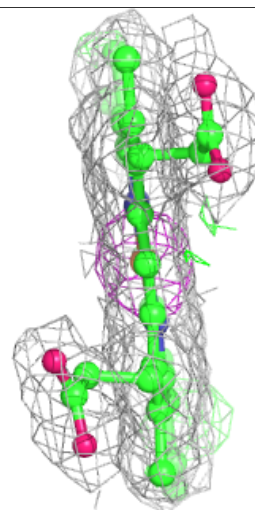
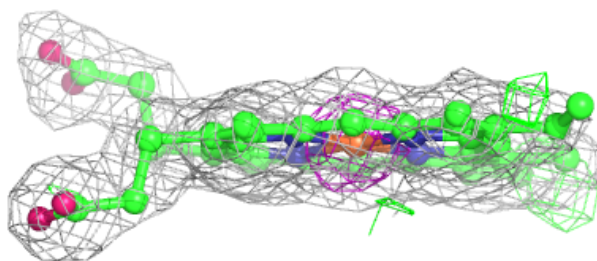
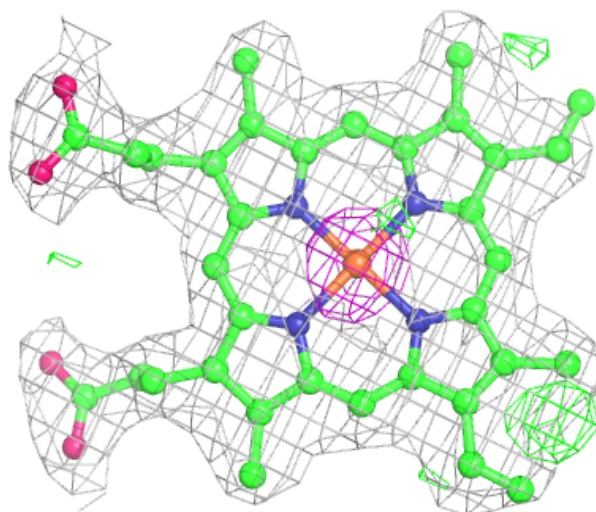
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





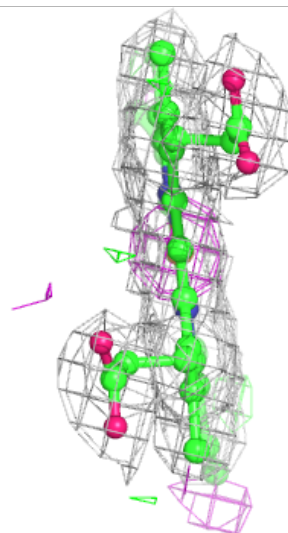
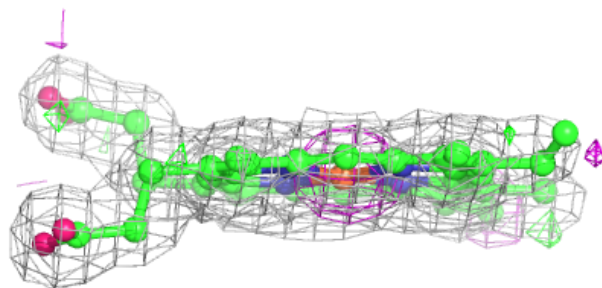
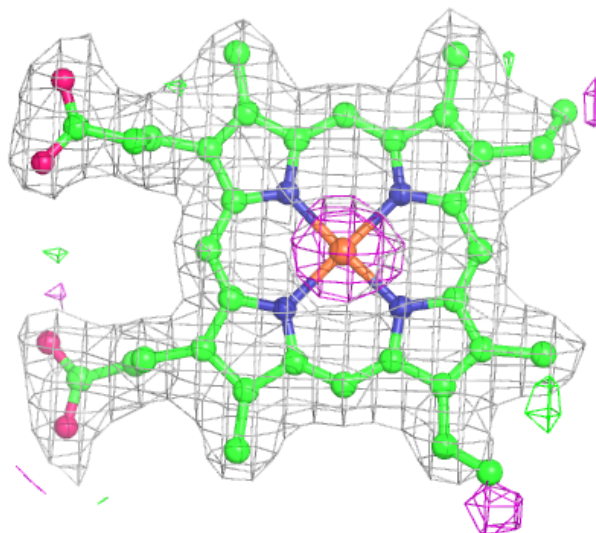
**Electron density around HEM P 205:**

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



**Electron density around HEM K 206:**

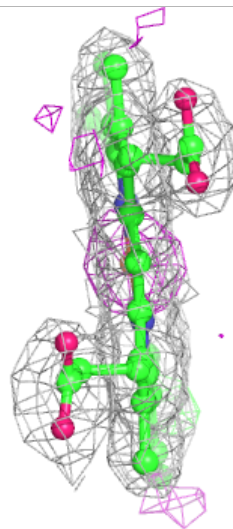
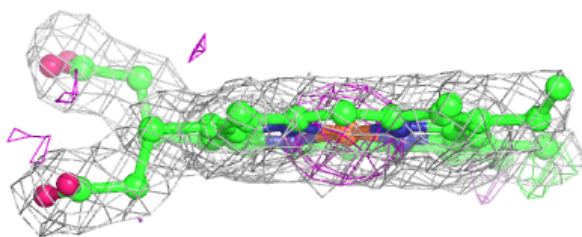
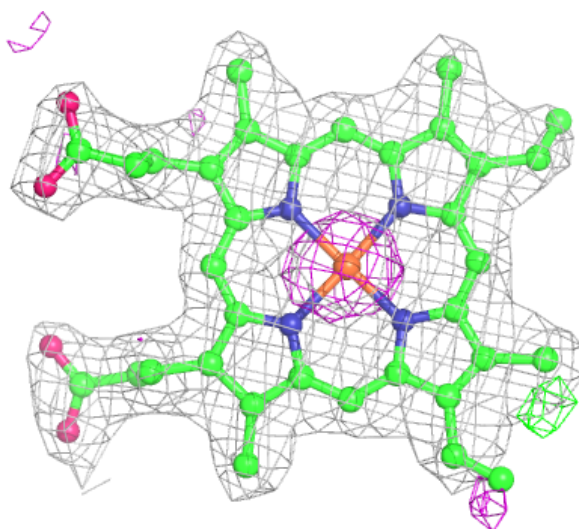
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





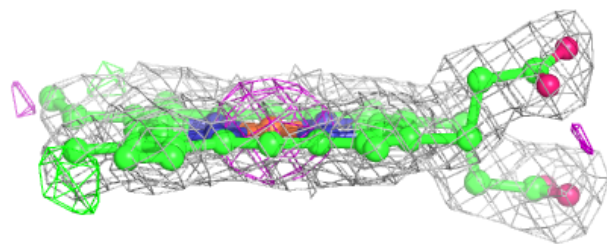
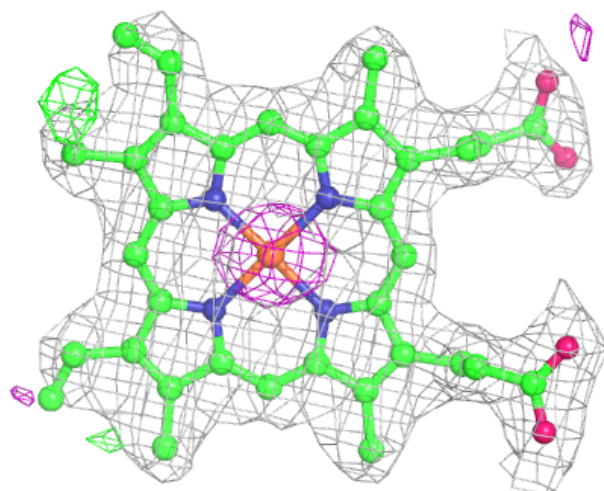
**Electron density around HEM C 205:**

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



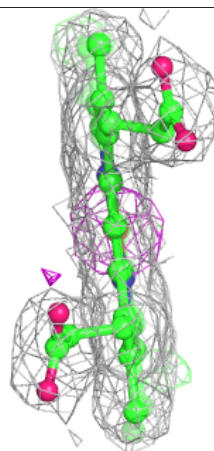
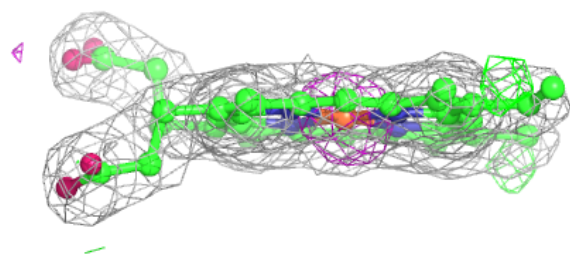
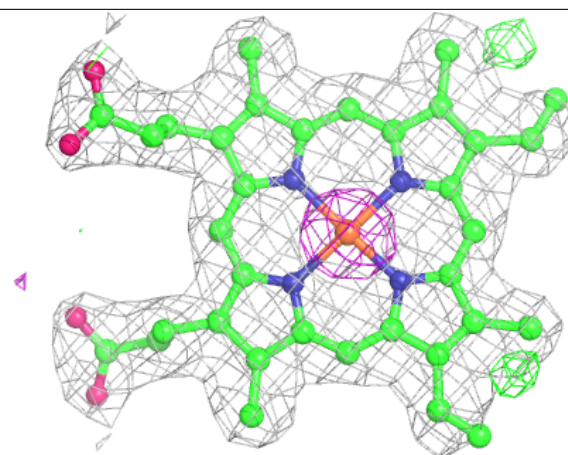
**Electron density around HEM M 206:**

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



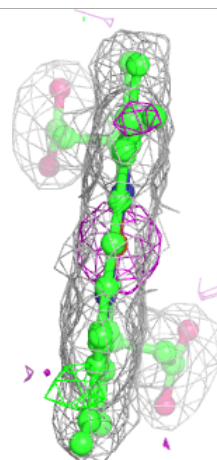
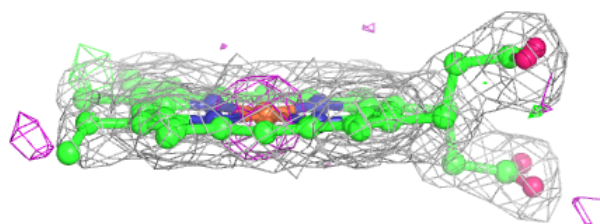
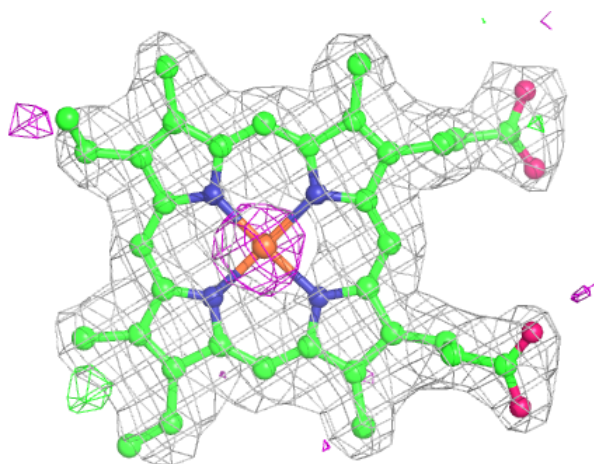
**Electron density around HEM H 206:**

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



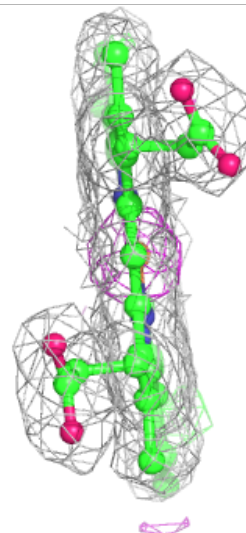
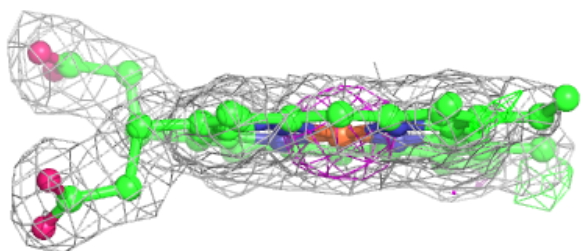
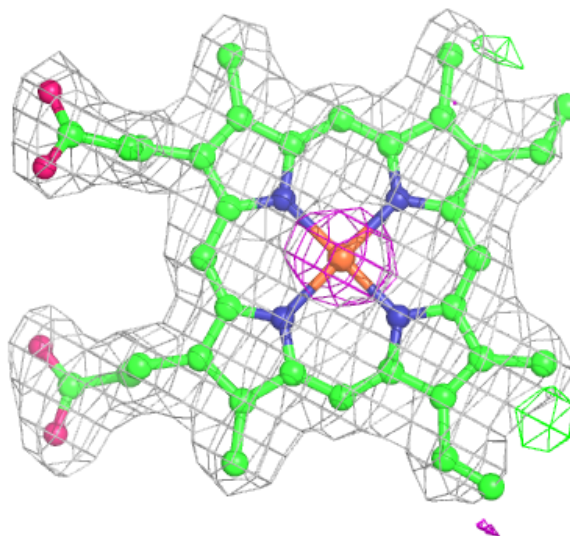
**Electron density around HEM A 207:**

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



**Electron density around HEM T 206:**

$2mF_o-DF_c$  (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.