



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 18, 2023 – 10:18 PM EDT

PDB ID : 5D8X  
Title : 1.50Å resolution structure of BfrB (L68A E81A) from Pseudomonas aeruginosa  
Authors : Lovell, S.; Battaile, K.P.; Wang, Y.; Yao, H.; Rivera, M.  
Deposited on : 2015-08-18  
Resolution : 1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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) : 2.35.1

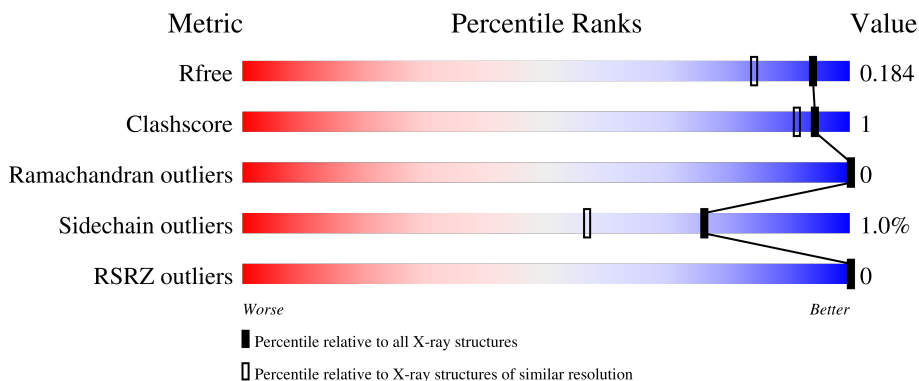
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\geq 3$ , 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	95%
1	B	158	95%
1	C	158	96%
1	D	158	95%
1	E	158	97%

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Mol	Chain	Length	Quality of chain
1	F	158	97% ..
1	G	158	96% ...
1	H	158	98% ..
1	I	158	97% ..
1	J	158	96% ..
1	K	158	96% ..
1	L	158	95% ..
1	M	158	95% ..
1	N	158	94% 5% ..
1	O	158	96% ...
1	P	158	95% ..
1	Q	158	96% ..
1	R	158	97% ...
1	S	158	97% ..
1	T	158	95% ...
1	U	158	95% ..
1	V	158	96% ..
1	W	158	97% ...
1	X	158	96% ..

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 35653 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 Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1293	817	220	249	7	0	5	0
1	B	156	1270	802	216	245	7	0	2	0
1	C	156	1278	807	218	246	7	0	3	0
1	D	156	1281	809	219	246	7	0	3	0
1	E	156	1271	802	217	245	7	0	2	0
1	F	156	1269	802	218	242	7	0	2	0
1	G	156	1285	812	219	247	7	0	4	0
1	H	156	1264	798	216	243	7	0	1	0
1	I	156	1269	801	217	244	7	0	2	0
1	J	156	1260	796	215	242	7	0	1	0
1	K	156	1267	800	217	243	7	0	1	0
1	L	156	1277	807	219	244	7	0	2	0
1	M	156	1281	810	218	246	7	0	3	0
1	N	156	1272	803	217	245	7	0	2	0
1	O	156	1281	809	218	247	7	0	4	0
1	P	156	1272	803	218	244	7	0	2	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	156	1272	803	217	245	7	0	2	0
1	R	156	1273	804	218	244	7	0	2	0
1	S	156	1275	805	218	245	7	0	2	0
1	T	156	1272	803	218	244	7	0	2	0
1	U	156	1266	800	216	243	7	0	2	0
1	V	156	1272	803	218	244	7	0	2	0
1	W	156	1276	806	218	245	7	0	3	0
1	X	156	1272	803	217	245	7	0	2	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ALA	LEU	engineered mutation	UNP Q9HY79
A	81	ALA	GLU	engineered mutation	UNP Q9HY79
B	68	ALA	LEU	engineered mutation	UNP Q9HY79
B	81	ALA	GLU	engineered mutation	UNP Q9HY79
C	68	ALA	LEU	engineered mutation	UNP Q9HY79
C	81	ALA	GLU	engineered mutation	UNP Q9HY79
D	68	ALA	LEU	engineered mutation	UNP Q9HY79
D	81	ALA	GLU	engineered mutation	UNP Q9HY79
E	68	ALA	LEU	engineered mutation	UNP Q9HY79
E	81	ALA	GLU	engineered mutation	UNP Q9HY79
F	68	ALA	LEU	engineered mutation	UNP Q9HY79
F	81	ALA	GLU	engineered mutation	UNP Q9HY79
G	68	ALA	LEU	engineered mutation	UNP Q9HY79
G	81	ALA	GLU	engineered mutation	UNP Q9HY79
H	68	ALA	LEU	engineered mutation	UNP Q9HY79
H	81	ALA	GLU	engineered mutation	UNP Q9HY79
I	68	ALA	LEU	engineered mutation	UNP Q9HY79
I	81	ALA	GLU	engineered mutation	UNP Q9HY79
J	68	ALA	LEU	engineered mutation	UNP Q9HY79
J	81	ALA	GLU	engineered mutation	UNP Q9HY79
K	68	ALA	LEU	engineered mutation	UNP Q9HY79
K	81	ALA	GLU	engineered mutation	UNP Q9HY79
L	68	ALA	LEU	engineered mutation	UNP Q9HY79

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Chain	Residue	Modelled	Actual	Comment	Reference
L	81	ALA	GLU	engineered mutation	UNP Q9HY79
M	68	ALA	LEU	engineered mutation	UNP Q9HY79
M	81	ALA	GLU	engineered mutation	UNP Q9HY79
N	68	ALA	LEU	engineered mutation	UNP Q9HY79
N	81	ALA	GLU	engineered mutation	UNP Q9HY79
O	68	ALA	LEU	engineered mutation	UNP Q9HY79
O	81	ALA	GLU	engineered mutation	UNP Q9HY79
P	68	ALA	LEU	engineered mutation	UNP Q9HY79
P	81	ALA	GLU	engineered mutation	UNP Q9HY79
Q	68	ALA	LEU	engineered mutation	UNP Q9HY79
Q	81	ALA	GLU	engineered mutation	UNP Q9HY79
R	68	ALA	LEU	engineered mutation	UNP Q9HY79
R	81	ALA	GLU	engineered mutation	UNP Q9HY79
S	68	ALA	LEU	engineered mutation	UNP Q9HY79
S	81	ALA	GLU	engineered mutation	UNP Q9HY79
T	68	ALA	LEU	engineered mutation	UNP Q9HY79
T	81	ALA	GLU	engineered mutation	UNP Q9HY79
U	68	ALA	LEU	engineered mutation	UNP Q9HY79
U	81	ALA	GLU	engineered mutation	UNP Q9HY79
V	68	ALA	LEU	engineered mutation	UNP Q9HY79
V	81	ALA	GLU	engineered mutation	UNP Q9HY79
W	68	ALA	LEU	engineered mutation	UNP Q9HY79
W	81	ALA	GLU	engineered mutation	UNP Q9HY79
X	68	ALA	LEU	engineered mutation	UNP Q9HY79
X	81	ALA	GLU	engineered mutation	UNP Q9HY79

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

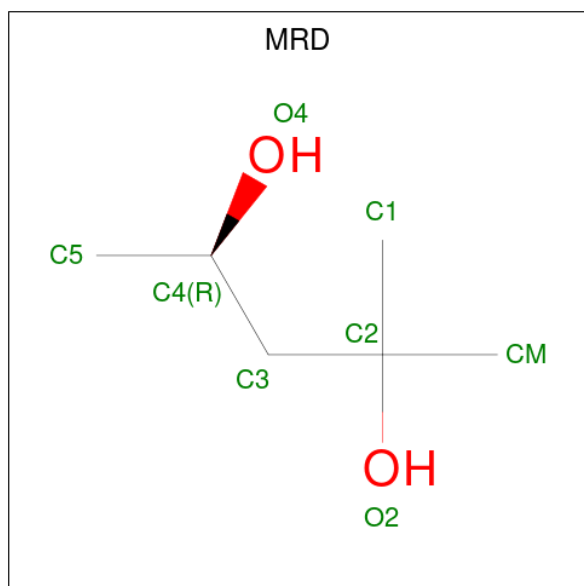


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0
3	D	1	Total K 1 1	0	0
3	E	1	Total K 1 1	0	0
3	G	1	Total K 1 1	0	0
3	L	1	Total K 1 1	0	0

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	D	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0
4	E	1	Total C O 8 6 2	0	0

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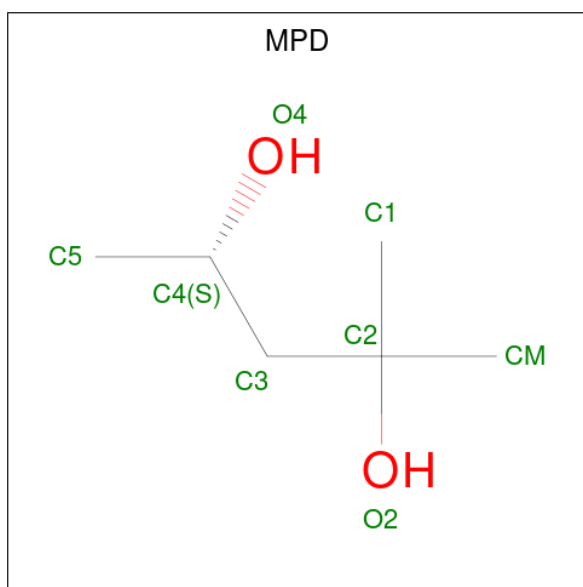
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	M	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	N	1	Total	C	O	0	0
			8	6	2		
4	O	1	Total	C	O	0	0
			8	6	2		
4	P	1	Total	C	O	0	0
			8	6	2		
4	R	1	Total	C	O	0	0
			8	6	2		
4	S	1	Total	C	O	0	0
			8	6	2		
4	T	1	Total	C	O	0	0
			8	6	2		
4	U	1	Total	C	O	0	0
			8	6	2		
4	V	1	Total	C	O	0	0
			8	6	2		
4	W	1	Total	C	O	0	0
			8	6	2		
4	X	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0
5	B	2	Total Na 2 2	0	0
5	C	1	Total Na 1 1	0	0
5	D	2	Total Na 2 2	0	0
5	E	2	Total Na 2 2	0	0
5	F	1	Total Na 1 1	0	0
5	G	2	Total Na 2 2	0	0
5	H	1	Total Na 1 1	0	0
5	I	1	Total Na 1 1	0	0
5	J	1	Total Na 1 1	0	0
5	K	1	Total Na 1 1	0	0
5	L	2	Total Na 2 2	0	0
5	M	1	Total Na 1 1	0	0
5	N	1	Total Na 1 1	0	0
5	R	1	Total Na 1 1	0	0
5	S	1	Total Na 1 1	0	0
5	T	1	Total Na 1 1	0	0
5	V	1	Total Na 1 1	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 8 6 2	0	0
6	I	1	Total C O 8 6 2	0	0
6	J	1	Total C O 8 6 2	0	0
6	K	1	Total C O 8 6 2	0	0
6	L	1	Total C O 8 6 2	0	0
6	Q	1	Total C O 8 6 2	0	0
6	Q	1	Total C O 8 6 2	0	0
6	R	1	Total C O 8 6 2	0	0
6	S	1	Total C O 8 6 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	179	Total O 179 179	0	0
7	B	180	Total O 180 180	0	0
7	C	182	Total O 182 182	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	183	Total 183	O 183	0	0
7	E	178	Total 178	O 178	0	0
7	F	167	Total 167	O 167	0	0
7	G	181	Total 181	O 181	0	0
7	H	184	Total 184	O 184	0	0
7	I	171	Total 171	O 171	0	0
7	J	165	Total 165	O 165	0	0
7	K	175	Total 175	O 175	0	0
7	L	173	Total 173	O 173	0	0
7	M	195	Total 195	O 195	0	0
7	N	191	Total 191	O 191	0	0
7	O	177	Total 177	O 177	0	0
7	P	163	Total 163	O 163	0	0
7	Q	200	Total 200	O 200	0	0
7	R	166	Total 166	O 166	0	0
7	S	188	Total 188	O 188	0	0
7	T	181	Total 181	O 181	0	0
7	U	168	Total 168	O 168	0	0
7	V	172	Total 172	O 172	0	0
7	W	176	Total 176	O 176	0	0
7	X	180	Total 180	O 180	0	0

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

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

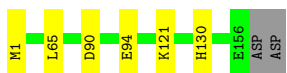
- Molecule 1: Ferroxidase

Chain A:  95%



- Molecule 1: Ferroxidase

Chain B:  95%



- Molecule 1: Ferroxidase

Chain C:  96%



- Molecule 1: Ferroxidase

Chain D:  95%



- Molecule 1: Ferroxidase

Chain E:  97%



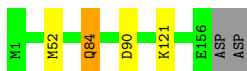
- Molecule 1: Ferroxidase

Chain F:  97%



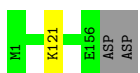
- Molecule 1: Ferroxidase

Chain G: 96%



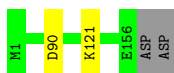
- Molecule 1: Ferroxidase

Chain H: 98%



- Molecule 1: Ferroxidase

Chain I: 97%



- Molecule 1: Ferroxidase

Chain J: 96%



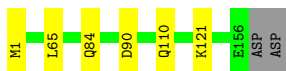
- Molecule 1: Ferroxidase

Chain K: 96%



- Molecule 1: Ferroxidase

Chain L: 95%



- Molecule 1: Ferroxidase

Chain M: 95%



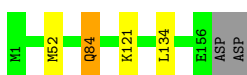
- Molecule 1: Ferroxidase

Chain N: 94% 5%



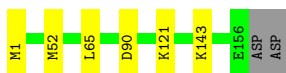
- Molecule 1: Ferroxidase

Chain O: 96%



- Molecule 1: Ferroxidase

Chain P: 95%



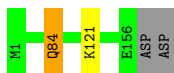
- Molecule 1: Ferroxidase

Chain Q: 96%



- Molecule 1: Ferroxidase

Chain R: 97%



- Molecule 1: Ferroxidase

Chain S: 97%



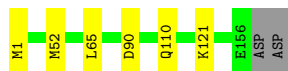
- Molecule 1: Ferroxidase

Chain T: 95%



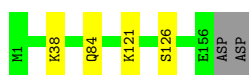
- Molecule 1: Ferroxidase

Chain U: 95%



- Molecule 1: Ferroxidase

Chain V: 96%



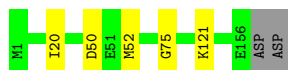
- Molecule 1: Ferroxidase

Chain W: 97%



- Molecule 1: Ferroxidase

Chain X: 96%





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.27Å 125.27Å 274.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.01 – 1.50 46.65 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.01-1.50) 99.9 (46.65-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.50Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.152 , 0.173 0.164 , 0.184	Depositor DCC
$R_{free}$ test set	39692 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.4	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l 0.019 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	35653	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: K, NA, MPD, HEM, MRD

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	0.43	0/1329	0.57	0/1791
1	B	0.39	0/1297	0.55	1/1750 (0.1%)
1	C	0.38	0/1308	0.55	0/1764
1	D	0.40	0/1311	0.55	1/1767 (0.1%)
1	E	0.42	0/1298	0.56	0/1751
1	F	0.41	0/1296	0.57	1/1748 (0.1%)
1	G	0.37	0/1318	0.56	1/1777 (0.1%)
1	H	0.38	0/1288	0.55	0/1738
1	I	0.39	0/1296	0.56	1/1749 (0.1%)
1	J	0.40	0/1284	0.55	0/1733
1	K	0.38	0/1291	0.55	0/1741
1	L	0.40	0/1304	0.58	1/1757 (0.1%)
1	M	0.41	0/1311	0.58	1/1767 (0.1%)
1	N	0.42	0/1299	0.56	1/1752 (0.1%)
1	O	0.40	0/1314	0.57	0/1773
1	P	0.38	0/1299	0.55	1/1752 (0.1%)
1	Q	0.40	0/1299	0.55	0/1752
1	R	0.39	0/1300	0.57	0/1753
1	S	0.39	0/1302	0.55	0/1755
1	T	0.40	0/1299	0.58	1/1752 (0.1%)
1	U	0.40	0/1293	0.53	1/1745 (0.1%)
1	V	0.40	0/1299	0.55	0/1752
1	W	0.38	0/1306	0.56	0/1762
1	X	0.39	0/1299	0.55	0/1752
All	All	0.40	0/31240	0.56	11/42133 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	90	ASP	CB-CG-OD1	6.44	124.10	118.30
1	M	90	ASP	CB-CG-OD1	6.16	123.84	118.30
1	P	90	ASP	CB-CG-OD1	5.99	123.69	118.30
1	F	90	ASP	CB-CG-OD1	5.90	123.61	118.30
1	L	90	ASP	CB-CG-OD1	5.69	123.42	118.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1293	0	1270	4	0
1	B	1270	0	1232	2	0
1	C	1278	0	1247	3	0
1	D	1281	0	1256	2	0
1	E	1271	0	1237	2	0
1	F	1269	0	1239	0	0
1	G	1285	0	1257	3	0
1	H	1264	0	1226	0	0
1	I	1269	0	1232	0	0
1	J	1260	0	1220	3	0
1	K	1267	0	1235	2	0
1	L	1277	0	1254	3	0
1	M	1281	0	1253	4	0
1	N	1272	0	1239	7	0
1	O	1281	0	1246	3	0
1	P	1272	0	1241	4	0
1	Q	1272	0	1239	2	0
1	R	1273	0	1243	1	0
1	S	1275	0	1248	3	0
1	T	1272	0	1241	4	0
1	U	1266	0	1228	3	0
1	V	1272	0	1241	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1276	0	1242	2	0
1	X	1272	0	1239	3	0
2	A	43	0	30	1	0
2	C	43	0	30	1	0
2	E	43	0	30	1	0
2	G	43	0	30	2	0
2	I	43	0	30	2	0
2	K	43	0	30	1	0
2	M	43	0	30	2	0
2	O	43	0	30	3	0
2	Q	43	0	30	2	0
2	S	43	0	30	1	0
2	U	43	0	30	2	0
2	W	43	0	30	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	L	1	0	0	0	0
4	A	8	0	14	0	0
4	B	8	0	14	0	0
4	D	8	0	14	0	0
4	E	16	0	28	0	0
4	F	8	0	14	0	0
4	G	8	0	14	0	0
4	H	8	0	14	0	0
4	I	8	0	14	0	0
4	J	8	0	14	0	0
4	K	8	0	14	0	0
4	M	16	0	28	0	0
4	N	16	0	28	5	0
4	O	8	0	14	0	0
4	P	8	0	14	0	0
4	R	8	0	14	0	0
4	S	8	0	14	3	0
4	T	8	0	14	0	0
4	U	8	0	14	0	0
4	V	8	0	14	0	0
4	W	8	0	14	0	0
4	X	8	0	14	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	2	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	T	1	0	0	0	0
5	V	1	0	0	0	0
6	C	8	0	14	1	0
6	I	8	0	14	0	0
6	J	8	0	14	4	0
6	K	8	0	14	1	0
6	L	8	0	14	0	0
6	Q	16	0	28	2	0
6	R	8	0	14	1	0
6	S	8	0	14	0	0
7	A	179	0	0	3	1
7	B	180	0	0	0	0
7	C	182	0	0	1	0
7	D	183	0	0	1	0
7	E	178	0	0	2	0
7	F	167	0	0	0	0
7	G	181	0	0	2	0
7	H	184	0	0	0	0
7	I	171	0	0	0	0
7	J	165	0	0	1	0
7	K	175	0	0	2	0
7	L	173	0	0	2	0
7	M	195	0	0	4	1
7	N	191	0	0	2	0
7	O	177	0	0	2	0
7	P	163	0	0	2	0
7	Q	200	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	166	0	0	1	0
7	S	188	0	0	1	0
7	T	181	0	0	4	0
7	U	168	0	0	1	0
7	V	172	0	0	2	0
7	W	176	0	0	2	0
7	X	180	0	0	1	0
All	All	35653	0	30627	81	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.

The worst 5 of 81 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50[B]:ASP:OD2	7:E:301:HOH:O	1.90	0.90
1:M:50[B]:ASP:OD2	7:M:301:HOH:O	1.90	0.88
1:N:50[B]:ASP:OD2	7:N:301:HOH:O	1.91	0.87
6:J:201:MPD:H13	7:J:331:HOH:O	1.75	0.86
1:T:126[A]:SER:OG	7:T:301:HOH:O	2.08	0.71

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)
7:A:360:HOH:O	7:M:405:HOH:O[2_554]	2.00	0.20

## 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	159/158 (101%)	158 (99%)	1 (1%)	0	100	100
1	B	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	C	157/158 (99%)	157 (100%)	0	0	100	100
1	D	157/158 (99%)	157 (100%)	0	0	100	100
1	E	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	F	156/158 (99%)	156 (100%)	0	0	100	100
1	G	158/158 (100%)	158 (100%)	0	0	100	100
1	H	155/158 (98%)	155 (100%)	0	0	100	100
1	I	156/158 (99%)	156 (100%)	0	0	100	100
1	J	155/158 (98%)	155 (100%)	0	0	100	100
1	K	155/158 (98%)	155 (100%)	0	0	100	100
1	L	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	M	157/158 (99%)	155 (99%)	2 (1%)	0	100	100
1	N	156/158 (99%)	156 (100%)	0	0	100	100
1	O	158/158 (100%)	158 (100%)	0	0	100	100
1	P	156/158 (99%)	156 (100%)	0	0	100	100
1	Q	156/158 (99%)	156 (100%)	0	0	100	100
1	R	156/158 (99%)	156 (100%)	0	0	100	100
1	S	156/158 (99%)	156 (100%)	0	0	100	100
1	T	156/158 (99%)	156 (100%)	0	0	100	100
1	U	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	V	156/158 (99%)	156 (100%)	0	0	100	100
1	W	157/158 (99%)	157 (100%)	0	0	100	100
1	X	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
All	All	3752/3792 (99%)	3744 (100%)	8 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	141/142 (99%)	140 (99%)	1 (1%)	84	69
1	B	136/142 (96%)	135 (99%)	1 (1%)	84	69
1	C	138/142 (97%)	138 (100%)	0	100	100
1	D	139/142 (98%)	137 (99%)	2 (1%)	67	42
1	E	137/142 (96%)	136 (99%)	1 (1%)	84	69
1	F	136/142 (96%)	135 (99%)	1 (1%)	84	69
1	G	139/142 (98%)	136 (98%)	3 (2%)	52	22
1	H	135/142 (95%)	134 (99%)	1 (1%)	84	69
1	I	136/142 (96%)	135 (99%)	1 (1%)	84	69
1	J	134/142 (94%)	133 (99%)	1 (1%)	84	69
1	K	136/142 (96%)	135 (99%)	1 (1%)	84	69
1	L	138/142 (97%)	137 (99%)	1 (1%)	84	69
1	M	138/142 (97%)	137 (99%)	1 (1%)	84	69
1	N	137/142 (96%)	135 (98%)	2 (2%)	65	39
1	O	138/142 (97%)	135 (98%)	3 (2%)	52	22
1	P	137/142 (96%)	136 (99%)	1 (1%)	84	69
1	Q	137/142 (96%)	135 (98%)	2 (2%)	65	39
1	R	137/142 (96%)	134 (98%)	3 (2%)	52	22
1	S	138/142 (97%)	137 (99%)	1 (1%)	84	69
1	T	137/142 (96%)	135 (98%)	2 (2%)	65	39
1	U	135/142 (95%)	134 (99%)	1 (1%)	84	69
1	V	137/142 (96%)	135 (98%)	2 (2%)	65	39
1	W	137/142 (96%)	134 (98%)	3 (2%)	52	22
1	X	137/142 (96%)	136 (99%)	1 (1%)	84	69
All	All	3290/3408 (96%)	3254 (99%)	36 (1%)	76	53

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	121	LYS
1	X	121	LYS
1	U	121	LYS
1	W	84[A]	GLN

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Mol	Chain	Res	Type
1	K	121	LYS

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

Mol	Chain	Res	Type
1	I	155	HIS
1	T	46	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 75 ligands modelled in this entry, 30 are monoatomic - leaving 45 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	$\# Z  > 2$
6	MPD	R	201	-	7,7,7	0.29	0	9,10,10	0.40	0
4	MRD	S	202	-	7,7,7	0.37	0	9,10,10	0.68	0
6	MPD	L	202	-	7,7,7	0.29	0	9,10,10	0.46	0
4	MRD	B	202	-	7,7,7	0.32	0	9,10,10	0.58	0
6	MPD	Q	202	-	7,7,7	0.35	0	9,10,10	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	M	201	1	41,50,50	1.42	4 (9%)	45,82,82	1.43	7 (15%)
4	MRD	U	202	-	7,7,7	0.32	0	9,10,10	0.48	0
2	HEM	E	201	1	41,50,50	1.37	3 (7%)	45,82,82	1.42	5 (11%)
6	MPD	J	201	-	7,7,7	0.45	0	9,10,10	0.63	0
4	MRD	N	201	-	7,7,7	0.32	0	9,10,10	0.51	0
2	HEM	A	201	1	41,50,50	1.32	3 (7%)	45,82,82	1.43	6 (13%)
2	HEM	K	201	1	41,50,50	1.38	4 (9%)	45,82,82	1.63	10 (22%)
4	MRD	J	202	-	7,7,7	0.52	0	9,10,10	1.02	0
4	MRD	N	202	-	7,7,7	0.40	0	9,10,10	0.74	0
4	MRD	G	203	-	7,7,7	0.34	0	9,10,10	0.28	0
6	MPD	I	202	-	7,7,7	0.31	0	9,10,10	0.59	0
4	MRD	E	204	-	7,7,7	0.44	0	9,10,10	0.93	0
6	MPD	K	203	-	7,7,7	0.36	0	9,10,10	0.57	0
4	MRD	K	202	-	7,7,7	0.34	0	9,10,10	0.43	0
2	HEM	W	201	1	41,50,50	1.34	4 (9%)	45,82,82	1.56	9 (20%)
2	HEM	I	203	1	41,50,50	1.41	4 (9%)	45,82,82	1.53	8 (17%)
4	MRD	R	202	-	7,7,7	0.38	0	9,10,10	0.75	0
6	MPD	S	201	-	7,7,7	0.40	0	9,10,10	0.40	0
6	MPD	Q	203	-	7,7,7	0.36	0	9,10,10	0.53	0
4	MRD	I	201	-	7,7,7	0.28	0	9,10,10	0.38	0
4	MRD	O	201	-	7,7,7	0.39	0	9,10,10	0.21	0
4	MRD	P	201	-	7,7,7	0.29	0	9,10,10	0.42	0
4	MRD	E	203	-	7,7,7	0.30	0	9,10,10	0.49	0
4	MRD	F	201	-	7,7,7	0.31	0	9,10,10	0.51	0
6	MPD	C	201	-	7,7,7	0.25	0	9,10,10	0.38	0
2	HEM	U	201	1	41,50,50	1.36	3 (7%)	45,82,82	1.70	11 (24%)
4	MRD	T	201	-	7,7,7	0.31	0	9,10,10	0.34	0
4	MRD	A	203	-	7,7,7	0.33	0	9,10,10	0.43	0
2	HEM	G	201	1	41,50,50	1.41	3 (7%)	45,82,82	1.50	6 (13%)
4	MRD	H	201	-	7,7,7	0.34	0	9,10,10	0.33	0
4	MRD	M	203	-	7,7,7	0.49	0	9,10,10	0.87	0
2	HEM	C	202	1	41,50,50	1.40	3 (7%)	45,82,82	1.58	6 (13%)
2	HEM	Q	201	1	41,50,50	1.43	4 (9%)	45,82,82	1.58	10 (22%)
4	MRD	X	201	-	7,7,7	0.31	0	9,10,10	0.38	0
2	HEM	O	202	1	41,50,50	1.36	3 (7%)	45,82,82	1.69	10 (22%)
4	MRD	M	202	-	7,7,7	0.26	0	9,10,10	0.44	0
4	MRD	V	201	-	7,7,7	0.28	0	9,10,10	0.46	0
2	HEM	S	204	1	41,50,50	1.35	3 (7%)	45,82,82	1.53	8 (17%)
4	MRD	W	202	-	7,7,7	0.25	0	9,10,10	0.37	0
4	MRD	D	202	-	7,7,7	0.28	0	9,10,10	0.39	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
6	MPD	R	201	-	-	1/5/5/5	-
4	MRD	S	202	-	-	1/5/5/5	-
6	MPD	L	202	-	-	0/5/5/5	-
4	MRD	B	202	-	-	0/5/5/5	-
6	MPD	Q	202	-	-	1/5/5/5	-
2	HEM	M	201	1	-	4/12/54/54	-
4	MRD	U	202	-	-	0/5/5/5	-
2	HEM	E	201	1	-	4/12/54/54	-
6	MPD	J	201	-	-	0/5/5/5	-
4	MRD	N	201	-	-	0/5/5/5	-
2	HEM	A	201	1	-	4/12/54/54	-
2	HEM	K	201	1	-	4/12/54/54	-
4	MRD	J	202	-	-	1/5/5/5	-
4	MRD	N	202	-	-	2/5/5/5	-
4	MRD	G	203	-	-	0/5/5/5	-
6	MPD	I	202	-	-	0/5/5/5	-
4	MRD	E	204	-	-	1/5/5/5	-
6	MPD	K	203	-	-	0/5/5/5	-
4	MRD	K	202	-	-	0/5/5/5	-
2	HEM	W	201	1	-	4/12/54/54	-
2	HEM	I	203	1	-	4/12/54/54	-
4	MRD	R	202	-	-	1/5/5/5	-
6	MPD	S	201	-	-	2/5/5/5	-
6	MPD	Q	203	-	-	0/5/5/5	-
4	MRD	I	201	-	-	0/5/5/5	-
4	MRD	O	201	-	-	0/5/5/5	-
4	MRD	P	201	-	-	0/5/5/5	-
4	MRD	E	203	-	-	0/5/5/5	-
4	MRD	F	201	-	-	0/5/5/5	-
6	MPD	C	201	-	-	2/5/5/5	-
2	HEM	U	201	1	-	4/12/54/54	-
4	MRD	T	201	-	-	0/5/5/5	-
4	MRD	A	203	-	-	0/5/5/5	-
2	HEM	G	201	1	-	4/12/54/54	-
4	MRD	H	201	-	-	0/5/5/5	-
4	MRD	M	203	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	202	1	-	4/12/54/54	-
2	HEM	Q	201	1	-	4/12/54/54	-
4	MRD	X	201	-	-	0/5/5/5	-
2	HEM	O	202	1	-	4/12/54/54	-
4	MRD	M	202	-	-	0/5/5/5	-
4	MRD	V	201	-	-	0/5/5/5	-
2	HEM	S	204	1	-	4/12/54/54	-
4	MRD	W	202	-	-	0/5/5/5	-
4	MRD	D	202	-	-	0/5/5/5	-

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	201	HEM	C3C-C2C	-4.62	1.34	1.40
2	G	201	HEM	C3C-C2C	-4.36	1.34	1.40
2	I	203	HEM	C3C-C2C	-4.25	1.34	1.40
2	M	201	HEM	C3C-C2C	-4.08	1.34	1.40
2	E	201	HEM	C3C-C2C	-4.06	1.34	1.40

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	201	HEM	CBA-CAA-C2A	-4.68	104.63	112.62
2	A	201	HEM	CMC-C2C-C3C	4.31	132.73	124.68
2	O	202	HEM	CMC-C2C-C3C	4.13	132.40	124.68
2	E	201	HEM	CBA-CAA-C2A	-4.11	105.60	112.62
2	M	201	HEM	CMC-C2C-C3C	3.91	131.99	124.68

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

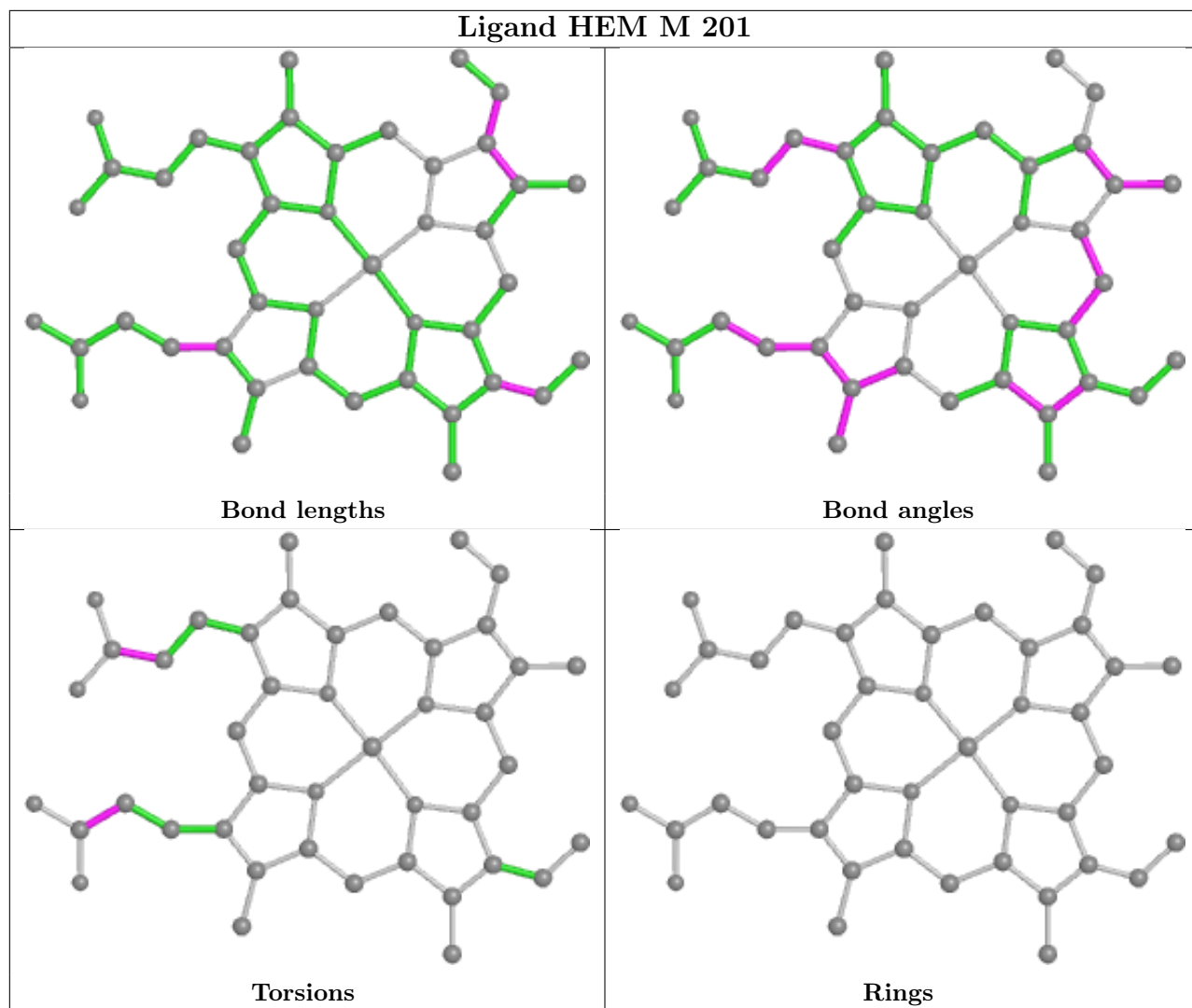
Mol	Chain	Res	Type	Atoms
4	E	204	MRD	C2-C3-C4-O4
4	R	202	MRD	C2-C3-C4-O4
4	N	202	MRD	C2-C3-C4-C5
6	S	201	MPD	C2-C3-C4-C5
2	G	201	HEM	CAD-CBD-CGD-O2D

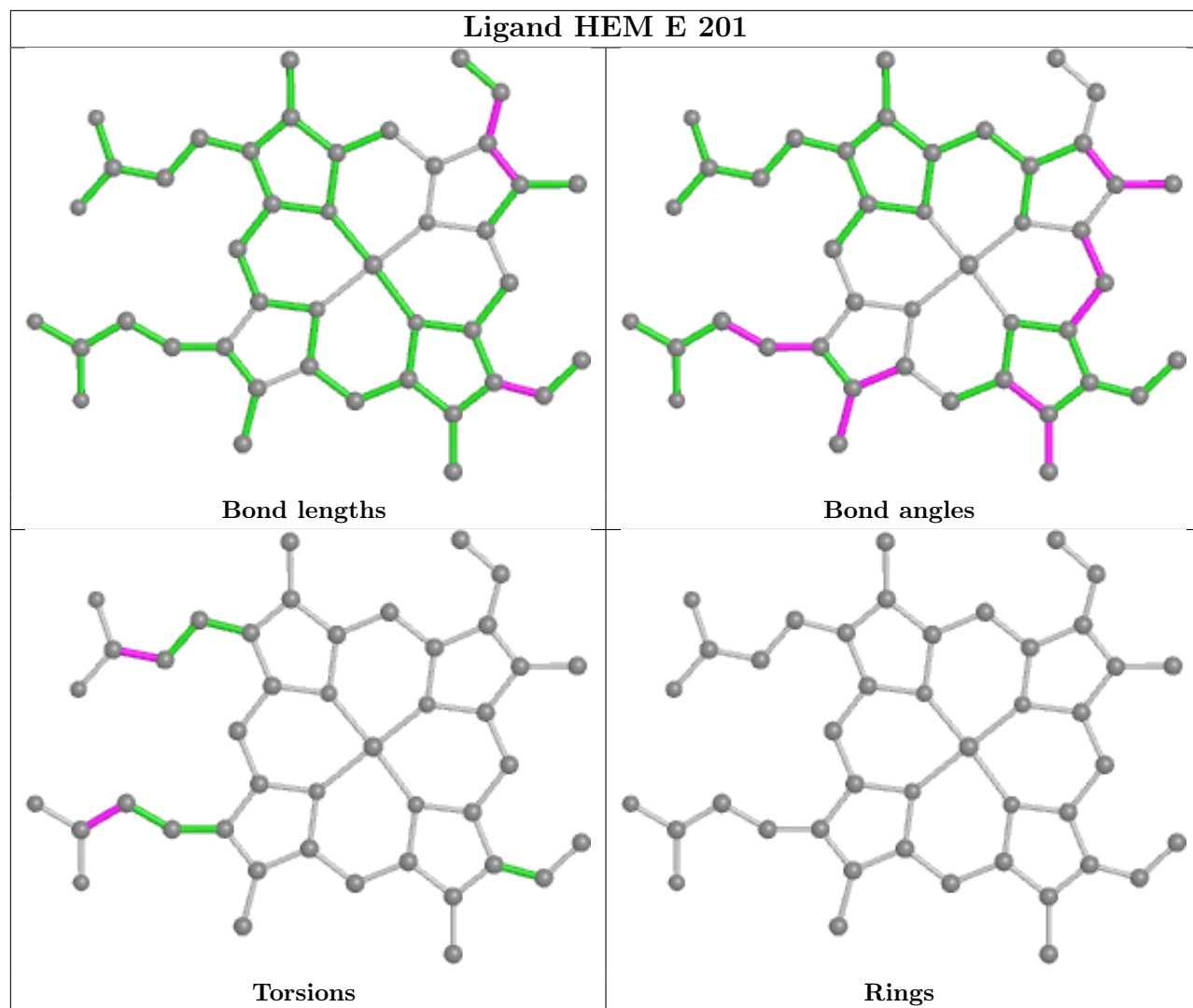
There are no ring outliers.

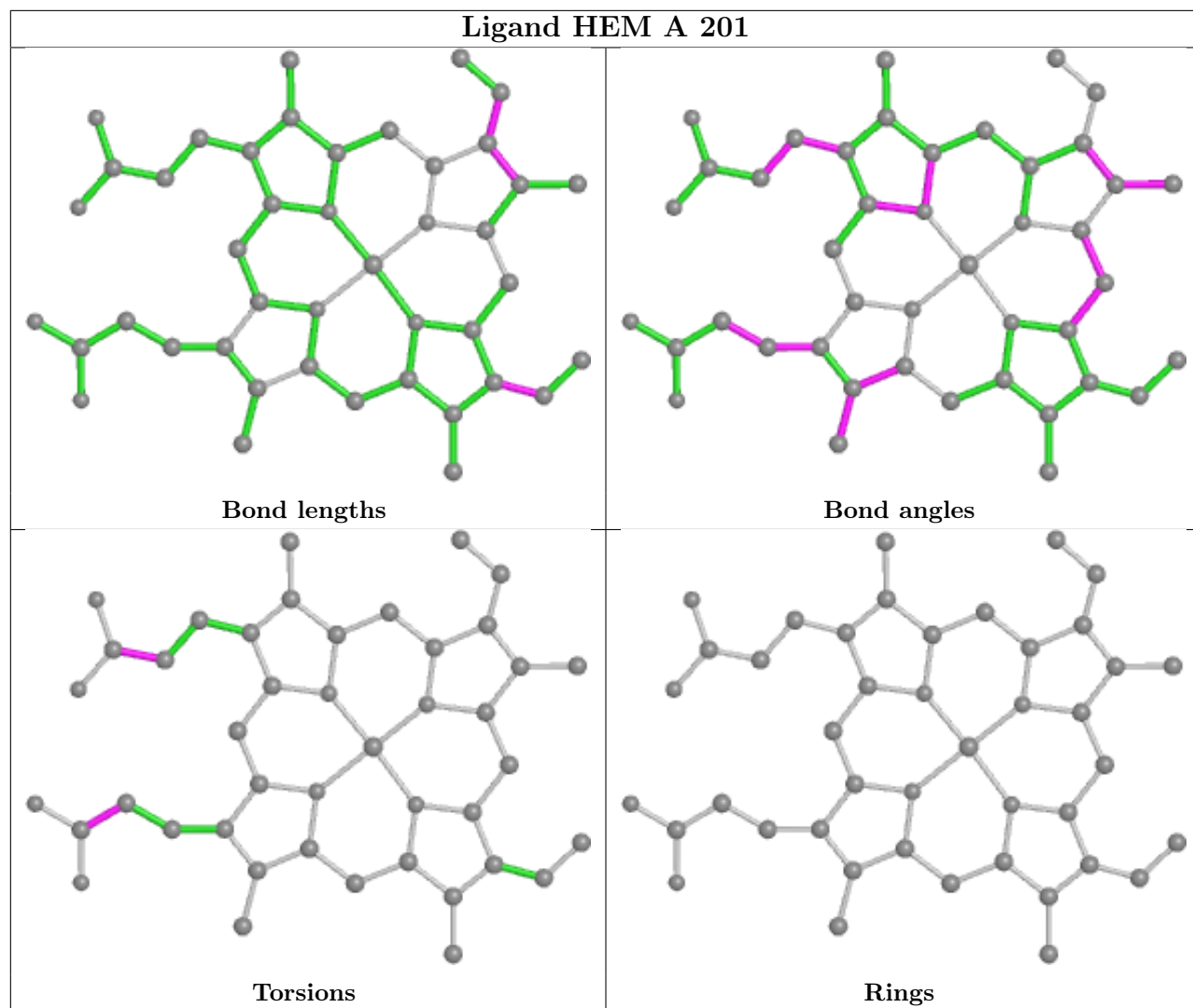
21 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	201	MPD	1	0
4	S	202	MRD	3	0
6	Q	202	MPD	1	0
2	M	201	HEM	2	0
2	E	201	HEM	1	0
6	J	201	MPD	4	0
4	N	201	MRD	1	0
2	A	201	HEM	1	0
2	K	201	HEM	1	0
4	N	202	MRD	4	0
6	K	203	MPD	1	0
2	W	201	HEM	1	0
2	I	203	HEM	2	0
6	Q	203	MPD	1	0
6	C	201	MPD	1	0
2	U	201	HEM	2	0
2	G	201	HEM	2	0
2	C	202	HEM	1	0
2	Q	201	HEM	2	0
2	O	202	HEM	3	0
2	S	204	HEM	1	0

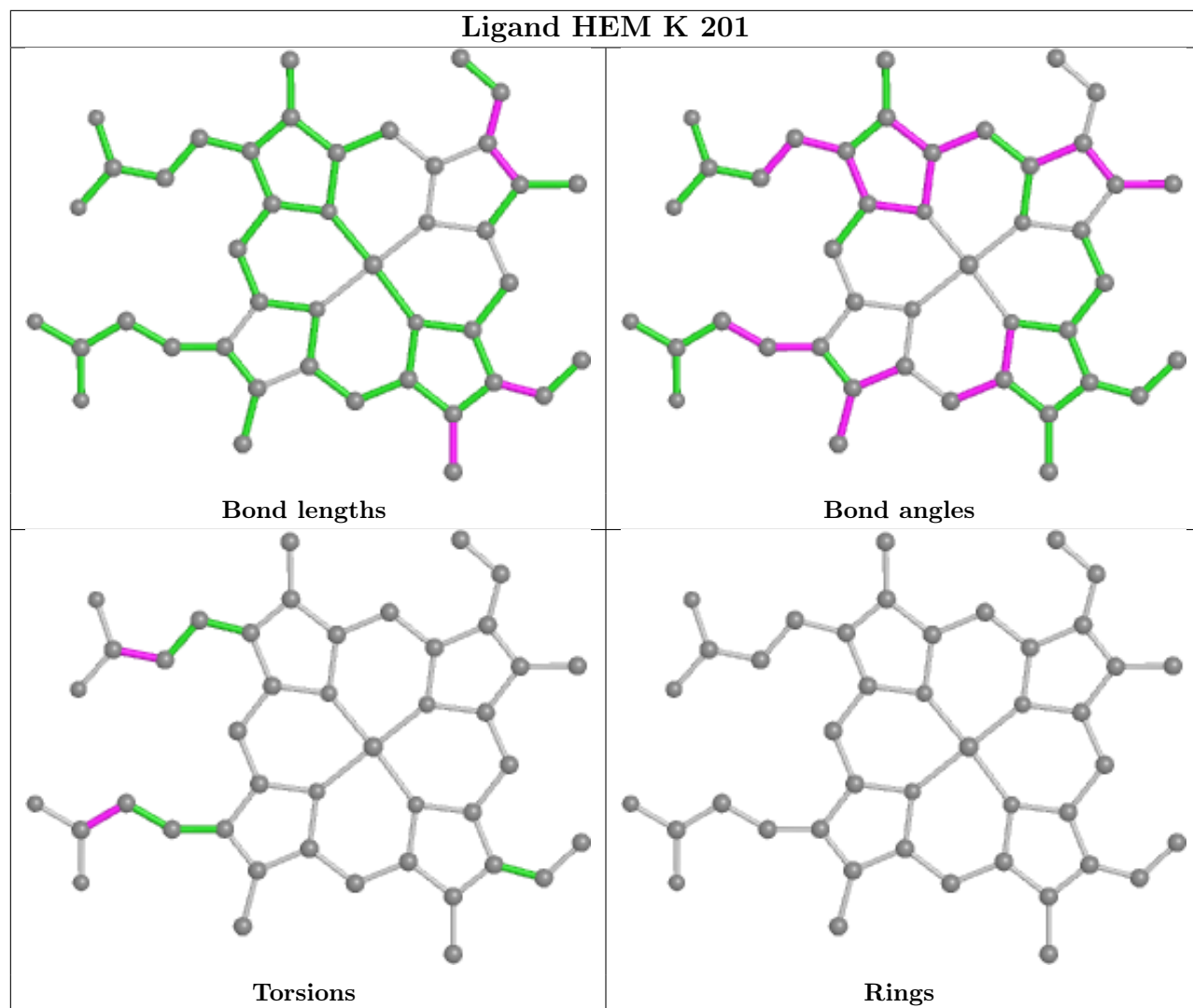
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

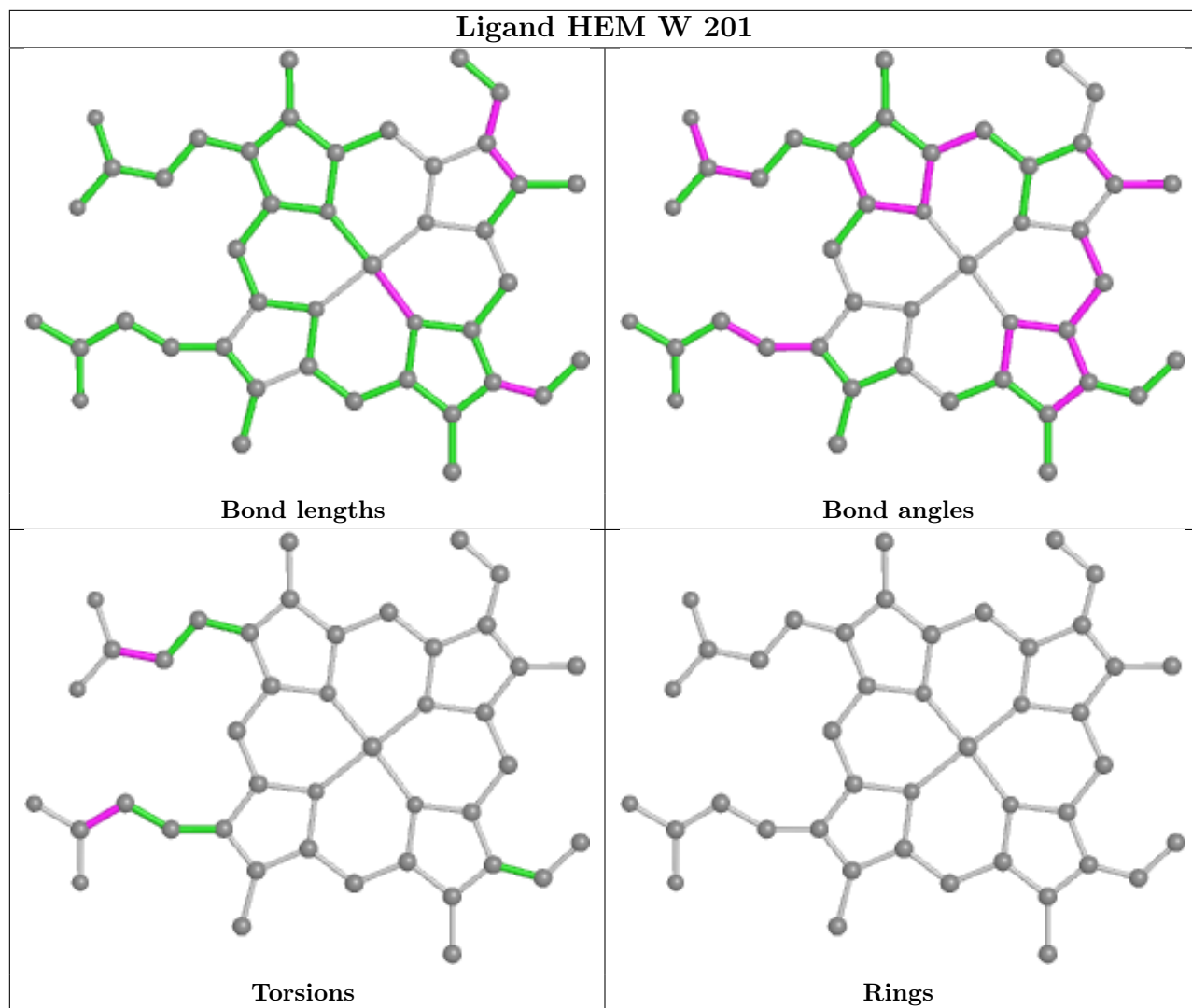


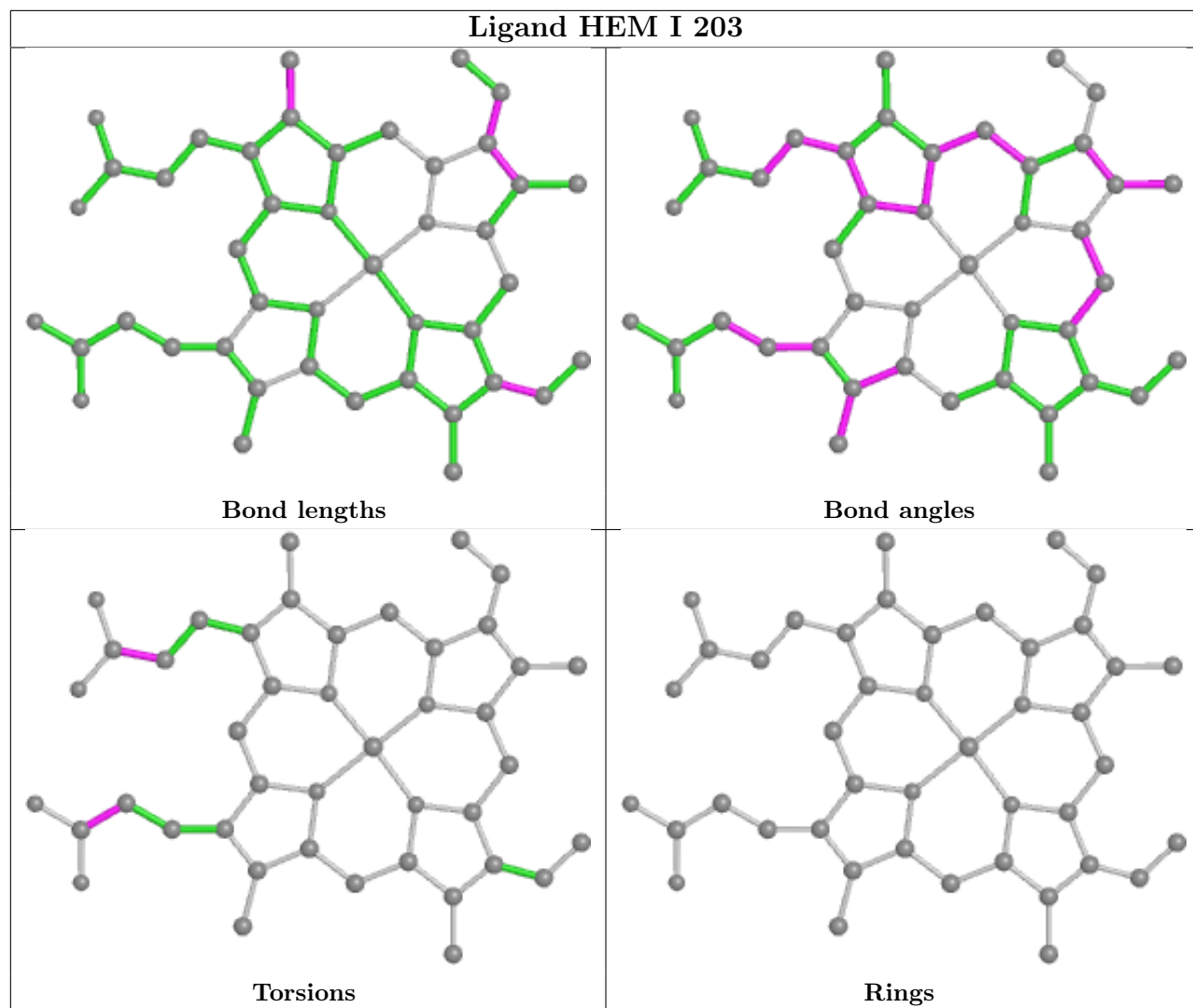


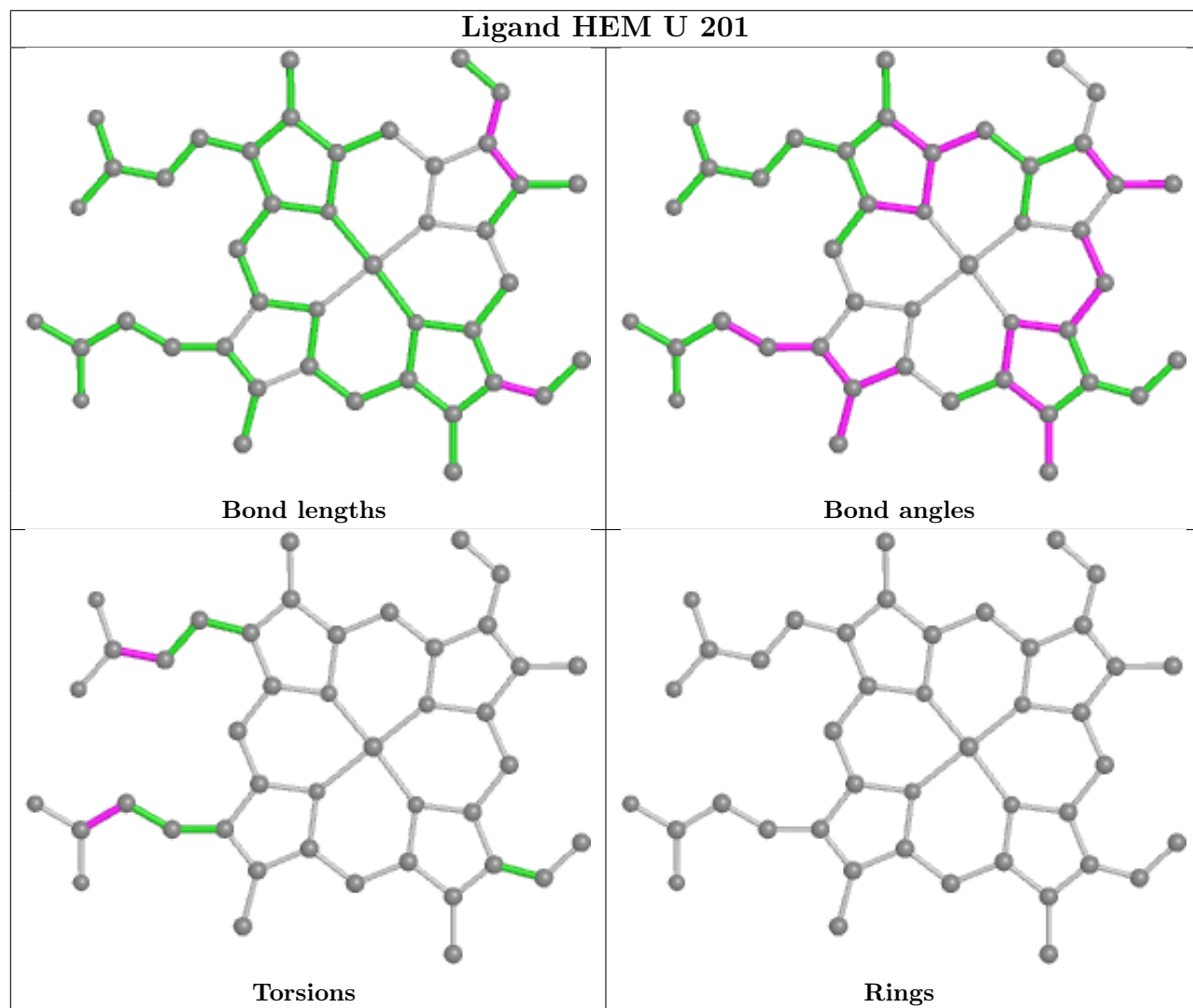


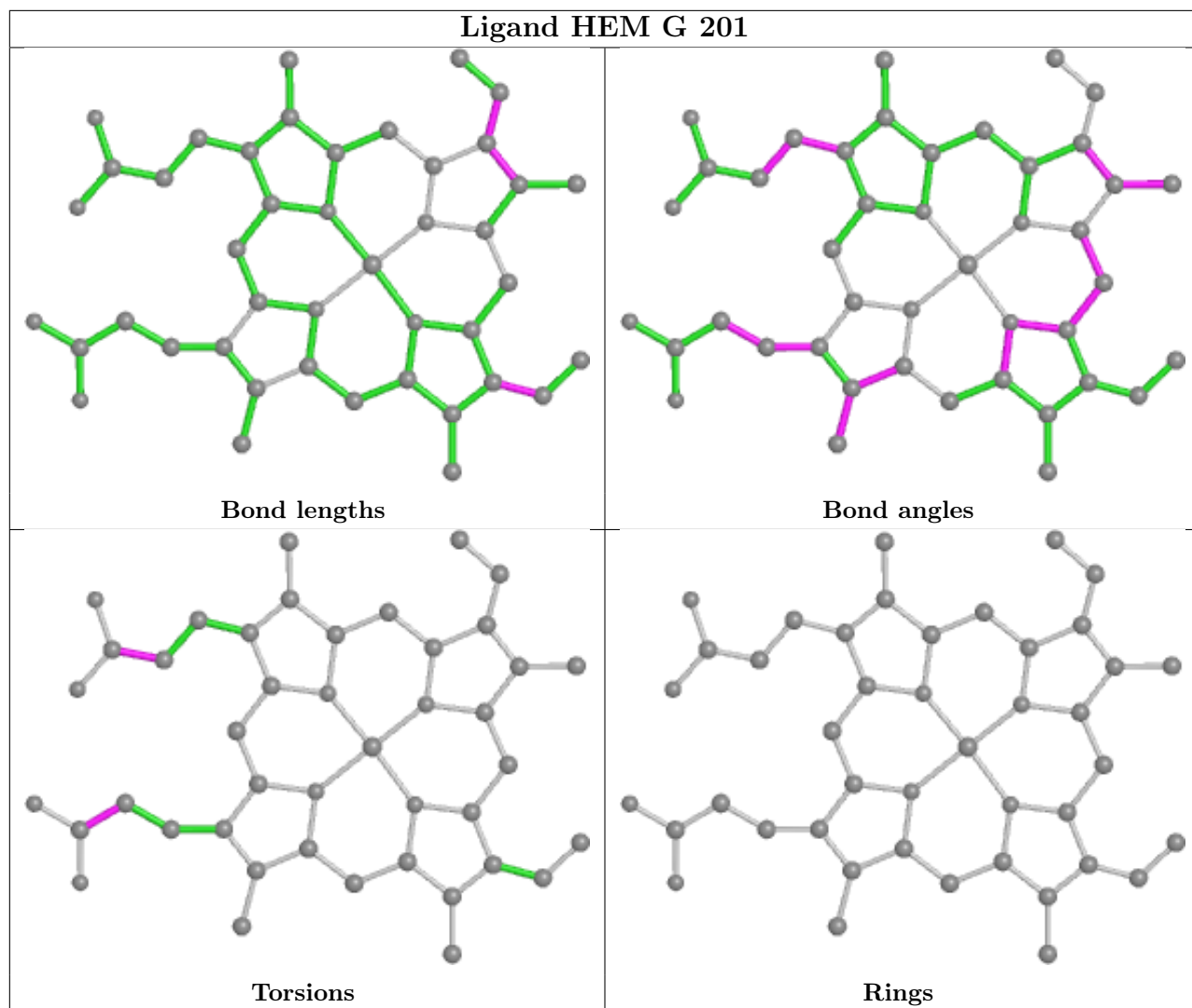


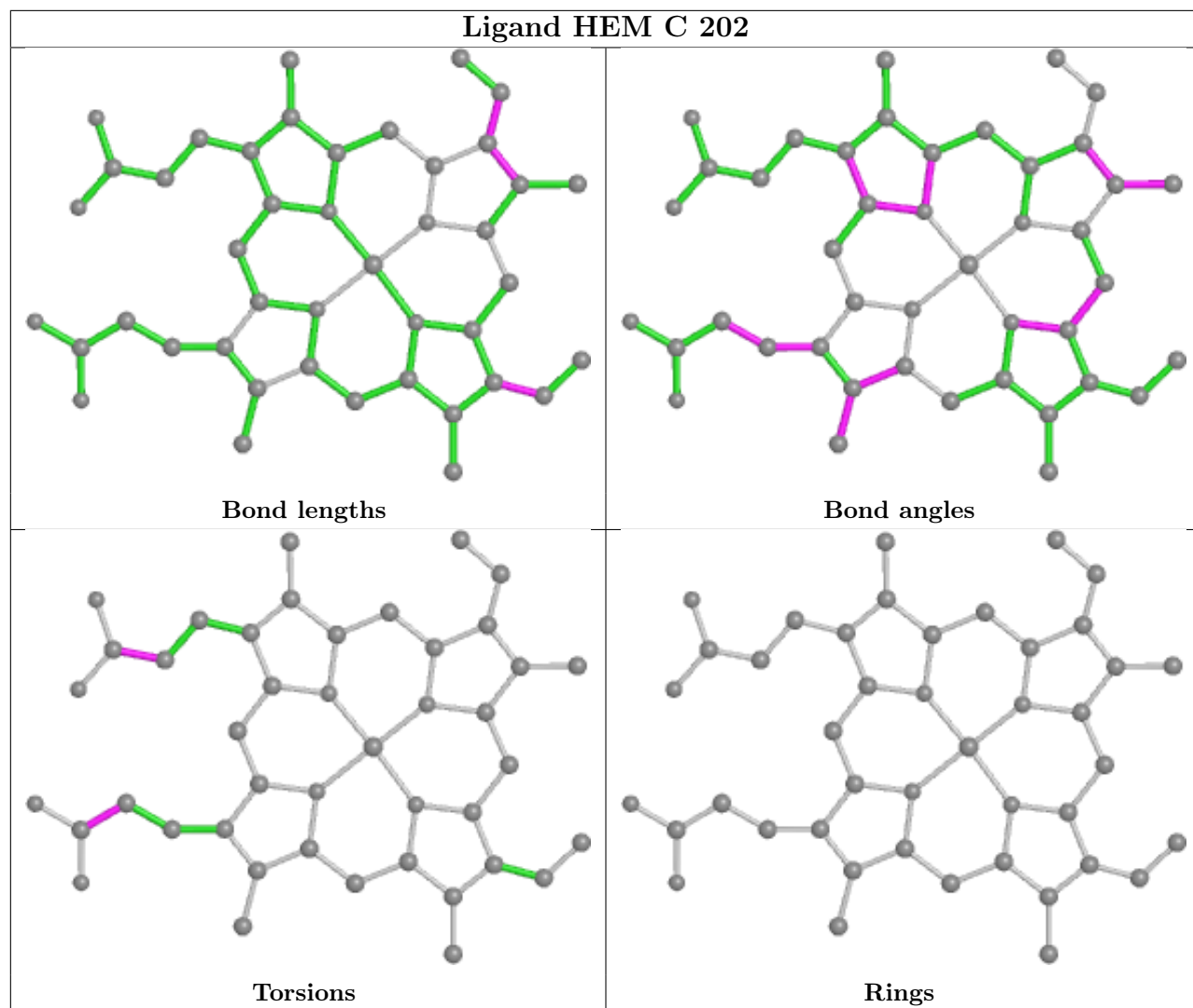


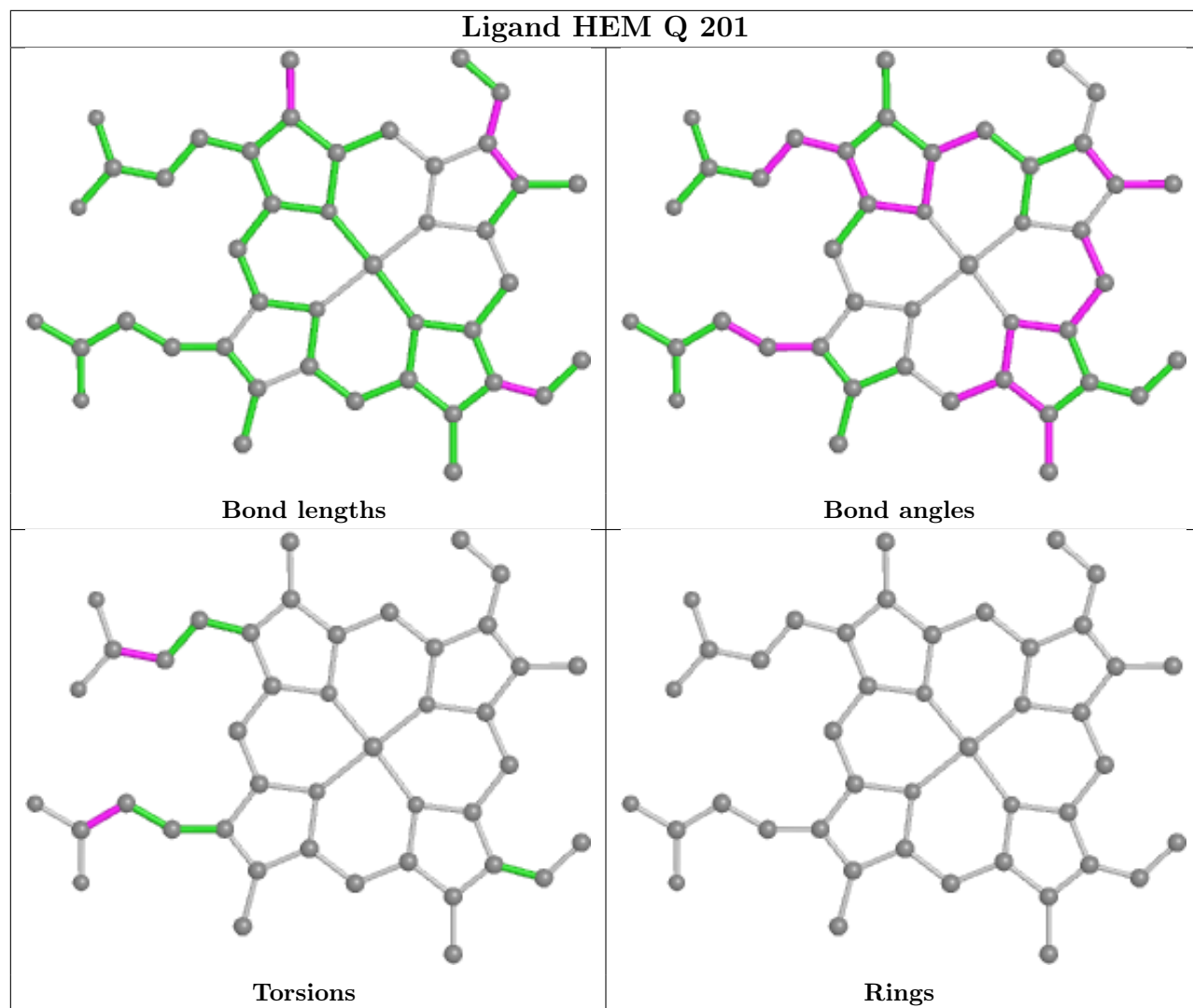


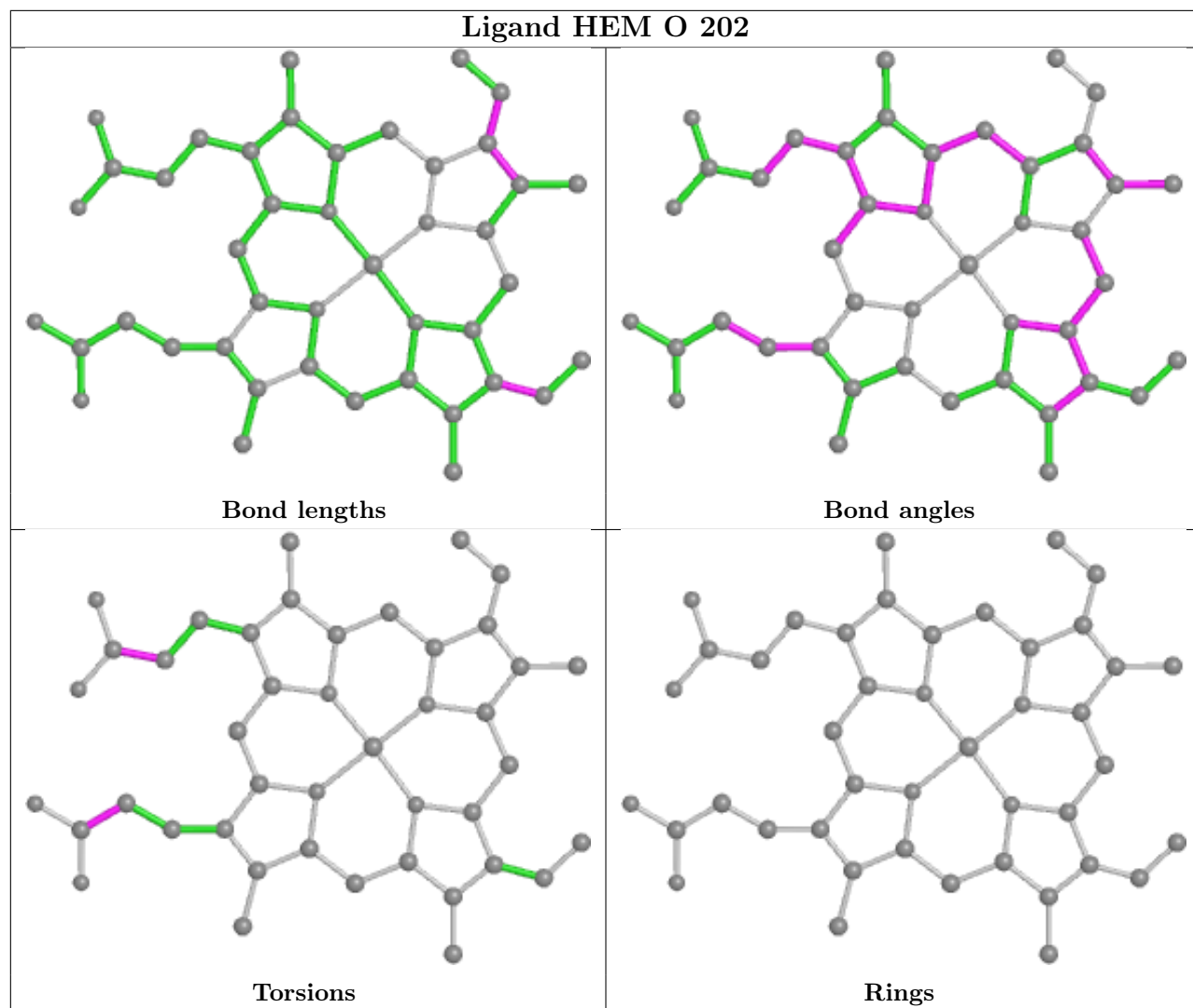




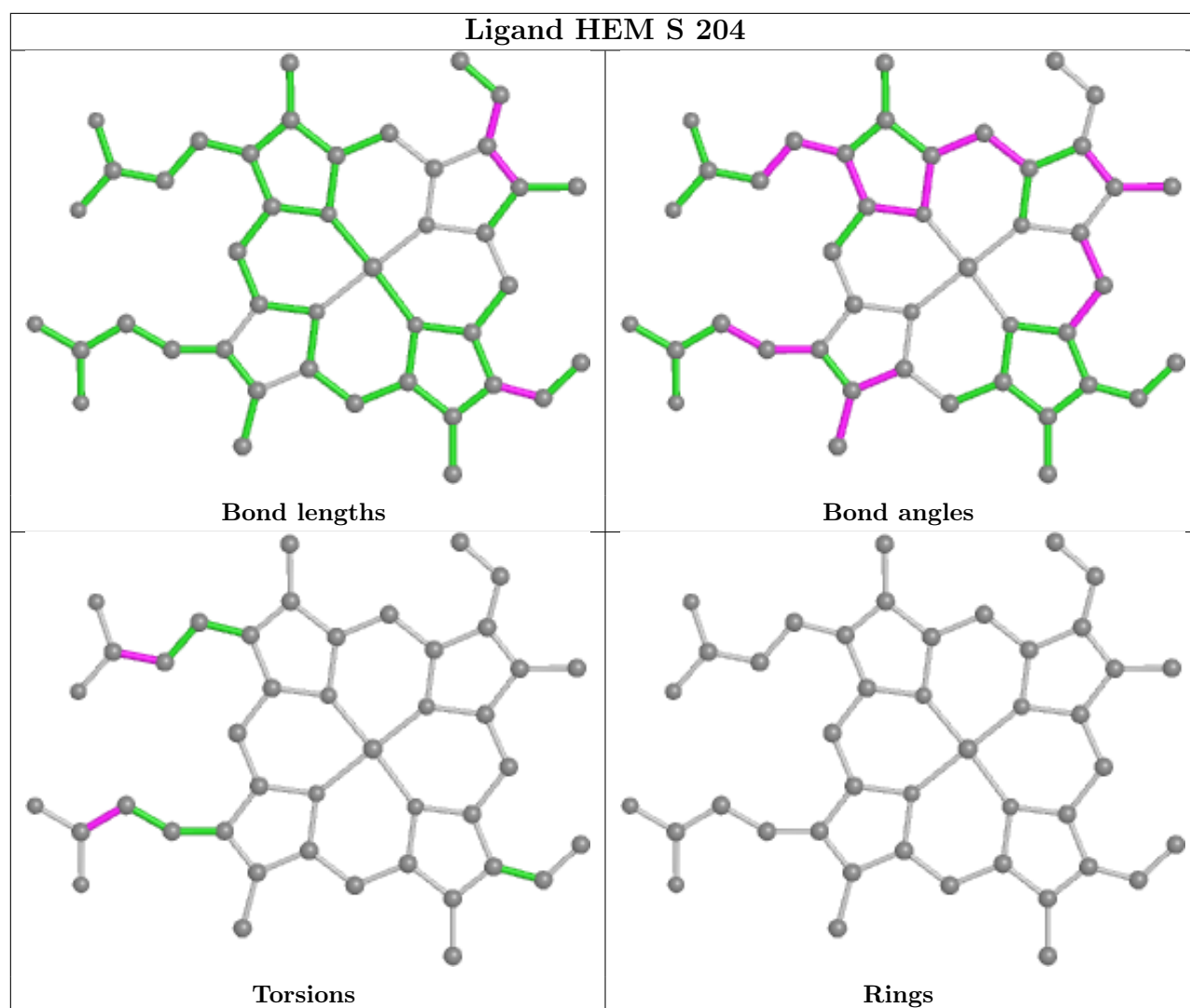












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	156/158 (98%)	-0.04	0 100 100	10, 14, 23, 35	0
1	B	156/158 (98%)	-0.17	0 100 100	11, 15, 24, 40	0
1	C	156/158 (98%)	-0.08	0 100 100	13, 17, 26, 38	0
1	D	156/158 (98%)	-0.11	0 100 100	13, 16, 24, 34	0
1	E	156/158 (98%)	-0.05	0 100 100	12, 16, 25, 37	0
1	F	156/158 (98%)	-0.10	0 100 100	12, 16, 25, 34	0
1	G	156/158 (98%)	-0.07	0 100 100	13, 17, 25, 37	0
1	H	156/158 (98%)	-0.09	0 100 100	12, 16, 25, 35	0
1	I	156/158 (98%)	-0.08	0 100 100	13, 17, 26, 38	0
1	J	156/158 (98%)	-0.09	0 100 100	13, 17, 26, 39	0
1	K	156/158 (98%)	-0.07	0 100 100	13, 16, 26, 38	0
1	L	156/158 (98%)	-0.15	0 100 100	12, 16, 25, 34	0
1	M	156/158 (98%)	0.01	0 100 100	11, 14, 23, 39	0
1	N	156/158 (98%)	-0.12	0 100 100	11, 15, 24, 34	0
1	O	156/158 (98%)	-0.03	0 100 100	13, 17, 25, 37	0
1	P	156/158 (98%)	-0.08	0 100 100	14, 17, 26, 36	0
1	Q	156/158 (98%)	-0.16	0 100 100	12, 15, 24, 34	0
1	R	156/158 (98%)	-0.11	0 100 100	12, 16, 24, 36	0
1	S	156/158 (98%)	-0.14	0 100 100	11, 15, 25, 36	0
1	T	156/158 (98%)	-0.11	0 100 100	12, 15, 26, 35	0
1	U	156/158 (98%)	-0.15	0 100 100	13, 17, 25, 38	0
1	V	156/158 (98%)	-0.11	0 100 100	14, 17, 26, 35	0
1	W	156/158 (98%)	-0.07	0 100 100	14, 17, 24, 35	0
1	X	156/158 (98%)	-0.06	0 100 100	12, 16, 25, 36	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3744/3792 (98%)	-0.09	0 100 100	10, 16, 25, 40	0

There are no RSRZ outliers to report.

## 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 monosaccharides 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
4	MRD	N	202	8/8	0.79	0.22	25,34,45,46	0
4	MRD	S	202	8/8	0.80	0.21	27,32,42,42	0
6	MPD	R	201	8/8	0.81	0.25	24,34,44,50	0
4	MRD	J	202	8/8	0.82	0.18	23,30,39,40	0
4	MRD	A	203	8/8	0.83	0.21	24,28,36,41	0
4	MRD	E	203	8/8	0.83	0.18	19,27,34,37	0
4	MRD	E	204	8/8	0.83	0.16	23,29,40,43	0
4	MRD	F	201	8/8	0.83	0.15	22,30,33,39	0
6	MPD	Q	203	8/8	0.84	0.16	25,32,39,40	0
6	MPD	C	201	8/8	0.84	0.16	22,30,35,45	0
4	MRD	B	202	8/8	0.86	0.15	20,24,33,34	0
4	MRD	M	203	8/8	0.86	0.21	21,30,41,41	0
6	MPD	I	202	8/8	0.86	0.17	26,34,43,45	0
6	MPD	K	203	8/8	0.86	0.20	23,35,41,42	0
4	MRD	I	201	8/8	0.86	0.20	23,30,38,39	0
4	MRD	R	202	8/8	0.86	0.18	24,33,39,41	0
5	NA	J	203	1/1	0.87	0.14	28,28,28,28	0
4	MRD	V	201	8/8	0.87	0.16	24,27,33,36	0
5	NA	D	203	1/1	0.87	0.16	26,26,26,26	0

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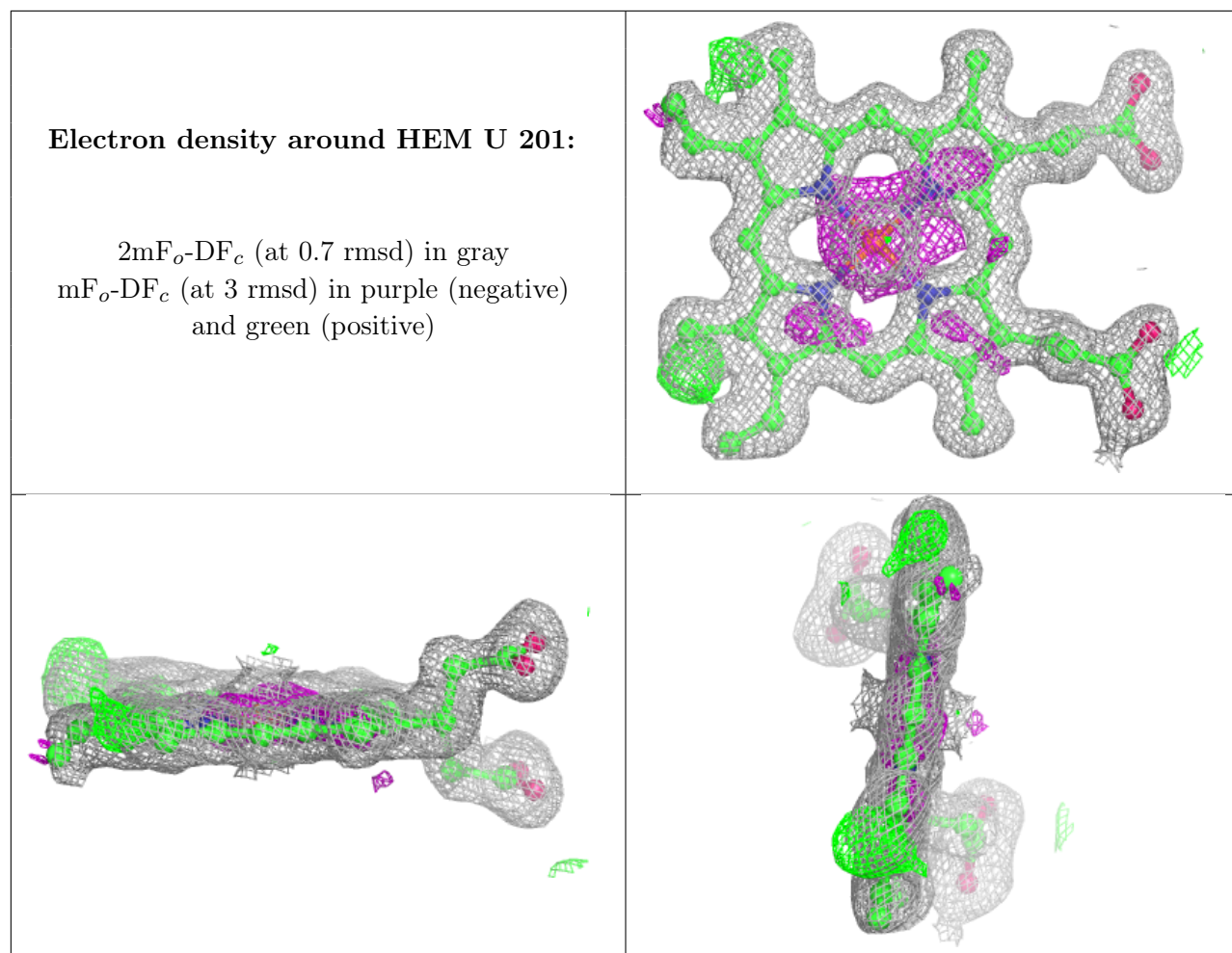
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MRD	O	201	8/8	0.88	0.14	25,28,37,37	0
4	MRD	P	201	8/8	0.88	0.14	24,30,37,38	0
4	MRD	W	202	8/8	0.88	0.16	20,27,32,33	0
4	MRD	X	201	8/8	0.88	0.15	24,32,36,37	0
6	MPD	L	202	8/8	0.88	0.22	22,30,41,48	0
6	MPD	Q	202	8/8	0.88	0.15	22,28,35,44	0
4	MRD	H	201	8/8	0.88	0.14	22,30,34,35	0
5	NA	I	204	1/1	0.88	0.10	30,30,30,30	0
5	NA	R	203	1/1	0.89	0.12	26,26,26,26	0
4	MRD	G	203	8/8	0.89	0.14	21,27,35,36	0
5	NA	E	206	1/1	0.89	0.14	26,26,26,26	0
5	NA	K	204	1/1	0.89	0.12	27,27,27,27	0
6	MPD	S	201	8/8	0.89	0.15	22,27,36,47	0
4	MRD	T	201	8/8	0.90	0.16	22,29,35,37	0
5	NA	B	204	1/1	0.90	0.10	27,27,27,27	0
4	MRD	U	202	8/8	0.90	0.12	20,25,30,33	0
5	NA	T	202	1/1	0.90	0.14	26,26,26,26	0
4	MRD	N	201	8/8	0.90	0.12	24,27,37,38	0
4	MRD	K	202	8/8	0.90	0.15	21,23,34,34	0
4	MRD	D	202	8/8	0.91	0.17	19,27,32,34	0
4	MRD	M	202	8/8	0.91	0.12	23,24,34,36	0
5	NA	E	205	1/1	0.91	0.14	28,28,28,28	0
5	NA	V	202	1/1	0.91	0.15	28,28,28,28	0
5	NA	G	204	1/1	0.92	0.12	26,26,26,26	0
5	NA	G	205	1/1	0.92	0.10	28,28,28,28	0
6	MPD	J	201	8/8	0.92	0.15	17,25,40,41	0
5	NA	D	204	1/1	0.93	0.10	28,28,28,28	0
5	NA	L	203	1/1	0.93	0.10	26,26,26,26	0
5	NA	M	204	1/1	0.93	0.12	24,24,24,24	0
5	NA	N	203	1/1	0.93	0.10	23,23,23,23	0
5	NA	S	203	1/1	0.94	0.11	26,26,26,26	0
5	NA	H	202	1/1	0.94	0.10	26,26,26,26	0
5	NA	L	204	1/1	0.94	0.12	29,29,29,29	0
2	HEM	U	201	43/43	0.94	0.15	16,19,31,31	0
5	NA	A	204	1/1	0.94	0.13	28,28,28,28	0
2	HEM	O	202	43/43	0.94	0.12	15,18,30,33	0
2	HEM	W	201	43/43	0.95	0.12	15,18,30,35	0
2	HEM	G	201	43/43	0.95	0.12	14,18,31,32	0
2	HEM	I	203	43/43	0.95	0.14	15,20,32,34	0
5	NA	F	202	1/1	0.95	0.12	27,27,27,27	0
2	HEM	K	201	43/43	0.95	0.13	14,19,31,33	0
2	HEM	M	201	43/43	0.95	0.14	13,16,26,31	0

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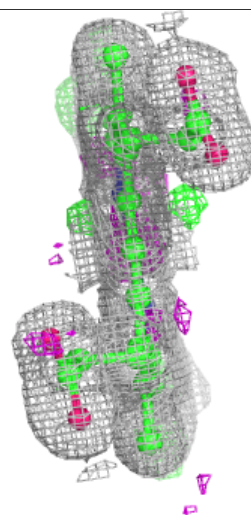
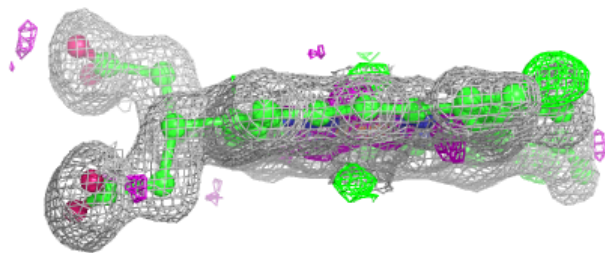
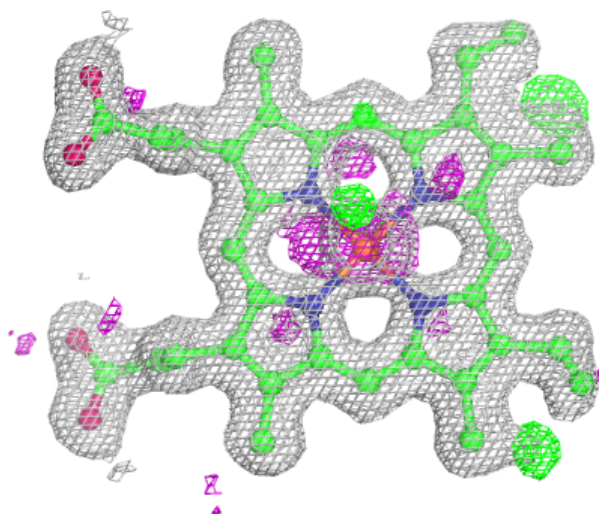
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	A	205	1/1	0.95	0.12	22,22,22,22	0
2	HEM	C	202	43/43	0.95	0.14	15,19,32,35	0
2	HEM	E	201	43/43	0.95	0.15	14,18,28,32	0
2	HEM	S	204	43/43	0.96	0.12	13,16,29,31	0
2	HEM	A	201	43/43	0.96	0.13	13,16,27,28	0
5	NA	B	203	1/1	0.96	0.15	24,24,24,24	0
2	HEM	Q	201	43/43	0.96	0.11	13,16,30,34	0
5	NA	C	203	1/1	0.97	0.10	29,29,29,29	0
3	K	B	201	1/1	0.99	0.07	15,15,15,15	0
3	K	E	202	1/1	0.99	0.07	14,14,14,14	0
3	K	G	202	1/1	0.99	0.08	13,13,13,13	0
3	K	A	202	1/1	1.00	0.09	11,11,11,11	0
3	K	D	201	1/1	1.00	0.09	13,13,13,13	0
3	K	L	201	1/1	1.00	0.08	12,12,12,12	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.



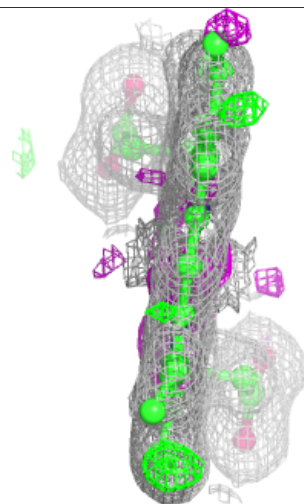
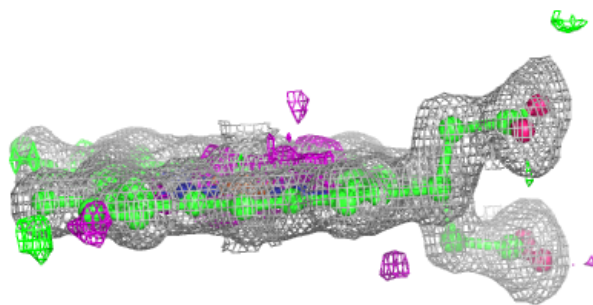
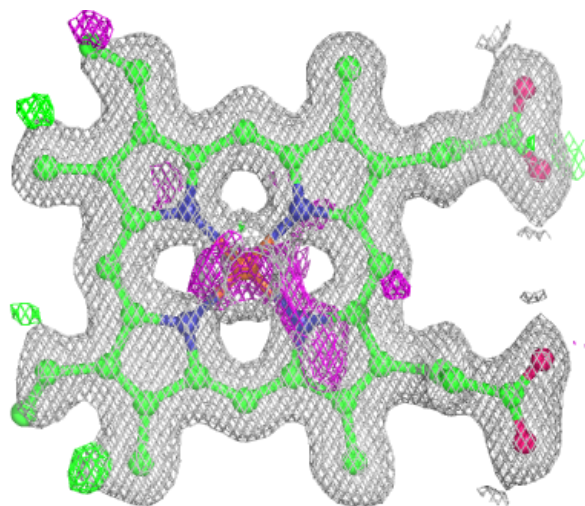
**Electron density around HEM O 202:**

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

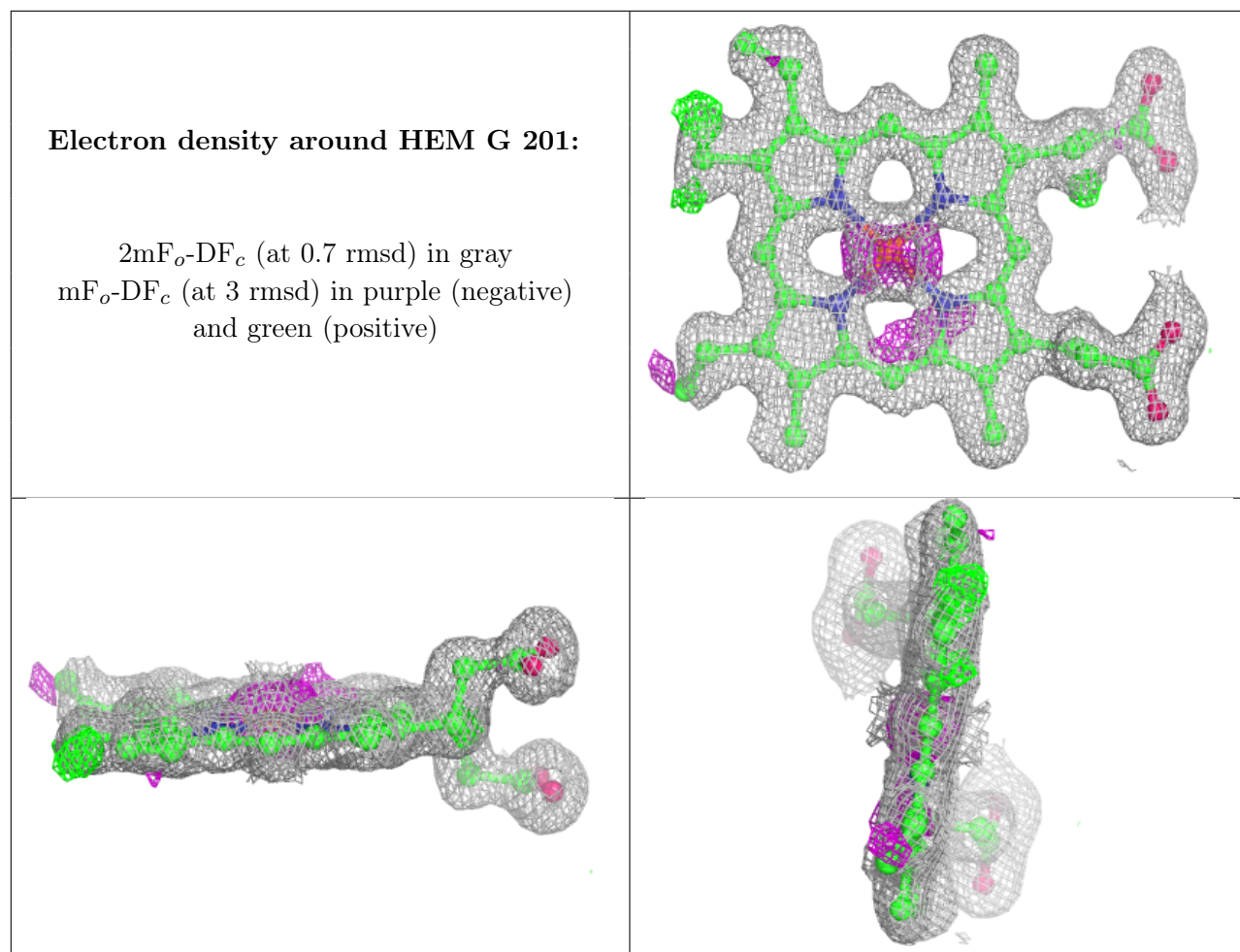


**Electron density around HEM W 201:**

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and green (positive)

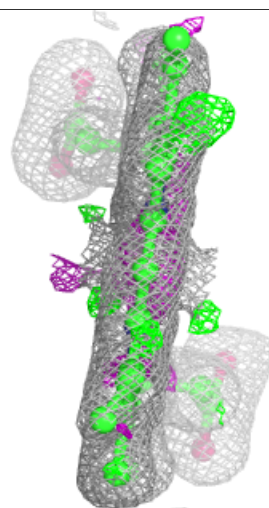
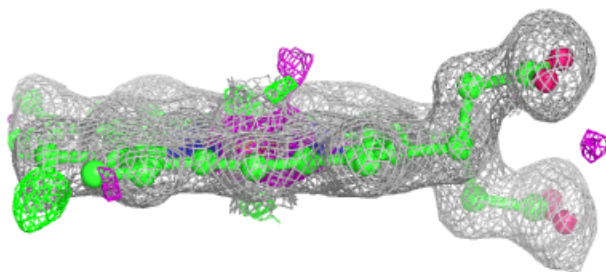
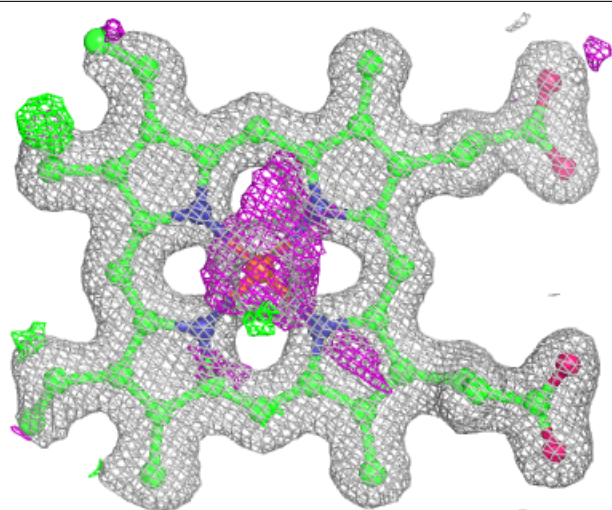






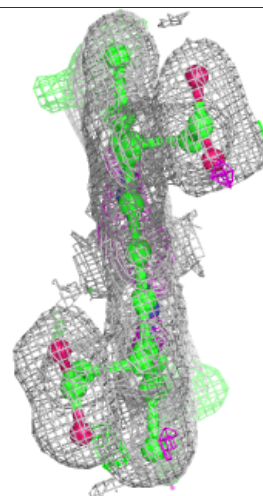
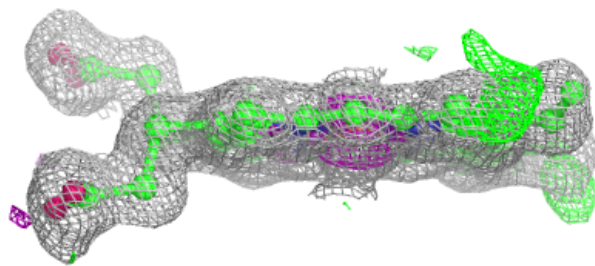
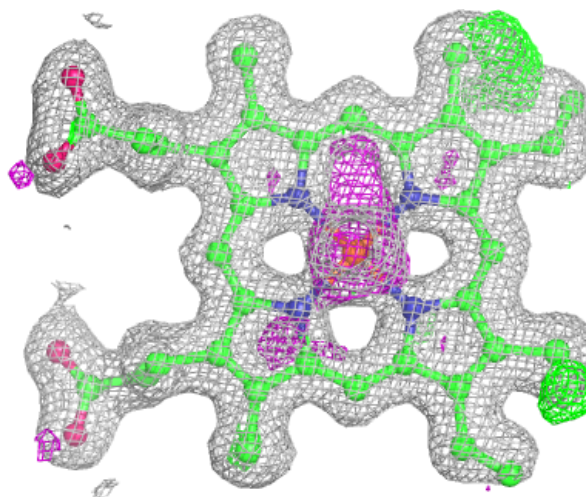
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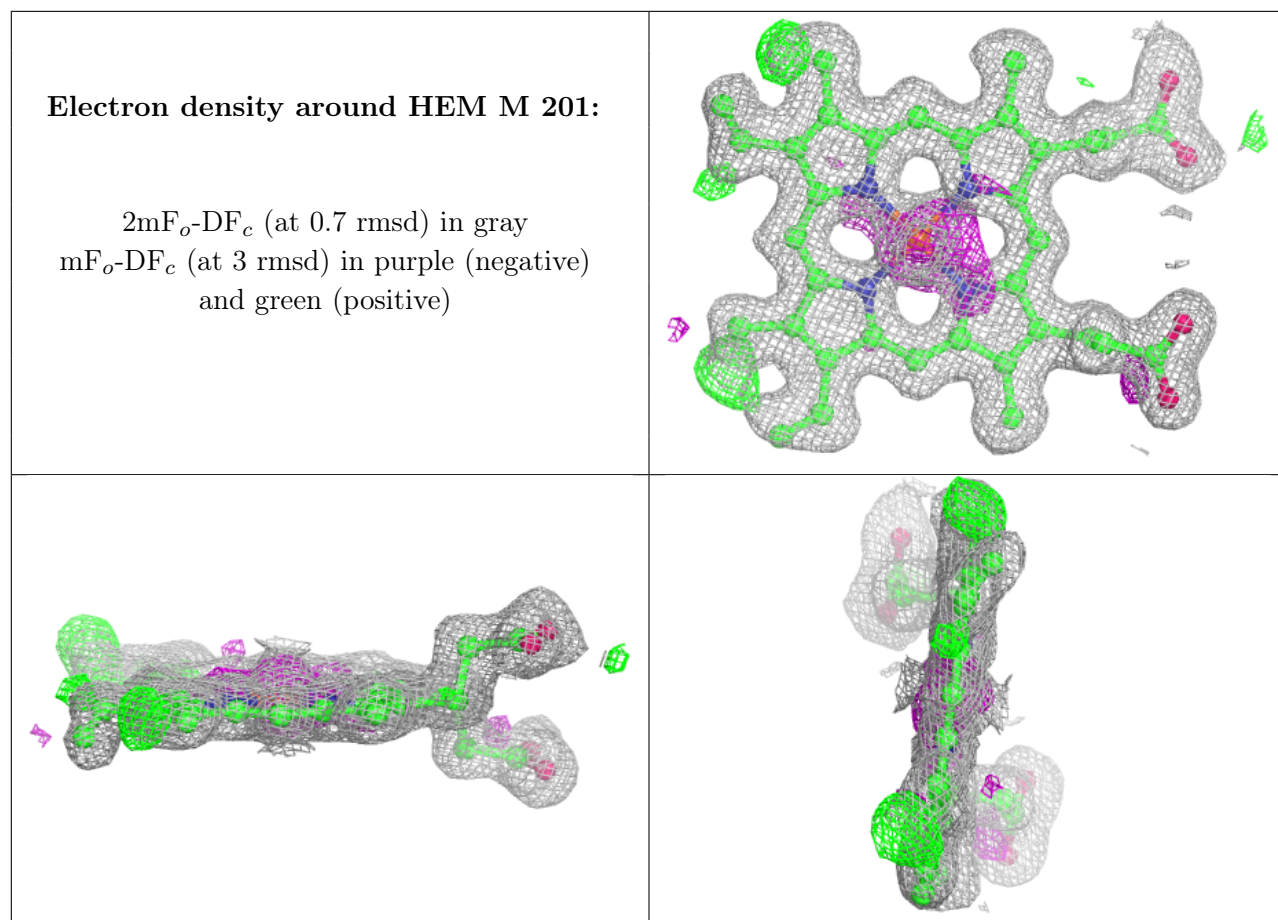
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and green (positive)



**Electron density around HEM K 201:**

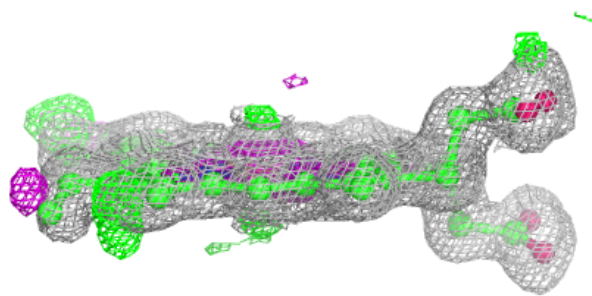
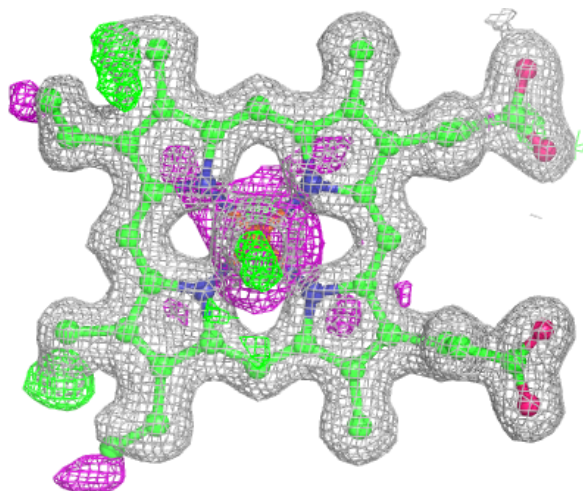
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





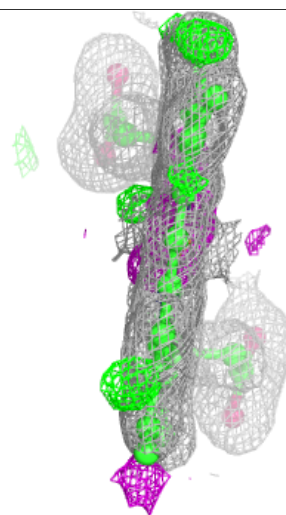
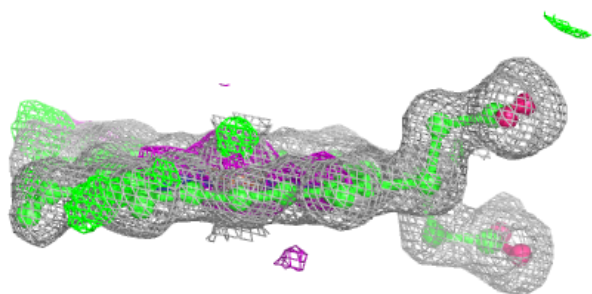
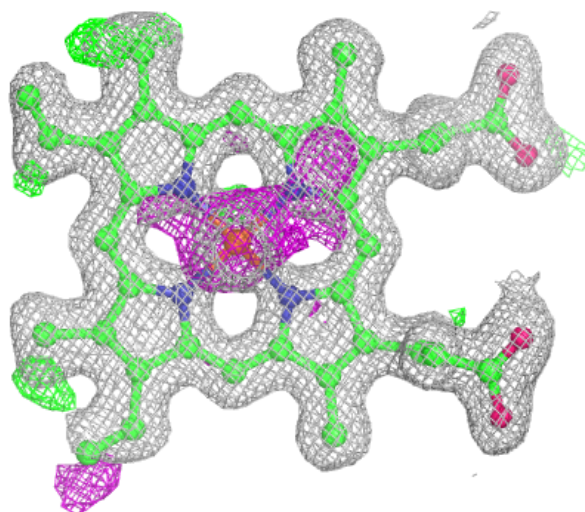
**Electron density around HEM C 202:**

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and green (positive)



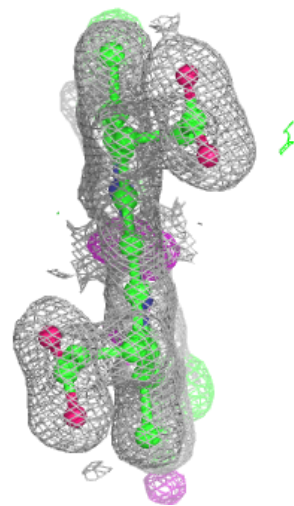
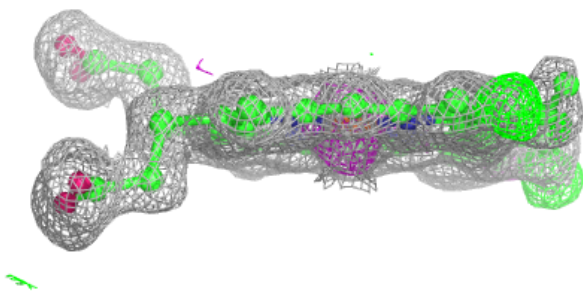
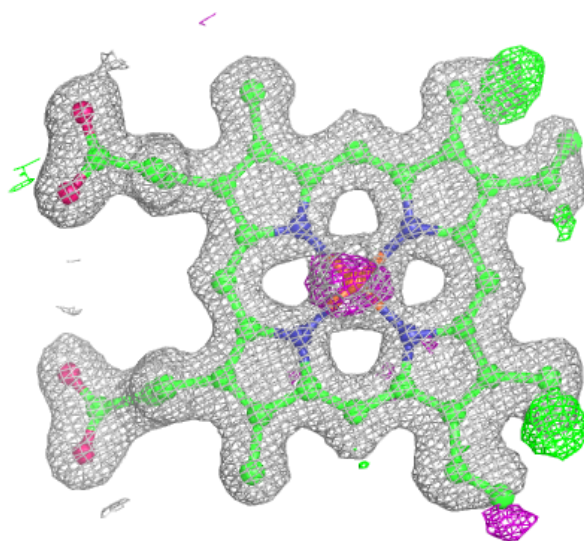
**Electron density around HEM E 201:**

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



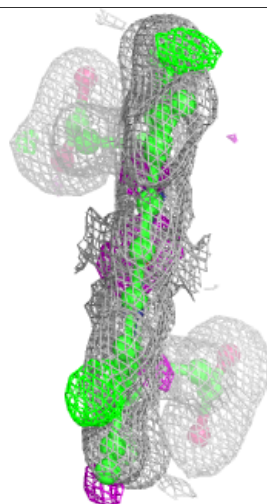
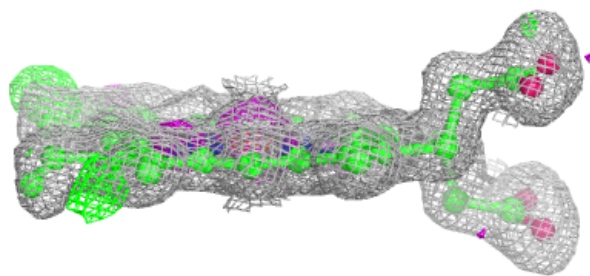
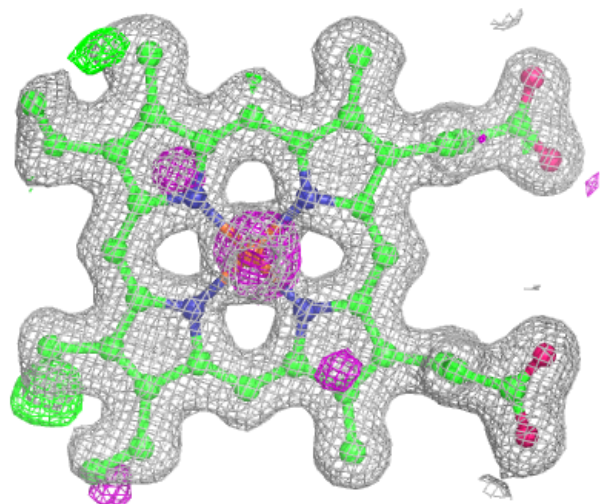
**Electron density around HEM S 204:**

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

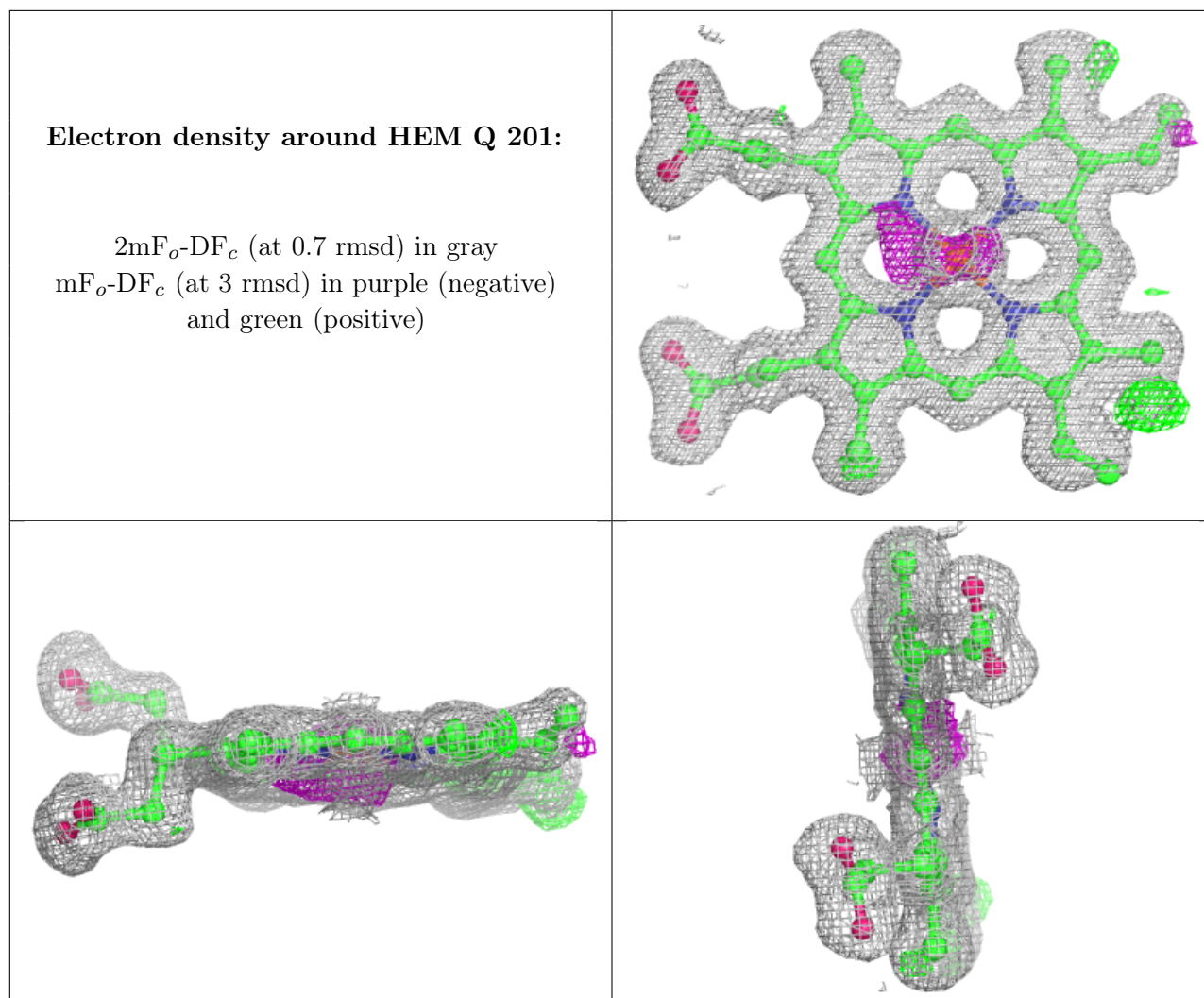


**Electron density around HEM A 201:**

$2mF_o-DF_c$  (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.