



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 11:19 am BST

PDB ID : 2PCC  
Title : CRYSTAL STRUCTURE OF A COMPLEX BETWEEN ELECTRON  
TRANSFER PARTNERS, CYTOCHROME C PEROXIDASE AND CY-  
TOCHROME C  
Authors : Pelletier, H.; Kraut, J.  
Deposited on : 1993-04-14  
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

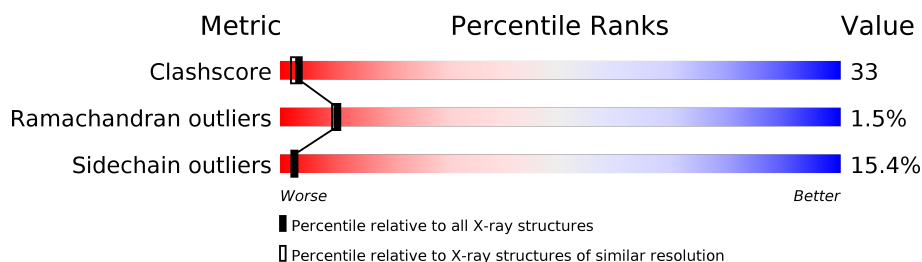
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	296	<div> <div style="width: 44%; background-color: green;"></div> <div style="width: 40%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 3%; background-color: grey;"></div> </div> <div>44% 40% 13% . .</div>
1	C	296	<div> <div style="width: 46%; background-color: green;"></div> <div style="width: 38%; background-color: yellow;"></div> <div style="width: 13%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> <div style="width: 3%; background-color: grey;"></div> </div> <div>46% 38% 13% . .</div>
2	B	108	<div> <div style="width: 39%; background-color: green;"></div> <div style="width: 45%; background-color: yellow;"></div> <div style="width: 15%; background-color: orange;"></div> <div style="width: 1%; background-color: red;"></div> </div> <div>39% 45% 15% .</div>
2	D	108	<div> <div style="width: 32%; background-color: green;"></div> <div style="width: 46%; background-color: yellow;"></div> <div style="width: 19%; background-color: orange;"></div> <div style="width: 3%; background-color: red;"></div> </div> <div>32% 46% 19% .</div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7115 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 CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2371	1514	395	456	6			
1	C	294	Total	C	N	O	S	0	0	0
			2371	1514	395	456	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	CONFLICT	UNP P00431
A	152	GLY	ASP	CONFLICT	UNP P00431
C	53	ILE	THR	CONFLICT	UNP P00431
C	152	GLY	ASP	CONFLICT	UNP P00431

- Molecule 2 is a protein called ISO-1-CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			847	534	151	157	5			
2	D	108	Total	C	N	O	S	0	0	0
			847	534	151	157	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			2	1	1		
3	C	1	Total	O	S	0	0
			2	1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

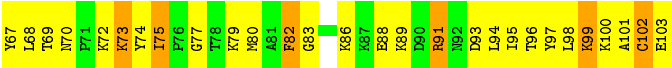
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total 203	O 203	0	0
5	B	46	Total 46	O 46	0	0
5	C	212	Total 212	O 212	0	0
5	D	42	Total 42	O 42	0	0





● Molecule 2: ISO-1-CYTOCHROME C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.40Å 118.60Å 45.10Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 35.89 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 87.4 (35.89-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.10 (at 2.24Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.167 , (Not available) 0.284 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 127.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.095 for -h-l,-k,l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	7115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 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	1.21	0/2438	2.08	74/3302 (2.2%)
1	C	1.18	2/2438 (0.1%)	2.09	97/3302 (2.9%)
2	B	0.93	0/865	1.71	4/1156 (0.3%)
2	D	0.93	0/865	1.73	11/1156 (1.0%)
All	All	1.13	2/6606 (0.0%)	2.00	186/8916 (2.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	3
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	SER	CA-CB	-5.76	1.44	1.52
1	C	181	HIS	CA-CB	5.43	1.65	1.53

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	TYR	CB-CG-CD2	15.44	130.26	121.00
1	A	155	ARG	NE-CZ-NH2	15.05	127.83	120.30
1	A	155	ARG	NE-CZ-NH1	-14.84	112.88	120.30
1	C	146	ASP	CB-CG-OD2	-14.44	105.31	118.30
1	A	130	ARG	NE-CZ-NH2	13.91	127.25	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	143	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	31	ARG	Sidechain
1	C	31	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2371	0	2252	105	1
1	C	2371	0	2252	136	5
2	B	847	0	851	75	1
2	D	847	0	851	103	0
3	A	2	0	0	1	0
3	C	2	0	0	1	0
4	A	43	0	30	0	0
4	B	43	0	30	16	0
4	C	43	0	30	4	0
4	D	43	0	30	19	0
5	A	203	0	0	12	4
5	B	46	0	0	5	0
5	C	212	0	0	23	1
5	D	42	0	0	11	0
All	All	7115	0	6326	423	6

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 33.

The worst 5 of 423 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)
2:B:14:CYS:SG	4:B:104:HEM:CAB	2.29	1.20
1:C:74:LYS:HE3	1:C:78:ASN:HD21	1.14	1.13

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:CYS:SG	4:B:104:HEM:CAC	2.39	1.10
2:B:8:THR:HA	2:B:11:LYS:HD2	1.34	1.08
2:D:17:CYS:SG	4:D:104:HEM:CAC	2.43	1.06

The worst 5 of 6 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)
1:C:221:GLU:OE2	5:A:549:HOH:O[1_656]	1.11	1.09
1:C:221:GLU:CD	5:A:549:HOH:O[1_656]	1.12	1.08
1:C:221:GLU:CG	5:A:549:HOH:O[1_656]	1.91	0.29
1:A:240:GLN:NE2	5:C:635:HOH:O[1_455]	2.15	0.05
2:B:54:LYS:CE	1:C:253:ASN:ND2[2_646]	2.15	0.05

## 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	292/296 (99%)	264 (90%)	27 (9%)	1 (0%)	41	50
1	C	292/296 (99%)	272 (93%)	19 (6%)	1 (0%)	41	50
2	B	106/108 (98%)	91 (86%)	9 (8%)	6 (6%)	1	1
2	D	106/108 (98%)	89 (84%)	13 (12%)	4 (4%)	3	1
All	All	796/808 (98%)	716 (90%)	68 (8%)	12 (2%)	10	10

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	-2	LYS
2	B	-1	ALA
2	B	56	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	2	THR
2	D	61	GLU

### 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	252/254 (99%)	221 (88%)	31 (12%)	4	5
1	C	252/254 (99%)	214 (85%)	38 (15%)	3	2
2	B	89/89 (100%)	73 (82%)	16 (18%)	1	1
2	D	89/89 (100%)	69 (78%)	20 (22%)	1	0
All	All	682/686 (99%)	577 (85%)	105 (15%)	2	2

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2	THR
1	C	97	LYS
2	D	63	ASN
1	C	5	VAL
1	C	47	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	20	GLN
1	C	62	ASN
2	D	26	HIS
1	C	24	ASN
1	C	38	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	HEM	A	296	1,3	27,50,50	2.32	9 (33%)	17,82,82	2.34	8 (47%)
3	SO4	A	299	4	0,1,4	0.00	-	-		
4	HEM	B	104	2	27,50,50	2.11	7 (25%)	17,82,82	1.96	7 (41%)
3	SO4	C	300	4	0,1,4	0.00	-	-		
4	HEM	D	104	2	27,50,50	1.85	5 (18%)	17,82,82	1.46	4 (23%)
4	HEM	C	296	1,3	27,50,50	1.85	6 (22%)	17,82,82	2.22	7 (41%)

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
4	HEM	D	104	2	-	0/6/54/54	-
4	HEM	A	296	1,3	-	0/6/54/54	-
4	HEM	B	104	2	-	0/6/54/54	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	C	296	1,3	-	0/6/54/54	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	296	HEM	C3B-C2B	-7.21	1.30	1.40
4	C	296	HEM	C3B-C2B	-5.96	1.32	1.40
4	B	104	HEM	C3C-C2C	-5.95	1.32	1.40
4	B	104	HEM	C3B-C2B	-4.34	1.34	1.40
4	B	104	HEM	C3C-CAC	4.19	1.56	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	296	HEM	CMD-C2D-C1D	-4.59	121.41	128.46
4	C	296	HEM	CMA-C3A-C4A	-4.22	121.98	128.46
4	A	296	HEM	CMA-C3A-C4A	-4.04	122.25	128.46
4	C	296	HEM	CMD-C2D-C1D	-3.85	122.55	128.46
4	A	296	HEM	CMD-C2D-C3D	3.67	131.85	124.94

There are no chirality outliers.

There are no torsion outliers.

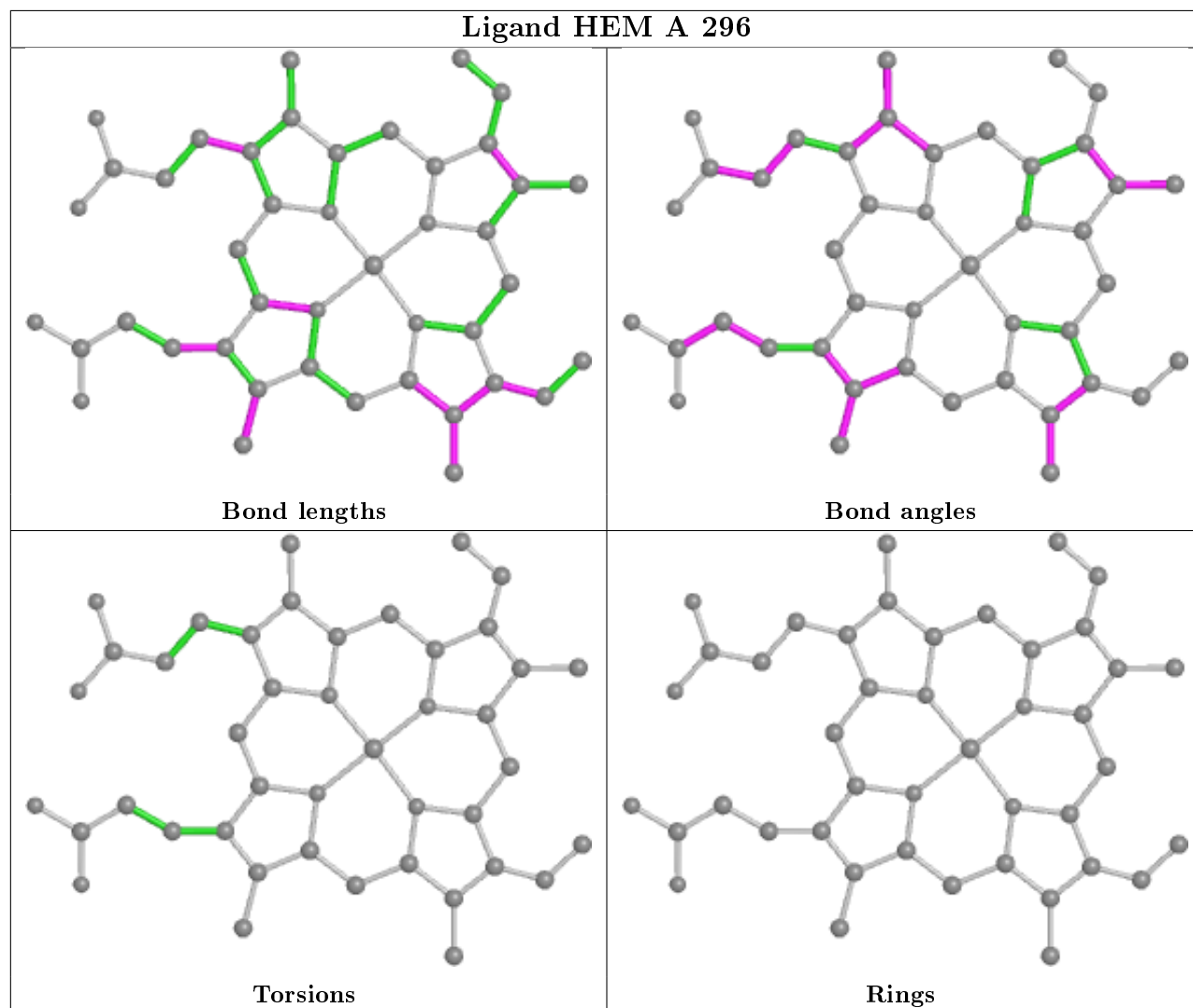
There are no ring outliers.

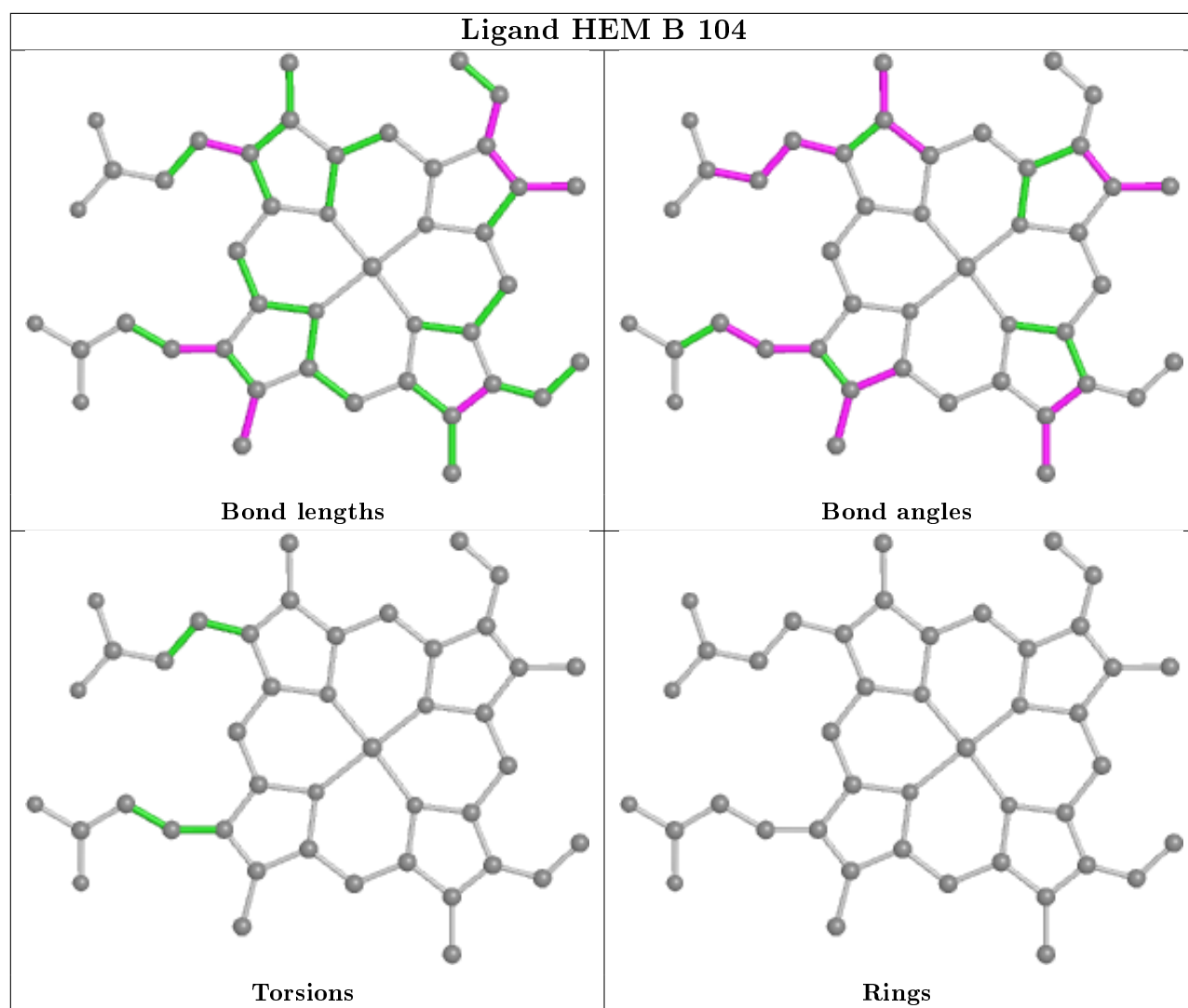
5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	299	SO4	1	0
4	B	104	HEM	16	0
3	C	300	SO4	1	0
4	D	104	HEM	19	0
4	C	296	HEM	4	0

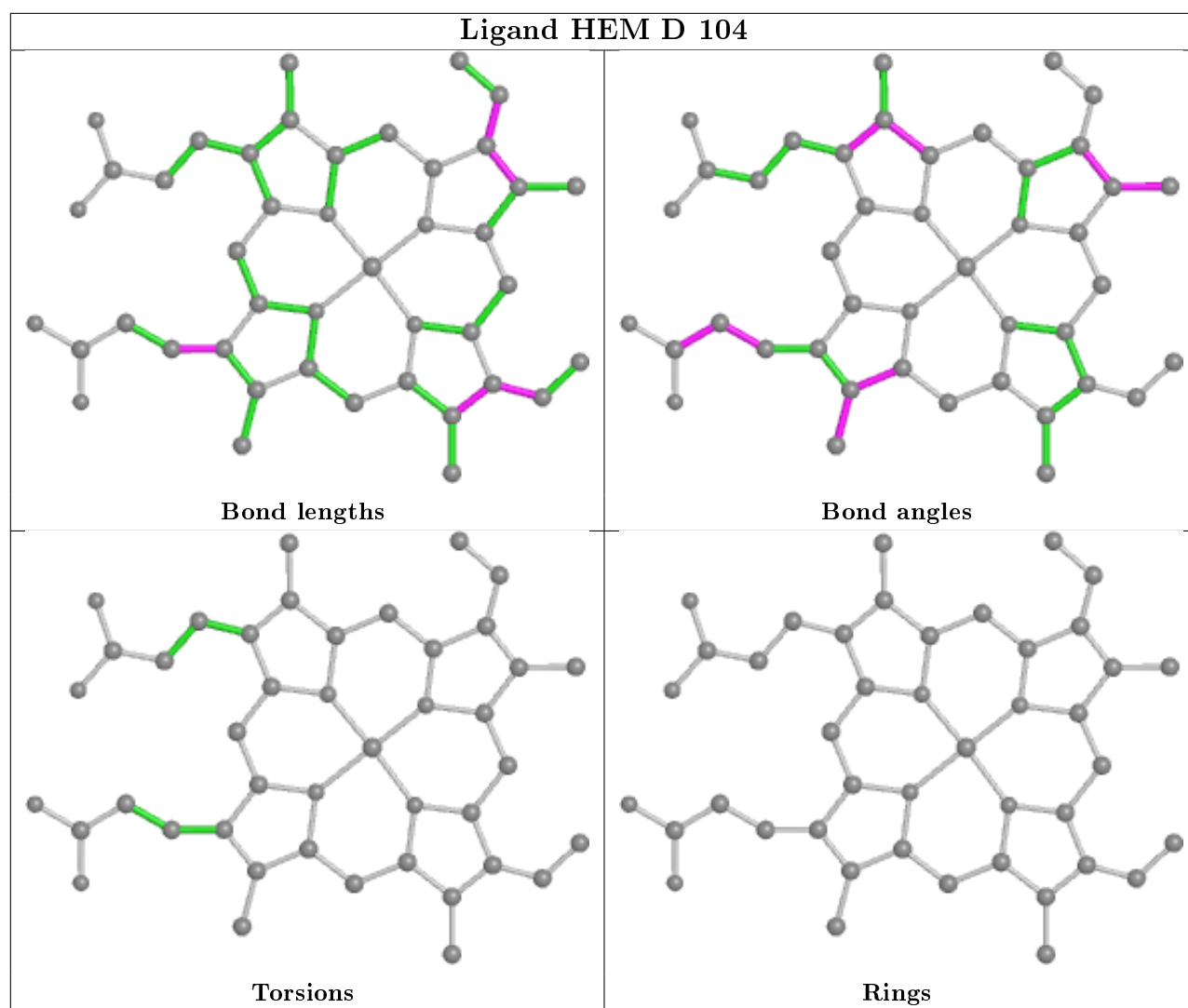
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

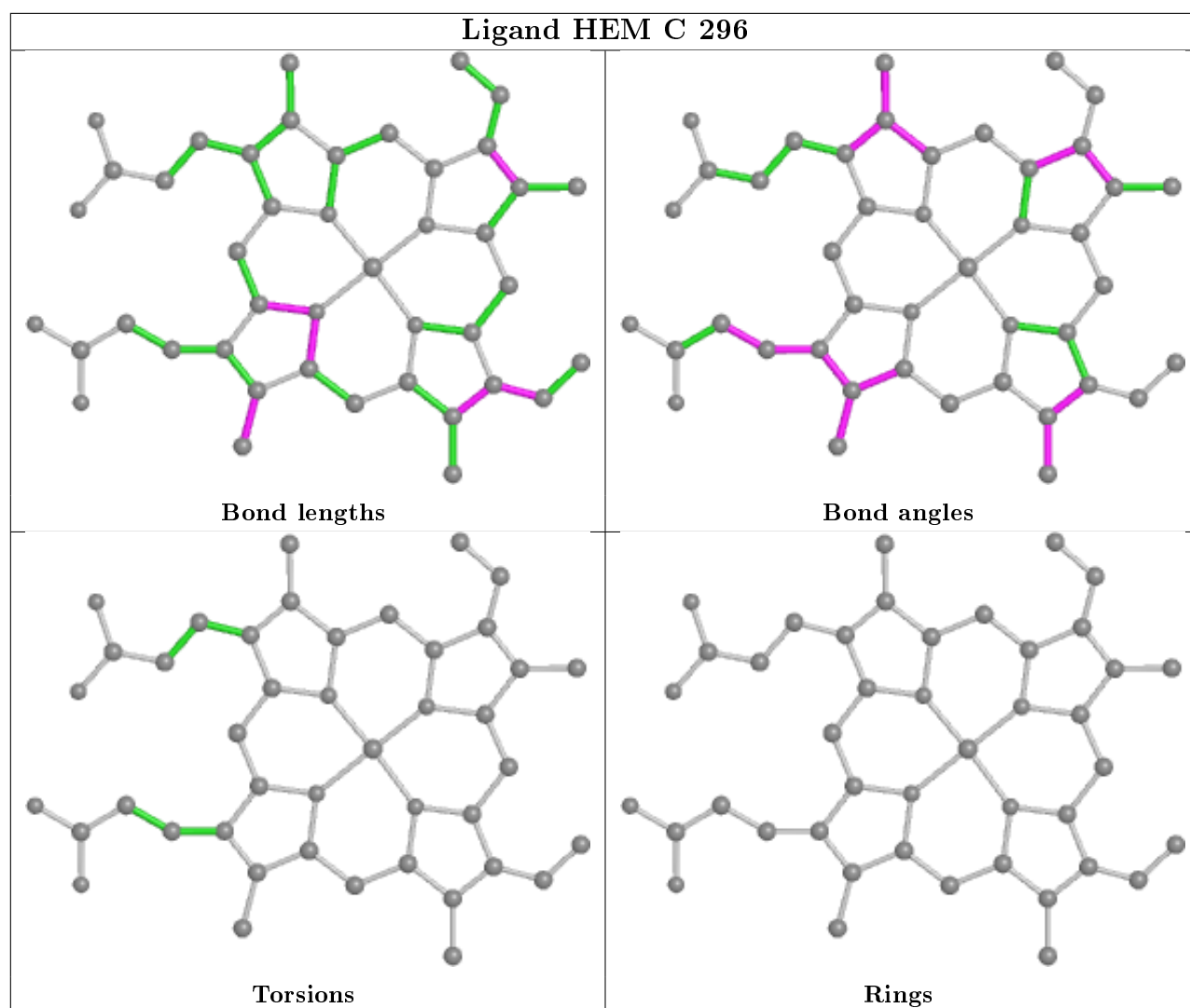
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

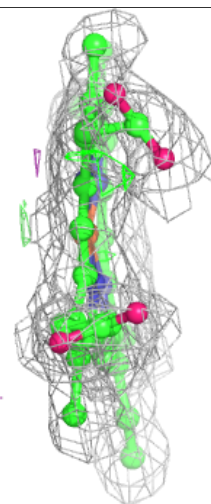
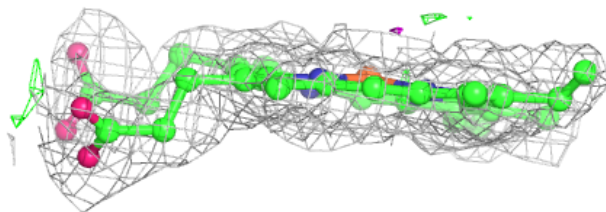
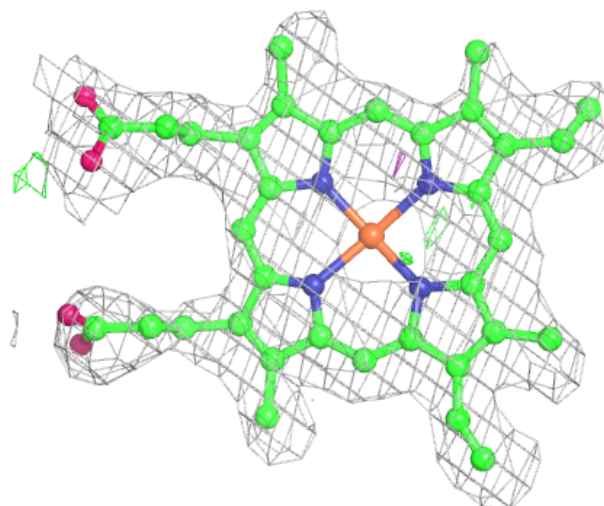
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

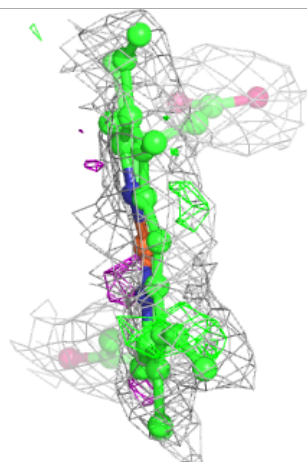
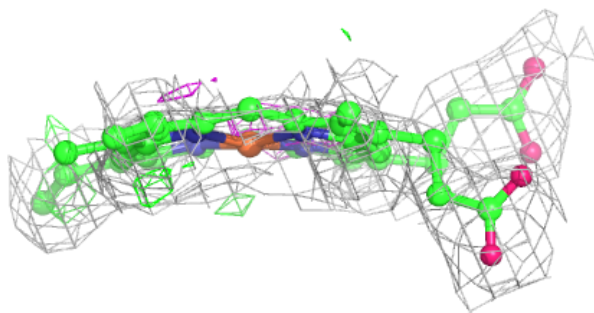
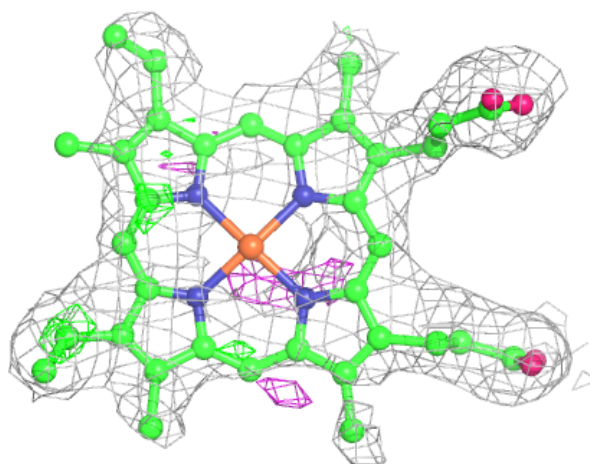
**Electron density around HEM A 296:**

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



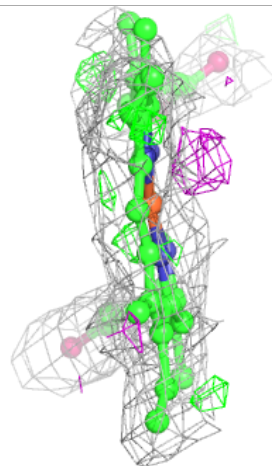
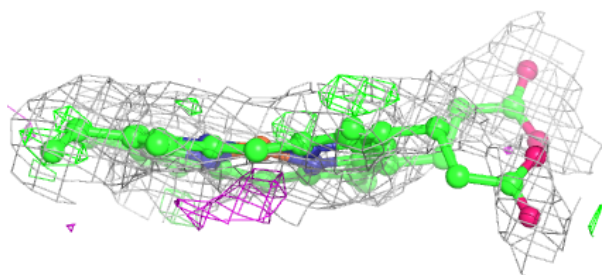
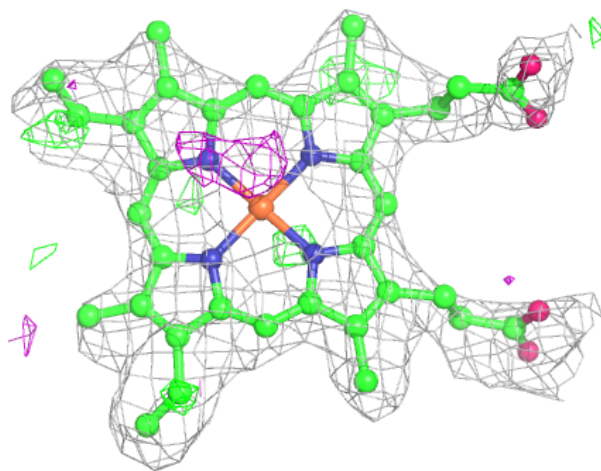
**Electron density around HEM B 104:**

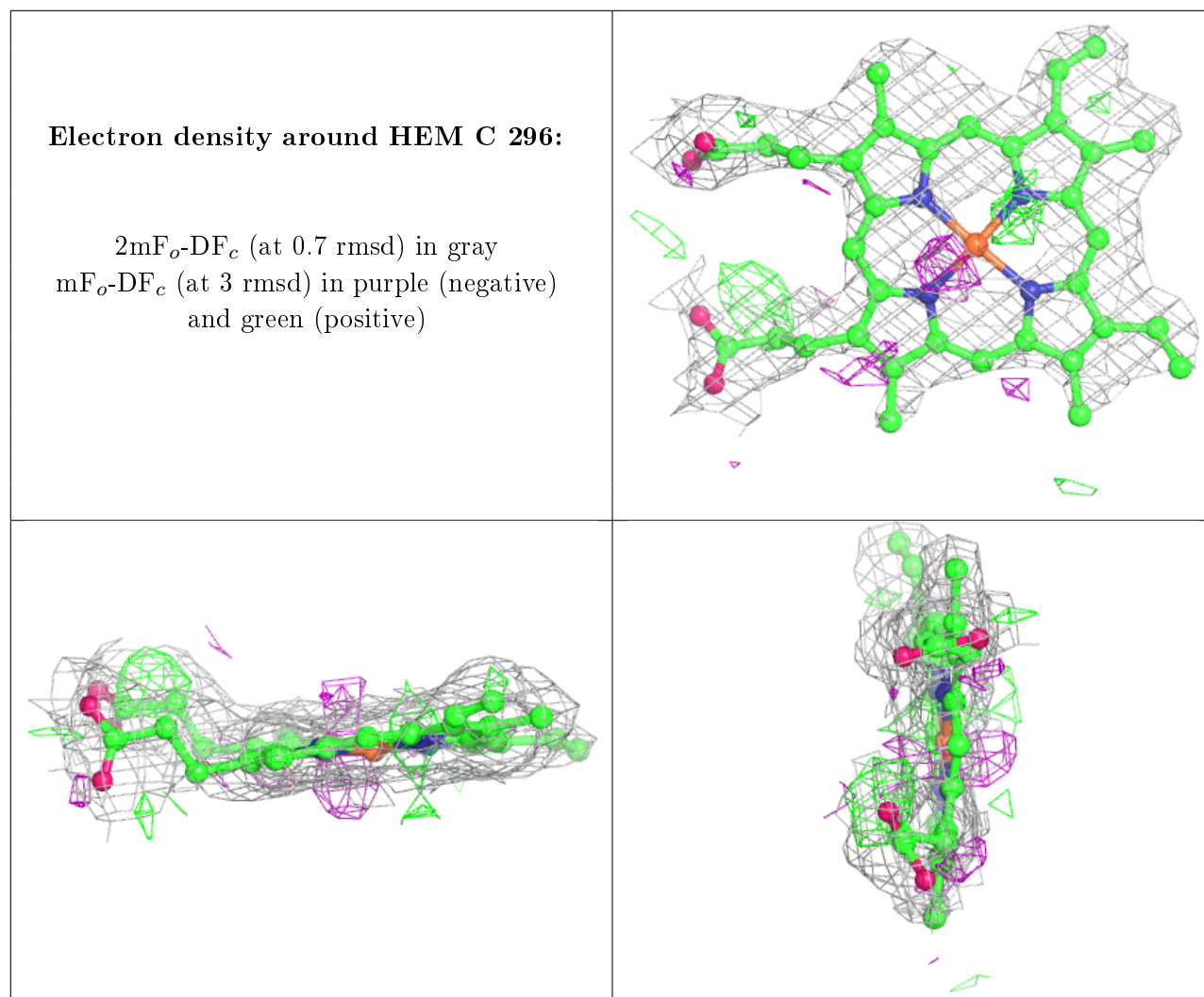
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM D 104:**

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





## 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.