



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 7, 2025 – 10:17 am BST

PDB ID : 9EWJ / pdb\_00009ewj  
Title : Dye-decolourising peroxidase DtpB (224 kGy)  
Authors : Lucic, M.; Worrall, J.A.R.; Hough, M.A.; Owen, R.L.; Strange, R.W.  
Deposited on : 2024-04-03  
Resolution : 1.92 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

<http://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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

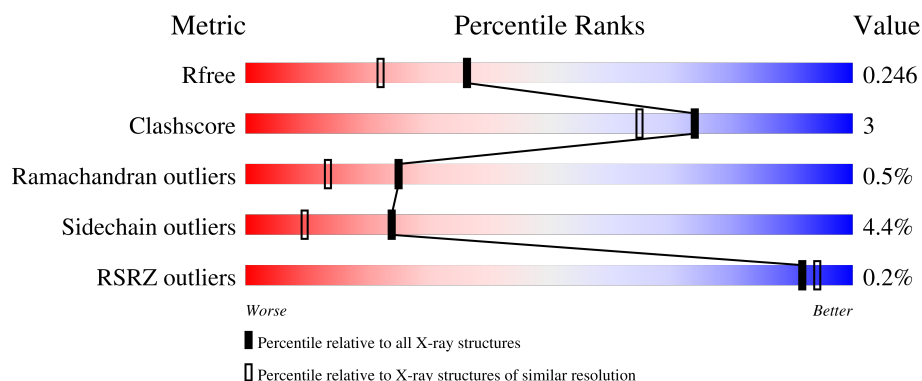
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	312	<div> <div>87%</div> <div>8%</div> <div>...</div> </div>
1	B	312	<div> <div>86%</div> <div>8%</div> <div>...</div> </div>
1	C	312	<div> <div>83%</div> <div>12%</div> <div>...</div> </div>
1	D	312	<div> <div>82%</div> <div>11%</div> <div>...</div> </div>
1	E	312	<div> <div>84%</div> <div>11%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	312	<div><div></div><div>82%</div><div>12%</div><div></div><div></div></div>

## 2 Entry composition [i](#)

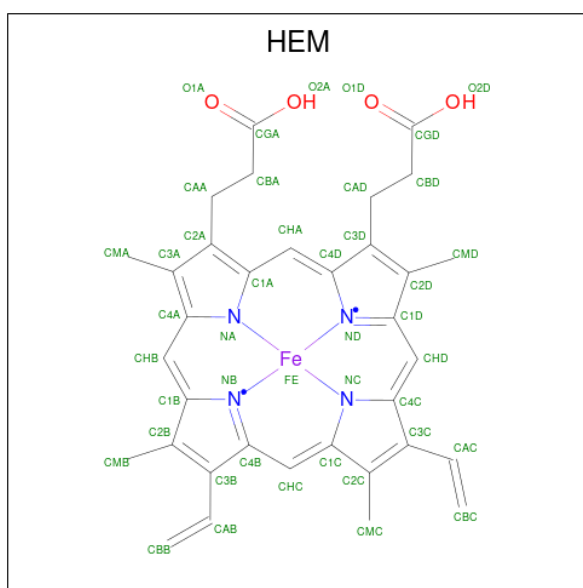
There are 6 unique types of molecules in this entry. The entry contains 14342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2313	1458	396	450	9			
1	B	305	Total	C	N	O	S	0	0	0
			2291	1447	389	446	9			
1	C	306	Total	C	N	O	S	0	0	0
			2311	1459	397	446	9			
1	D	306	Total	C	N	O	S	0	0	0
			2301	1452	396	444	9			
1	E	306	Total	C	N	O	S	0	0	0
			2305	1456	396	444	9			
1	F	306	Total	C	N	O	S	0	0	0
			2303	1454	392	448	9			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



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

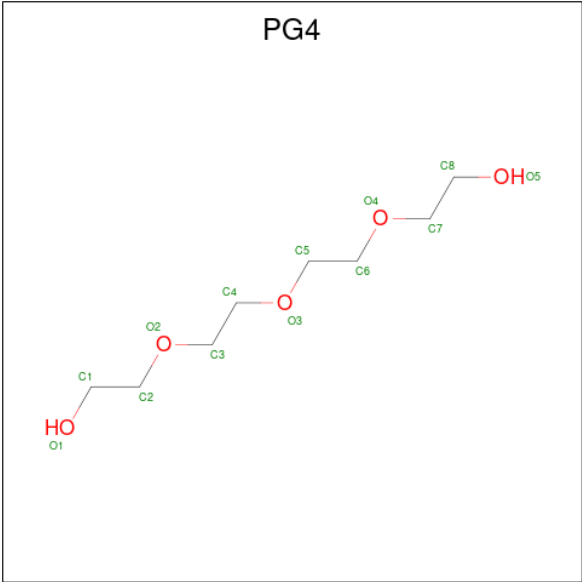
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	8	5		

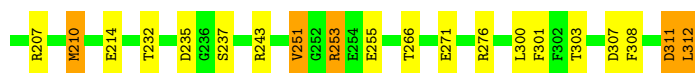
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total	O	0	0
			58	58		
6	B	29	Total	O	0	0
			29	29		
6	C	41	Total	O	0	0
			41	41		
6	D	49	Total	O	0	0
			49	49		
6	E	30	Total	O	0	0
			30	30		
6	F	36	Total	O	0	0
			36	36		

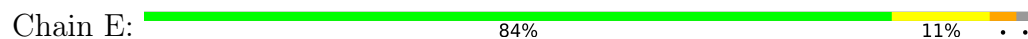


- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup

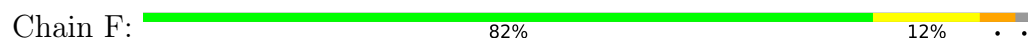




- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup



- Molecule 1: Putative dye-decolorizing peroxidase (DyP), encapsulated subgroup





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.85Å 121.90Å 199.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.11 – 1.92 40.11 – 1.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.11-1.92) 100.0 (40.11-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.208 , 0.245 0.213 , 0.246	Depositor DCC
$R_{free}$ test set	8044 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 26.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14342	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 2.79% 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: MG, PG4, HEM, O

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	0.86	3/2363 (0.1%)	1.35	31/3210 (1.0%)
1	B	0.75	1/2341 (0.0%)	1.27	21/3183 (0.7%)
1	C	0.87	4/2361 (0.2%)	1.33	28/3209 (0.9%)
1	D	0.86	4/2351 (0.2%)	1.37	32/3196 (1.0%)
1	E	0.79	2/2355 (0.1%)	1.29	24/3202 (0.7%)
1	F	0.78	3/2353 (0.1%)	1.35	31/3200 (1.0%)
All	All	0.82	17/14124 (0.1%)	1.33	167/19200 (0.9%)

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	7
1	B	0	5
1	C	0	8
1	D	0	7
1	E	0	8
1	F	0	7
All	All	0	42

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	GLU	CD-OE1	9.30	1.35	1.25
1	C	199	GLU	CD-OE2	9.12	1.35	1.25
1	D	199	GLU	CD-OE2	8.60	1.35	1.25
1	E	199	GLU	CD-OE1	7.49	1.33	1.25
1	A	47	GLU	CD-OE1	-6.28	1.18	1.25

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	ARG	NE-CZ-NH2	12.93	126.77	120.30
1	E	87	ARG	CG-CD-NE	-11.22	88.23	111.80
1	D	276	ARG	NE-CZ-NH1	-10.55	115.02	120.30
1	A	125	ARG	NE-CZ-NH2	9.92	125.26	120.30
1	A	232	THR	CA-CB-OG1	-9.91	88.18	109.00

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	A	127	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	37	ARG	Sidechain
1	A	95	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	2313	0	2235	17	0
1	B	2291	0	2201	14	0
1	C	2311	0	2232	17	0
1	D	2301	0	2216	19	0
1	E	2305	0	2224	15	0
1	F	2303	0	2214	9	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
2	E	43	0	30	2	0
2	F	43	0	30	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	13	0	18	1	0
6	A	58	0	0	1	0
6	B	29	0	0	0	0
6	C	41	0	0	1	0
6	D	49	0	0	0	0
6	E	30	0	0	1	0
6	F	36	0	0	2	0
All	All	14342	0	13520	82	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 3.

The worst 5 of 82 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:F:125:ARG:HD3	6:F:522:HOH:O	1.72	0.90
1:D:53:ARG:HG2	1:D:53:ARG:HH11	1.45	0.81
1:A:210:MET:HE1	1:D:210:MET:HB2	1.66	0.77
1:B:53:ARG:HG2	1:B:53:ARG:NH1	1.99	0.77
1:A:53:ARG:HH11	1:A:53:ARG:HG2	1.49	0.76

There are no symmetry-related clashes.

## 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	303/312 (97%)	296 (98%)	5 (2%)	2 (1%)	19 9
1	B	303/312 (97%)	294 (97%)	8 (3%)	1 (0%)	37 26
1	C	304/312 (97%)	293 (96%)	9 (3%)	2 (1%)	19 9
1	D	304/312 (97%)	297 (98%)	6 (2%)	1 (0%)	37 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	304/312 (97%)	298 (98%)	5 (2%)	1 (0%)	37	26
1	F	304/312 (97%)	295 (97%)	6 (2%)	3 (1%)	13	4
All	All	1822/1872 (97%)	1773 (97%)	39 (2%)	10 (0%)	25	13

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	PHE
1	C	142	PHE
1	F	235	ASP
1	D	16	PRO
1	B	16	PRO

### 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	240/249 (96%)	233 (97%)	7 (3%)	37	20
1	B	235/249 (94%)	225 (96%)	10 (4%)	25	10
1	C	238/249 (96%)	229 (96%)	9 (4%)	28	13
1	D	236/249 (95%)	220 (93%)	16 (7%)	13	3
1	E	237/249 (95%)	228 (96%)	9 (4%)	28	13
1	F	237/249 (95%)	226 (95%)	11 (5%)	23	9
All	All	1423/1494 (95%)	1361 (96%)	62 (4%)	24	10

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	19	SER
1	F	111	ARG
1	D	210	MET
1	F	92	PRO
1	F	234	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\# Z  > 2$
2	HEM	D	401	4,1	41,50,50	1.85	13 (31%)	45,82,82	3.42	22 (48%)
2	HEM	A	401	4,1	41,50,50	1.80	13 (31%)	45,82,82	2.24	16 (35%)
5	PG4	D	403	-	12,12,12	0.89	0	11,11,11	0.76	0
2	HEM	C	401	6,1	41,50,50	1.63	7 (17%)	45,82,82	2.90	20 (44%)
2	HEM	E	401	6,1	41,50,50	1.65	10 (24%)	45,82,82	2.61	23 (51%)
2	HEM	F	401	6,1	41,50,50	1.77	8 (19%)	45,82,82	2.48	19 (42%)
2	HEM	B	501	1	41,50,50	1.59	7 (17%)	45,82,82	2.26	21 (46%)

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
2	HEM	D	401	4,1	-	4/12/54/54	-
2	HEM	A	401	4,1	-	5/12/54/54	-
5	PG4	D	403	-	-	7/10/10/10	-
2	HEM	C	401	6,1	-	5/12/54/54	-
2	HEM	E	401	6,1	-	6/12/54/54	-
2	HEM	F	401	6,1	-	4/12/54/54	-
2	HEM	B	501	1	-	7/12/54/54	-

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1B-NB	-4.94	1.31	1.40
2	C	401	HEM	CHA-C4D	4.76	1.47	1.35
2	A	401	HEM	C4D-ND	-4.63	1.32	1.40
2	F	401	HEM	C4D-C3D	4.52	1.52	1.45
2	F	401	HEM	C3C-C2C	-4.36	1.34	1.40

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	HEM	O2D-CGD-CBD	11.07	149.59	114.03
2	D	401	HEM	O1D-CGD-CBD	-10.65	88.87	123.08
2	C	401	HEM	CHC-C4B-NB	9.33	134.57	124.43
2	A	401	HEM	C1B-NB-C4B	7.09	112.40	105.07
2	B	501	HEM	O2D-CGD-CBD	6.07	133.55	114.03

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	HEM	C2A-CAA-CBA-CGA
5	D	403	PG4	O3-C5-C6-O4
2	A	401	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C2B-C3B-CAB-CBB
2	E	401	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

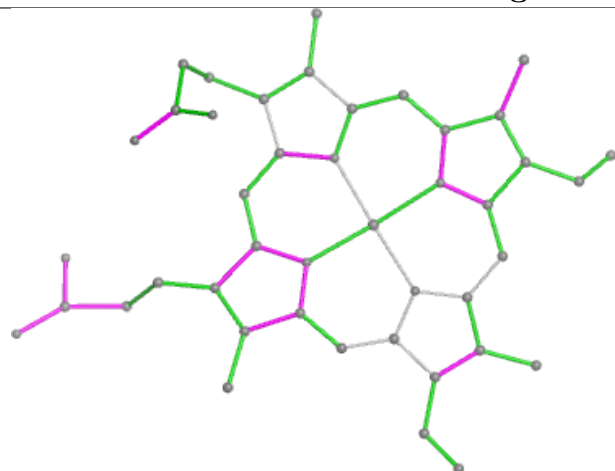
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	1	0
5	D	403	PG4	1	0
2	E	401	HEM	2	0
2	B	501	HEM	1	0

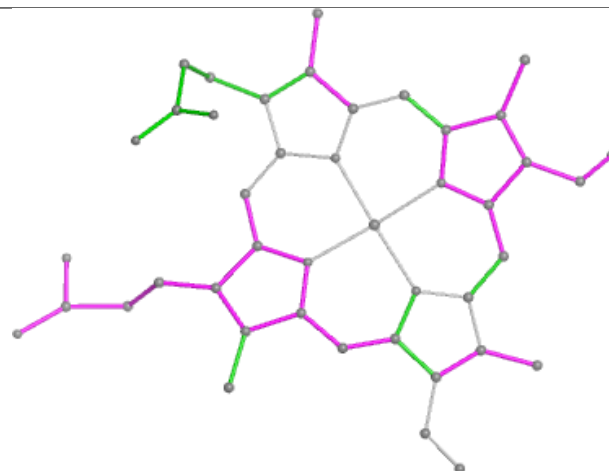
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



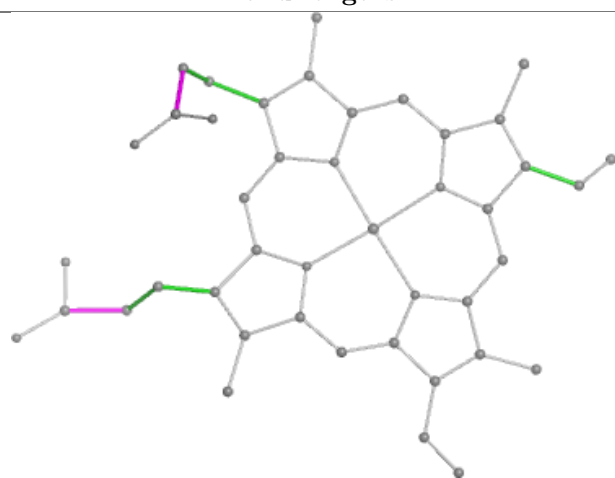
## Ligand HEM D 401



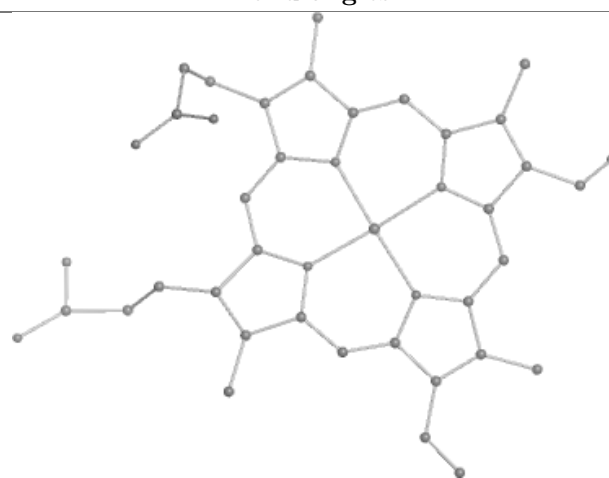
Bond lengths



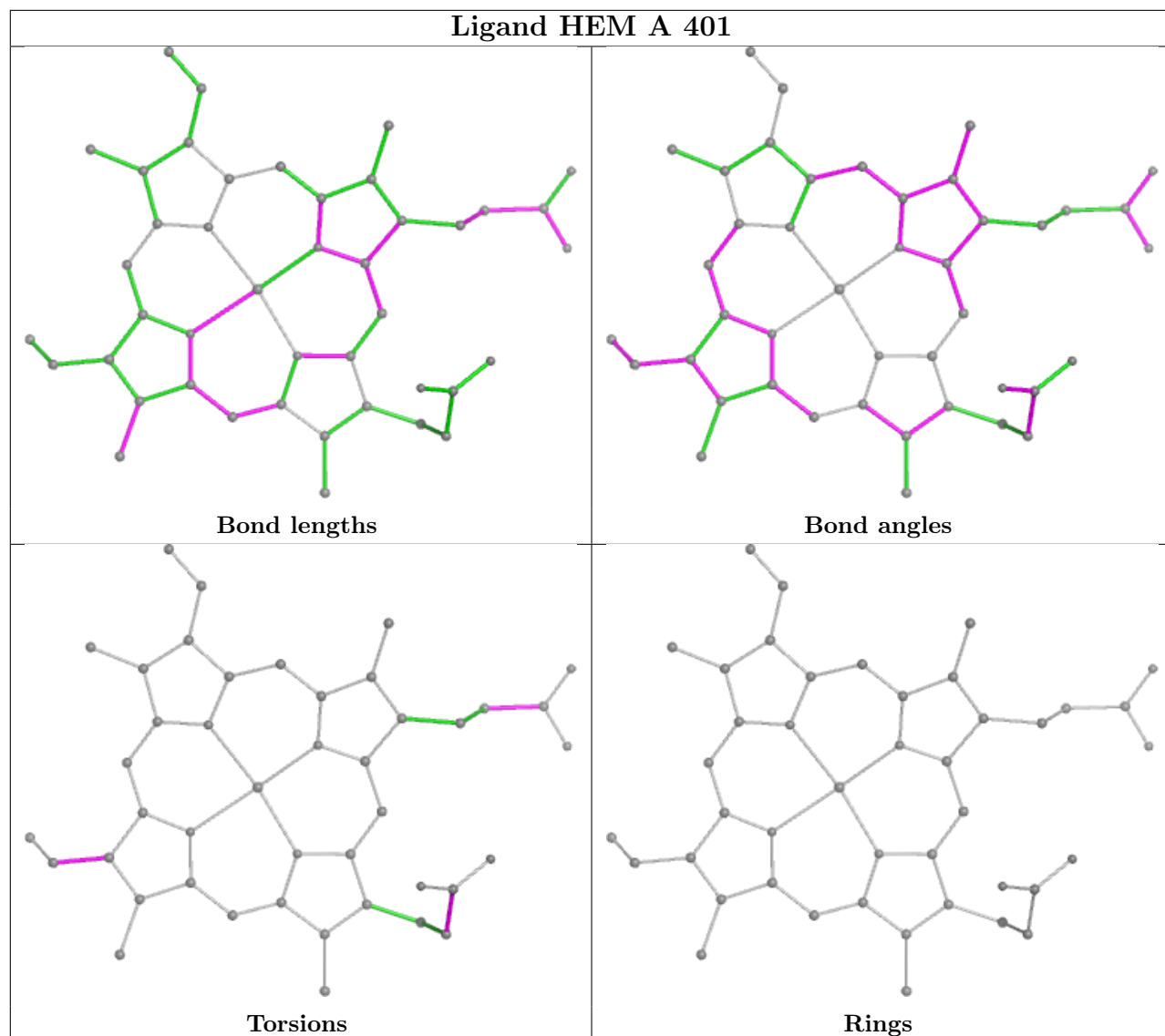
Bond angles

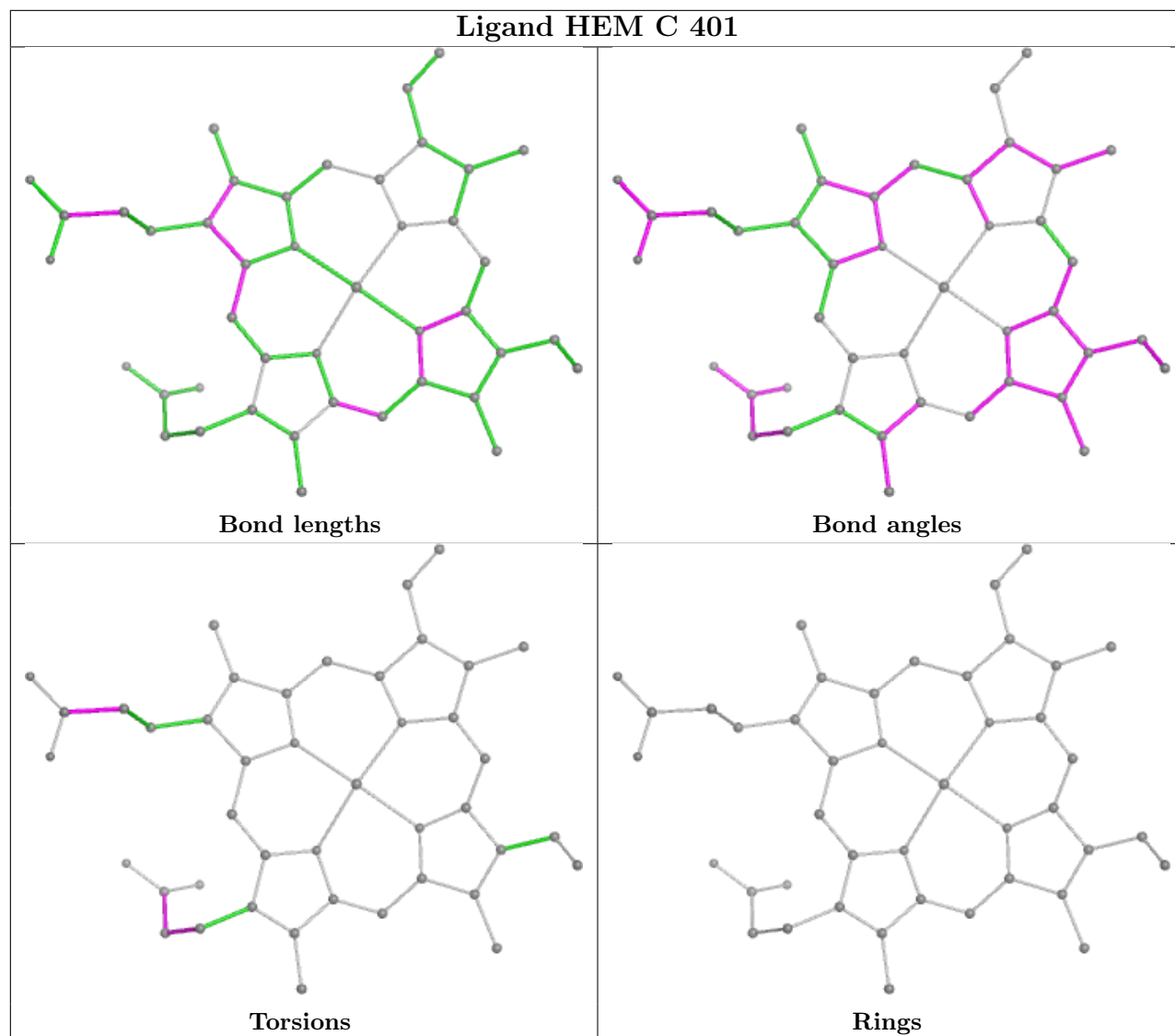


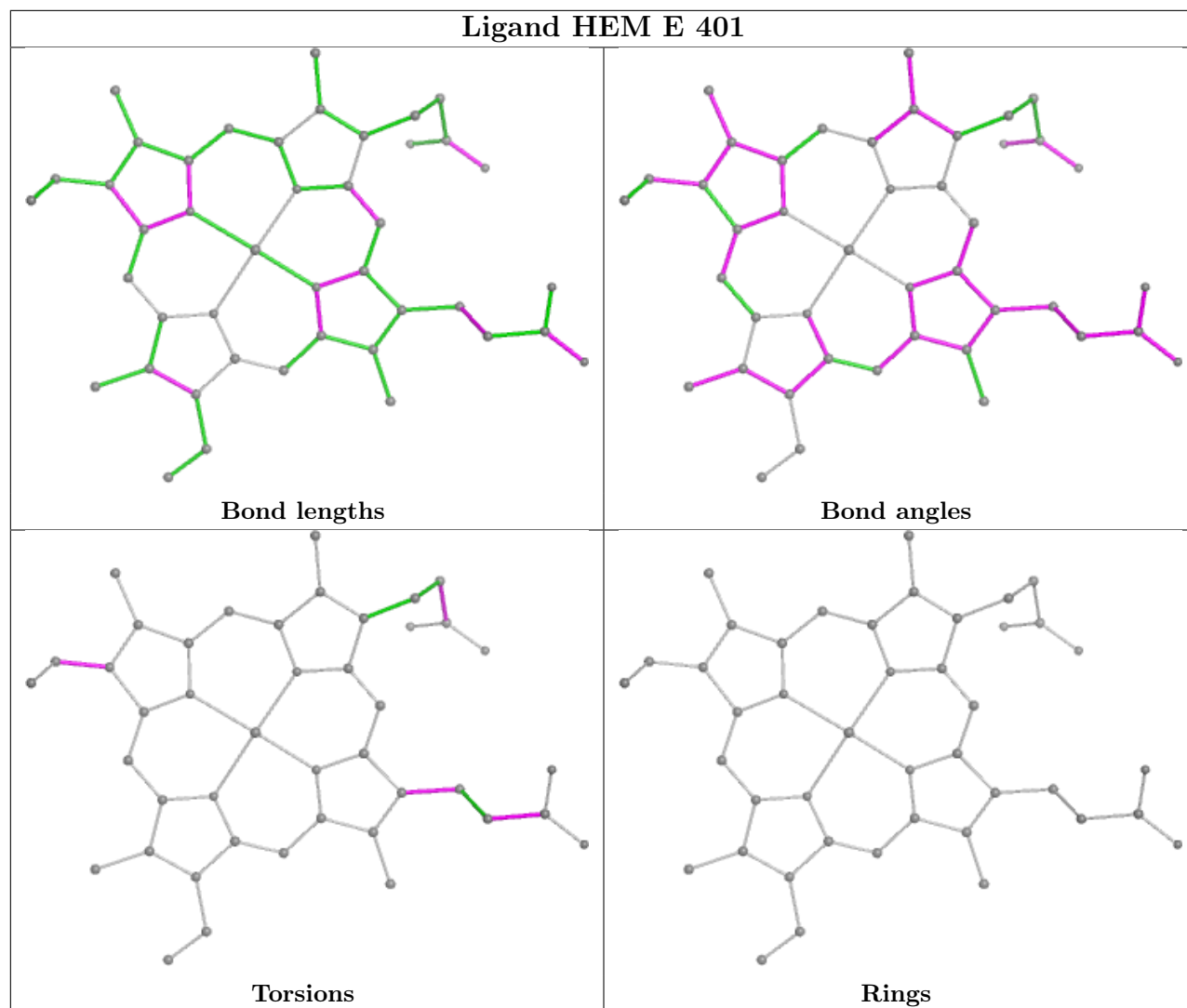
Torsions

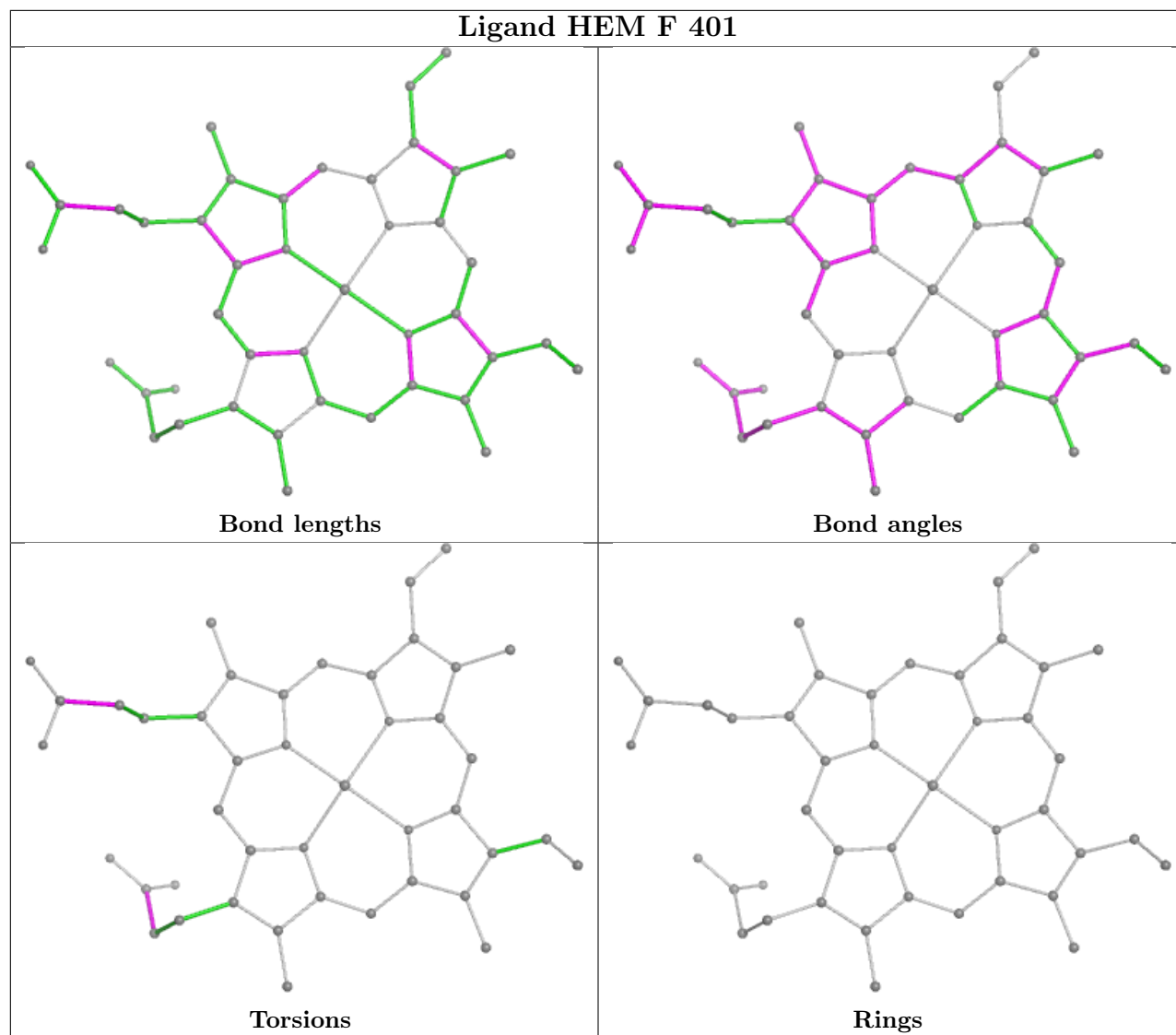


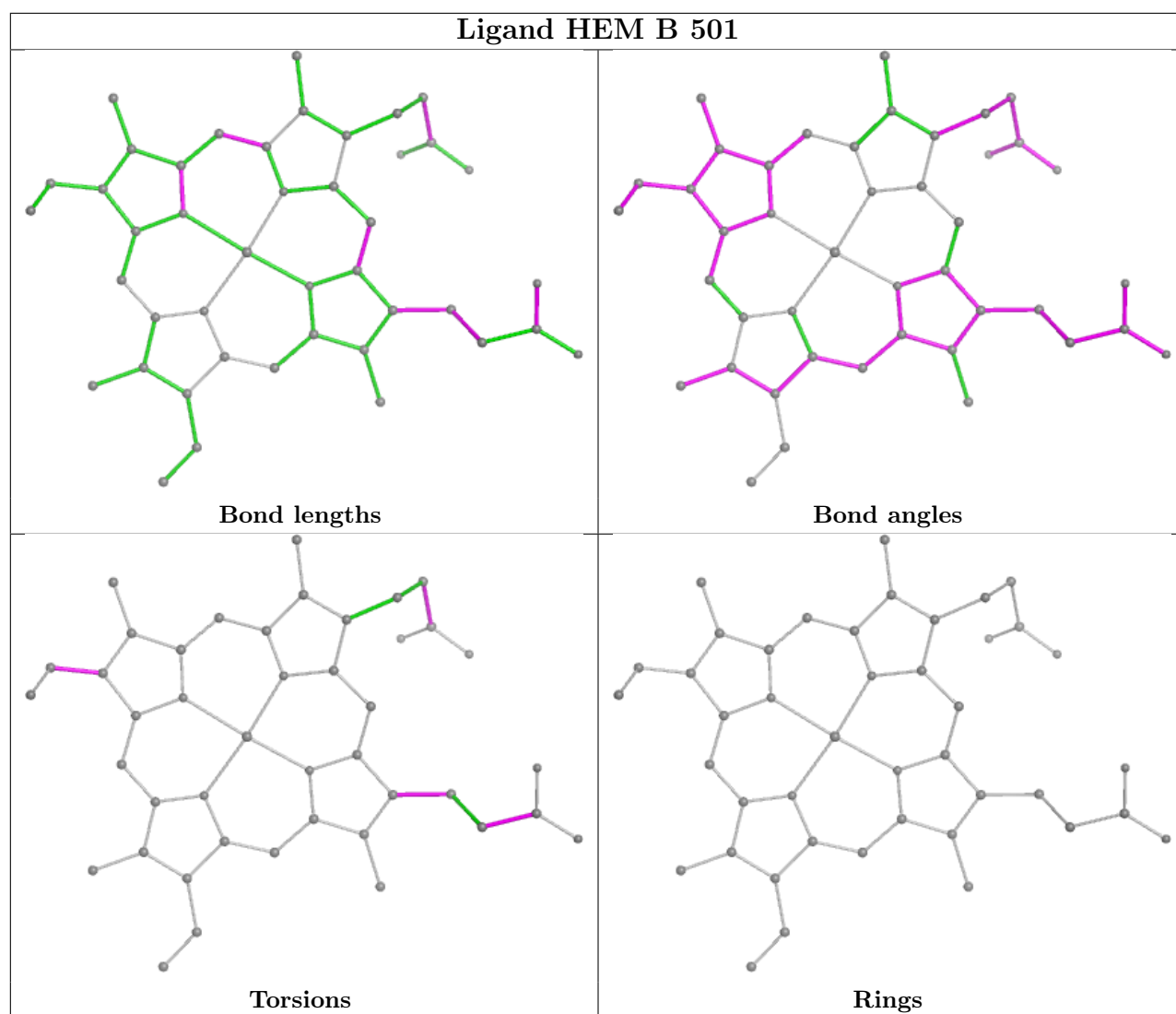
Rings











## 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	305/312 (97%)	-0.83	1 (0%) 90 93	19, 27, 54, 76	0
1	B	305/312 (97%)	-0.67	0 100 100	23, 33, 60, 91	0
1	C	306/312 (98%)	-0.75	1 (0%) 90 93	18, 30, 62, 97	0
1	D	306/312 (98%)	-0.78	1 (0%) 90 93	18, 28, 58, 98	0
1	E	306/312 (98%)	-0.71	0 100 100	20, 30, 62, 111	0
1	F	306/312 (98%)	-0.74	1 (0%) 90 93	19, 30, 60, 104	0
All	All	1834/1872 (97%)	-0.75	4 (0%) 92 94	18, 30, 61, 111	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	142	PHE	5.0
1	D	142	PHE	2.5
1	A	312	LEU	2.2
1	C	312	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

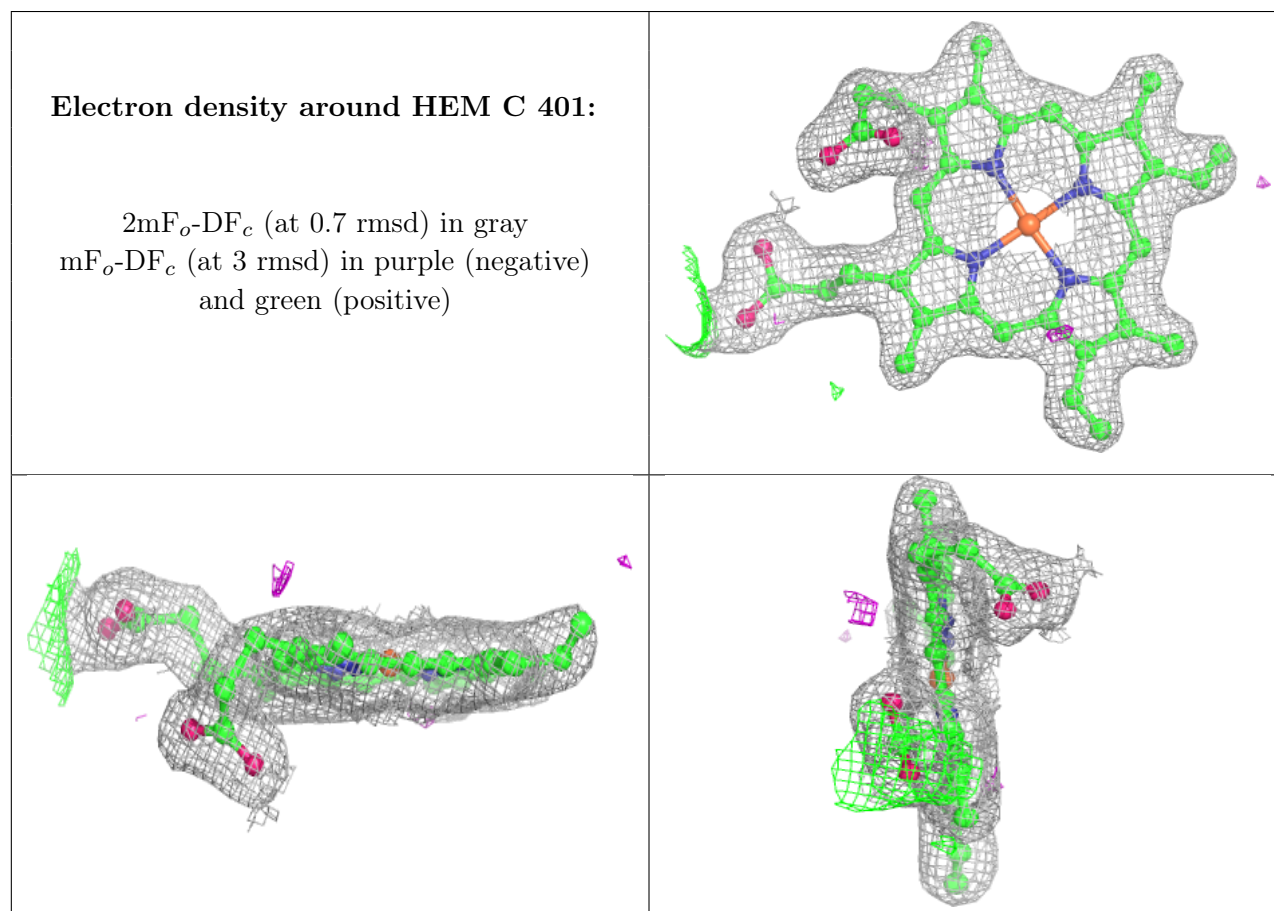
### 6.4 Ligands [i](#)

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
5	PG4	D	403	13/13	0.83	0.14	46,62,84,85	0
3	MG	D	402	1/1	0.96	0.05	47,47,47,47	0
2	HEM	C	401	43/43	0.99	0.05	22,28,32,40	0
2	HEM	D	401	43/43	0.99	0.04	15,20,25,37	0
2	HEM	E	401	43/43	0.99	0.04	20,25,30,39	0
2	HEM	F	401	43/43	0.99	0.04	20,24,30,41	0
2	HEM	A	401	43/43	0.99	0.04	21,26,31,33	0
4	O	A	403	1/1	0.99	0.04	21,21,21,21	1
4	O	D	404	1/1	0.99	0.08	22,22,22,22	1
2	HEM	B	501	43/43	0.99	0.04	19,23,30,50	0
3	MG	A	402	1/1	1.00	0.03	24,24,24,24	0

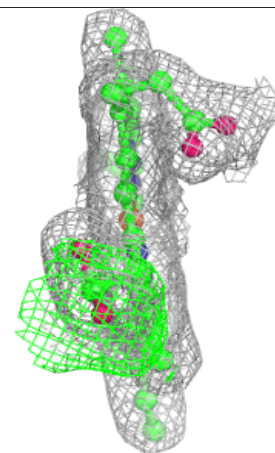
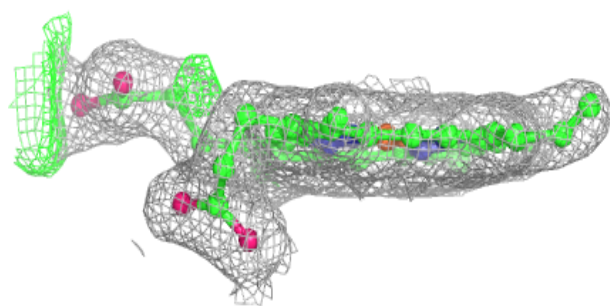
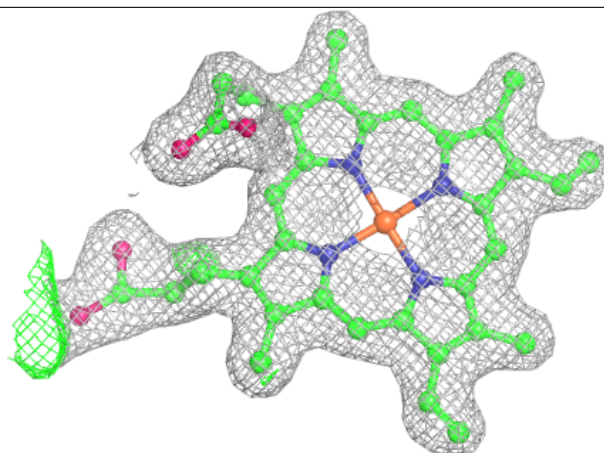
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





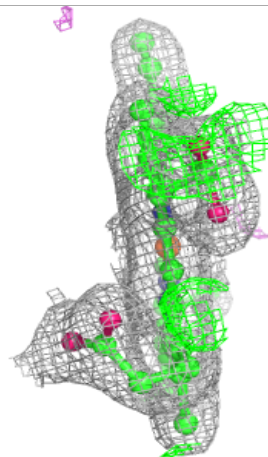
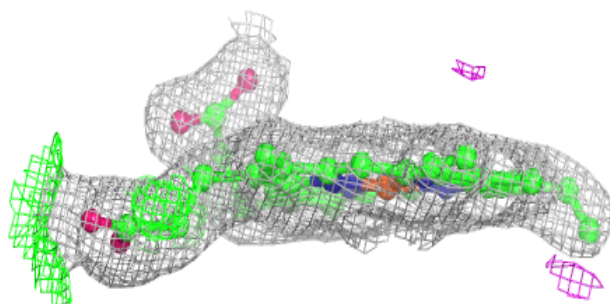
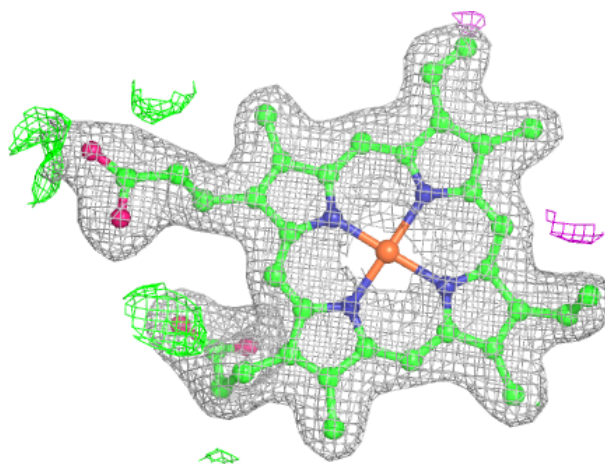
**Electron density around HEM D 401:**

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



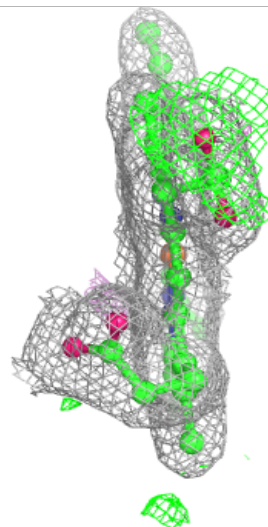
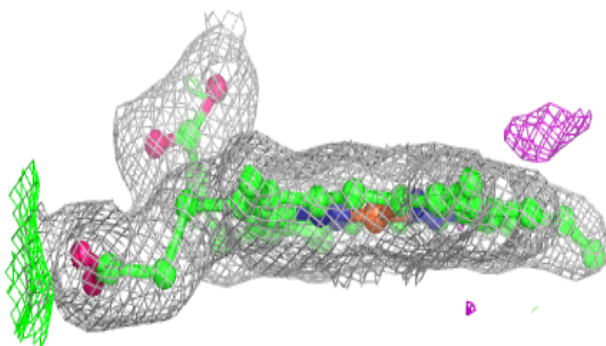
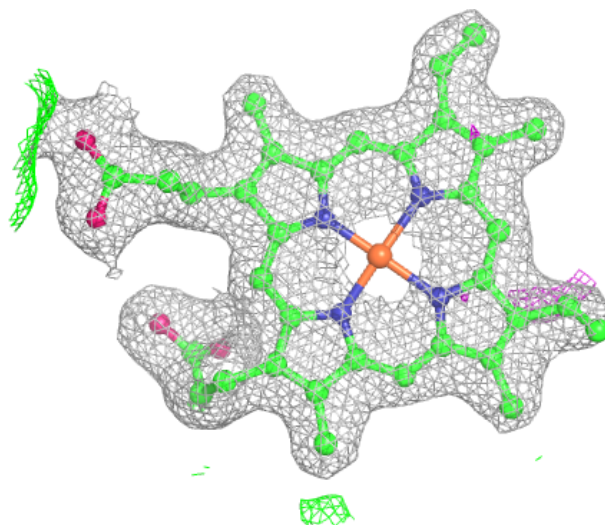
**Electron density around HEM E 401:**

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



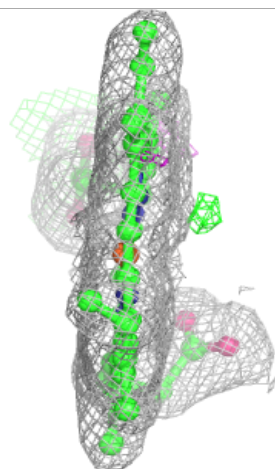
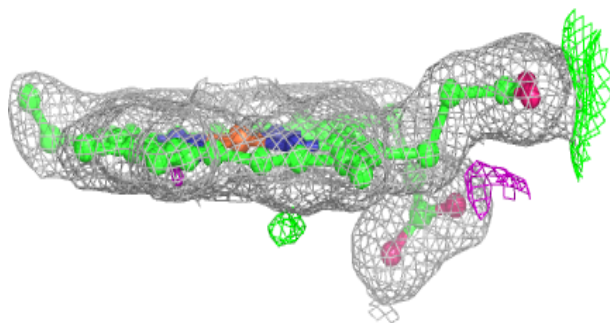
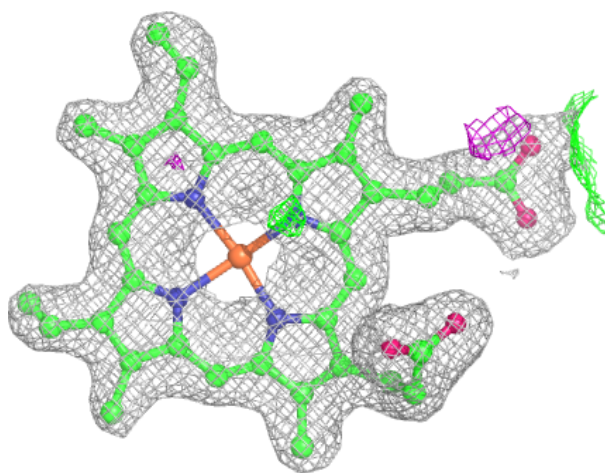
**Electron density around HEM F 401:**

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



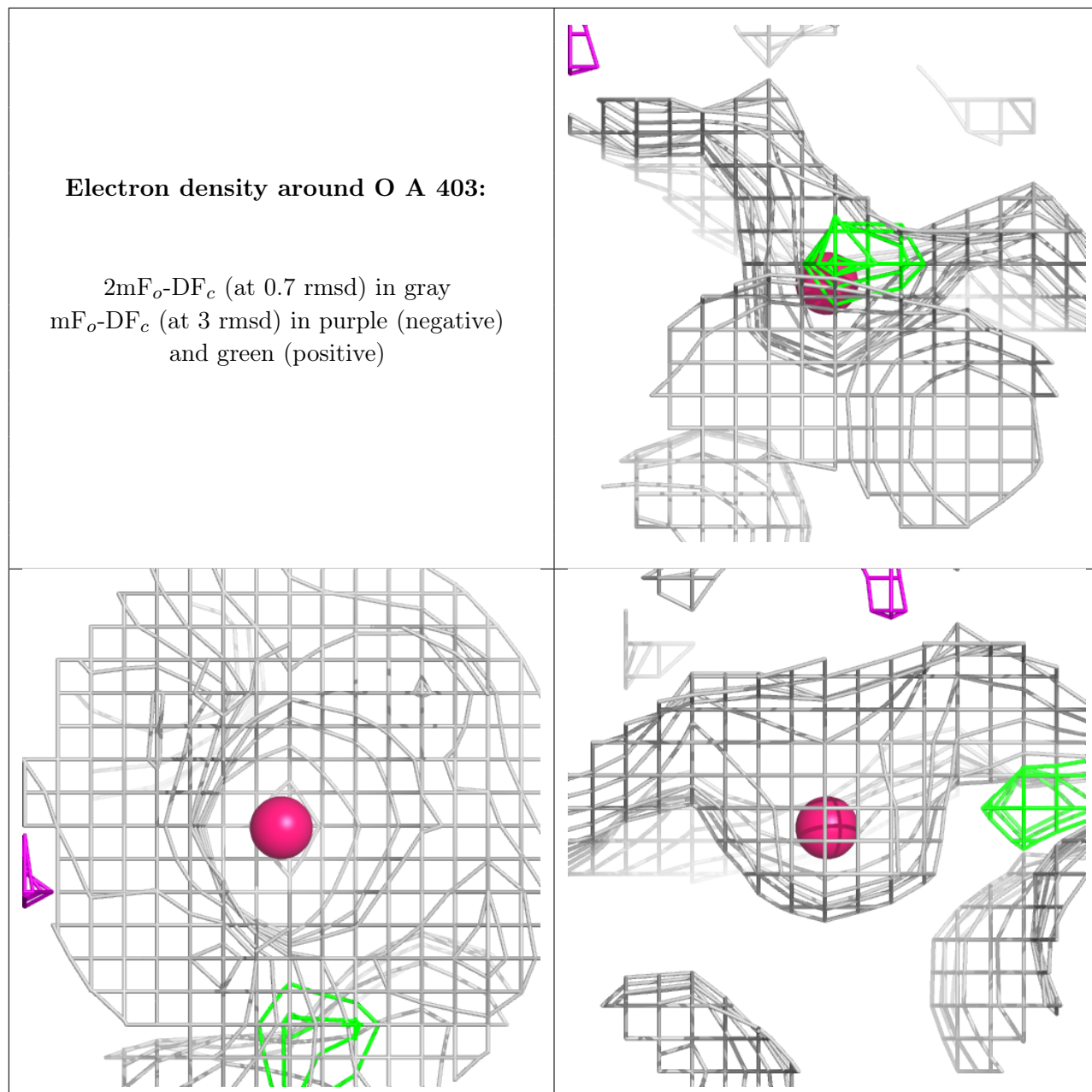
**Electron density around HEM A 401:**

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



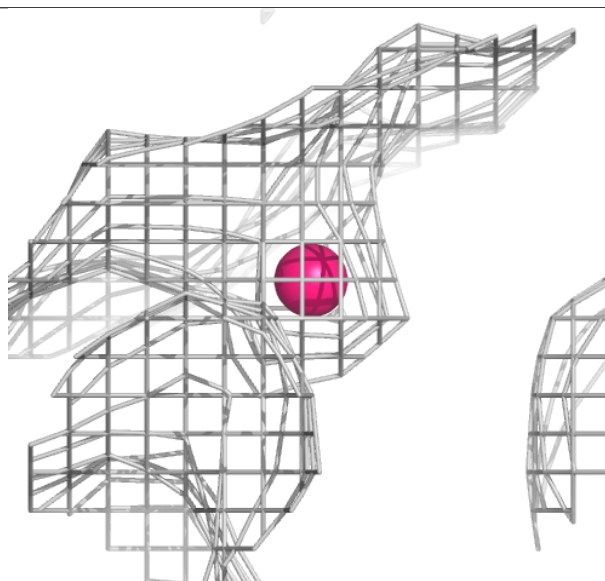
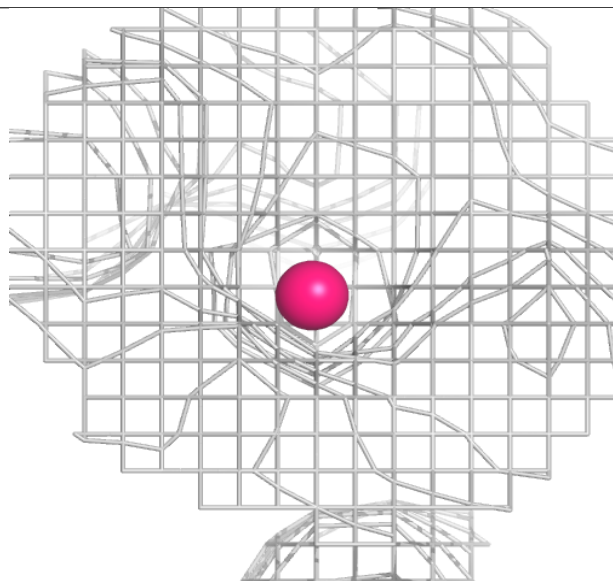
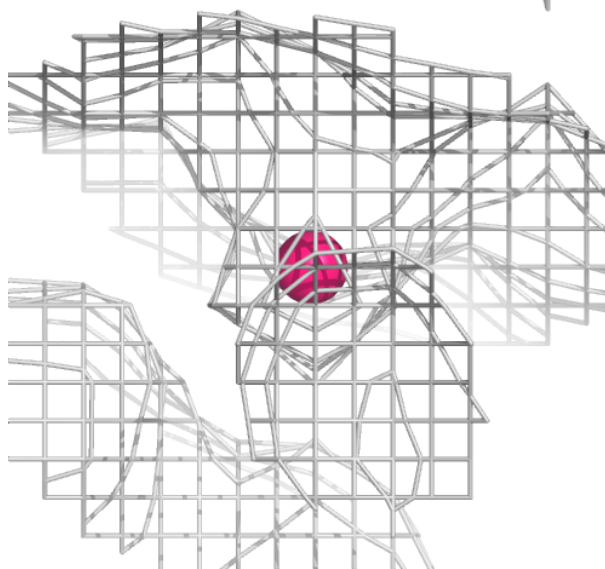
**Electron density around O A 403:**

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



**Electron density around O D 404:**

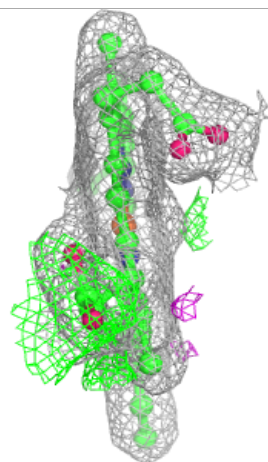
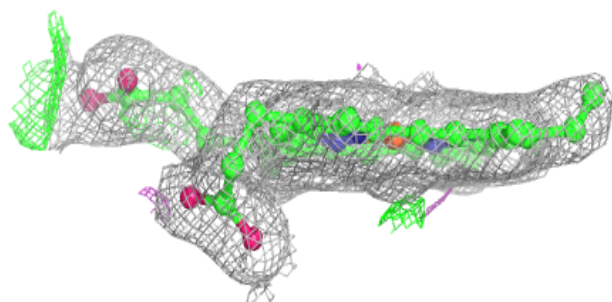
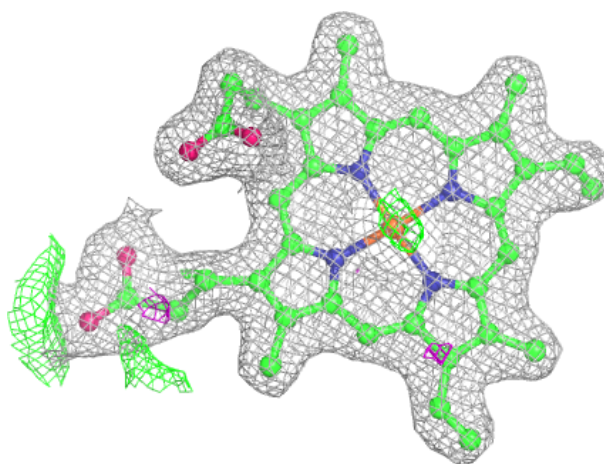
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM B 501:**

$2mF_o-DF_c$  (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.