



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 03:08 AM UTC

PDB ID : 24RQ / pdb\_000024rq  
Title : Crystal structure of Pseudomonas fluorescens peroxidase EfeB  
Authors : Okumura, K.; Ogura, K.; Mikami, B.; Hashimoto, W.  
Deposited on : 2026-03-18  
Resolution : 2.11 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

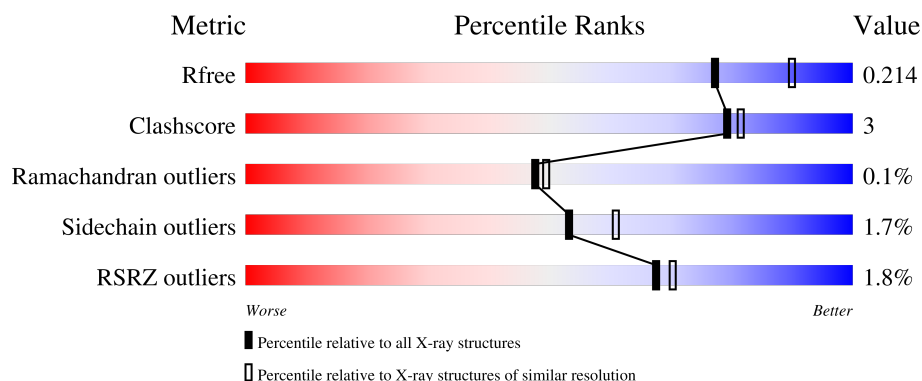
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>89%</span> <span>7%</span> </div> </div>
1	B	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>89%</span> <span>7%</span> </div> </div>
1	C	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>90%</span> <span>6%</span> </div> </div>
1	D	404	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>90%</span> <span>6%</span> </div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13434 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 Deferrochelataase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	2	0
			3040	1913	543	575	9			
1	B	389	Total	C	N	O	S	0	2	0
			3040	1912	541	578	9			
1	C	389	Total	C	N	O	S	0	3	0
			3053	1920	547	577	9			
1	D	389	Total	C	N	O	S	0	2	0
			3037	1911	542	575	9			

There are 28 discrepancies between the modelled and reference sequences:

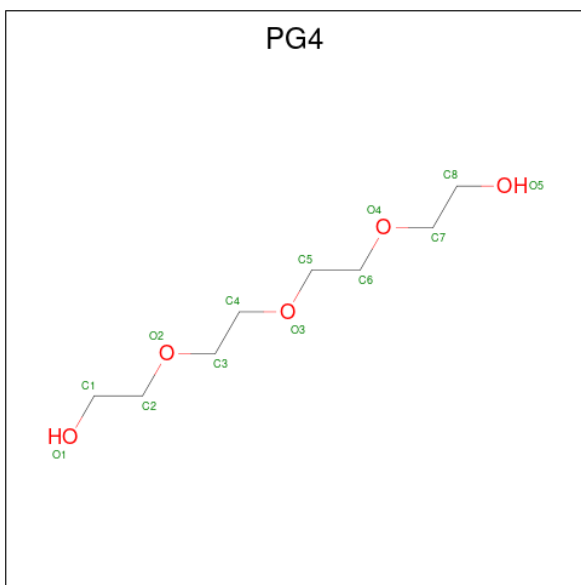
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP A0A3M3XL07
A	439	HIS	-	expression tag	UNP A0A3M3XL07
A	440	HIS	-	expression tag	UNP A0A3M3XL07
A	441	HIS	-	expression tag	UNP A0A3M3XL07
A	442	HIS	-	expression tag	UNP A0A3M3XL07
A	443	HIS	-	expression tag	UNP A0A3M3XL07
A	444	HIS	-	expression tag	UNP A0A3M3XL07
B	41	MET	-	initiating methionine	UNP A0A3M3XL07
B	439	HIS	-	expression tag	UNP A0A3M3XL07
B	440	HIS	-	expression tag	UNP A0A3M3XL07
B	441	HIS	-	expression tag	UNP A0A3M3XL07
B	442	HIS	-	expression tag	UNP A0A3M3XL07
B	443	HIS	-	expression tag	UNP A0A3M3XL07
B	444	HIS	-	expression tag	UNP A0A3M3XL07
C	41	MET	-	initiating methionine	UNP A0A3M3XL07
C	439	HIS	-	expression tag	UNP A0A3M3XL07
C	440	HIS	-	expression tag	UNP A0A3M3XL07
C	441	HIS	-	expression tag	UNP A0A3M3XL07
C	442	HIS	-	expression tag	UNP A0A3M3XL07
C	443	HIS	-	expression tag	UNP A0A3M3XL07
C	444	HIS	-	expression tag	UNP A0A3M3XL07

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Chain	Residue	Modelled	Actual	Comment	Reference
D	41	MET	-	initiating methionine	UNP A0A3M3XL07
D	439	HIS	-	expression tag	UNP A0A3M3XL07
D	440	HIS	-	expression tag	UNP A0A3M3XL07
D	441	HIS	-	expression tag	UNP A0A3M3XL07
D	442	HIS	-	expression tag	UNP A0A3M3XL07
D	443	HIS	-	expression tag	UNP A0A3M3XL07
D	444	HIS	-	expression tag	UNP A0A3M3XL07

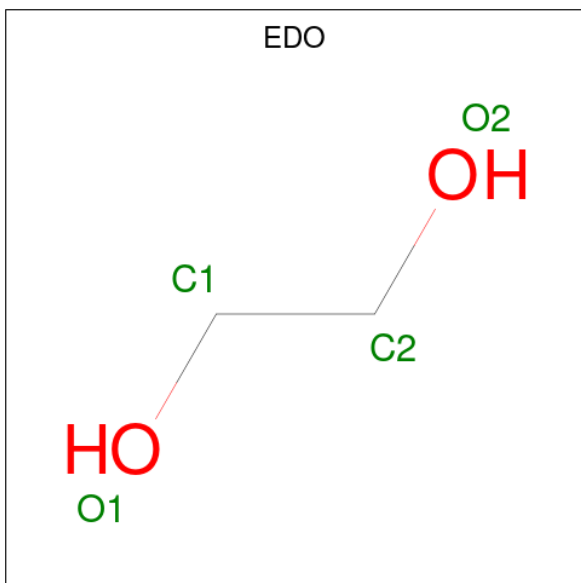
- # HEM

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula:  $C_8H_{18}O_5$ ).



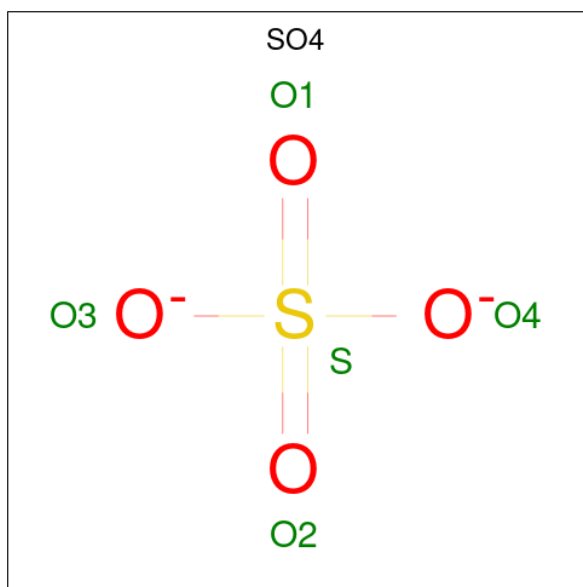
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



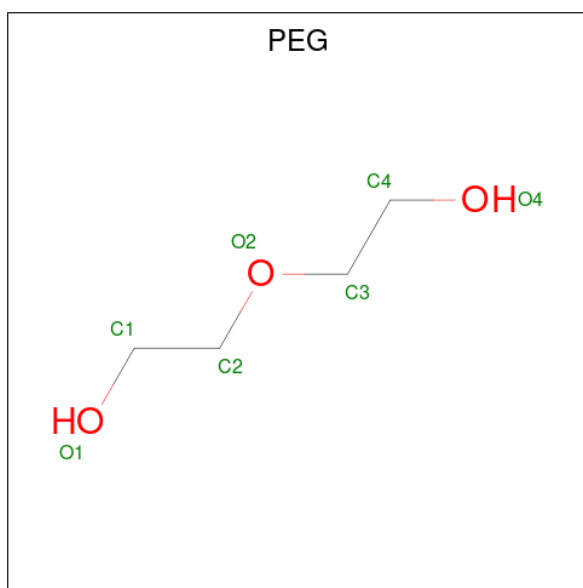
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

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

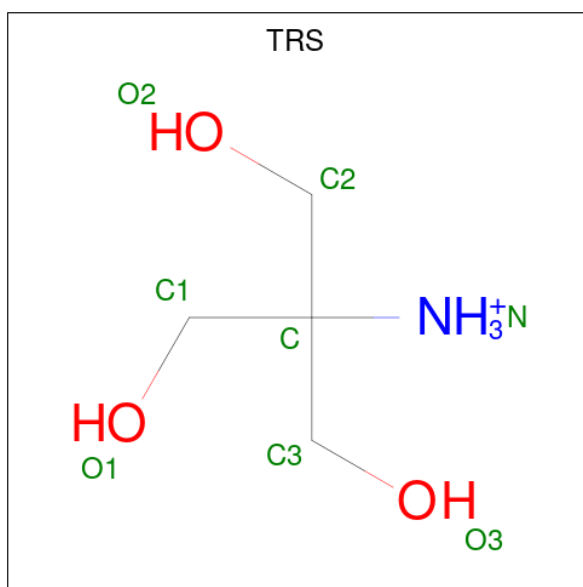
- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

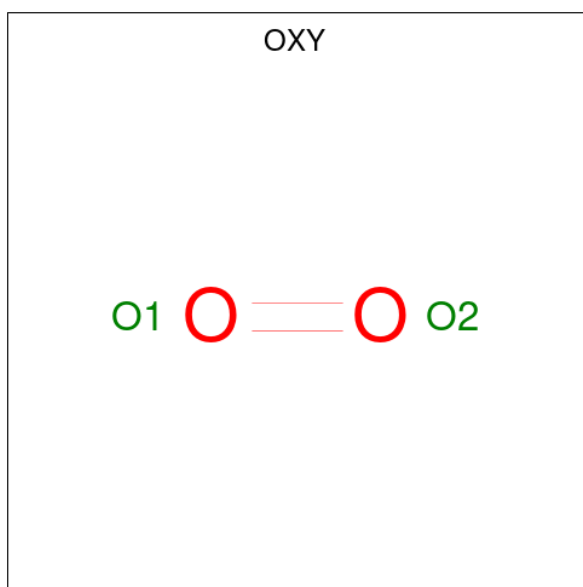
- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula:  $C_4H_{12}NO_3$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O<sub>2</sub>).



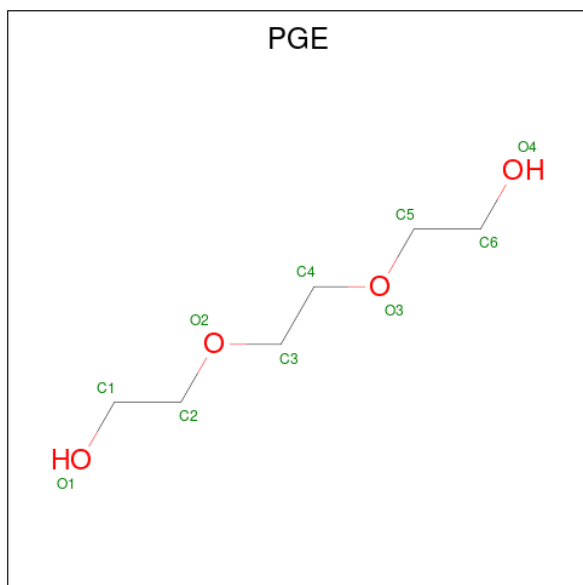
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	O	0	0
			2	2		
8	C	1	Total	O	0	0
			2	2		
8	D	1	Total	O	0	0
			2	2		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	245	Total	O	0	0
			245	245		
10	B	219	Total	O	0	0
			219	219		
10	C	181	Total	O	0	0
			181	181		
10	D	169	Total	O	0	0
			169	169		



E395	T411	T430	H431	PRO	GLN	THR	THR	ALA	ASN	THR	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.66Å 136.66Å 217.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.71 – 2.11 49.71 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.71-2.11) 100.0 (49.71-2.11)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.181 , 0.216 0.181 , 0.214	Depositor DCC
$R_{free}$ test set	6775 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13434	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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: SO4, EDO, PEG, TRS, HEM, PGE, OXY, PG4

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	0.30	0/3114	0.54	0/4234
1	B	0.33	0/3114	0.52	0/4235
1	C	0.29	0/3128	0.47	0/4253
1	D	0.29	0/3114	0.50	0/4235
All	All	0.30	0/12470	0.51	0/16957

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3040	0	3011	20	0
1	B	3040	0	3002	17	0
1	C	3053	0	3017	14	0
1	D	3037	0	3007	16	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	13	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	36	3	0
3	D	13	0	18	1	0
4	A	8	0	12	3	0
4	B	8	0	12	2	0
4	C	8	0	12	0	0
4	D	12	0	18	1	0
5	A	35	0	0	0	0
5	B	45	0	0	0	0
5	C	25	0	0	0	0
5	D	15	0	0	0	0
6	A	21	0	30	4	0
6	B	7	0	10	3	0
7	A	8	0	12	2	0
7	B	8	0	12	0	0
7	D	8	0	12	1	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	C	10	0	14	0	0
10	A	245	0	0	2	0
10	B	219	0	0	2	0
10	C	181	0	0	0	0
10	D	169	0	0	1	0
All	All	13434	0	12373	68	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 68 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:B:282:ARG:HH12	4:B:504:EDO:H12	1.54	0.72
1:A:419:LYS:NZ	6:B:515:PEG:H41	2.11	0.66
1:A:419:LYS:HZ3	6:B:515:PEG:H41	1.66	0.61
1:C:159:LYS:HG3	1:C:160:ARG:HD3	1.83	0.61
1:B:69:ILE:HD11	1:B:411:THR:HG21	1.84	0.60

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/404 (96%)	380 (98%)	9 (2%)	0	100	100
1	B	389/404 (96%)	377 (97%)	12 (3%)	0	100	100
1	C	390/404 (96%)	374 (96%)	16 (4%)	0	100	100
1	D	389/404 (96%)	372 (96%)	16 (4%)	1 (0%)	36	36
All	All	1557/1616 (96%)	1503 (96%)	53 (3%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	226	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	333/344 (97%)	327 (98%)	6 (2%)	51	59
1	B	333/344 (97%)	324 (97%)	9 (3%)	39	44
1	C	334/344 (97%)	328 (98%)	6 (2%)	51	59
1	D	333/344 (97%)	329 (99%)	4 (1%)	63	71
All	All	1333/1376 (97%)	1308 (98%)	25 (2%)	53	57

5 of 25 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	B	431	HIS
1	C	111	THR
1	D	378	GLN
1	C	58[B]	HIS
1	C	194	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	65	HIS
1	C	214	GLN
1	D	393	ASN
1	C	360	ASN
1	D	176	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

53 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PG4	B	502	-	12,12,12	0.31	0	11,11,11	0.19	0
5	SO4	B	506	-	4,4,4	0.79	0	6,6,6	0.22	0
7	TRS	B	516	-	7,7,7	0.41	0	9,9,9	1.19	0
4	EDO	D	503	-	3,3,3	0.25	0	2,2,2	0.17	0
5	SO4	B	509	-	4,4,4	0.73	0	6,6,6	0.15	0
4	EDO	A	504	-	3,3,3	0.26	0	2,2,2	0.36	0
5	SO4	B	513	-	4,4,4	0.71	0	6,6,6	0.20	0
5	SO4	B	507	-	4,4,4	0.65	0	6,6,6	0.35	0
6	PEG	A	512	-	6,6,6	0.20	0	5,5,5	0.43	0
5	SO4	A	505	-	4,4,4	0.62	0	6,6,6	0.49	0
3	PG4	A	502	-	12,12,12	0.27	0	11,11,11	0.37	0
7	TRS	A	515	-	7,7,7	0.40	0	9,9,9	0.55	0
4	EDO	B	504	-	3,3,3	0.26	0	2,2,2	0.29	0
2	HEM	C	501	1,8	50,50,50	1.49	9 (18%)	67,82,82	1.18	4 (5%)
2	HEM	B	501	1,8	50,50,50	1.47	9 (18%)	67,82,82	1.23	6 (8%)
5	SO4	A	508	-	4,4,4	0.75	0	6,6,6	0.39	0
5	SO4	A	506	-	4,4,4	0.66	0	6,6,6	0.21	0
2	HEM	D	501	1	50,50,50	1.49	7 (14%)	67,82,82	1.17	5 (7%)
4	EDO	D	504	-	3,3,3	0.22	0	2,2,2	0.29	0
5	SO4	B	511	-	4,4,4	0.73	0	6,6,6	0.13	0
4	EDO	A	503	-	3,3,3	0.27	0	2,2,2	0.13	0
8	OXY	A	516	2	1,1,1	0.02	0	-		
7	TRS	D	509	-	7,7,7	0.42	0	9,9,9	0.65	0
5	SO4	B	512	-	4,4,4	0.74	0	6,6,6	0.10	0
5	SO4	C	506	-	4,4,4	0.79	0	6,6,6	0.19	0
6	PEG	A	513	-	6,6,6	0.25	0	5,5,5	0.52	0
5	SO4	B	514	-	4,4,4	0.76	0	6,6,6	0.19	0
5	SO4	D	506	-	4,4,4	0.71	0	6,6,6	0.17	0
4	EDO	C	502	-	3,3,3	0.27	0	2,2,2	0.11	0
5	SO4	C	507	-	4,4,4	0.77	0	6,6,6	0.15	0
2	HEM	A	501	1,8	50,50,50	1.42	6 (12%)	67,82,82	1.22	8 (11%)
5	SO4	C	505	-	4,4,4	0.72	0	6,6,6	0.15	0
8	OXY	B	517	2	1,1,1	0.05	0	-		
5	SO4	D	508	-	4,4,4	0.73	0	6,6,6	0.08	0
5	SO4	B	510	-	4,4,4	0.69	0	6,6,6	0.25	0
3	PG4	D	502	-	12,12,12	0.30	0	11,11,11	0.21	0
5	SO4	C	508	-	4,4,4	0.60	0	6,6,6	0.41	0
9	PGE	C	509	-	9,9,9	0.34	0	8,8,8	0.66	0
5	SO4	D	507	-	4,4,4	0.73	0	6,6,6	0.31	0
4	EDO	B	505	-	3,3,3	0.25	0	2,2,2	0.35	0
6	PEG	B	515	-	6,6,6	0.35	0	5,5,5	0.34	0
8	OXY	D	510	-	1,1,1	0.13	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	510	-	4,4,4	0.71	0	6,6,6	0.16	0
5	SO4	A	511	-	4,4,4	0.70	0	6,6,6	0.13	0
4	EDO	C	503	-	3,3,3	0.24	0	2,2,2	0.47	0
5	SO4	B	508	-	4,4,4	0.61	0	6,6,6	0.37	0
6	PEG	A	514	-	6,6,6	0.25	0	5,5,5	0.21	0
3	PG4	B	503	-	12,12,12	0.32	0	11,11,11	0.37	0
5	SO4	C	504	-	4,4,4	0.68	0	6,6,6	0.30	0
4	EDO	D	505	-	3,3,3	0.23	0	2,2,2	0.52	0
5	SO4	A	507	-	4,4,4	0.70	0	6,6,6	0.32	0
5	SO4	A	509	-	4,4,4	0.69	0	6,6,6	0.23	0
8	OXY	C	510	2	1,1,1	0.07	0	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG4	B	502	-	-	3/10/10/10	-
7	TRS	B	516	-	-	3/9/9/9	-
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
6	PEG	A	512	-	-	1/4/4/4	-
3	PG4	A	502	-	-	1/10/10/10	-
7	TRS	A	515	-	-	9/9/9/9	-
4	EDO	B	504	-	-	0/1/1/1	-
2	HEM	C	501	1,8	-	2/14/54/54	-
2	HEM	B	501	1,8	-	2/14/54/54	-
2	HEM	D	501	1	-	2/14/54/54	-
4	EDO	D	504	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
7	TRS	D	509	-	-	9/9/9/9	-
6	PEG	A	513	-	-	1/4/4/4	-
4	EDO	C	502	-	-	0/1/1/1	-
2	HEM	A	501	1,8	-	4/14/54/54	-
3	PG4	D	502	-	-	7/10/10/10	-
9	PGE	C	509	-	-	3/7/7/7	-
4	EDO	B	505	-	-	1/1/1/1	-
6	PEG	B	515	-	-	2/4/4/4	-
6	PEG	A	514	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	503	-	-	1/1/1/1	-
3	PG4	B	503	-	-	4/10/10/10	-
4	EDO	D	505	-	-	1/1/1/1	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	FE-ND	5.04	2.10	1.94
2	D	501	HEM	FE-NB	4.63	2.09	1.94
2	B	501	HEM	FE-ND	4.58	2.09	1.94
2	D	501	HEM	FE-ND	4.10	2.07	1.94
2	A	501	HEM	FE-NC	4.09	2.08	1.95

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CHD-C4C-NC	3.65	128.43	124.45
2	B	501	HEM	C1B-NB-C4B	3.06	108.84	105.21
2	B	501	HEM	C4D-ND-C1D	2.89	108.63	105.21
2	A	501	HEM	C4D-ND-C1D	2.68	108.38	105.21
2	C	501	HEM	C4D-ND-C1D	2.67	108.37	105.21

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	515	TRS	C2-C-C1-O1
7	A	515	TRS	C3-C-C1-O1
7	A	515	TRS	N-C-C1-O1
7	A	515	TRS	C1-C-C2-O2
7	A	515	TRS	N-C-C2-O2

There are no ring outliers.

15 monomers are involved in 22 short contacts:

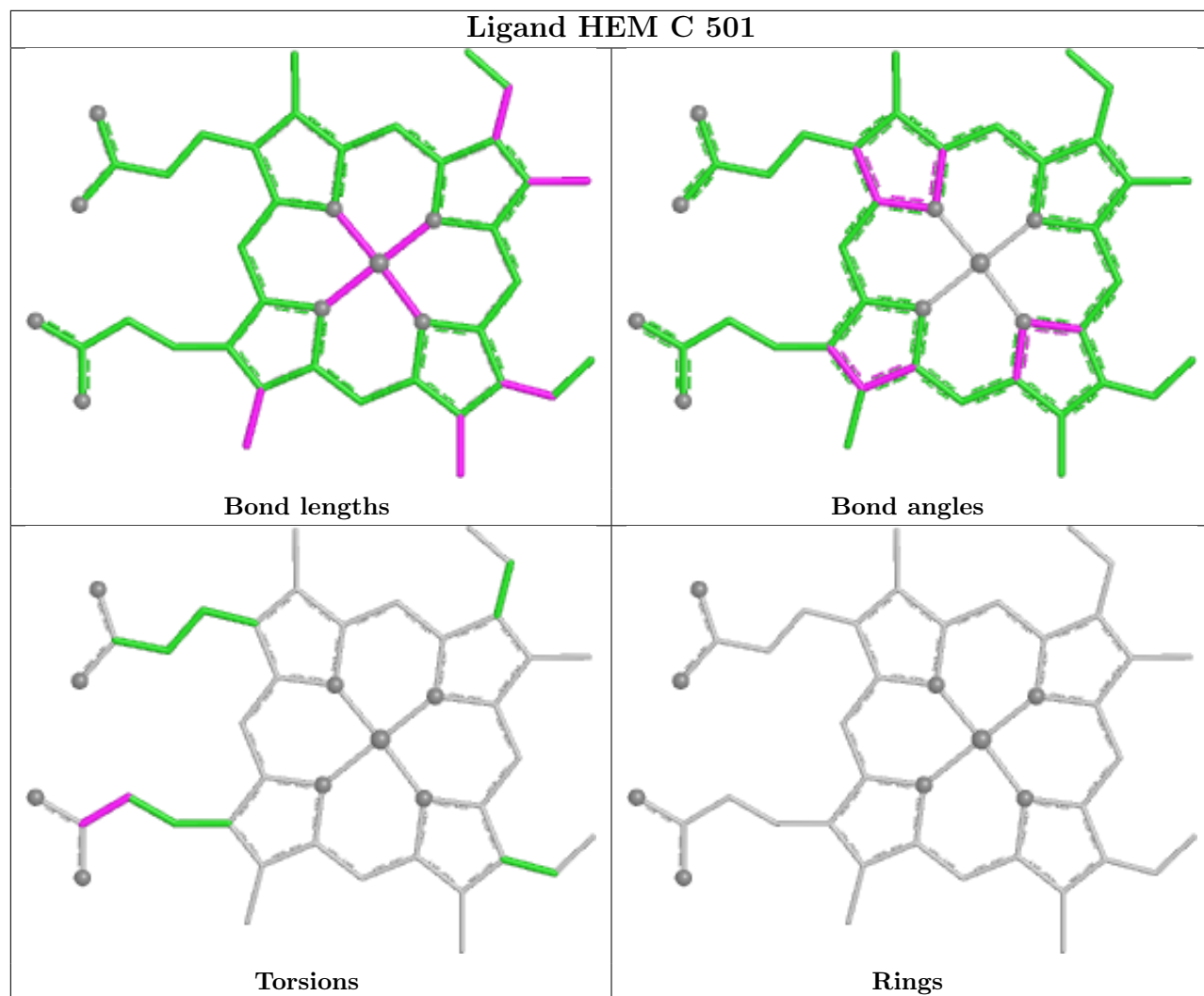
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	PG4	2	0
4	A	504	EDO	3	0
6	A	512	PEG	1	0
3	A	502	PG4	1	0
7	A	515	TRS	2	0

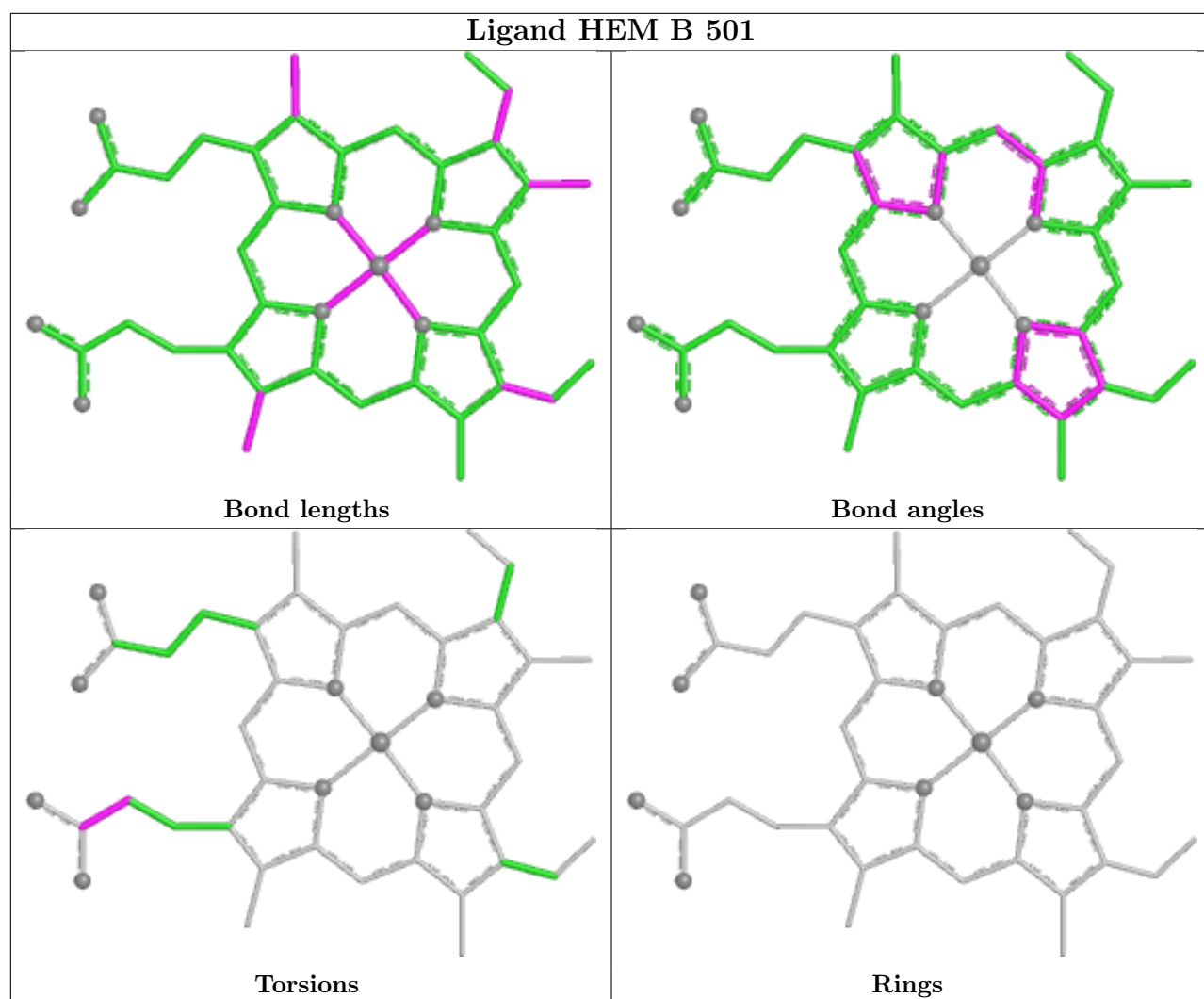
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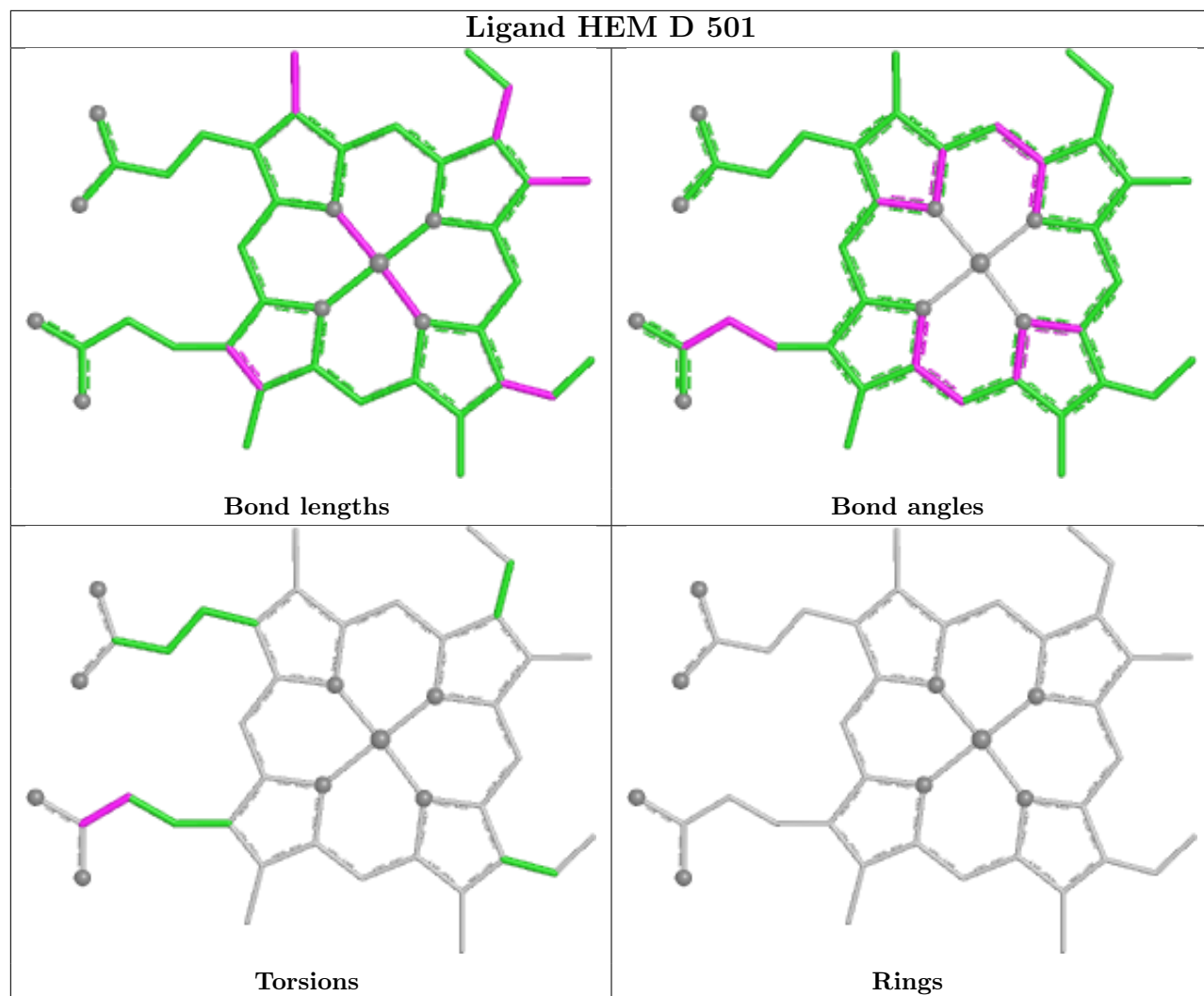
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	EDO	1	0
2	B	501	HEM	1	0
7	D	509	TRS	1	0
6	A	513	PEG	2	0
3	D	502	PG4	1	0
4	B	505	EDO	1	0
6	B	515	PEG	3	0
6	A	514	PEG	1	0
3	B	503	PG4	1	0
4	D	505	EDO	1	0

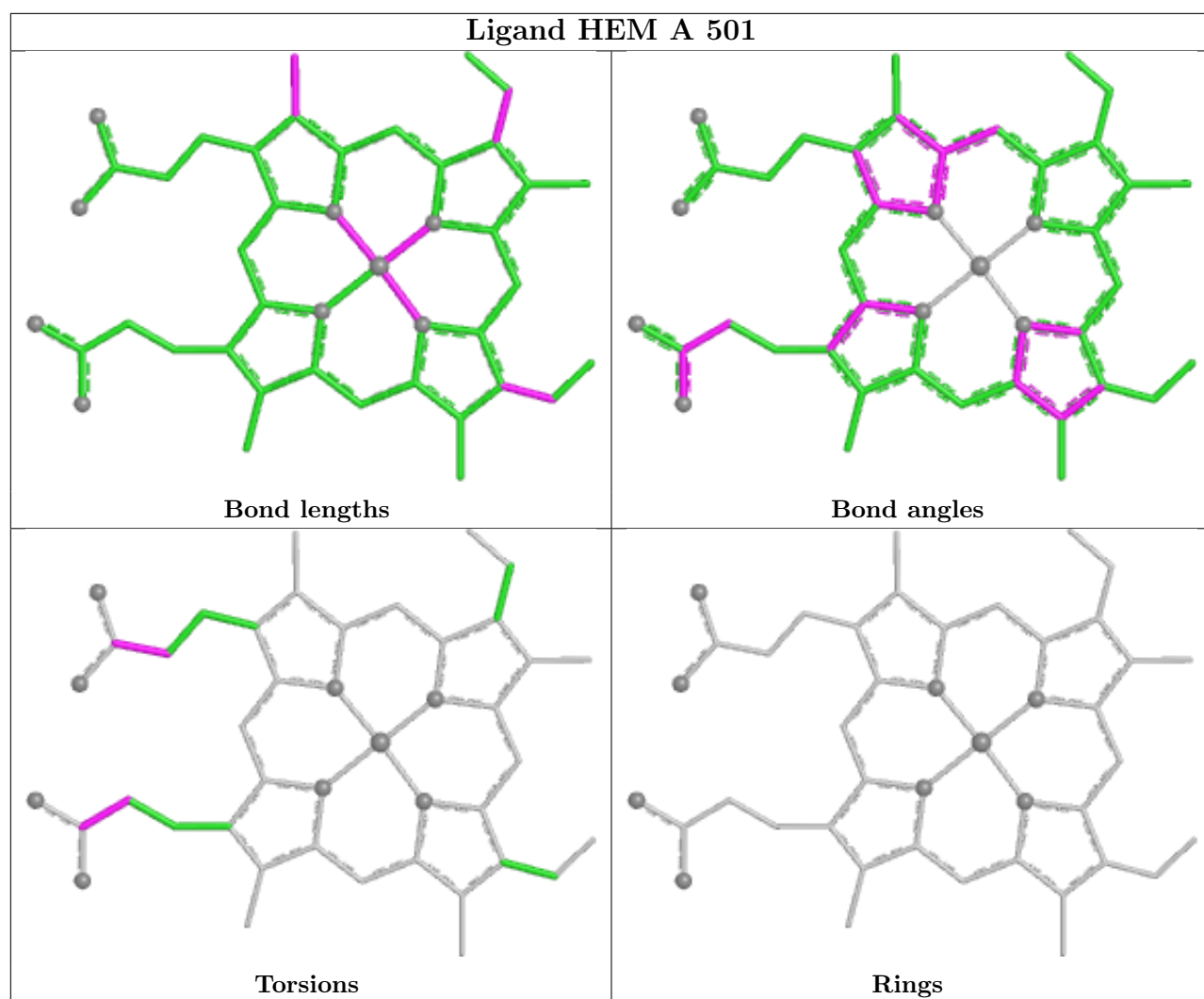
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	389/404 (96%)	-0.32	5 (1%) 75 77	18, 35, 52, 81	2 (0%)
1	B	389/404 (96%)	-0.23	3 (0%) 82 85	22, 36, 51, 67	2 (0%)
1	C	389/404 (96%)	-0.09	5 (1%) 75 77	22, 38, 52, 89	3 (0%)
1	D	389/404 (96%)	0.26	15 (3%) 43 46	29, 44, 62, 91	2 (0%)
All	All	1556/1616 (96%)	-0.09	28 (1%) 67 70	18, 38, 56, 91	9 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	PRO	4.9
1	C	226	PRO	4.7
1	A	43	ALA	3.9
1	D	227	GLY	3.9
1	C	58[A]	HIS	3.8

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [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( $\text{\AA}^2$ )	Q<0.9
7	TRS	A	515	8/8	0.63	0.19	56,61,68,75	0
5	SO4	D	507	5/5	0.73	0.12	67,69,84,86	0
5	SO4	C	508	5/5	0.73	0.29	37,38,42,43	5
5	SO4	B	514	5/5	0.76	0.12	63,75,89,89	0
5	SO4	B	512	5/5	0.76	0.11	70,80,92,92	0
5	SO4	A	511	5/5	0.77	0.11	72,75,91,103	0
5	SO4	A	510	5/5	0.77	0.11	71,78,88,92	0
4	EDO	B	505	4/4	0.78	0.19	53,53,54,66	0
5	SO4	C	506	5/5	0.79	0.12	51,59,71,73	0
6	PEG	A	513	7/7	0.79	0.16	52,55,58,59	0
3	PG4	D	502	13/13	0.79	0.17	53,58,70,71	0
4	EDO	D	503	4/4	0.80	0.23	48,48,50,54	0
4	EDO	C	502	4/4	0.82	0.17	43,50,50,50	0
5	SO4	C	507	5/5	0.82	0.10	60,68,83,90	0
6	PEG	B	515	7/7	0.82	0.17	37,44,47,53	0
5	SO4	A	508	5/5	0.82	0.11	51,57,76,77	0
7	TRS	B	516	8/8	0.82	0.17	46,55,57,62	0
6	PEG	A	514	7/7	0.83	0.17	44,51,54,57	0
4	EDO	B	504	4/4	0.83	0.16	60,62,63,66	0
9	PGE	C	509	10/10	0.83	0.16	53,57,59,59	0
5	SO4	B	511	5/5	0.85	0.10	62,67,78,84	0
5	SO4	D	508	5/5	0.85	0.10	63,71,79,83	0
3	PG4	B	503	13/13	0.85	0.15	42,51,54,57	0
5	SO4	A	509	5/5	0.85	0.11	64,75,81,84	0
4	EDO	C	503	4/4	0.86	0.16	55,56,58,59	0
4	EDO	A	503	4/4	0.86	0.15	53,54,56,58	0
7	TRS	D	509	8/8	0.86	0.16	45,58,66,66	0
4	EDO	D	505	4/4	0.86	0.14	41,43,53,59	0
4	EDO	A	504	4/4	0.87	0.17	38,45,49,52	0
5	SO4	B	507	5/5	0.88	0.12	54,57,61,69	0
6	PEG	A	512	7/7	0.89	0.14	37,47,58,60	0
8	OXY	B	517	2/2	0.89	0.12	36,36,36,37	0
4	EDO	D	504	4/4	0.89	0.13	49,51,53,62	0
8	OXY	C	510	2/2	0.90	0.11	39,39,39,43	0
5	SO4	A	507	5/5	0.91	0.17	47,51,60,61	0
5	SO4	B	510	5/5	0.91	0.10	54,59,65,68	0
5	SO4	C	505	5/5	0.92	0.08	55,56,65,67	0
3	PG4	B	502	13/13	0.92	0.11	37,40,52,54	0
5	SO4	B	513	5/5	0.92	0.13	41,42,43,46	5
3	PG4	A	502	13/13	0.92	0.10	35,39,56,57	0
5	SO4	D	506	5/5	0.93	0.08	53,60,62,68	0
8	OXY	A	516	2/2	0.94	0.08	30,30,30,33	0
5	SO4	A	505	5/5	0.94	0.10	52,54,56,61	0

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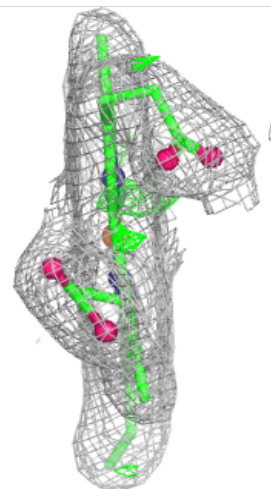
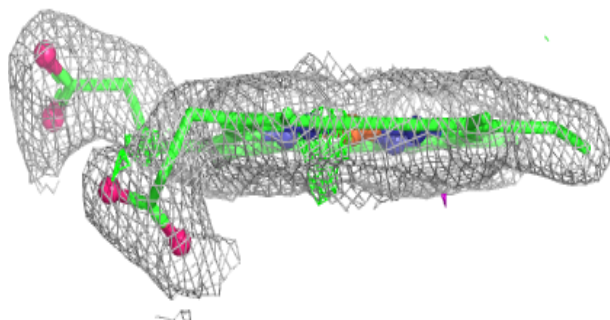
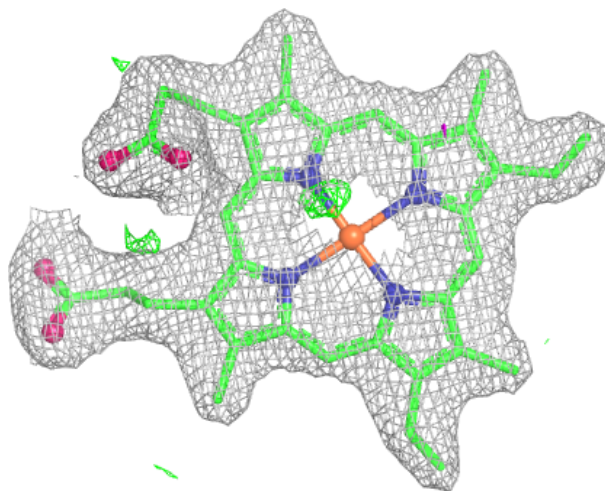
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	B	508	5/5	0.95	0.08	52,56,65,66	0
8	OXY	D	510	2/2	0.95	0.09	42,42,42,45	0
5	SO4	A	506	5/5	0.95	0.07	54,55,64,66	0
5	SO4	B	509	5/5	0.96	0.10	53,53,60,64	0
5	SO4	C	504	5/5	0.97	0.09	43,52,56,58	0
5	SO4	B	506	5/5	0.97	0.10	39,46,50,51	0
2	HEM	D	501	43/43	0.98	0.08	32,38,43,45	0
2	HEM	B	501	43/43	0.98	0.06	28,32,35,35	0
2	HEM	A	501	43/43	0.99	0.05	23,29,34,36	0
2	HEM	C	501	43/43	0.99	0.05	30,34,36,37	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.

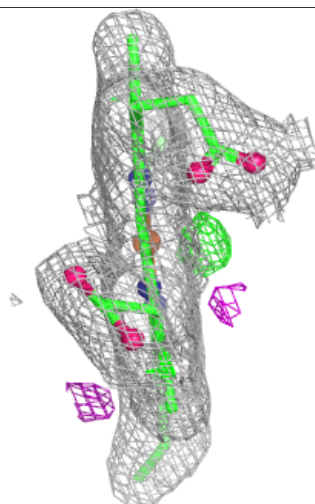
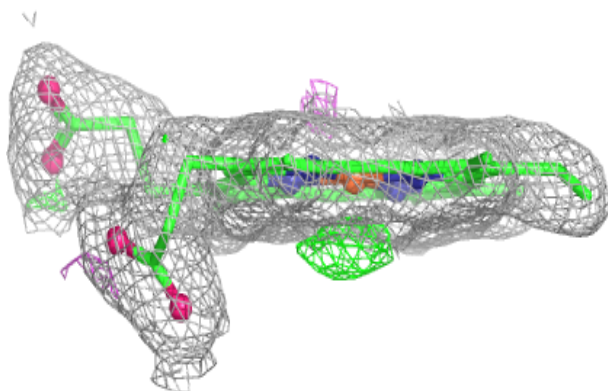
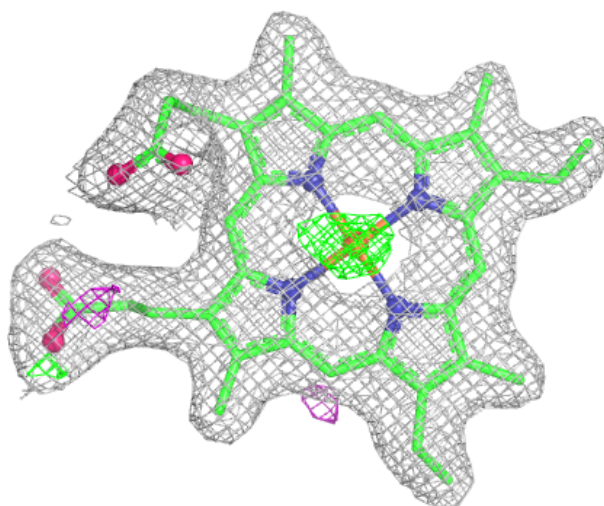
#### Electron density around HEM D 501:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)



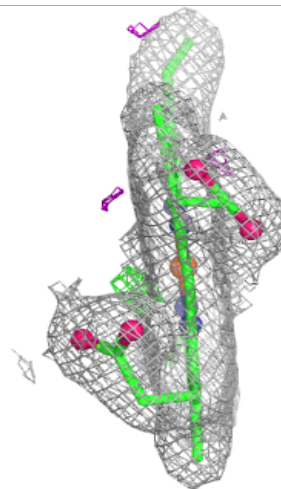
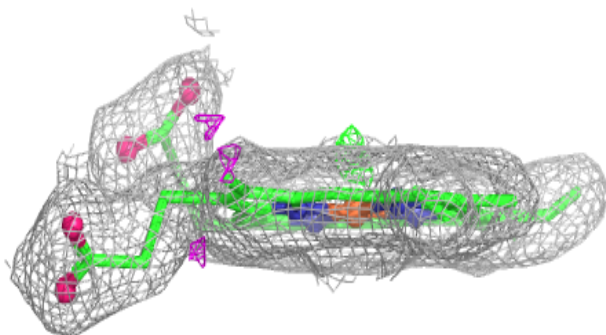
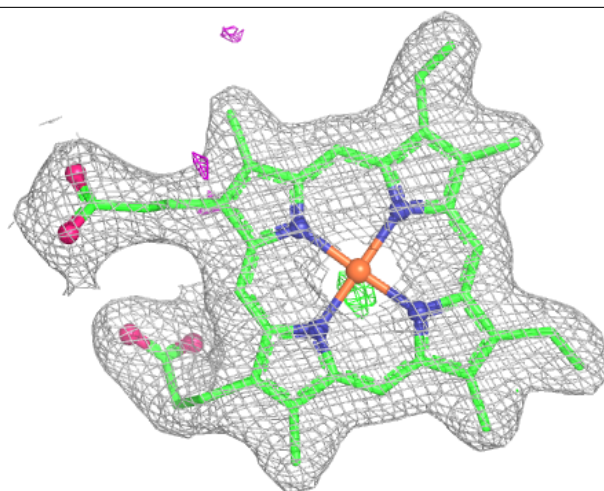
**Electron density around HEM B 501:**

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



**Electron density around HEM A 501:**

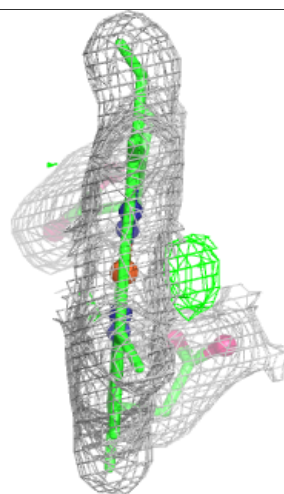
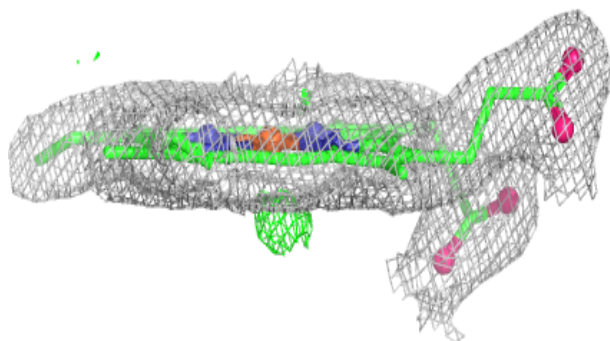
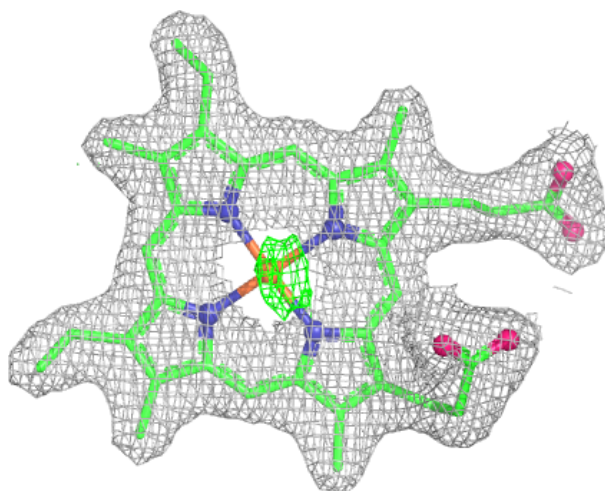
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM C 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.