



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:28 AM UTC

PDB ID : 8DSG / pdb\_00008dsg  
Title : P411-PFA carbene transferase  
Authors : Maggiolo, A.O.; Porter, N.J.; Zhang, J.; Arnold, F.H.  
Deposited on : 2022-07-22  
Resolution : 1.87 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

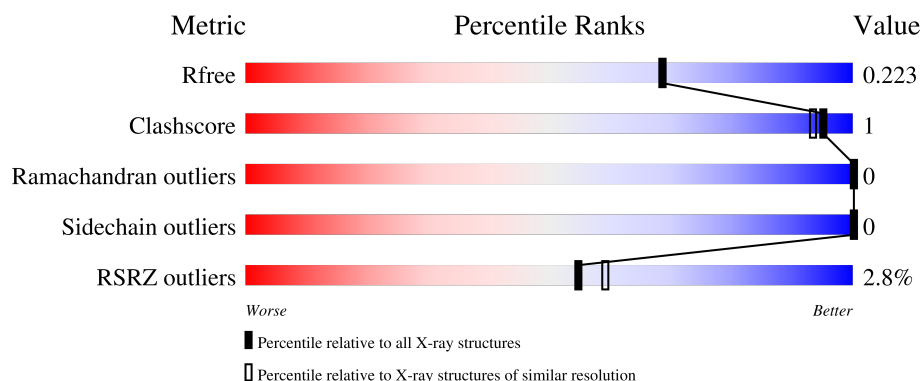
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

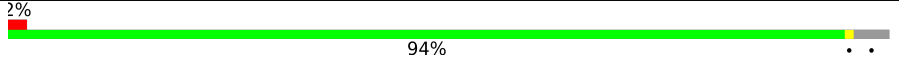
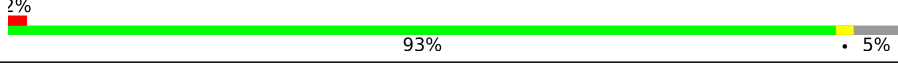
The reported resolution of this entry is 1.87 Å.

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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	472	 2% 92% 5%
1	B	472	 2% 94% 2%
1	C	472	 5% 92% 6%
1	D	472	 2% 93% 5%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15955 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 P450-BM3 variant P411-PFA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	7	0
			3678	2355	624	682	17			
1	B	451	Total	C	N	O	S	0	9	0
			3695	2366	626	686	17			
1	C	445	Total	C	N	O	S	0	8	0
			3652	2340	620	676	16			
1	D	449	Total	C	N	O	S	0	8	0
			3679	2355	624	683	17			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	THR	ASN	engineered mutation	UNP F2Q7T0
A	74	GLY	ALA	engineered mutation	UNP F2Q7T0
A	78	LEU	VAL	engineered mutation	UNP F2Q7T0
A	82	LEU	ALA	engineered mutation	UNP F2Q7T0
A	87	ALA	PHE	engineered mutation	UNP F2Q7T0
A	118	SER	MET	engineered mutation	UNP F2Q7T0
A	142	SER	PRO	engineered mutation	UNP F2Q7T0
A	175	ILE	THR	engineered mutation	UNP F2Q7T0
A	184	VAL	ALA	engineered mutation	UNP F2Q7T0
A	226	THR	SER	engineered mutation	UNP F2Q7T0
A	236	GLN	HIS	engineered mutation	UNP F2Q7T0
A	252	GLY	GLU	engineered mutation	UNP F2Q7T0
A	263	TYR	ILE	engineered mutation	UNP F2Q7T0
A	266	VAL	HIS	engineered mutation	UNP F2Q7T0
A	268	GLY	THR	engineered mutation	UNP F2Q7T0
A	290	VAL	ALA	engineered mutation	UNP F2Q7T0
A	327	VAL	THR	engineered mutation	UNP F2Q7T0
A	328	VAL	ALA	engineered mutation	UNP F2Q7T0
A	330	VAL	ALA	engineered mutation	UNP F2Q7T0
A	353	VAL	LEU	engineered mutation	UNP F2Q7T0
A	366	VAL	ILE	engineered mutation	UNP F2Q7T0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	400	SER	CYS	engineered mutation	UNP F2Q7T0
A	401	PRO	ILE	engineered mutation	UNP F2Q7T0
A	436	LEU	THR	engineered mutation	UNP F2Q7T0
A	437	GLN	LEU	engineered mutation	UNP F2Q7T0
A	442	LYS	GLU	engineered mutation	UNP F2Q7T0
A	464	LEU	-	expression tag	UNP F2Q7T0
A	465	GLU	-	expression tag	UNP F2Q7T0
A	466	HIS	-	expression tag	UNP F2Q7T0
A	467	HIS	-	expression tag	UNP F2Q7T0
A	468	HIS	-	expression tag	UNP F2Q7T0
A	469	HIS	-	expression tag	UNP F2Q7T0
A	470	HIS	-	expression tag	UNP F2Q7T0
A	471	HIS	-	expression tag	UNP F2Q7T0
B	70	THR	ASN	engineered mutation	UNP F2Q7T0
B	74	GLY	ALA	engineered mutation	UNP F2Q7T0
B	78	LEU	VAL	engineered mutation	UNP F2Q7T0
B	82	LEU	ALA	engineered mutation	UNP F2Q7T0
B	87	ALA	PHE	engineered mutation	UNP F2Q7T0
B	118	SER	MET	engineered mutation	UNP F2Q7T0
B	142	SER	PRO	engineered mutation	UNP F2Q7T0
B	175	ILE	THR	engineered mutation	UNP F2Q7T0
B	184	VAL	ALA	engineered mutation	UNP F2Q7T0
B	226	THR	SER	engineered mutation	UNP F2Q7T0
B	236	GLN	HIS	engineered mutation	UNP F2Q7T0
B	252	GLY	GLU	engineered mutation	UNP F2Q7T0
B	263	TYR	ILE	engineered mutation	UNP F2Q7T0
B	266	VAL	HIS	engineered mutation	UNP F2Q7T0
B	268	GLY	THR	engineered mutation	UNP F2Q7T0
B	290	VAL	ALA	engineered mutation	UNP F2Q7T0
B	327	VAL	THR	engineered mutation	UNP F2Q7T0
B	328	VAL	ALA	engineered mutation	UNP F2Q7T0
B	330	VAL	ALA	engineered mutation	UNP F2Q7T0
B	353	VAL	LEU	engineered mutation	UNP F2Q7T0
B	366	VAL	ILE	engineered mutation	UNP F2Q7T0
B	400	SER	CYS	engineered mutation	UNP F2Q7T0
B	401	PRO	ILE	engineered mutation	UNP F2Q7T0
B	436	LEU	THR	engineered mutation	UNP F2Q7T0
B	437	GLN	LEU	engineered mutation	UNP F2Q7T0
B	442	LYS	GLU	engineered mutation	UNP F2Q7T0
B	464	LEU	-	expression tag	UNP F2Q7T0
B	465	GLU	-	expression tag	UNP F2Q7T0
B	466	HIS	-	expression tag	UNP F2Q7T0

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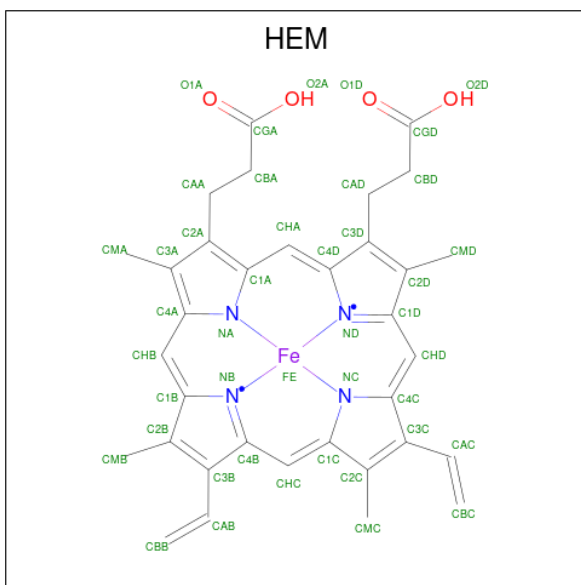
Chain	Residue	Modelled	Actual	Comment	Reference
B	467	HIS	-	expression tag	UNP F2Q7T0
B	468	HIS	-	expression tag	UNP F2Q7T0
B	469	HIS	-	expression tag	UNP F2Q7T0
B	470	HIS	-	expression tag	UNP F2Q7T0
B	471	HIS	-	expression tag	UNP F2Q7T0
C	70	THR	ASN	engineered mutation	UNP F2Q7T0
C	74	GLY	ALA	engineered mutation	UNP F2Q7T0
C	78	LEU	VAL	engineered mutation	UNP F2Q7T0
C	82	LEU	ALA	engineered mutation	UNP F2Q7T0
C	87	ALA	PHE	engineered mutation	UNP F2Q7T0
C	118	SER	MET	engineered mutation	UNP F2Q7T0
C	142	SER	PRO	engineered mutation	UNP F2Q7T0
C	175	ILE	THR	engineered mutation	UNP F2Q7T0
C	184	VAL	ALA	engineered mutation	UNP F2Q7T0
C	226	THR	SER	engineered mutation	UNP F2Q7T0
C	236	GLN	HIS	engineered mutation	UNP F2Q7T0
C	252	GLY	GLU	engineered mutation	UNP F2Q7T0
C	263	TYR	ILE	engineered mutation	UNP F2Q7T0
C	266	VAL	HIS	engineered mutation	UNP F2Q7T0
C	268	GLY	THR	engineered mutation	UNP F2Q7T0
C	290	VAL	ALA	engineered mutation	UNP F2Q7T0
C	327	VAL	THR	engineered mutation	UNP F2Q7T0
C	328	VAL	ALA	engineered mutation	UNP F2Q7T0
C	330	VAL	ALA	engineered mutation	UNP F2Q7T0
C	353	VAL	LEU	engineered mutation	UNP F2Q7T0
C	366	VAL	ILE	engineered mutation	UNP F2Q7T0
C	400	SER	CYS	engineered mutation	UNP F2Q7T0
C	401	PRO	ILE	engineered mutation	UNP F2Q7T0
C	436	LEU	THR	engineered mutation	UNP F2Q7T0
C	437	GLN	LEU	engineered mutation	UNP F2Q7T0
C	442	LYS	GLU	engineered mutation	UNP F2Q7T0
C	464	LEU	-	expression tag	UNP F2Q7T0
C	465	GLU	-	expression tag	UNP F2Q7T0
C	466	HIS	-	expression tag	UNP F2Q7T0
C	467	HIS	-	expression tag	UNP F2Q7T0
C	468	HIS	-	expression tag	UNP F2Q7T0
C	469	HIS	-	expression tag	UNP F2Q7T0
C	470	HIS	-	expression tag	UNP F2Q7T0
C	471	HIS	-	expression tag	UNP F2Q7T0
D	70	THR	ASN	engineered mutation	UNP F2Q7T0
D	74	GLY	ALA	engineered mutation	UNP F2Q7T0
D	78	LEU	VAL	engineered mutation	UNP F2Q7T0

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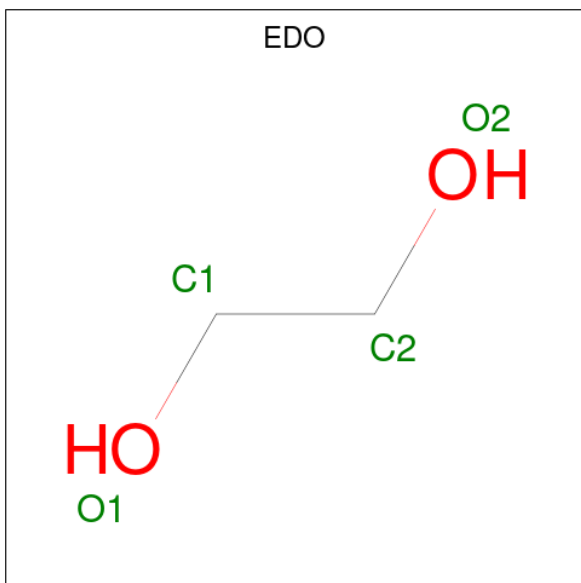
Chain	Residue	Modelled	Actual	Comment	Reference
D	82	LEU	ALA	engineered mutation	UNP F2Q7T0
D	87	ALA	PHE	engineered mutation	UNP F2Q7T0
D	118	SER	MET	engineered mutation	UNP F2Q7T0
D	142	SER	PRO	engineered mutation	UNP F2Q7T0
D	175	ILE	THR	engineered mutation	UNP F2Q7T0
D	184	VAL	ALA	engineered mutation	UNP F2Q7T0
D	226	THR	SER	engineered mutation	UNP F2Q7T0
D	236	GLN	HIS	engineered mutation	UNP F2Q7T0
D	252	GLY	GLU	engineered mutation	UNP F2Q7T0
D	263	TYR	ILE	engineered mutation	UNP F2Q7T0
D	266	VAL	HIS	engineered mutation	UNP F2Q7T0
D	268	GLY	THR	engineered mutation	UNP F2Q7T0
D	290	VAL	ALA	engineered mutation	UNP F2Q7T0
D	327	VAL	THR	engineered mutation	UNP F2Q7T0
D	328	VAL	ALA	engineered mutation	UNP F2Q7T0
D	330	VAL	ALA	engineered mutation	UNP F2Q7T0
D	353	VAL	LEU	engineered mutation	UNP F2Q7T0
D	366	VAL	ILE	engineered mutation	UNP F2Q7T0
D	400	SER	CYS	engineered mutation	UNP F2Q7T0
D	401	PRO	ILE	engineered mutation	UNP F2Q7T0
D	436	LEU	THR	engineered mutation	UNP F2Q7T0
D	437	GLN	LEU	engineered mutation	UNP F2Q7T0
D	442	LYS	GLU	engineered mutation	UNP F2Q7T0
D	464	LEU	-	expression tag	UNP F2Q7T0
D	465	GLU	-	expression tag	UNP F2Q7T0
D	466	HIS	-	expression tag	UNP F2Q7T0
D	467	HIS	-	expression tag	UNP F2Q7T0
D	468	HIS	-	expression tag	UNP F2Q7T0
D	469	HIS	-	expression tag	UNP F2Q7T0
D	470	HIS	-	expression tag	UNP F2Q7T0
D	471	HIS	-	expression tag	UNP F2Q7T0

- 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).



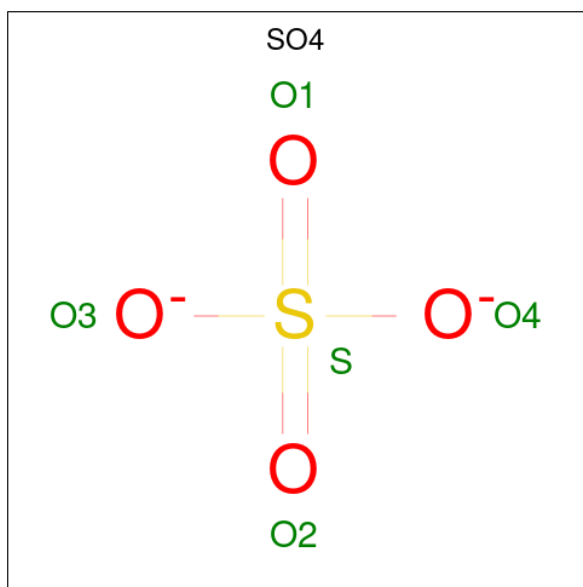
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

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



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

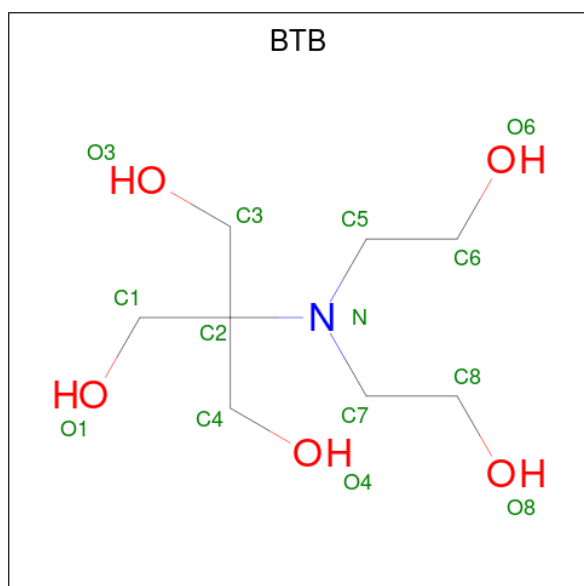
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	262	Total	O	0	0
			262	262		
6	B	260	Total	O	0	0
			260	260		
6	C	175	Total	O	0	0
			175	175		
6	D	288	Total	O	0	0
			288	288		

### 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: Cytochrome P450-BM3 variant P411-PFA

Chain A: 



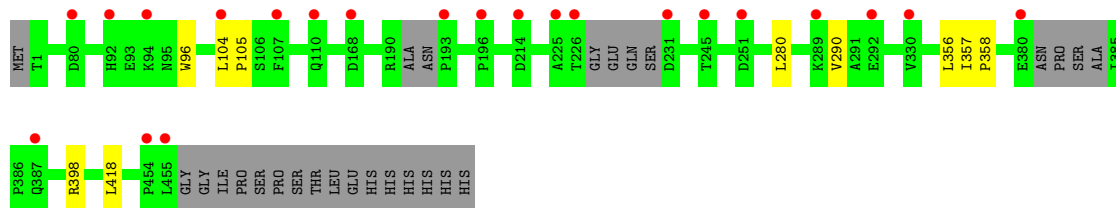
- Molecule 1: Cytochrome P450-BM3 variant P411-PFA

Chain B: 




- Molecule 1: Cytochrome P450-BM3 variant P411-PFA

Chain C: 



- Molecule 1: Cytochrome P450-BM3 variant P411-PFA

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.25Å 172.46Å 225.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.60 – 1.87 38.60 – 1.87	Depositor EDS
% Data completeness (in resolution range)	91.8 (38.60-1.87) 91.9 (38.60-1.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.187 , 0.218 0.195 , 0.223	Depositor DCC
$R_{free}$ test set	7853 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: BTB, SO4, EDO, HEM

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	0.97	0/3763	1.35	2/5084 (0.0%)
1	B	0.98	0/3783	1.36	2/5112 (0.0%)
1	C	0.98	0/3737	1.40	2/5043 (0.0%)
1	D	0.98	0/3763	1.35	2/5082 (0.0%)
All	All	0.97	0/15046	1.37	8/20321 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	356	LEU	CA-C-N	6.45	124.30	120.24
1	C	356	LEU	C-N-CA	6.45	124.30	120.24
1	A	356	LEU	CA-C-N	6.07	124.06	120.24
1	A	356	LEU	C-N-CA	6.07	124.06	120.24
1	D	356	LEU	CA-C-N	5.90	123.96	120.24

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	3678	0	3676	11	0
1	B	3695	0	3699	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3652	0	3660	6	0
1	D	3679	0	3674	5	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	8	0	12	0	0
3	B	12	0	18	0	0
3	C	8	0	12	0	0
3	D	8	0	12	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
5	A	14	0	19	0	0
5	B	14	0	19	0	0
6	A	262	0	0	0	0
6	B	260	0	0	0	0
6	C	175	0	0	0	0
6	D	288	0	0	1	0
All	All	15955	0	14921	35	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 1.

The worst 5 of 35 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:A:290:VAL:CG1	1:A:418:LEU:HD13	2.26	0.65
2:C:1102:HEM:HBC2	2:C:1102:HEM:HMC2	1.84	0.60
1:C:290:VAL:CG1	1:C:418:LEU:HD13	2.36	0.55
2:C:1102:HEM:HMB2	2:C:1102:HEM:HBB2	1.89	0.55
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.89	0.54

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	453/472 (96%)	443 (98%)	10 (2%)	0	100	100
1	B	456/472 (97%)	445 (98%)	11 (2%)	0	100	100
1	C	445/472 (94%)	431 (97%)	14 (3%)	0	100	100
1	D	451/472 (96%)	442 (98%)	9 (2%)	0	100	100
All	All	1805/1888 (96%)	1761 (98%)	44 (2%)	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	404/416 (97%)	404 (100%)	0	100	100
1	B	407/416 (98%)	407 (100%)	0	100	100
1	C	402/416 (97%)	402 (100%)	0	100	100
1	D	405/416 (97%)	405 (100%)	0	100	100
All	All	1618/1664 (97%)	1618 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	204	GLN
1	D	310	GLN
1	D	359	GLN
1	D	285	HIS
1	B	381	ASN

### 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](#)

21 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	EDO	A	503	-	3,3,3	0.10	0	2,2,2	0.17	0
2	HEM	B	501	1	50,50,50	1.51	5 (10%)	67,82,82	1.53	14 (20%)
3	EDO	D	502	-	3,3,3	0.08	0	2,2,2	0.17	0
4	SO4	A	504	-	4,4,4	0.34	0	6,6,6	0.06	0
3	EDO	D	503	-	3,3,3	0.08	0	2,2,2	0.19	0
3	EDO	B	504	-	3,3,3	0.06	0	2,2,2	0.17	0
4	SO4	D	505	-	4,4,4	0.34	0	6,6,6	0.08	0
2	HEM	A	501	1	50,50,50	1.53	5 (10%)	67,82,82	1.44	12 (17%)
5	BTB	A	506	-	13,13,13	0.66	0	7,16,16	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	C	1102	1	50,50,50	1.58	7 (14%)	67,82,82	1.47	13 (19%)
4	SO4	D	504	-	4,4,4	0.33	0	6,6,6	0.07	0
3	EDO	C	1103	-	3,3,3	0.09	0	2,2,2	0.09	0
3	EDO	C	1104	-	3,3,3	0.11	0	2,2,2	0.25	0
3	EDO	A	502	-	3,3,3	0.10	0	2,2,2	0.18	0
4	SO4	A	505	-	4,4,4	0.34	0	6,6,6	0.11	0
3	EDO	B	502	-	3,3,3	0.08	0	2,2,2	0.15	0
4	SO4	B	506	-	4,4,4	0.36	0	6,6,6	0.09	0
5	BTB	B	505	-	13,13,13	1.03	1 (7%)	7,16,16	0.14	0
2	HEM	D	501	1	50,50,50	1.52	6 (12%)	67,82,82	1.47	12 (17%)
3	EDO	B	503	-	3,3,3	0.07	0	2,2,2	0.14	0
4	SO4	C	1101	-	4,4,4	0.34	0	6,6,6	0.06	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	EDO	A	503	-	-	0/1/1/1	-
5	BTB	B	505	-	-	1/21/21/21	-
2	HEM	B	501	1	-	2/14/54/54	-
3	EDO	D	502	-	-	0/1/1/1	-
2	HEM	D	501	1	-	2/14/54/54	-
5	BTB	A	506	-	-	4/21/21/21	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
3	EDO	C	1103	-	-	0/1/1/1	-
3	EDO	C	1104	-	-	1/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
2	HEM	C	1102	1	-	2/14/54/54	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
2	HEM	A	501	1	-	2/14/54/54	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1102	HEM	FE-NB	5.53	2.11	1.94
2	A	501	HEM	FE-NB	5.35	2.11	1.94

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	FE-NB	5.23	2.11	1.94
2	D	501	HEM	FE-NB	5.11	2.10	1.94
2	C	1102	HEM	FE-NC	4.44	2.09	1.95

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CHC-C4B-NB	4.87	129.66	124.42
2	B	501	HEM	CHC-C4B-NB	4.81	129.60	124.42
2	C	1102	HEM	CHC-C4B-NB	4.63	129.41	124.42
2	A	501	HEM	CHC-C4B-NB	4.31	129.06	124.42
2	A	501	HEM	CHD-C1D-ND	3.77	128.48	124.42

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	506	BTB	C1-C2-C4-O4
5	A	506	BTB	C3-C2-C4-O4
5	A	506	BTB	N-C2-C4-O4
5	A	506	BTB	N-C7-C8-O8
3	C	1104	EDO	O1-C1-C2-O2

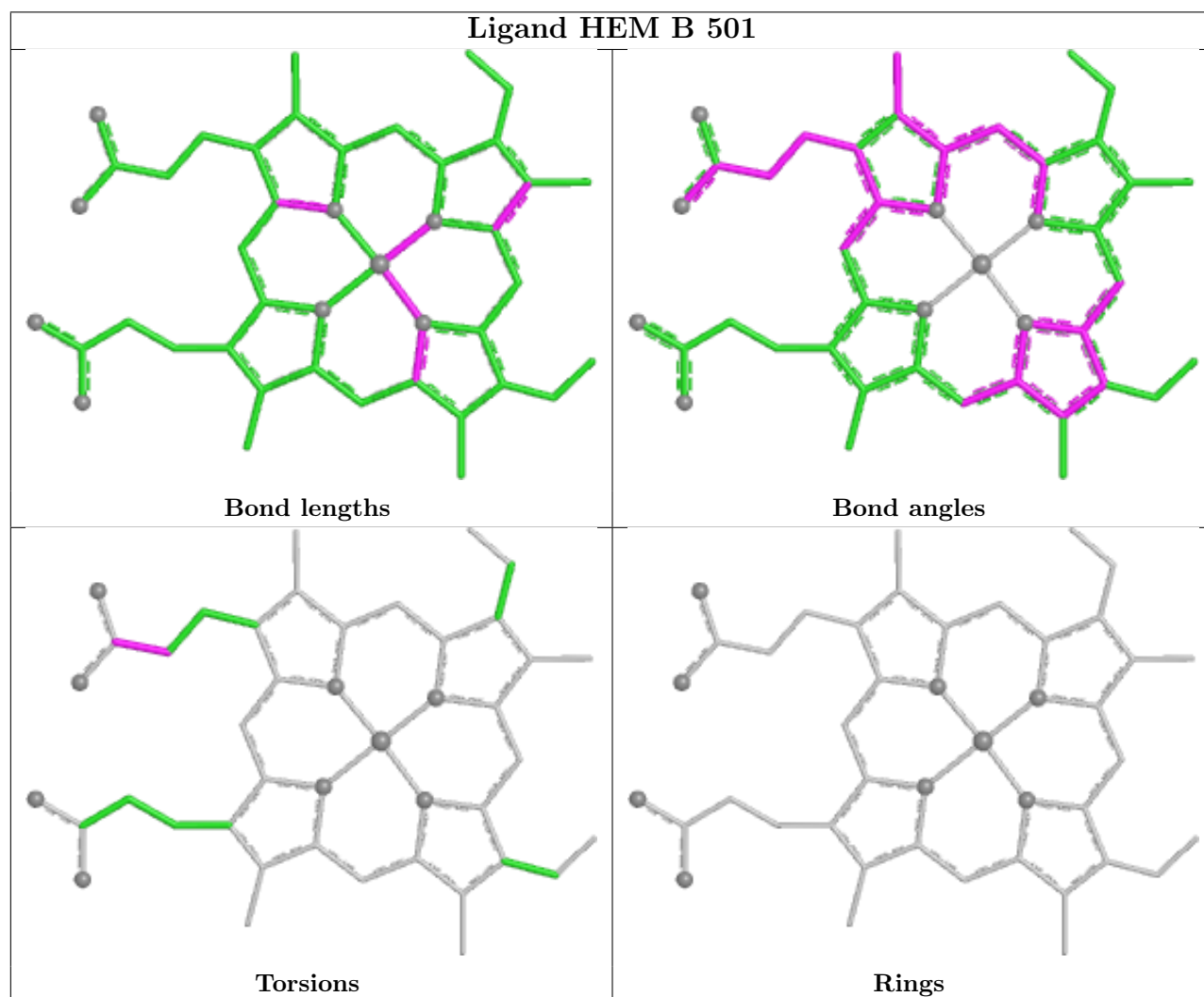
There are no ring outliers.

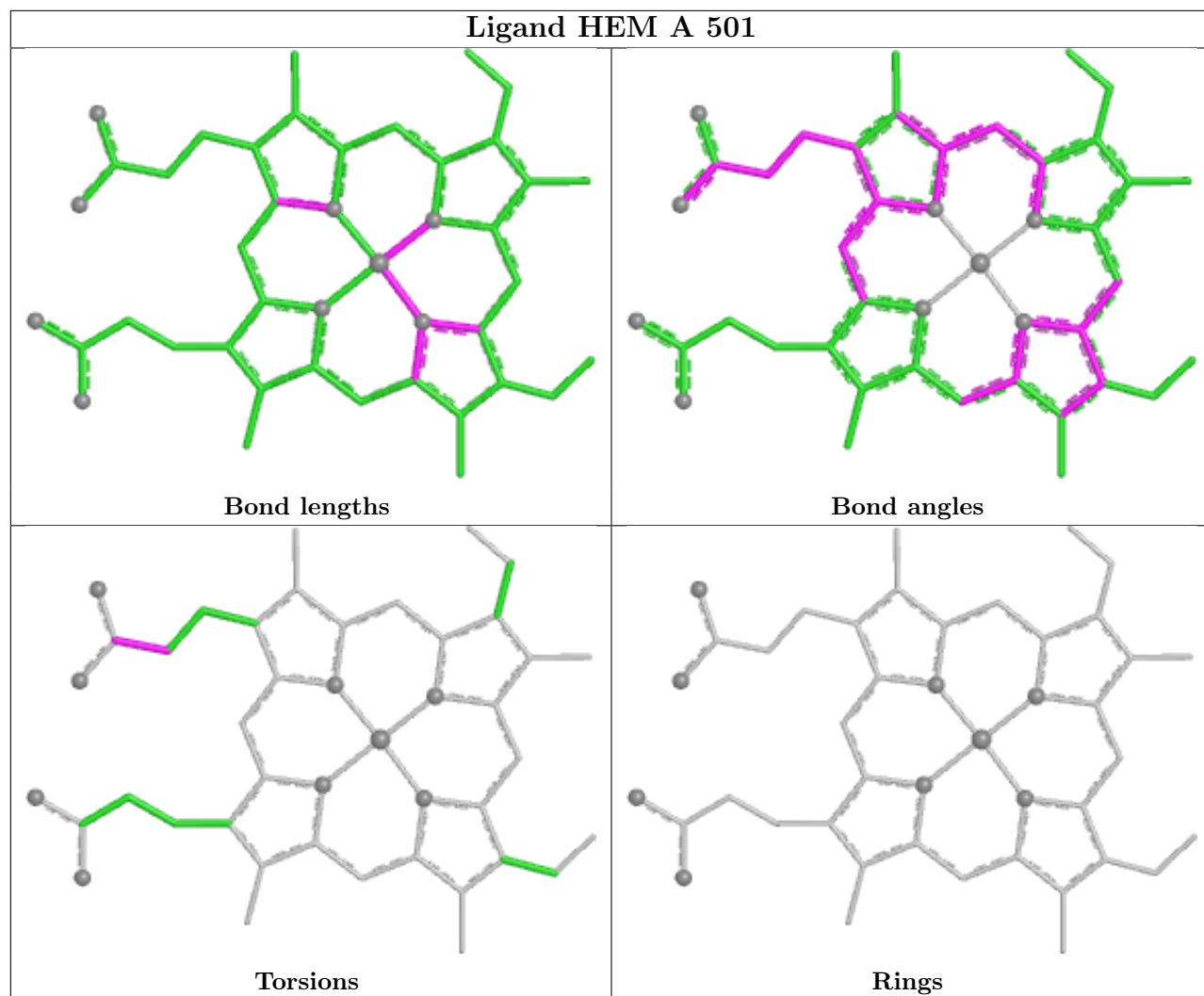
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	3	0
2	A	501	HEM	2	0
2	C	1102	HEM	3	0
2	D	501	HEM	2	0

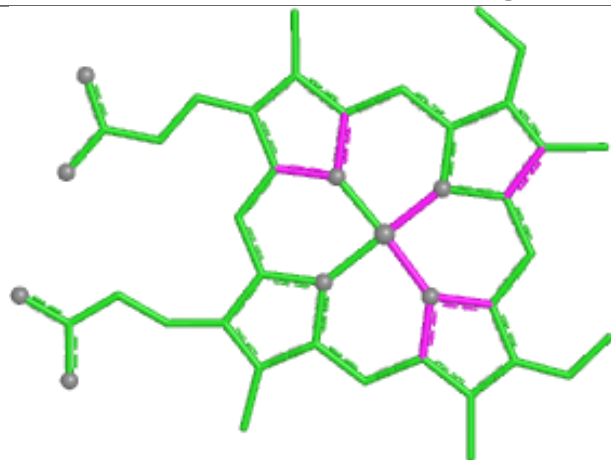
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

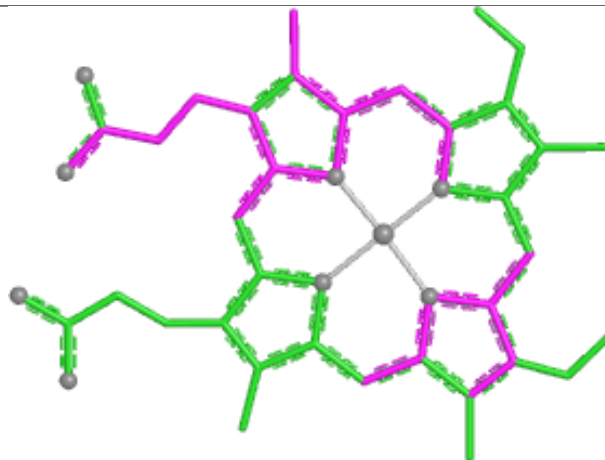




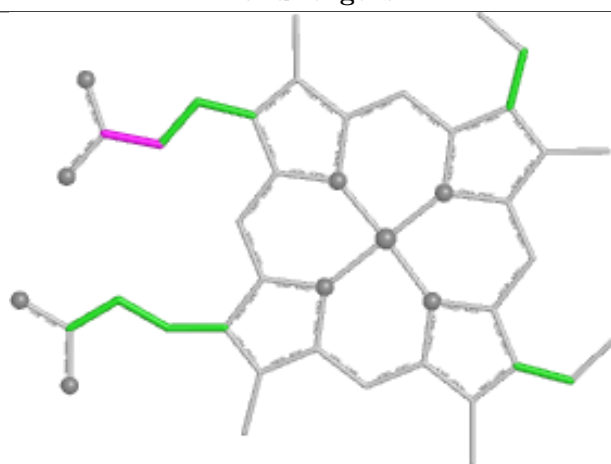
## Ligand HEM C 1102



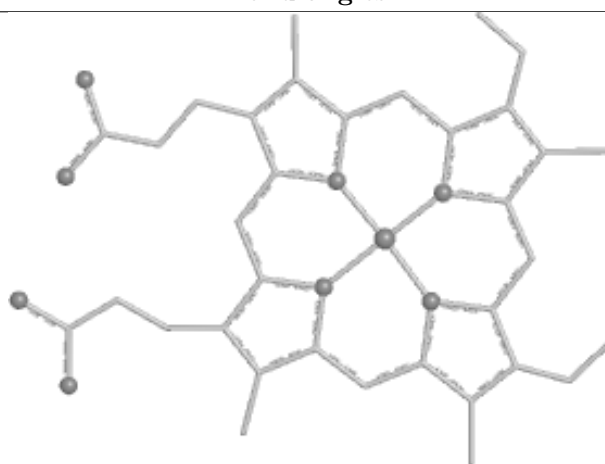
Bond lengths



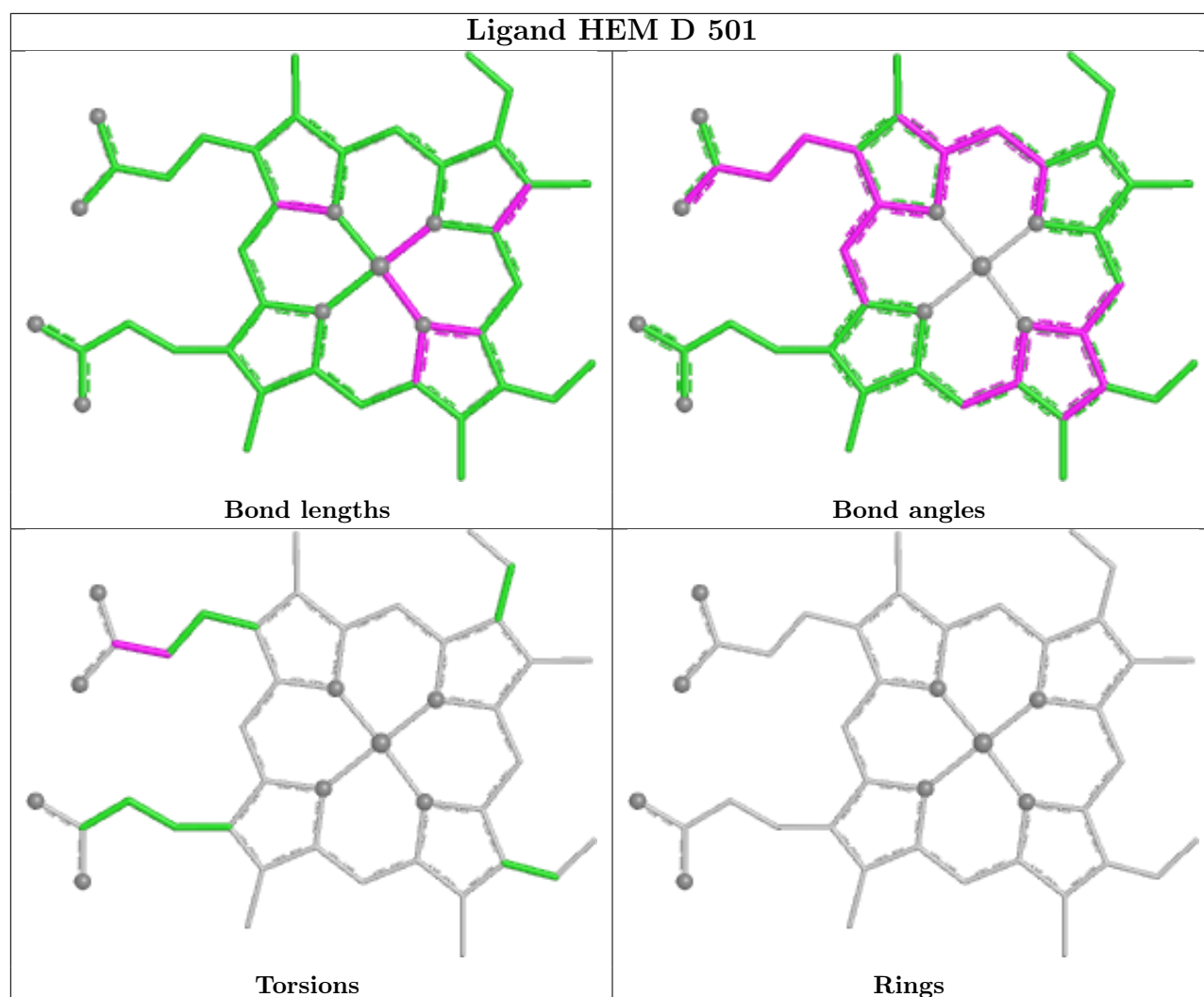
Bond angles



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	450/472 (95%)	0.14	8 (1%) 67 73	7, 19, 33, 53	66 (14%)
1	B	451/472 (95%)	0.13	9 (1%) 65 71	6, 19, 32, 49	70 (15%)
1	C	445/472 (94%)	0.52	22 (4%) 35 37	8, 25, 39, 57	61 (13%)
1	D	449/472 (95%)	0.08	11 (2%) 59 66	6, 18, 31, 45	57 (12%)
All	All	1795/1888 (95%)	0.21	50 (2%) 55 59	6, 20, 35, 57	254 (14%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	LEU	5.0
1	B	231	ASP	4.5
1	A	2	ILE	4.2
1	D	104	LEU	3.7
1	B	383	SER	3.7

### 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](#)

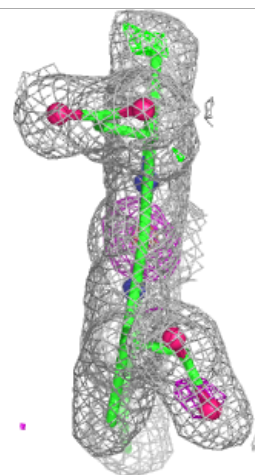
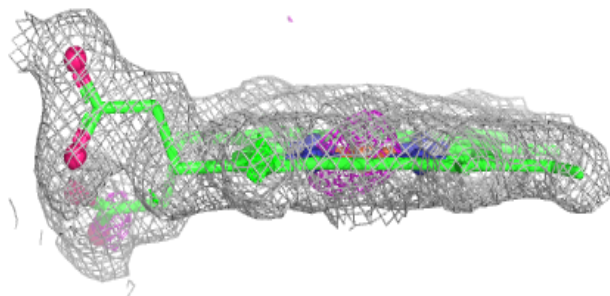
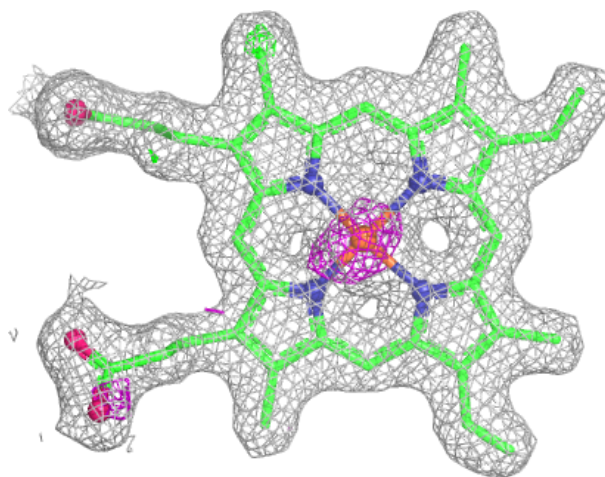
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
5	BTB	A	506	14/14	0.66	0.28	28,29,30,30	14
3	EDO	B	503	4/4	0.73	0.23	48,48,48,50	0
4	SO4	D	504	5/5	0.74	0.15	63,63,63,64	0
5	BTB	B	505	14/14	0.75	0.15	39,40,40,41	0
3	EDO	D	502	4/4	0.77	0.20	38,39,39,39	0
3	EDO	C	1104	4/4	0.78	0.18	38,39,39,40	0
3	EDO	A	503	4/4	0.81	0.16	33,33,34,34	0
4	SO4	D	505	5/5	0.82	0.12	67,68,70,70	0
3	EDO	B	502	4/4	0.86	0.13	29,30,30,31	0
3	EDO	D	503	4/4	0.86	0.13	30,32,32,34	0
4	SO4	C	1101	5/5	0.88	0.11	63,63,63,65	0
3	EDO	B	504	4/4	0.89	0.12	33,35,35,35	0
4	SO4	A	505	5/5	0.90	0.10	45,45,47,47	0
4	SO4	A	504	5/5	0.92	0.09	49,49,50,50	0
3	EDO	A	502	4/4	0.93	0.09	22,23,23,23	0
4	SO4	B	506	5/5	0.95	0.11	34,35,37,37	0
3	EDO	C	1103	4/4	0.96	0.06	28,29,29,30	0
2	HEM	C	1102	43/43	0.96	0.08	17,19,21,22	0
2	HEM	A	501	43/43	0.96	0.07	13,14,15,16	0
2	HEM	D	501	43/43	0.97	0.07	12,13,14,14	0
2	HEM	B	501	43/43	0.97	0.07	11,13,13,15	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 C 1102:**

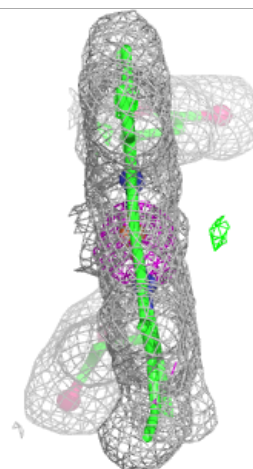
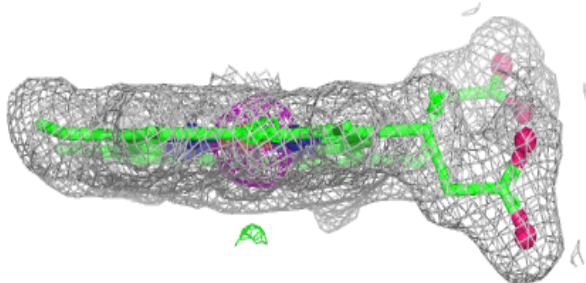
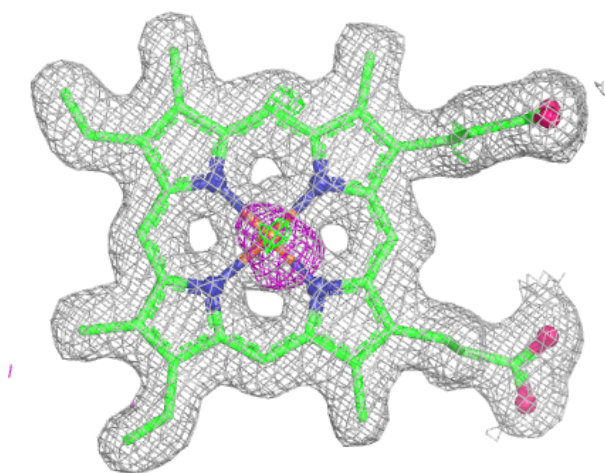
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





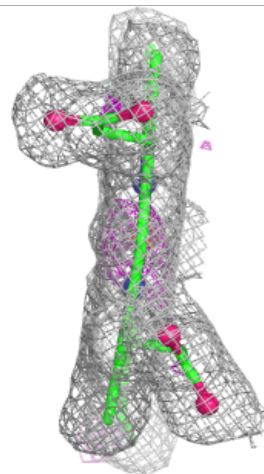
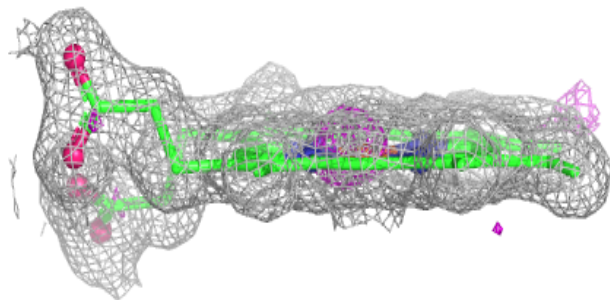
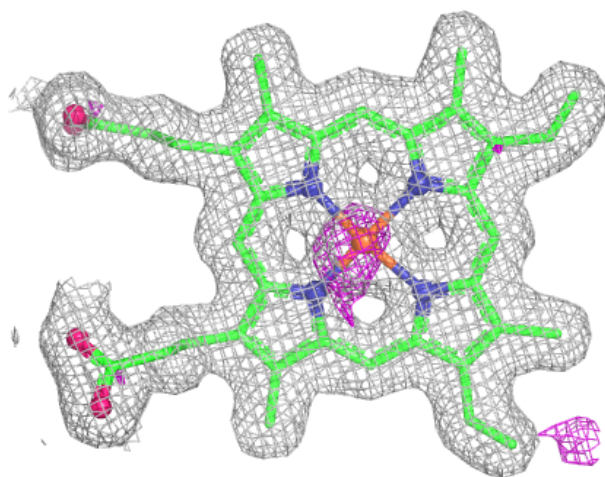
**Electron density around HEM A 501:**

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



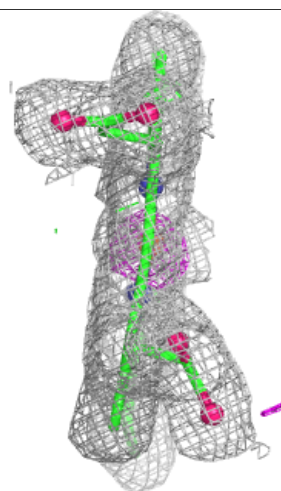
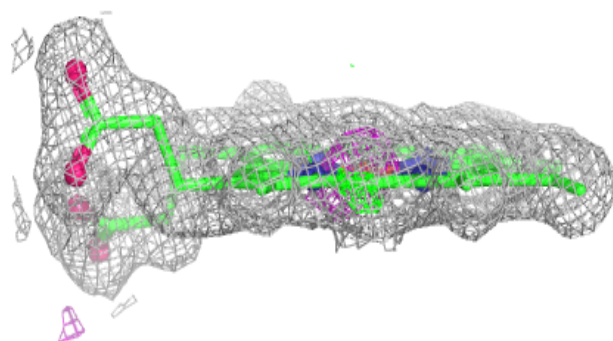
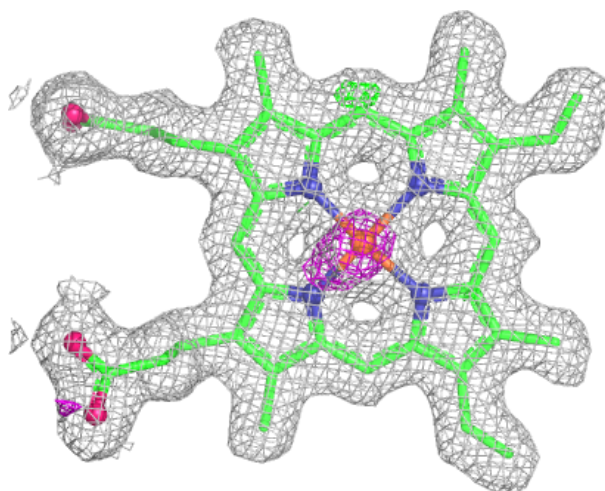
**Electron density around HEM D 501:**

$2mF_o-DF_c$  (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.