



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 03:38 PM JST

PDB ID : 7Y0T / pdb_00007y0t
Title : Crystal structure of the P450 BM3 heme domain mutant F87A in complex with N-imidazolyl-hexanoyl-L-phenylalanyl-L-phenylalanine
Authors : Jiang, Y.; Dong, S.; Feng, Y.; Cong, Z.
Deposited on : 2022-06-06
Resolution : 1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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

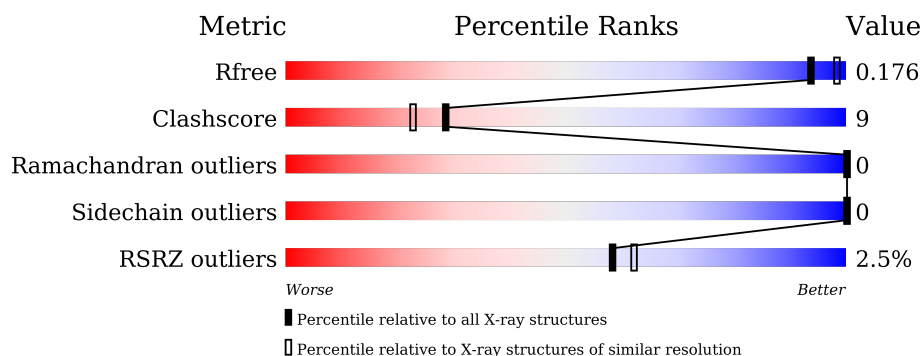
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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.



2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7890 atoms, of which 0 are hydrogens and 0 are deuteriums.

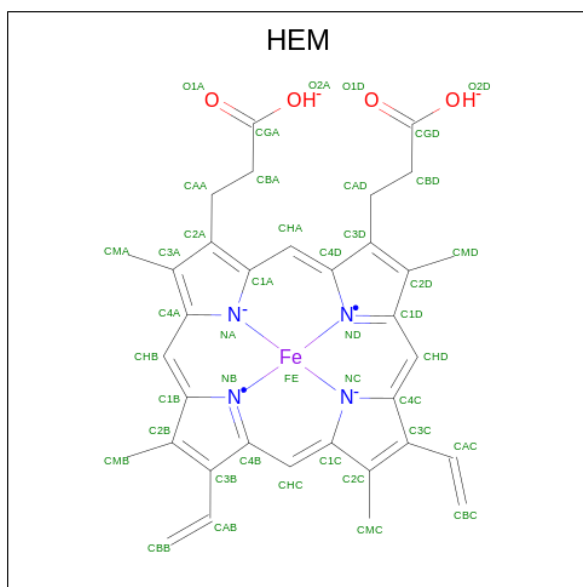
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	446	Total	C	N	O	S	0	2	0
			3541	2268	603	652	18			
1	A	447	Total	C	N	O	S	3	3	0
			3550	2274	602	656	18	</		

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			35	27	4	4			
2	D	3	Total	C	N	O	0	0	0
			35	27	4	4			

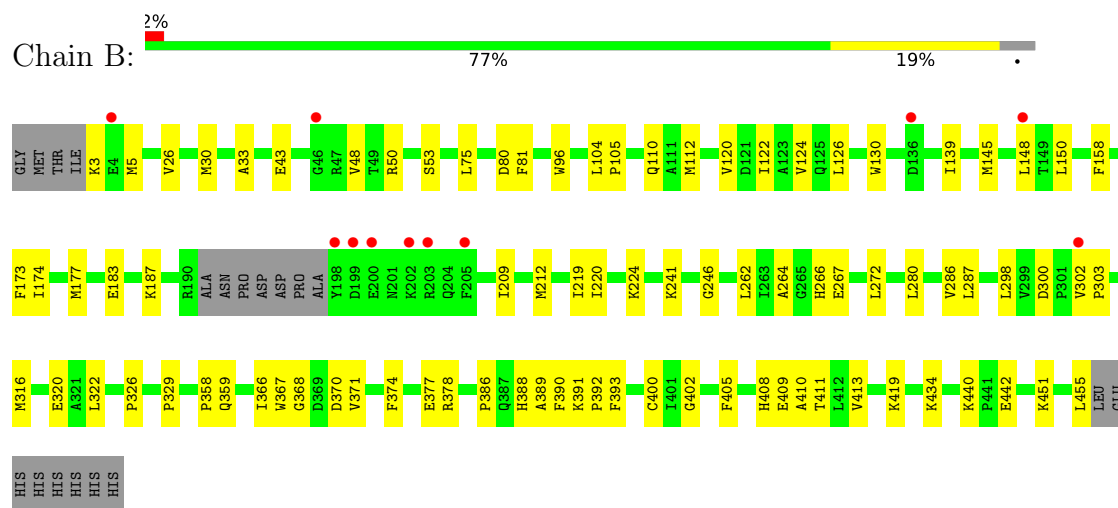
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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: Bifunctional cytochrome P450/NADPH-P450 reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.48Å 144.35Å 63.24Å 90.00° 100.34° 90.00°	Depositor
Resolution (Å)	38.90 – 1.89 38.90 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.6 (38.90-1.89) 96.6 (38.90-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.168 , 0.198 0.171 , 0.176	Depositor DCC
R_{free} test set	3983 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage

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: HEM, I7X

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	0.56	3/3640 (0.1%)	0.69	0/4927
1	B	0.57	5/3628 (0.1%)	0.68	0/4911
2	C	1.69	1/24 (4.2%)	1.31	0/29
2	D	1.75	1/24 (4.2%)	1.37	

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	3550	0	3486	63	0
1	B	3541	0	3481	65	0
2	C	35	0	17	2	0
2	D	35	0	17	0	0
3	A	43	0	30	2	0
3	B	43	0	30	3	0
4	A	322	0	0	4	0
4	B	321	0	0	4	0
All	All	7890	0	7061	126	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 9.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:CD2	1:B:413:VAL:HG11	2.32	0.60
1:B:150:LEU:HD13	1:B:174:ILE:HD13	1.84	0.60
1:A:298:LEU:HD22	1:A:303:PRO:HB3	1.84	0.59
1:B:434:LYS:HB2	1:B:442:GLU:HB2	1.85	0.59
3:A:501:HEM:HMC2	3:A:501:HEM:HBC2	1.87	0.57
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.87	0.57
1:A:148:LEU:CD1	1:A:413:VAL:HG11	2.35	0.57
1:A:43:GLU:HG2	1:A:48:VAL:HG22	1.88	0.56
1:A:312:LYS:NZ	4:A:612:HOH:O	2.38	0.55
1:B:126:LEU:HD21	1:B:145:MET:HE1	1.90	0.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLN:H	1:B:110:GLN:CD	2.24	0.46
1:B:390:PHE:CZ	1:B:392:PRO:HG3	2.50	0.46
1:B:30:MET:HG2	1:B:359:GLN:HG2	1.98	0.45
1:B:366:ILE:HD12	1:B:386:PRO:HG2	1.99	0.45
1:A:52:LEU:HD11	1:A:353:LEU:HD13	1.98	0.45
1:B:80:ASP:OD2	4:B:601:HOH:O	2.20	0.45
1:B:150:LEU:HD21	1:B:177:MET:HE1	1.99	0.45
1:B:33:ALA:HB3	1:B:359:GLN:HG3	1.99	0.45
1:B:148:LEU:HD23	1:B:413:VAL:HG11	1.98	0.45
1:A:253:ASN:O	1:A:257:GLN:HG2	2.17	

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:VAL:CG2	2:C:2:PHE:HB3	2.50	0.42
1:B:434:LYS:HD3	1:B:440:LYS:HE3	2.02	0.41
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.91	0.41
1:A:104:LEU:HB3	1:A:105:PRO:HD3	2.03	0.41
1:A:139:ILE:O	1:A:445:VAL:HA	2.19	0.41
1:A:177:MET:HE2	1:A:177:MET:HB3	1.89	0.41
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.85	0.41
1:B:402:GLY:HA3	3:B:501:HEM:C3C	2.56	0.41
1:A:39:ILE:HA	1:A:51:TYR:O	2.21	0.41
1:A:278:TYR:HA	1:A:444:PHE:CZ	2.56	0.41
1			

There are no Ramachandran outliers to report.

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	377/407 (93%)	377 (100%)	0	100	100
1	B	376/407 (92%)	376 (100%)	0	100	100
2	C	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100
All	All	757/818 (92%)	757 (100%)	0	100	100

There

5.6 Ligand geometry

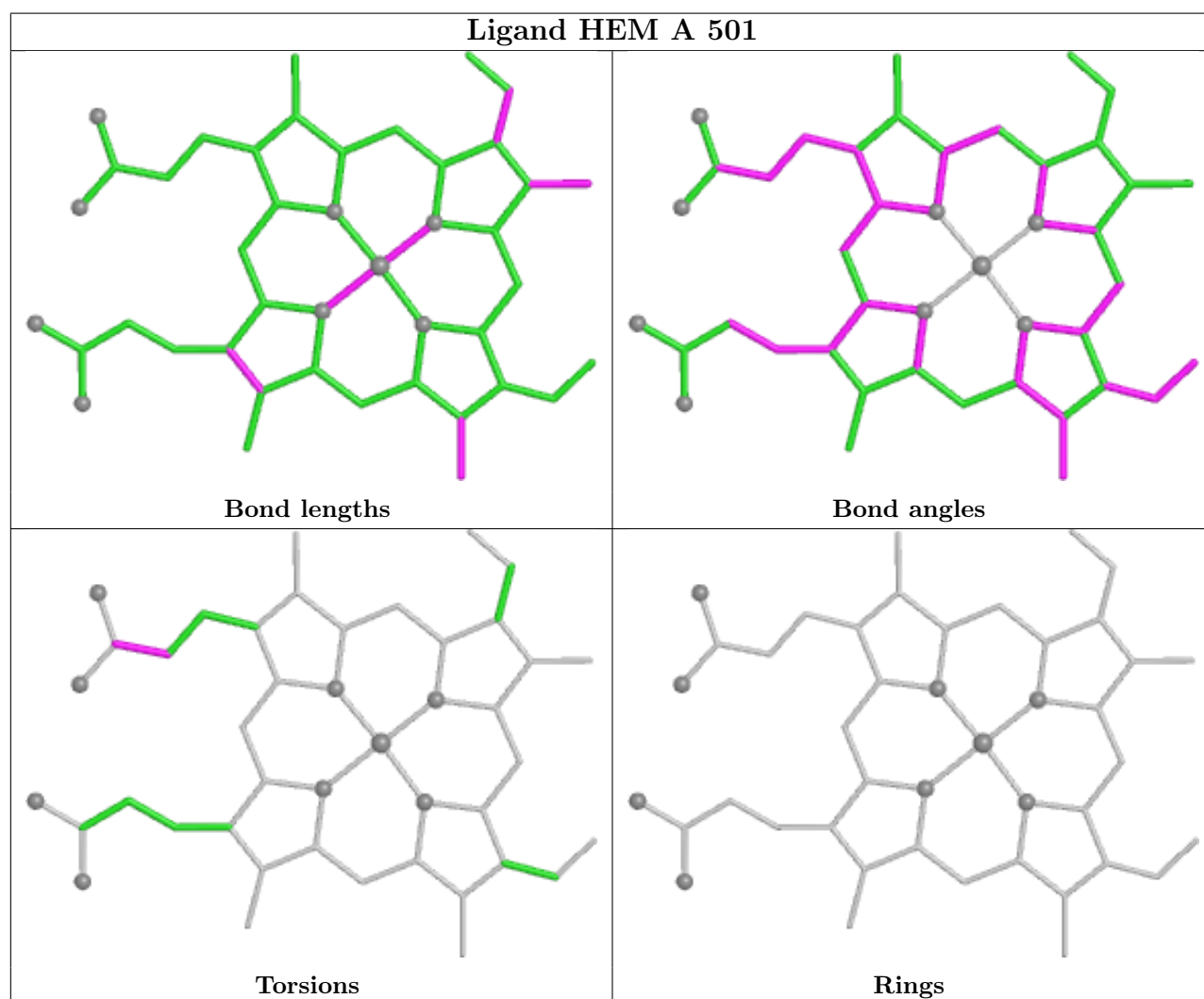
2 ligands are modelled in this entry.

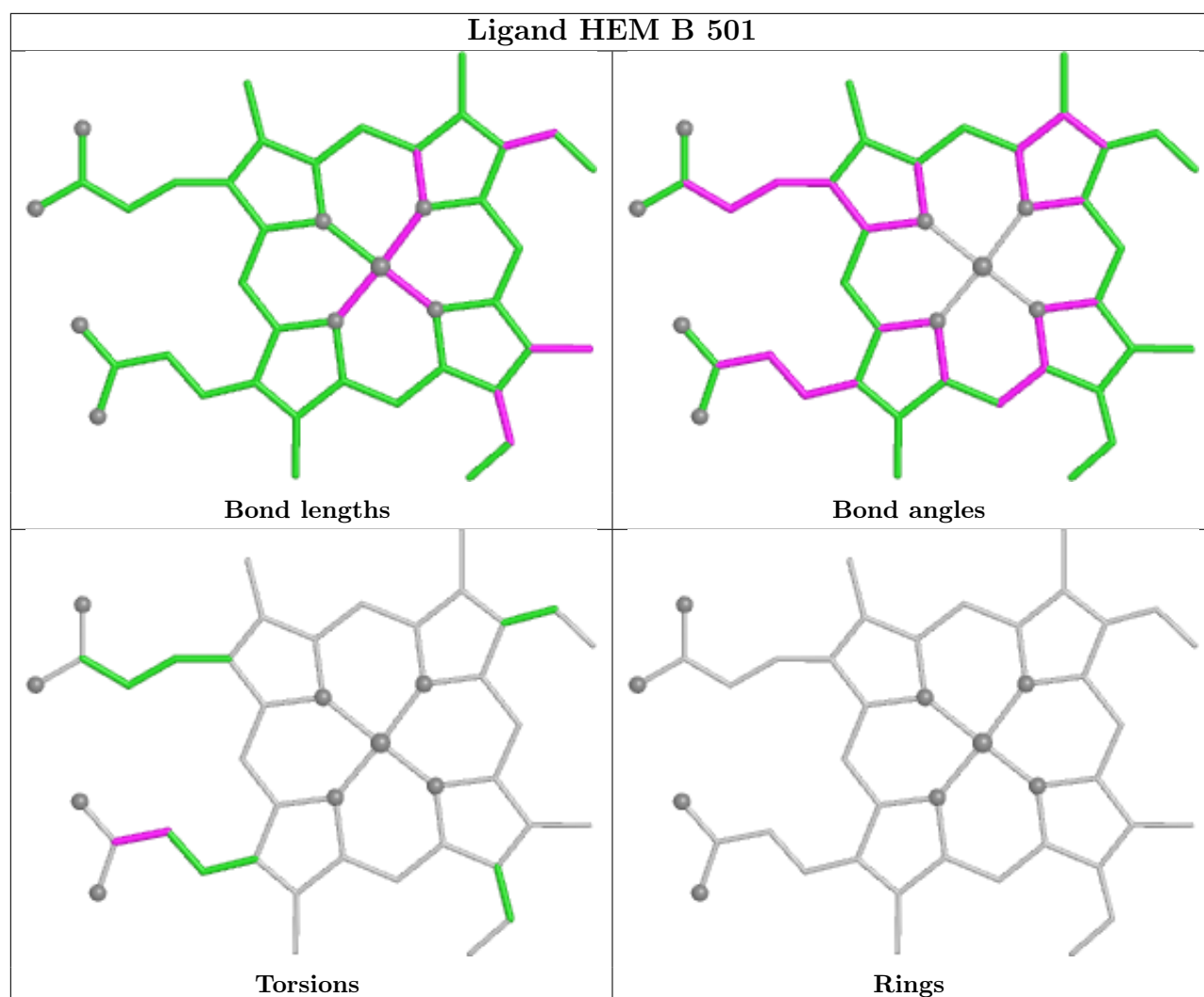
In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists 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	HEM	A	501	1,4	50,50,50	1.30	6 (12%)	66,82,82	1.46	14 (21%)

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	HEM	CBA-CAA-C2A	-3.48	102.95	112.63
3	B	501	HEM	C4A-NA-C1A	3.15	108.44	105.35
3	B	501	HEM	CHD-C4C-NC	3.04	127.73	124.44
3	A	501	HEM	CHD-C1D-ND	3.02	127.70	124.42
3	A	501	HEM	CBA-CAA-C2A	-3.00	104.30	112.63
3	A	501	HEM	C1B-NB-C4B	2.97	108.14	105.07
3	B	501	HEM	CBD-CAD-C3D	-2.82	104.80	112.63
3	A	501	HEM	CHC-C4B-NB	2.78	127.44	124.42
3	A	501	HEM	C4C			

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	447/465 (96%)	0.11	11 (2%) 58 62	19, 33, 51, 75	3 (0%)
1	B	446/465 (95%)	0.12	11 (2%) 58 62	19, 33, 53, 75	2 (0%)
2	C	2/3 (66%)	0.23	0 100 100	35, 35, 35, 37	0
2	D					

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](#)

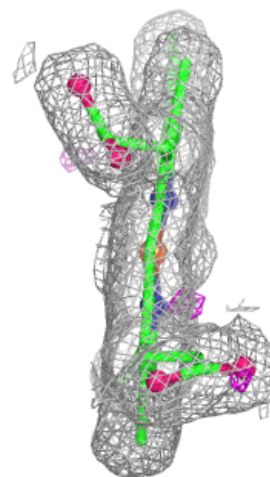
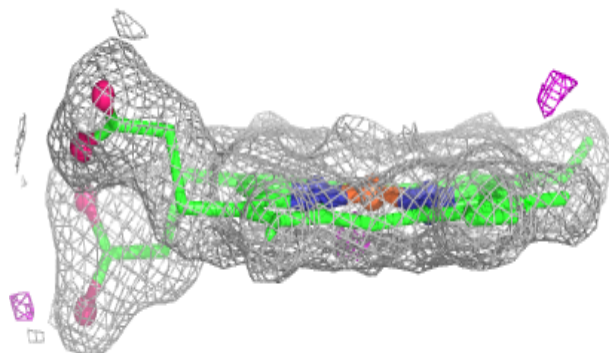
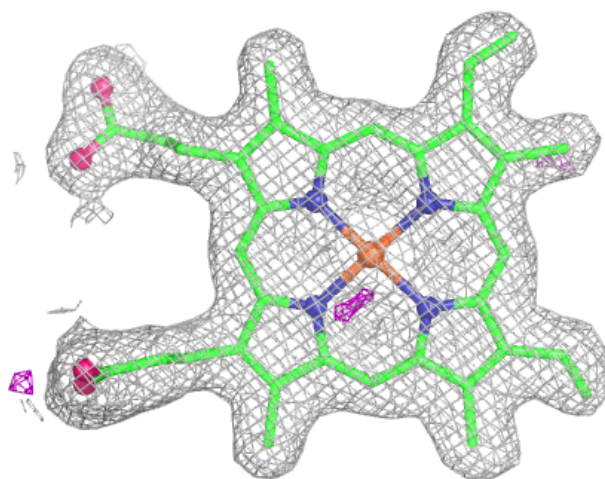
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	HEM	B	501	43/43	0.98	0.06	19,24,28,34	0
3	HEM	A	501	43/43	0.99	0.04	22,25,27,33	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

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)



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)

