wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 08:44 PM EDT

PDB ID	:	1QF7
Title	:	STRUCTURE OF THE MUTANT HIS392GLN OF CATALASE HPII FROM E. COLI
Authors	:	Mate, M.J.; Loewen, P.C.; Fita, I.
Deposited on	:	1999-03-26
Resolution	:	2.20 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

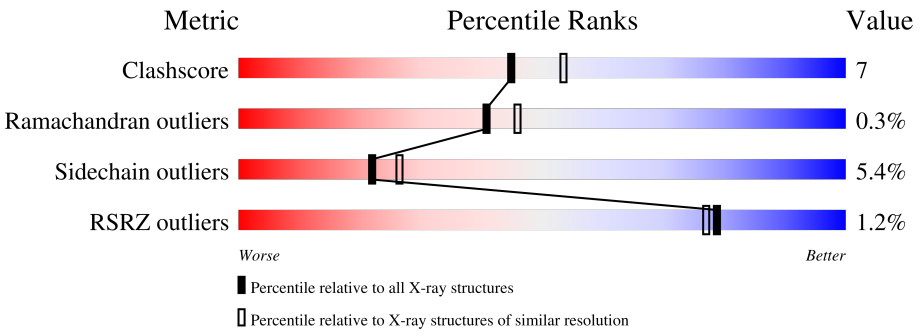
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 >=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 <=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	753	% 76% 16% • • •
1	B	753	% 75% 18% • • •
1	C	753	% 75% 17% • • •
1	D	753	% 76% 17% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25843 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.

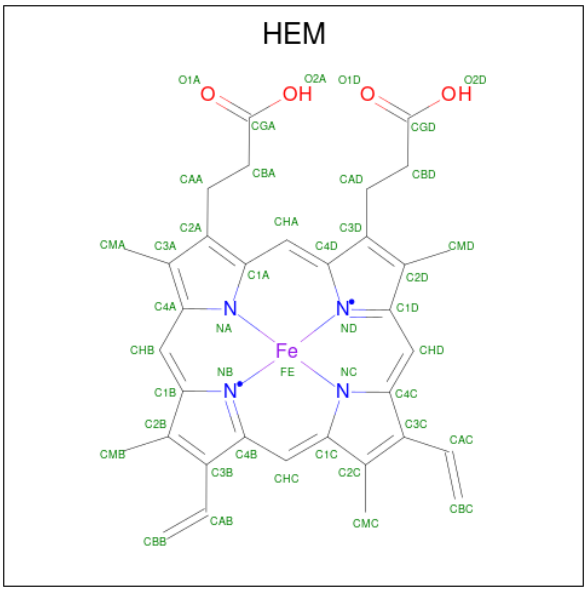
- Molecule 1 is a protein called PROTEIN (CATALASE HPII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	5748	3650	1004	1082	12	0	1	0
1	B	727	5748	3650	1004	1082	12	0	1	0
1	C	727	5748	3650	1004	1082	12	0	1	0
1	D	727	5748	3650	1004	1082	12	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLN	HIS	engineered mutation	UNP P21179
B	392	GLN	HIS	engineered mutation	UNP P21179
C	392	GLN	HIS	engineered mutation	UNP P21179
D	392	GLN	HIS	engineered mutation	UNP P21179

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is water.

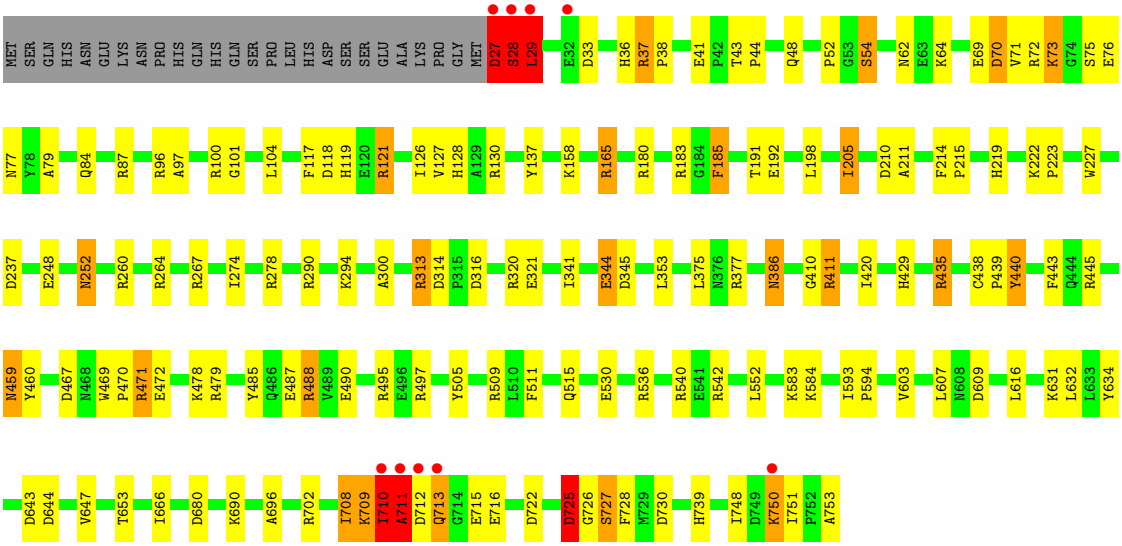
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	728	728	728	0	0
			Total	O		
3	B	625	625	625	0	0
			Total	O		
3	C	634	634	634	0	0
			Total	O		
3	D	692	692	692	0	0

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.

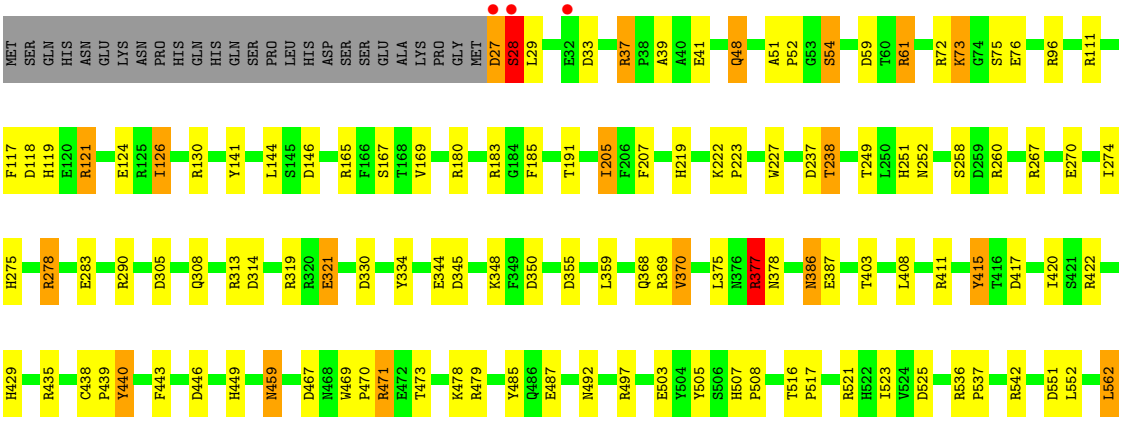
• Molecule 1: PROTEIN (CATALASE HPII)

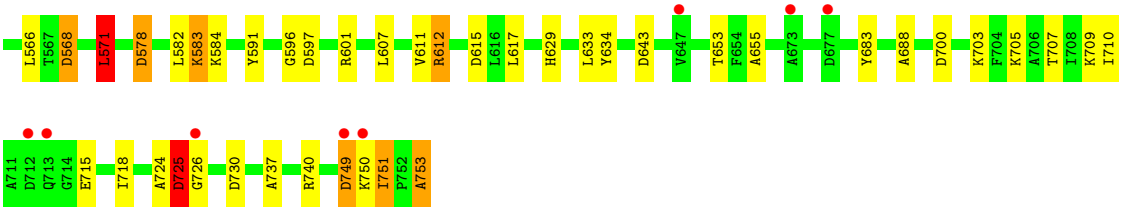
Chain A:



• Molecule 1: PROTEIN (CATALASE HPII)

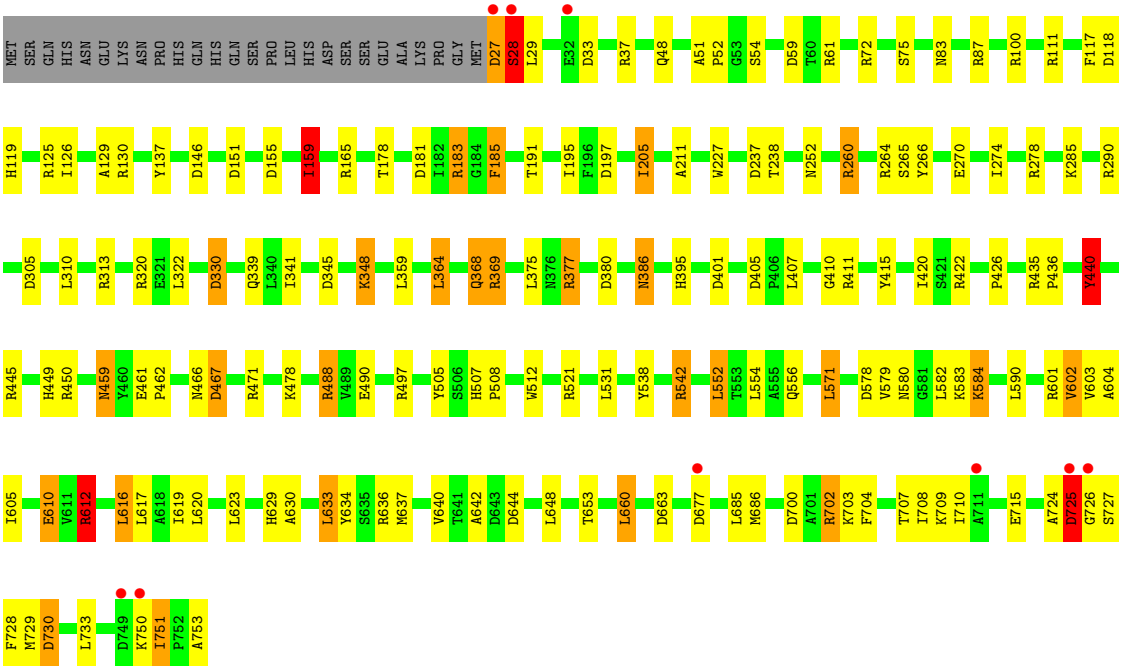
Chain B:





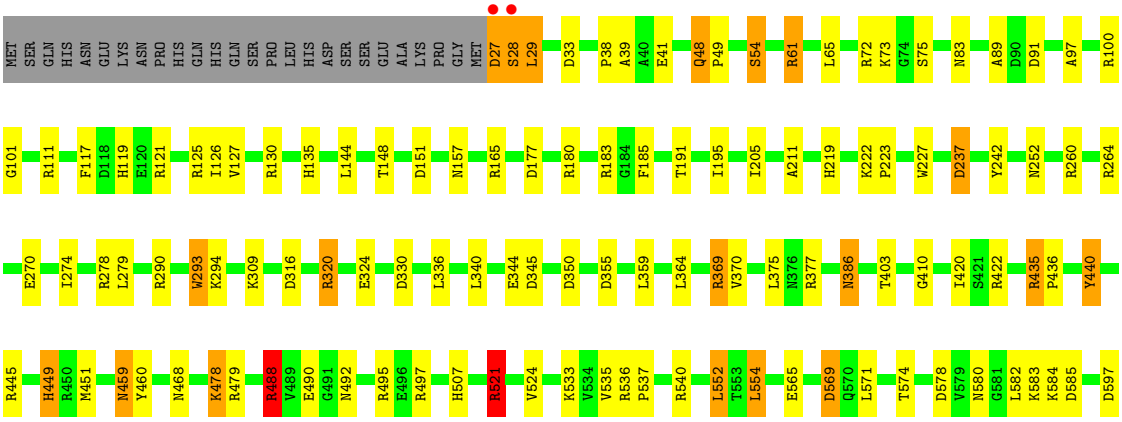
• Molecule 1: PROTEIN (CATALASE HPII)

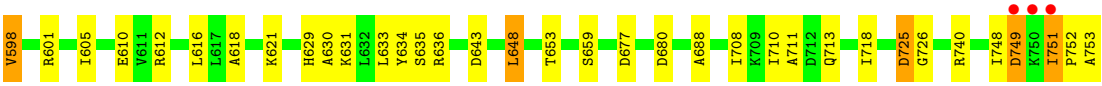
Chain C:



• Molecule 1: PROTEIN (CATALASE HPII)

Chain D:




V598
R601
I605
E610
V611
R612
L616
L617
A618
K621
H629
A630
K631
L632
L633
Y634
S635
R636
D643
L648
T653
S659
D677
D680
A688
I708
K709
I710
A711
D712
Q713
I718
D725
G726
R740
I748
D749
K750
I751
P752
A753

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.40Å 132.92Å 121.67Å 90.00° 109.47° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.04 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.20) 92.4 (20.04-2.19)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.210 0.143 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	12.3	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25843	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.77	1/5907 (0.0%)	1.70	117/8032 (1.5%)
1	B	0.74	1/5907 (0.0%)	1.64	109/8032 (1.4%)
1	C	0.75	1/5907 (0.0%)	1.65	84/8032 (1.0%)
1	D	0.73	0/5907	1.66	100/8032 (1.2%)
All	All	0.75	3/23628 (0.0%)	1.66	410/32128 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	D	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	725	ASP	CA-CB	6.15	1.67	1.53
1	A	28	SER	CA-CB	5.47	1.61	1.52
1	B	753	ALA	C-O	5.05	1.32	1.23

The worst 5 of 410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	542	ARG	CD-NE-CZ	37.39	175.94	123.60
1	D	488	ARG	CD-NE-CZ	24.67	158.14	123.60
1	D	61	ARG	CD-NE-CZ	23.79	156.90	123.60
1	A	27	ASP	CA-CB-CG	20.44	158.37	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	377	ARG	NE-CZ-NH1	-19.28	110.66	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ASP	Peptide,Mainchain
1	A	28	SER	Mainchain
1	A	711	ALA	Mainchain
1	D	157	ASN	Mainchain

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	5748	0	5586	81	0
1	B	5748	0	5586	84	0
1	C	5748	0	5586	86	0
1	D	5748	0	5586	85	1
2	A	43	0	30	4	0
2	B	43	0	30	6	0
2	C	43	0	30	4	0
2	D	43	0	30	7	0
3	A	728	0	0	7	2
3	B	625	0	0	14	0
3	C	634	0	0	13	1
3	D	692	0	0	10	2
All	All	25843	0	22464	298	3

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 7.

The worst 5 of 298 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:C:725:ASP:HB2	1:C:728:PHE:HB3	1.30	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:LYS:HE2	1:B:583:LYS:H	1.25	0.98
1:C:724:ALA:O	1:C:725:ASP:HB3	1.65	0.96
1:B:415:TYR:HB2	3:B:1378:HOH:O	1.64	0.95
1:D:369:ARG:HB2	3:D:1392:HOH:O	1.76	0.86

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1360:HOH:O	3:D:1418:HOH:O[1_455]	2.06	0.14
1:D:28:SER:CA	3:C:1326:HOH:O[2_555]	2.07	0.13
3:A:1133:HOH:O	3:D:1418:HOH:O[1_455]	2.12	0.08

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	726/753 (96%)	703 (97%)	19 (3%)	4 (1%)	25	26
1	B	726/753 (96%)	701 (97%)	22 (3%)	3 (0%)	34	37
1	C	726/753 (96%)	705 (97%)	19 (3%)	2 (0%)	41	46
1	D	726/753 (96%)	700 (96%)	25 (3%)	1 (0%)	51	60
All	All	2904/3012 (96%)	2809 (97%)	85 (3%)	10 (0%)	41	46

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	725	ASP
1	A	711	ALA
1	B	725	ASP
1	C	75	SER
1	A	75	SER

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	613/636 (96%)	587 (96%)	26 (4%)	30	38
1	B	613/636 (96%)	580 (95%)	33 (5%)	22	26
1	C	613/636 (96%)	572 (93%)	41 (7%)	16	18
1	D	613/636 (96%)	579 (94%)	34 (6%)	21	26
All	All	2452/2544 (96%)	2318 (94%)	134 (6%)	22	26

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	386	ASN
1	D	488	ARG
1	D	648	LEU
1	B	478	LYS
1	B	459	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	386	ASN
1	D	546	GLN
1	C	556	GLN
1	D	459	ASN
1	C	507	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	HEM	C	754	1	41,50,50	1.59	9 (21%)	45,82,82	1.28	3 (6%)
2	HEM	A	754	1	41,50,50	1.50	6 (14%)	45,82,82	1.09	2 (4%)
2	HEM	D	754	1	41,50,50	1.60	6 (14%)	45,82,82	1.17	5 (11%)
2	HEM	B	754	1,3	41,50,50	1.66	6 (14%)	45,82,82	1.32	4 (8%)

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	C	754	1	-	2/12/54/54	-
2	HEM	A	754	1	-	2/12/54/54	-
2	HEM	D	754	1	-	2/12/54/54	-
2	HEM	B	754	1,3	-	2/12/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	754	HEM	C3C-C2C	-4.86	1.33	1.40
2	D	754	HEM	C3C-C2C	-4.15	1.34	1.40
2	A	754	HEM	C3C-C2C	-3.84	1.35	1.40
2	D	754	HEM	C3C-CAC	3.66	1.55	1.47
2	B	754	HEM	C3C-CAC	3.65	1.55	1.47

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	754	HEM	O1A-CGA-CBA	-3.43	112.07	123.08
2	C	754	HEM	O2A-CGA-O1A	3.15	131.16	123.30
2	D	754	HEM	CBA-CAA-C2A	2.70	117.23	112.62
2	B	754	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
2	A	754	HEM	CMA-C3A-C4A	-2.59	124.49	128.46

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	754	HEM	CAA-CBA-CGA-O2A
2	B	754	HEM	CAA-CBA-CGA-O1A
2	D	754	HEM	CAA-CBA-CGA-O2A
2	A	754	HEM	CAA-CBA-CGA-O1A
2	C	754	HEM	CAA-CBA-CGA-O2A

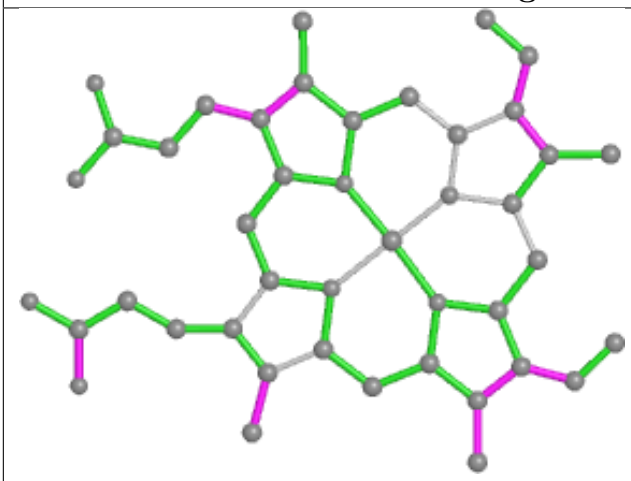
There are no ring outliers.

4 monomers are involved in 21 short contacts:

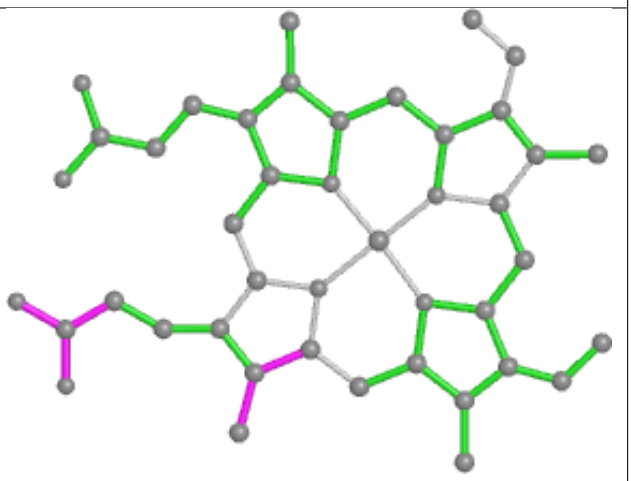
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	754	HEM	4	0
2	A	754	HEM	4	0
2	D	754	HEM	7	0
2	B	754	HEM	6	0

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 then 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.

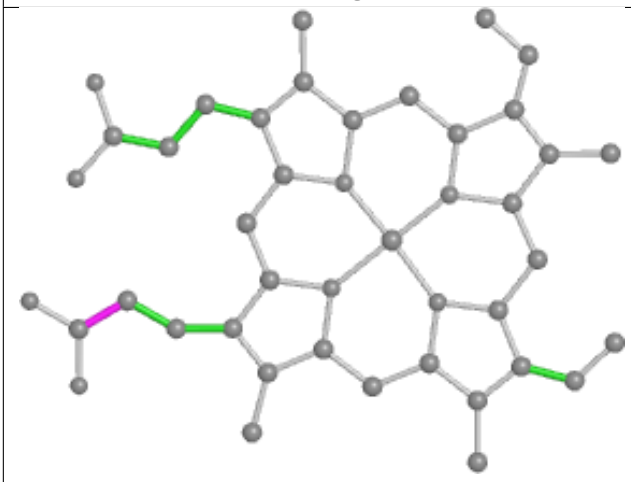
Ligand HEM C 754



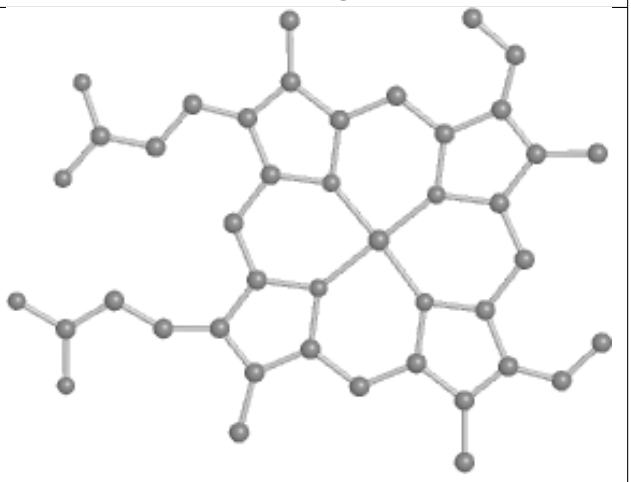
Bond lengths



Bond angles

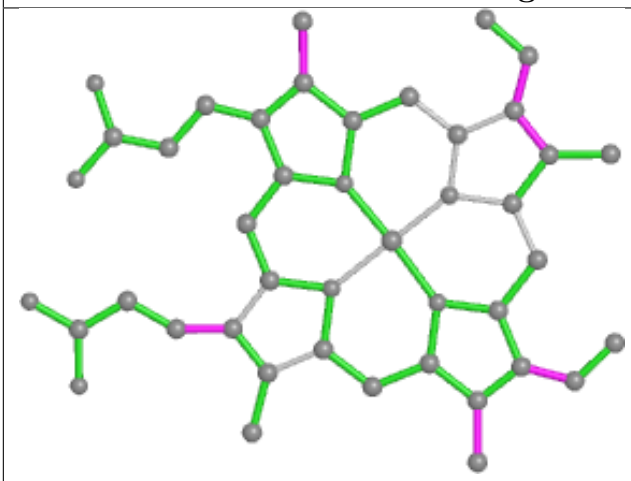


Torsions

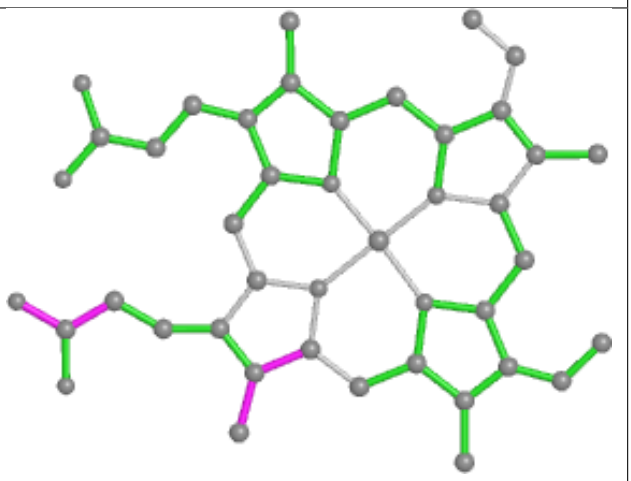


Rings

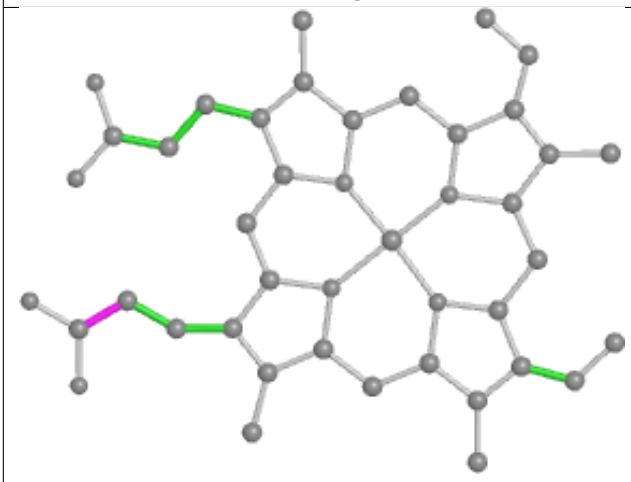
Ligand HEM A 754



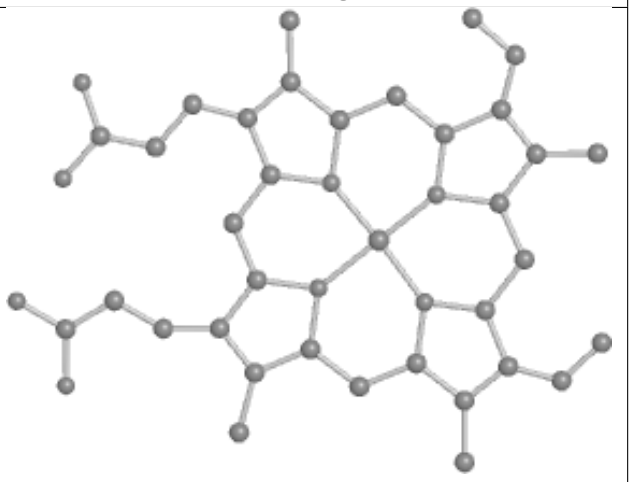
Bond lengths



Bond angles

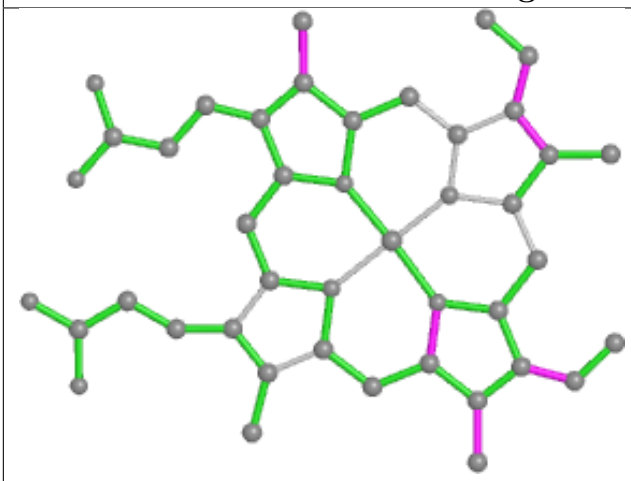


Torsions

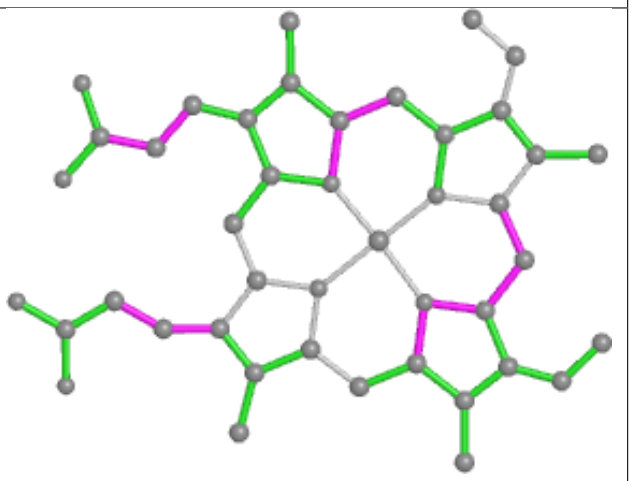


Rings

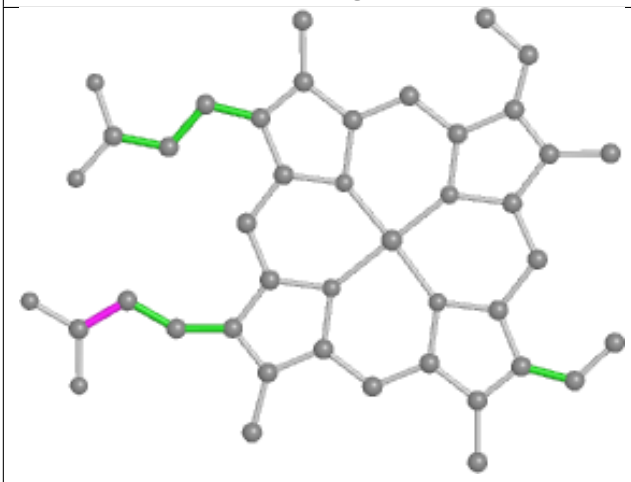
Ligand HEM D 754



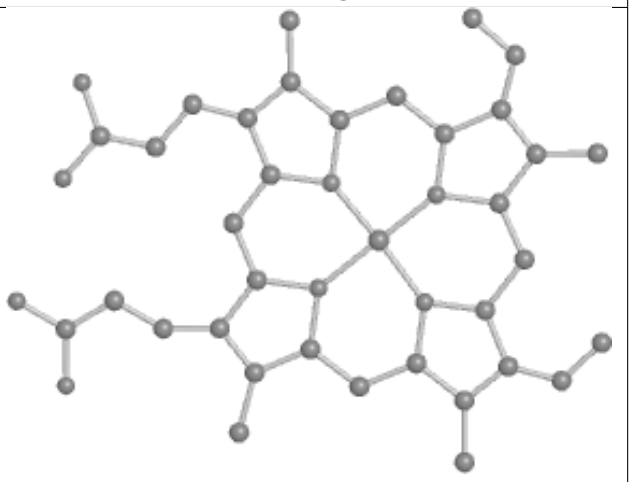
Bond lengths



Bond angles

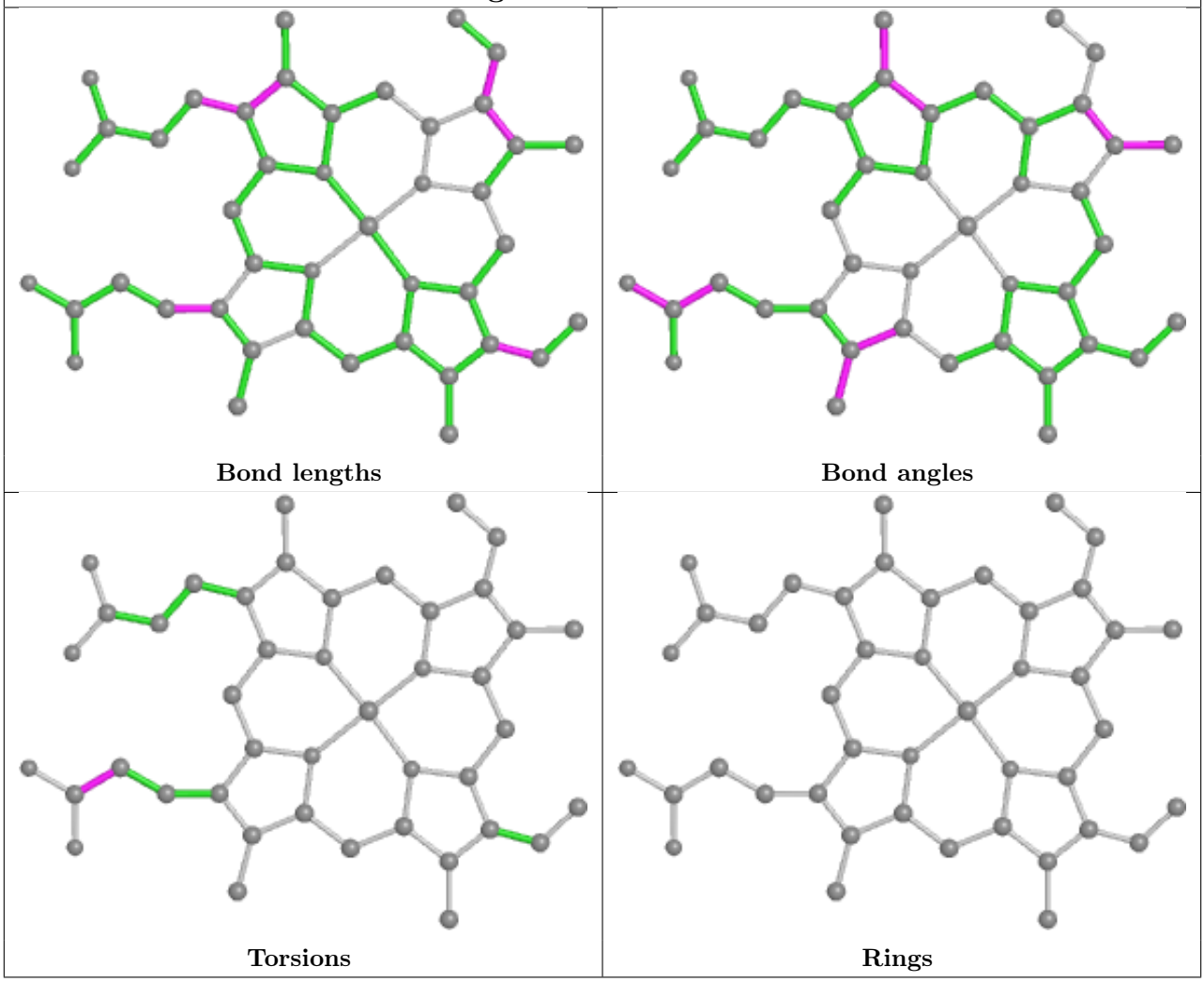


Torsions



Rings

Ligand HEM B 754



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, 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	727/753 (96%)	-0.70	9 (1%)	79	77	8, 16, 34, 64	0
1	B	727/753 (96%)	-0.63	11 (1%)	73	72	9, 17, 35, 63	0
1	C	727/753 (96%)	-0.66	9 (1%)	79	77	9, 17, 35, 63	0
1	D	727/753 (96%)	-0.75	5 (0%)	87	86	10, 16, 34, 62	0
All	All	2908/3012 (96%)	-0.68	34 (1%)	79	77	8, 16, 35, 64	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	ASP	8.7
1	A	28	SER	8.3
1	C	27	ASP	7.1
1	A	27	ASP	7.0
1	A	712	ASP	5.7

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 monosaccharides in this entry.

6.4 Ligands (i)

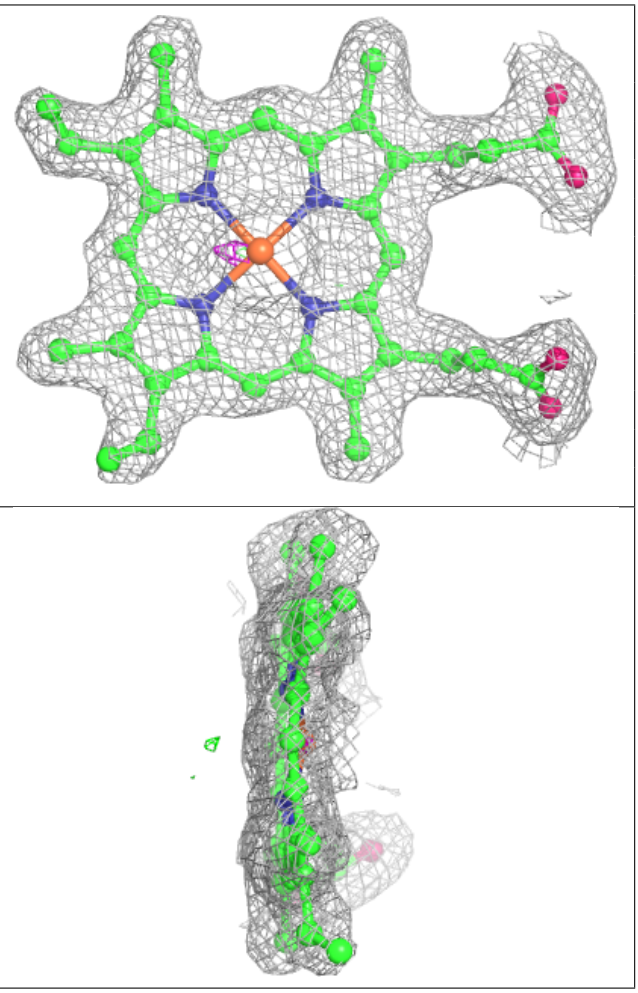
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	C	754	43/43	0.97	0.09	10,15,19,27	0
2	HEM	D	754	43/43	0.97	0.09	11,14,19,28	0
2	HEM	A	754	43/43	0.98	0.09	11,14,19,28	0
2	HEM	B	754	43/43	0.98	0.09	10,15,19,27	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.

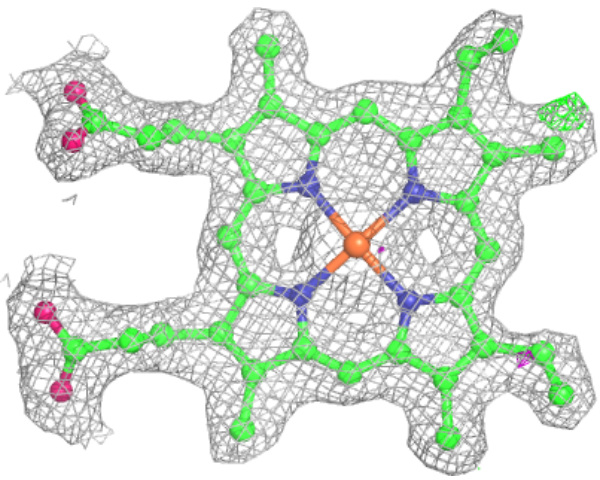
Electron density around HEM C 754:

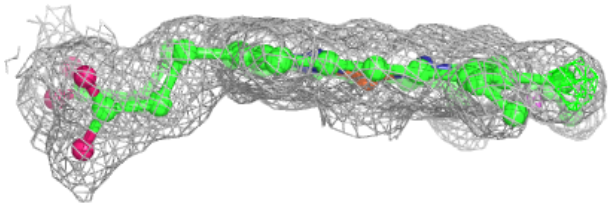
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

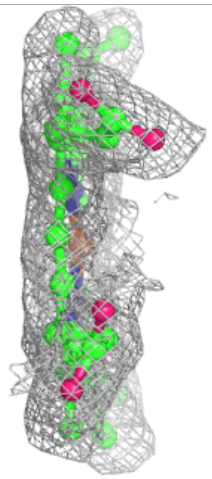


Electron density around HEM D 754:

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

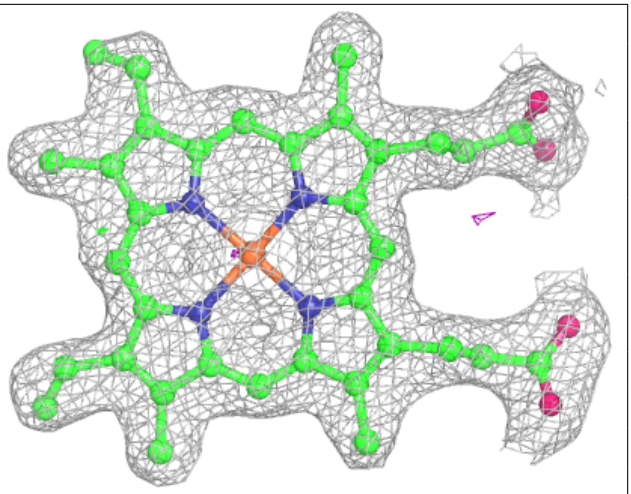


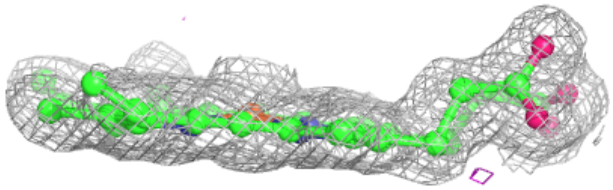


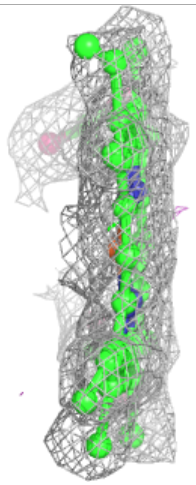


Electron density around HEM A 754:

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

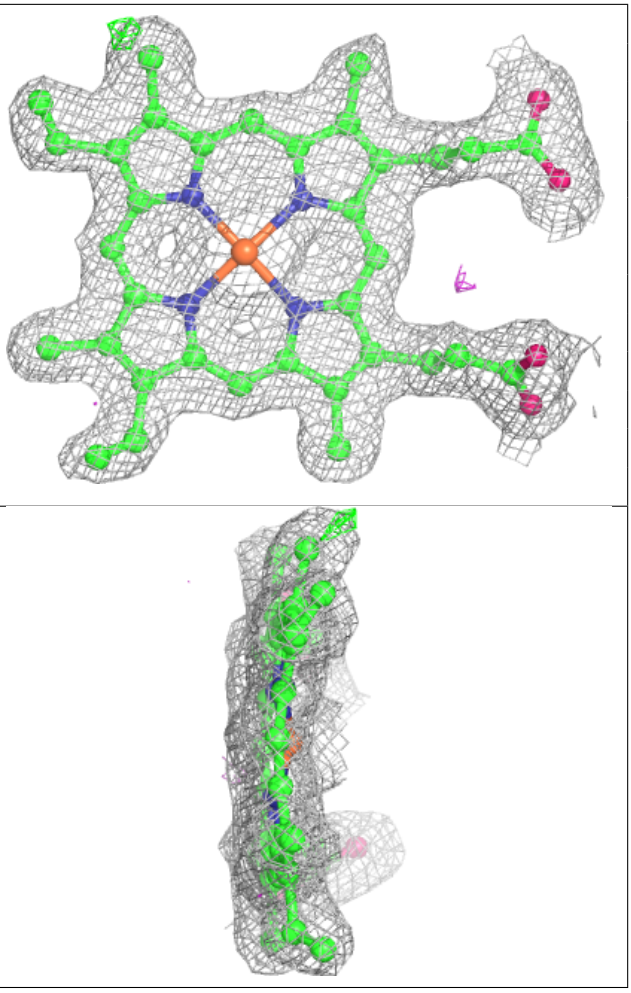






Electron density around HEM B 754:

$2mF_o$-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.