wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 12:11 PM EDT

PDB ID	:	1GGF / pdb_00001ggf
Title	:	CRYSTAL STRUCTURE OF CATALASE HPII FROM ESCHERICHIA COLI, VARIANT HIS128ASN, COMPLEX WITH HYDROGEN PEROXIDE.
Authors	:	Melik-Adamyan, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.
Deposited on	:	2000-08-21
Resolution	:	2.28 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:

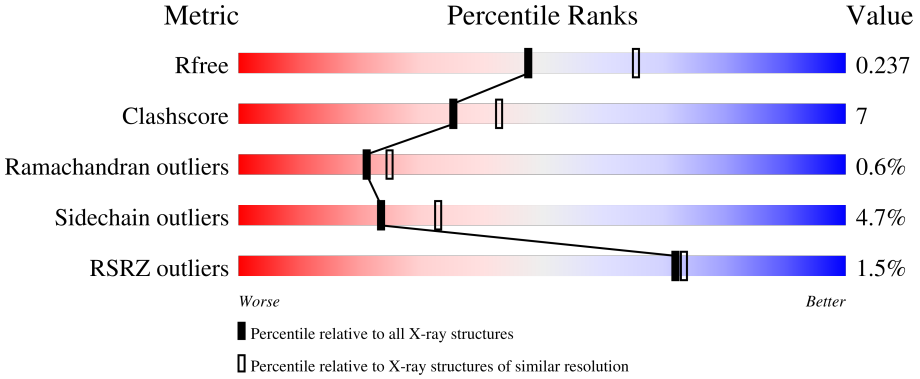
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	2% 74% 19% • •
1	B	753	2% 68% 23% 5% • •
1	C	753	% 74% 19% • •
1	D	753	% 72% 21% • • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEO	A	3002	-	-	X	-
3	PEO	A	3003	-	-	X	-
3	PEO	D	6002	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25199 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.

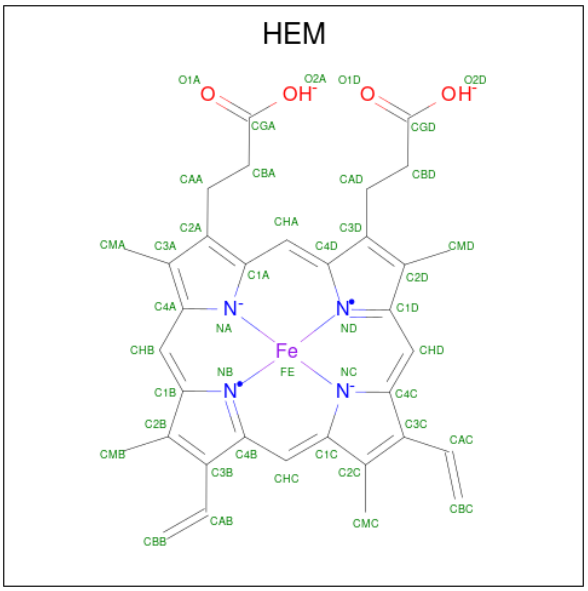
- Molecule 1 is a protein called CATALASE HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	5744	3645	1004	1083	12	0	0	0
1	B	727	5744	3645	1004	1083	12	0	0	0
1	C	727	5744	3645	1004	1083	12	0	0	0
1	D	727	5744	3645	1004	1083	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

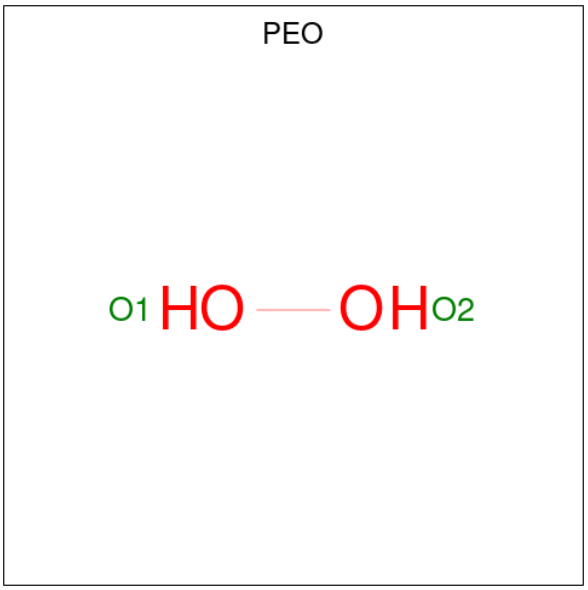
Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ASN	HIS	engineered mutation	UNP P21179
B	128	ASN	HIS	engineered mutation	UNP P21179
C	128	ASN	HIS	engineered mutation	UNP P21179
D	128	ASN	HIS	engineered mutation	UNP P21179

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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 HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



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

- Molecule 4 is water.

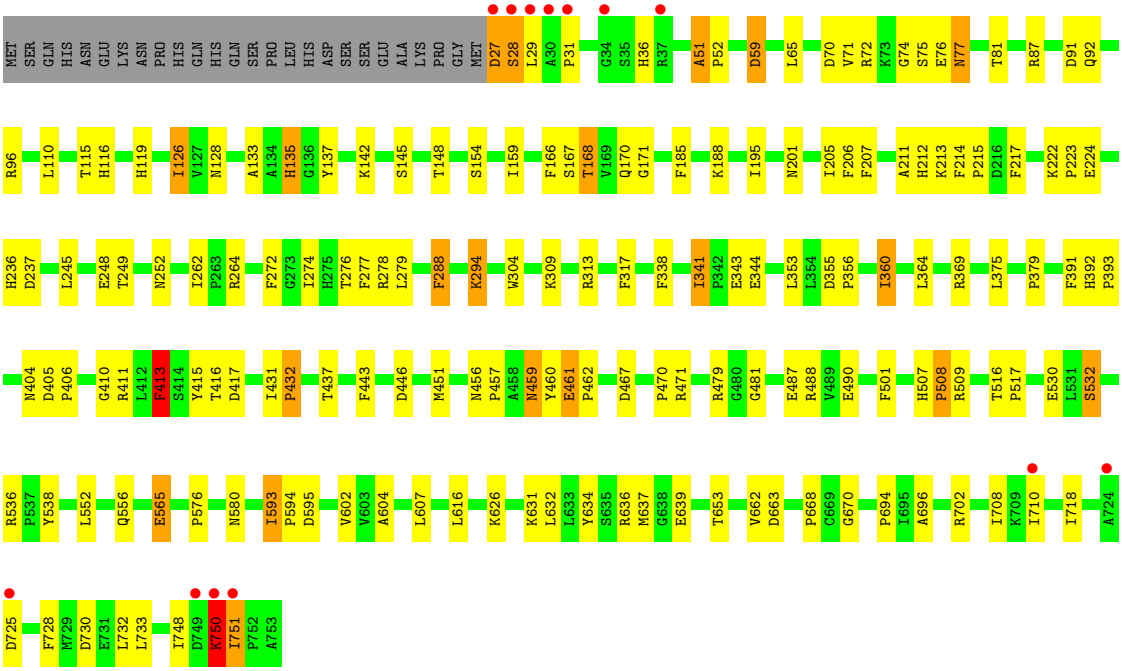
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	581	Total O 581 581	0	0
4	B	440	Total O 440 440	0	0
4	C	474	Total O 474 474	0	0
4	D	530	Total O 530 530	0	0

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.

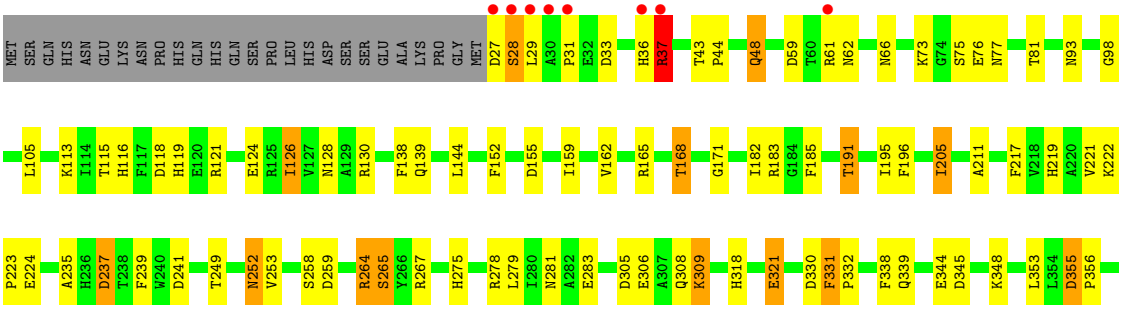
• Molecule 1: CATALASE HPII

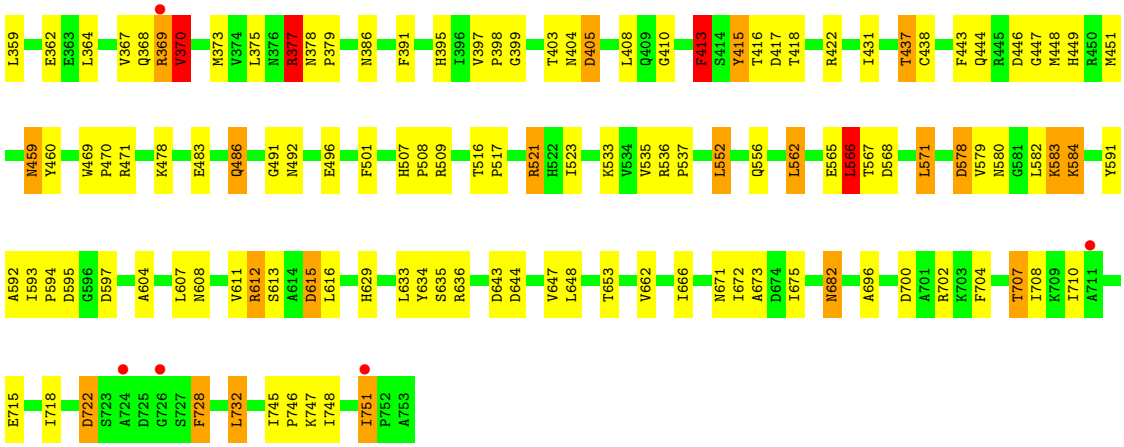
Chain A:



• Molecule 1: CATALASE HPII

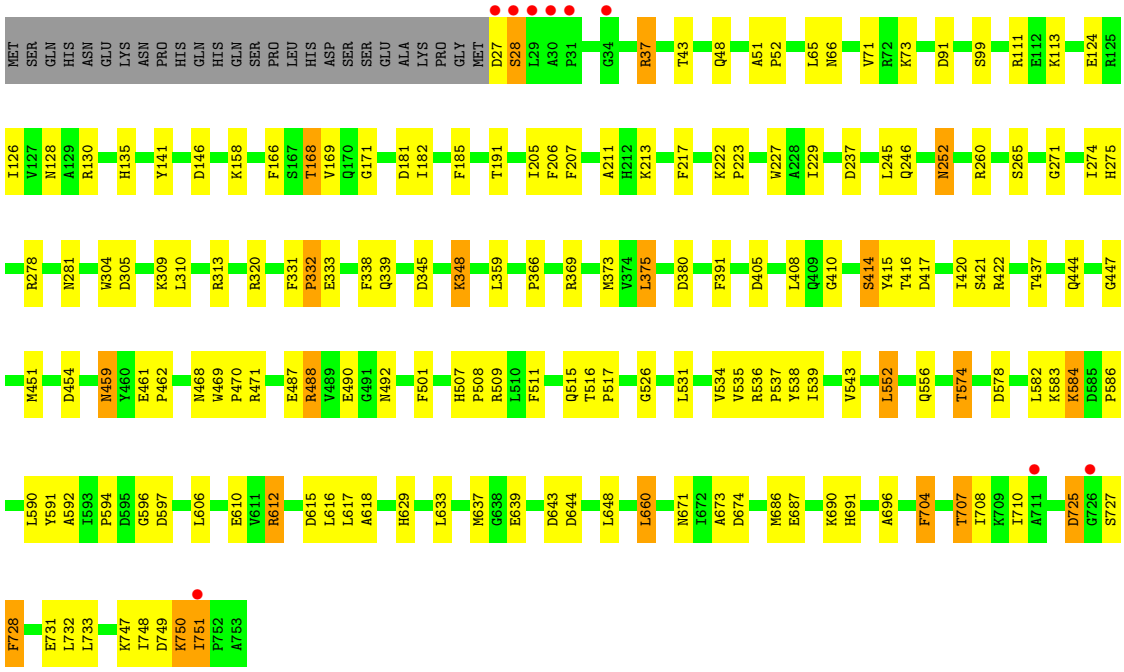
Chain B:





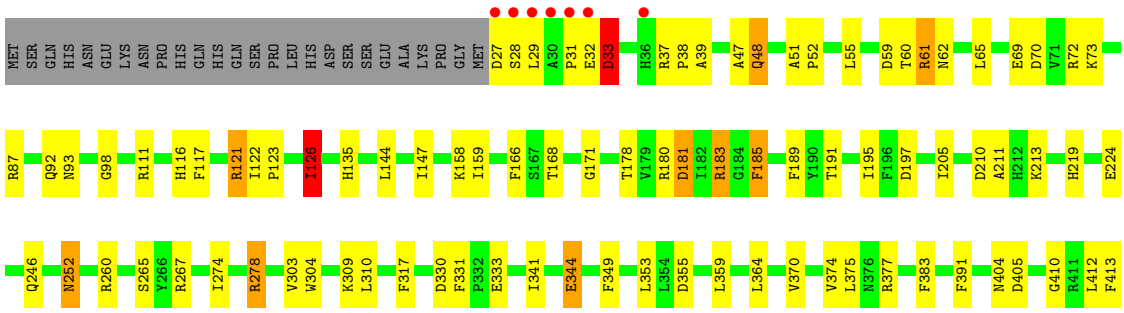
• Molecule 1: CATALASE HPII

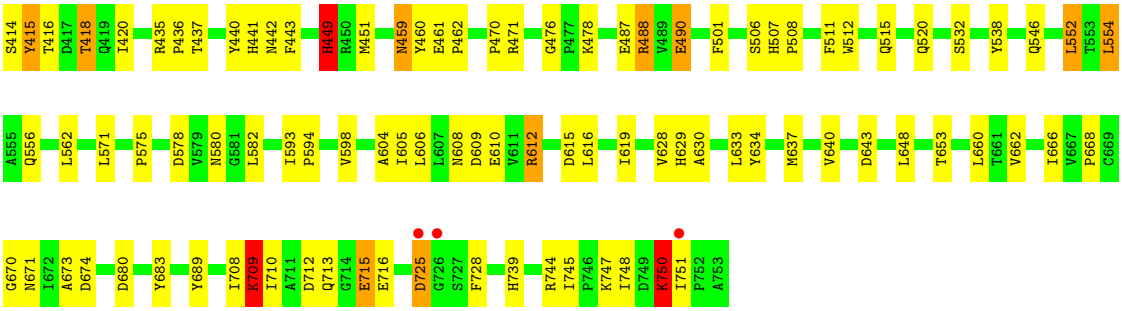
Chain C:



• Molecule 1: CATALASE HPII

Chain D:




S414 Y415 T416 D417 T418 Q419 I420 R435 P436 T437 Y440 H441 N442 F443 H449 R450 M451 N459 Y460 E461 P462 P470 R471 G476 P477 K478 E487 R488 V489 E490 F501 S506 H507 P508 F511 W512 Q515 Q520 S532 Y538 Q546 L552 T553 L554
A555 Q556 L562 L571 P575 D578 V579 N580 G581 L582 I593 P594 V598 A604 I605 L606 L607 N608 D609 E610 V611 R612 D615 L616 I619 V628 H629 A630 L633 Y634 M637 V640 D643 L648 T653 L660 T661 V662 I666 V667 P668 C669
G670 N671 I672 A673 D674 D680 Y683 Y689 I708 K709 I710 A711 D712 Q713 G714 E715 E716 D725 G726 S727 F728 H739 R744 I745 P746 K747 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	93.37Å 133.41Å 121.92Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	87.95 – 2.28 87.95 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.3 (87.95-2.28) 98.3 (87.95-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.28Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.254 0.171 , 0.237	Depositor DCC
R_{free} test set	6348 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25199	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, PEO

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	0.67	0/5899	1.66	80/8020 (1.0%)
1	B	0.64	0/5899	1.68	86/8020 (1.1%)
1	C	0.64	0/5899	1.62	61/8020 (0.8%)
1	D	0.66	0/5899	1.67	76/8020 (0.9%)
All	All	0.65	0/23596	1.66	303/32080 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

The worst 5 of 303 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	449	HIS	CA-CB-CG	16.40	130.20	113.80
1	D	488	ARG	CD-NE-CZ	13.96	143.95	124.40
1	B	37	ARG	CD-NE-CZ	11.18	140.05	124.40
1	B	722	ASP	CA-CB-CG	-10.41	102.19	112.60
1	D	33	ASP	CA-CB-CG	10.27	122.87	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	207	PHE	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	5744	0	5577	77	1
1	B	5744	0	5577	111	1
1	C	5744	0	5577	80	0
1	D	5744	0	5577	94	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	4	0
3	A	6	0	0	5	0
3	B	6	0	0	3	0
3	C	6	0	0	2	0
3	D	8	0	0	4	0
4	A	581	0	0	5	0
4	B	440	0	0	12	0
4	C	474	0	0	8	0
4	D	530	0	0	7	0
All	All	25199	0	22428	335	1

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 335 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)
3:C:5003:PEO:O2	3:C:5003:PEO:O1	1.53	1.27
3:A:3002:PEO:O2	3:A:3002:PEO:O1	1.53	1.26
3:C:5001:PEO:O2	3:C:5001:PEO:O1	1.52	1.26
3:A:3003:PEO:O2	3:A:3003:PEO:O1	1.53	1.25
3:D:6002:PEO:O1	3:D:6002:PEO:O2	1.52	1.25

All (1) 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)
1:A:59:ASP:OD1	1:B:369:ARG:NH2[2_545]	2.17	0.03

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	725/753 (96%)	701 (97%)	21 (3%)	3 (0%)	30	36
1	B	725/753 (96%)	686 (95%)	34 (5%)	5 (1%)	18	21
1	C	725/753 (96%)	698 (96%)	23 (3%)	4 (1%)	21	25
1	D	725/753 (96%)	699 (96%)	22 (3%)	4 (1%)	21	25
All	All	2900/3012 (96%)	2784 (96%)	100 (3%)	16 (1%)	21	25

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	B	28	SER
1	C	28	SER
1	C	725	ASP
1	D	33	ASP

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	612/636 (96%)	589 (96%)	23 (4%)	29	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	612/636 (96%)	581 (95%)	31 (5%)	21	29
1	C	612/636 (96%)	581 (95%)	31 (5%)	21	29
1	D	612/636 (96%)	583 (95%)	29 (5%)	23	33
All	All	2448/2544 (96%)	2334 (95%)	114 (5%)	23	33

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	99	SER
1	D	713	GLN
1	C	574	THR
1	D	709	LYS
1	D	459	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	556	GLN
1	D	507	HIS
1	C	629	HIS
1	D	252	ASN
1	D	671	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)

17 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	PEO	D	6003	-	1,1,1	0.83	0	-		
3	PEO	B	4002	2	1,1,1	0.81	0	-		
3	PEO	A	3001	-	1,1,1	0.60	0	-		
2	HEM	C	760	1	50,50,50	1.41	9 (18%)	67,82,82	1.12	6 (8%)
3	PEO	A	3002	-	1,1,1	0.74	0	-		
3	PEO	D	3004	-	1,1,1	0.86	0	-		
3	PEO	D	6002	-	1,1,1	0.72	0	-		
3	PEO	B	4003	-	1,1,1	0.79	0	-		
3	PEO	D	6001	-	1,1,1	0.67	0	-		
3	PEO	C	5001	-	1,1,1	0.69	0	-		
2	HEM	A	760	1	50,50,50	1.46	9 (18%)	67,82,82	1.05	5 (7%)
3	PEO	A	3003	-	1,1,1	0.77	0	-		
3	PEO	B	4001	-	1,1,1	0.80	0	-		
3	PEO	C	5002	-	1,1,1	0.67	0	-		
2	HEM	D	760	1	50,50,50	1.38	9 (18%)	67,82,82	0.86	3 (4%)
3	PEO	C	5003	-	1,1,1	0.72	0	-		
2	HEM	B	760	3,1	50,50,50	1.37	10 (20%)	67,82,82	1.05	6 (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	B	760	3,1	-	2/14/54/54	-
2	HEM	D	760	1	-	4/14/54/54	-
2	HEM	C	760	1	-	2/14/54/54	-
2	HEM	A	760	1	-	2/14/54/54	-

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	CAC-C3C	3.42	1.56	1.47
2	A	760	HEM	FE-NB	3.32	2.05	1.94
2	C	760	HEM	CAC-C3C	3.30	1.56	1.47
2	D	760	HEM	CAB-C3B	2.98	1.55	1.47
2	C	760	HEM	FE-NB	2.88	2.03	1.94

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760	HEM	CHC-C1C-NC	3.29	128.04	124.45
2	C	760	HEM	O1A-CGA-CBA	-3.27	112.72	123.09
2	B	760	HEM	CMA-C3A-C4A	-3.01	120.83	125.42
2	B	760	HEM	CBA-CAA-C2A	2.79	120.24	112.53
2	A	760	HEM	CHC-C4B-NB	2.70	127.33	124.42

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	760	HEM	C2C-C3C-CAC-CBC
2	C	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	D	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

16 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	6003	PEO	1	0
3	B	4002	PEO	1	0
3	A	3001	PEO	1	0
2	C	760	HEM	3	0
3	A	3002	PEO	3	0
3	D	3004	PEO	1	0
3	D	6002	PEO	2	0
3	B	4003	PEO	1	0
3	D	6001	PEO	1	0
3	C	5001	PEO	1	0
2	A	760	HEM	2	0
3	A	3003	PEO	2	0
3	B	4001	PEO	1	0

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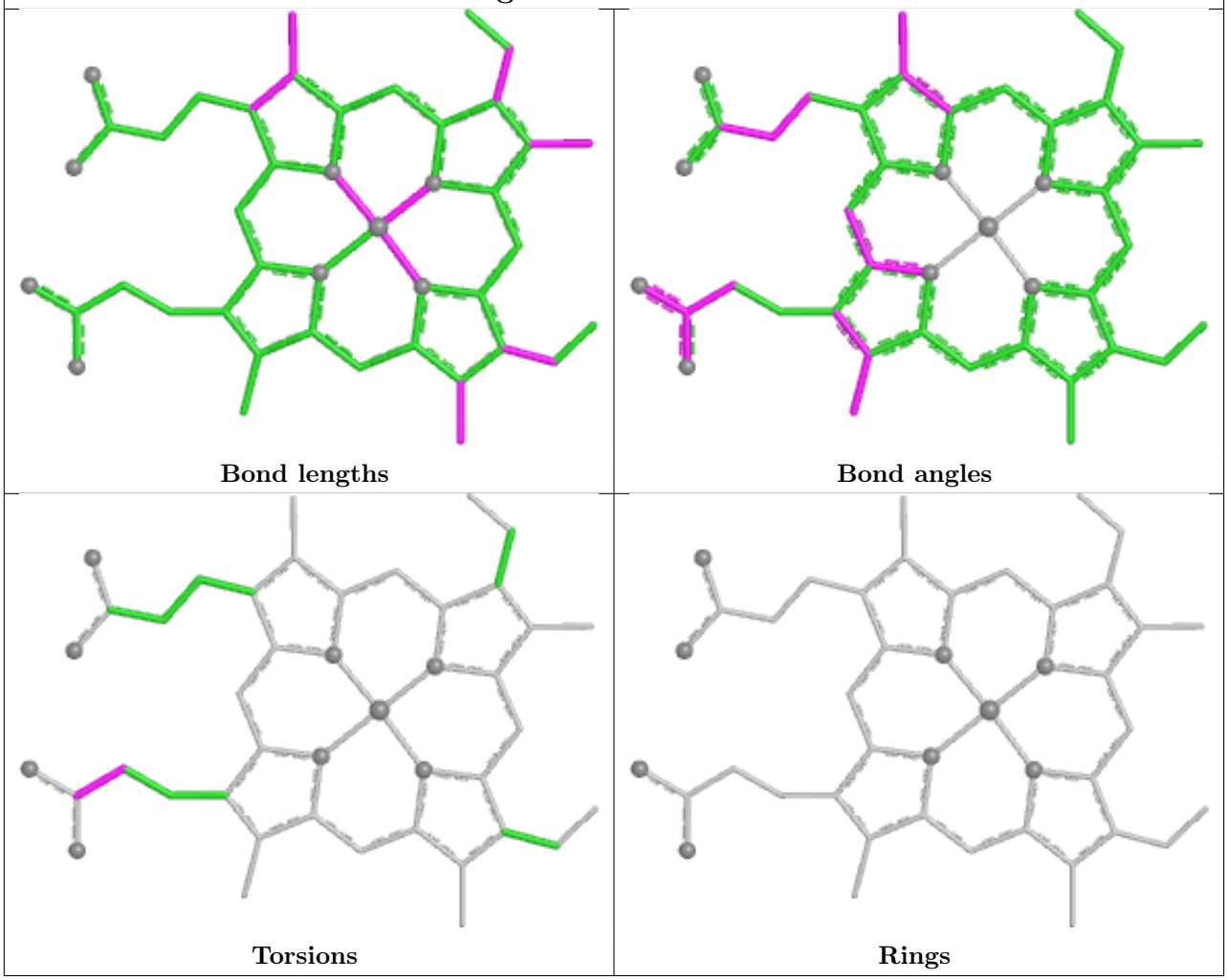
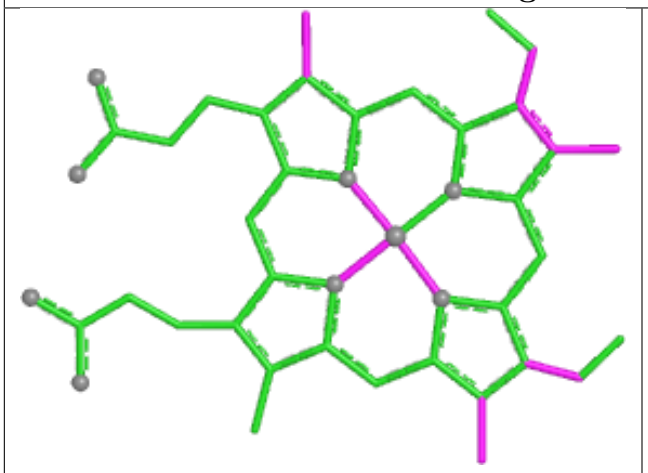
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760	HEM	4	0
3	C	5003	PEO	1	0
2	B	760	HEM	3	0

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.

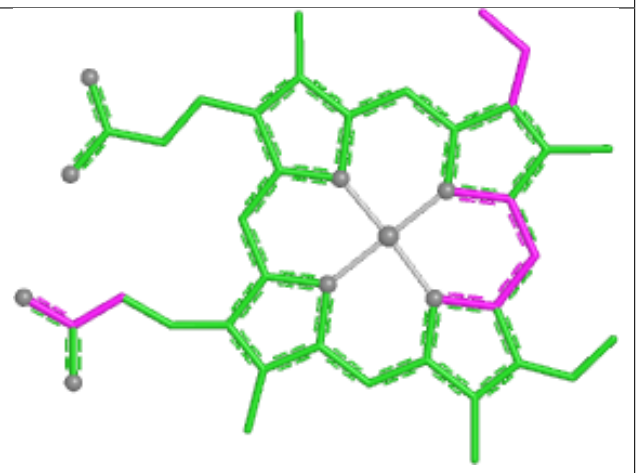
Ligand HEM C 760



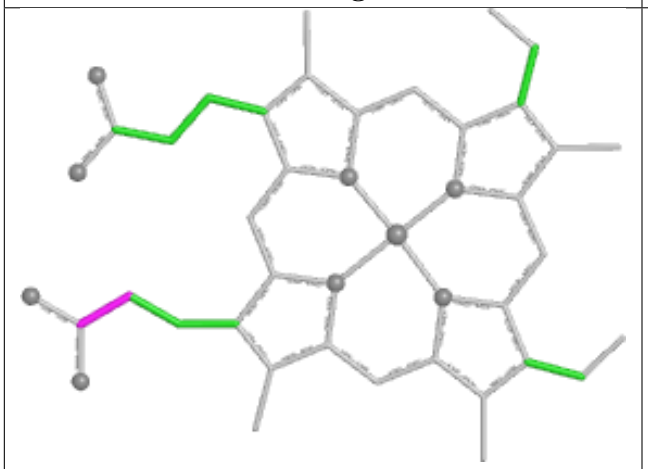
Ligand HEM A 760



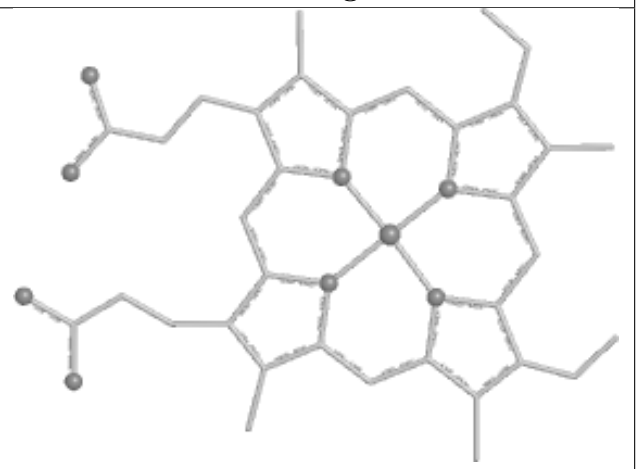
Bond lengths



Bond angles

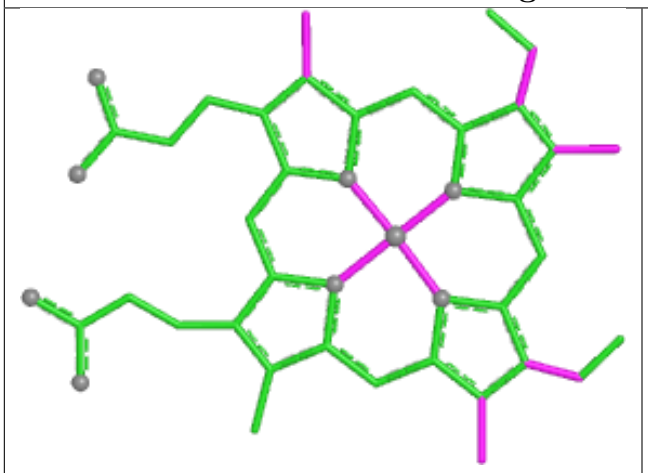


Torsions

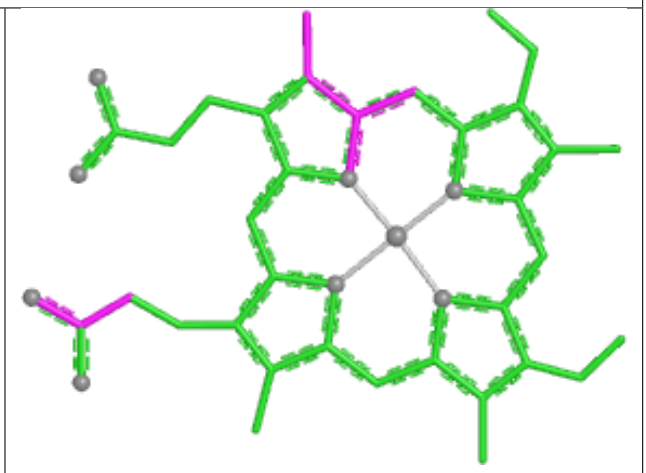


Rings

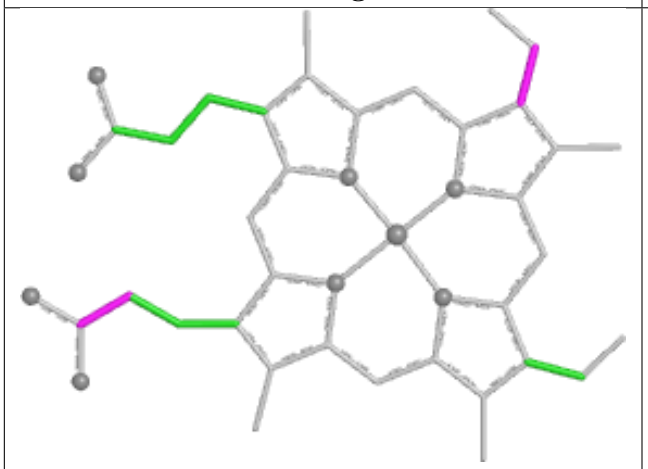
Ligand HEM D 760



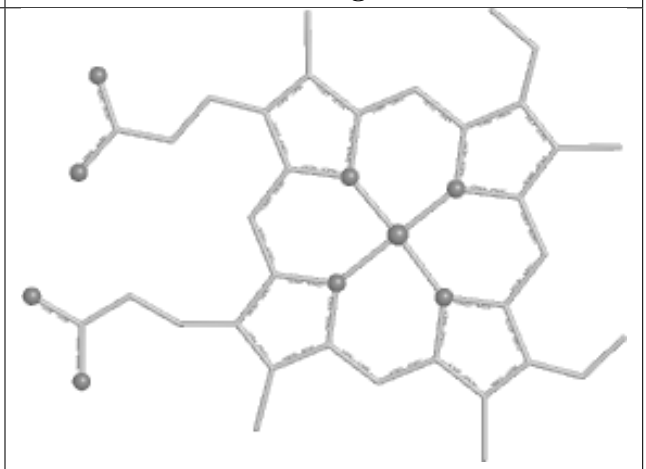
Bond lengths



Bond angles

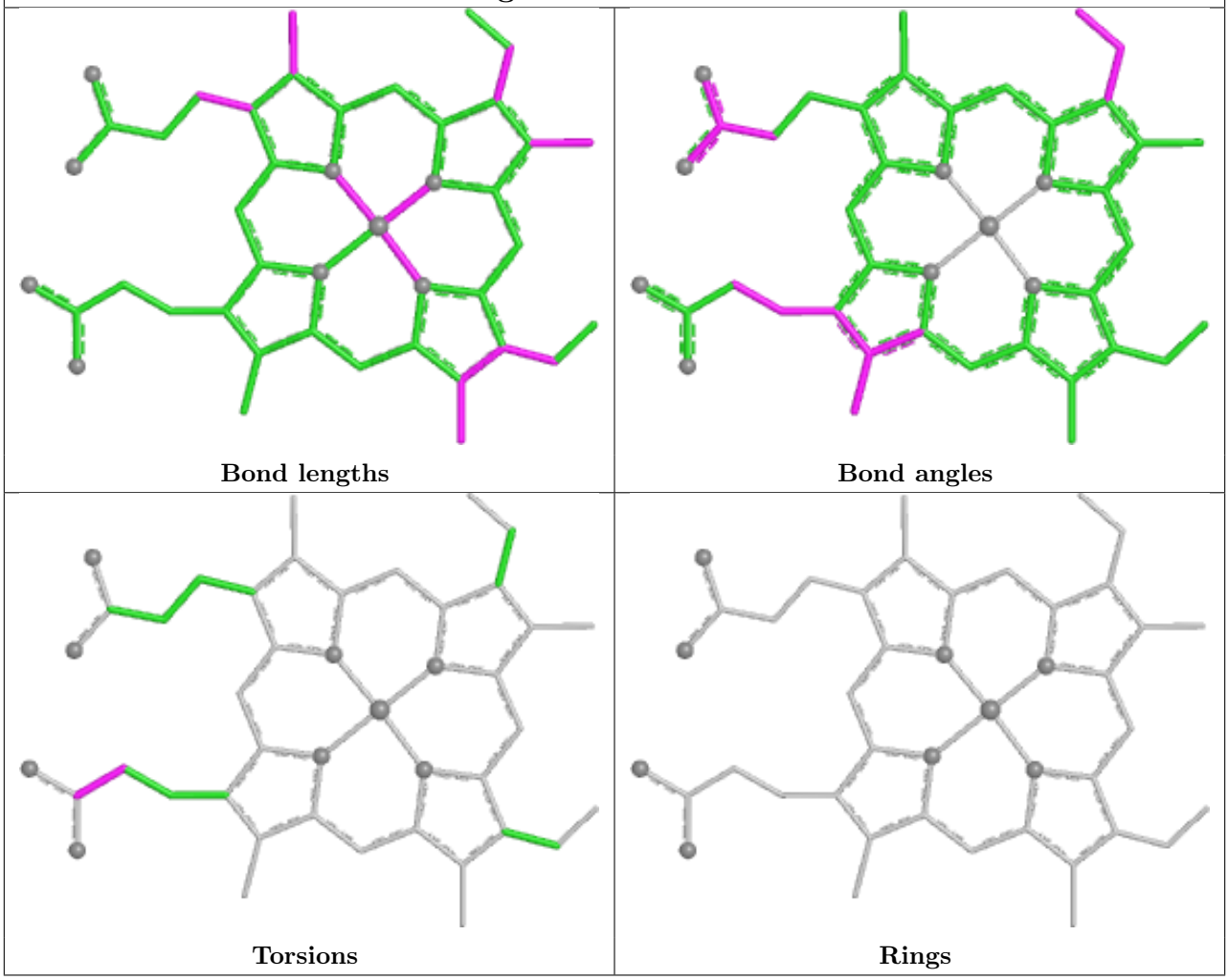


Torsions



Rings

Ligand HEM B 760



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%)	-0.28	13 (1%)	67	69	10, 20, 43, 91	1 (0%)
1	B	727/753 (96%)	-0.18	13 (1%)	67	69	13, 22, 46, 91	1 (0%)
1	C	727/753 (96%)	-0.18	9 (1%)	76	78	11, 22, 45, 90	1 (0%)
1	D	727/753 (96%)	-0.26	10 (1%)	73	75	11, 20, 44, 92	1 (0%)
All	All	2908/3012 (96%)	-0.23	45 (1%)	72	73	10, 21, 45, 92	4 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	726	GLY	7.6
1	D	27	ASP	6.5
1	A	29	LEU	5.9
1	B	27	ASP	5.7
1	A	27	ASP	5.1

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)

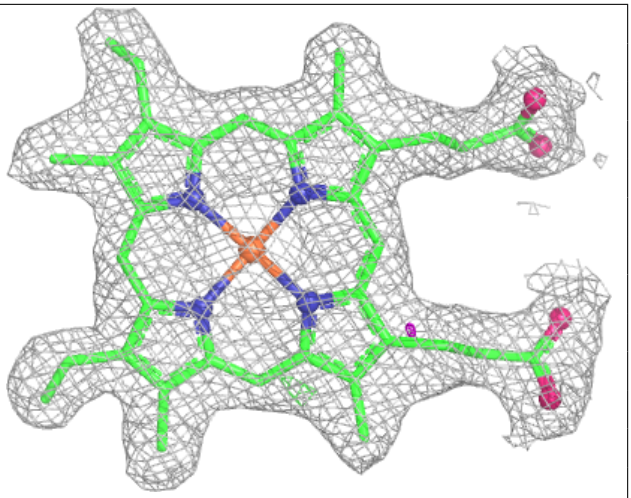
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

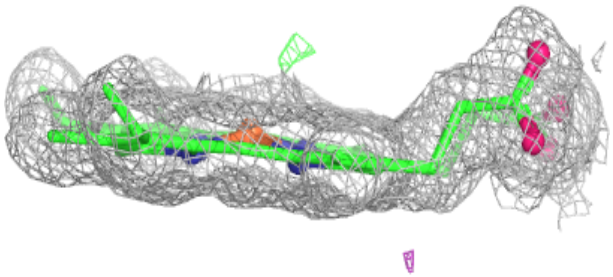
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEO	D	3004	2/2	0.83	0.14	33,33,33,34	0
3	PEO	B	4002	2/2	0.93	0.15	25,25,25,28	0
3	PEO	B	4003	2/2	0.95	0.06	31,31,31,32	0
3	PEO	A	3001	2/2	0.95	0.10	29,29,29,29	0
3	PEO	D	6002	2/2	0.95	0.09	18,18,18,18	0
3	PEO	D	6003	2/2	0.95	0.09	21,21,21,23	0
3	PEO	B	4001	2/2	0.96	0.06	17,17,17,19	0
3	PEO	D	6001	2/2	0.96	0.08	21,21,21,22	0
2	HEM	D	760	43/43	0.97	0.06	10,15,16,18	0
3	PEO	A	3002	2/2	0.97	0.07	13,13,13,16	0
3	PEO	A	3003	2/2	0.97	0.05	22,22,22,25	0
3	PEO	C	5003	2/2	0.97	0.07	18,18,18,18	0
2	HEM	B	760	43/43	0.98	0.05	12,16,18,18	0
2	HEM	C	760	43/43	0.98	0.06	16,18,19,21	0
2	HEM	A	760	43/43	0.98	0.05	9,14,16,18	0
3	PEO	C	5002	2/2	0.98	0.07	34,34,34,35	0
3	PEO	C	5001	2/2	0.98	0.05	20,20,20,21	0

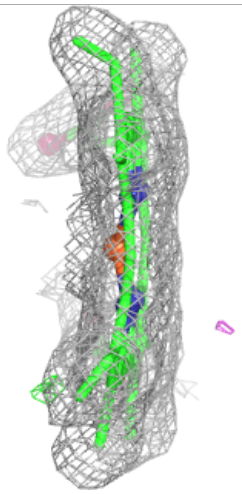
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM D 760:

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

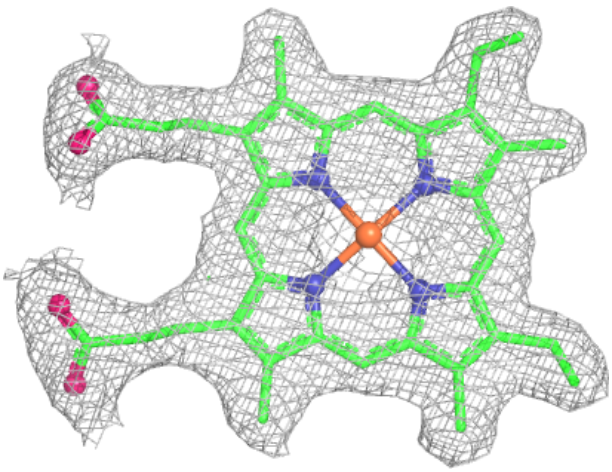


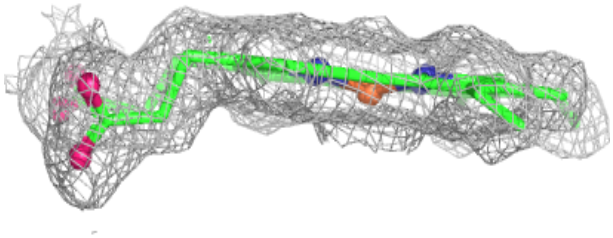


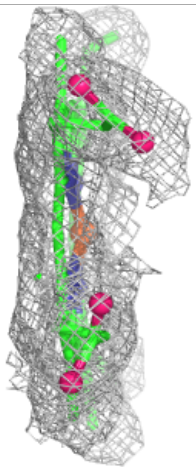


Electron density around HEM B 760:

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

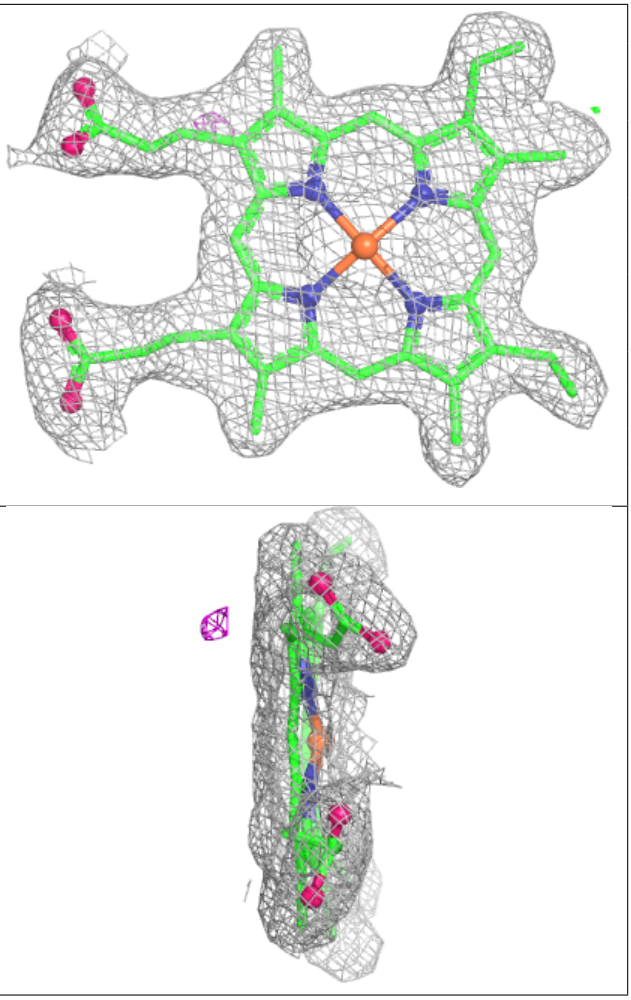






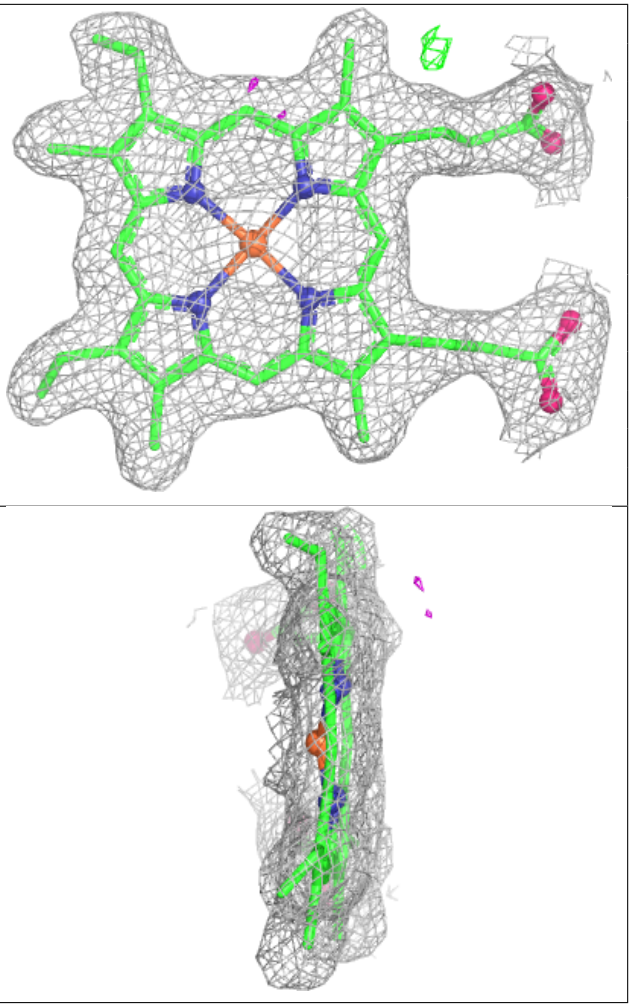
Electron density around HEM C 760:

$2mF_o$-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 760:

$2mF_o$-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.