wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 10:16 PM EDT

PDB ID	:	3BK9 / pdb_00003bk9
Title	:	H55A mutant of tryptophan 2,3-dioxygenase from Xanthomonas campestris
Authors	:	Bruckmann, C.; Mowat, C.G.
Deposited on	:	2007-12-06
Resolution	:	2.15 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:

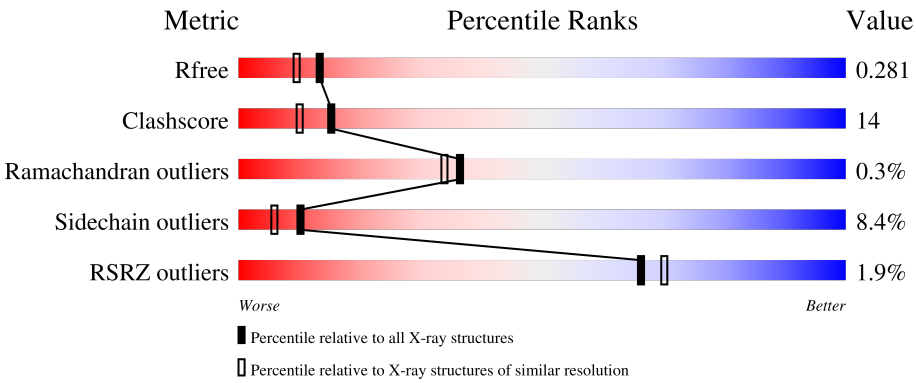
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	306	% 60% 23% 6% • 9%
1	B	306	56% 28% 7% • 8%
1	C	306	3% 53% 30% 6% 11%
1	D	306	55% 24% 6% 14%
1	E	306	% 50% 27% 7% • 15%

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Mol	Chain	Length	Quality of chain
1	F	306	2% 53% 24% 5% 18%
1	G	306	% 48% 32% 5% • 14%
1	H	306	4% 56% 25% • 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19073 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2285	1462	404	412	7	0	0	0
1	B	280	2308	1475	408	418	7	0	0	0
1	C	272	2244	1437	395	405	7	0	0	0
1	D	262	2165	1389	381	388	7	0	0	0
1	E	260	2153	1381	379	386	7	0	0	0
1	F	250	2071	1330	362	372	7	0	0	0
1	G	262	2172	1393	384	388	7	0	0	0
1	H	257	2120	1362	372	379	7	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	HIS	engineered mutation	UNP Q8PDA8
A	299	LEU	-	expression tag	UNP Q8PDA8
A	300	GLU	-	expression tag	UNP Q8PDA8
A	301	HIS	-	expression tag	UNP Q8PDA8
A	302	HIS	-	expression tag	UNP Q8PDA8
A	303	HIS	-	expression tag	UNP Q8PDA8
A	304	HIS	-	expression tag	UNP Q8PDA8
A	305	HIS	-	expression tag	UNP Q8PDA8
A	306	HIS	-	expression tag	UNP Q8PDA8
B	55	ALA	HIS	engineered mutation	UNP Q8PDA8
B	299	LEU	-	expression tag	UNP Q8PDA8
B	300	GLU	-	expression tag	UNP Q8PDA8
B	301	HIS	-	expression tag	UNP Q8PDA8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP Q8PDA8
B	303	HIS	-	expression tag	UNP Q8PDA8
B	304	HIS	-	expression tag	UNP Q8PDA8
B	305	HIS	-	expression tag	UNP Q8PDA8
B	306	HIS	-	expression tag	UNP Q8PDA8
C	55	ALA	HIS	engineered mutation	UNP Q8PDA8
C	299	LEU	-	expression tag	UNP Q8PDA8
C	300	GLU	-	expression tag	UNP Q8PDA8
C	301	HIS	-	expression tag	UNP Q8PDA8
C	302	HIS	-	expression tag	UNP Q8PDA8
C	303	HIS	-	expression tag	UNP Q8PDA8
C	304	HIS	-	expression tag	UNP Q8PDA8
C	305	HIS	-	expression tag	UNP Q8PDA8
C	306	HIS	-	expression tag	UNP Q8PDA8
D	55	ALA	HIS	engineered mutation	UNP Q8PDA8
D	299	LEU	-	expression tag	UNP Q8PDA8
D	300	GLU	-	expression tag	UNP Q8PDA8
D	301	HIS	-	expression tag	UNP Q8PDA8
D	302	HIS	-	expression tag	UNP Q8PDA8
D	303	HIS	-	expression tag	UNP Q8PDA8
D	304	HIS	-	expression tag	UNP Q8PDA8
D	305	HIS	-	expression tag	UNP Q8PDA8
D	306	HIS	-	expression tag	UNP Q8PDA8
E	55	ALA	HIS	engineered mutation	UNP Q8PDA8
E	299	LEU	-	expression tag	UNP Q8PDA8
E	300	GLU	-	expression tag	UNP Q8PDA8
E	301	HIS	-	expression tag	UNP Q8PDA8
E	302	HIS	-	expression tag	UNP Q8PDA8
E	303	HIS	-	expression tag	UNP Q8PDA8
E	304	HIS	-	expression tag	UNP Q8PDA8
E	305	HIS	-	expression tag	UNP Q8PDA8
E	306	HIS	-	expression tag	UNP Q8PDA8
F	55	ALA	HIS	engineered mutation	UNP Q8PDA8
F	299	LEU	-	expression tag	UNP Q8PDA8
F	300	GLU	-	expression tag	UNP Q8PDA8
F	301	HIS	-	expression tag	UNP Q8PDA8
F	302	HIS	-	expression tag	UNP Q8PDA8
F	303	HIS	-	expression tag	UNP Q8PDA8
F	304	HIS	-	expression tag	UNP Q8PDA8
F	305	HIS	-	expression tag	UNP Q8PDA8
F	306	HIS	-	expression tag	UNP Q8PDA8
G	55	ALA	HIS	engineered mutation	UNP Q8PDA8

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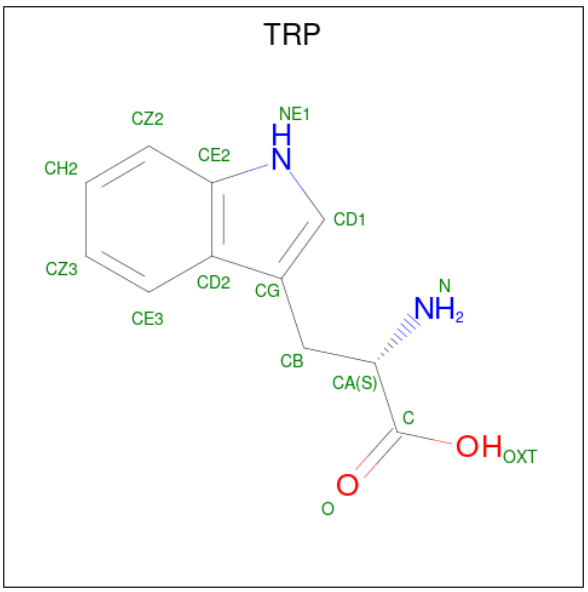
Chain	Residue	Modelled	Actual	Comment	Reference
G	299	LEU	-	expression tag	UNP Q8PDA8
G	300	GLU	-	expression tag	UNP Q8PDA8
G	301	HIS	-	expression tag	UNP Q8PDA8
G	302	HIS	-	expression tag	UNP Q8PDA8
G	303	HIS	-	expression tag	UNP Q8PDA8
G	304	HIS	-	expression tag	UNP Q8PDA8
G	305	HIS	-	expression tag	UNP Q8PDA8
G	306	HIS	-	expression tag	UNP Q8PDA8
H	55	ALA	HIS	engineered mutation	UNP Q8PDA8
H	299	LEU	-	expression tag	UNP Q8PDA8
H	300	GLU	-	expression tag	UNP Q8PDA8
H	301	HIS	-	expression tag	UNP Q8PDA8
H	302	HIS	-	expression tag	UNP Q8PDA8
H	303	HIS	-	expression tag	UNP Q8PDA8
H	304	HIS	-	expression tag	UNP Q8PDA8
H	305	HIS	-	expression tag	UNP Q8PDA8
H	306	HIS	-	expression tag	UNP Q8PDA8

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	11	2	2	0	0
			Total	C	N	O		
2	A	1	15	11	2	2	0	0
			Total	C	N	O		
2	B	1	15	11	2	2	0	0

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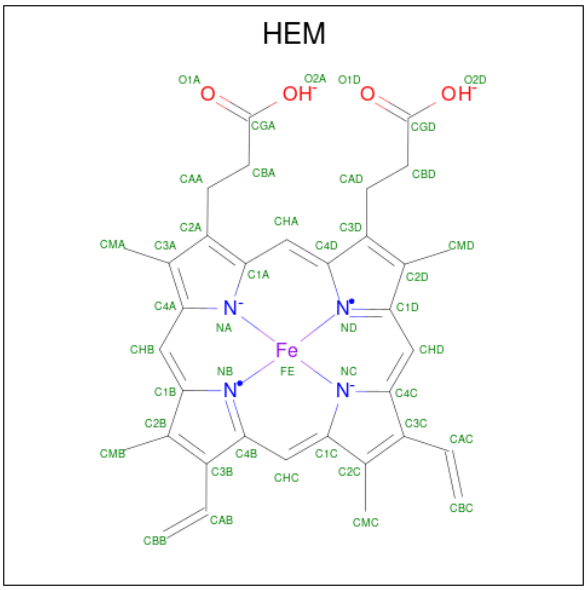
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	15	11	2	2	0	0
2	C	1	15	11	2	2	0	0
2	C	1	15	11	2	2	0	0
2	D	1	15	11	2	2	0	0
2	D	1	15	11	2	2	0	0
2	E	1	15	11	2	2	0	0
2	E	1	15	11	2	2	0	0
2	F	1	15	11	2	2	0	0
2	G	1	15	11	2	2	0	0
2	H	1	15	11	2	2	0	0

- Molecule 3 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		
3	A	1	43	34	1	4	4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
3	C	1	43	34	1	4	4	0	0
3	D	1	43	34	1	4	4	0	0
3	E	1	43	34	1	4	4	0	0
3	F	1	43	34	1	4	4	0	0
3	G	1	43	34	1	4	4	0	0
3	H	1	43	34	1	4	4	0	0

- Molecule 4 is water.

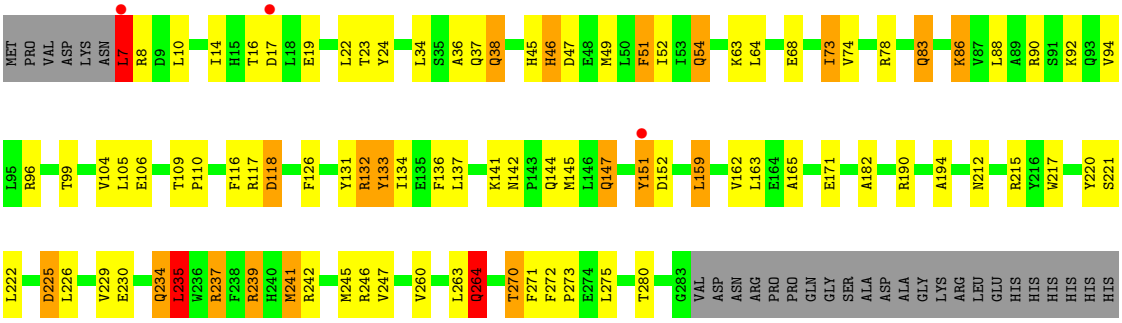
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	170	170	170	0	0
4	B	152	152	152	0	0
4	C	129	129	129	0	0
4	D	124	124	124	0	0
4	E	133	133	133	0	0
4	F	96	96	96	0	0
4	G	113	113	113	0	0
4	H	99	99	99	0	0

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.

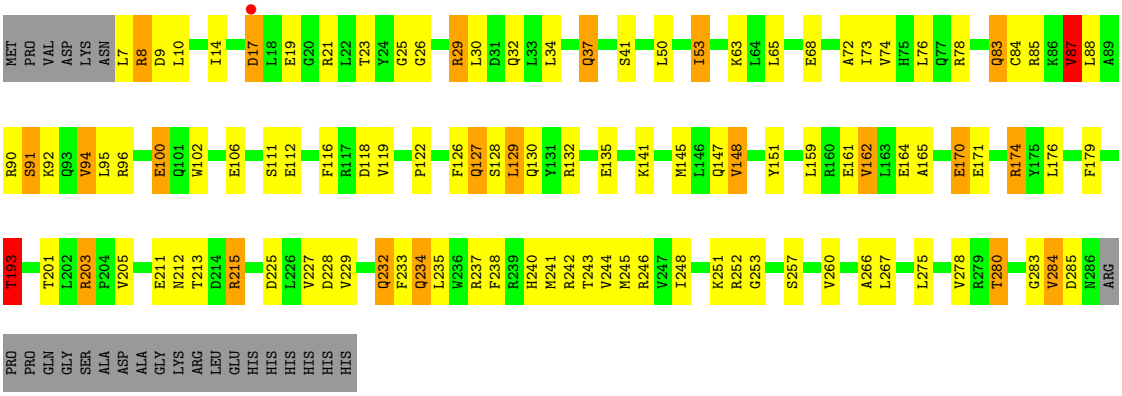
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain A:



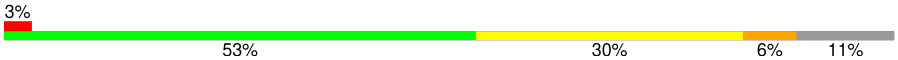
• Molecule 1: Tryptophan 2,3-dioxygenase

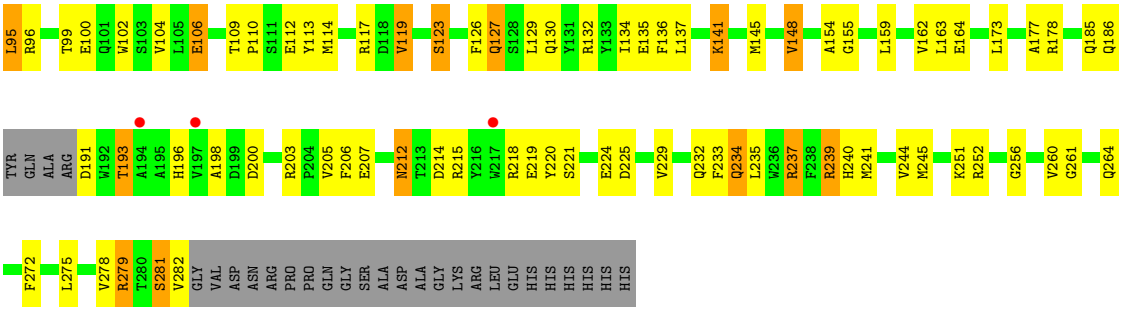
Chain B:



• Molecule 1: Tryptophan 2,3-dioxygenase

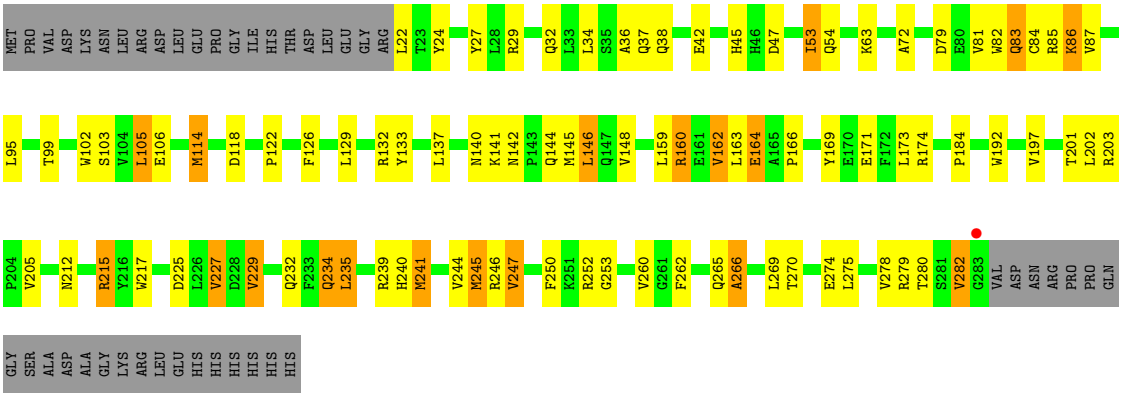
Chain C:





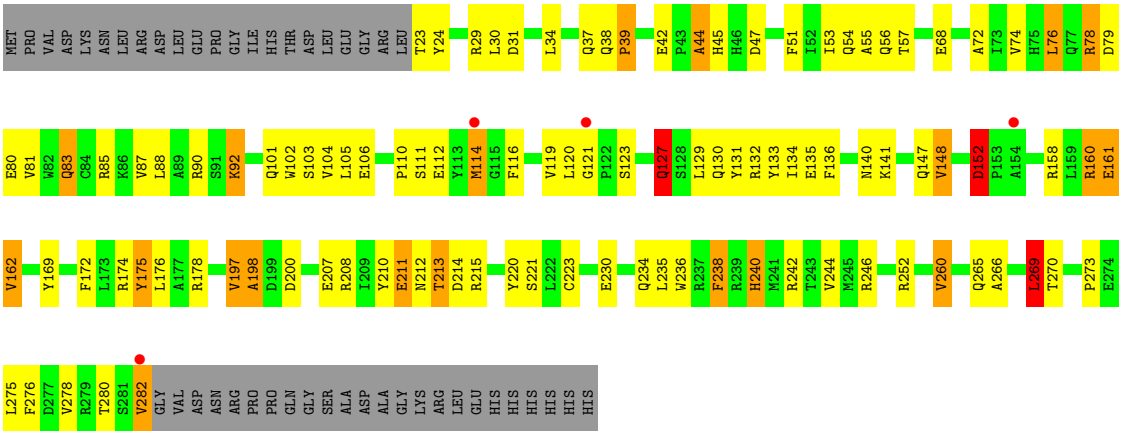
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain D:



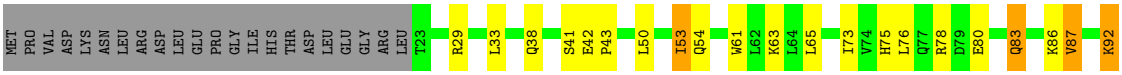
- Molecule 1: Tryptophan 2,3-dioxygenase

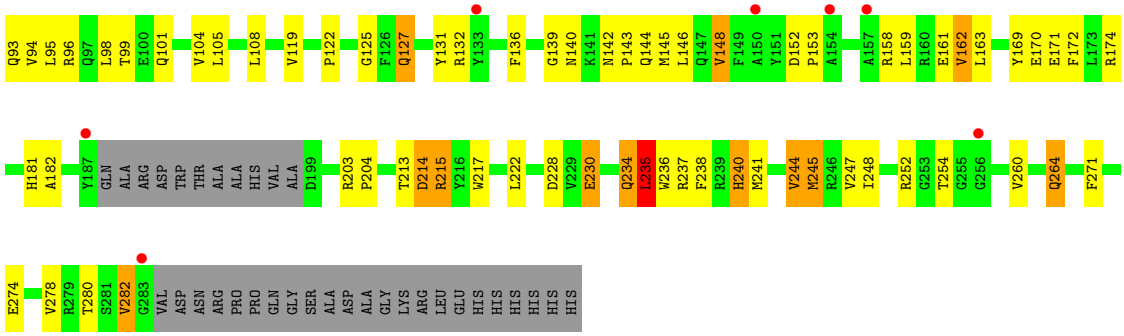
Chain E:



- Molecule 1: Tryptophan 2,3-dioxygenase

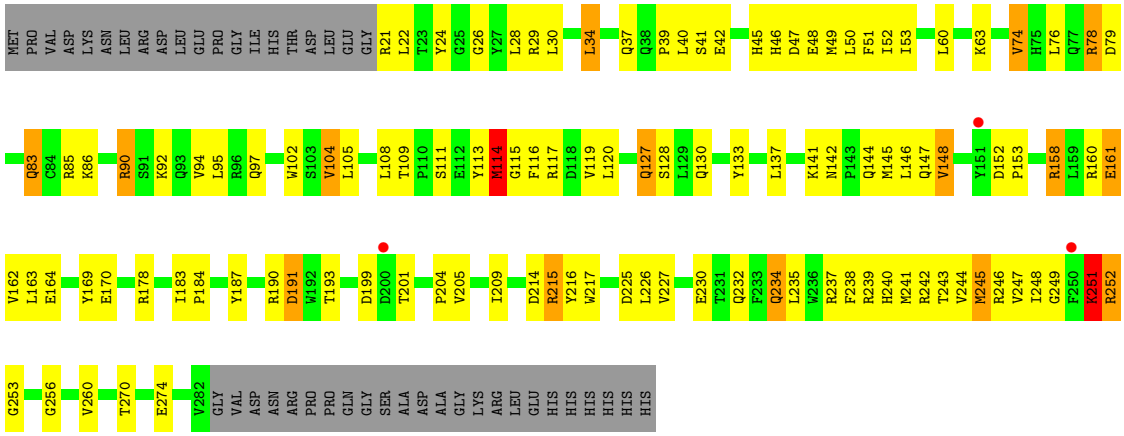
Chain F:





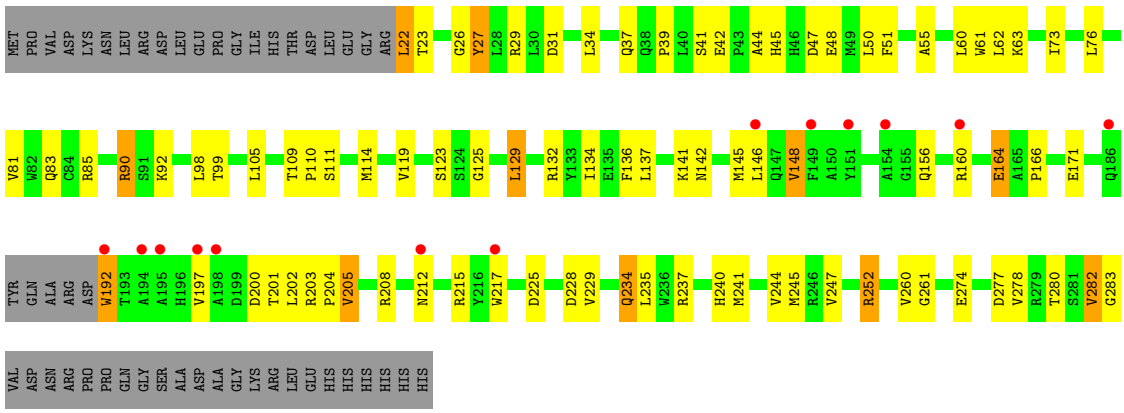
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain G:



- Molecule 1: Tryptophan 2,3-dioxygenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.22Å 117.61Å 139.28Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	54.13 – 2.15 54.13 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.7 (54.13-2.15) 96.7 (54.13-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.285 0.201 , 0.281	Depositor DCC
R_{free} test set	6624 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19073	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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	1.76	27/2342 (1.2%)	1.57	28/3174 (0.9%)
1	B	1.80	30/2365 (1.3%)	1.66	35/3206 (1.1%)
1	C	1.62	23/2299 (1.0%)	1.54	24/3115 (0.8%)
1	D	1.64	24/2220 (1.1%)	1.51	16/3009 (0.5%)
1	E	1.64	18/2208 (0.8%)	1.52	25/2993 (0.8%)
1	F	1.55	16/2122 (0.8%)	1.45	14/2872 (0.5%)
1	G	1.56	16/2227 (0.7%)	1.52	23/3018 (0.8%)
1	H	1.41	9/2173 (0.4%)	1.41	11/2944 (0.4%)
All	All	1.63	163/17956 (0.9%)	1.53	176/24331 (0.7%)

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	1	0
1	B	0	1
1	G	0	1
All	All	1	2

The worst 5 of 163 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	97	GLN	C-O	-11.13	1.11	1.24
1	E	104	VAL	C-O	-10.11	1.12	1.24
1	E	148	VAL	CA-CB	8.95	1.67	1.54
1	E	141	LYS	N-CA	8.87	1.57	1.46
1	C	218	ARG	C-O	8.73	1.34	1.24

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	252	ARG	NE-CZ-NH2	-11.75	108.62	119.20
1	B	252	ARG	CG-CD-NE	-9.23	91.69	112.00
1	H	229	VAL	N-CA-C	8.80	118.84	110.30
1	B	252	ARG	CD-NE-CZ	8.68	136.56	124.40
1	A	152	ASP	CA-C-N	8.60	128.59	119.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	17	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	283	GLY	Peptide
1	G	251	LYS	Peptide

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	2285	0	2240	72	0
1	B	2308	0	2259	63	0
1	C	2244	0	2201	70	0
1	D	2165	0	2123	66	0
1	E	2153	0	2109	70	0
1	F	2071	0	2033	57	0
1	G	2172	0	2133	79	0
1	H	2120	0	2083	61	0
2	A	30	0	18	3	0
2	B	30	0	18	0	0
2	C	30	0	18	3	0
2	D	30	0	18	0	0
2	E	30	0	18	1	0
2	F	15	0	9	0	0
2	G	15	0	9	1	0
2	H	15	0	9	2	0
3	A	43	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	30	4	0
3	C	43	0	30	2	0
3	D	43	0	30	4	0
3	E	43	0	30	7	0
3	F	43	0	30	5	0
3	G	43	0	30	3	0
3	H	43	0	30	5	0
4	A	170	0	0	3	0
4	B	152	0	0	6	0
4	C	129	0	0	7	0
4	D	124	0	0	5	0
4	E	133	0	0	6	0
4	F	96	0	0	2	0
4	G	113	0	0	11	0
4	H	99	0	0	1	0
All	All	19073	0	17538	483	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 14.

The worst 5 of 483 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:E:114:MET:SD	1:H:283:GLY:HA2	1.77	1.24
1:E:38:GLN:NE2	1:F:29:ARG:HH11	1.37	1.23
1:C:241:MET:SD	1:C:245:MET:HE3	1.79	1.22
1:F:241:MET:SD	1:F:245:MET:HE1	1.78	1.22
1:E:38:GLN:HE22	1:F:29:ARG:NH1	1.38	1.20

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	275/306 (90%)	269 (98%)	5 (2%)	1 (0%)	30	26
1	B	278/306 (91%)	268 (96%)	9 (3%)	1 (0%)	30	26
1	C	268/306 (88%)	258 (96%)	9 (3%)	1 (0%)	30	26
1	D	260/306 (85%)	250 (96%)	9 (4%)	1 (0%)	30	26
1	E	258/306 (84%)	245 (95%)	13 (5%)	0	100	100
1	F	246/306 (80%)	235 (96%)	9 (4%)	2 (1%)	16	10
1	G	260/306 (85%)	247 (95%)	12 (5%)	1 (0%)	30	26
1	H	253/306 (83%)	241 (95%)	12 (5%)	0	100	100
All	All	2098/2448 (86%)	2013 (96%)	78 (4%)	7 (0%)	36	34

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	VAL
1	A	118	ASP
1	G	114	MET
1	C	198	ALA
1	D	184	PRO

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	241/266 (91%)	227 (94%)	14 (6%)	18	14
1	B	244/266 (92%)	223 (91%)	21 (9%)	10	5
1	C	238/266 (90%)	216 (91%)	22 (9%)	8	4
1	D	228/266 (86%)	211 (92%)	17 (8%)	12	8
1	E	227/266 (85%)	200 (88%)	27 (12%)	5	2
1	F	220/266 (83%)	202 (92%)	18 (8%)	10	6
1	G	229/266 (86%)	213 (93%)	16 (7%)	14	9
1	H	224/266 (84%)	205 (92%)	19 (8%)	10	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1851/2128 (87%)	1697 (92%)	154 (8%)	10 6

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	234	GLN
1	H	129	LEU
1	G	21	ARG
1	G	234	GLN
1	H	234	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	185	GLN
1	H	45	HIS
1	F	234	GLN
1	G	142	ASN
1	H	130	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	HEM	G	401	1	50,50,50	2.22	10 (20%)	67,82,82	2.01	20 (29%)
2	TRP	G	402	-	15,16,16	1.62	2 (13%)	18,22,22	0.71	1 (5%)
3	HEM	C	401	1	50,50,50	2.13	13 (26%)	67,82,82	1.82	18 (26%)
3	HEM	F	401	1	50,50,50	2.67	10 (20%)	67,82,82	2.06	17 (25%)
3	HEM	B	401	1,4	50,50,50	2.07	16 (32%)	67,82,82	1.84	19 (28%)
2	TRP	C	402	-	15,16,16	2.05	3 (20%)	18,22,22	0.93	1 (5%)
3	HEM	H	401	1	50,50,50	2.39	10 (20%)	67,82,82	2.00	24 (35%)
2	TRP	H	402	-	15,16,16	1.59	3 (20%)	18,22,22	0.73	0
2	TRP	A	402	-	15,16,16	2.13	3 (20%)	18,22,22	1.15	1 (5%)
2	TRP	D	402	-	15,16,16	2.19	4 (26%)	18,22,22	1.00	1 (5%)
2	TRP	E	403	-	15,16,16	1.76	5 (33%)	18,22,22	0.49	0
3	HEM	A	401	1,4	50,50,50	2.07	14 (28%)	67,82,82	2.00	19 (28%)
2	TRP	B	402	-	15,16,16	2.12	5 (33%)	18,22,22	0.75	0
3	HEM	D	401	1,4	50,50,50	2.06	14 (28%)	67,82,82	1.81	23 (34%)
2	TRP	A	403	-	15,16,16	1.55	2 (13%)	18,22,22	0.51	0
3	HEM	E	401	1,4	50,50,50	2.54	11 (22%)	67,82,82	2.09	18 (26%)
2	TRP	B	403	-	15,16,16	1.04	1 (6%)	18,22,22	0.79	1 (5%)
2	TRP	E	402	-	15,16,16	1.97	4 (26%)	18,22,22	1.22	2 (11%)
2	TRP	C	403	-	15,16,16	1.44	2 (13%)	18,22,22	0.79	1 (5%)
2	TRP	D	403	-	15,16,16	1.60	4 (26%)	18,22,22	0.90	1 (5%)
2	TRP	F	402	-	15,16,16	1.62	4 (26%)	18,22,22	1.10	1 (5%)

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	HEM	G	401	1	-	4/14/54/54	-
2	TRP	G	402	-	-	5/8/8/8	0/2/2/2
3	HEM	C	401	1	-	2/14/54/54	-
3	HEM	F	401	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	401	1,4	-	6/14/54/54	-
2	TRP	C	402	-	-	6/8/8/8	0/2/2/2
3	HEM	H	401	1	-	5/14/54/54	-
2	TRP	H	402	-	-	5/8/8/8	0/2/2/2
2	TRP	A	402	-	-	5/8/8/8	0/2/2/2
2	TRP	D	402	-	-	5/8/8/8	0/2/2/2
2	TRP	E	403	-	-	1/8/8/8	0/2/2/2
3	HEM	A	401	1,4	-	6/14/54/54	-
2	TRP	B	402	-	-	5/8/8/8	0/2/2/2
3	HEM	D	401	1,4	-	3/14/54/54	-
2	TRP	A	403	-	-	0/8/8/8	0/2/2/2
3	HEM	E	401	1,4	-	4/14/54/54	-
2	TRP	B	403	-	-	0/8/8/8	0/2/2/2
2	TRP	E	402	-	-	3/8/8/8	0/2/2/2
2	TRP	C	403	-	-	0/8/8/8	0/2/2/2
2	TRP	D	403	-	-	0/8/8/8	0/2/2/2
2	TRP	F	402	-	-	6/8/8/8	0/2/2/2

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	HEM	FE-ND	10.61	2.27	1.94
3	E	401	HEM	FE-ND	10.32	2.26	1.94
3	H	401	HEM	C3D-C2D	8.76	1.55	1.36
3	F	401	HEM	C3D-C2D	8.66	1.55	1.36
3	E	401	HEM	C3D-C2D	8.29	1.54	1.36

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	401	HEM	C4D-ND-C1D	8.55	115.33	105.21
3	E	401	HEM	C4D-ND-C1D	7.70	114.33	105.21
3	G	401	HEM	C4D-ND-C1D	7.27	113.81	105.21
3	E	401	HEM	C3B-C4B-NB	-7.11	104.36	109.47
3	H	401	HEM	C4D-ND-C1D	7.04	113.54	105.21

There are no chirality outliers.

5 of 75 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	HEM	C2B-C3B-CAB-CBB
3	B	401	HEM	C2B-C3B-CAB-CBB
3	E	401	HEM	C2B-C3B-CAB-CBB
3	E	401	HEM	C4B-C3B-CAB-CBB
3	H	401	HEM	C2C-C3C-CAC-CBC

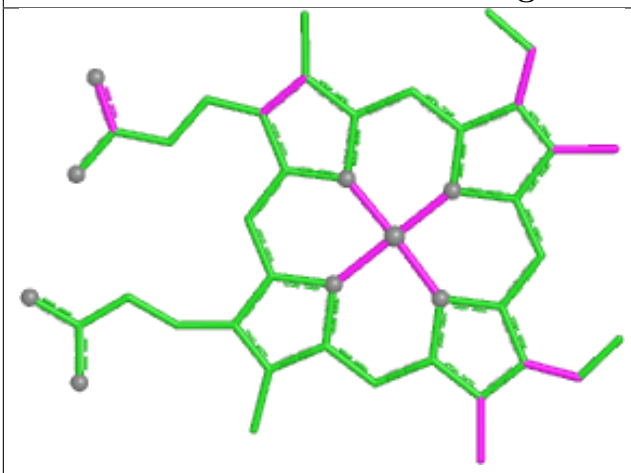
There are no ring outliers.

14 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	HEM	3	0
2	G	402	TRP	1	0
3	C	401	HEM	2	0
3	F	401	HEM	5	0
3	B	401	HEM	4	0
2	C	402	TRP	3	0
3	H	401	HEM	5	0
2	H	402	TRP	2	0
2	A	402	TRP	2	0
2	E	403	TRP	1	0
3	A	401	HEM	1	0
3	D	401	HEM	4	0
2	A	403	TRP	1	0
3	E	401	HEM	7	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 G 401



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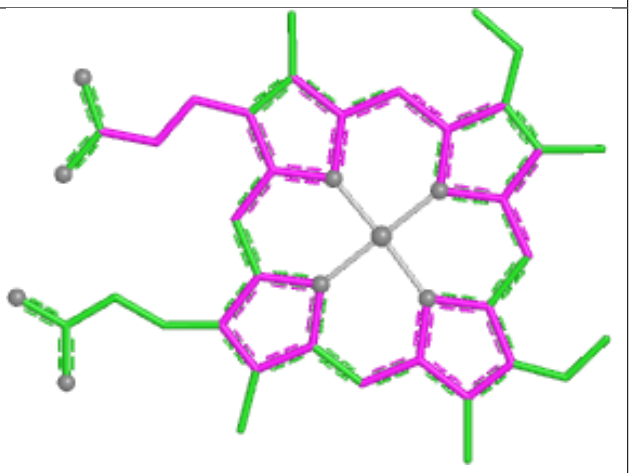

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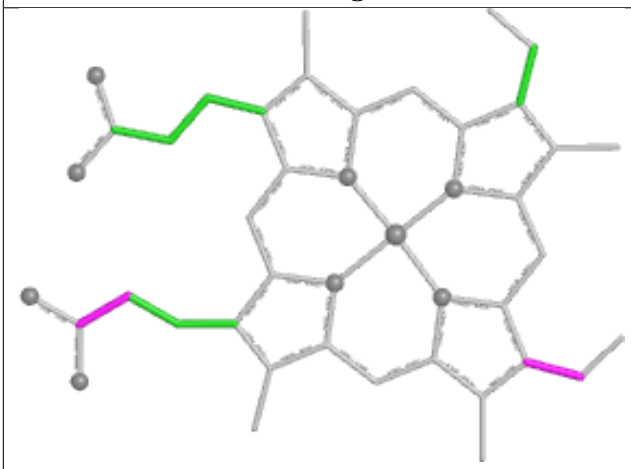
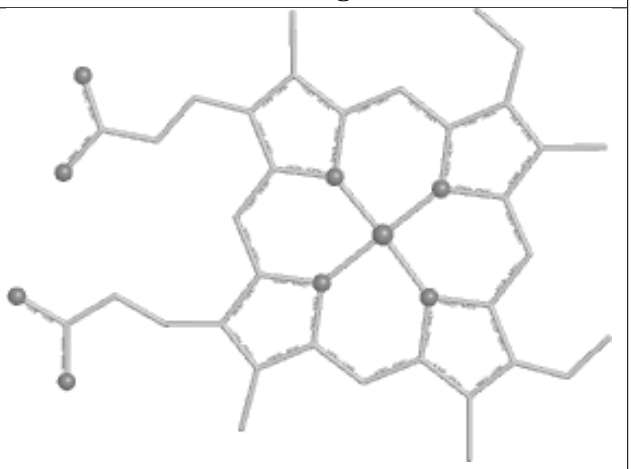
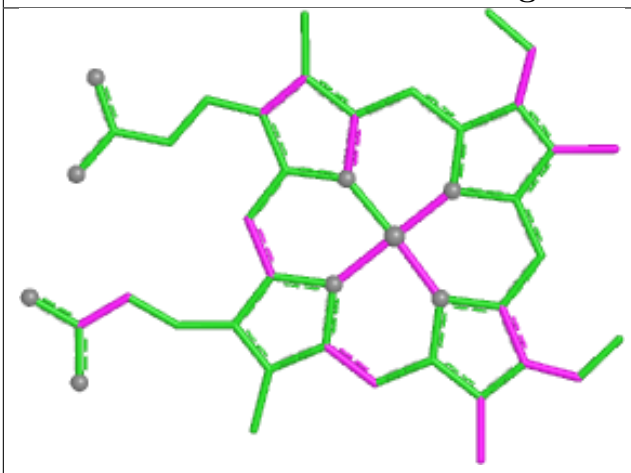


Torsions



Rings

Ligand HEM C 401



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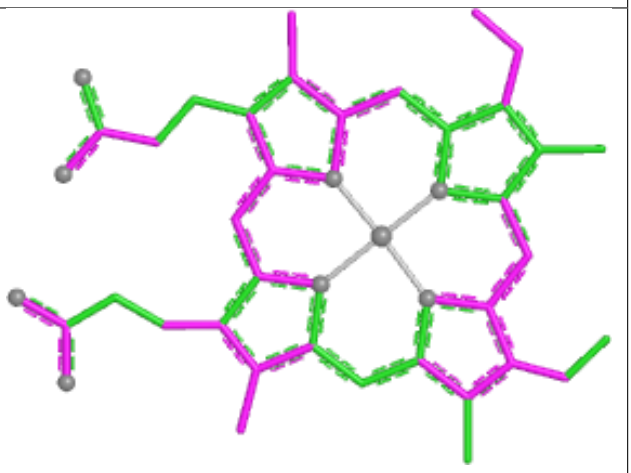

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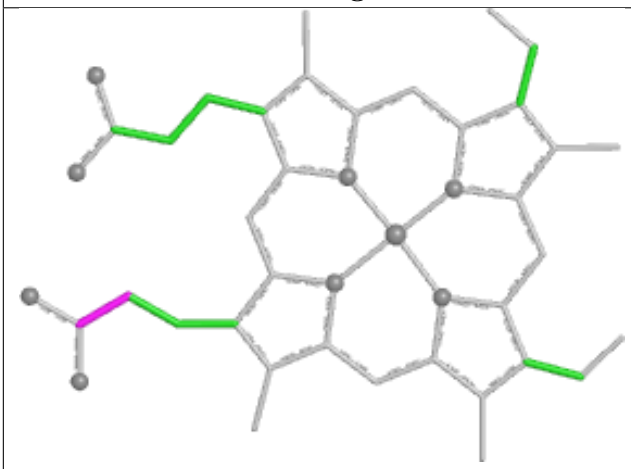

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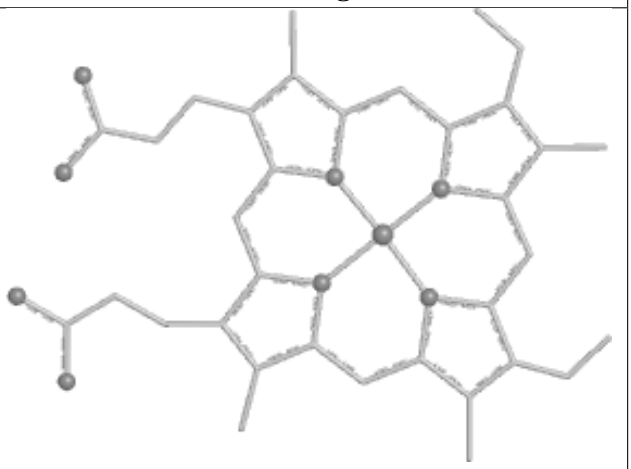

Rings

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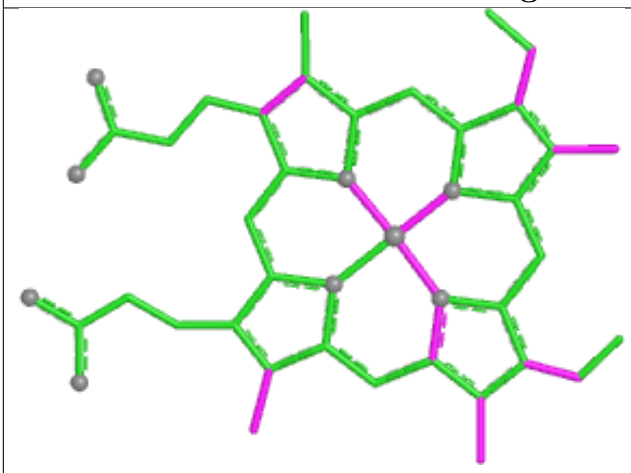

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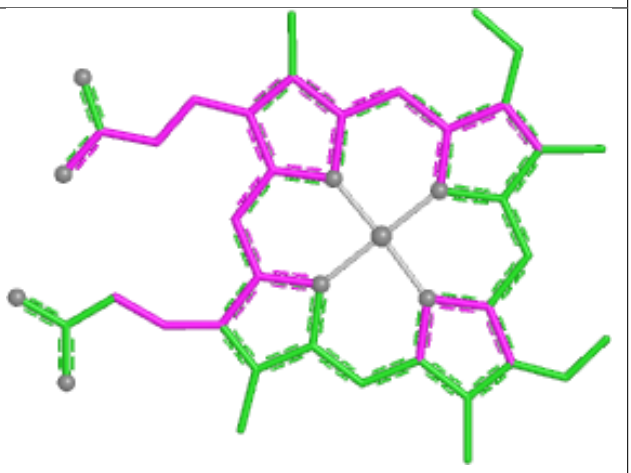

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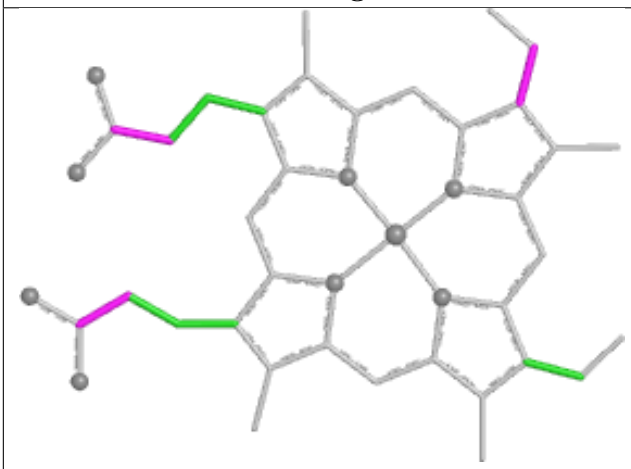

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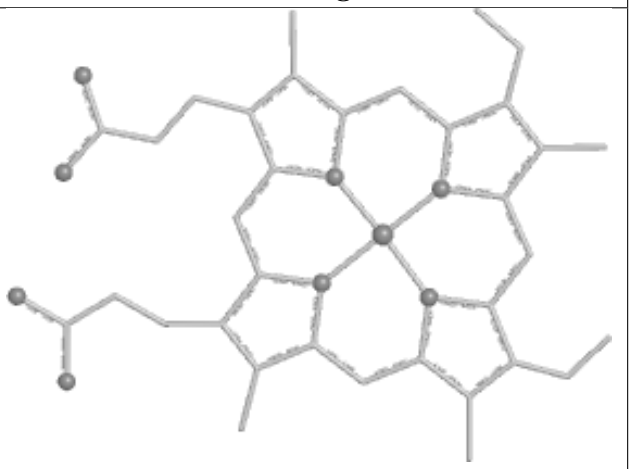

Rings

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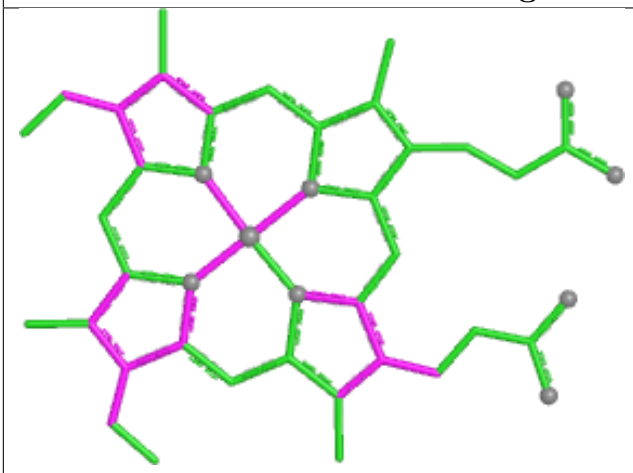

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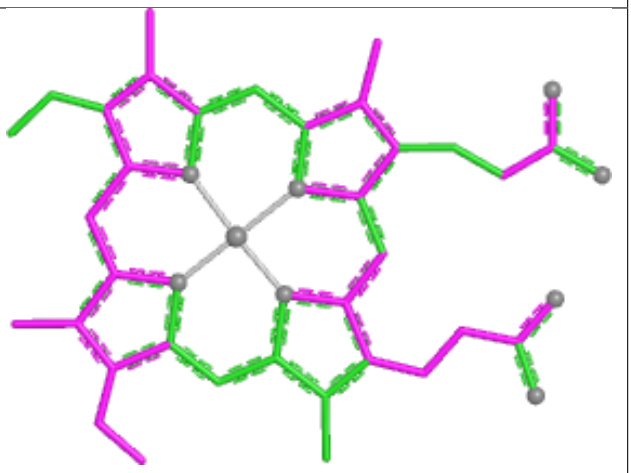

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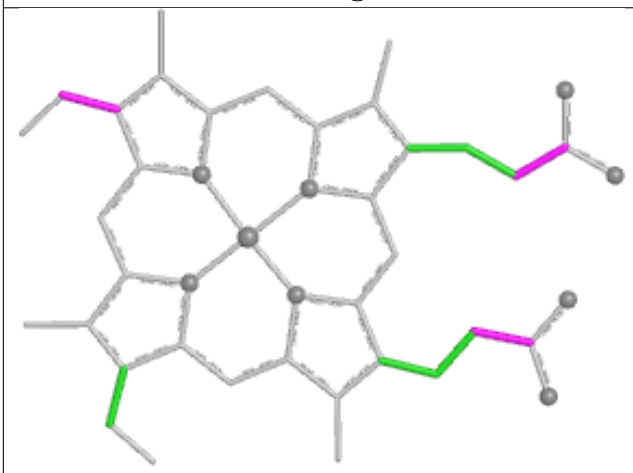

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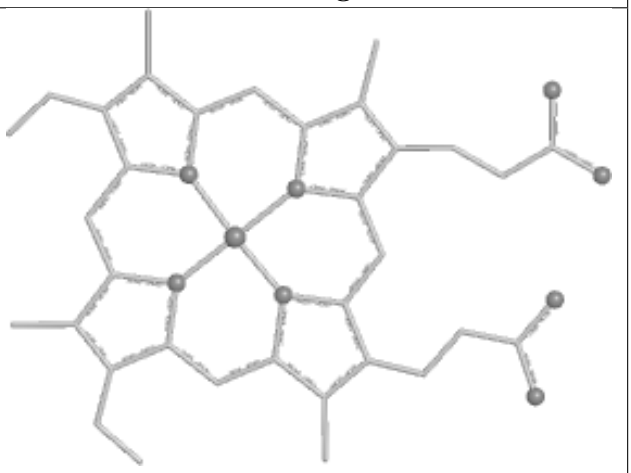

Rings

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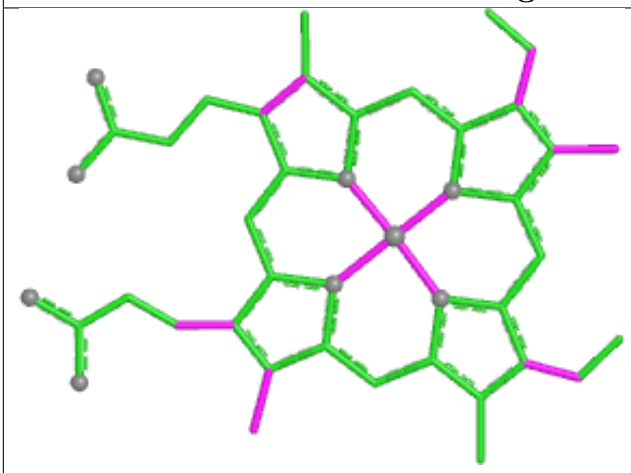

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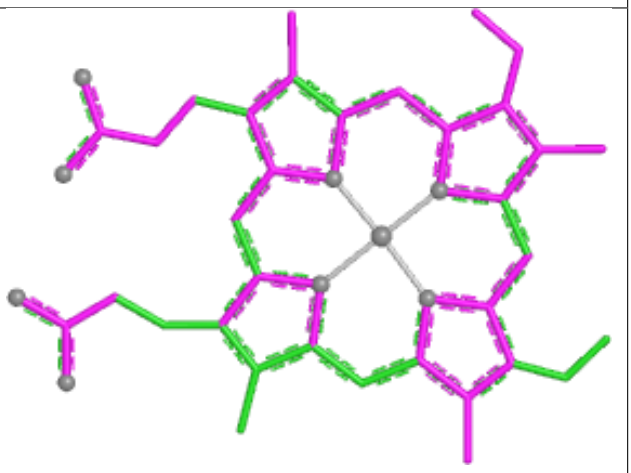

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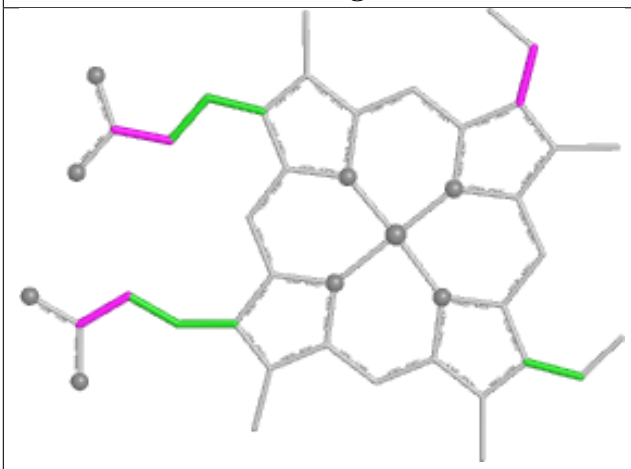

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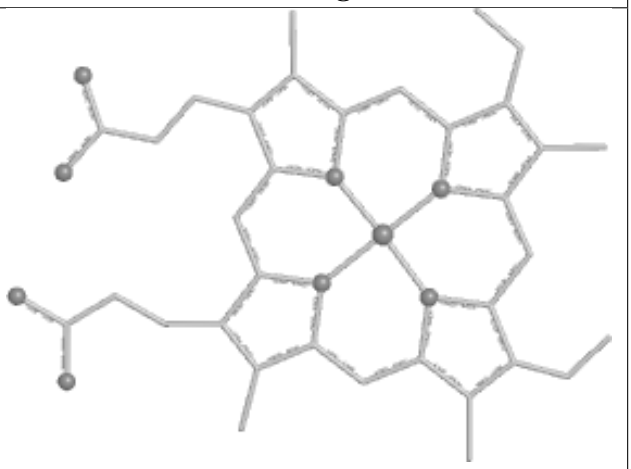
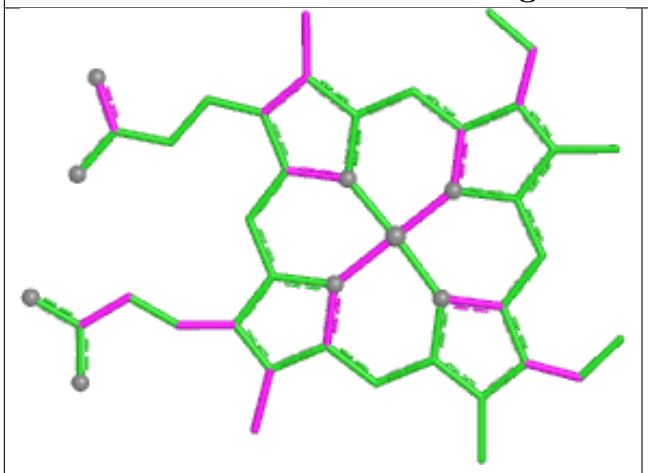


Rings

Ligand HEM A 401



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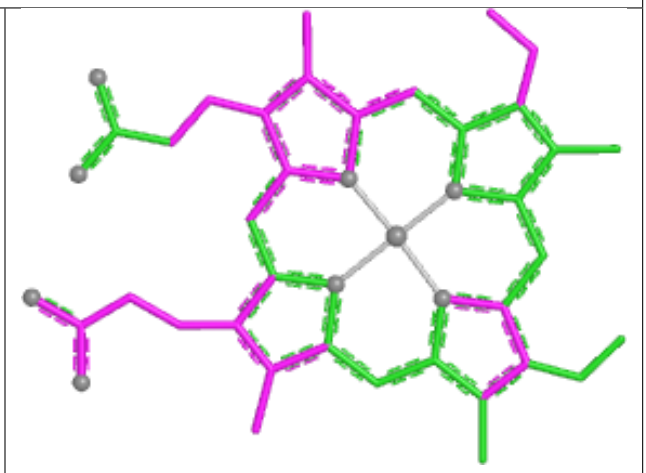
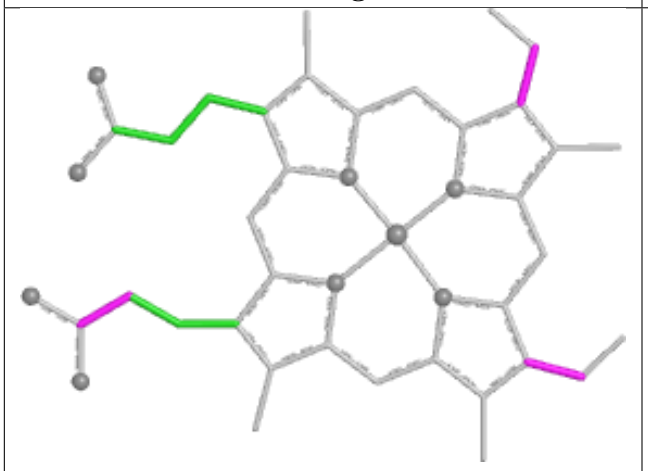


Bond angles



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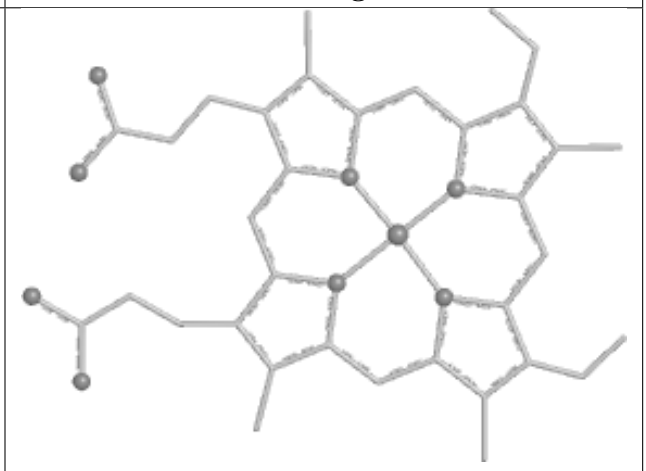
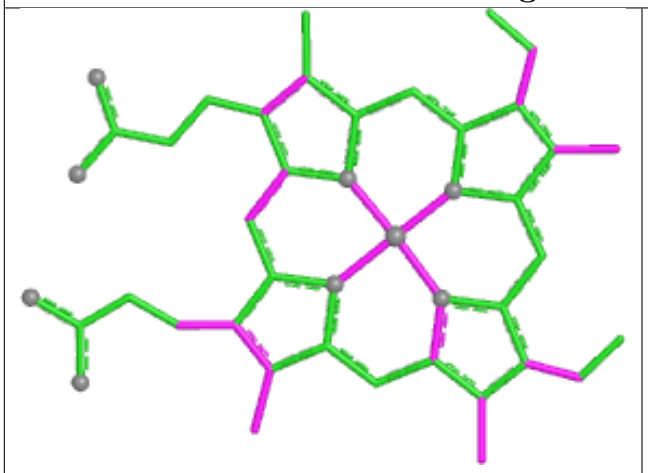


Rings

Ligand HEM D 401



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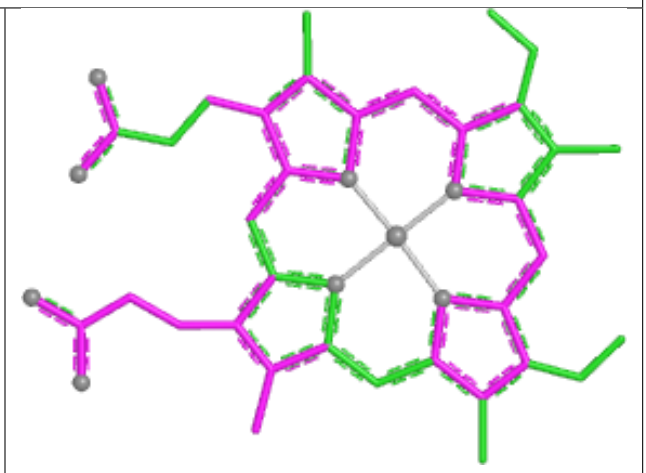
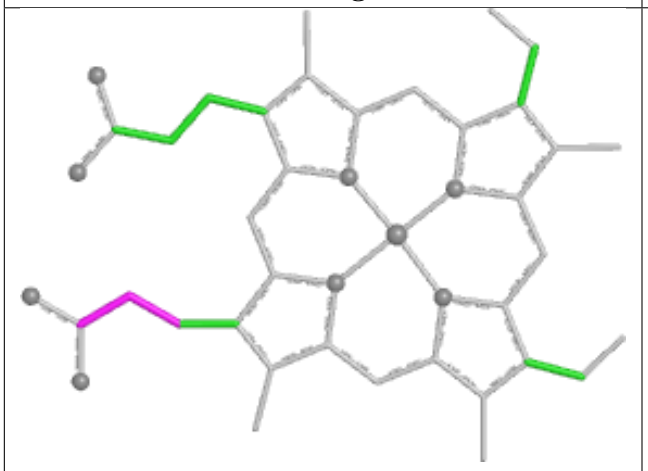
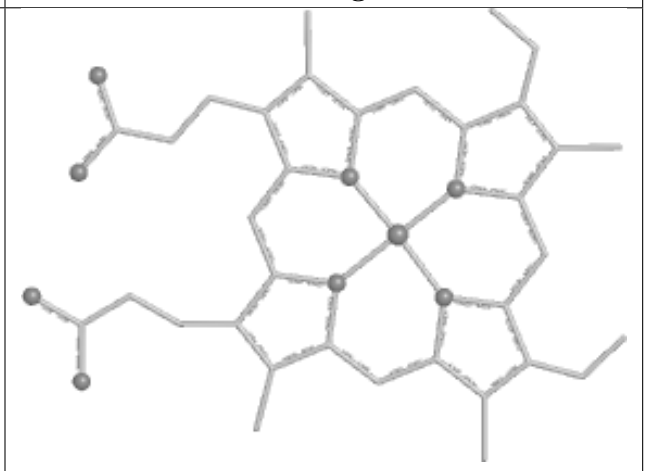


Bond angles

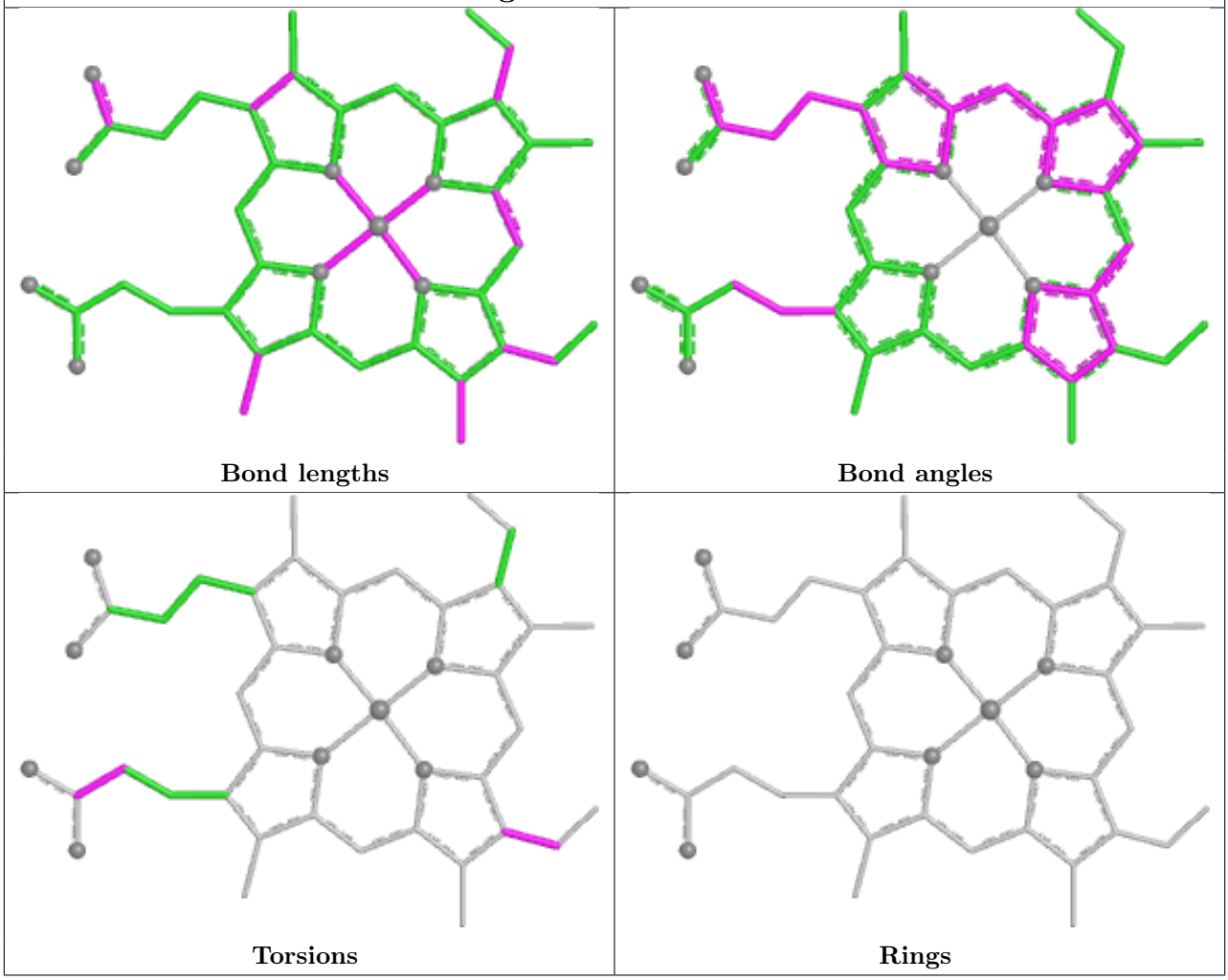


Torsions



Rings

Ligand HEM E 401



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	277/306 (90%)	-0.32	3 (1%)	78	80	5, 15, 27, 45	0
1	B	280/306 (91%)	-0.27	1 (0%)	88	90	4, 15, 31, 42	0
1	C	272/306 (88%)	-0.06	8 (2%)	53	57	10, 19, 41, 54	0
1	D	262/306 (85%)	-0.16	1 (0%)	88	90	9, 19, 38, 44	0
1	E	260/306 (84%)	-0.02	4 (1%)	72	76	9, 24, 37, 43	0
1	F	250/306 (81%)	0.19	7 (2%)	55	59	15, 26, 45, 55	0
1	G	262/306 (85%)	0.08	3 (1%)	78	80	9, 25, 42, 47	0
1	H	257/306 (83%)	0.37	13 (5%)	33	37	16, 31, 52, 63	0
All	All	2120/2448 (86%)	-0.03	40 (1%)	66	70	4, 22, 41, 63	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	LEU	4.4
1	C	19	GLU	3.8
1	H	192	TRP	3.6
1	A	7	LEU	3.4
1	G	250	PHE	3.3

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)

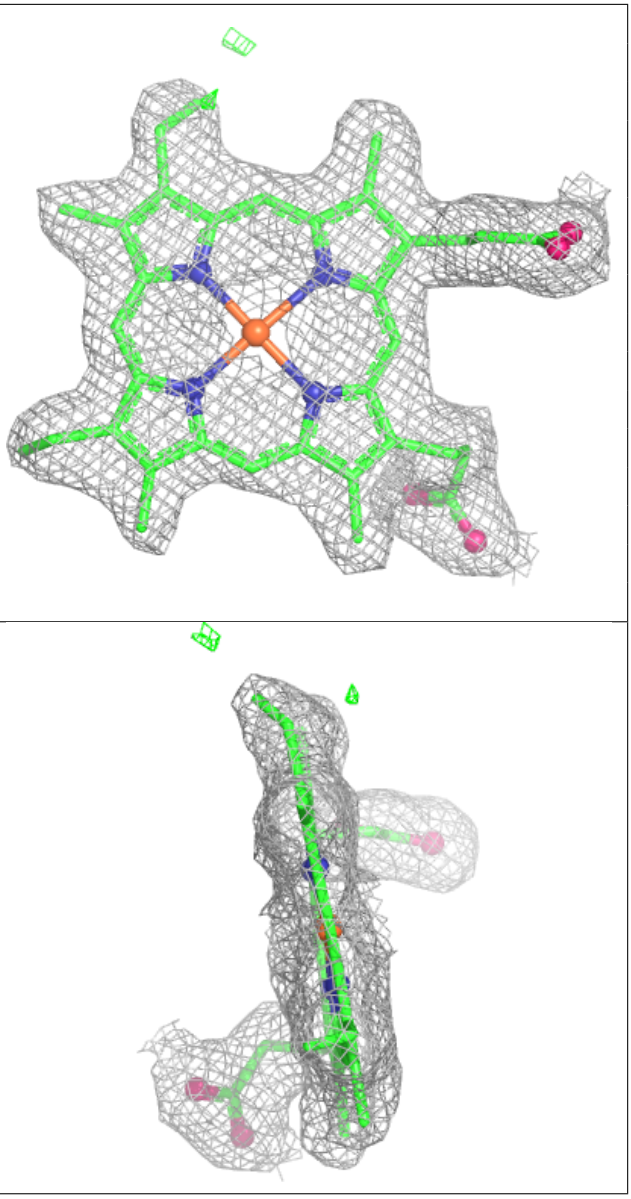
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRP	H	402	15/15	0.79	0.16	32,36,40,41	0
2	TRP	E	402	15/15	0.82	0.13	29,31,33,36	0
2	TRP	G	402	15/15	0.84	0.13	30,35,40,43	0
2	TRP	E	403	15/15	0.86	0.11	24,27,38,39	0
2	TRP	F	402	15/15	0.91	0.09	25,27,32,35	0
2	TRP	C	403	15/15	0.91	0.08	14,18,27,28	0
2	TRP	D	402	15/15	0.91	0.09	14,18,25,26	0
2	TRP	B	403	15/15	0.92	0.07	12,20,26,26	0
2	TRP	C	402	15/15	0.92	0.09	13,21,28,31	0
2	TRP	A	402	15/15	0.92	0.08	14,16,23,25	0
2	TRP	A	403	15/15	0.93	0.08	14,21,28,28	0
2	TRP	D	403	15/15	0.94	0.07	11,15,27,30	0
2	TRP	B	402	15/15	0.95	0.07	7,9,18,18	0
3	HEM	E	401	43/43	0.96	0.07	11,23,27,34	0
3	HEM	F	401	43/43	0.96	0.08	13,20,27,34	0
3	HEM	G	401	43/43	0.96	0.07	20,25,31,38	0
3	HEM	H	401	43/43	0.96	0.07	17,23,27,28	0
3	HEM	A	401	43/43	0.98	0.06	2,8,13,17	0
3	HEM	B	401	43/43	0.98	0.05	2,5,10,13	0
3	HEM	C	401	43/43	0.98	0.06	4,10,16,19	0
3	HEM	D	401	43/43	0.98	0.05	2,9,17,21	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.

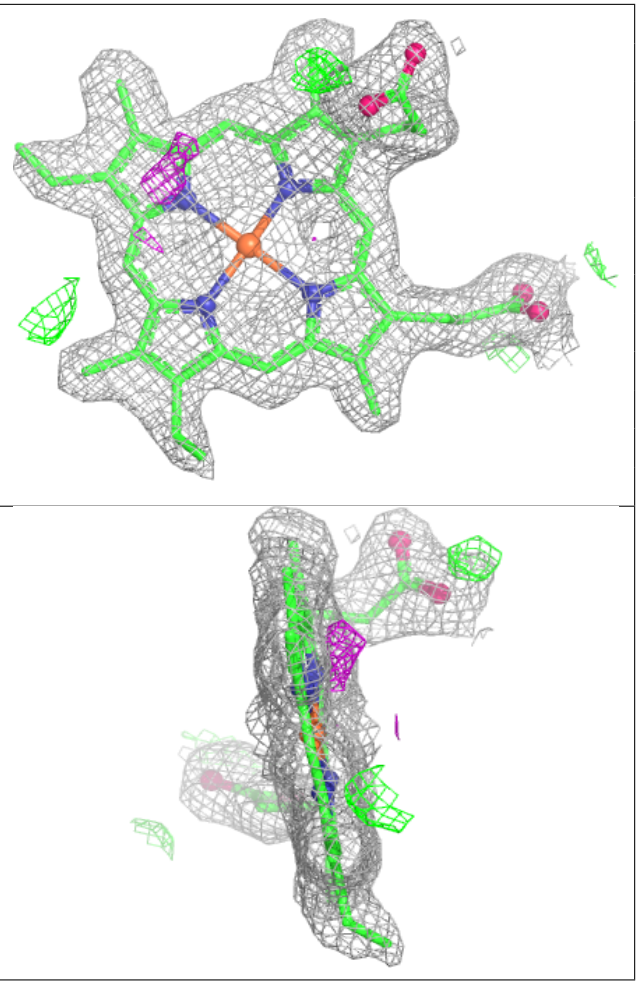
Electron density around HEM E 401:

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



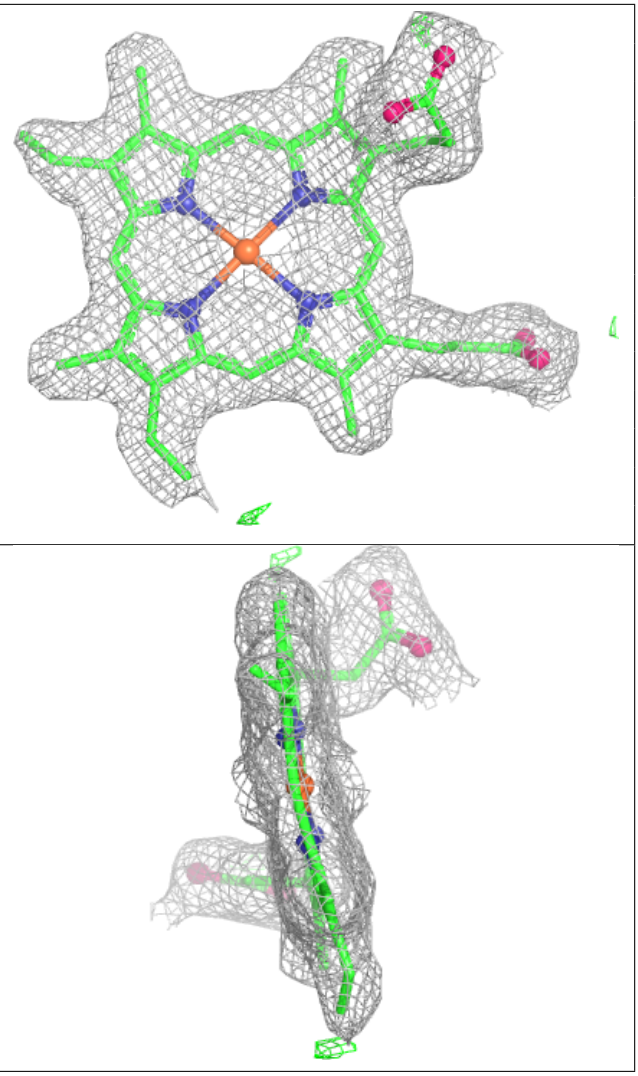
Electron density around HEM F 401:

$2mF_o$-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 G 401:

$2mF_o$-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 H 401:

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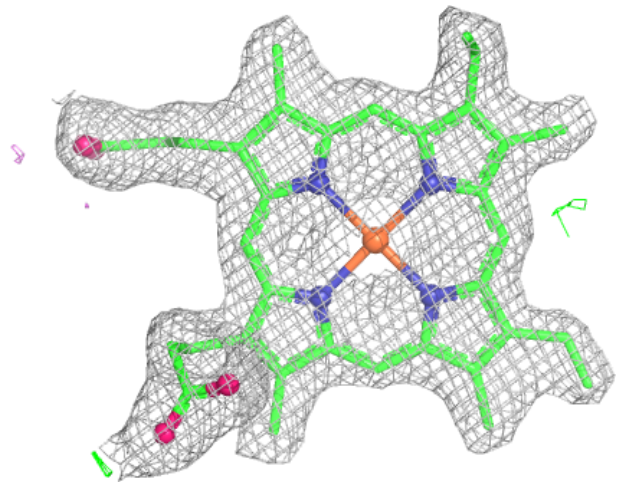
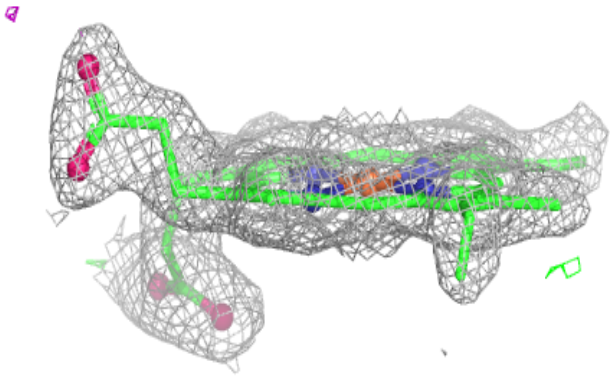
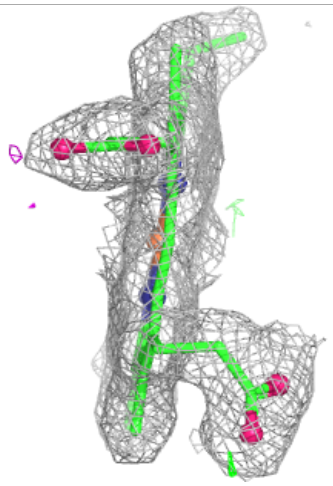
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

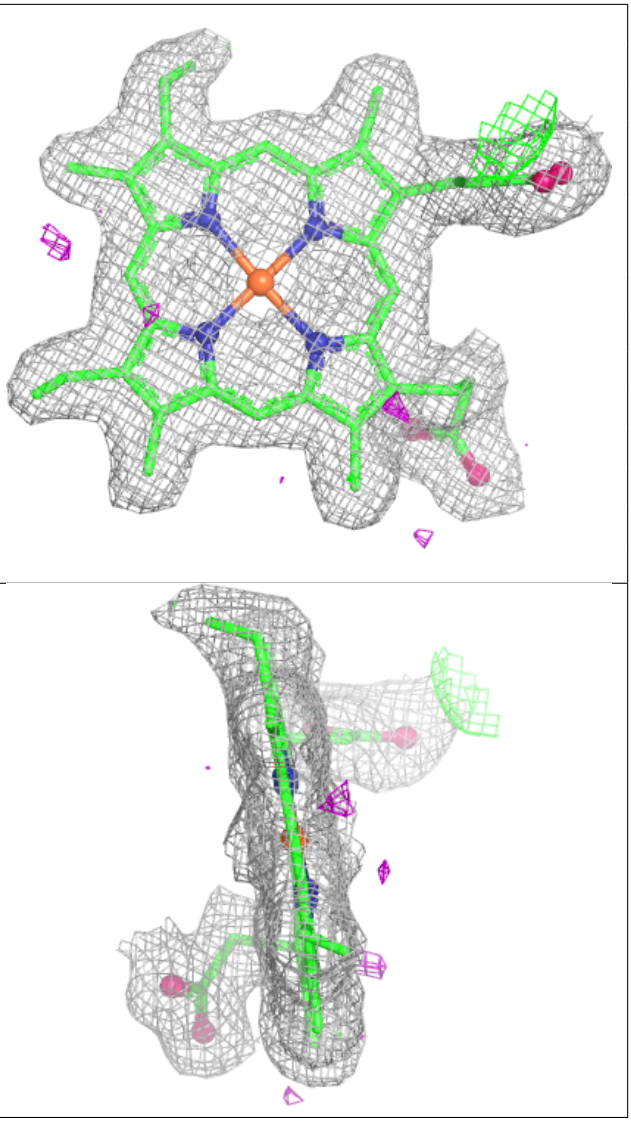






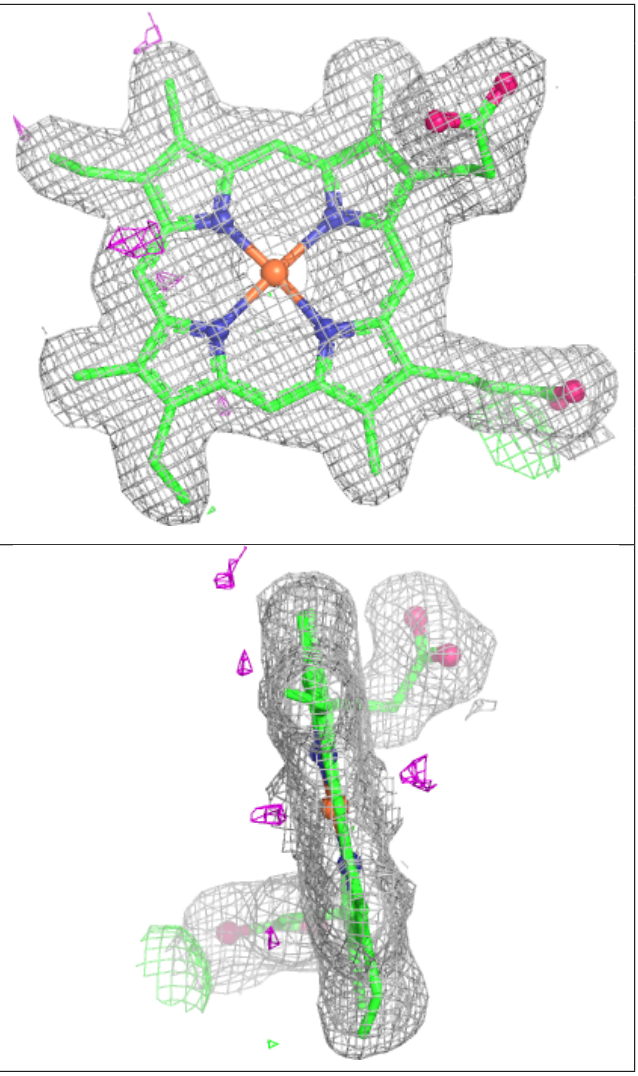
Electron density around HEM A 401:

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



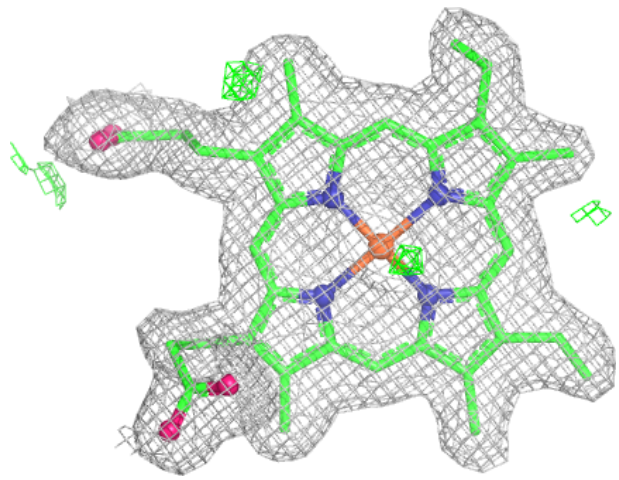
Electron density around HEM B 401:

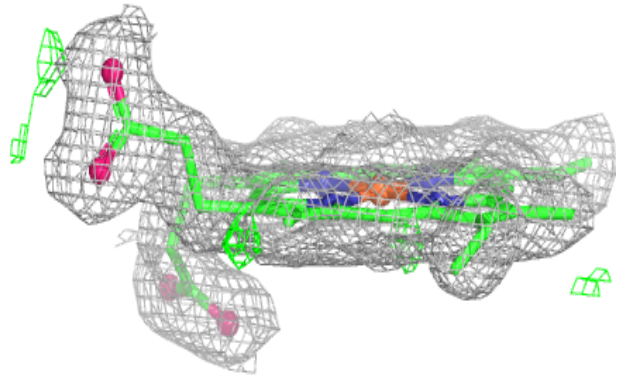
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

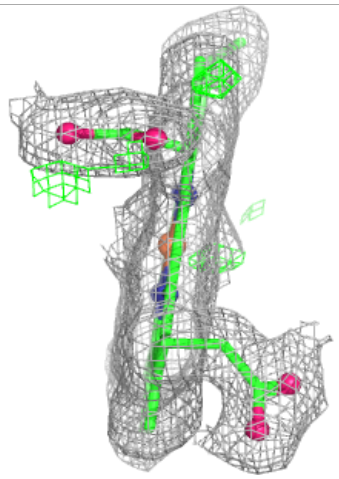


Electron density around HEM C 401:

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

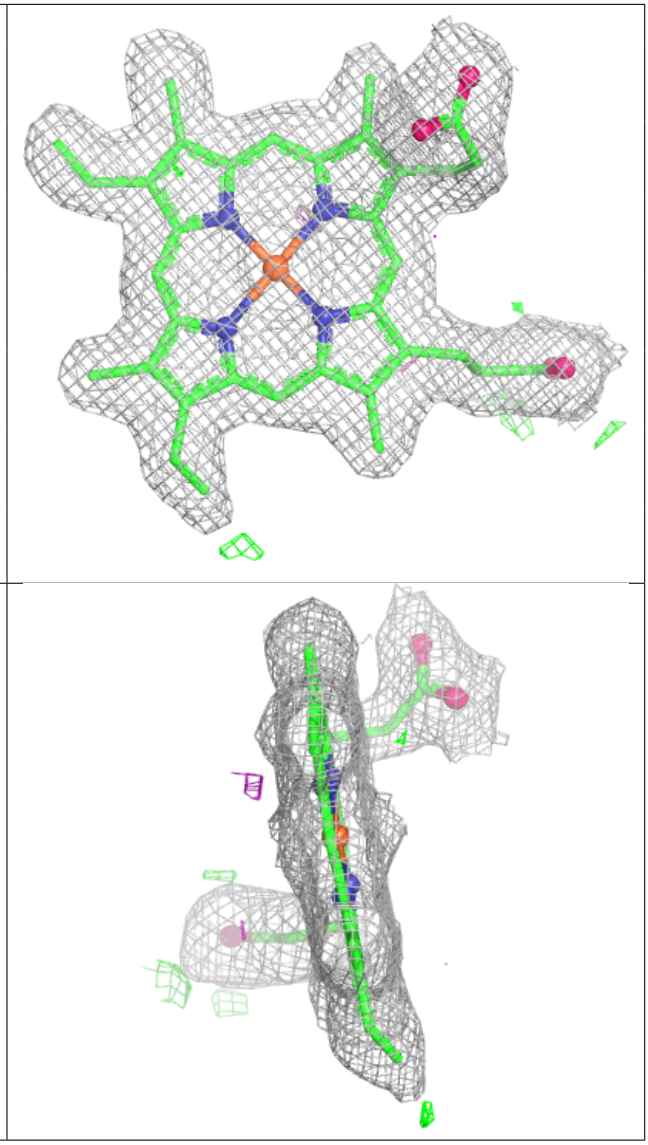






Electron density around HEM D 401:

$2mF_o$-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.