Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 03:07 AM JST

PDB ID	:	5IT1 / pdb_00005it1
Title	:	Streptomyces peucetius CYP105P2 complex with biphenyl compound
Authors	:	Lee, C.W.; Lee, J.H.
Deposited on	:	2016-03-16
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

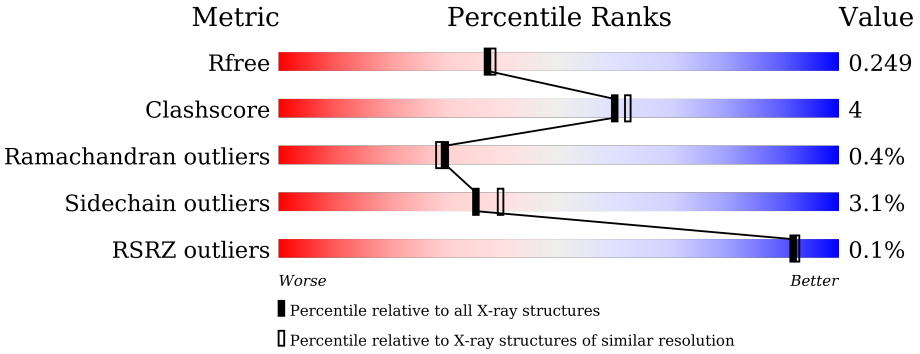
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	399	87% 10% • •
1	B	399	87% 11% • •
1	C	399	89% 9% • •
1	D	399	86% 13% • •

2 Entry composition (i)

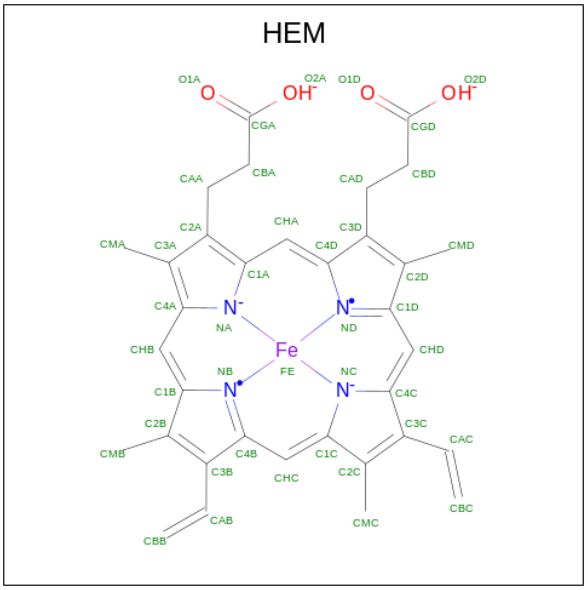
There are 4 unique types of molecules in this entry. The entry contains 13065 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	395	3042	1922	544	564	12	0	0	0
1	B	395	3042	1922	544	564	12	0	0	0
1	C	395	3042	1922	544	564	12	0	0	0
1	D	395	3042	1922	544	564	12	0	0	0

- 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
2	B	1	43	34	1	4	4	0	0

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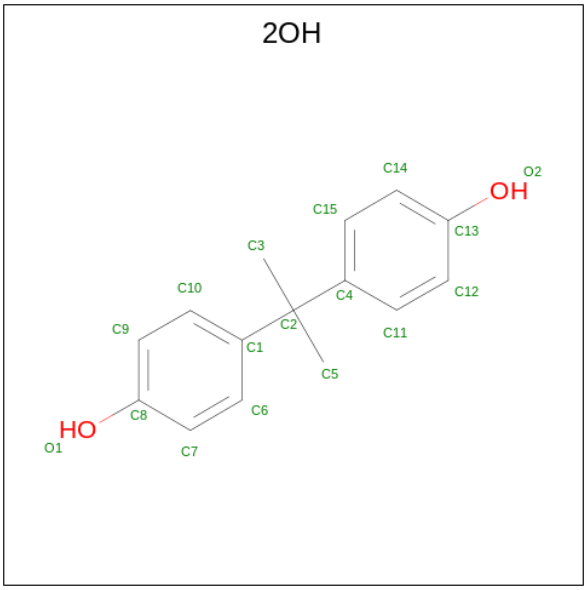
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is 4,4'-PROPANE-2,2-DIYLDIPHENOL (CCD ID: 2OH) (formula: $C_{15}H_{16}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	17	15	2	0	0
			Total	C	O		
3	B	1	17	15	2	0	0
			Total	C	O		
3	C	1	17	15	2	0	0
			Total	C	O		
3	D	1	17	15	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	155	155	155	0	0
			Total	O		
4	B	177	177	177	0	0
			Total	O		
4	C	164	164	164	0	0

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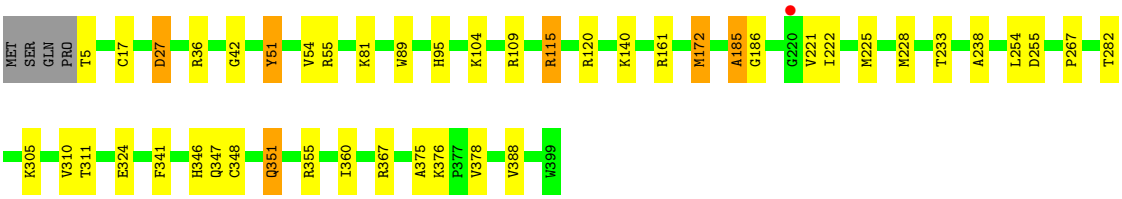
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	161	161	161	0	0

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.

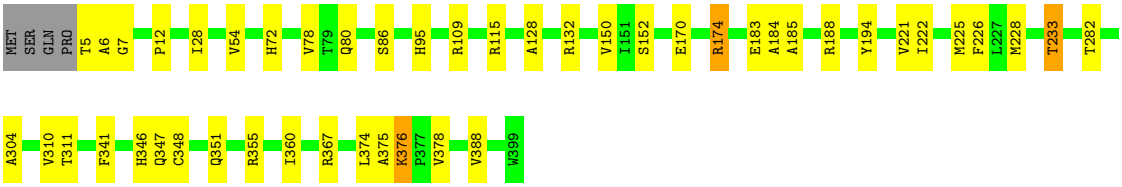
• Molecule 1: Putative cytochrome P450

Chain A:



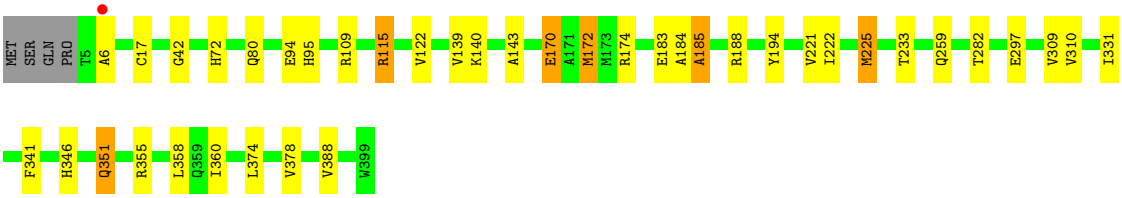
• Molecule 1: Putative cytochrome P450

Chain B:



• Molecule 1: Putative cytochrome P450

Chain C:



• Molecule 1: Putative cytochrome P450

Chain D:

G232
T233
D255
R256
P257
D258
T282
V310
T311
D325
F341
G344
A345
H346
Q347
G350
Q351
R355
L358
R367
K376
R382
V388
E394
L395
W399

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.02Å 122.94Å 193.29Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.10) 98.9 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.45 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.200 , 0.243 0.208 , 0.249	Depositor DCC
R_{free} test set	8315 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.428 for k,h,-l 0.437 for -k,-h,-l 0.460 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13065	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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, 2OH

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	1.29	6/3106 (0.2%)	1.21	5/4224 (0.1%)
1	B	1.28	7/3106 (0.2%)	1.21	3/4224 (0.1%)
1	C	1.29	4/3106 (0.1%)	1.20	6/4224 (0.1%)
1	D	1.29	11/3106 (0.4%)	1.22	9/4224 (0.2%)
All	All	1.29	28/12424 (0.2%)	1.21	23/16896 (0.1%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	TYR	CA-C	-7.02	1.44	1.52
1	D	36	ARG	CA-C	-6.81	1.44	1.52
1	C	388	VAL	CA-C	6.33	1.60	1.52
1	D	51	TYR	CA-C	-6.00	1.45	1.52
1	B	367	ARG	C-O	-5.99	1.17	1.24
1	C	358	LEU	CA-C	5.91	1.60	1.52
1	D	325	ASP	CA-C	5.89	1.57	1.53
1	A	367	ARG	C-O	-5.87	1.17	1.24
1	A	310	VAL	CA-CB	-5.85	1.46	1.53
1	D	70	ALA	N-CA	-5.83	1.38	1.46
1	D	367	ARG	C-O	-5.79	1.17	1.24
1	D	78	VAL	C-O	-5.78	1.18	1.24
1	C	309	VAL	CA-CB	-5.76	1.47	1.54
1	B	388	VAL	CA-C	5.74	1.60	1.52
1	A	388	VAL	CA-C	5.71	1.60	1.52
1	D	310	VAL	CA-CB	-5.56	1.47	1.53
1	C	310	VAL	CA-CB	-5.48	1.47	1.54
1	B	78	VAL	C-O	-5.44	1.18	1.24
1	B	150	VAL	CA-C	-5.43	1.46	1.52
1	D	388	VAL	CA-C	5.39	1.59	1.52
1	B	310	VAL	CA-CB	-5.39	1.47	1.54
1	B	348	CYS	C-O	-5.25	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	358	LEU	CA-C	5.23	1.59	1.52
1	A	36	ARG	CA-C	-5.17	1.46	1.52
1	D	231	ALA	CA-C	-5.14	1.46	1.52
1	D	38	THR	CA-C	-5.11	1.46	1.52
1	B	233	THR	CB-CG2	-5.10	1.35	1.52
1	A	120	ARG	C-O	-5.00	1.18	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	233	THR	N-CA-CB	7.87	122.47	110.28
1	A	347	GLN	CB-CA-C	-7.22	98.20	109.61
1	D	17	CYS	CA-C-N	6.79	126.42	119.56
1	D	17	CYS	C-N-CA	6.79	126.42	119.56
1	C	351	GLN	CB-CA-C	-6.74	100.03	110.81
1	D	172	MET	CG-SD-CE	-6.36	86.92	100.90
1	D	258	ASP	N-CA-CB	-6.35	100.48	109.94
1	A	42	GLY	N-CA-C	-6.27	106.77	114.92
1	B	185	ALA	N-CA-C	-5.77	105.12	111.82
1	C	185	ALA	N-CA-C	-5.77	105.13	111.82
1	A	351	GLN	CB-CA-C	-5.76	101.59	110.81
1	B	222	ILE	CB-CA-C	-5.63	105.14	111.23
1	C	225	MET	CG-SD-CE	-5.60	88.58	100.90
1	D	350	GLY	CA-C-N	5.40	127.83	120.54
1	D	350	GLY	C-N-CA	5.40	127.83	120.54
1	C	42	GLY	N-CA-C	-5.37	108.23	115.21
1	D	71	LEU	N-CA-C	5.24	117.74	111.71
1	D	256	ARG	CA-C-N	5.24	125.55	119.47
1	D	256	ARG	C-N-CA	5.24	125.55	119.47
1	A	172	MET	CG-SD-CE	-5.20	89.45	100.90
1	C	172	MET	CG-SD-CE	-5.16	89.54	100.90
1	A	185	ALA	N-CA-C	-5.16	105.84	111.82
1	C	122	VAL	N-CA-C	5.13	115.35	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3042	0	3032	22	0
1	B	3042	0	3032	39	0
1	C	3042	0	3032	36	0
1	D	3042	0	3032	23	0
2	A	43	0	30	5	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	2	0
3	C	17	0	15	0	0
3	D	17	0	15	0	0
4	A	155	0	0	2	0
4	B	177	0	0	2	0
4	C	164	0	0	5	0
4	D	161	0	0	3	0
All	All	13065	0	12308	105	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 4.

All (105) 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:B:225:MET:HE1	1:C:184:ALA:HA	1.35	1.08
1:B:184:ALA:HA	1:C:225:MET:HE1	1.46	0.96
1:B:351:GLN:HE21	1:B:355:ARG:HH12	1.19	0.90
1:D:351:GLN:HE21	1:D:355:ARG:HH12	1.21	0.87
1:C:351:GLN:HE21	1:C:355:ARG:HH12	1.19	0.86
1:B:184:ALA:CA	1:C:225:MET:HE1	2.06	0.85
1:A:172:MET:HE1	1:A:185:ALA:C	2.00	0.85
1:C:172:MET:HE1	1:C:185:ALA:C	2.02	0.83
1:A:17:CYS:HB3	4:A:636:HOH:O	1.79	0.81
1:A:351:GLN:HE21	1:A:355:ARG:HH12	1.29	0.81
1:B:225:MET:CE	1:C:184:ALA:HA	2.11	0.81
1:B:225:MET:HE1	1:C:184:ALA:CA	2.11	0.80
1:B:233:THR:HG22	3:B:402:2OH:O2	1.83	0.79
1:C:17:CYS:HB3	4:C:645:HOH:O	1.83	0.78
1:C:95:HIS:HD2	4:C:567:HOH:O	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:MET:CE	1:C:184:ALA:CA	2.67	0.72
1:D:172:MET:HE1	1:D:185:ALA:C	2.15	0.72
1:B:95:HIS:HD2	4:B:545:HOH:O	1.75	0.69
1:B:225:MET:CE	1:C:184:ALA:N	2.54	0.69
1:B:86:SER:O	1:B:233:THR:HG21	1.92	0.68
1:B:184:ALA:N	1:C:225:MET:HE1	2.09	0.67
1:B:225:MET:HE3	1:C:183:GLU:C	2.19	0.67
1:A:95:HIS:HD2	4:A:569:HOH:O	1.76	0.66
1:D:95:HIS:HD2	4:D:532:HOH:O	1.77	0.66
1:B:184:ALA:N	1:C:225:MET:CE	2.59	0.65
1:B:225:MET:HE3	1:C:184:ALA:N	2.11	0.65
1:C:297:GLU:HG2	4:C:509:HOH:O	1.98	0.63
1:C:72:HIS:HD2	4:C:513:HOH:O	1.80	0.63
1:D:255:ASP:OD2	1:D:256:ARG:NH1	2.34	0.61
1:C:115:ARG:HG2	1:C:360:ILE:HD11	1.82	0.60
1:C:351:GLN:HE21	1:C:355:ARG:NH1	1.96	0.58
1:C:170:GLU:OE2	1:C:174:ARG:NH2	2.37	0.58
1:D:192:LEU:C	1:D:192:LEU:HD23	2.29	0.58
1:A:346:HIS:HD2	2:A:401:HEM:O2A	1.87	0.57
1:B:225:MET:CE	1:C:183:GLU:C	2.77	0.57
1:D:72:HIS:HD2	4:D:509:HOH:O	1.87	0.57
1:B:72:HIS:HD2	4:B:512:HOH:O	1.87	0.56
1:A:172:MET:HE1	1:A:186:GLY:N	2.22	0.54
1:C:346:HIS:HD2	2:C:401:HEM:O1A	1.91	0.54
1:B:184:ALA:CA	1:C:225:MET:CE	2.84	0.54
2:C:401:HEM:HMC1	2:C:401:HEM:HBC2	1.89	0.53
1:D:54:VAL:HG13	1:D:311:THR:HB	1.92	0.52
1:D:382:ARG:HH12	1:D:394:GLU:HG2	1.74	0.52
1:D:172:MET:HE2	1:D:172:MET:CA	2.38	0.52
1:B:80:GLN:HG2	1:C:80:GLN:NE2	2.24	0.52
1:B:115:ARG:HG2	1:B:360:ILE:HD11	1.91	0.52
1:D:382:ARG:NH1	1:D:394:GLU:HG2	2.26	0.51
1:B:346:HIS:HD2	2:B:401:HEM:O1D	1.94	0.51
1:B:5:THR:O	1:B:6:ALA:HB3	2.11	0.51
1:C:341:PHE:CG	1:C:351:GLN:HG2	2.46	0.51
1:A:225:MET:HA	1:A:228:MET:HE3	1.94	0.50
1:C:259:GLN:NE2	1:C:331:ILE:H	2.09	0.49
1:D:82:PRO:HD3	1:D:181:ALA:HB2	1.94	0.49
1:A:375:ALA:O	1:A:376:LYS:HG3	2.12	0.49
1:A:172:MET:HA	1:A:172:MET:HE2	1.93	0.49
1:C:172:MET:HE1	1:C:185:ALA:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PRO:HB2	1:B:304:ALA:HB1	1.93	0.49
1:C:351:GLN:NE2	1:C:355:ARG:HH12	1.99	0.49
1:A:172:MET:HE2	1:A:172:MET:CA	2.43	0.49
1:B:225:MET:HA	1:B:228:MET:HE3	1.95	0.49
1:B:12:PRO:HG2	1:B:28:ILE:HD12	1.95	0.48
1:B:174:ARG:CG	1:B:174:ARG:HH11	2.26	0.48
1:B:194:TYR:CE1	1:C:188:ARG:HD2	2.48	0.48
1:A:95:HIS:HE1	2:A:401:HEM:O1A	1.96	0.48
1:B:183:GLU:C	1:C:225:MET:CE	2.87	0.48
1:D:346:HIS:HD2	2:D:401:HEM:O1D	1.96	0.48
1:A:115:ARG:HG2	1:A:360:ILE:HD11	1.95	0.48
1:B:183:GLU:C	1:C:225:MET:HE1	2.38	0.48
2:D:401:HEM:HMC2	2:D:401:HEM:HBC2	1.95	0.48
1:D:168:ILE:HD12	1:D:192:LEU:HD12	1.95	0.47
1:D:95:HIS:HE1	2:D:401:HEM:O2D	1.96	0.46
1:A:140:LYS:HE3	1:A:140:LYS:HA	1.97	0.46
1:D:344:GLY:O	1:D:347:GLN:HB2	2.16	0.46
1:B:128:ALA:O	1:B:132:ARG:HG2	2.17	0.45
1:C:172:MET:CA	1:C:172:MET:HE2	2.46	0.45
1:B:54:VAL:HG13	1:B:311:THR:HB	1.98	0.45
1:B:95:HIS:HE1	2:B:401:HEM:O2D	1.99	0.45
1:C:94:GLU:HG3	4:C:551:HOH:O	2.17	0.45
1:B:188:ARG:HD2	1:C:194:TYR:CE1	2.52	0.44
1:C:139:VAL:HA	1:C:143:ALA:HB3	2.00	0.44
1:B:341:PHE:CD2	1:B:351:GLN:HG2	2.52	0.44
1:A:341:PHE:CG	1:A:351:GLN:HG2	2.52	0.44
1:D:5:THR:OG1	1:D:6:ALA:HA	2.17	0.44
1:D:172:MET:HE2	1:D:172:MET:HA	1.99	0.44
1:B:174:ARG:CG	1:B:174:ARG:NH1	2.81	0.44
1:D:94:GLU:HG3	4:D:578:HOH:O	2.17	0.43
1:C:95:HIS:HE1	2:C:401:HEM:O2A	2.01	0.43
2:A:401:HEM:HMC1	2:A:401:HEM:HBC2	2.00	0.42
1:A:81:LYS:HD2	1:A:89:TRP:CD2	2.54	0.42
1:B:233:THR:HG23	3:B:402:2OH:H12	2.01	0.42
2:D:401:HEM:CMB	2:D:401:HEM:HBB2	2.49	0.42
1:A:27:ASP:OD1	1:A:27:ASP:N	2.38	0.42
1:A:255:ASP:O	1:A:255:ASP:CG	2.63	0.42
1:A:54:VAL:HG13	1:A:311:THR:HB	2.01	0.42
1:A:238:ALA:HB2	2:A:401:HEM:HMB1	2.00	0.42
1:A:348:CYS:HB2	2:A:401:HEM:ND	2.34	0.42
1:B:375:ALA:O	1:B:376:LYS:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:GLU:CD	1:D:174:ARG:HH21	2.28	0.42
1:A:51:TYR:CE1	1:A:55:ARG:HD2	2.55	0.42
1:D:117:ASN:H	1:D:117:ASN:HD22	1.69	0.41
1:D:341:PHE:CD2	1:D:351:GLN:HG2	2.55	0.41
1:B:226:PHE:CD1	1:B:226:PHE:C	2.98	0.41
1:D:395:LEU:HD12	1:D:395:LEU:HA	1.93	0.41
1:B:5:THR:HG23	1:B:7:GLY:H	1.84	0.41
1:D:139:VAL:HA	1:D:143:ALA:HB3	2.04	0.40

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	393/399 (98%)	383 (98%)	9 (2%)	1 (0%)	36	36
1	B	393/399 (98%)	380 (97%)	11 (3%)	2 (0%)	24	22
1	C	393/399 (98%)	381 (97%)	10 (2%)	2 (0%)	24	22
1	D	393/399 (98%)	381 (97%)	11 (3%)	1 (0%)	36	36
All	All	1572/1596 (98%)	1525 (97%)	41 (3%)	6 (0%)	30	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	THR
1	B	282	THR
1	C	6	ALA
1	C	282	THR
1	D	282	THR
1	B	347	GLN

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	316/320 (99%)	303 (96%)	13 (4%)	27	29
1	B	316/320 (99%)	308 (98%)	8 (2%)	42	48
1	C	316/320 (99%)	307 (97%)	9 (3%)	38	43
1	D	316/320 (99%)	307 (97%)	9 (3%)	38	43
All	All	1264/1280 (99%)	1225 (97%)	39 (3%)	35	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	27	ASP
1	A	104	LYS
1	A	109	ARG
1	A	115	ARG
1	A	161	ARG
1	A	221	VAL
1	A	222	ILE
1	A	233	THR
1	A	254	LEU
1	A	305	LYS
1	A	324	GLU
1	A	378	VAL
1	B	109	ARG
1	B	152	SER
1	B	170	GLU
1	B	174	ARG
1	B	221	VAL
1	B	374	LEU
1	B	376	LYS
1	B	378	VAL
1	C	109	ARG
1	C	115	ARG
1	C	140	LYS

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Mol	Chain	Res	Type
1	C	170	GLU
1	C	221	VAL
1	C	222	ILE
1	C	233	THR
1	C	374	LEU
1	C	378	VAL
1	D	27	ASP
1	D	74	GLN
1	D	153	ASP
1	D	161	ARG
1	D	170	GLU
1	D	221	VAL
1	D	222	ILE
1	D	233	THR
1	D	376	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	80	GLN
1	A	95	HIS
1	A	272	ASN
1	A	346	HIS
1	A	347	GLN
1	A	351	GLN
1	B	72	HIS
1	B	95	HIS
1	B	117	ASN
1	B	346	HIS
1	B	347	GLN
1	B	351	GLN
1	C	72	HIS
1	C	95	HIS
1	C	112	GLN
1	C	259	GLN
1	C	264	GLN
1	C	346	HIS
1	C	347	GLN
1	C	351	GLN
1	C	393	HIS
1	D	72	HIS

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Mol	Chain	Res	Type
1	D	95	HIS
1	D	112	GLN
1	D	117	ASN
1	D	346	HIS
1	D	351	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)

8 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	D	401	1	50,50,50	1.41	7 (14%)	66,82,82	1.57	14 (21%)
2	HEM	B	401	1	50,50,50	1.46	8 (16%)	66,82,82	1.79	18 (27%)
3	2OH	A	402	-	18,18,18	1.00	1 (5%)	26,26,26	1.13	0
3	2OH	B	402	-	18,18,18	1.03	1 (5%)	26,26,26	0.98	1 (3%)
2	HEM	C	401	1	50,50,50	1.64	10 (20%)	66,82,82	1.82	22 (33%)
3	2OH	D	402	-	18,18,18	1.00	1 (5%)	26,26,26	0.73	0
2	HEM	A	401	1	50,50,50	1.60	10 (20%)	66,82,82	1.79	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	2OH	C	402	-	18,18,18	0.86	0	26,26,26	1.11	1 (3%)

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	D	401	1	-	0/14/54/54	-
2	HEM	B	401	1	-	0/14/54/54	-
3	2OH	A	402	-	-	0/12/12/12	0/2/2/2
3	2OH	B	402	-	-	0/12/12/12	0/2/2/2
2	HEM	C	401	1	-	0/14/54/54	-
3	2OH	D	402	-	-	0/12/12/12	0/2/2/2
2	HEM	A	401	1	-	0/14/54/54	-
3	2OH	C	402	-	-	0/12/12/12	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C1B-NB	-4.68	1.32	1.40
2	C	401	HEM	FE-NB	4.65	2.09	1.94
2	A	401	HEM	C1B-NB	-4.65	1.32	1.40
2	B	401	HEM	FE-NC	4.37	2.10	1.95
2	D	401	HEM	FE-NC	4.30	2.09	1.95
2	A	401	HEM	FE-NB	4.22	2.07	1.94
2	A	401	HEM	C4B-NB	-3.55	1.31	1.38
2	C	401	HEM	C4D-ND	-3.51	1.34	1.40
2	B	401	HEM	C4C-NC	-3.27	1.33	1.39
2	A	401	HEM	C1C-C2C	-3.12	1.39	1.45
2	D	401	HEM	C1B-NB	-3.11	1.34	1.40
2	C	401	HEM	C4B-NB	-3.00	1.32	1.38
2	D	401	HEM	FE-NB	2.99	2.04	1.94
2	B	401	HEM	FE-NA	2.94	2.05	1.95
3	B	402	2OH	C5-C2	-2.89	1.49	1.54
3	D	402	2OH	C3-C2	-2.86	1.49	1.54
2	B	401	HEM	C1C-NC	-2.82	1.34	1.39
2	B	401	HEM	C1B-NB	-2.72	1.35	1.40
2	D	401	HEM	CHA-C4D	2.68	1.44	1.38
2	B	401	HEM	C1D-ND	-2.68	1.33	1.38
2	D	401	HEM	FE-NA	2.65	2.04	1.95
2	B	401	HEM	FE-NB	2.60	2.02	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	HEM	C1C-C2C	-2.58	1.40	1.45
2	C	401	HEM	O2D-CGD	-2.52	1.22	1.30
2	A	401	HEM	CMB-C2B	2.51	1.56	1.50
2	C	401	HEM	CMB-C2B	2.49	1.56	1.50
2	C	401	HEM	FE-NC	2.47	2.03	1.95
2	A	401	HEM	FE-NC	2.39	2.03	1.95
2	A	401	HEM	C3C-C4C	-2.32	1.42	1.46
2	D	401	HEM	C1C-NC	-2.22	1.35	1.39
2	C	401	HEM	C3D-C2D	-2.22	1.32	1.36
2	D	401	HEM	C4C-NC	-2.21	1.35	1.39
2	A	401	HEM	C4D-ND	-2.15	1.36	1.40
2	B	401	HEM	C4B-NB	-2.15	1.34	1.38
3	A	402	2OH	C5-C2	-2.12	1.51	1.54
2	C	401	HEM	C4C-NC	-2.03	1.35	1.39
2	A	401	HEM	C3D-C2D	-2.02	1.32	1.36
2	A	401	HEM	CMC-C2C	2.01	1.55	1.50

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	HEM	C1B-NB-C4B	4.94	110.17	105.07
2	B	401	HEM	CHC-C4B-NB	4.57	129.38	124.42
2	A	401	HEM	C3B-C2B-C1B	-4.01	103.51	106.49
2	D	401	HEM	CMB-C2B-C1B	3.80	130.83	125.04
2	C	401	HEM	CHC-C4B-NB	3.73	128.47	124.42
2	D	401	HEM	CMD-C2D-C1D	3.70	130.68	125.04
2	C	401	HEM	C1B-NB-C4B	3.70	108.89	105.07
2	C	401	HEM	CMD-C2D-C1D	3.66	130.62	125.04
2	C	401	HEM	C4C-C3C-C2C	3.57	109.68	106.75
2	D	401	HEM	CHC-C4B-NB	3.55	128.27	124.42
2	A	401	HEM	CMB-C2B-C1B	3.43	130.27	125.04
2	B	401	HEM	CMD-C2D-C1D	3.39	130.21	125.04
2	C	401	HEM	C3B-C2B-C1B	-3.37	103.98	106.49
2	A	401	HEM	CMD-C2D-C1D	3.33	130.11	125.04
2	C	401	HEM	CAD-CBD-CGD	-3.24	106.63	113.60
2	B	401	HEM	C4C-NC-C1C	3.23	108.51	105.35
2	A	401	HEM	CHC-C4B-NB	3.19	127.89	124.42
2	A	401	HEM	C1B-NB-C4B	3.18	108.35	105.07
2	D	401	HEM	C1B-NB-C4B	3.18	108.35	105.07
2	C	401	HEM	CHD-C4C-NC	3.15	127.85	124.44
2	B	401	HEM	CHA-C4D-ND	3.14	128.25	124.37
2	C	401	HEM	CMC-C2C-C1C	3.14	130.24	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	HEM	CHA-C4D-C3D	-3.05	119.61	125.33
2	B	401	HEM	CHA-C4D-C3D	-3.03	119.64	125.33
2	D	401	HEM	CHC-C1C-NC	-3.00	121.19	124.44
2	B	401	HEM	C1A-CHA-C4D	-2.98	119.27	126.34
2	B	401	HEM	CMB-C2B-C1B	2.97	129.56	125.04
2	B	401	HEM	CAA-CBA-CGA	-2.96	107.23	113.60
2	A	401	HEM	CAA-CBA-CGA	2.96	119.98	113.60
2	C	401	HEM	C4C-NC-C1C	2.88	108.17	105.35
2	C	401	HEM	C3C-C2C-C1C	-2.88	104.33	107.08
2	B	401	HEM	CHD-C1D-C2D	-2.83	120.56	124.98
2	C	401	HEM	CHD-C1D-C2D	-2.79	120.62	124.98
2	A	401	HEM	CHD-C4C-NC	2.78	127.45	124.44
2	C	401	HEM	CHA-C4D-C3D	-2.78	120.11	125.33
2	D	401	HEM	C1A-CHA-C4D	-2.78	119.75	126.34
2	A	401	HEM	C4C-C3C-C2C	2.77	109.03	106.75
2	A	401	HEM	CAD-CBD-CGD	-2.77	107.65	113.60
3	B	402	2OH	C5-C2-C3	-2.76	104.17	107.58
2	A	401	HEM	C4D-ND-C1D	-2.73	102.25	105.07
2	B	401	HEM	CHB-C1B-NB	2.72	127.73	124.37
2	A	401	HEM	CHD-C1D-C2D	-2.68	120.80	124.98
2	A	401	HEM	C1A-CHA-C4D	-2.65	120.06	126.34
2	C	401	HEM	C3D-C4D-ND	2.60	113.06	110.17
2	A	401	HEM	CHA-C4D-C3D	-2.59	120.46	125.33
2	D	401	HEM	C3B-C2B-C1B	-2.56	104.59	106.49
2	B	401	HEM	O2A-CGA-CBA	2.56	122.25	114.03
2	D	401	HEM	CHA-C4D-ND	2.54	127.51	124.37
2	A	401	HEM	C2D-C1D-ND	2.53	112.91	109.88
2	A	401	HEM	CMC-C2C-C1C	2.53	129.16	124.71
2	A	401	HEM	CAD-C3D-C4D	2.52	129.07	124.66
2	B	401	HEM	CAD-C3D-C4D	2.51	129.04	124.66
2	A	401	HEM	C3D-C4D-ND	2.49	112.94	110.17
2	D	401	HEM	CAD-C3D-C4D	2.47	128.98	124.66
2	C	401	HEM	C1A-CHA-C4D	-2.46	120.49	126.34
2	D	401	HEM	C4D-ND-C1D	-2.46	102.53	105.07
2	C	401	HEM	CAA-CBA-CGA	2.43	118.84	113.60
2	B	401	HEM	CAC-C3C-C4C	-2.33	119.26	124.90
2	C	401	HEM	CAD-C3D-C4D	2.27	128.63	124.66
2	C	401	HEM	C4D-ND-C1D	-2.26	102.74	105.07
2	A	401	HEM	C4C-NC-C1C	2.25	107.55	105.35
2	B	401	HEM	C2D-C1D-ND	2.25	112.58	109.88
2	C	401	HEM	CAC-C3C-C4C	-2.25	119.47	124.90
2	D	401	HEM	C3C-C2C-C1C	-2.21	104.97	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	HEM	C3C-C2C-C1C	-2.19	104.98	107.08
2	C	401	HEM	O2A-CGA-O1A	-2.18	117.86	123.30
2	D	401	HEM	CHD-C1D-C2D	-2.16	121.61	124.98
2	D	401	HEM	CAA-CBA-CGA	-2.13	109.01	113.60
2	A	401	HEM	CAC-C3C-C4C	-2.13	119.76	124.90
2	C	401	HEM	C2D-C1D-ND	2.12	112.42	109.88
2	B	401	HEM	O2D-CGD-CBD	2.12	120.83	114.03
2	C	401	HEM	CBB-CAB-C3B	-2.11	117.11	127.62
3	C	402	2OH	C3-C2-C4	2.09	115.30	109.84
2	A	401	HEM	CHC-C1C-NC	-2.07	122.20	124.44
2	A	401	HEM	O2A-CGA-O1A	-2.04	118.21	123.30
2	C	401	HEM	O2A-CGA-CBA	2.03	120.56	114.03
2	B	401	HEM	CHC-C1C-NC	-2.02	122.25	124.44

There are no chirality outliers.

There are no torsion outliers.

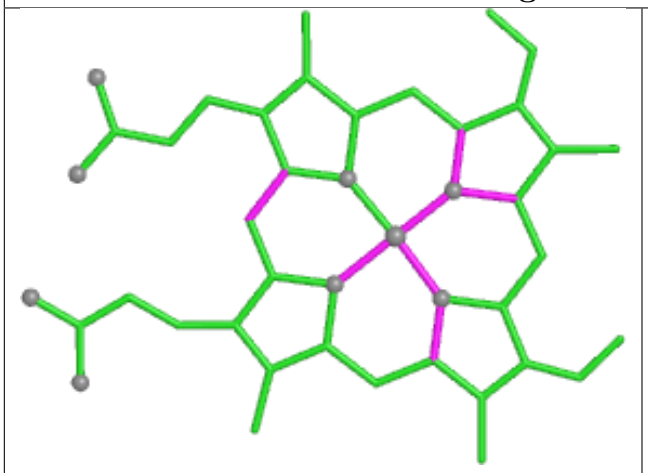
There are no ring outliers.

5 monomers are involved in 16 short contacts:

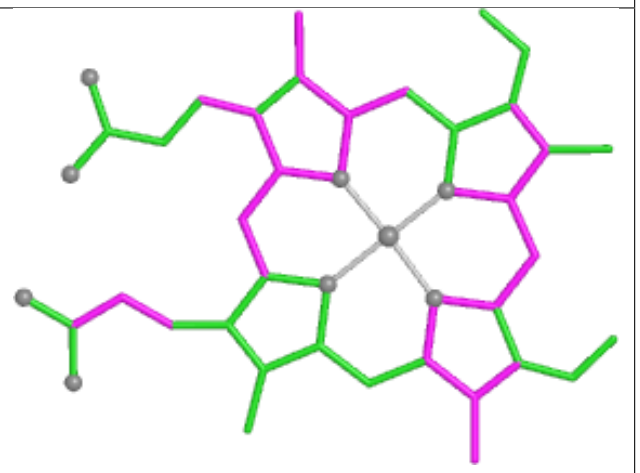
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	HEM	4	0
2	B	401	HEM	2	0
3	B	402	2OH	2	0
2	C	401	HEM	3	0
2	A	401	HEM	5	0

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.

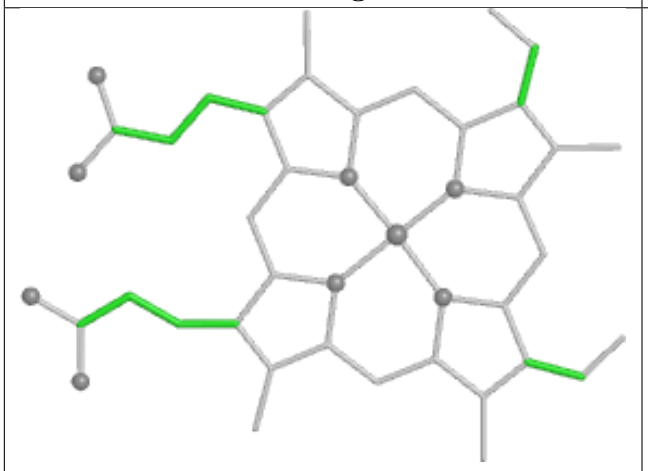
Ligand HEM D 401



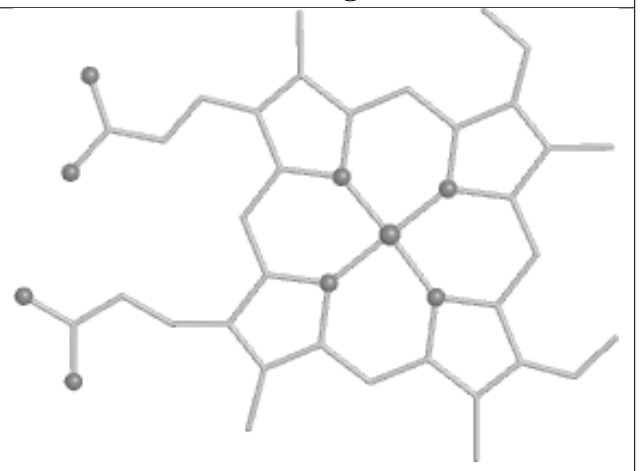
Bond lengths



Bond angles

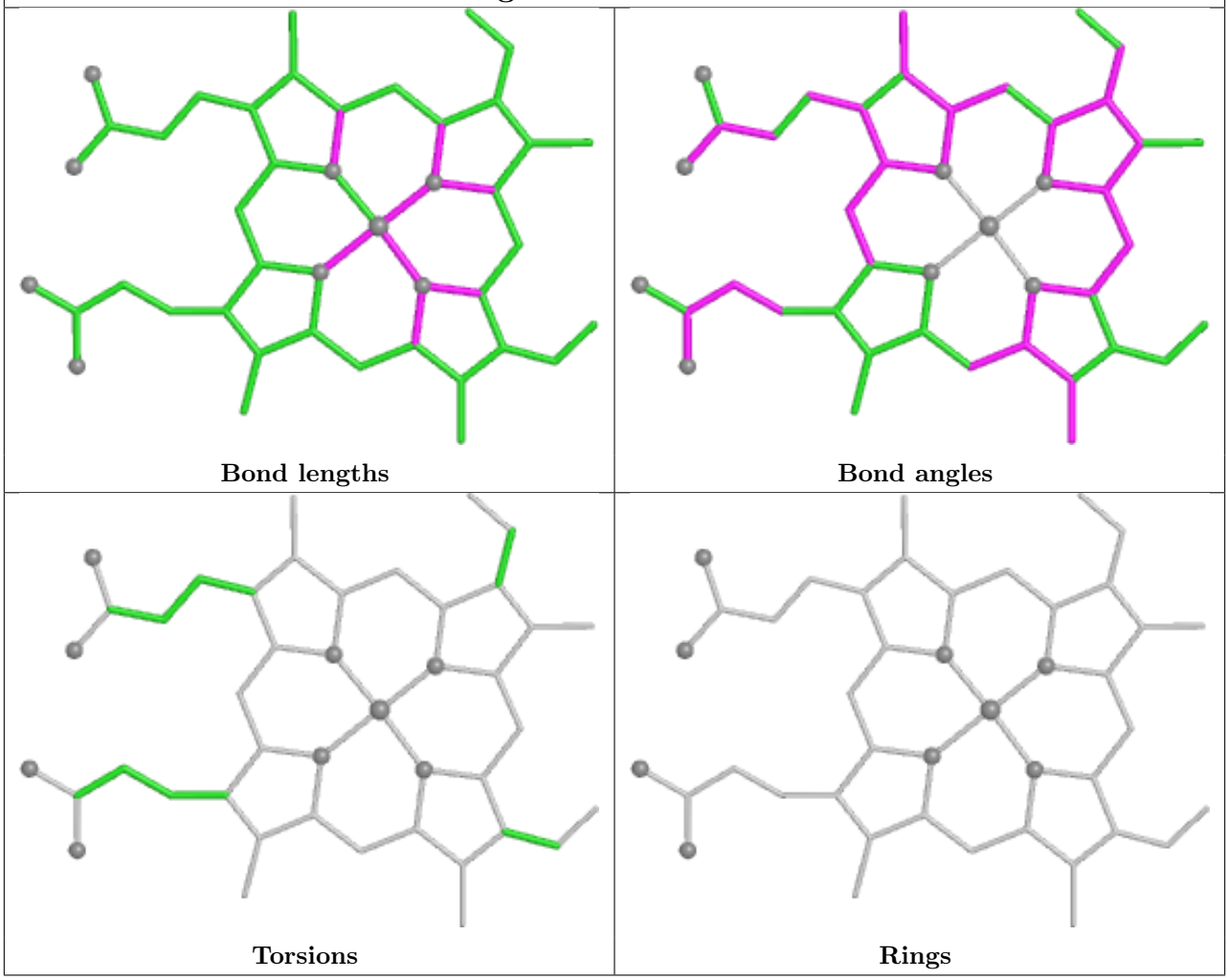


Torsions

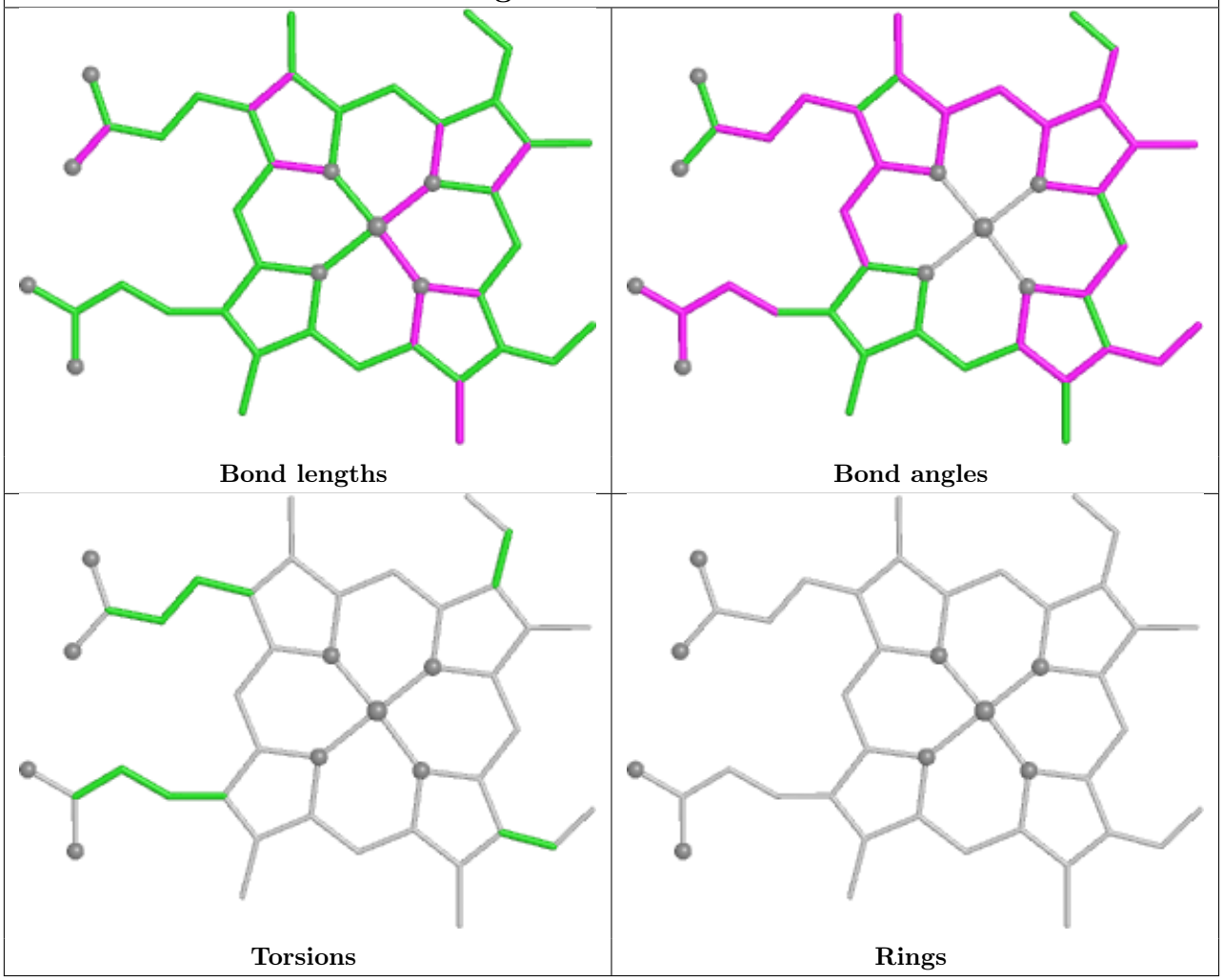


Rings

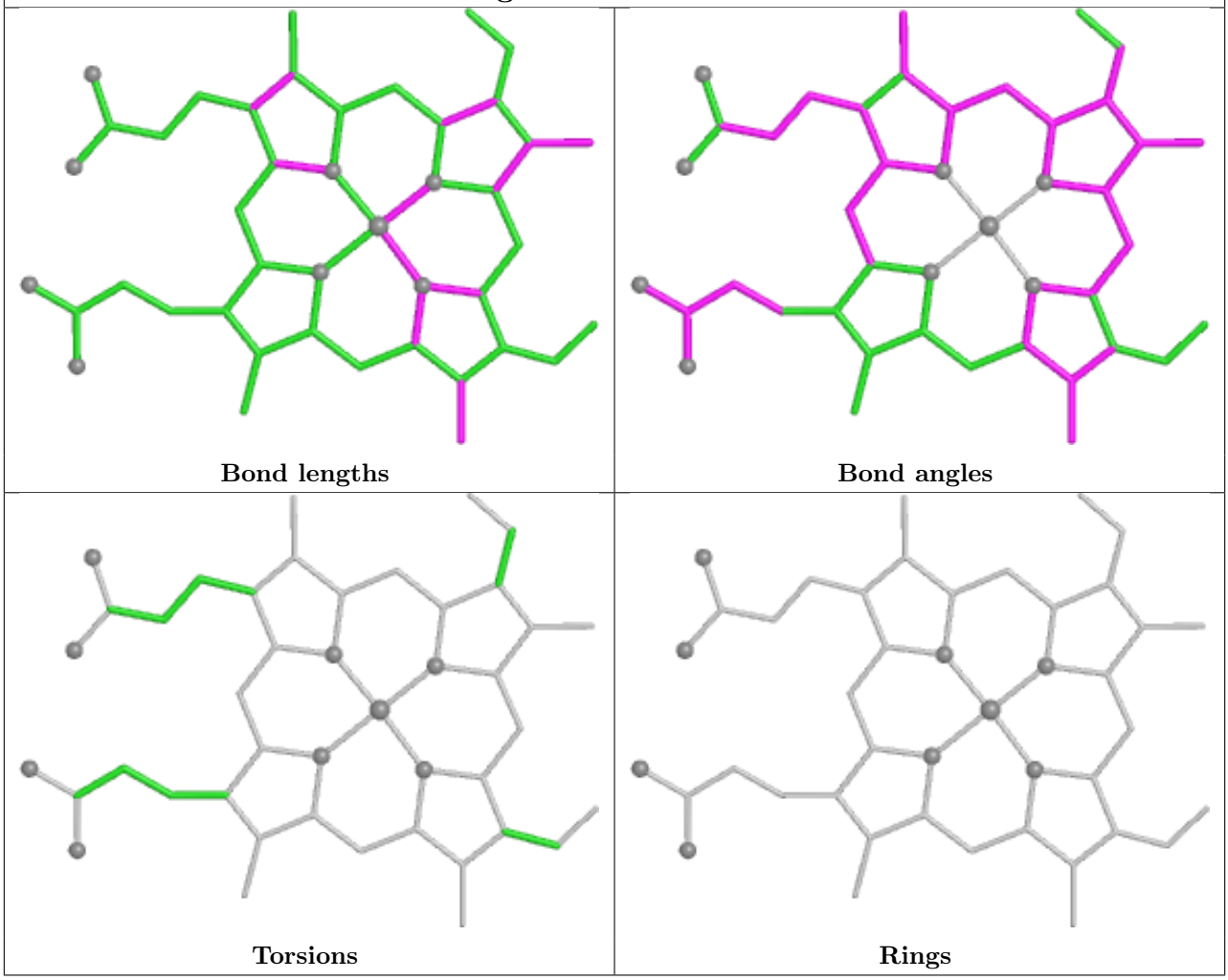
Ligand HEM B 401



Ligand HEM C 401



Ligand HEM A 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	395/399 (98%)	-0.54	1 (0%) 90 91	33, 45, 69, 103	0
1	B	395/399 (98%)	-0.57	0 100 100	34, 45, 69, 102	0
1	C	395/399 (98%)	-0.60	1 (0%) 90 91	33, 45, 70, 103	0
1	D	395/399 (98%)	-0.55	0 100 100	33, 45, 69, 103	0
All	All	1580/1596 (98%)	-0.57	2 (0%) 92 92	33, 45, 70, 103	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	GLY	3.5
1	C	6	ALA	2.0

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)

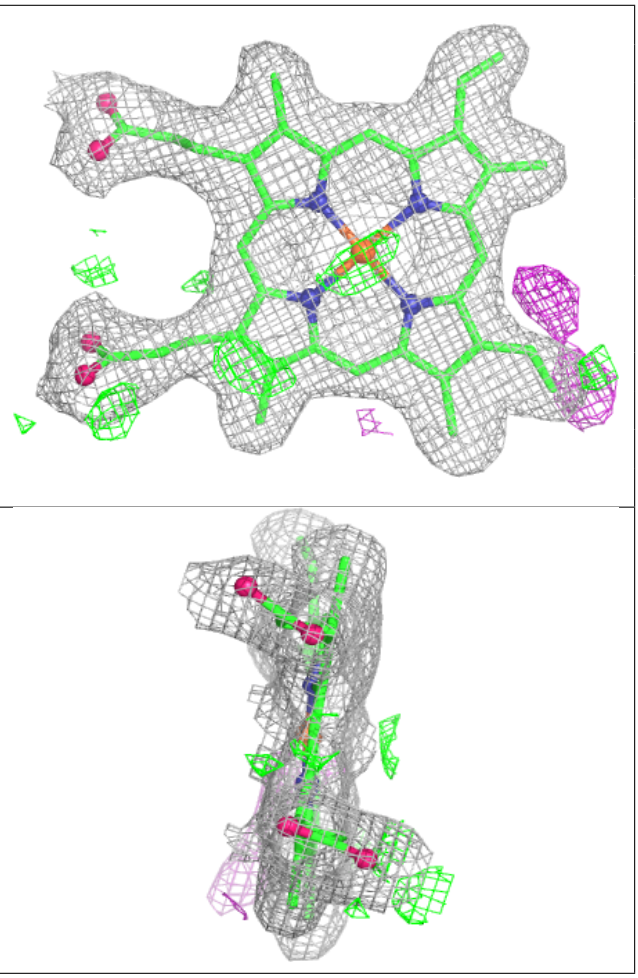
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	2OH	C	402	17/17	0.97	0.07	39,46,52,59	0
3	2OH	B	402	17/17	0.98	0.06	36,42,51,64	0
3	2OH	D	402	17/17	0.98	0.06	36,43,53,62	0
2	HEM	D	401	43/43	0.99	0.05	31,36,41,43	0
3	2OH	A	402	17/17	0.99	0.05	36,43,52,60	0
2	HEM	A	401	43/43	0.99	0.05	34,37,43,53	0
2	HEM	B	401	43/43	0.99	0.04	28,36,42,48	0
2	HEM	C	401	43/43	0.99	0.05	30,37,42,55	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.

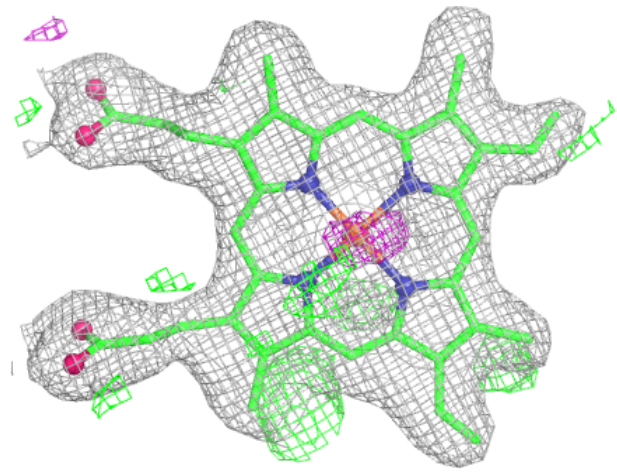
Electron density around HEM D 401:

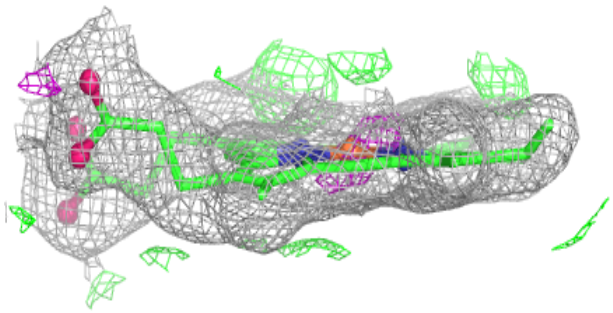
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

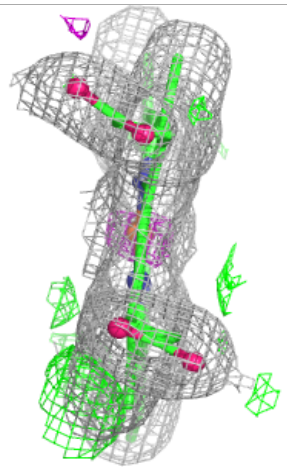


Electron density around HEM A 401:

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

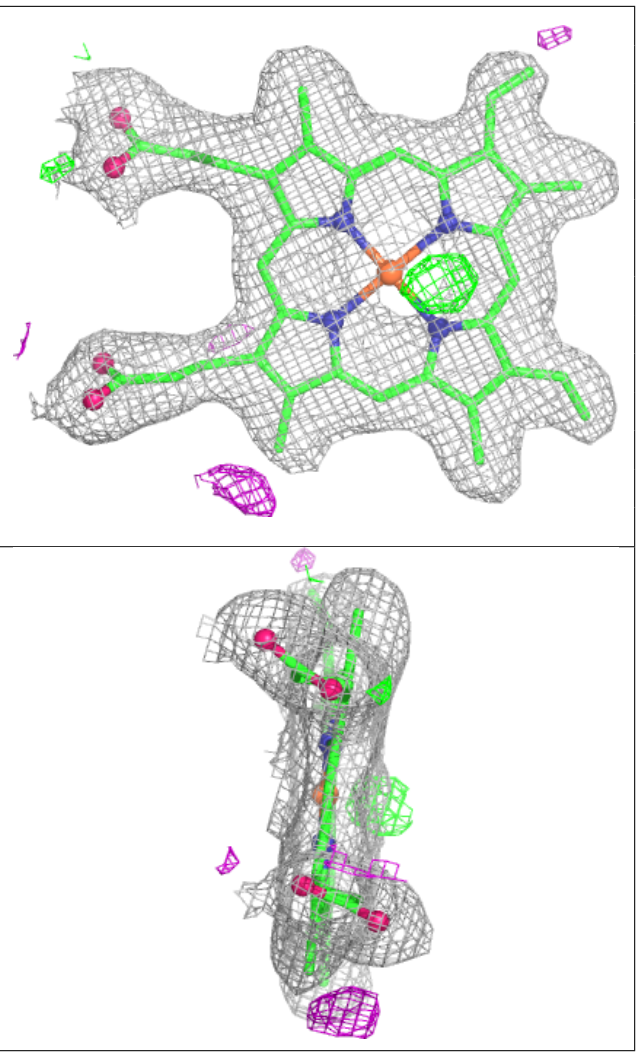






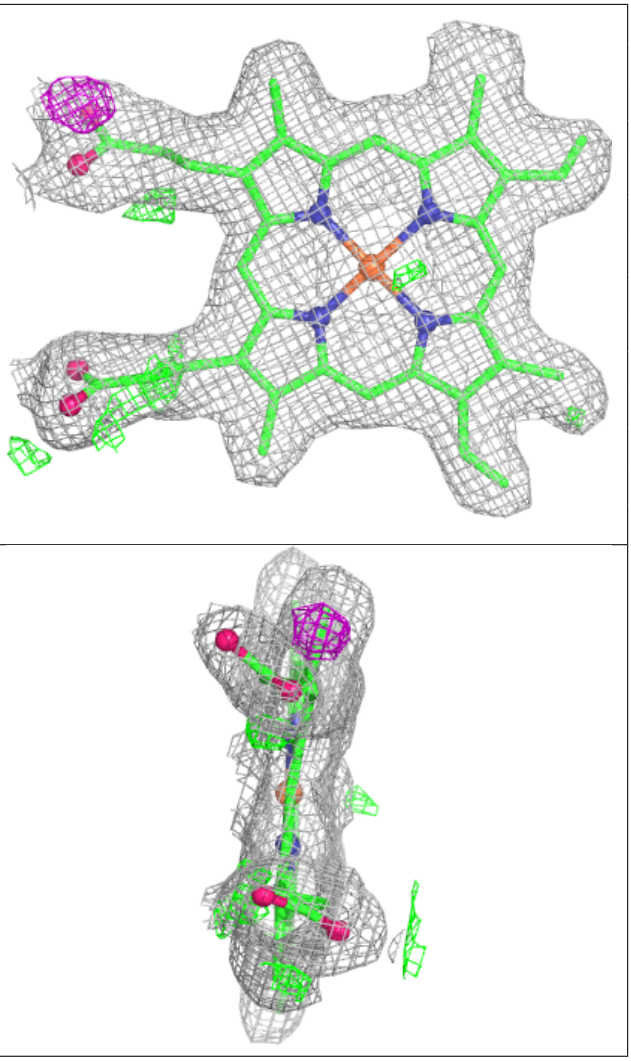
Electron density around HEM B 401:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.