Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 10:05 am BST

PDB ID	:	4QOO
Title	:	Structure of Bacillus pumilus catalase with resorcinol bound.
Authors	:	Loewen, P.C.
Deposited on	:	2014-06-20
Resolution	:	1.75 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 following versions of software and data (see references (i)) were used in the production of this report:

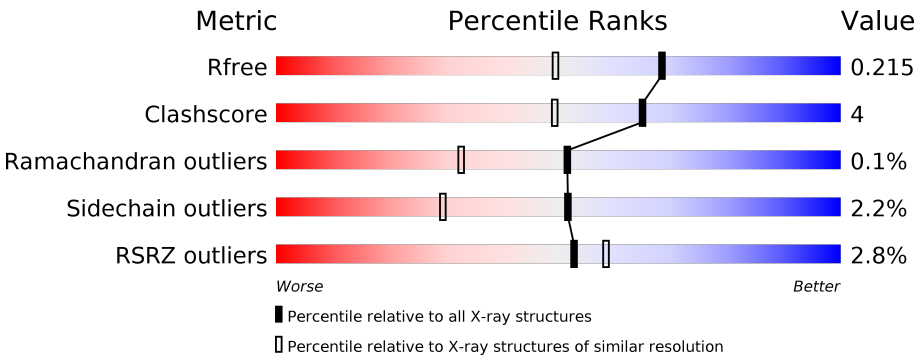
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on 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	491	4% 90% 7% •
1	B	491	% 89% 8% •
1	C	491	3% 90% 7% •
1	D	491	3% 90% 7% • •

2 Entry composition (i)

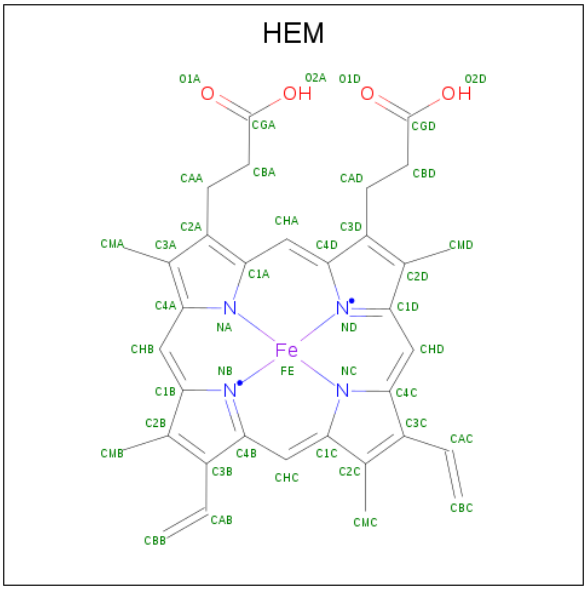
There are 6 unique types of molecules in this entry. The entry contains 17842 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	480	3960	2497	694	755	14	0	7	0
1	B	480	3959	2496	691	756	16	0	7	0
1	C	480	3971	2505	696	755	15	0	8	0
1	D	480	3961	2497	693	757	14	0	6	0

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



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

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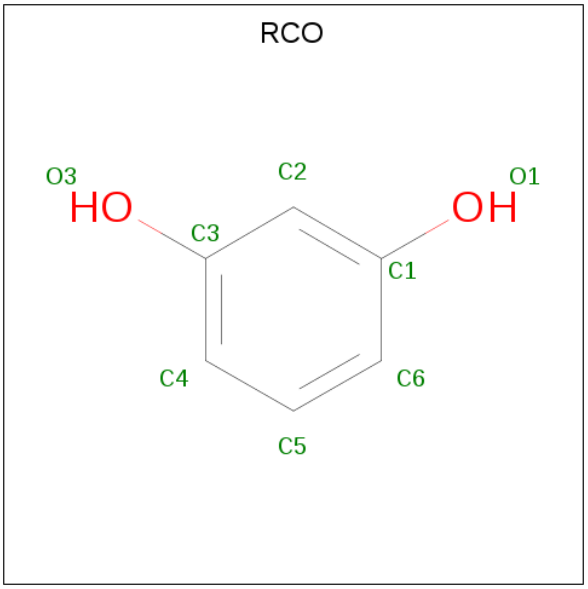
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	1
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	1
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	1
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	1
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	1
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	1

- Molecule 3 is RESORCINOL (three-letter code: RCO) (formula: $C_6H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	8	6	2	0	0
			Total	C	O		
3	B	1	8	6	2	0	0
			Total	C	O		
3	C	1	8	6	2	0	0
			Total	C	O		
3	D	1	8	6	2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	2	Total Cl 2 2	0	0
4	D	1	Total Cl 1 1	0	0
4	C	2	Total Cl 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Na 1 1	0	0
5	A	1	Total Na 1 1	0	0

- Molecule 6 is water.

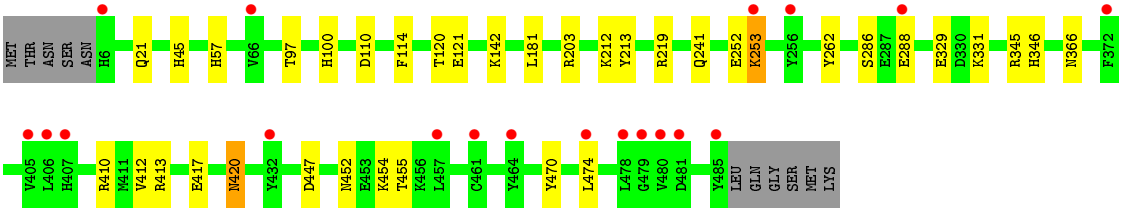
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	401	Total O 401 401	0	0
6	B	395	Total O 395 395	0	0
6	C	418	Total O 418 418	0	0
6	D	393	Total O 393 393	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

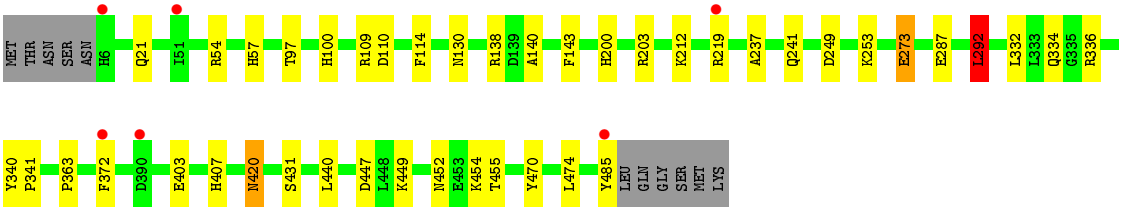
- Molecule 1: Catalase

Chain A:



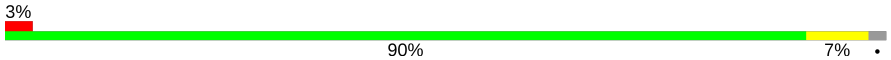
- Molecule 1: Catalase

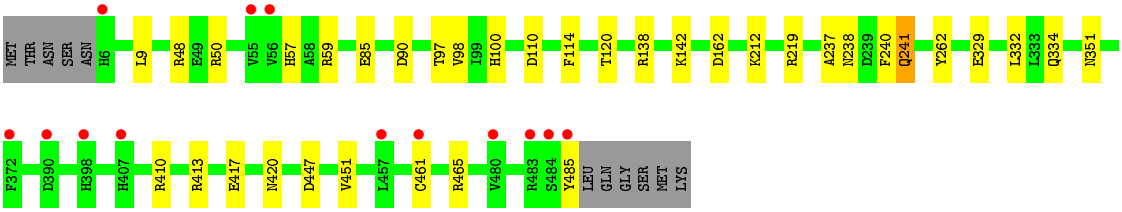
Chain B:



- Molecule 1: Catalase

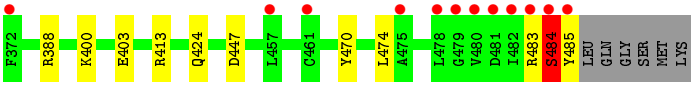
Chain C:





- Molecule 1: Catalase

Chain D:


F372
R388
K400
E403
R413
Q424
D447
L457
C461
Y470
L474
A475
L478
G479
V480
D481
I482
R483
S484
Y485
LEU
GLN
GLY
SER
MET
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.91Å 108.60Å 103.52Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	103.46 – 1.75 46.74 – 1.75	Depositor EDS
% Data completeness (in resolution range)	96.4 (103.46-1.75) 96.4 (46.74-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.179 , 0.209 0.188 , 0.215	Depositor DCC
R_{free} test set	9664 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.887	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.089 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17842	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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, CL, RCO, NA

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	0.88	0/4086	0.88	6/5541 (0.1%)
1	B	0.93	0/4083	0.90	5/5535 (0.1%)
1	C	1.01	1/4095 (0.0%)	0.93	9/5550 (0.2%)
1	D	0.88	0/4079	0.89	5/5529 (0.1%)
All	All	0.92	1/16343 (0.0%)	0.90	25/22155 (0.1%)

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	B	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	329	GLU	CG-CD	5.45	1.60	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	413	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	C	413	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	D	388	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	109	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	413	ARG	NE-CZ-NH1	-6.02	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	B	138	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	50	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	138	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	138	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	54	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	203	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	292	LEU	CB-CG-CD2	5.45	120.26	111.00
1	C	238	ASN	CB-CA-C	-5.36	99.68	110.40
1	C	59	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	48	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	C	50	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	203	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	345	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	50	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	59	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	203	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	48	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	121	GLU	OE1-CD-OE2	5.08	129.40	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	HIS	Peptide
1	D	484	SER	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	3960	0	3764	27	1
1	B	3959	0	3765	30	1
1	C	3971	0	3789	23	1
1	D	3961	0	3766	23	4
2	A	86	0	60	10	0
2	B	86	0	60	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	86	0	60	11	0
2	D	86	0	60	9	0
3	A	8	0	5	1	0
3	B	8	0	6	0	0
3	C	8	0	5	0	0
3	D	8	0	5	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
6	A	401	0	0	10	1
6	B	395	0	0	9	3
6	C	418	0	0	10	1
6	D	393	0	0	13	0
All	All	17842	0	15345	129	6

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 (129) 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)
2:B:502[B]:HEM:CMC	2:B:502[B]:HEM:HBC2	1.97	0.95
2:B:501[A]:HEM:HMB2	2:B:501[A]:HEM:HBB2	1.53	0.89
1:A:219:ARG:HD2	6:A:851:HOH:O	1.70	0.89
1:C:461[B]:CYS:SG	1:C:465:ARG:NH2	2.52	0.83
2:B:502[B]:HEM:HMC1	2:B:502[B]:HEM:HBC2	1.62	0.80
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:CMC	2.10	0.80
2:C:501[A]:HEM:CMB	2:C:501[A]:HEM:HBB2	2.14	0.78
2:B:502[B]:HEM:HMC1	2:B:502[B]:HEM:CBC	2.14	0.77
1:B:449:LYS:HE3	6:B:922:HOH:O	1.83	0.77
1:B:212:LYS:NZ	6:B:886:HOH:O	2.18	0.76
1:C:212:LYS:NZ	6:C:903:HOH:O	2.18	0.75
2:A:501[A]:HEM:CMB	2:A:501[A]:HEM:HBB2	2.16	0.74
2:C:501[A]:HEM:HMB2	2:C:501[A]:HEM:HBB2	1.68	0.74
1:B:249[B]:ASP:OD2	1:B:253:LYS:HE3	1.88	0.74
1:D:212:LYS:HE2	6:D:712:HOH:O	1.87	0.72
1:B:449:LYS:CE	6:B:922:HOH:O	2.39	0.71
1:B:431:SER:OG	6:B:633:HOH:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASN:HD22	1:A:455:THR:H	1.40	0.70
1:B:372[A]:PHE:CE2	6:D:887:HOH:O	2.45	0.70
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:HBB2	1.74	0.69
1:A:45:HIS:HE1	1:C:351:ASN:OD1	1.75	0.69
1:B:140:ALA:HA	2:B:501[A]:HEM:HBB1	1.74	0.68
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:HMC2	1.75	0.68
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:CMC	2.22	0.67
1:B:334:GLN:HG3	6:C:706:HOH:O	1.96	0.65
2:C:501[A]:HEM:HMB2	2:C:501[A]:HEM:CBB	2.28	0.64
1:D:207:LYS:NZ	6:D:841:HOH:O	2.30	0.64
1:A:212:LYS:HE2	6:A:698:HOH:O	1.96	0.64
2:B:501[A]:HEM:CMB	2:B:501[A]:HEM:HBB2	2.20	0.64
1:B:452:ASN:HD22	1:B:455:THR:H	1.44	0.64
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:HMC2	1.80	0.64
2:D:501[A]:HEM:CMC	2:D:501[A]:HEM:HBC2	2.27	0.64
5:A:506:NA:NA	6:A:836:HOH:O	1.71	0.62
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:CMC	2.29	0.62
1:C:219:ARG:HD3	1:C:262:TYR:CE1	2.35	0.61
2:C:502[B]:HEM:HBC2	2:C:502[B]:HEM:HMC1	1.83	0.61
1:D:483:ARG:O	1:D:484:SER:CB	2.49	0.60
2:D:501[A]:HEM:HMC2	2:D:501[A]:HEM:HBC2	1.81	0.60
1:A:100:HIS:HE1	6:D:672:HOH:O	1.84	0.60
1:A:286:SER:OG	1:A:288:GLU:HG2	2.03	0.59
1:D:332:LEU:HD12	2:D:501[A]:HEM:HBB1	1.85	0.59
1:B:100:HIS:HE1	6:C:705:HOH:O	1.86	0.58
2:C:501[A]:HEM:CBC	2:C:501[A]:HEM:HMC2	2.33	0.58
1:A:366:ASN:HA	1:C:9[B]:LEU:CD2	2.33	0.58
2:C:501[A]:HEM:CBC	2:C:501[A]:HEM:CMC	2.80	0.57
1:C:461[B]:CYS:SG	1:C:465:ARG:CZ	2.91	0.57
1:A:219:ARG:HD3	1:A:262:TYR:CE1	2.40	0.57
1:A:219:ARG:CD	6:A:851:HOH:O	2.42	0.56
2:C:502[B]:HEM:HBC2	2:C:502[B]:HEM:CMC	2.35	0.56
1:C:85:GLU:OE1	6:C:905:HOH:O	2.18	0.56
1:A:452:ASN:HD21	1:A:454:LYS:HB3	1.69	0.56
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:CBB	2.35	0.56
2:A:502[B]:HEM:HBB2	2:A:502[B]:HEM:CMB	2.36	0.55
1:A:346:HIS:CE1	6:D:887:HOH:O	2.60	0.55
1:A:417:GLU:HG2	1:D:28:HIS:CD2	2.41	0.55
1:D:400:LYS:NZ	6:D:953:HOH:O	1.95	0.54
2:D:502[B]:HEM:HBC2	2:D:502[B]:HEM:CMC	2.36	0.54
1:A:346:HIS:HE1	6:D:887:HOH:O	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:GLN:HG3	6:D:809:HOH:O	2.08	0.54
1:D:483:ARG:O	1:D:484:SER:HB3	2.08	0.53
2:B:502[B]:HEM:HMC3	2:B:502[B]:HEM:HBC2	1.86	0.53
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:HMC2	1.91	0.53
1:B:372[A]:PHE:CD2	6:D:887:HOH:O	2.60	0.52
1:B:452:ASN:HD21	1:B:454:LYS:HB3	1.75	0.52
1:C:410:ARG:NH2	1:D:403:GLU:O	2.42	0.52
1:A:219:ARG:CG	6:A:851:HOH:O	2.57	0.52
1:B:287:GLU:HG2	1:B:292:LEU:HD21	1.91	0.52
1:A:412[A]:VAL:HG13	1:B:403:GLU:OE2	2.09	0.52
1:A:213:TYR:OH	1:A:329:GLU:OE2	2.18	0.51
2:A:501[A]:HEM:CBC	2:A:501[A]:HEM:CMC	2.89	0.51
2:A:502[B]:HEM:HMB1	2:A:502[B]:HEM:HBB2	1.91	0.51
2:D:501[A]:HEM:HMC2	2:D:501[A]:HEM:CBC	2.40	0.50
1:B:287:GLU:HG2	1:B:292:LEU:CD2	2.41	0.50
1:A:181:LEU:HD21	3:A:503:RCO:C6	2.42	0.49
1:B:287:GLU:CD	1:B:292:LEU:HD21	2.32	0.49
1:C:212:LYS:HE2	6:C:902:HOH:O	2.12	0.49
2:A:502[B]:HEM:CMC	2:A:502[B]:HEM:HBC2	2.43	0.49
1:A:45:HIS:HD2	6:A:686:HOH:O	1.96	0.48
1:C:162:ASP:HA	1:C:451:VAL:HG22	1.96	0.48
1:D:219:ARG:HG3	1:D:219:ARG:HH11	1.79	0.48
2:D:502[B]:HEM:HMC1	2:D:502[B]:HEM:HBC2	1.95	0.48
1:B:143:PHE:HB2	2:B:501[A]:HEM:CBB	2.44	0.48
1:B:219:ARG:CG	6:B:982:HOH:O	2.61	0.48
1:C:219:ARG:HD2	6:C:991:HOH:O	2.12	0.48
2:A:501[A]:HEM:CBC	2:A:501[A]:HEM:HMC2	2.44	0.47
1:B:287:GLU:CG	1:B:292:LEU:HD21	2.44	0.47
1:B:219:ARG:HG3	6:B:982:HOH:O	2.15	0.46
1:D:234:GLU:HG3	6:D:772:HOH:O	2.15	0.46
6:A:960:HOH:O	1:D:334:GLN:HG3	2.16	0.45
1:D:75[A]:LYS:HG2	1:D:76:HIS:CE1	2.52	0.45
1:C:219:ARG:HD3	1:C:262:TYR:CD1	2.52	0.45
1:C:90:ASP:HB3	6:C:900:HOH:O	2.16	0.45
1:D:143:PHE:CD2	2:D:501[A]:HEM:CMB	2.99	0.45
1:B:332:LEU:HD12	2:B:501[A]:HEM:HBB1	1.99	0.44
1:D:57:HIS:HA	1:D:97:THR:O	2.17	0.44
2:C:501[A]:HEM:HMC3	2:C:501[A]:HEM:HBC2	1.97	0.44
6:B:828:HOH:O	1:C:334:GLN:HG3	2.18	0.44
1:C:240:PHE:C	1:C:241:GLN:HG3	2.36	0.44
2:D:501[A]:HEM:HBB2	2:D:501[A]:HEM:CMB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ASN:ND2	6:A:739:HOH:O	2.42	0.44
1:C:332:LEU:HD12	2:C:501[A]:HEM:HBB1	2.00	0.44
1:D:219:ARG:HD2	6:D:783:HOH:O	2.17	0.43
1:A:57:HIS:HA	1:A:97:THR:O	2.17	0.43
1:A:21:GLN:HA	1:D:142:LYS:HD3	2.00	0.43
1:A:142:LYS:HD3	1:D:21:GLN:HA	2.01	0.43
1:B:407:HIS:CD2	6:C:899:HOH:O	2.72	0.43
1:B:340:TYR:HB2	1:B:341:PRO:HD3	2.01	0.42
1:C:57:HIS:HA	1:C:97:THR:O	2.19	0.42
1:B:420:ASN:ND2	6:B:725:HOH:O	2.46	0.42
1:A:452:ASN:ND2	1:A:455:THR:H	2.13	0.42
1:B:237:ALA:HB2	1:C:237:ALA:HB2	2.01	0.42
1:B:57:HIS:HA	1:B:97:THR:O	2.20	0.42
6:A:982:HOH:O	1:D:304:PRO:HB2	2.20	0.42
1:D:234:GLU:CG	6:D:772:HOH:O	2.67	0.42
1:B:336:ARG:HG2	2:B:502[B]:HEM:C2C	2.55	0.41
6:B:730:HOH:O	1:C:100:HIS:HE1	2.01	0.41
1:A:410:ARG:NH2	1:B:403:GLU:O	2.54	0.41
1:C:57:HIS:CE1	1:C:98:VAL:HG22	2.55	0.41
1:B:130:ASN:CG	2:B:502[B]:HEM:HMB2	2.40	0.41
6:A:796:HOH:O	1:D:100:HIS:HE1	2.03	0.41
1:B:21:GLN:HA	1:C:142:LYS:HD3	2.02	0.41
1:D:343:THR:HG21	2:D:501[A]:HEM:HAA2	2.03	0.41
1:C:219:ARG:CD	6:C:991:HOH:O	2.68	0.41
1:C:219:ARG:NE	6:C:991:HOH:O	2.54	0.41
1:D:181:LEU:HD21	3:D:503:RCO:C6	2.51	0.41
2:B:501[A]:HEM:HMC2	2:B:501[A]:HEM:CBC	2.49	0.40
1:A:219:ARG:HD3	1:A:262:TYR:CD1	2.56	0.40
1:A:331:LYS:HG2	6:D:876:HOH:O	2.21	0.40

All (6) 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:D:225:ARG:NH1	6:B:975:HOH:O[2_655]	1.66	0.54
1:B:273:GLU:OE1	1:C:417:GLU:OE2[1_455]	1.79	0.41
6:A:944:HOH:O	6:C:730:HOH:O[2_656]	1.87	0.33
1:D:234:GLU:OE2	6:B:872:HOH:O[2_655]	1.89	0.31
1:D:225:ARG:CZ	6:B:975:HOH:O[2_655]	1.96	0.24
1:A:417:GLU:OE2	1:D:273:GLU:OE1[1_455]	2.06	0.14

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	485/491 (99%)	476 (98%)	9 (2%)	0	100	100
1	B	485/491 (99%)	474 (98%)	11 (2%)	0	100	100
1	C	486/491 (99%)	476 (98%)	10 (2%)	0	100	100
1	D	484/491 (99%)	469 (97%)	14 (3%)	1 (0%)	47	29
All	All	1940/1964 (99%)	1895 (98%)	44 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	484	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	428/432 (99%)	419 (98%)	9 (2%)	53	31
1	B	428/432 (99%)	416 (97%)	12 (3%)	43	20
1	C	429/432 (99%)	422 (98%)	7 (2%)	62	45
1	D	427/432 (99%)	417 (98%)	10 (2%)	50	28
All	All	1712/1728 (99%)	1674 (98%)	38 (2%)	52	29

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	114	PHE
1	A	120	THR
1	A	241	GLN
1	A	253	LYS
1	A	420	ASN
1	A	447	ASP
1	A	470	TYR
1	A	474	LEU
1	B	110	ASP
1	B	114	PHE
1	B	241	GLN
1	B	273	GLU
1	B	292	LEU
1	B	363	PRO
1	B	420	ASN
1	B	440	LEU
1	B	447	ASP
1	B	470	TYR
1	B	474	LEU
1	B	485	TYR
1	C	110	ASP
1	C	114	PHE
1	C	120	THR
1	C	241	GLN
1	C	420	ASN
1	C	447	ASP
1	C	485	TYR
1	D	75[A]	LYS
1	D	75[B]	LYS
1	D	114	PHE
1	D	234	GLU
1	D	241	GLN
1	D	273	GLU
1	D	447	ASP
1	D	470	TYR
1	D	474	LEU
1	D	485	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS

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Mol	Chain	Res	Type
1	A	100	HIS
1	A	157	ASN
1	A	226	ASN
1	A	346	HIS
1	A	407	HIS
1	A	420	ASN
1	A	452	ASN
1	B	100	HIS
1	B	157	ASN
1	B	226	ASN
1	B	420	ASN
1	B	452	ASN
1	C	100	HIS
1	C	226	ASN
1	C	420	ASN
1	D	100	HIS
1	D	157	ASN
1	D	226	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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	RCO	D	503	-	8,8,8	0.86	0	10,10,10	1.55	3 (30%)
2	HEM	A	502[B]	1	27,50,50	1.10	2 (7%)	17,82,82	1.86	4 (23%)
2	HEM	C	501[A]	1	27,50,50	1.27	3 (11%)	17,82,82	1.76	4 (23%)
2	HEM	A	501[A]	1	27,50,50	1.36	5 (18%)	17,82,82	2.19	7 (41%)
3	RCO	C	503	-	8,8,8	1.10	0	10,10,10	2.15	4 (40%)
3	RCO	A	503	-	8,8,8	1.24	1 (12%)	10,10,10	1.44	3 (30%)
2	HEM	D	502[B]	1	27,50,50	1.23	3 (11%)	17,82,82	2.50	7 (41%)
2	HEM	D	501[A]	1,6	27,50,50	1.09	3 (11%)	17,82,82	1.90	5 (29%)
3	RCO	B	503	-	8,8,8	1.15	1 (12%)	10,10,10	1.95	2 (20%)
2	HEM	B	501[A]	1,6	27,50,50	1.14	2 (7%)	17,82,82	1.49	3 (17%)
2	HEM	C	502[B]	1	27,50,50	1.13	3 (11%)	17,82,82	2.99	14 (82%)
2	HEM	B	502[B]	1,6	27,50,50	1.11	3 (11%)	17,82,82	2.45	10 (58%)

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	RCO	D	503	-	-	-	0/1/1/1
2	HEM	A	502[B]	1	-	0/6/54/54	-
2	HEM	C	501[A]	1	-	0/6/54/54	-
2	HEM	A	501[A]	1	-	0/6/54/54	-
3	RCO	C	503	-	-	-	0/1/1/1
3	RCO	A	503	-	-	-	0/1/1/1
2	HEM	D	502[B]	1	-	0/6/54/54	-
2	HEM	D	501[A]	1,6	-	2/6/54/54	-
3	RCO	B	503	-	-	-	0/1/1/1
2	HEM	B	501[A]	1,6	-	0/6/54/54	-
2	HEM	C	502[B]	1	-	0/6/54/54	-
2	HEM	B	502[B]	1,6	-	0/6/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501[A]	HEM	C3B-C2B	-4.40	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	HEM	C3B-C2B	-4.14	1.34	1.40
2	D	501[A]	HEM	C4D-C3D	3.51	1.50	1.42
2	D	502[B]	HEM	C1A-NA	3.43	1.43	1.36
2	B	502[B]	HEM	C4D-C3D	3.12	1.49	1.42
2	C	502[B]	HEM	C3C-C2C	-3.00	1.36	1.40
3	A	503	RCO	C2-C3	2.98	1.43	1.39
2	A	501[A]	HEM	C4D-C3D	2.74	1.48	1.42
2	B	501[A]	HEM	C4D-C3D	2.62	1.48	1.42
2	C	501[A]	HEM	C3C-C2C	-2.49	1.36	1.40
2	D	501[A]	HEM	C3B-C2B	-2.45	1.37	1.40
2	B	502[B]	HEM	C3C-C2C	-2.45	1.37	1.40
2	A	502[B]	HEM	C4D-C3D	2.45	1.48	1.42
2	A	501[A]	HEM	C4B-NB	-2.40	1.31	1.36
2	C	501[A]	HEM	C4D-C3D	2.37	1.47	1.42
2	A	502[B]	HEM	C3B-C2B	-2.34	1.37	1.40
2	D	501[A]	HEM	C3C-C2C	-2.29	1.37	1.40
3	B	503	RCO	C2-C1	-2.29	1.35	1.39
2	B	501[A]	HEM	C3B-C2B	-2.26	1.37	1.40
2	A	501[A]	HEM	C3C-C2C	-2.25	1.37	1.40
2	A	501[A]	HEM	C3C-CAC	-2.25	1.43	1.47
2	C	502[B]	HEM	C3C-CAC	-2.21	1.43	1.47
2	D	502[B]	HEM	C1A-CHA	-2.06	1.35	1.41
2	C	502[B]	HEM	C1A-NA	2.06	1.40	1.36
2	D	502[B]	HEM	C4D-C3D	2.01	1.47	1.42
2	B	502[B]	HEM	C1A-NA	2.01	1.40	1.36

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502[B]	HEM	C4A-C3A-C2A	6.36	111.42	107.00
2	C	502[B]	HEM	CBD-CAD-C3D	-5.58	102.20	112.48
2	B	502[B]	HEM	C4A-C3A-C2A	4.52	110.14	107.00
2	A	501[A]	HEM	CMD-C2D-C1D	-4.29	121.87	128.46
2	D	501[A]	HEM	CAD-CBD-CGD	-4.24	105.55	112.67
2	C	502[B]	HEM	C1D-C2D-C3D	-4.24	104.05	107.00
2	B	502[B]	HEM	CMB-C2B-C3B	4.17	132.49	124.68
3	B	503	RCO	C6-C1-C2	-4.17	115.61	120.17
2	A	502[B]	HEM	CAA-CBA-CGA	-4.13	105.74	112.67
2	B	502[B]	HEM	CAD-CBD-CGD	4.02	119.41	112.67
2	C	502[B]	HEM	CMD-C2D-C3D	3.88	132.26	124.94
2	A	501[A]	HEM	CMD-C2D-C3D	3.80	132.11	124.94
3	B	503	RCO	C3-C2-C1	3.72	123.65	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	503	RCO	C6-C1-C2	-3.71	116.11	120.17
3	C	503	RCO	C6-C5-C4	3.70	125.50	120.25
2	B	501[A]	HEM	C3B-C4B-NB	-3.63	104.52	109.21
2	D	502[B]	HEM	CMD-C2D-C1D	-3.53	123.04	128.46
2	C	501[A]	HEM	CMA-C3A-C4A	-3.50	123.08	128.46
2	C	502[B]	HEM	C4A-C3A-C2A	3.42	109.37	107.00
2	D	502[B]	HEM	CBD-CAD-C3D	-3.34	106.32	112.48
2	A	502[B]	HEM	CBD-CAD-C3D	-3.32	106.36	112.48
2	C	502[B]	HEM	CMD-C2D-C1D	-3.27	123.43	128.46
2	C	502[B]	HEM	CMA-C3A-C2A	-3.19	118.92	124.94
2	D	502[B]	HEM	CMA-C3A-C4A	-3.16	123.60	128.46
2	A	501[A]	HEM	CAA-CBA-CGA	3.07	117.82	112.67
2	C	501[A]	HEM	C4C-C3C-C2C	3.04	109.02	106.90
2	A	502[B]	HEM	CMC-C2C-C3C	3.02	130.32	124.68
2	A	501[A]	HEM	CAD-CBD-CGD	-3.01	107.62	112.67
2	A	501[A]	HEM	CBA-CAA-C2A	-3.00	106.95	112.49
2	C	502[B]	HEM	CAA-C2A-C3A	-3.00	118.63	127.25
2	C	502[B]	HEM	C4C-C3C-C2C	2.98	108.98	106.90
2	D	502[B]	HEM	CMD-C2D-C3D	2.92	130.46	124.94
2	D	501[A]	HEM	CBA-CAA-C2A	-2.87	107.19	112.49
2	B	502[B]	HEM	CMA-C3A-C4A	-2.82	124.12	128.46
3	C	503	RCO	C3-C2-C1	2.79	122.55	119.20
2	D	502[B]	HEM	CBA-CAA-C2A	2.78	117.61	112.49
2	B	502[B]	HEM	C1D-C2D-C3D	-2.77	105.07	107.00
2	D	502[B]	HEM	CMB-C2B-C3B	2.71	129.75	124.68
2	D	501[A]	HEM	CMD-C2D-C1D	-2.70	124.31	128.46
2	B	501[A]	HEM	CAD-CBD-CGD	-2.70	108.15	112.67
2	D	501[A]	HEM	CMB-C2B-C3B	2.68	129.70	124.68
2	A	502[B]	HEM	C3C-C4C-NC	-2.66	105.91	110.94
2	C	501[A]	HEM	CAA-CBA-CGA	2.63	117.08	112.67
3	C	503	RCO	C5-C4-C3	-2.61	115.62	119.31
3	D	503	RCO	C4-C3-C2	2.55	122.96	120.17
2	C	502[B]	HEM	CAD-CBD-CGD	2.51	116.88	112.67
3	D	503	RCO	C6-C1-C2	-2.50	117.43	120.17
3	D	503	RCO	C5-C6-C1	2.48	122.82	119.31
2	C	502[B]	HEM	C3B-C4B-NB	-2.48	106.00	109.21
2	B	502[B]	HEM	C4C-C3C-C2C	2.47	108.62	106.90
2	C	501[A]	HEM	CMA-C3A-C2A	2.45	129.57	124.94
3	A	503	RCO	C6-C1-C2	-2.42	117.53	120.17
2	B	502[B]	HEM	C3B-C4B-NB	-2.36	106.16	109.21
2	B	502[B]	HEM	C3C-C4C-NC	-2.31	106.58	110.94
2	A	501[A]	HEM	C3B-C4B-NB	-2.27	106.27	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	502[B]	HEM	C3C-C4C-NC	-2.27	106.66	110.94
3	A	503	RCO	O1-C1-C2	2.26	125.71	119.84
2	D	501[A]	HEM	C3B-C4B-NB	-2.22	106.34	109.21
3	A	503	RCO	C5-C6-C1	2.21	122.43	119.31
2	C	502[B]	HEM	CMC-C2C-C3C	2.19	128.77	124.68
2	B	502[B]	HEM	CBD-CAD-C3D	-2.18	108.46	112.48
2	A	501[A]	HEM	C3C-C4C-NC	-2.13	106.93	110.94
2	C	502[B]	HEM	CMB-C2B-C3B	2.13	128.65	124.68
2	C	502[B]	HEM	CMA-C3A-C4A	2.11	131.70	128.46
2	B	502[B]	HEM	CMD-C2D-C3D	2.04	128.79	124.94
2	B	501[A]	HEM	CMB-C2B-C3B	2.00	128.43	124.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501[A]	HEM	C1A-C2A-CAA-CBA
2	D	501[A]	HEM	C3A-C2A-CAA-CBA

There are no ring outliers.

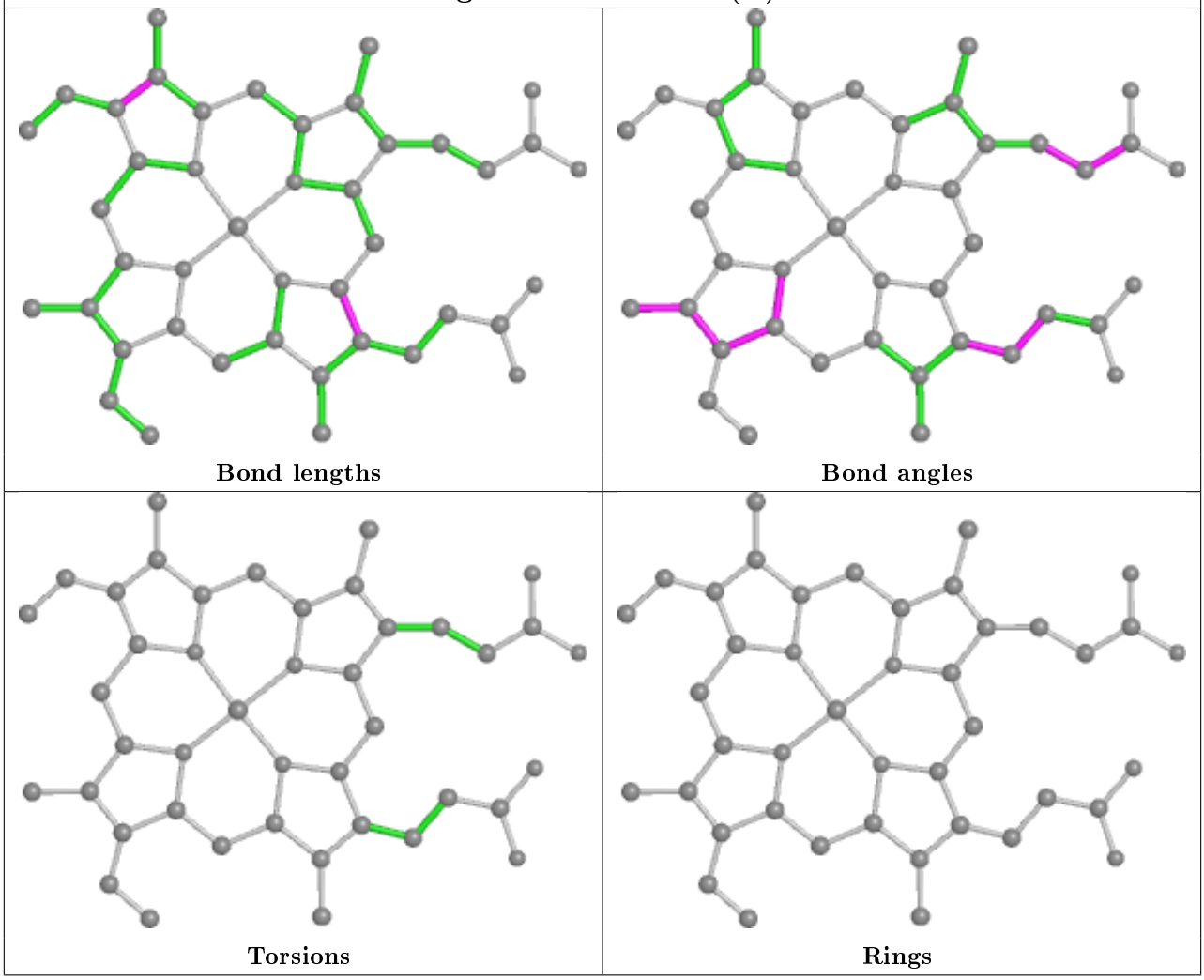
10 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	503	RCO	1	0
2	A	502[B]	HEM	3	0
2	C	501[A]	HEM	9	0
2	A	501[A]	HEM	7	0
3	A	503	RCO	1	0
2	D	502[B]	HEM	2	0
2	D	501[A]	HEM	7	0
2	B	501[A]	HEM	8	0
2	C	502[B]	HEM	2	0
2	B	502[B]	HEM	6	0

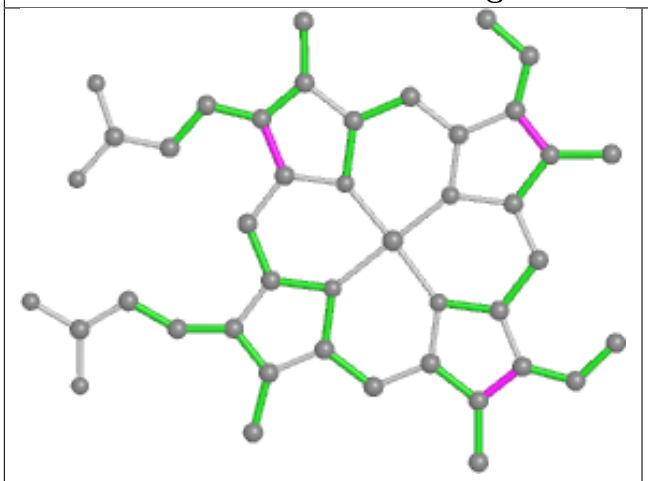
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

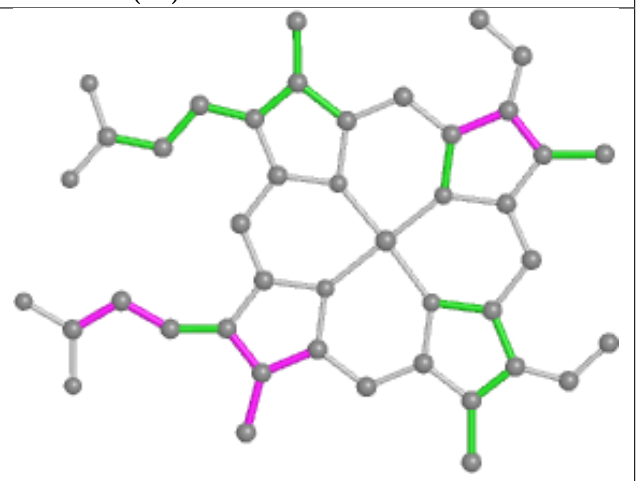
Ligand HEM A 502 (B)



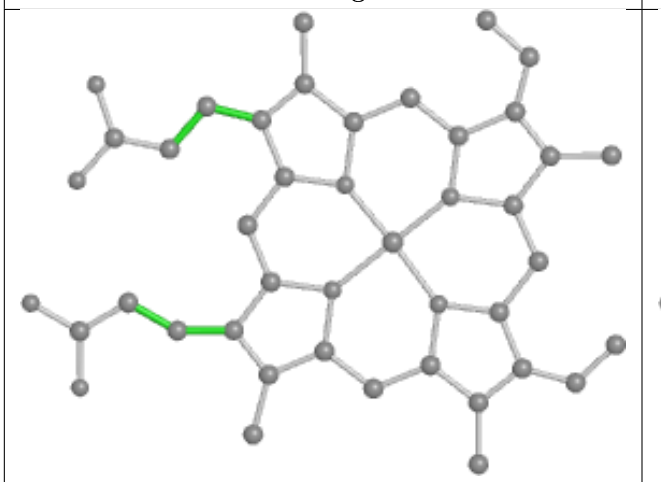
Ligand HEM C 501 (A)



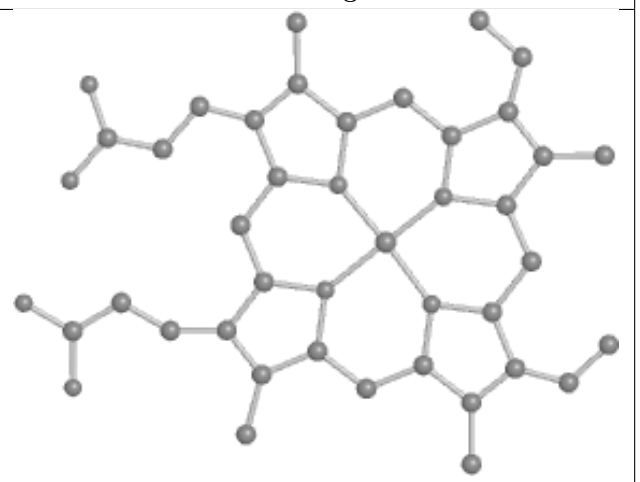
Bond lengths



Bond angles

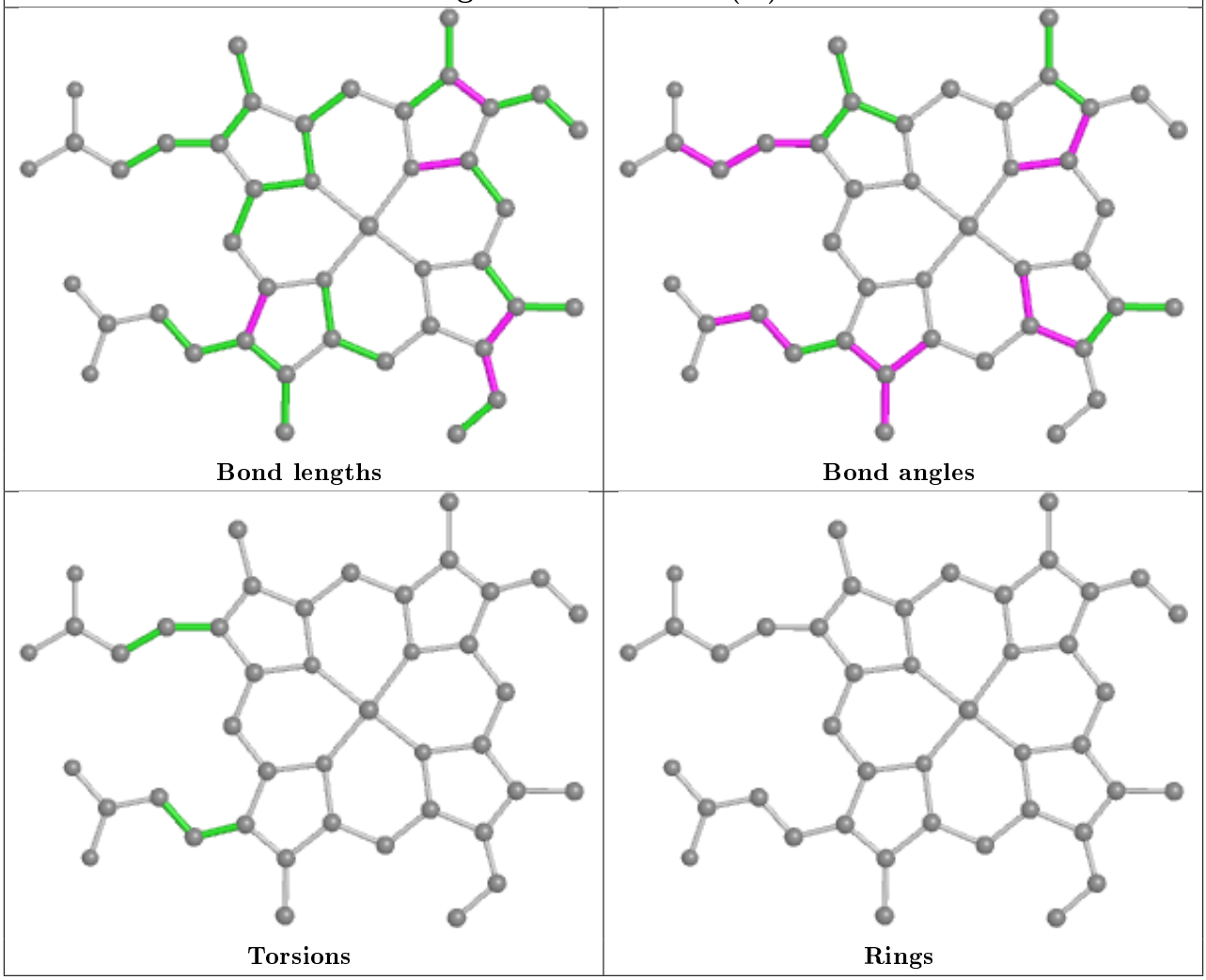


Torsions

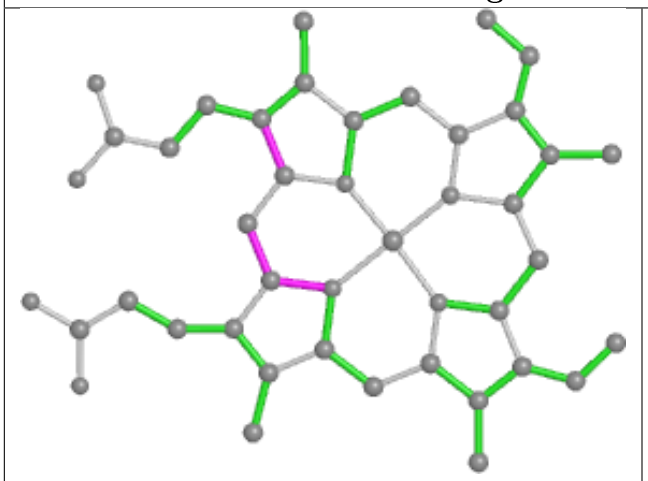


Rings

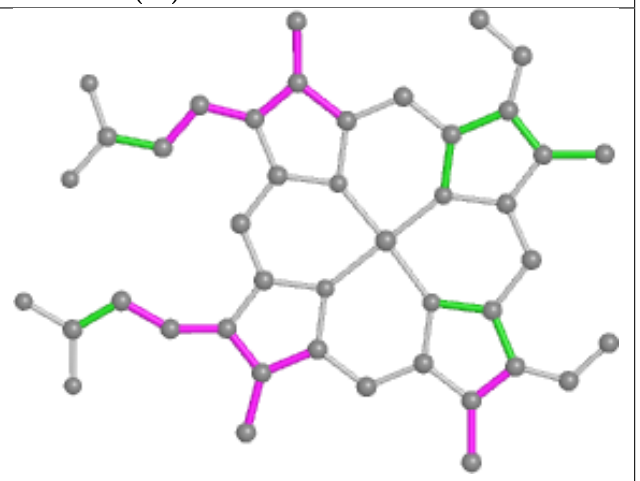
Ligand HEM A 501 (A)



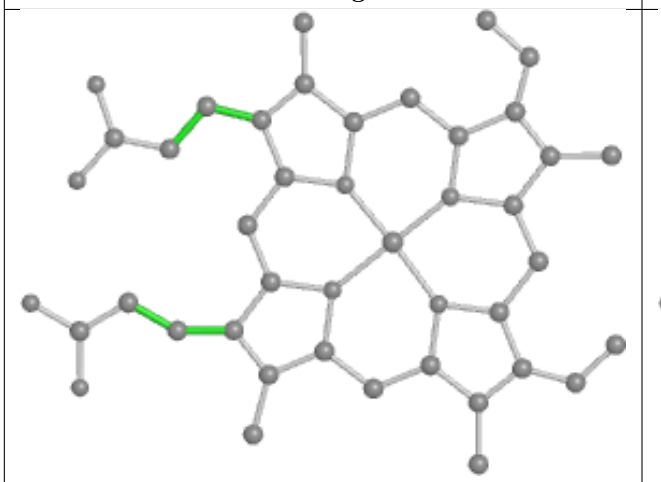
Ligand HEM D 502 (B)



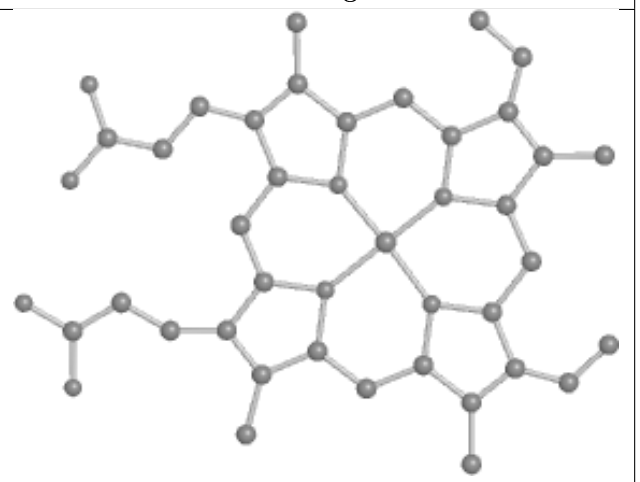
Bond lengths



Bond angles

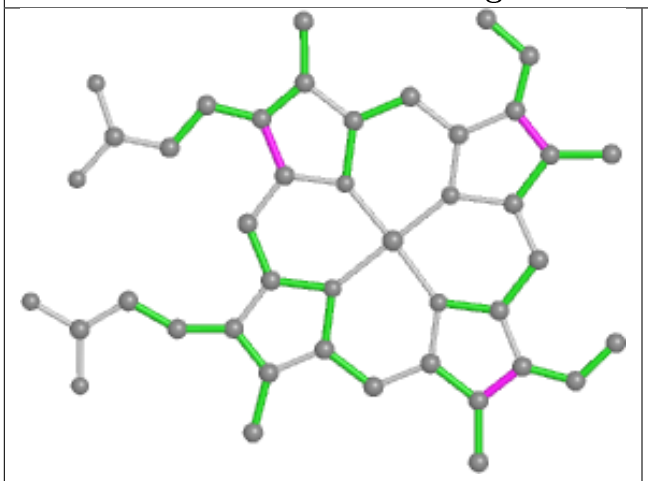


Torsions

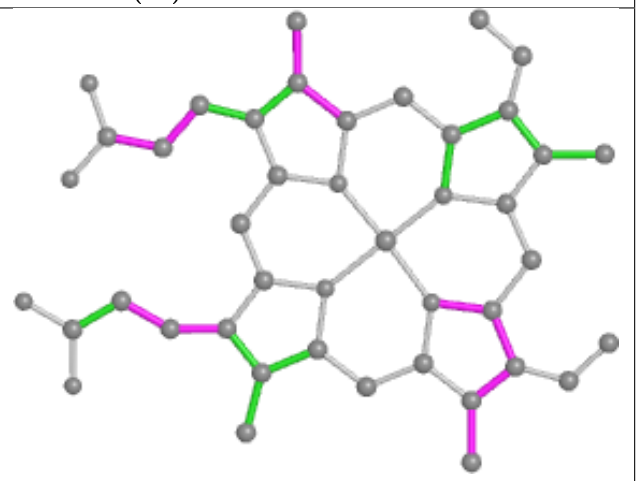


Rings

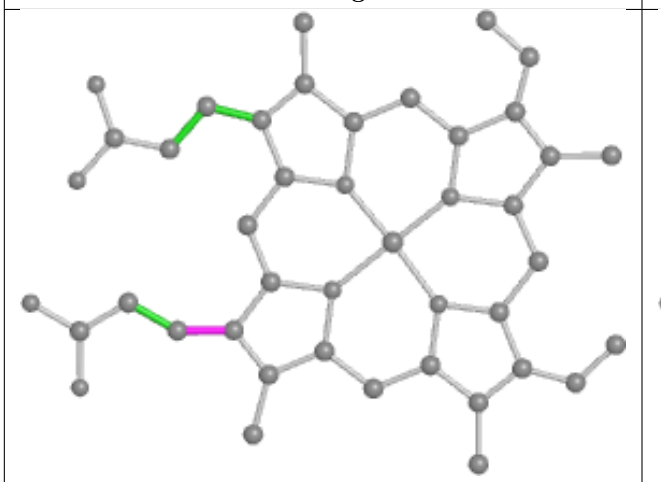
Ligand HEM D 501 (A)



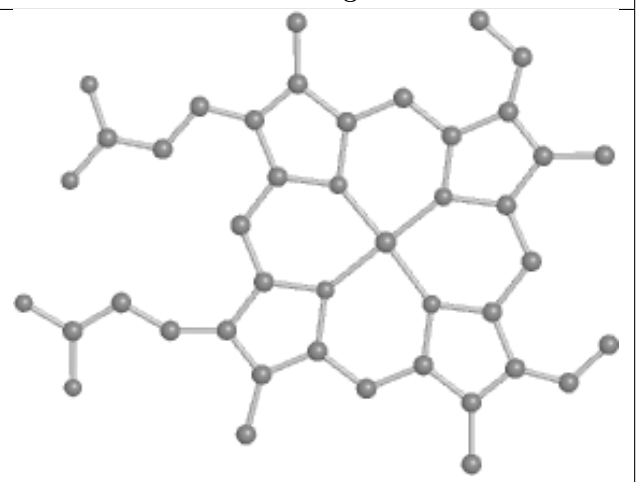
Bond lengths



Bond angles

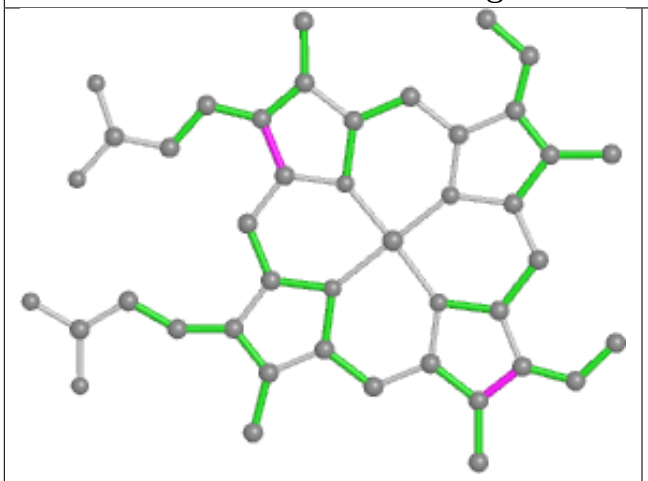


Torsions

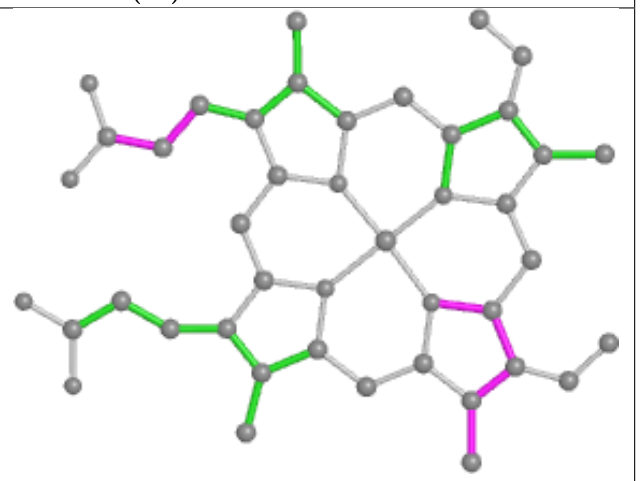


Rings

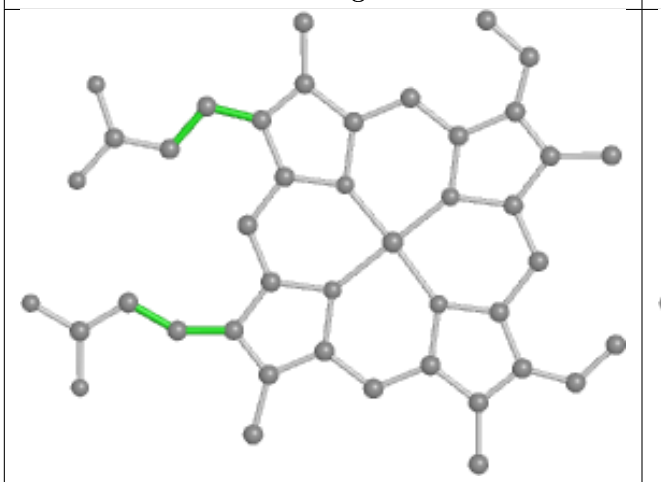
Ligand HEM B 501 (A)



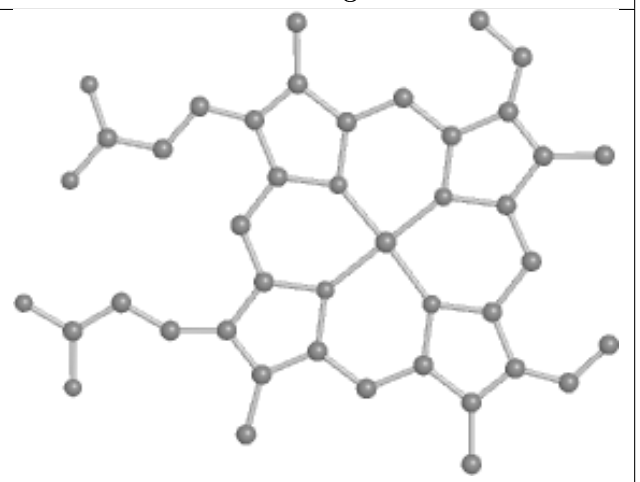
Bond lengths



Bond angles

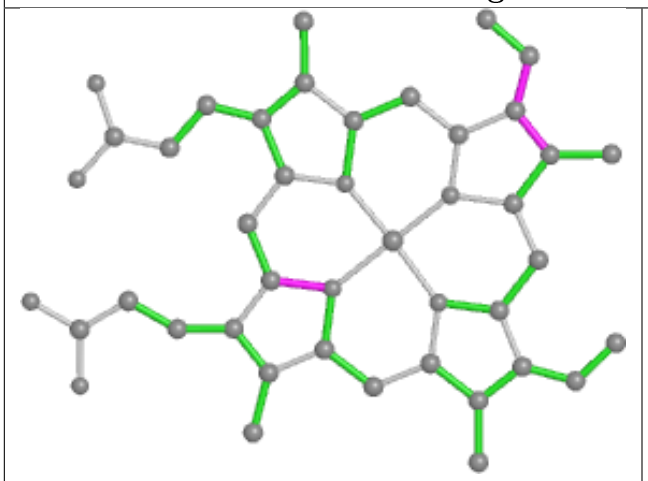


Torsions

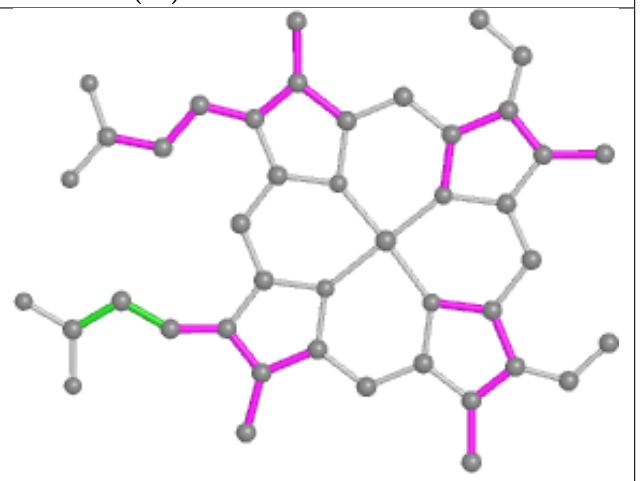


Rings

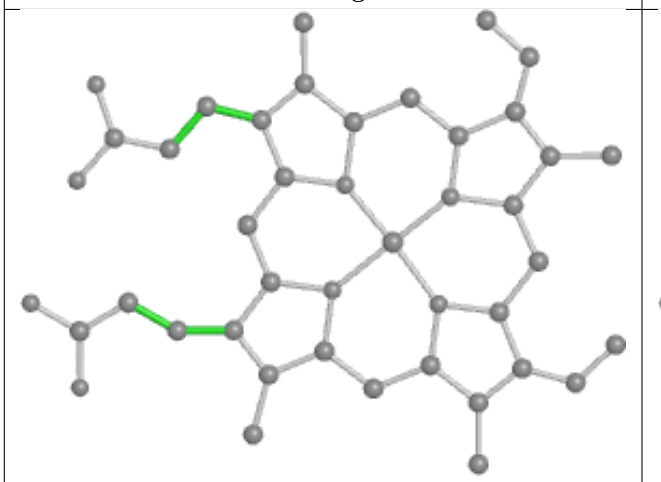
Ligand HEM C 502 (B)



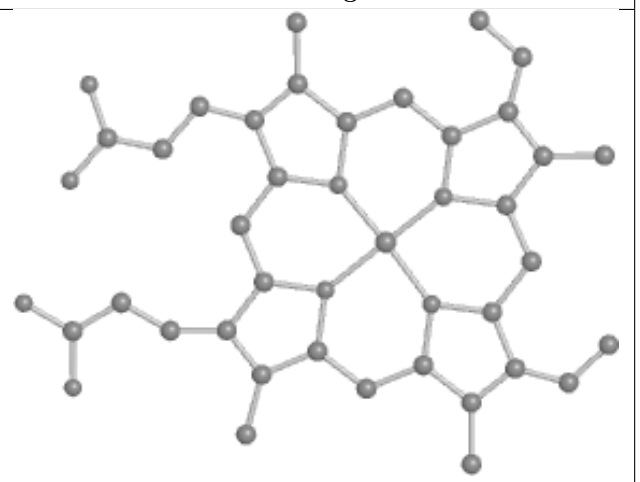
Bond lengths



Bond angles

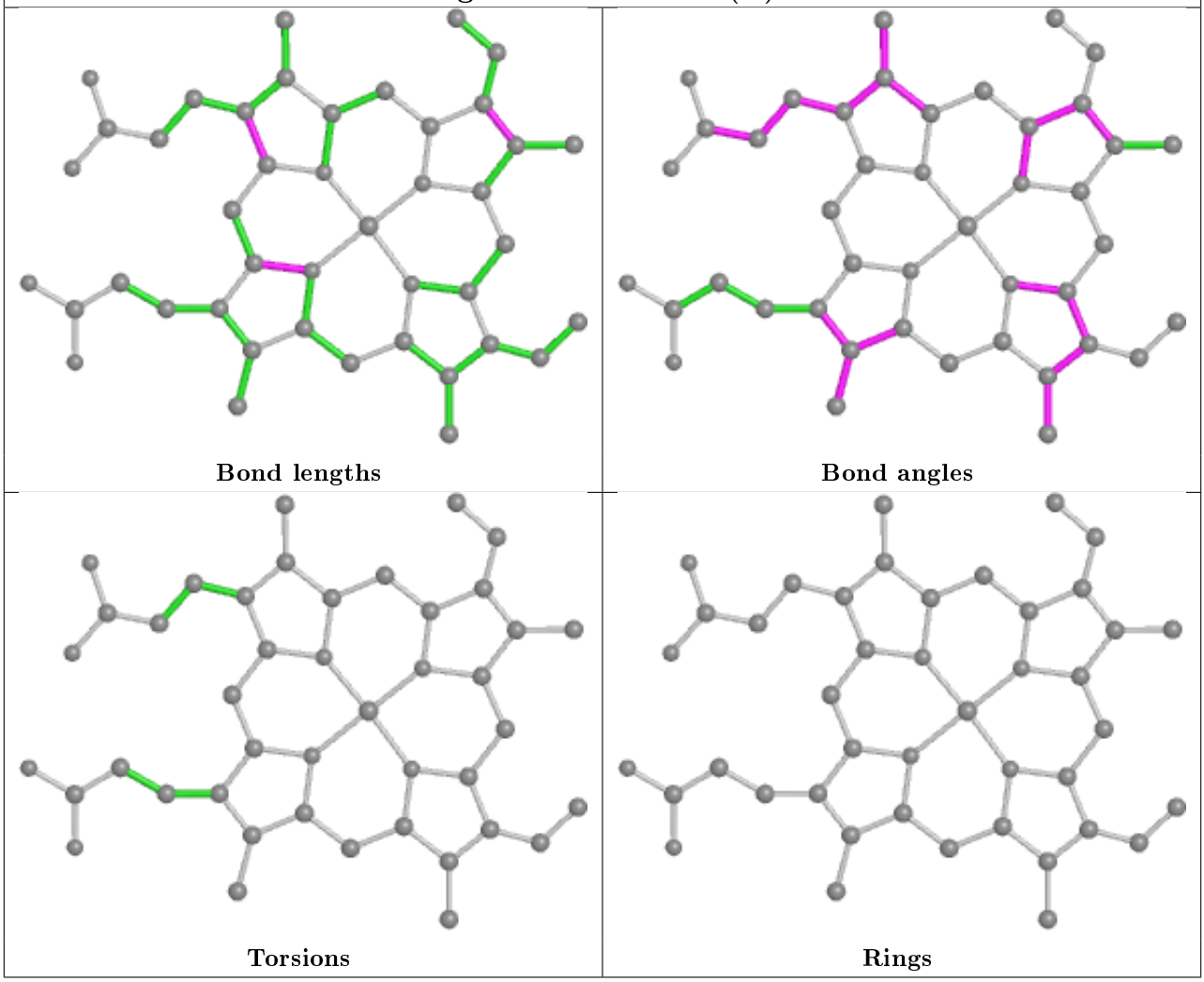


Torsions



Rings

Ligand HEM B 502 (B)



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	480/491 (97%)	0.22	19 (3%)	38	45	15, 26, 42, 72	0
1	B	480/491 (97%)	0.05	6 (1%)	77	83	15, 23, 38, 60	0
1	C	480/491 (97%)	0.16	13 (2%)	54	60	14, 21, 39, 70	0
1	D	480/491 (97%)	0.27	16 (3%)	46	53	15, 25, 42, 91	0
All	All	1920/1964 (97%)	0.17	54 (2%)	53	58	14, 24, 42, 91	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	485	TYR	8.8
1	C	485	TYR	7.0
1	A	485	TYR	6.8
1	D	484	SER	5.0
1	D	372[A]	PHE	4.9
1	C	484	SER	4.8
1	D	483	ARG	4.3
1	B	372[A]	PHE	4.2
1	A	372[A]	PHE	3.9
1	C	372[A]	PHE	3.9
1	A	6	HIS	3.8
1	D	480	VAL	3.6
1	A	288	GLU	3.5
1	D	479	GLY	3.4
1	C	483	ARG	3.4
1	A	479	GLY	3.3
1	B	485	TYR	3.3
1	D	482	ILE	3.2
1	D	481	ASP	3.0
1	C	6	HIS	3.0
1	A	481	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	6	HIS	2.9
1	A	457	LEU	2.9
1	D	478	LEU	2.9
1	A	474	LEU	2.8
1	B	219	ARG	2.8
1	C	461[A]	CYS	2.8
1	A	478	LEU	2.7
1	D	475	ALA	2.6
1	A	253	LYS	2.6
1	D	457	LEU	2.5
1	A	464	TYR	2.5
1	A	407	HIS	2.5
1	D	461	CYS	2.4
1	B	390	ASP	2.4
1	C	55	VAL	2.3
1	C	56	VAL	2.3
1	C	480	VAL	2.3
1	D	350	ALA	2.3
1	A	461	CYS	2.3
1	D	86	GLY	2.3
1	A	405	VAL	2.2
1	C	398	HIS	2.2
1	A	256	TYR	2.2
1	A	406	LEU	2.2
1	B	51	ILE	2.2
1	C	390	ASP	2.1
1	D	240	PHE	2.1
1	A	480	VAL	2.1
1	C	457	LEU	2.1
1	C	407	HIS	2.1
1	A	66[A]	VAL	2.1
1	B	6	HIS	2.0
1	A	432	TYR	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 carbohydrates in this entry.

6.4 Ligands (i)

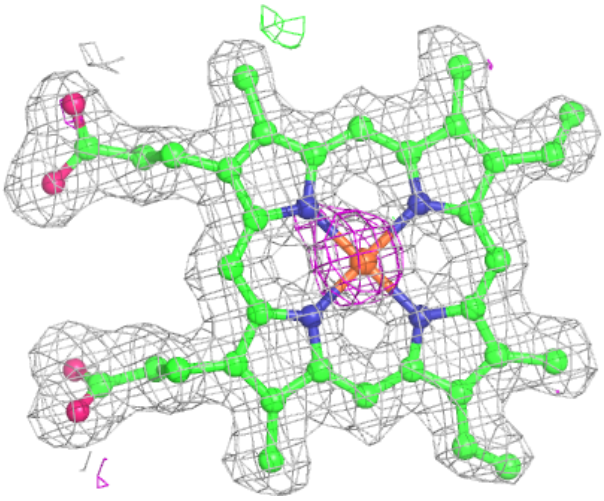
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

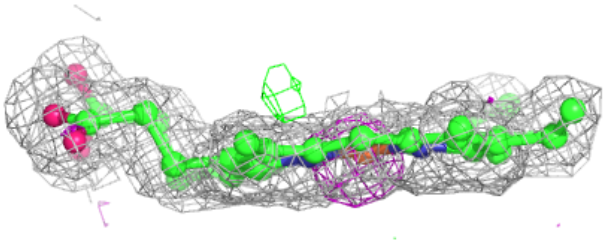
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RCO	A	503	8/8	0.85	0.12	32,33,35,37	0
3	RCO	C	503	8/8	0.93	0.11	22,23,26,27	0
5	NA	B	505	1/1	0.93	0.11	20,20,20,20	0
3	RCO	D	503	8/8	0.95	0.08	27,29,30,30	0
3	RCO	B	503	8/8	0.95	0.08	24,26,27,29	0
2	HEM	C	502[B]	43/43	0.96	0.12	11,12,13,14	43
2	HEM	D	502[B]	43/43	0.97	0.11	12,14,15,16	43
2	HEM	A	501[A]	43/43	0.97	0.10	12,16,18,19	43
2	HEM	D	501[A]	43/43	0.97	0.12	18,20,22,26	43
2	HEM	A	502[B]	43/43	0.97	0.10	16,20,24,27	43
2	HEM	B	501[A]	43/43	0.97	0.11	15,16,19,23	43
2	HEM	C	501[A]	43/43	0.97	0.11	15,17,20,25	43
2	HEM	B	502[B]	43/43	0.97	0.11	10,12,14,15	43
4	CL	B	504	1/1	0.98	0.09	22,22,22,22	0
5	NA	A	506	1/1	0.98	0.12	9,9,9,9	0
4	CL	C	504	1/1	0.98	0.11	26,26,26,26	0
4	CL	A	505	1/1	0.99	0.04	20,20,20,20	0
4	CL	D	504	1/1	0.99	0.06	20,20,20,20	0
4	CL	A	504	1/1	1.00	0.14	28,28,28,28	0
4	CL	C	505	1/1	1.00	0.04	23,23,23,23	0

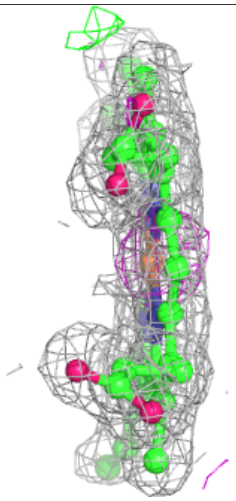
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

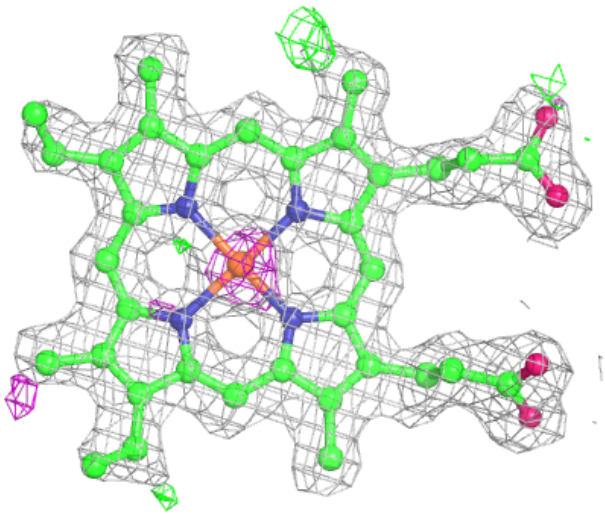
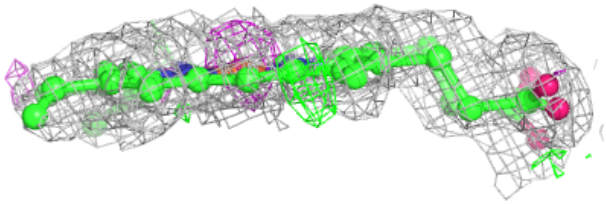
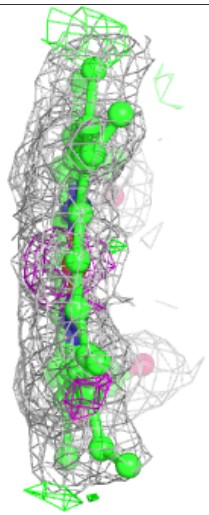
Electron density around HEM C 502 (B):

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



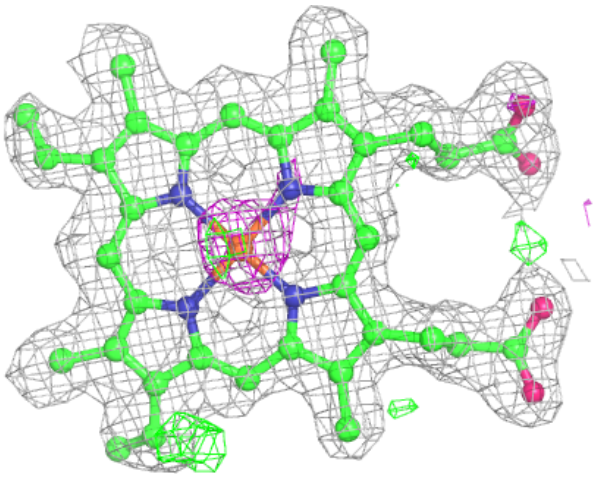


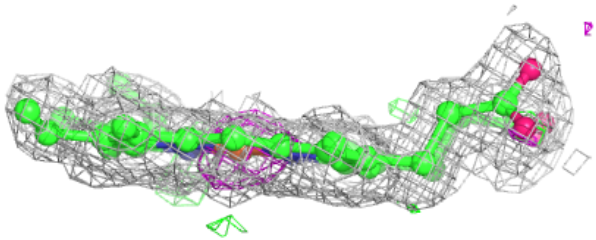


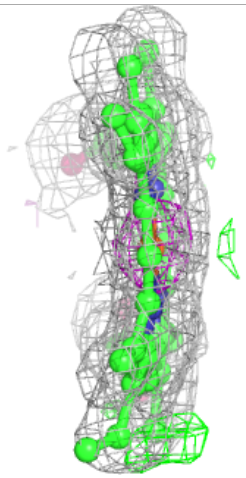
Electron density around HEM D 502 (B): 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around HEM A 501 (A):

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

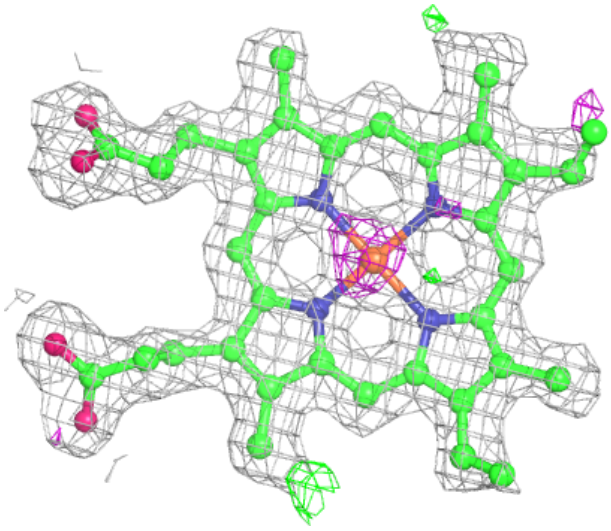


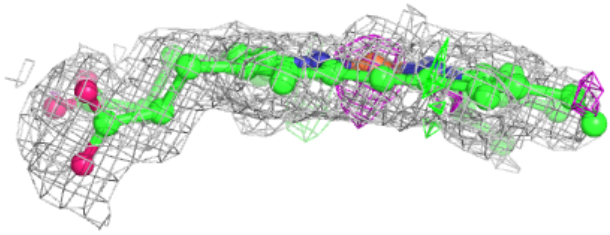


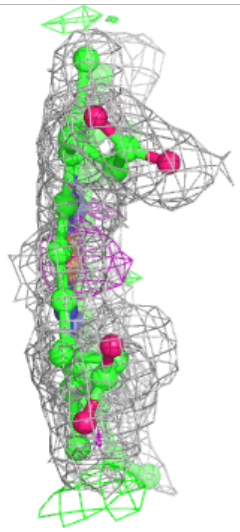


Electron density around HEM D 501 (A):

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

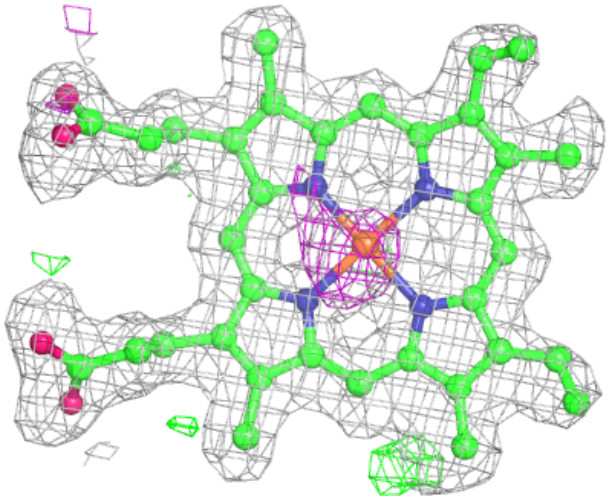


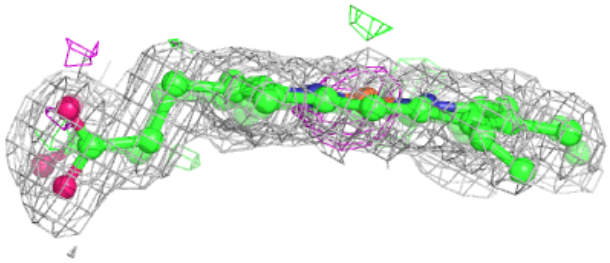




Electron density around HEM A 502 (B):

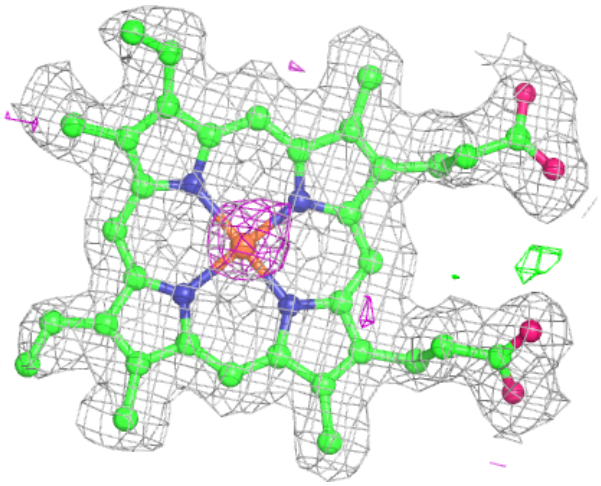
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

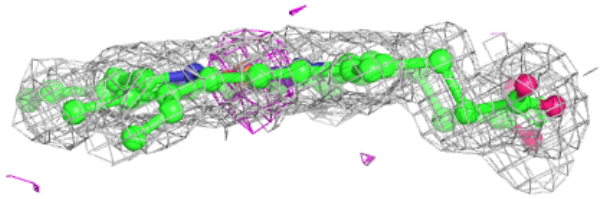


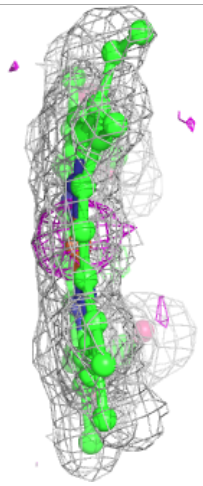


Electron density around HEM B 501 (A):

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

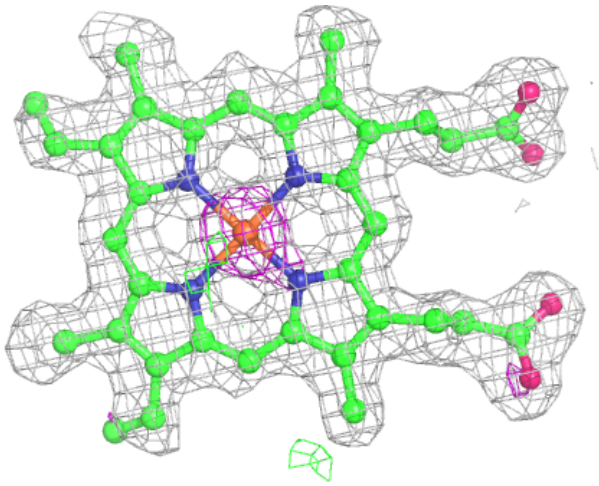


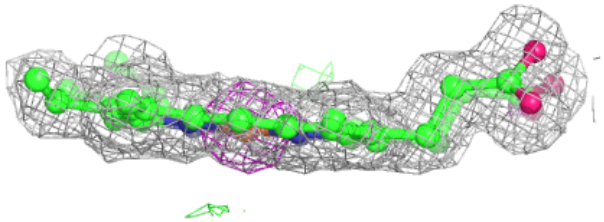


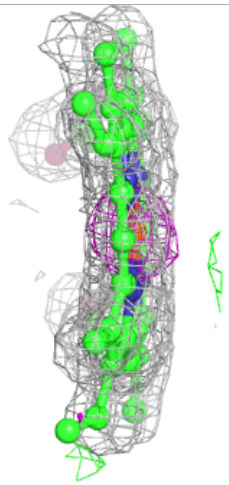


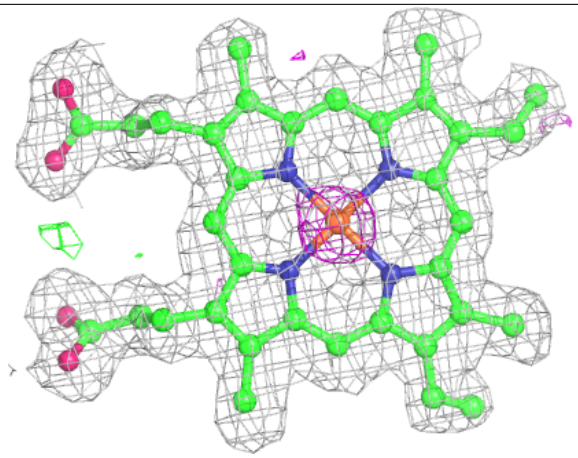
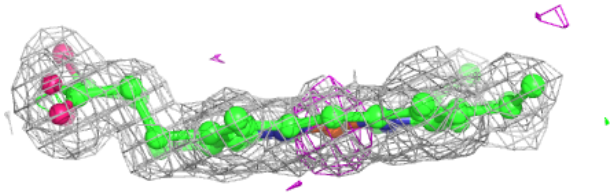
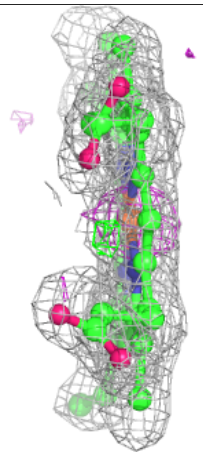
Electron density around HEM C 501 (A):

$2mF_o$-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 502 (B): $2mF_o$-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.