Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 02:14 AM EDT

PDB ID	:	4QOL
Title	:	Structure of Bacillus pumilus catalase
Authors	:	Loewen, P.C.
Deposited on	:	2014-06-20
Resolution	:	1.65 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:

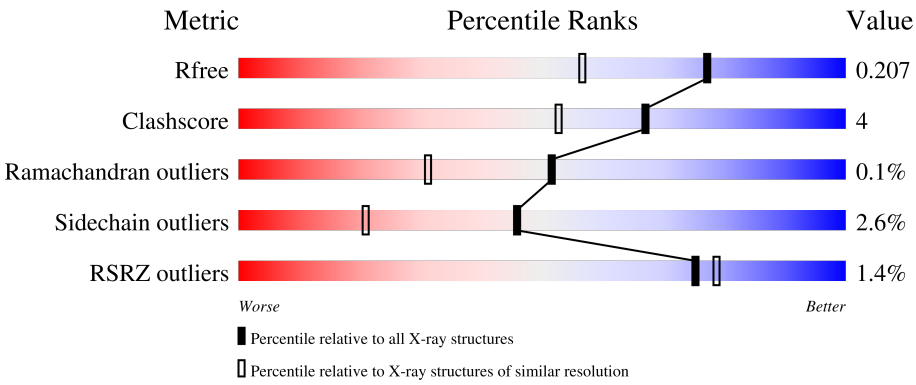
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	491	.% 88% 9% •
1	B	491	.% 90% 8% • •
1	C	491	.% 90% 7% •
1	D	491	2% 89% 9% • •

2 Entry composition (i)

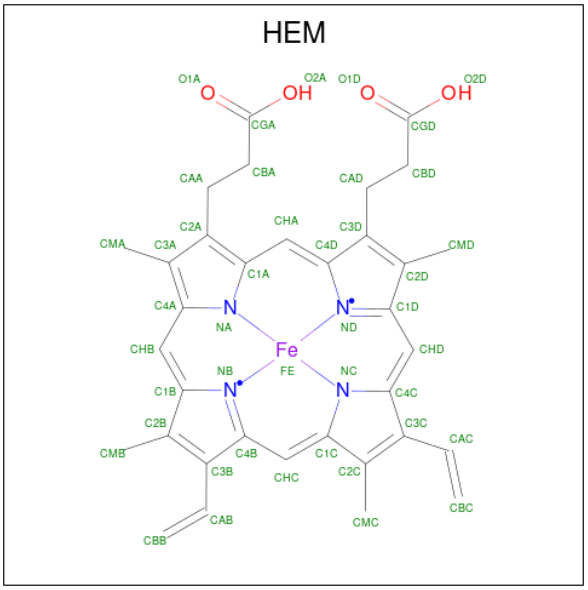
There are 6 unique types of molecules in this entry. The entry contains 17939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	3949	2488	692	755	14	0	5	0
1	B	480	3951	2491	691	754	15	0	5	0
1	C	480	3962	2498	695	755	14	0	6	0
1	D	480	3958	2494	692	758	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

Continued on next page...

Continued from previous page...

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

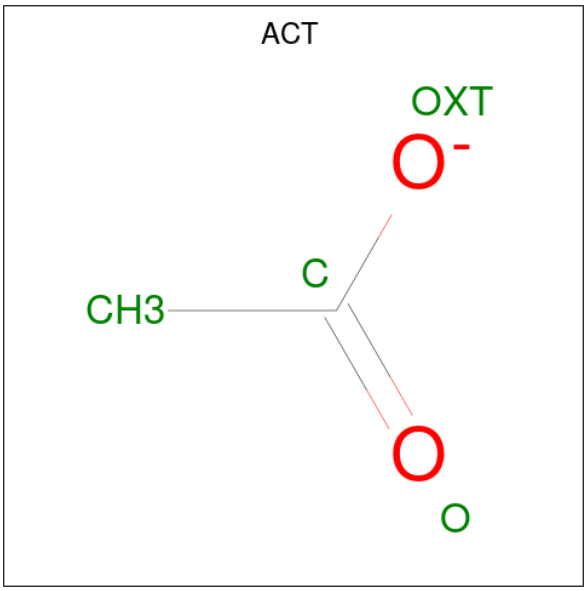
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

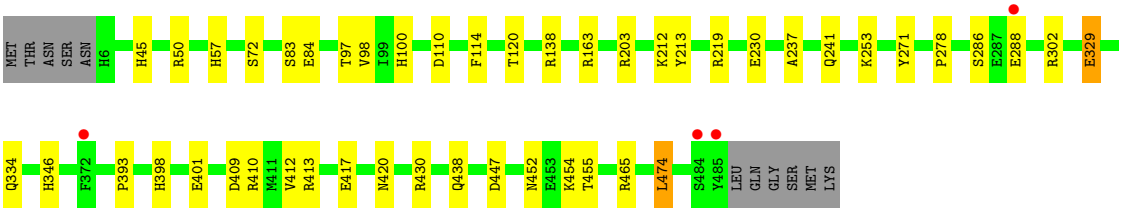
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	472	472	472	0	0
6	B	423	423	423	0	0
6	C	425	425	425	0	0
6	D	431	431	431	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

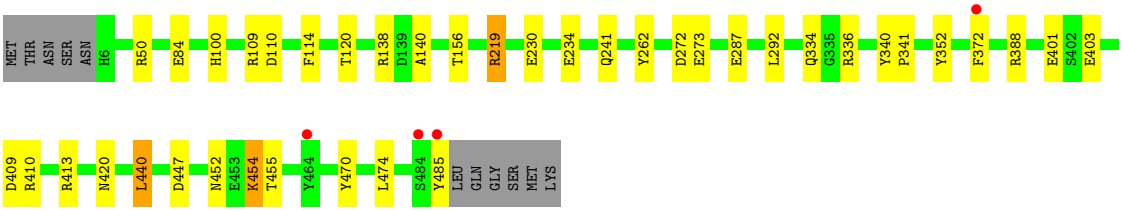
• Molecule 1: Catalase

Chain A:



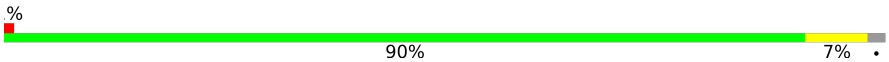
• Molecule 1: Catalase

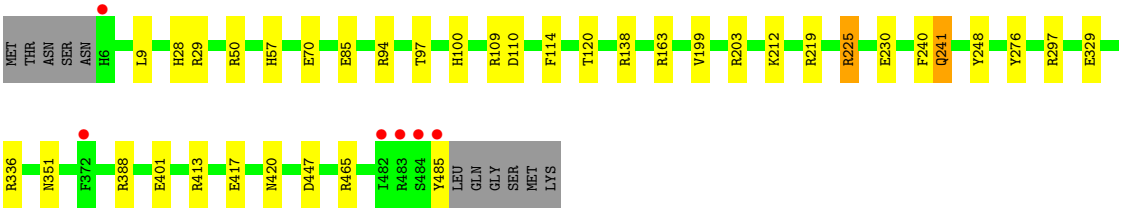
Chain B:



• Molecule 1: Catalase

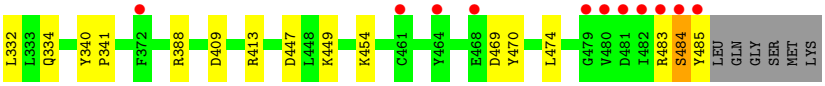
Chain C:





• Molecule 1: Catalase

Chain D:


L332
L333
Q334
Y340
P341
F372
R388
D409
R413
D447
L448
K449
K454
C461
Y464
E468
D469
Y470
L474
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	91.65Å 109.19Å 102.83Å 90.00° 91.67° 90.00°	Depositor
Resolution (Å)	102.79 – 1.65 48.22 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.4 (102.79-1.65) 96.4 (48.22-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.171 , 0.199 0.181 , 0.207	Depositor DCC
R_{free} test set	11569 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17939	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, NA, ACT, CL

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	0.92	1/4068 (0.0%)	0.95	15/5516 (0.3%)
1	B	0.92	1/4069 (0.0%)	0.93	6/5516 (0.1%)
1	C	0.94	2/4080 (0.0%)	1.01	17/5531 (0.3%)
1	D	0.90	0/4076	0.92	11/5526 (0.2%)
All	All	0.92	4/16293 (0.0%)	0.95	49/22089 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLU	CG-CD	6.63	1.61	1.51
1	C	329	GLU	CG-CD	5.97	1.60	1.51
1	B	352	TYR	CD1-CE1	5.93	1.48	1.39
1	C	276	TYR	CE1-CZ	5.25	1.45	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	ARG	NE-CZ-NH1	-14.95	112.83	120.30
1	C	225	ARG	NE-CZ-NH2	13.04	126.82	120.30
1	C	465	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	C	413	ARG	NE-CZ-NH1	-9.94	115.33	120.30
1	D	413	ARG	NE-CZ-NH1	-9.41	115.59	120.30
1	A	465	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	C	50	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	C	50	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	465	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	A	465	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	50	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	329	GLU	OE1-CD-OE2	-7.88	113.84	123.30
1	A	50	ARG	NE-CZ-NH1	7.83	124.21	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	50	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	50	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	413	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	A	413	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	C	225	ARG	CG-CD-NE	-7.08	96.92	111.80
1	D	50	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	D	388	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	B	138	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	203	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	203	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	D	272	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	D	388	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	163	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	C	329	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	B	440	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	388	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	413	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	C	203	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	109	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	138	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	430	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	440	LEU	CB-CG-CD2	5.49	120.33	111.00
1	C	94	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	302	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	109	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	329	GLU	CG-CD-OE1	5.37	129.04	118.30
1	A	203	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	109	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	163	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	C	297	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	163	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	138	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	138	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	474	LEU	CB-CG-CD2	5.14	119.73	111.00
1	A	410	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	D	297	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	3949	0	3748	32	1
1	B	3951	0	3756	22	1
1	C	3962	0	3771	21	1
1	D	3958	0	3758	24	2
2	A	86	0	60	5	0
2	B	86	0	60	11	0
2	C	86	0	60	12	0
2	D	86	0	60	12	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
5	D	4	0	3	0	0
6	A	472	0	0	15	0
6	B	423	0	0	6	1
6	C	425	0	0	10	0
6	D	431	0	0	17	0
All	All	17939	0	15285	124	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (124) 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:388:ARG:HD2	6:B:1010:HOH:O	1.42	1.17
1:D:72[B]:SER:OG	1:D:74:GLU:OE1	1.77	1.01
1:A:329:GLU:HG3	6:D:1001:HOH:O	1.61	0.99
1:C:219:ARG:CD	6:C:727:HOH:O	2.14	0.95
1:B:372[A]:PHE:CE2	6:D:911:HOH:O	2.20	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:HIS:ND1	6:C:840:HOH:O	2.06	0.87
1:A:219:ARG:CD	6:A:869:HOH:O	2.23	0.86
1:D:469:ASP:OD1	6:D:1024:HOH:O	1.94	0.85
1:C:219:ARG:HD3	6:C:727:HOH:O	1.75	0.85
1:A:230:GLU:OE2	6:A:872:HOH:O	2.02	0.78
1:A:452:ASN:HD22	1:A:455:THR:H	1.33	0.77
1:B:452:ASN:HD22	1:B:455:THR:H	1.34	0.75
1:D:231:GLU:OE2	6:D:915:HOH:O	2.04	0.75
1:D:449:LYS:NZ	6:D:834:HOH:O	2.20	0.71
1:D:454:LYS:HE3	6:D:1022:HOH:O	1.90	0.71
1:A:346:HIS:HE1	6:D:911:HOH:O	1.73	0.71
2:C:501[A]:HEM:CMB	2:C:501[A]:HEM:HBB2	2.21	0.71
1:C:29:ARG:HD3	6:C:900:HOH:O	1.91	0.71
1:A:393:PRO:HB2	1:C:9[B]:LEU:HD23	1.74	0.68
1:D:28:HIS:CD2	6:D:995:HOH:O	2.46	0.68
1:A:83:SER:OG	6:A:981:HOH:O	2.11	0.67
2:D:501[A]:HEM:CMB	2:D:501[A]:HEM:HBB2	2.25	0.67
2:C:501[A]:HEM:HBB2	2:C:501[A]:HEM:HMB2	1.77	0.66
1:B:372[A]:PHE:CD2	6:D:911:HOH:O	2.45	0.66
1:A:213:TYR:OH	1:A:329:GLU:OE2	2.13	0.64
1:A:219:ARG:HD2	6:A:869:HOH:O	1.90	0.64
1:C:219:ARG:HD2	6:C:727:HOH:O	1.89	0.64
2:B:502[B]:HEM:CMC	2:B:502[B]:HEM:HBC2	2.28	0.63
1:D:483:ARG:O	1:D:484:SER:CB	2.46	0.63
2:D:501[A]:HEM:HBB2	2:D:501[A]:HEM:HMB2	1.81	0.63
1:A:438:GLN:HG2	6:A:1009:HOH:O	1.99	0.63
6:A:1005:HOH:O	1:D:334:GLN:HG3	1.99	0.62
1:A:45:HIS:HE1	1:C:351:ASN:OD1	1.81	0.62
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:HBB2	1.82	0.61
2:A:501[A]:HEM:HBB2	2:A:501[A]:HEM:CMB	2.30	0.61
2:D:502[B]:HEM:CMC	2:D:502[B]:HEM:HBC2	2.31	0.61
1:A:219:ARG:HD3	6:A:869:HOH:O	1.96	0.60
1:A:454:LYS:HE3	6:A:1060:HOH:O	2.01	0.59
1:C:28:HIS:CE1	6:C:840:HOH:O	2.51	0.59
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:CMC	2.33	0.58
1:A:219:ARG:HD2	6:A:842:HOH:O	2.02	0.58
1:B:140:ALA:HA	2:B:501[A]:HEM:HBB1	1.84	0.58
1:D:252:GLU:OE1	6:D:678:HOH:O	2.16	0.58
2:A:501[A]:HEM:CMC	2:A:501[A]:HEM:HBC2	2.32	0.58
1:A:286:SER:OG	1:A:288:GLU:HG2	2.04	0.58
2:B:501[A]:HEM:CMC	2:B:501[A]:HEM:HBC2	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HE2	6:A:700:HOH:O	2.04	0.57
1:C:199:VAL:HG11	2:C:502[B]:HEM:HBB1	1.86	0.57
1:B:388:ARG:CD	6:B:1010:HOH:O	2.20	0.57
1:B:410:ARG:NH1	6:B:931:HOH:O	2.38	0.56
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:HMC2	1.87	0.56
1:A:398:HIS:HB2	6:A:949:HOH:O	2.06	0.55
2:C:501[A]:HEM:HBC2	2:C:501[A]:HEM:HMC2	1.88	0.55
1:B:100:HIS:HE1	6:C:702:HOH:O	1.88	0.55
1:A:334:GLN:HG3	6:D:892:HOH:O	2.06	0.55
6:B:736:HOH:O	1:C:100:HIS:HE1	1.89	0.55
2:C:501[A]:HEM:HMB2	2:C:501[A]:HEM:CBB	2.37	0.55
1:C:212:LYS:HE2	6:C:904:HOH:O	2.05	0.54
1:D:85:GLU:CD	6:D:923:HOH:O	2.46	0.54
6:A:809:HOH:O	1:D:100:HIS:HE1	1.91	0.53
1:B:219:ARG:NH2	1:B:262:TYR:OH	2.43	0.52
1:C:219:ARG:HD2	6:C:1007:HOH:O	2.10	0.51
1:D:219:ARG:HG2	6:D:859:HOH:O	2.08	0.51
1:A:45:HIS:HD2	6:A:688:HOH:O	1.93	0.51
1:D:332:LEU:HD12	2:D:501[A]:HEM:HBB1	1.91	0.51
1:D:483:ARG:O	1:D:484:SER:HB3	2.09	0.51
1:A:219:ARG:HG3	6:A:1045:HOH:O	2.10	0.51
1:B:287:GLU:CD	1:B:292:LEU:HD21	2.32	0.51
1:A:100:HIS:HE1	6:D:676:HOH:O	1.93	0.51
2:C:501[A]:HEM:CMB	2:C:501[A]:HEM:CBB	2.89	0.50
2:A:502[B]:HEM:HBC2	2:A:502[B]:HEM:CMC	2.41	0.50
1:D:230:GLU:CD	1:D:230:GLU:H	2.14	0.50
1:B:287:GLU:CG	1:B:292:LEU:HD21	2.42	0.49
2:B:501[A]:HEM:HMB2	2:B:501[A]:HEM:HBB2	1.94	0.49
1:A:452:ASN:ND2	1:A:455:THR:H	2.07	0.49
2:C:502[B]:HEM:CMB	2:C:502[B]:HEM:HBB2	2.42	0.49
2:B:502[B]:HEM:HBC2	2:B:502[B]:HEM:HMC1	1.94	0.49
2:B:501[A]:HEM:HBB2	2:B:501[A]:HEM:CMB	2.42	0.49
2:D:501[A]:HEM:CMC	2:D:501[A]:HEM:HBC2	2.42	0.49
1:B:452:ASN:HD21	1:B:454:LYS:HB2	1.78	0.48
1:B:336:ARG:HG2	2:B:502[B]:HEM:C2C	2.49	0.48
1:C:199:VAL:HG11	2:C:502[B]:HEM:CBB	2.44	0.48
2:D:501[A]:HEM:HMB2	2:D:501[A]:HEM:CBB	2.44	0.47
1:B:452:ASN:ND2	1:B:455:THR:H	2.06	0.47
2:D:502[B]:HEM:CMC	2:D:502[B]:HEM:CBC	2.90	0.47
1:A:393:PRO:HB2	1:C:9[B]:LEU:CD2	2.44	0.47
1:B:272:ASP:HB2	6:B:915:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:HIS:HD2	6:D:995:HOH:O	1.92	0.46
2:D:502[B]:HEM:CBC	2:D:502[B]:HEM:HMC1	2.46	0.46
1:C:336:ARG:HG2	2:C:502[B]:HEM:C2C	2.51	0.46
2:D:501[A]:HEM:CMB	2:D:501[A]:HEM:CBB	2.94	0.46
1:C:240:PHE:C	1:C:241:GLN:HG3	2.22	0.45
2:A:501[A]:HEM:CMC	2:A:501[A]:HEM:CBC	2.95	0.45
1:B:84:GLU:OE1	6:B:996:HOH:O	2.21	0.45
1:A:84:GLU:OE1	6:A:983:HOH:O	2.21	0.44
1:D:340:TYR:HB2	1:D:341:PRO:HD3	1.99	0.44
1:A:72:SER:HB3	1:A:84:GLU:HA	2.00	0.44
1:D:57:HIS:HA	1:D:97:THR:O	2.18	0.44
1:A:57:HIS:HA	1:A:97:THR:O	2.17	0.44
1:B:334:GLN:HG3	6:C:704:HOH:O	2.17	0.44
1:B:156:THR:HG22	1:C:248:TYR:CZ	2.53	0.44
1:C:230:GLU:H	1:C:230:GLU:CD	2.21	0.43
1:A:230:GLU:H	1:A:230:GLU:CD	2.20	0.43
2:B:501[A]:HEM:HMC2	2:B:501[A]:HEM:CBC	2.49	0.43
2:B:502[B]:HEM:HMC1	2:B:502[B]:HEM:CBC	2.50	0.42
1:A:346:HIS:CE1	6:D:911:HOH:O	2.57	0.42
1:C:70:GLU:O	1:C:85:GLU:HG3	2.19	0.42
1:D:321:LEU:HD12	6:D:841:HOH:O	2.18	0.42
2:C:502[B]:HEM:CMC	2:C:502[B]:HEM:HBC2	2.50	0.42
1:A:271:TYR:CD1	1:A:278:PRO:HD2	2.55	0.42
1:D:75:LYS:HG2	1:D:76:HIS:CE1	2.55	0.42
1:C:57:HIS:HA	1:C:97:THR:O	2.19	0.42
1:B:287:GLU:HG2	1:B:292:LEU:HD21	2.02	0.41
1:A:57:HIS:CE1	1:A:98:VAL:HG22	2.56	0.41
1:D:134[B]:ILE:H	1:D:134[B]:ILE:HD13	1.84	0.41
2:D:501[A]:HEM:HBC2	2:D:501[A]:HEM:HMC2	2.02	0.41
1:A:237:ALA:HB2	1:D:237:ALA:HB2	2.03	0.41
1:C:57:HIS:CD2	2:C:501[A]:HEM:C4D	3.09	0.41
1:D:199:VAL:HG11	2:D:502[B]:HEM:CBB	2.50	0.41
1:A:412[A]:VAL:HG13	1:B:403:GLU:OE2	2.21	0.41
2:B:502[B]:HEM:CMC	2:B:502[B]:HEM:CBC	2.96	0.41
1:B:340:TYR:HB2	1:B:341:PRO:HD3	2.02	0.41
1:B:230:GLU:O	1:B:234:GLU:HG3	2.21	0.41
1:D:57:HIS:CD2	2:D:501[A]:HEM:C4D	3.09	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:GLU:OE1	1:C:417:GLU:OE2[1_455]	1.96	0.24
1:D:234:GLU:OE2	6:B:886:HOH:O[2_655]	2.08	0.12
1:A:417:GLU:OE2	1:D:273:GLU:OE1[1_455]	2.16	0.04

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	483/491 (98%)	469 (97%)	14 (3%)	0	100	100
1	B	483/491 (98%)	470 (97%)	13 (3%)	0	100	100
1	C	484/491 (99%)	469 (97%)	15 (3%)	0	100	100
1	D	484/491 (99%)	468 (97%)	15 (3%)	1 (0%)	47	28
All	All	1934/1964 (98%)	1876 (97%)	57 (3%)	1 (0%)	51	31

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	426/432 (99%)	416 (98%)	10 (2%)	50	25
1	B	426/432 (99%)	412 (97%)	14 (3%)	38	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	427/432 (99%)	418 (98%)	9 (2%)	53	29
1	D	427/432 (99%)	416 (97%)	11 (3%)	46	21
All	All	1706/1728 (99%)	1662 (97%)	44 (3%)	46	21

All (44) 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	401	GLU
1	A	409	ASP
1	A	420	ASN
1	A	447	ASP
1	A	474	LEU
1	B	110	ASP
1	B	114	PHE
1	B	120	THR
1	B	219	ARG
1	B	241	GLN
1	B	401	GLU
1	B	409	ASP
1	B	420	ASN
1	B	440	LEU
1	B	447	ASP
1	B	454	LYS
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	225	ARG
1	C	241	GLN
1	C	401	GLU
1	C	420	ASN
1	C	447	ASP
1	C	485	TYR
1	D	75	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	110	ASP
1	D	114	PHE
1	D	120	THR
1	D	234	GLU
1	D	241	GLN
1	D	409	ASP
1	D	447	ASP
1	D	470	TYR
1	D	474	LEU
1	D	485	TYR

Sometimes 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
1	A	100	HIS
1	A	157	ASN
1	A	226	ASN
1	A	346	HIS
1	A	367	ASN
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	28	HIS
1	D	100	HIS
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 monosaccharides 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	$\#\|Z\| > 2$
5	ACT	A	506	-	3,3,3	0.60	0	3,3,3	1.59	1 (33%)
2	HEM	D	501[A]	1,6	41,50,50	1.28	7 (17%)	45,82,82	2.29	17 (37%)
5	ACT	C	504	-	3,3,3	0.92	0	3,3,3	0.30	0
2	HEM	D	502[B]	1	41,50,50	1.63	8 (19%)	45,82,82	2.27	12 (26%)
2	HEM	B	501[A]	1,6	41,50,50	1.72	12 (29%)	45,82,82	2.40	14 (31%)
2	HEM	A	502[B]	1	41,50,50	1.46	9 (21%)	45,82,82	2.06	15 (33%)
2	HEM	C	501[A]	1,6	41,50,50	1.36	6 (14%)	45,82,82	2.65	18 (40%)
2	HEM	C	502[B]	1,6	41,50,50	1.61	6 (14%)	45,82,82	2.49	17 (37%)
5	ACT	D	505	-	3,3,3	0.79	0	3,3,3	0.49	0
2	HEM	A	501[A]	1	41,50,50	1.38	6 (14%)	45,82,82	2.65	18 (40%)
5	ACT	B	505	-	3,3,3	0.68	0	3,3,3	1.17	0
2	HEM	B	502[B]	1,6	41,50,50	1.46	7 (17%)	45,82,82	2.34	17 (37%)

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	501[A]	1,6	-	2/12/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	502[B]	1	-	2/12/54/54	-
2	HEM	B	501[A]	1,6	-	2/12/54/54	-
2	HEM	A	502[B]	1	-	2/12/54/54	-
2	HEM	C	501[A]	1,6	-	2/12/54/54	-
2	HEM	C	502[B]	1,6	-	4/12/54/54	-
2	HEM	A	501[A]	1	-	2/12/54/54	-
2	HEM	B	502[B]	1,6	-	3/12/54/54	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502[B]	HEM	C1B-NB	-5.05	1.31	1.40
2	B	502[B]	HEM	C1B-NB	-4.55	1.32	1.40
2	D	502[B]	HEM	C1B-NB	-4.09	1.33	1.40
2	A	502[B]	HEM	C1B-NB	-3.98	1.33	1.40
2	D	502[B]	HEM	CHB-C1B	3.84	1.44	1.35
2	C	502[B]	HEM	C4D-ND	-3.78	1.33	1.40
2	D	502[B]	HEM	C4D-C3D	3.76	1.51	1.45
2	B	501[A]	HEM	C1B-NB	-3.69	1.33	1.40
2	D	502[B]	HEM	C3C-C2C	-3.51	1.35	1.40
2	C	502[B]	HEM	CHB-C1B	3.50	1.43	1.35
2	B	501[A]	HEM	C1D-C2D	3.50	1.51	1.44
2	C	501[A]	HEM	C1B-NB	-3.49	1.34	1.40
2	B	502[B]	HEM	C4D-ND	-3.10	1.35	1.40
2	A	501[A]	HEM	C1B-NB	-3.05	1.35	1.40
2	A	501[A]	HEM	CHB-C1B	3.04	1.42	1.35
2	D	501[A]	HEM	C1B-NB	-2.99	1.35	1.40
2	B	501[A]	HEM	C4B-NB	-2.99	1.32	1.38
2	C	501[A]	HEM	CHB-C1B	2.98	1.42	1.35
2	A	502[B]	HEM	C4D-C3D	2.93	1.50	1.45
2	D	502[B]	HEM	C1A-NA	2.92	1.42	1.36
2	B	501[A]	HEM	CAA-C2A	-2.80	1.47	1.52
2	A	501[A]	HEM	C3C-C2C	-2.77	1.36	1.40
2	B	501[A]	HEM	C4D-C3D	2.70	1.49	1.45
2	A	502[B]	HEM	C1B-C2B	-2.68	1.39	1.44
2	A	502[B]	HEM	CHB-C1B	2.67	1.41	1.35
2	A	501[A]	HEM	C1D-ND	-2.67	1.33	1.38
2	D	501[A]	HEM	CHB-C1B	2.60	1.41	1.35
2	B	501[A]	HEM	C4D-ND	-2.59	1.35	1.40
2	D	502[B]	HEM	C3B-C4B	2.58	1.50	1.44
2	B	502[B]	HEM	C1D-C2D	2.56	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502[B]	HEM	CHA-C4D	2.55	1.41	1.35
2	B	502[B]	HEM	FE-NB	2.54	2.09	1.96
2	B	502[B]	HEM	CAA-C2A	2.48	1.55	1.52
2	D	501[A]	HEM	C4B-NB	-2.46	1.33	1.38
2	C	502[B]	HEM	FE-NB	2.45	2.09	1.96
2	D	501[A]	HEM	C1D-ND	-2.43	1.33	1.38
2	A	501[A]	HEM	C3C-CAC	-2.42	1.42	1.47
2	C	502[B]	HEM	C4D-C3D	2.36	1.49	1.45
2	A	502[B]	HEM	FE-NB	2.35	2.08	1.96
2	B	502[B]	HEM	C4B-NB	-2.35	1.34	1.38
2	D	502[B]	HEM	C4D-ND	-2.35	1.36	1.40
2	C	501[A]	HEM	C4A-NA	2.32	1.40	1.36
2	A	501[A]	HEM	FE-NB	2.31	2.08	1.96
2	B	501[A]	HEM	FE-NB	2.28	2.08	1.96
2	B	501[A]	HEM	CBD-CGD	2.23	1.55	1.50
2	B	501[A]	HEM	O2D-CGD	-2.23	1.23	1.30
2	B	501[A]	HEM	CHB-C1B	2.20	1.40	1.35
2	B	501[A]	HEM	CHA-C4D	2.20	1.40	1.35
2	D	501[A]	HEM	FE-NB	2.13	2.07	1.96
2	D	502[B]	HEM	FE-NB	2.13	2.07	1.96
2	C	502[B]	HEM	CAA-C2A	2.09	1.55	1.52
2	B	501[A]	HEM	C3C-C2C	-2.09	1.37	1.40
2	A	502[B]	HEM	O1A-CGA	2.08	1.29	1.22
2	D	501[A]	HEM	C4D-C3D	2.08	1.48	1.45
2	B	502[B]	HEM	CBD-CAD	2.08	1.58	1.52
2	D	501[A]	HEM	O2D-CGD	-2.08	1.23	1.30
2	C	501[A]	HEM	CAD-C3D	2.08	1.56	1.51
2	C	501[A]	HEM	C4B-NB	-2.08	1.34	1.38
2	A	502[B]	HEM	C1D-C2D	2.07	1.48	1.44
2	C	501[A]	HEM	FE-NB	2.04	2.07	1.96
2	A	502[B]	HEM	C1A-NA	2.00	1.40	1.36

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501[A]	HEM	C1B-NB-C4B	8.20	113.55	105.07
2	A	501[A]	HEM	C1B-NB-C4B	7.63	112.96	105.07
2	C	501[A]	HEM	CHC-C4B-NB	6.97	132.00	124.43
2	C	501[A]	HEM	C1B-NB-C4B	6.94	112.24	105.07
2	B	501[A]	HEM	CHC-C4B-NB	6.64	131.65	124.43
2	A	501[A]	HEM	CHC-C4B-NB	6.60	131.60	124.43
2	D	501[A]	HEM	CHC-C4B-NB	6.58	131.58	124.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502[B]	HEM	CHC-C4B-NB	6.57	131.57	124.43
2	C	502[B]	HEM	C1B-NB-C4B	6.44	111.72	105.07
2	C	501[A]	HEM	CAD-C3D-C4D	6.38	135.80	124.66
2	D	501[A]	HEM	C1B-NB-C4B	6.02	111.29	105.07
2	B	502[B]	HEM	C1B-NB-C4B	5.81	111.08	105.07
2	D	502[B]	HEM	C1B-NB-C4B	5.75	111.01	105.07
2	B	502[B]	HEM	CHC-C4B-NB	5.69	130.61	124.43
2	A	501[A]	HEM	CHB-C1B-NB	5.69	131.41	124.38
2	D	502[B]	HEM	C4A-C3A-C2A	5.48	110.81	107.00
2	C	502[B]	HEM	CHD-C1D-C2D	-5.28	116.74	124.98
2	C	502[B]	HEM	CMA-C3A-C4A	-5.22	120.44	128.46
2	C	502[B]	HEM	CHD-C1D-ND	5.08	129.95	124.43
2	C	502[B]	HEM	CHC-C4B-NB	4.97	129.83	124.43
2	C	502[B]	HEM	C4A-C3A-C2A	4.85	110.37	107.00
2	A	501[A]	HEM	CMA-C3A-C4A	-4.71	121.23	128.46
2	D	502[B]	HEM	CHD-C1D-C2D	-4.69	117.65	124.98
2	D	502[B]	HEM	CHD-C1D-ND	4.56	129.39	124.43
2	C	501[A]	HEM	CHB-C1B-NB	4.53	129.98	124.38
2	A	501[A]	HEM	CAD-CBD-CGD	-4.39	104.16	113.60
2	A	502[B]	HEM	C1B-NB-C4B	4.31	109.53	105.07
2	D	501[A]	HEM	C2C-C3C-C4C	4.25	109.86	106.90
2	A	502[B]	HEM	C4A-C3A-C2A	4.21	109.93	107.00
2	B	501[A]	HEM	CHD-C1D-ND	4.11	128.89	124.43
2	C	501[A]	HEM	CHD-C1D-ND	4.07	128.85	124.43
2	B	501[A]	HEM	C4A-C3A-C2A	-4.00	104.21	107.00
2	A	501[A]	HEM	CBA-CAA-C2A	-4.00	105.80	112.62
2	C	501[A]	HEM	CAD-C3D-C2D	-3.92	120.57	127.88
2	D	501[A]	HEM	CMD-C2D-C1D	3.84	130.89	125.04
2	A	502[B]	HEM	CMC-C2C-C3C	3.80	131.79	124.68
2	C	501[A]	HEM	C3B-C2B-C1B	3.79	109.30	106.49
2	A	502[B]	HEM	C2D-C1D-ND	3.76	114.39	109.88
2	A	501[A]	HEM	CHD-C1D-ND	3.72	128.47	124.43
2	A	501[A]	HEM	CMA-C3A-C2A	3.68	131.88	124.94
2	A	502[B]	HEM	CHC-C4B-NB	3.67	128.42	124.43
2	A	502[B]	HEM	C4D-ND-C1D	-3.65	101.31	105.07
2	B	501[A]	HEM	CHB-C1B-NB	3.65	128.89	124.38
2	B	501[A]	HEM	CHA-C4D-ND	3.44	128.63	124.38
2	B	502[B]	HEM	O2D-CGD-CBD	3.43	125.06	114.03
2	D	501[A]	HEM	CHA-C4D-ND	3.43	128.62	124.38
2	B	501[A]	HEM	CAD-C3D-C4D	3.41	130.61	124.66
2	A	501[A]	HEM	C2C-C3C-C4C	3.40	109.27	106.90
2	B	501[A]	HEM	CHA-C4D-C3D	-3.38	118.99	125.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501[A]	HEM	CHA-C4D-ND	3.37	128.55	124.38
2	B	502[B]	HEM	C2C-C3C-C4C	3.30	109.20	106.90
2	A	502[B]	HEM	CHD-C1D-C2D	-3.27	119.87	124.98
2	B	502[B]	HEM	CAD-CBD-CGD	3.27	120.64	113.60
2	B	502[B]	HEM	C4A-C3A-C2A	3.21	109.23	107.00
2	B	502[B]	HEM	C3C-C4C-NC	-3.17	104.97	110.94
2	D	501[A]	HEM	CBA-CAA-C2A	-3.14	107.25	112.62
2	C	501[A]	HEM	C2B-C1B-NB	-3.13	106.13	109.84
2	B	502[B]	HEM	CHA-C4D-C3D	-3.11	119.48	125.33
2	C	501[A]	HEM	O2D-CGD-CBD	3.10	124.00	114.03
2	A	502[B]	HEM	CMA-C3A-C4A	-3.08	123.74	128.46
2	C	502[B]	HEM	C2C-C3C-C4C	3.00	108.99	106.90
2	B	502[B]	HEM	C1D-C2D-C3D	-2.99	103.81	106.96
2	D	501[A]	HEM	CHB-C1B-NB	2.98	128.06	124.38
2	C	501[A]	HEM	CHA-C4D-C3D	-2.94	119.80	125.33
2	D	501[A]	HEM	O2A-CGA-CBA	2.93	123.44	114.03
2	D	502[B]	HEM	O2D-CGD-CBD	2.90	123.36	114.03
2	D	501[A]	HEM	CAD-C3D-C4D	2.87	129.68	124.66
2	C	502[B]	HEM	C2D-C1D-ND	2.84	113.29	109.88
2	A	502[B]	HEM	C3D-C4D-ND	2.81	113.29	110.17
2	C	501[A]	HEM	C2C-C3C-C4C	2.80	108.85	106.90
2	C	502[B]	HEM	CMD-C2D-C3D	2.77	133.64	126.12
2	D	502[B]	HEM	CMA-C3A-C2A	-2.76	119.73	124.94
2	B	502[B]	HEM	CAA-CBA-CGA	-2.76	106.02	113.76
2	B	501[A]	HEM	O2D-CGD-CBD	2.74	122.82	114.03
2	B	502[B]	HEM	C2D-C1D-ND	2.71	113.13	109.88
2	C	501[A]	HEM	O1D-CGD-CBD	-2.69	114.44	123.08
2	A	501[A]	HEM	C2B-C1B-NB	-2.66	106.69	109.84
2	D	501[A]	HEM	CHA-C4D-C3D	-2.64	120.36	125.33
2	D	502[B]	HEM	C3B-C2B-C1B	2.61	108.42	106.49
2	B	502[B]	HEM	CHA-C4D-ND	2.60	127.59	124.38
2	C	501[A]	HEM	C1D-C2D-C3D	2.58	109.67	106.96
2	C	501[A]	HEM	CBA-CAA-C2A	-2.57	108.24	112.62
2	B	501[A]	HEM	CAD-CBD-CGD	-2.55	108.11	113.60
2	D	502[B]	HEM	C2D-C1D-ND	2.55	112.94	109.88
2	D	502[B]	HEM	CAA-CBA-CGA	-2.54	106.64	113.76
2	C	502[B]	HEM	CMD-C2D-C1D	-2.50	121.23	125.04
2	B	502[B]	HEM	C3D-C4D-ND	2.48	112.93	110.17
2	A	501[A]	HEM	CHA-C4D-ND	2.48	127.44	124.38
2	C	502[B]	HEM	CBD-CAD-C3D	-2.46	105.78	112.63
2	D	501[A]	HEM	CMB-C2B-C1B	2.46	128.78	125.04
2	C	502[B]	HEM	C4C-CHD-C1D	-2.46	119.31	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501[A]	HEM	CMC-C2C-C3C	2.45	129.27	124.68
2	C	501[A]	HEM	CHD-C1D-C2D	-2.45	121.15	124.98
2	A	502[B]	HEM	C3C-C4C-NC	-2.44	106.33	110.94
2	A	501[A]	HEM	O2D-CGD-CBD	2.44	121.87	114.03
2	A	501[A]	HEM	CHD-C1D-C2D	-2.41	121.21	124.98
2	A	502[B]	HEM	C4B-C3B-C2B	-2.41	105.20	107.11
2	B	502[B]	HEM	C4C-CHD-C1D	2.39	125.72	122.56
2	A	502[B]	HEM	O2A-CGA-CBA	2.39	121.72	114.03
2	B	502[B]	HEM	CMB-C2B-C1B	-2.39	121.40	125.04
2	D	501[A]	HEM	O2D-CGD-CBD	2.34	121.56	114.03
2	C	501[A]	HEM	C4D-C3D-C2D	-2.33	103.50	106.90
2	A	501[A]	HEM	CBD-CAD-C3D	-2.32	106.17	112.63
2	C	502[B]	HEM	CMC-C2C-C3C	2.31	129.00	124.68
2	B	501[A]	HEM	O2D-CGD-O1D	-2.31	117.54	123.30
2	A	501[A]	HEM	O2A-CGA-CBA	2.30	121.44	114.03
2	B	502[B]	HEM	CHB-C1B-NB	2.28	127.20	124.38
2	A	502[B]	HEM	CAA-CBA-CGA	-2.28	107.36	113.76
2	A	501[A]	HEM	C3C-C4C-NC	-2.28	106.65	110.94
2	A	501[A]	HEM	CHA-C4D-C3D	-2.24	121.13	125.33
2	D	502[B]	HEM	C4B-C3B-C2B	-2.23	105.35	107.11
2	D	502[B]	HEM	O2D-CGD-O1D	-2.21	117.78	123.30
2	C	502[B]	HEM	CMA-C3A-C2A	2.21	129.11	124.94
2	B	502[B]	HEM	O2D-CGD-O1D	-2.19	117.83	123.30
2	C	502[B]	HEM	C3D-C4D-ND	2.18	112.59	110.17
2	C	502[B]	HEM	CAA-CBA-CGA	-2.17	107.68	113.76
2	D	501[A]	HEM	CHD-C1D-ND	2.16	126.78	124.43
5	A	506	ACT	OXT-C-CH3	2.15	124.05	115.18
2	D	501[A]	HEM	CHD-C1D-C2D	-2.12	121.66	124.98
2	D	501[A]	HEM	C2B-C1B-NB	-2.12	107.33	109.84
2	B	501[A]	HEM	CHD-C1D-C2D	-2.12	121.67	124.98
2	B	501[A]	HEM	CBA-CAA-C2A	-2.06	109.10	112.62
2	D	501[A]	HEM	O2A-CGA-O1A	-2.04	118.21	123.30
2	B	501[A]	HEM	C3B-C2B-C1B	-2.04	104.98	106.49
2	C	502[B]	HEM	CAA-C2A-C3A	-2.03	121.42	127.25
2	A	502[B]	HEM	O2D-CGD-CBD	2.01	120.47	114.03
2	C	501[A]	HEM	O2A-CGA-CBA	2.01	120.47	114.03
2	A	502[B]	HEM	CMB-C2B-C1B	-2.00	121.99	125.04
2	D	501[A]	HEM	CMB-C2B-C3B	-2.00	123.40	128.30

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	502[B]	HEM	CAA-CBA-CGA-O2A
2	C	502[B]	HEM	CAA-CBA-CGA-O1A
2	B	501[A]	HEM	CAD-CBD-CGD-O2D
2	A	502[B]	HEM	CAA-CBA-CGA-O1A
2	D	502[B]	HEM	CAA-CBA-CGA-O2A
2	B	501[A]	HEM	CAD-CBD-CGD-O1D
2	B	502[B]	HEM	CAA-CBA-CGA-O2A
2	D	502[B]	HEM	CAA-CBA-CGA-O1A
2	A	502[B]	HEM	CAA-CBA-CGA-O2A
2	B	502[B]	HEM	CAA-CBA-CGA-O1A
2	A	501[A]	HEM	CAD-CBD-CGD-O1D
2	A	501[A]	HEM	CAD-CBD-CGD-O2D
2	C	501[A]	HEM	CAD-CBD-CGD-O2D
2	D	501[A]	HEM	CAD-CBD-CGD-O2D
2	D	501[A]	HEM	CAD-CBD-CGD-O1D
2	C	501[A]	HEM	CAD-CBD-CGD-O1D
2	C	502[B]	HEM	CAD-CBD-CGD-O2D
2	B	502[B]	HEM	CAD-CBD-CGD-O2D
2	C	502[B]	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

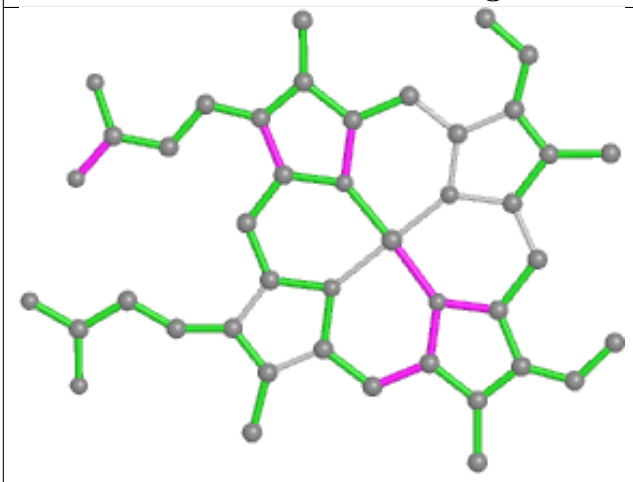
8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501[A]	HEM	8	0
2	D	502[B]	HEM	4	0
2	B	501[A]	HEM	6	0
2	A	502[B]	HEM	1	0
2	C	501[A]	HEM	7	0
2	C	502[B]	HEM	5	0
2	A	501[A]	HEM	4	0
2	B	502[B]	HEM	5	0

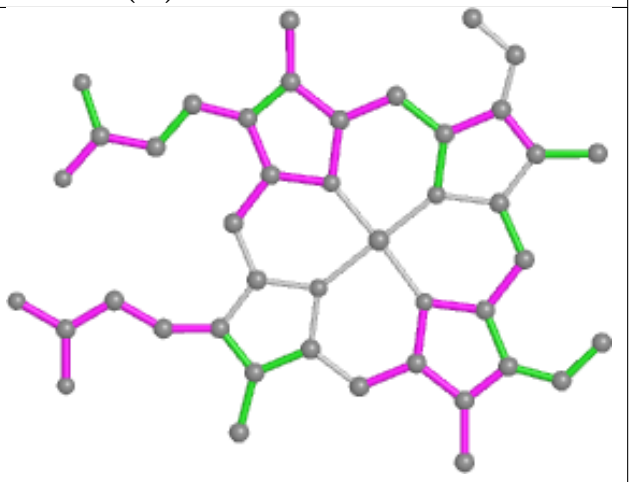
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

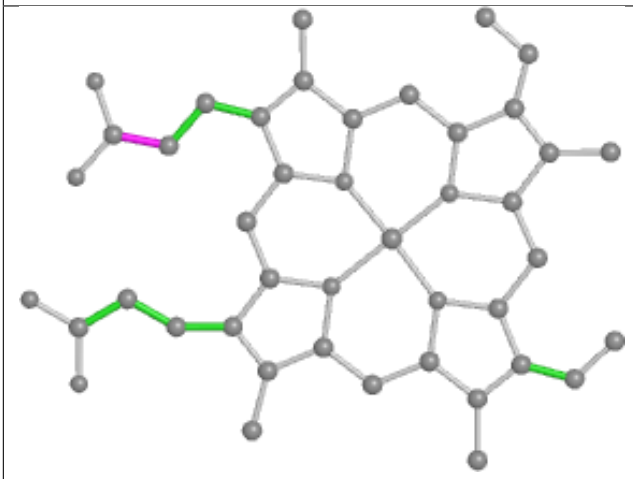
Ligand HEM D 501 (A)



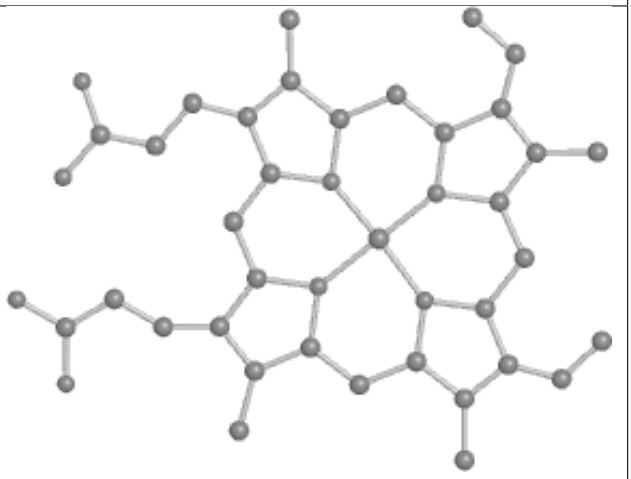
Bond lengths



Bond angles

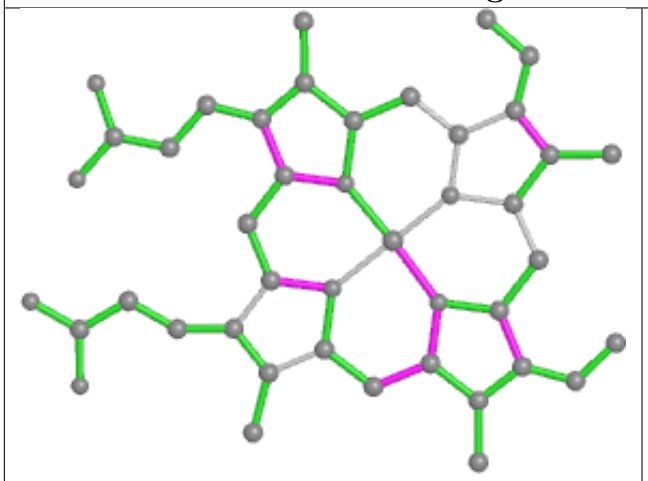


Torsions

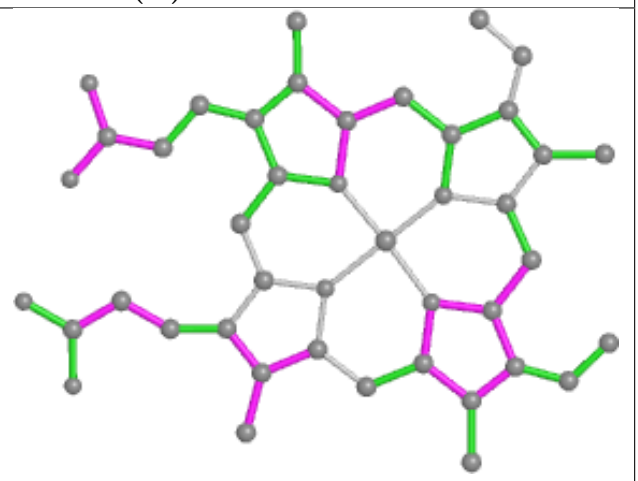


Rings

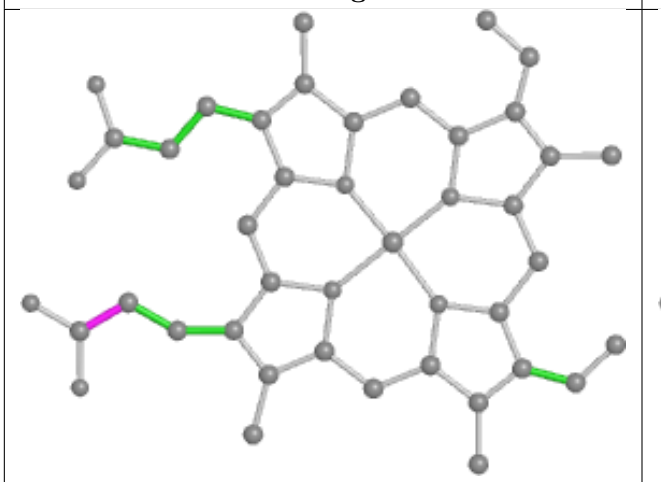
Ligand HEM D 502 (B)



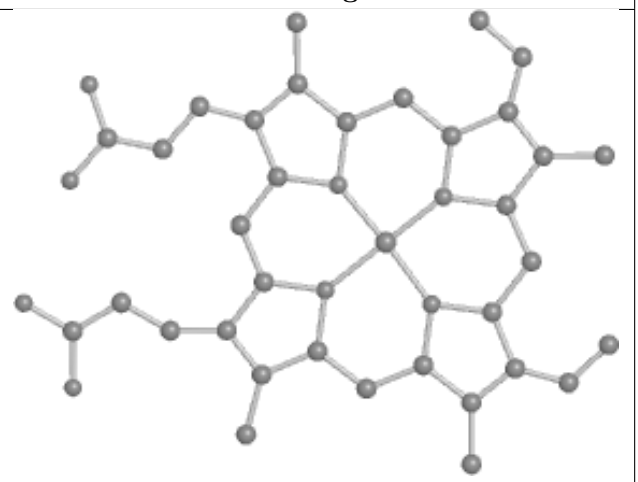
Bond lengths



Bond angles

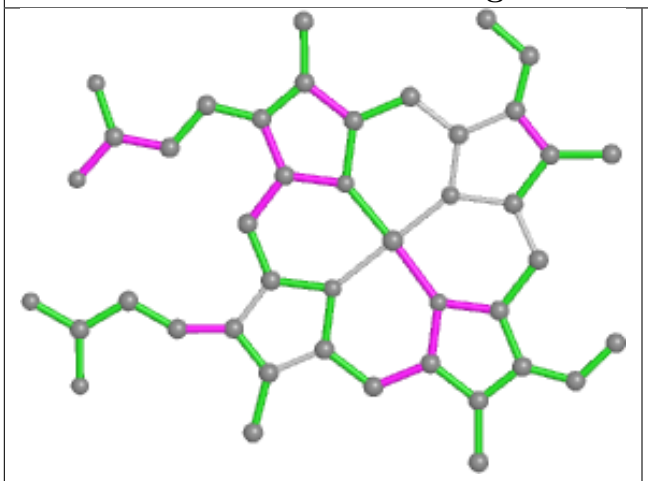


Torsions

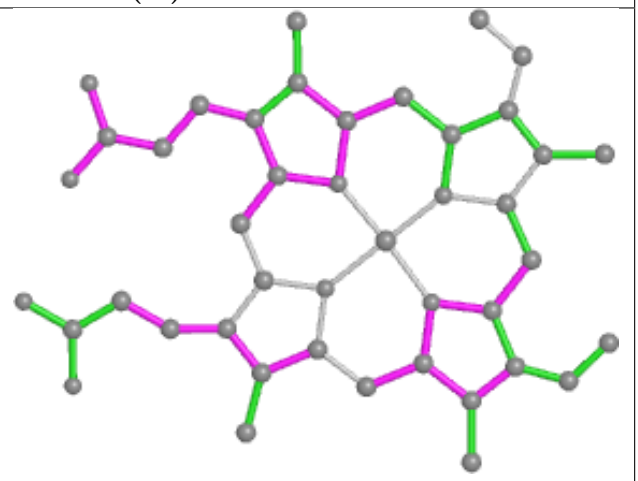


Rings

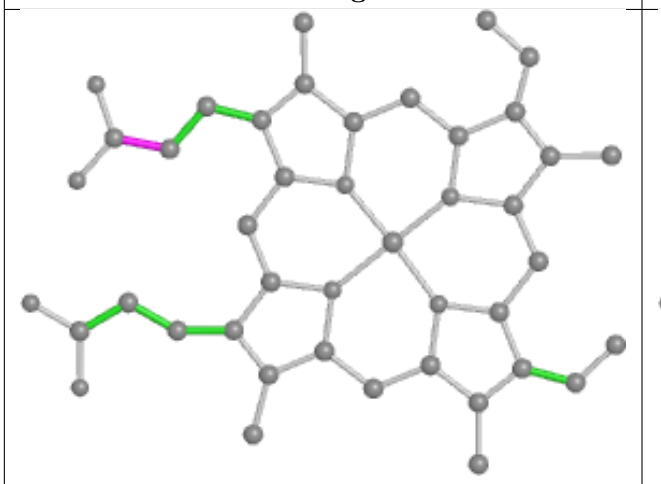
Ligand HEM B 501 (A)



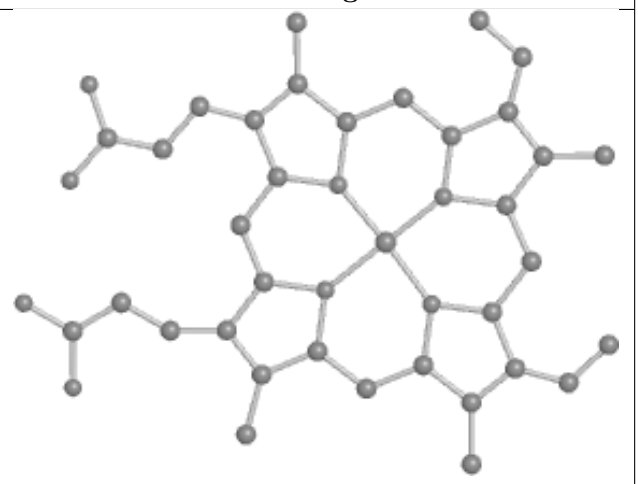
Bond lengths



Bond angles

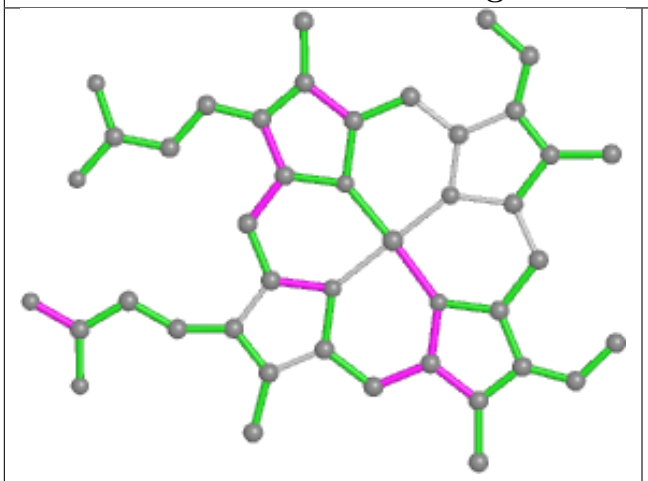


Torsions

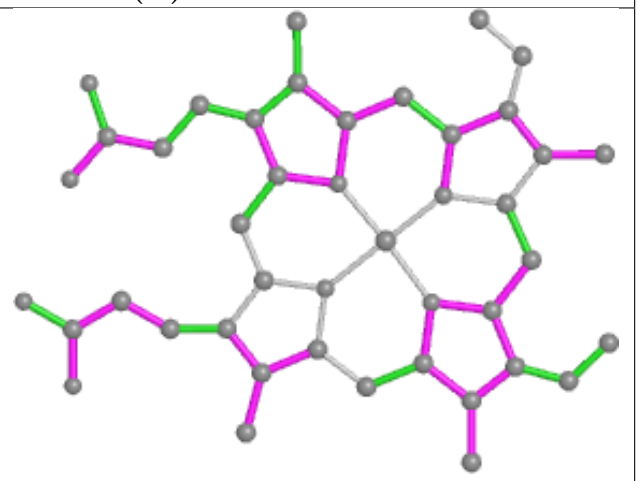


Rings

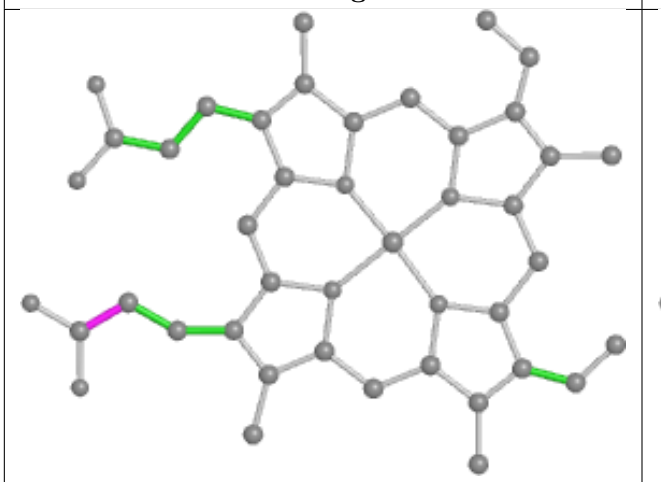
Ligand HEM A 502 (B)



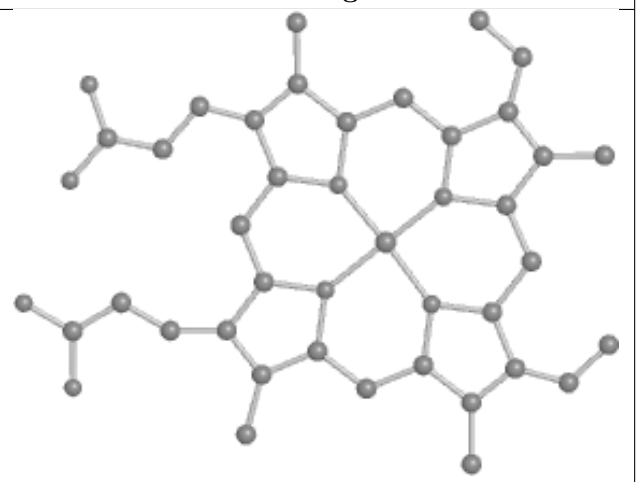
Bond lengths



Bond angles

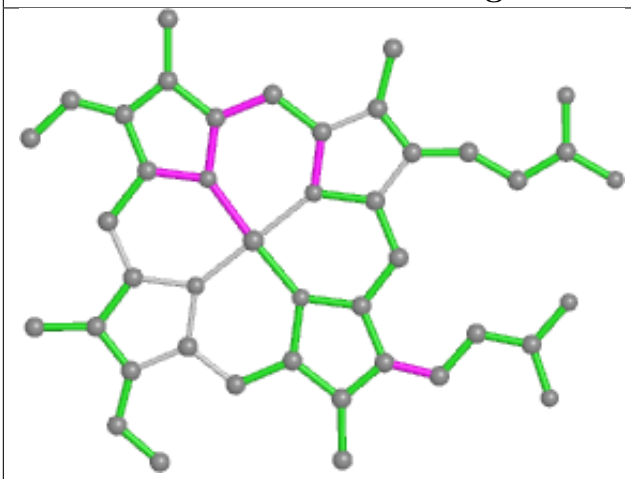


Torsions

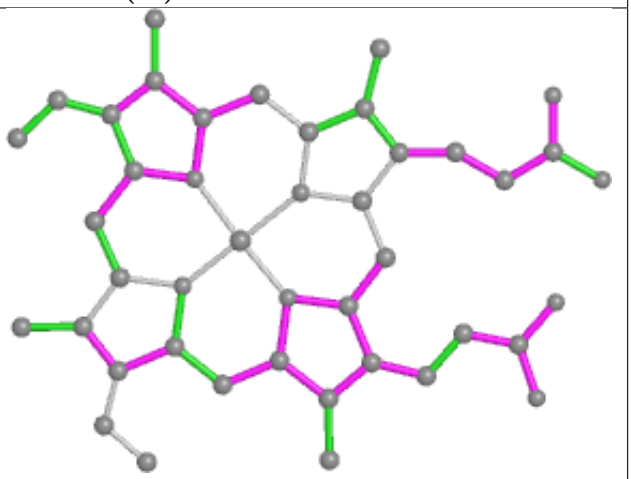


Rings

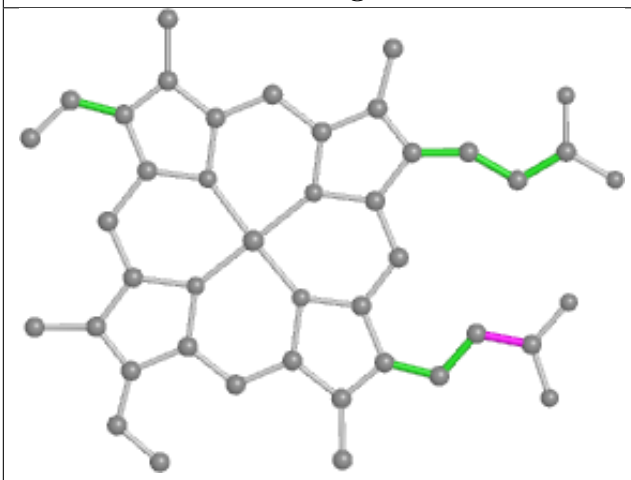
Ligand HEM C 501 (A)



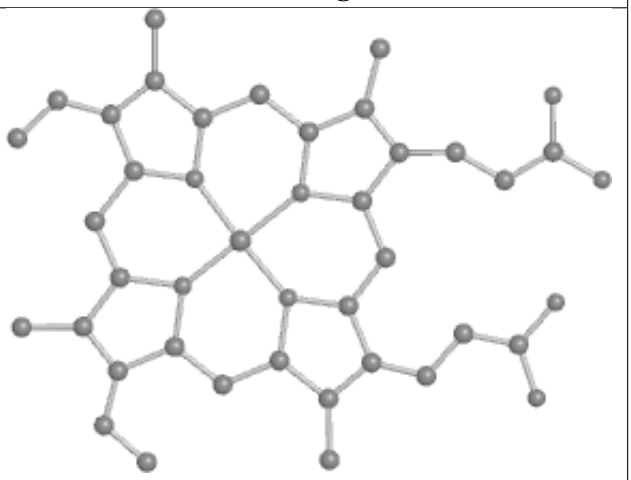
Bond lengths



Bond angles

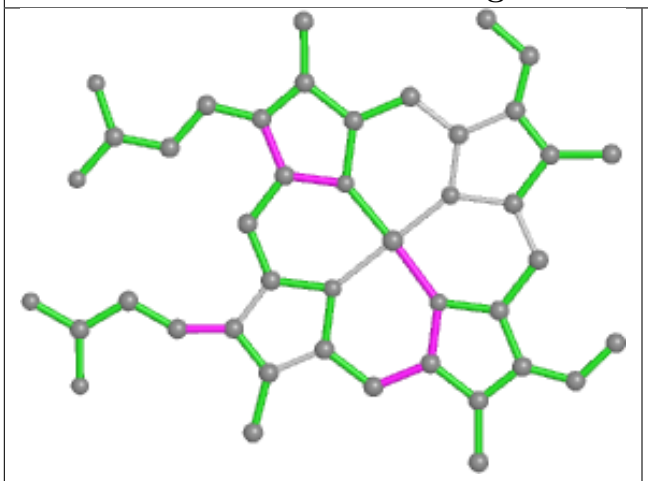


Torsions

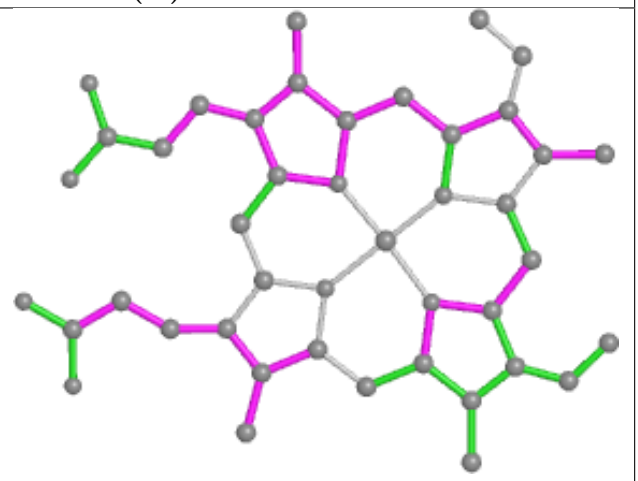


Rings

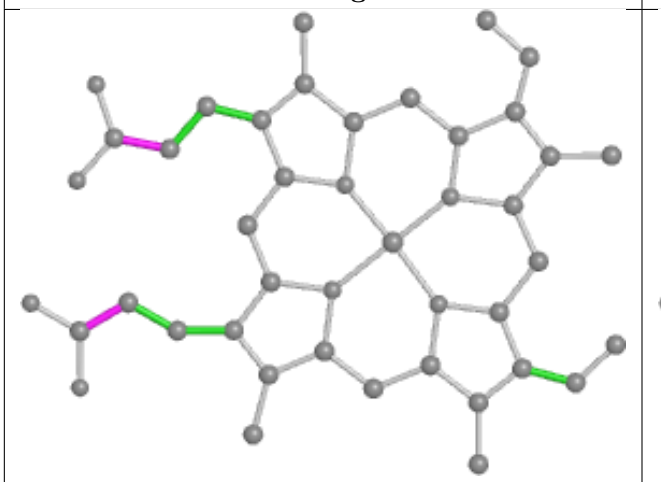
Ligand HEM C 502 (B)



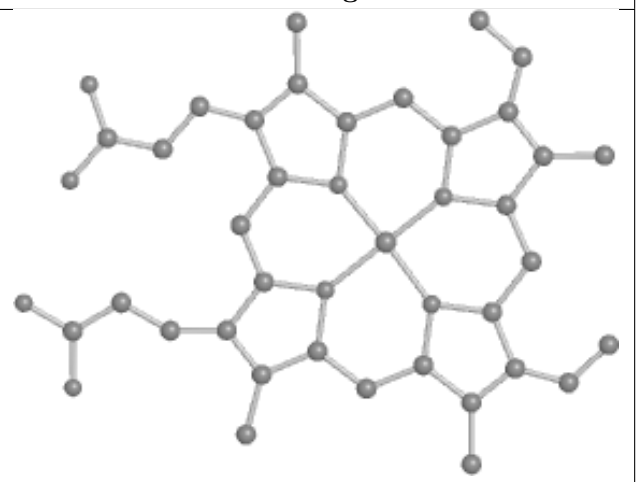
Bond lengths



Bond angles

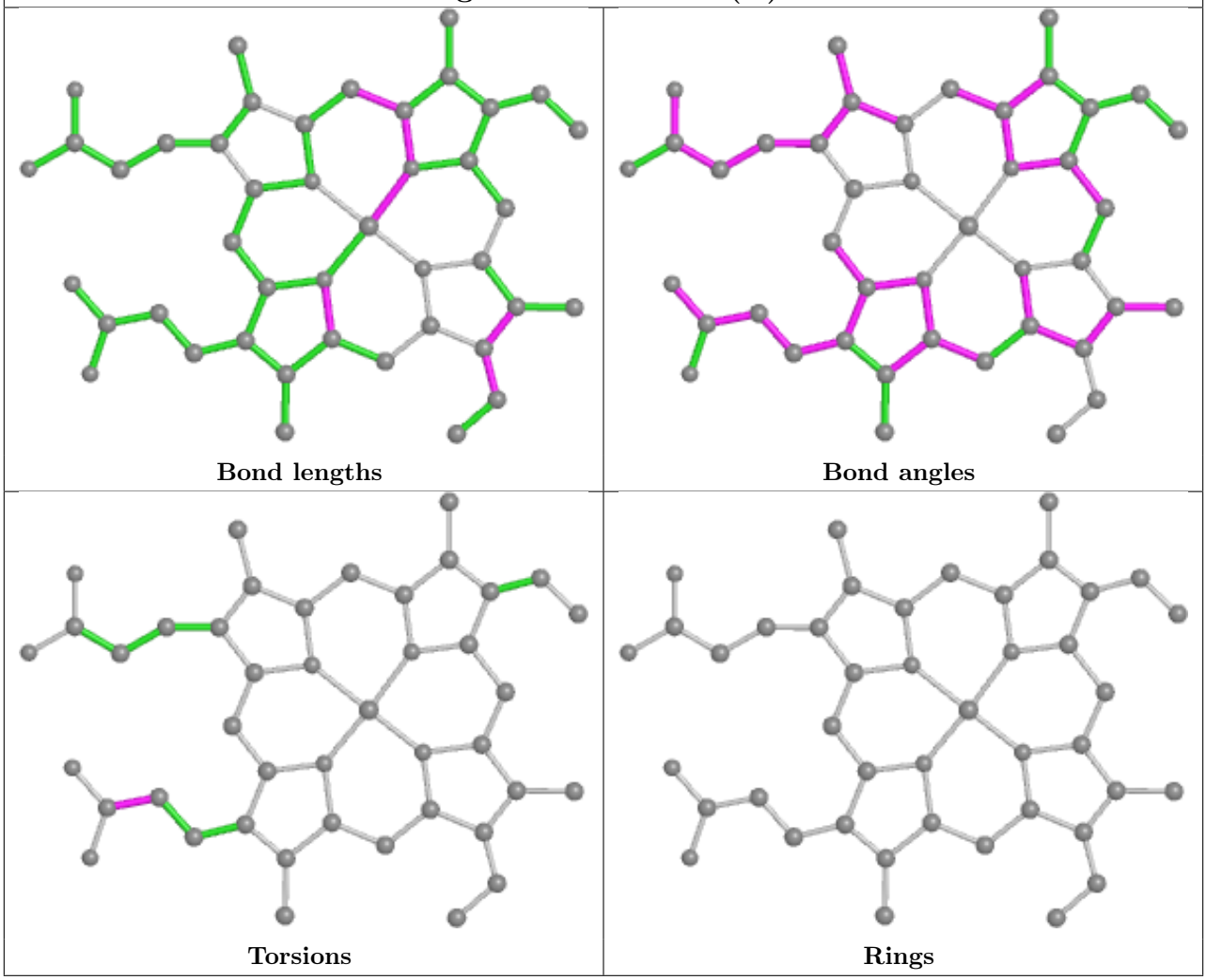


Torsions

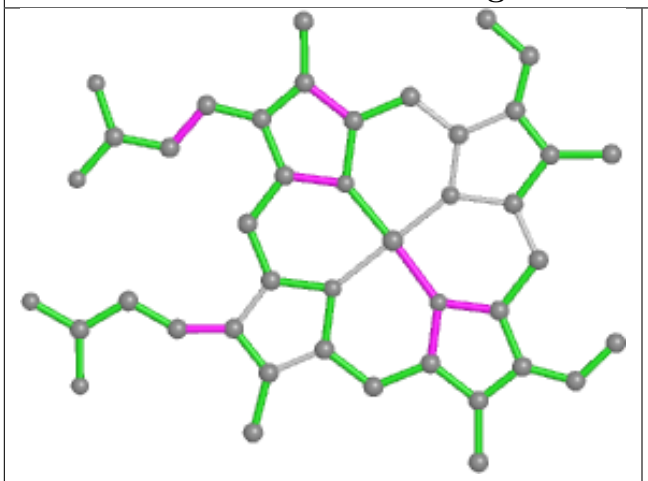


Rings

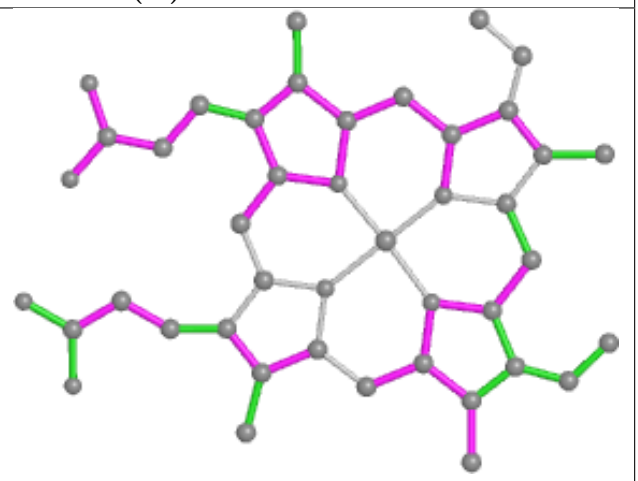
Ligand HEM A 501 (A)



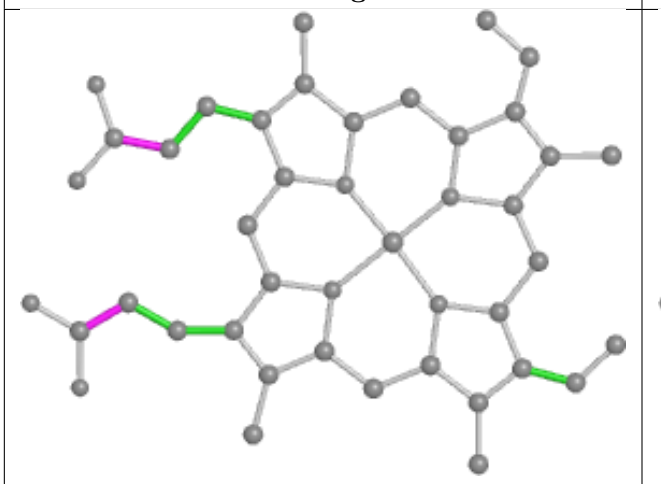
Ligand HEM B 502 (B)



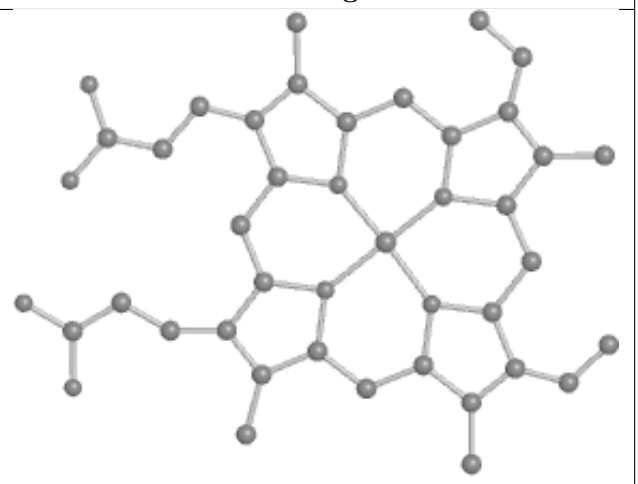
Bond lengths



Bond angles



Torsions



Rings

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%)	-0.13	4 (0%)	86	88	12, 18, 32, 45	0
1	B	480/491 (97%)	-0.16	4 (0%)	86	88	10, 18, 33, 66	0
1	C	480/491 (97%)	-0.16	6 (1%)	77	80	10, 16, 31, 77	0
1	D	480/491 (97%)	-0.02	12 (2%)	57	58	11, 19, 34, 84	0
All	All	1920/1964 (97%)	-0.12	26 (1%)	75	79	10, 18, 33, 84	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	485	TYR	7.8
1	C	485	TYR	7.2
1	C	372[A]	PHE	4.8
1	D	483	ARG	4.7
1	B	485	TYR	4.2
1	C	483	ARG	3.8
1	B	372[A]	PHE	3.7
1	A	372[A]	PHE	3.7
1	A	485	TYR	3.6
1	D	484	SER	3.6
1	D	481	ASP	3.3
1	D	372[A]	PHE	3.2
1	D	482	ILE	3.1
1	D	464	TYR	2.9
1	C	484	SER	2.8
1	D	461	CYS	2.7
1	B	464	TYR	2.6
1	A	484	SER	2.6
1	D	479	GLY	2.5
1	B	484	SER	2.4
1	D	468	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	6	HIS	2.3
1	A	288	GLU	2.2
1	D	480	VAL	2.2
1	C	6	HIS	2.1
1	C	482	ILE	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	C	504	4/4	0.89	0.12	25,26,26,27	0
5	ACT	B	505	4/4	0.90	0.12	28,30,30,31	0
5	ACT	A	506	4/4	0.92	0.09	26,27,29,30	0
5	ACT	D	505	4/4	0.94	0.10	30,34,38,38	0
4	NA	B	504	1/1	0.95	0.04	30,30,30,30	0
2	HEM	B	501[A]	43/43	0.96	0.10	10,13,14,18	43
2	HEM	D	501[A]	43/43	0.97	0.09	12,15,17,20	43
2	HEM	D	502[B]	43/43	0.97	0.09	7,9,10,10	43
4	NA	A	505	1/1	0.97	0.05	15,15,15,15	0
2	HEM	A	502[B]	43/43	0.97	0.09	9,10,11,13	43
2	HEM	A	501[A]	43/43	0.97	0.09	10,11,12,14	43
2	HEM	B	502[B]	43/43	0.97	0.10	8,11,12,12	43
2	HEM	C	501[A]	43/43	0.97	0.10	10,12,14,17	43
2	HEM	C	502[B]	43/43	0.97	0.11	7,8,9,10	43
3	CL	B	503	1/1	0.99	0.06	15,15,15,15	0
3	CL	D	503	1/1	0.99	0.09	21,21,21,21	0
3	CL	A	503	1/1	0.99	0.14	24,24,24,24	0
3	CL	A	504	1/1	0.99	0.04	18,18,18,18	0

Continued on next page...

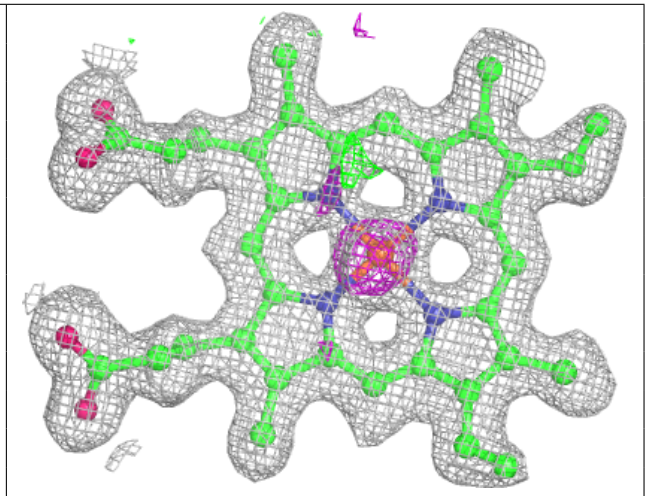
Continued from previous page...

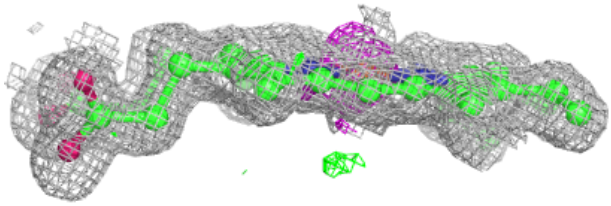
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	C	503	1/1	1.00	0.06	17,17,17,17	0
3	CL	D	504	1/1	1.00	0.04	13,13,13,13	0

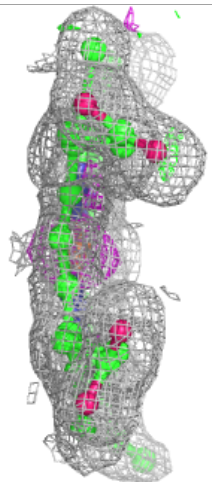
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM 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)

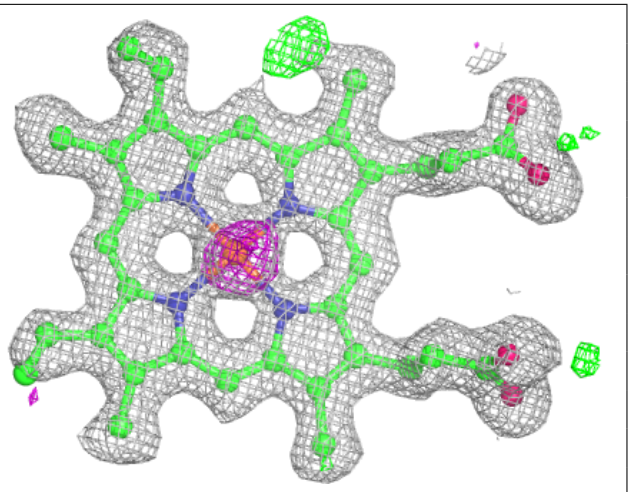


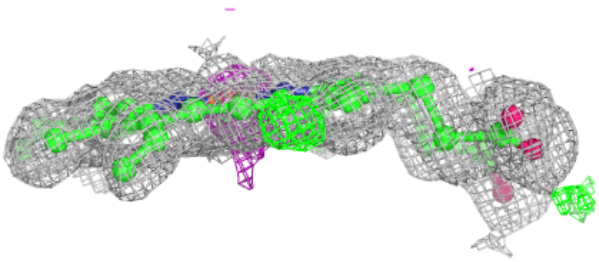


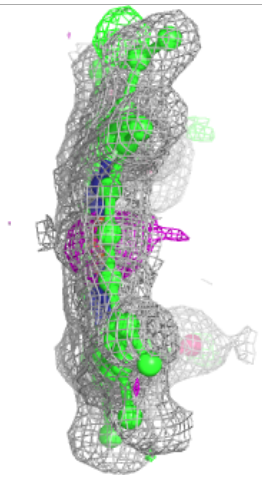


Electron density around HEM D 501 (A):

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

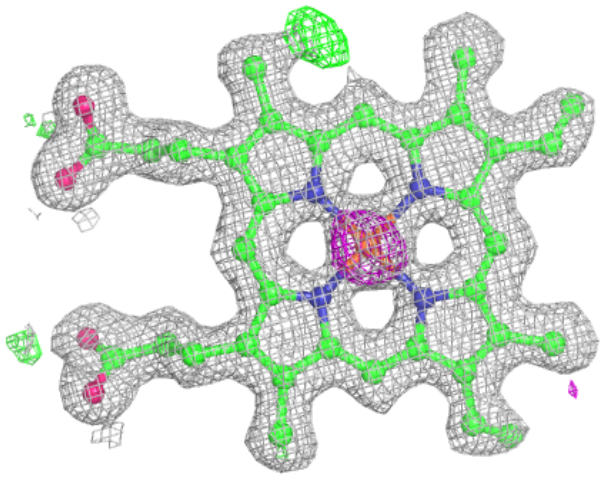


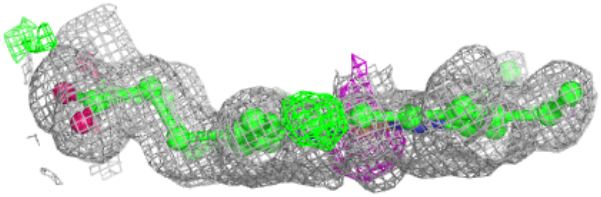


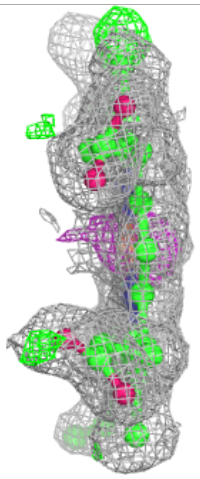


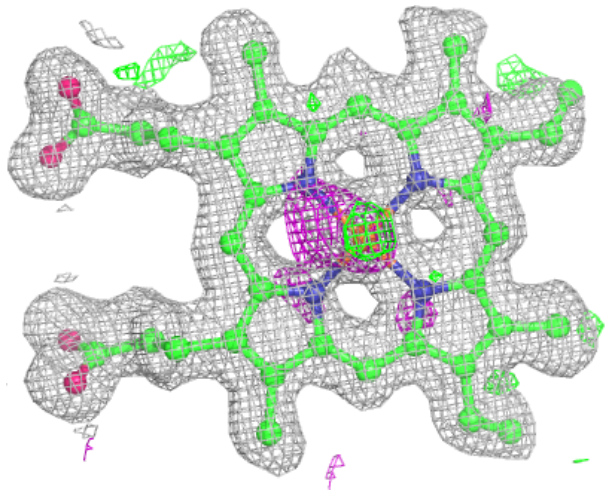
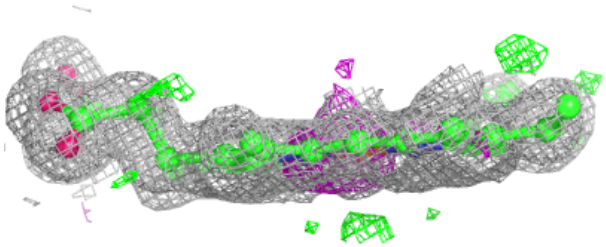
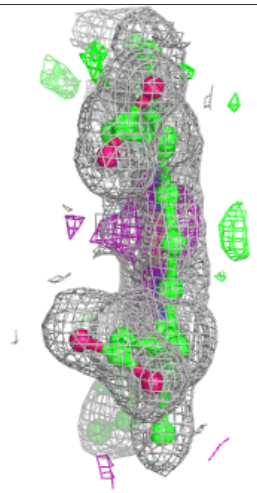
Electron density around HEM D 502 (B):

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



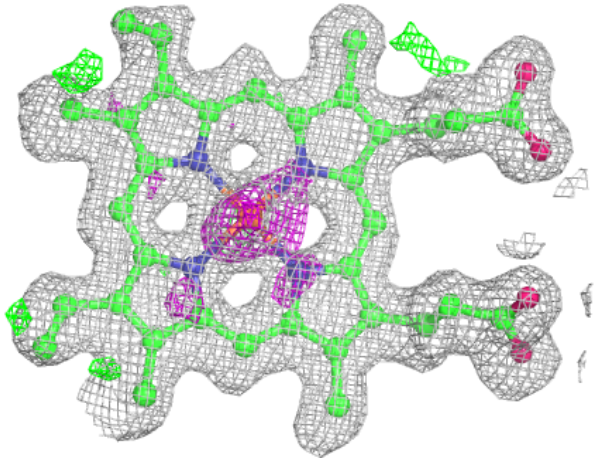


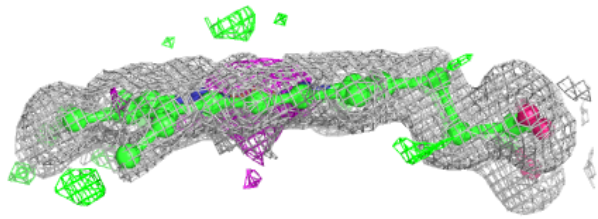


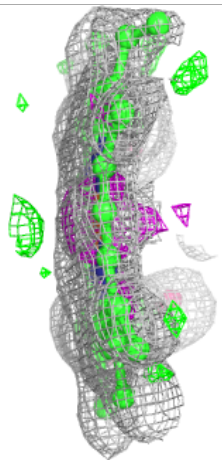
Electron density around HEM A 502 (B): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

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)

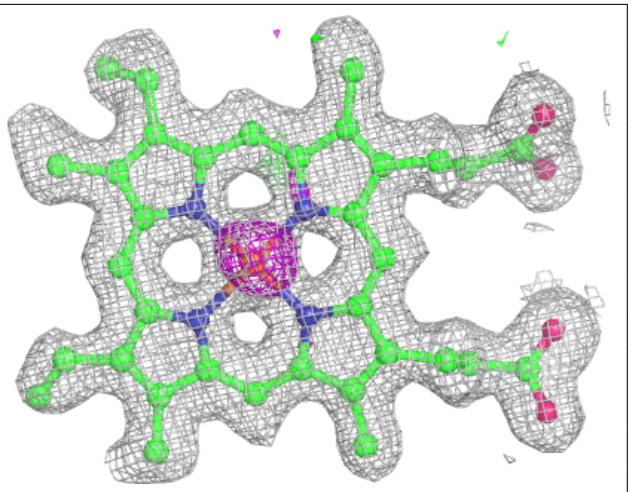


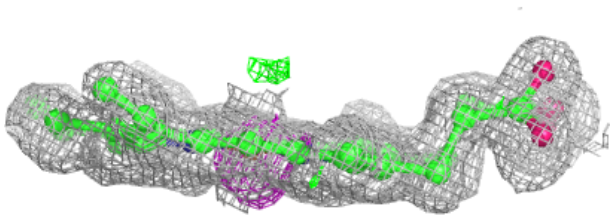


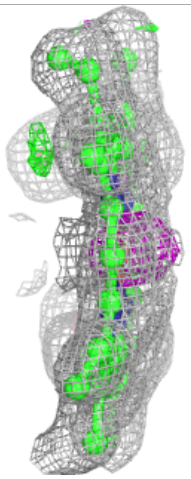


Electron density around HEM B 502 (B):

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

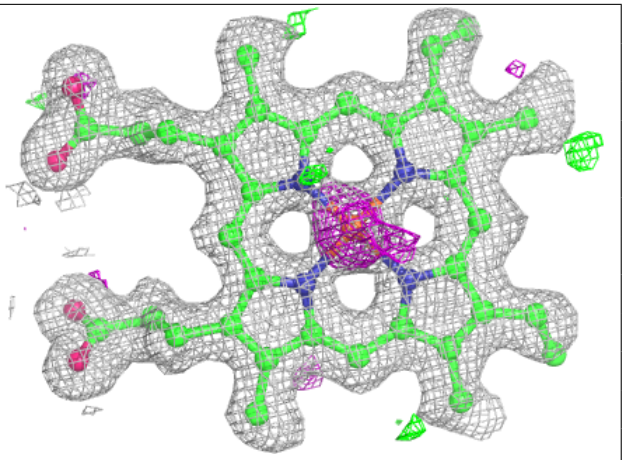


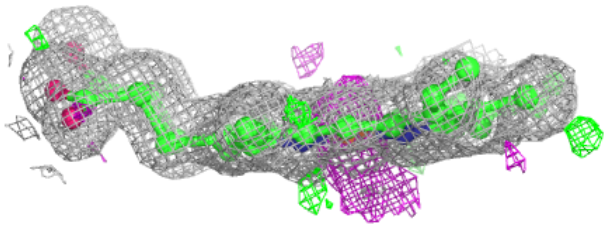


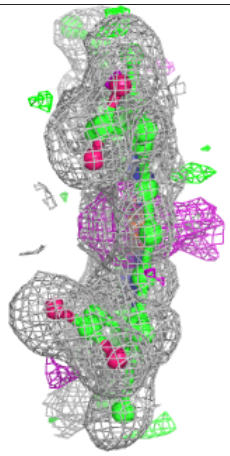


Electron density around HEM C 501 (A):

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

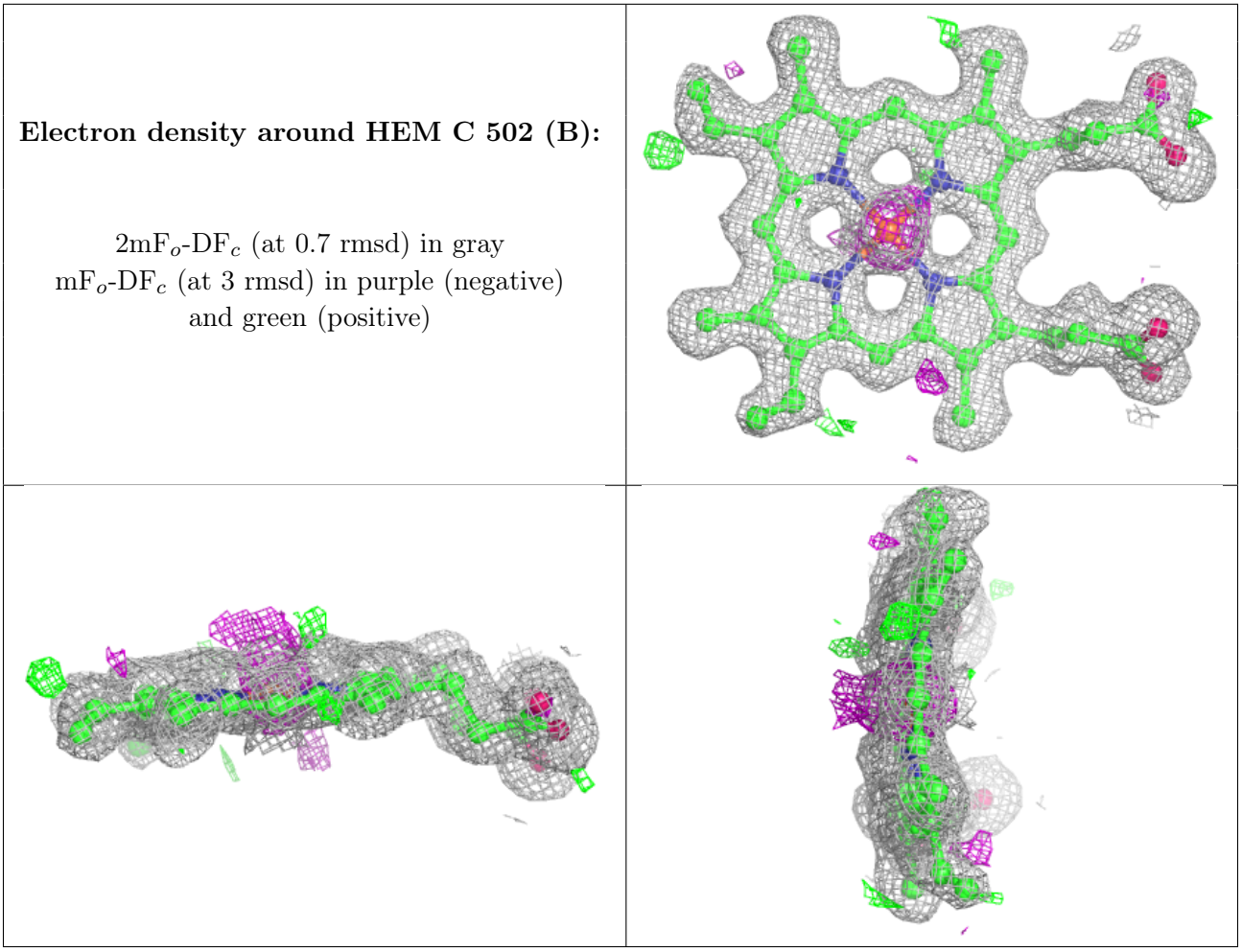






Electron density around HEM C 502 (B):

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



6.5 Other polymers (i)

There are no such residues in this entry.