Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:57 pm BST

PDB ID	:	6N6Q
Title	:	Crystal structure of a Cytochrome P450 (CYP102L1)
Authors	:	Follmer, A.H.; Poulos, T.L.
Deposited on	:	2018-11-26
Resolution	:	2.50 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 ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

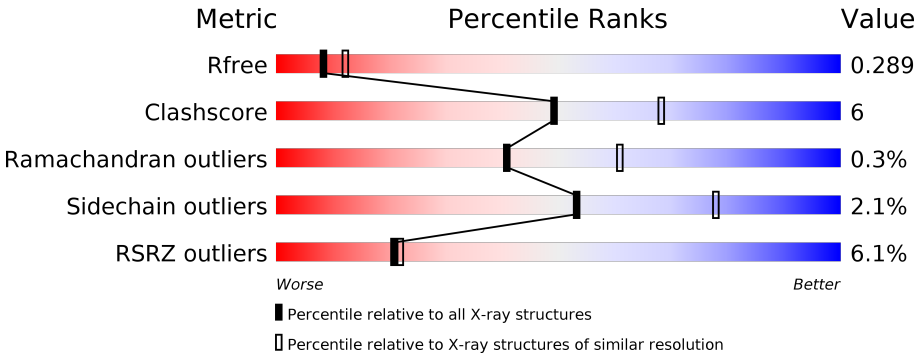
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	471	3% 82% 13% 5%
1	B	471	5% 79% 15% • 5%
1	C	471	6% 81% 13% 6%
1	D	471	9% 75% 17% • 7%

2 Entry composition

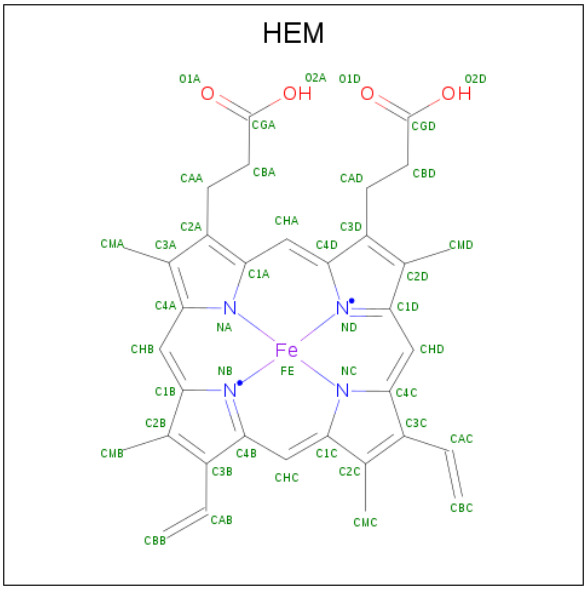
There are 4 unique types of molecules in this entry. The entry contains 14644 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P450 (CYP102L1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3594	2274	656	655	9			
1	B	448	Total	C	N	O	S	0	0	0
			3605	2279	666	651	9			
1	C	443	Total	C	N	O	S	0	0	0
			3578	2264	653	652	9			
1	D	440	Total	C	N	O	S	0	0	0
			3549	2244	647	649	9			

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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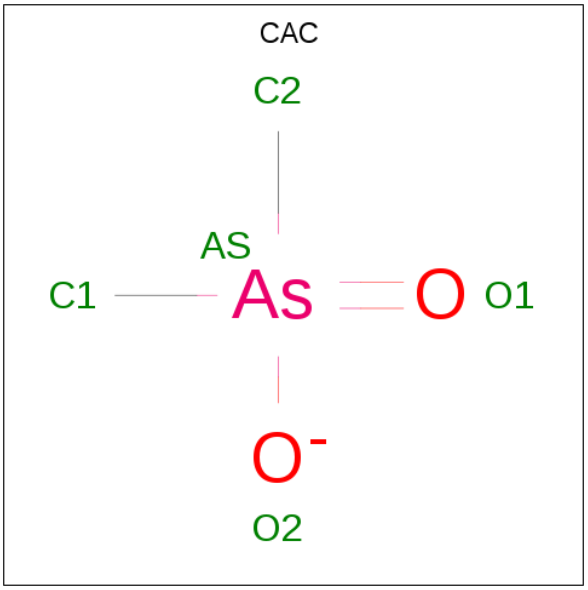
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	20	Total	O	0	0
			20	20		

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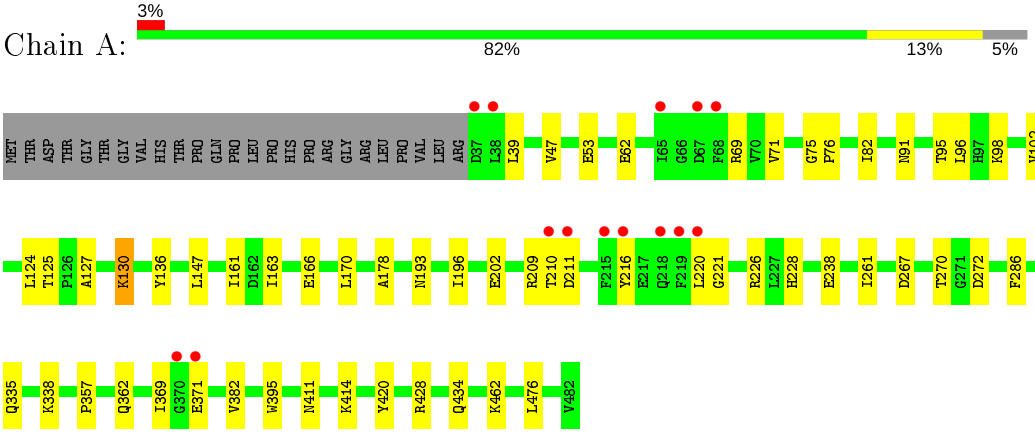
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	20	Total O 20 20	0	0
4	D	30	Total O 30 30	0	0

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.

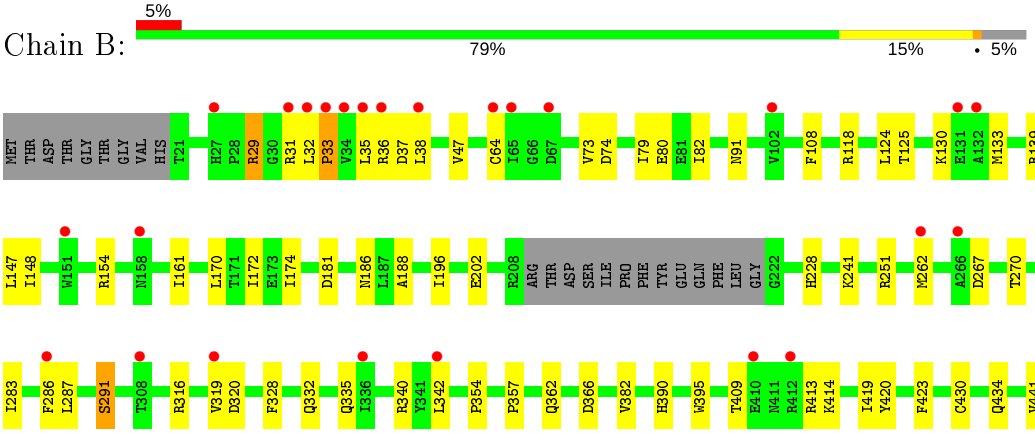
- Molecule 1: Cytochrome P450 (CYP102L1)

Chain A:



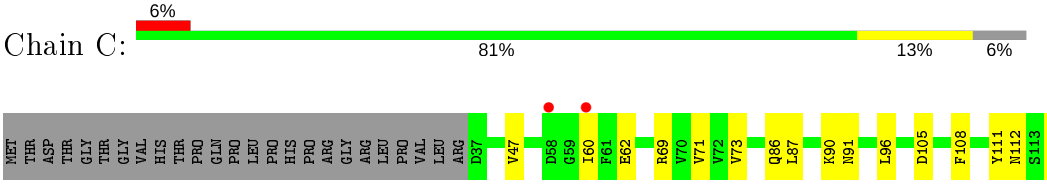
- Molecule 1: Cytochrome P450 (CYP102L1)

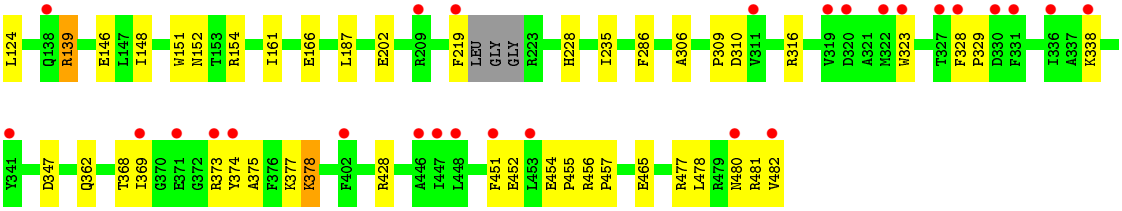
Chain B:



- Molecule 1: Cytochrome P450 (CYP102L1)

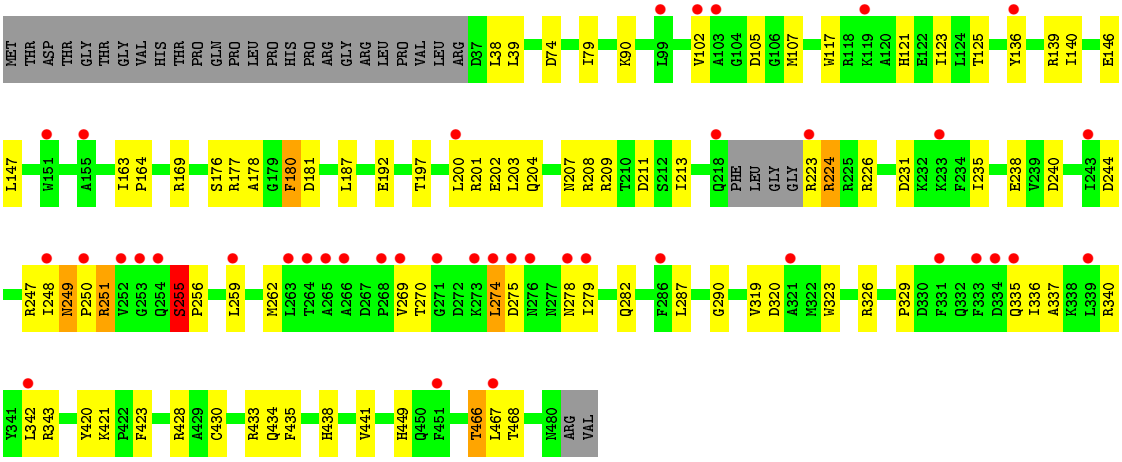
Chain C:





- Molecule 1: Cytochrome P450 (CYP102L1)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.90Å 174.09Å 203.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.56 – 2.50 66.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (66.56-2.50) 99.2 (66.56-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.230 , 0.289 0.230 , 0.289	Depositor DCC
R_{free} test set	3764 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14644	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.24	0/3679	0.39	0/4991
1	B	0.24	0/3691	0.40	0/5009
1	C	0.24	0/3662	0.40	0/4967
1	D	0.24	0/3632	0.40	0/4927
All	All	0.24	0/14664	0.40	0/19894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3594	0	3538	38	1
1	B	3605	0	3568	42	0
1	C	3578	0	3521	34	1
1	D	3549	0	3490	53	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	51	0	0	0	0
4	B	20	0	0	1	0
4	C	20	0	0	0	0
4	D	30	0	0	1	0
All	All	14644	0	14237	169	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (169) 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:D:249:ASN:HD21	1:D:251:ARG:HG2	1.35	0.88
1:A:209:ARG:HE	1:A:210:THR:H	1.25	0.84
1:B:332:GLN:H	1:B:335:GLN:HE21	1.34	0.76
1:D:123:ILE:HG21	1:D:274:LEU:HD11	1.71	0.72
1:A:220:LEU:HD13	1:D:201:ARG:HG3	1.71	0.71
2:A:501:HEM:HBC2	2:A:501:HEM:HHD	1.74	0.69
1:D:249:ASN:ND2	1:D:251:ARG:HG2	2.08	0.68
1:B:241:LYS:NZ	4:B:602:HOH:O	2.27	0.67
1:D:336:ILE:HG21	1:D:438:HIS:HD2	1.59	0.67
1:D:337:ALA:HA	1:D:343:ARG:HH12	1.62	0.64
1:A:69:ARG:NH1	1:D:39:LEU:O	2.31	0.64
1:D:223:ARG:HB3	1:D:224:ARG:HE	1.62	0.64
1:D:147:LEU:HB2	1:D:187:LEU:HD13	1.78	0.64
1:B:82:ILE:HD13	1:B:382:VAL:HG21	1.79	0.64
1:D:105:ASP:OD1	1:D:278:ASN:ND2	2.25	0.63
1:D:269:VAL:HG23	1:D:270:THR:HG23	1.80	0.63
1:A:270:THR:HG23	1:A:272:ASP:H	1.63	0.62
1:B:139:ARG:NH1	1:B:181:ASP:OD1	2.33	0.61
1:A:221:GLY:O	1:A:226:ARG:NH1	2.33	0.61
1:A:220:LEU:HD21	1:D:200:LEU:HB2	1.82	0.61
1:B:124:LEU:HD21	1:B:262:MET:HG2	1.83	0.60
1:B:35:LEU:HD13	1:B:38:LEU:HD23	1.84	0.60
1:D:326:ARG:NH1	1:D:449:HIS:O	2.34	0.60
2:D:501:HEM:HMB2	2:D:501:HEM:HBB2	1.84	0.60
1:C:86:GLN:HG3	1:C:87:LEU:HG	1.83	0.59
1:D:139:ARG:HH11	1:D:177:ARG:HB3	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:VAL:HG21	1:D:203:LEU:HD23	1.84	0.59
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.84	0.58
2:C:501:HEM:HMB2	2:C:501:HEM:HBB2	1.85	0.57
1:D:201:ARG:NH1	1:D:231:ASP:OD2	2.37	0.57
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.86	0.57
1:B:154:ARG:HD3	1:B:161:ILE:HG12	1.86	0.57
1:D:169:ARG:NH1	1:D:192:GLU:OE1	2.39	0.56
1:C:202:GLU:OE1	1:C:228:HIS:ND1	2.35	0.55
1:A:47:VAL:HG11	1:A:357:PRO:HB2	1.87	0.55
1:A:209:ARG:NE	1:A:210:THR:H	1.99	0.55
1:D:121:HIS:O	1:D:125:THR:OG1	2.19	0.55
1:C:454:GLU:OE1	1:C:477:ARG:NH1	2.39	0.55
1:A:335:GLN:HA	1:A:338:LYS:HE2	1.88	0.55
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.88	0.55
1:B:181:ASP:OD2	1:B:251:ARG:NH1	2.40	0.54
1:A:202:GLU:OE1	1:A:228:HIS:ND1	2.39	0.54
1:B:172:ILE:HD13	1:B:196:ILE:HD12	1.90	0.54
1:B:316:ARG:HA	1:B:319:VAL:HG22	1.90	0.54
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.89	0.54
1:B:124:LEU:HD13	1:B:286:PHE:HZ	1.73	0.53
1:D:180:PHE:HB3	1:D:259:LEU:HD22	1.91	0.53
1:B:47:VAL:HG11	1:B:357:PRO:HB2	1.91	0.53
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.91	0.53
1:B:33:PRO:HD2	1:B:37:ASP:H	1.74	0.53
1:B:423:PHE:HB3	1:B:430:CYS:HB3	1.91	0.53
1:D:176:SER:HB3	1:D:287:LEU:HD21	1.90	0.53
1:B:118:ARG:NH2	1:B:267:ASP:OD1	2.42	0.52
1:C:112:ASN:OD1	1:C:428:ARG:NH1	2.43	0.52
1:C:146:GLU:HG2	1:C:187:LEU:HB2	1.92	0.52
1:A:193:ASN:HB3	1:A:196:ILE:HG22	1.90	0.52
1:C:161:ILE:HG22	1:C:166:GLU:HG3	1.92	0.52
1:C:60:ILE:HD13	1:C:73:VAL:HG22	1.91	0.52
1:A:371:GLU:OE2	1:A:371:GLU:N	2.43	0.51
1:C:105:ASP:OD2	1:C:116:ASN:ND2	2.29	0.51
1:D:423:PHE:HB3	1:D:430:CYS:HB3	1.93	0.51
1:A:127:ALA:HB2	1:A:261:ILE:HD12	1.93	0.50
1:D:136:TYR:HB3	1:D:178:ALA:HB1	1.93	0.50
1:D:247:ARG:HG3	1:D:248:ILE:HG13	1.92	0.50
1:D:335:GLN:O	1:D:335:GLN:HG3	2.12	0.50
1:D:180:PHE:HD2	1:D:259:LEU:HB2	1.76	0.50
1:D:262:MET:HB3	1:D:279:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ASP:OD1	1:D:247:ARG:NH2	2.45	0.50
1:A:91:ASN:HB2	1:A:362:GLN:HB3	1.94	0.49
1:C:316:ARG:HH12	1:C:452:GLU:HA	1.77	0.49
1:A:117:TRP:CZ2	1:A:428:ARG:HG2	2.47	0.49
1:A:323:TRP:CG	1:A:329:PRO:HB3	2.47	0.49
1:B:118:ARG:HH22	1:B:270:THR:HG23	1.76	0.49
1:D:323:TRP:CG	1:D:329:PRO:HB3	2.47	0.49
1:A:147:LEU:HD22	1:A:170:LEU:HD22	1.94	0.49
1:B:108:PHE:HA	2:B:501:HEM:HAD1	1.95	0.49
1:B:202:GLU:OE2	1:B:228:HIS:ND1	2.45	0.49
1:C:323:TRP:CG	1:C:329:PRO:HB3	2.48	0.49
1:A:323:TRP:NE1	1:A:335:GLN:OE1	2.45	0.48
1:C:456:ARG:HD2	1:C:457:PRO:HD2	1.94	0.48
1:A:95:THR:HA	1:A:98:LYS:HD3	1.94	0.48
1:D:275:ASP:O	1:D:279:ILE:HG12	2.13	0.48
1:C:368:THR:HG22	1:C:375:ALA:HA	1.96	0.48
1:B:278:ASN:O	1:B:282:GLN:HG2	2.14	0.48
1:C:111:TYR:HB2	1:C:114:GLU:HG3	1.96	0.48
1:B:147:LEU:HD22	1:B:170:LEU:HD22	1.95	0.48
1:B:148:ILE:HG13	1:B:328:PHE:HE1	1.79	0.48
1:B:29:ARG:CZ	1:B:32:LEU:HD13	2.44	0.47
1:A:136:TYR:HB3	1:A:178:ALA:HB1	1.97	0.47
1:A:163:ILE:HD11	1:A:476:LEU:HB2	1.95	0.47
1:C:151:TRP:HA	1:C:154:ARG:HG3	1.95	0.47
1:D:466:THR:HG23	1:D:468:THR:H	1.78	0.47
1:B:74:ASP:HA	1:B:79:ILE:HD11	1.96	0.47
1:B:395:TRP:HZ2	1:B:420:TYR:HB2	1.79	0.47
1:A:102:VAL:HG22	1:A:202:GLU:HG3	1.96	0.47
1:C:451:PHE:HB3	1:C:478:LEU:HB3	1.96	0.47
1:D:290:GLY:HA2	2:D:501:HEM:C2C	2.50	0.47
1:C:310:ASP:N	1:C:310:ASP:OD1	2.46	0.46
1:A:216:TYR:H	1:D:204:GLN:HE21	1.63	0.46
1:B:73:VAL:HG11	1:B:82:ILE:HD12	1.97	0.46
1:B:31:ARG:HD2	1:B:31:ARG:N	2.31	0.46
1:A:124:LEU:HD13	1:A:286:PHE:HZ	1.81	0.46
1:D:320:ASP:OD2	1:D:326:ARG:NH2	2.49	0.46
1:D:208:ARG:NH1	1:D:213:ILE:HG22	2.31	0.46
1:B:130:LYS:HB2	1:B:434:GLN:HG2	1.97	0.46
1:B:354:PRO:HG3	1:B:390:HIS:HD1	1.80	0.46
1:C:96:LEU:HD21	1:C:108:PHE:CE1	2.51	0.45
1:D:146:GLU:HG2	1:D:187:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ARG:HD3	1:B:328:PHE:CD2	2.51	0.45
1:A:62:GLU:HG3	1:D:38:LEU:HD22	1.98	0.45
1:B:37:ASP:HB2	1:B:64:CYS:O	2.17	0.45
1:C:124:LEU:HD13	1:C:286:PHE:HZ	1.82	0.45
1:A:82:ILE:HD11	1:A:369:ILE:HD13	1.98	0.45
1:D:107:MET:HB2	1:D:282:GLN:HE22	1.82	0.45
1:D:117:TRP:CZ2	1:D:428:ARG:HG2	2.51	0.45
1:A:395:TRP:HZ2	1:A:420:TYR:HB2	1.82	0.45
1:B:186:ASN:HD21	1:B:188:ALA:HB3	1.81	0.45
1:B:91:ASN:HB2	1:B:362:GLN:HB3	1.99	0.45
1:D:278:ASN:O	1:D:282:GLN:HG2	2.17	0.45
1:B:29:ARG:NH1	1:B:37:ASP:OD2	2.50	0.44
1:C:91:ASN:HB2	1:C:362:GLN:HB3	1.99	0.44
1:A:161:ILE:HG23	1:A:166:GLU:HG3	1.99	0.44
1:D:140:ILE:HD11	1:D:435:PHE:CE1	2.51	0.44
1:A:130:LYS:HD3	1:A:434:GLN:HG2	2.00	0.43
1:A:211:ASP:OD2	1:D:209:ARG:NH2	2.51	0.43
1:B:140:ILE:HG12	1:B:174:ILE:HG23	1.99	0.43
1:D:433:ARG:NH2	1:D:434:GLN:OE1	2.51	0.43
1:D:90:LYS:NZ	4:D:602:HOH:O	2.34	0.43
1:A:71:VAL:HB	1:A:382:VAL:HG12	2.00	0.43
1:C:62:GLU:HB3	1:C:71:VAL:HG12	2.00	0.43
1:C:96:LEU:HD21	1:C:108:PHE:HE1	1.82	0.43
1:C:96:LEU:HA	1:C:96:LEU:HD23	1.82	0.43
1:C:373:ARG:HG3	1:C:374:TYR:CD2	2.54	0.43
1:D:202:GLU:HG3	1:D:235:ILE:HD12	2.01	0.43
1:B:320:ASP:OD2	1:B:481:ARG:NH2	2.43	0.42
1:D:197:THR:HG22	1:D:201:ARG:HH21	1.84	0.42
1:C:377:LYS:HB3	1:C:378:LYS:H	1.46	0.42
1:D:342:LEU:HD23	1:D:441:VAL:HG13	2.01	0.42
1:C:369:ILE:HD12	1:C:369:ILE:HA	1.84	0.42
1:C:90:LYS:HB3	1:C:428:ARG:HG3	2.02	0.42
1:B:133:MET:HE3	1:B:434:GLN:HB3	2.02	0.42
1:C:202:GLU:HG3	1:C:235:ILE:HD12	2.02	0.42
1:D:420:TYR:O	1:D:421:LYS:HD2	2.20	0.42
1:A:107:MET:O	1:A:428:ARG:NH2	2.53	0.42
1:C:369:ILE:CG2	1:C:374:TYR:HB2	2.49	0.42
1:A:267:ASP:HB3	1:A:270:THR:HG22	2.02	0.41
1:B:342:LEU:HD23	1:B:441:VAL:HG13	2.01	0.41
1:C:139:ARG:H	1:C:139:ARG:HD2	1.85	0.41
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ARG:HA	1:D:226:ARG:HD3	1.71	0.41
1:C:47:VAL:HG22	1:C:465:GLU:CD	2.40	0.41
1:A:209:ARG:HE	1:A:210:THR:HG22	1.86	0.41
1:A:411:ASN:HA	1:A:414:LYS:HD3	2.02	0.41
1:B:340:ARG:HH22	1:B:409:THR:H	1.68	0.41
1:C:306:ALA:HB1	1:C:455:PRO:HG3	2.03	0.41
1:D:466:THR:OG1	1:D:467:LEU:N	2.54	0.41
1:D:74:ASP:HA	1:D:79:ILE:HD11	2.02	0.41
1:C:316:ARG:HH11	1:C:482:VAL:HG11	1.84	0.41
1:B:287:LEU:O	1:B:291:SER:HB3	2.21	0.41
1:B:80:GLU:HG3	1:B:419:ILE:HD11	2.02	0.41
1:D:163:ILE:HB	1:D:164:PRO:HD3	2.02	0.41
1:D:262:MET:HE1	1:D:282:GLN:HB2	2.03	0.41
1:C:148:ILE:HG13	1:C:328:PHE:HE1	1.86	0.41
1:A:221:GLY:HA3	1:A:226:ARG:HH11	1.87	0.40
1:C:480:ASN:HB3	1:C:481:ARG:H	1.64	0.40
1:A:75:GLY:HA2	1:A:76:PRO:HD3	1.98	0.40
1:B:262:MET:HE2	1:B:279:ILE:HG12	2.03	0.40
1:B:279:ILE:O	1:B:283:ILE:HG12	2.20	0.40
1:D:255:SER:OG	1:D:256:PRO:O	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLU:OE2	1:C:69:ARG:NH2[7_555]	2.18	0.02

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	444/471 (94%)	433 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	444/471 (94%)	428 (96%)	14 (3%)	2 (0%)	29 48
1	C	439/471 (93%)	412 (94%)	26 (6%)	1 (0%)	47 68
1	D	436/471 (93%)	416 (95%)	18 (4%)	2 (0%)	29 48
All	All	1763/1884 (94%)	1689 (96%)	69 (4%)	5 (0%)	41 61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	ARG
1	C	378	LYS
1	D	250	PRO
1	B	33	PRO
1	D	255	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	376/398 (94%)	371 (99%)	5 (1%)	69 87
1	B	378/398 (95%)	372 (98%)	6 (2%)	62 84
1	C	375/398 (94%)	369 (98%)	6 (2%)	62 84
1	D	372/398 (94%)	358 (96%)	14 (4%)	33 58
All	All	1501/1592 (94%)	1470 (98%)	31 (2%)	53 78

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	125	THR
1	A	130	LYS
1	A	238	GLU
1	A	462	LYS
1	B	29	ARG

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Mol	Chain	Res	Type
1	B	125	THR
1	B	291	SER
1	B	366	ASP
1	B	413	ARG
1	B	414	LYS
1	C	139	ARG
1	C	152	ASN
1	C	219	PHE
1	C	309	PRO
1	C	338	LYS
1	C	347	ASP
1	D	180	PHE
1	D	181	ASP
1	D	207	ASN
1	D	211	ASP
1	D	224	ARG
1	D	238	GLU
1	D	240	ASP
1	D	249	ASN
1	D	251	ARG
1	D	255	SER
1	D	274	LEU
1	D	319	VAL
1	D	340	ARG
1	D	466	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	B	138	GLN
1	B	335	GLN
1	B	437	GLN
1	D	63	GLN
1	D	168	ASN
1	D	204	GLN
1	D	218	GLN
1	D	249	ASN
1	D	282	GLN
1	D	438	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	B	501	-	27,50,50	1.81	4 (14%)	17,82,82	1.52	3 (17%)
3	CAC	A	502	-	0,4,4	0.00	-	0,6,6	0.00	-
2	HEM	D	501	-	27,50,50	1.81	4 (14%)	17,82,82	1.51	4 (23%)
3	CAC	D	502	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	B	502	-	0,4,4	0.00	-	0,6,6	0.00	-
2	HEM	A	501	-	27,50,50	1.88	4 (14%)	17,82,82	1.42	2 (11%)
2	HEM	C	501	4	27,50,50	1.83	5 (18%)	17,82,82	1.48	3 (17%)
3	CAC	B	503	-	0,4,4	0.00	-	0,6,6	0.00	-
3	CAC	C	502	-	0,4,4	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	-	-	0/6/54/54	-
2	HEM	A	501	-	-	0/6/54/54	-
2	HEM	D	501	-	-	0/6/54/54	-
2	HEM	C	501	4	-	0/6/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-4.66	1.33	1.40
2	C	501	HEM	C3C-CAC	3.86	1.55	1.47
2	B	501	HEM	C3C-CAC	3.83	1.55	1.47
2	C	501	HEM	C3B-CAB	3.83	1.55	1.47
2	D	501	HEM	C3C-CAC	3.80	1.55	1.47
2	A	501	HEM	C3B-CAB	3.77	1.55	1.47
2	B	501	HEM	C3B-CAB	3.76	1.55	1.47
2	D	501	HEM	C3B-CAB	3.74	1.55	1.47
2	C	501	HEM	C3C-C2C	-3.71	1.35	1.40
2	B	501	HEM	C3C-C2C	-3.70	1.35	1.40
2	D	501	HEM	C3B-C2B	-3.70	1.35	1.40
2	A	501	HEM	C3B-C2B	-3.67	1.35	1.40
2	B	501	HEM	C3B-C2B	-3.67	1.35	1.40
2	D	501	HEM	C3C-C2C	-3.67	1.35	1.40
2	C	501	HEM	C3B-C2B	-3.65	1.35	1.40
2	A	501	HEM	C3C-CAC	3.64	1.55	1.47
2	C	501	HEM	CAA-C2A	2.04	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CMB-C2B-C3B	2.32	129.01	124.68
2	D	501	HEM	CMB-C2B-C3B	2.31	129.01	124.68
2	B	501	HEM	CBA-CAA-C2A	-2.28	108.27	112.49
2	B	501	HEM	CMC-C2C-C3C	2.23	128.86	124.68
2	C	501	HEM	CMC-C2C-C3C	2.23	128.85	124.68
2	A	501	HEM	CMB-C2B-C3B	2.21	128.81	124.68
2	D	501	HEM	CAA-CBA-CGA	-2.18	109.01	112.67
2	D	501	HEM	CBD-CAD-C3D	-2.18	108.47	112.48
2	C	501	HEM	CMB-C2B-C3B	2.15	128.70	124.68
2	A	501	HEM	CBA-CAA-C2A	-2.14	108.54	112.49
2	D	501	HEM	CMC-C2C-C3C	2.12	128.65	124.68
2	C	501	HEM	CAD-CBD-CGD	-2.10	109.15	112.67

There are no chirality outliers.

There are no torsion outliers.

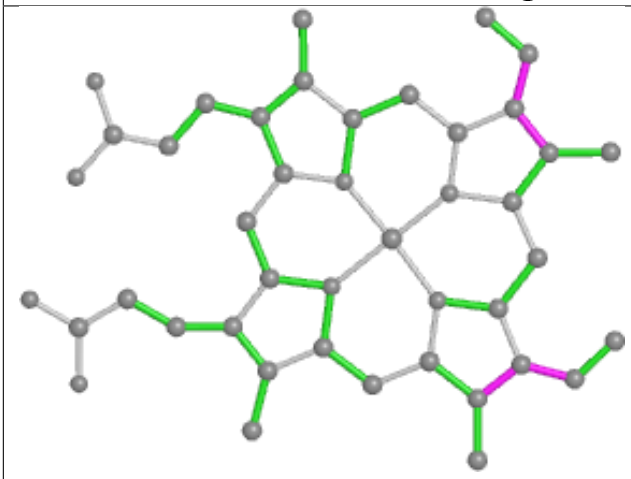
There are no ring outliers.

4 monomers are involved in 10 short contacts:

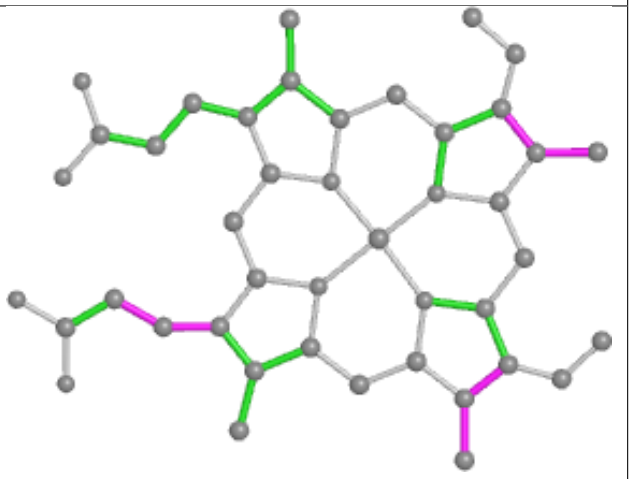
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	3	0
2	D	501	HEM	3	0
2	A	501	HEM	2	0
2	C	501	HEM	2	0

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.

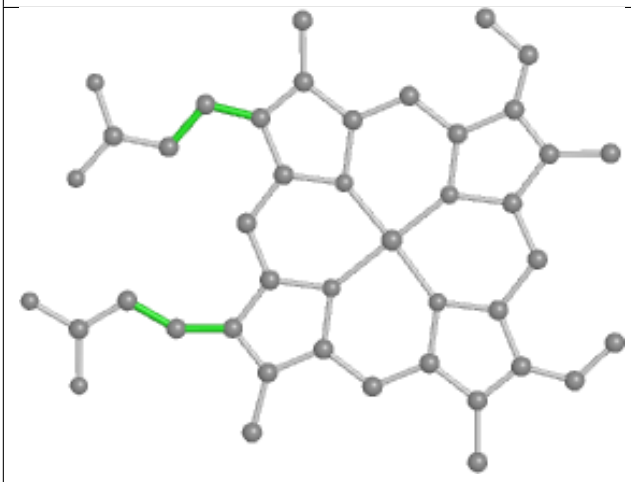
Ligand HEM B 501



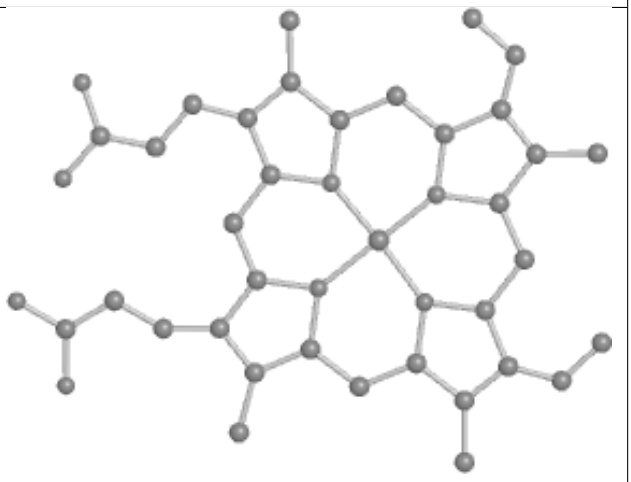
Bond lengths



Bond angles

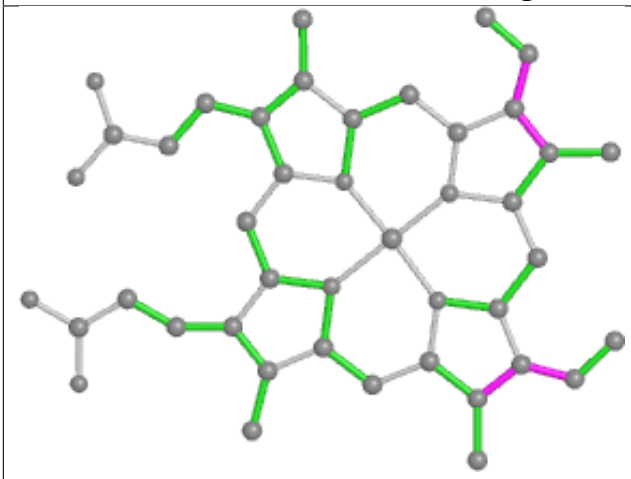


Torsions

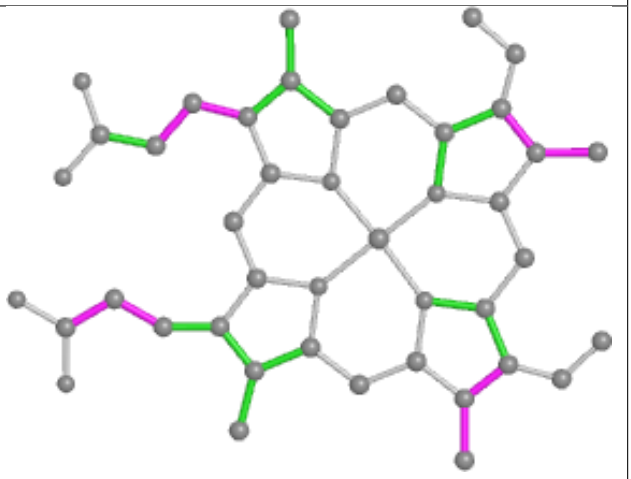


Rings

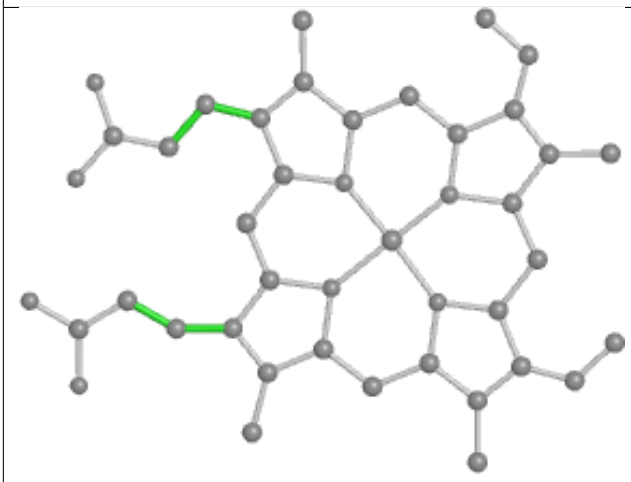
Ligand HEM D 501



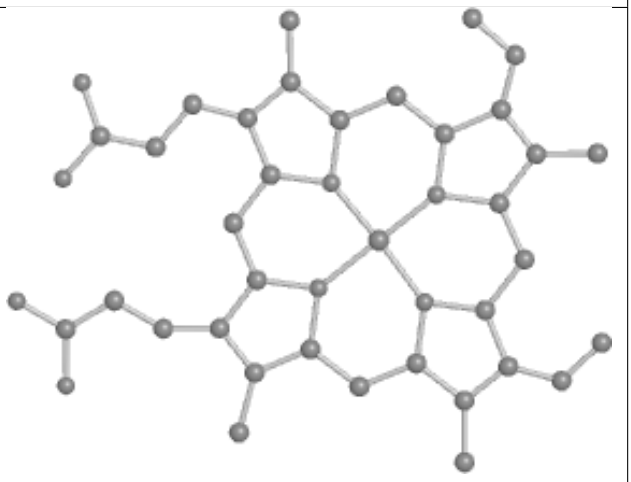
Bond lengths



Bond angles

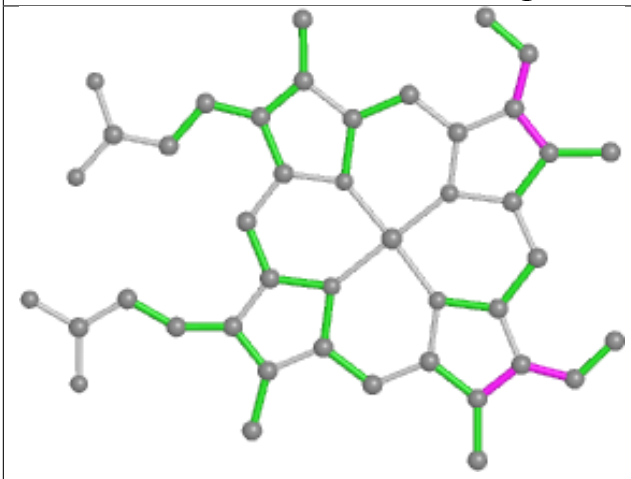


Torsions

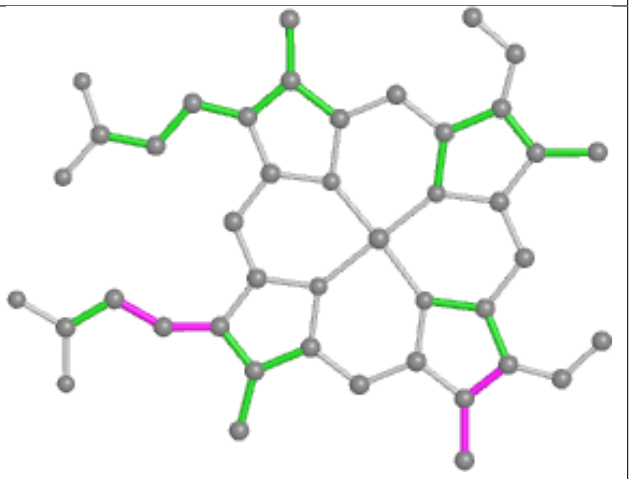


Rings

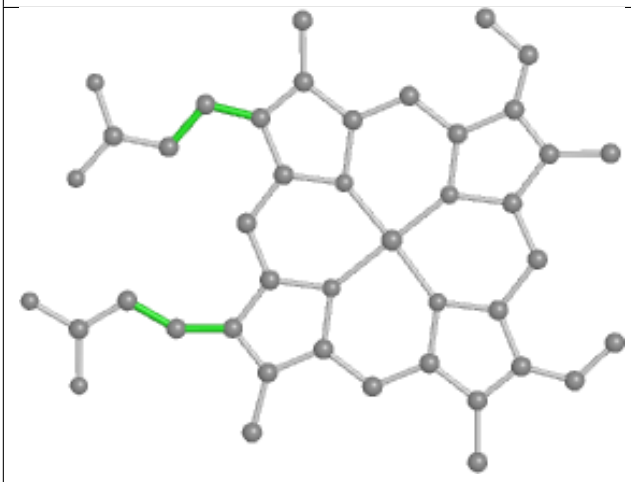
Ligand HEM A 501



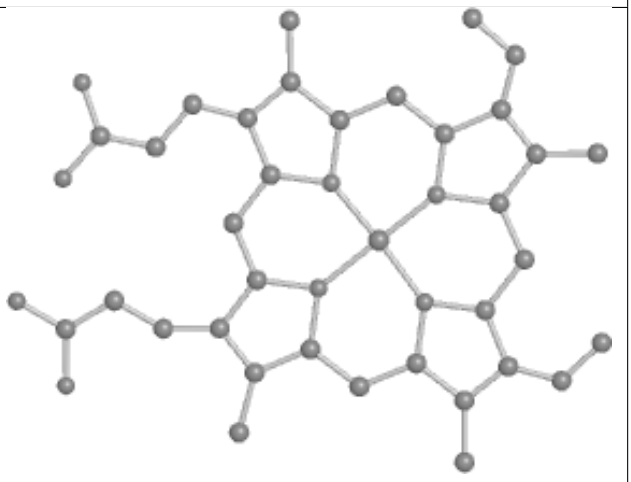
Bond lengths



Bond angles

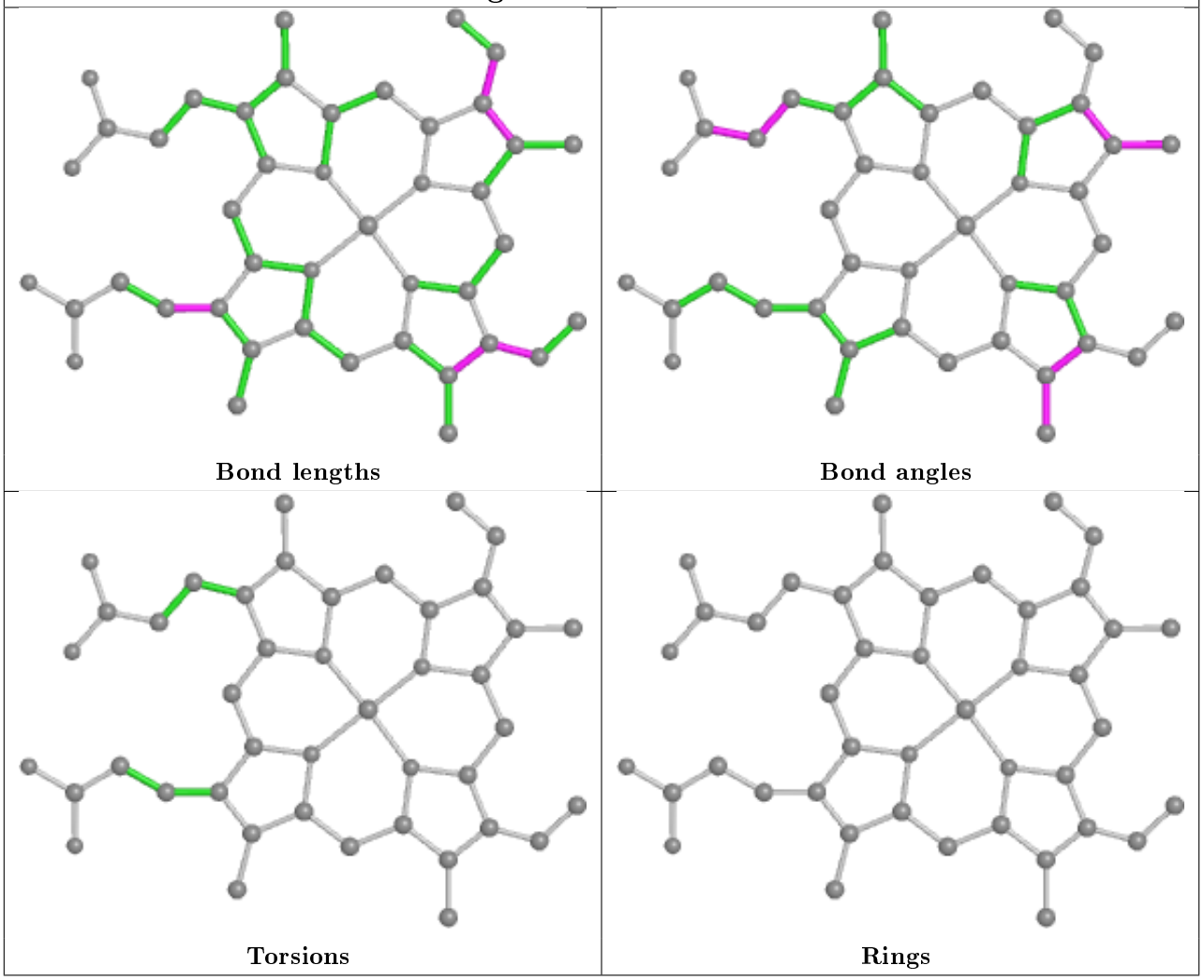


Torsions



Rings

Ligand HEM C 501



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	446/471 (94%)	0.33	14 (3%) 49 52	41, 56, 79, 104	0
1	B	448/471 (95%)	0.47	25 (5%) 24 25	44, 69, 94, 108	0
1	C	443/471 (94%)	0.67	29 (6%) 18 19	44, 70, 101, 118	0
1	D	440/471 (93%)	0.70	41 (9%) 8 8	42, 73, 105, 128	0
All	All	1777/1884 (94%)	0.54	109 (6%) 21 22	41, 66, 99, 128	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	254	GLN	6.8
1	C	480	ASN	6.3
1	C	453	LEU	6.3
1	D	271	GLY	5.9
1	D	268	PRO	5.7
1	B	35	LEU	5.4
1	D	279	ILE	5.1
1	C	482	VAL	5.1
1	C	323	TRP	5.1
1	C	373	ARG	5.0
1	A	220	LEU	4.8
1	D	269	VAL	4.8
1	A	219	PHE	4.7
1	D	266	ALA	4.6
1	D	253	GLY	4.6
1	A	370	GLY	4.6
1	B	32	LEU	4.5
1	C	319	VAL	4.2
1	B	31	ARG	4.2
1	D	252	VAL	4.1
1	B	33	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	265	ALA	3.9
1	D	335	GLN	3.9
1	C	322	MET	3.7
1	B	132	ALA	3.6
1	D	286	PHE	3.6
1	B	34	VAL	3.6
1	B	410	GLU	3.5
1	C	448	LEU	3.4
1	D	263	LEU	3.4
1	B	342	LEU	3.4
1	C	60	ILE	3.3
1	A	211	ASP	3.3
1	A	216	TYR	3.3
1	C	446	ALA	3.2
1	C	369	ILE	3.2
1	C	331	PHE	3.2
1	C	336	ILE	3.1
1	A	37	ASP	3.1
1	D	155	ALA	3.1
1	D	264	THR	3.1
1	D	250	PRO	3.1
1	D	274	LEU	3.1
1	A	218	GLN	3.1
1	C	219	PHE	3.0
1	C	447	ILE	2.9
1	B	131	GLU	2.9
1	B	64	CYS	2.9
1	C	374	TYR	2.9
1	C	58	ASP	2.9
1	D	467	LEU	2.9
1	D	339	LEU	2.8
1	D	331	PHE	2.8
1	C	311	VAL	2.7
1	A	215	PHE	2.7
1	B	67	ASP	2.7
1	D	273	LYS	2.7
1	C	451	PHE	2.7
1	D	278	ASN	2.7
1	B	286	PHE	2.7
1	A	38	LEU	2.6
1	B	412	ARG	2.6
1	A	210	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	151	TRP	2.6
1	A	67	ASP	2.6
1	B	266	ALA	2.5
1	D	218	GLN	2.5
1	D	243	ILE	2.5
1	D	223	ARG	2.5
1	D	333	PHE	2.5
1	C	209	ARG	2.4
1	D	136	TYR	2.4
1	D	342	LEU	2.4
1	D	233	LYS	2.4
1	D	275	ASP	2.4
1	C	371	GLU	2.4
1	B	27	HIS	2.3
1	D	248	ILE	2.3
1	C	341	TYR	2.3
1	D	334	ASP	2.3
1	D	103	ALA	2.3
1	B	38	LEU	2.3
1	B	336	ILE	2.3
1	D	276	ASN	2.3
1	D	119	LYS	2.3
1	D	200	LEU	2.3
1	B	151	TRP	2.3
1	B	308	THR	2.3
1	A	371	GLU	2.3
1	C	138	GLN	2.2
1	B	102	VAL	2.2
1	D	451	PHE	2.2
1	C	328	PHE	2.2
1	C	338	LYS	2.1
1	B	65	ILE	2.1
1	D	99	LEU	2.1
1	D	259	LEU	2.1
1	D	102	VAL	2.1
1	A	68	PHE	2.1
1	D	321	ALA	2.1
1	C	327	THR	2.1
1	A	65	ILE	2.1
1	B	319	VAL	2.1
1	B	158	ASN	2.1
1	C	330	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	402	PHE	2.0
1	C	320	ASP	2.0
1	B	262	MET	2.0
1	B	36	ARG	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)

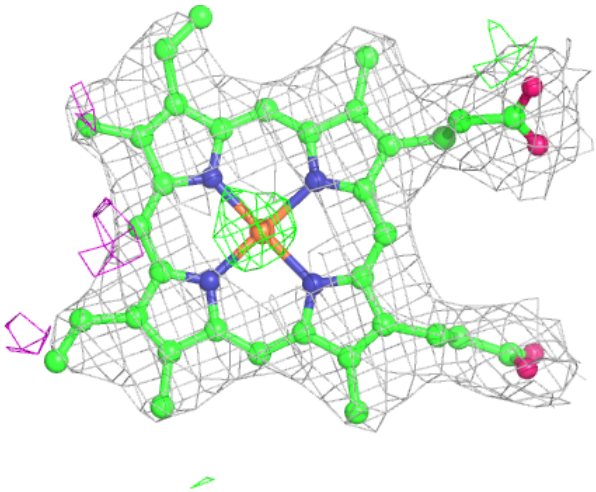
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

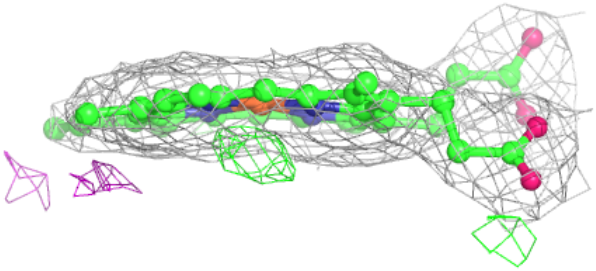
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CAC	B	503	5/5	0.91	0.29	92,93,94,94	5
2	HEM	A	501	43/43	0.96	0.16	32,45,53,54	0
3	CAC	C	502	5/5	0.96	0.15	54,66,77,92	0
2	HEM	B	501	43/43	0.97	0.16	44,53,62,67	0
2	HEM	C	501	43/43	0.97	0.17	38,52,60,65	0
2	HEM	D	501	43/43	0.97	0.17	41,53,62,66	0
3	CAC	D	502	5/5	0.97	0.11	70,83,89,106	0
3	CAC	A	502	5/5	0.98	0.18	52,58,64,67	5
3	CAC	B	502	5/5	0.98	0.12	71,72,85,98	0

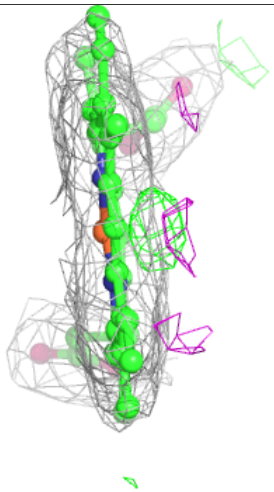
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 501:

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

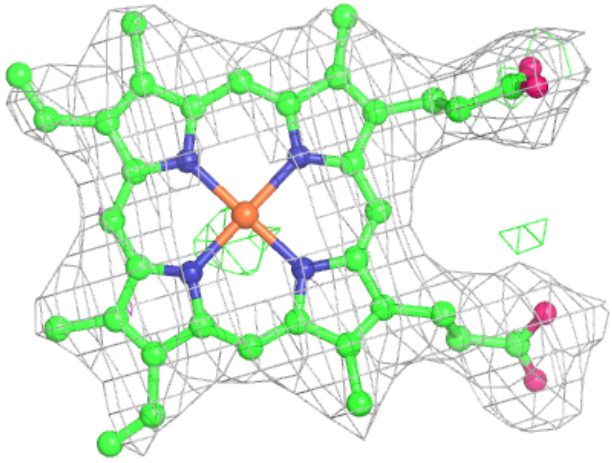


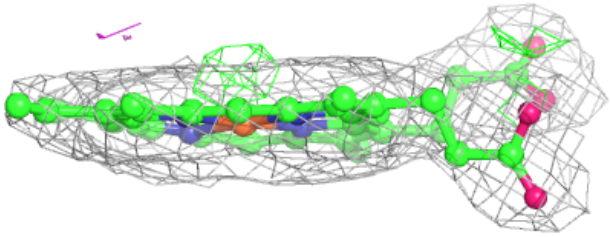


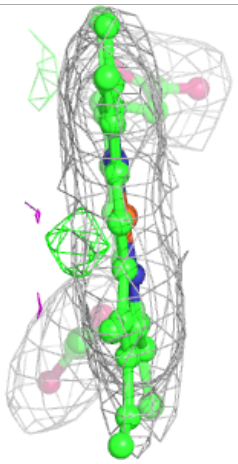


Electron density around HEM B 501:

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

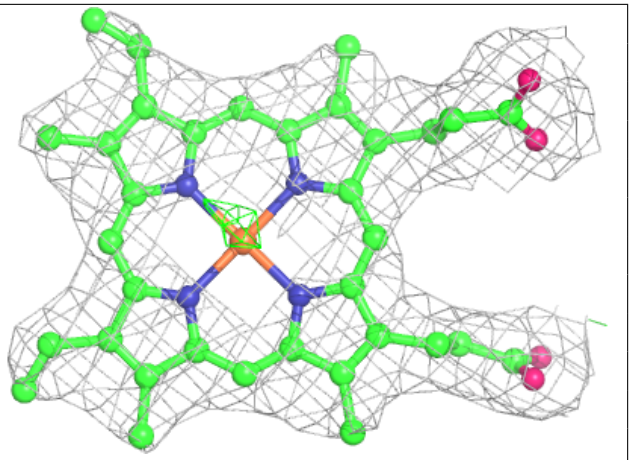


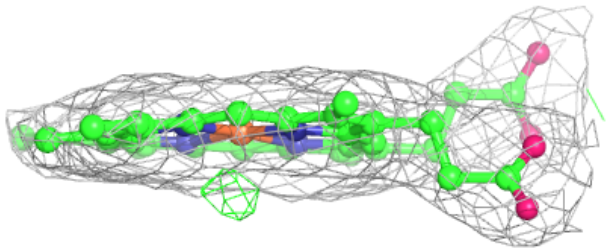


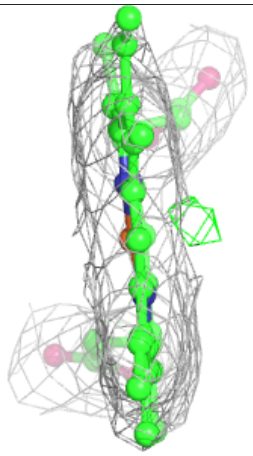


Electron density around HEM C 501:

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

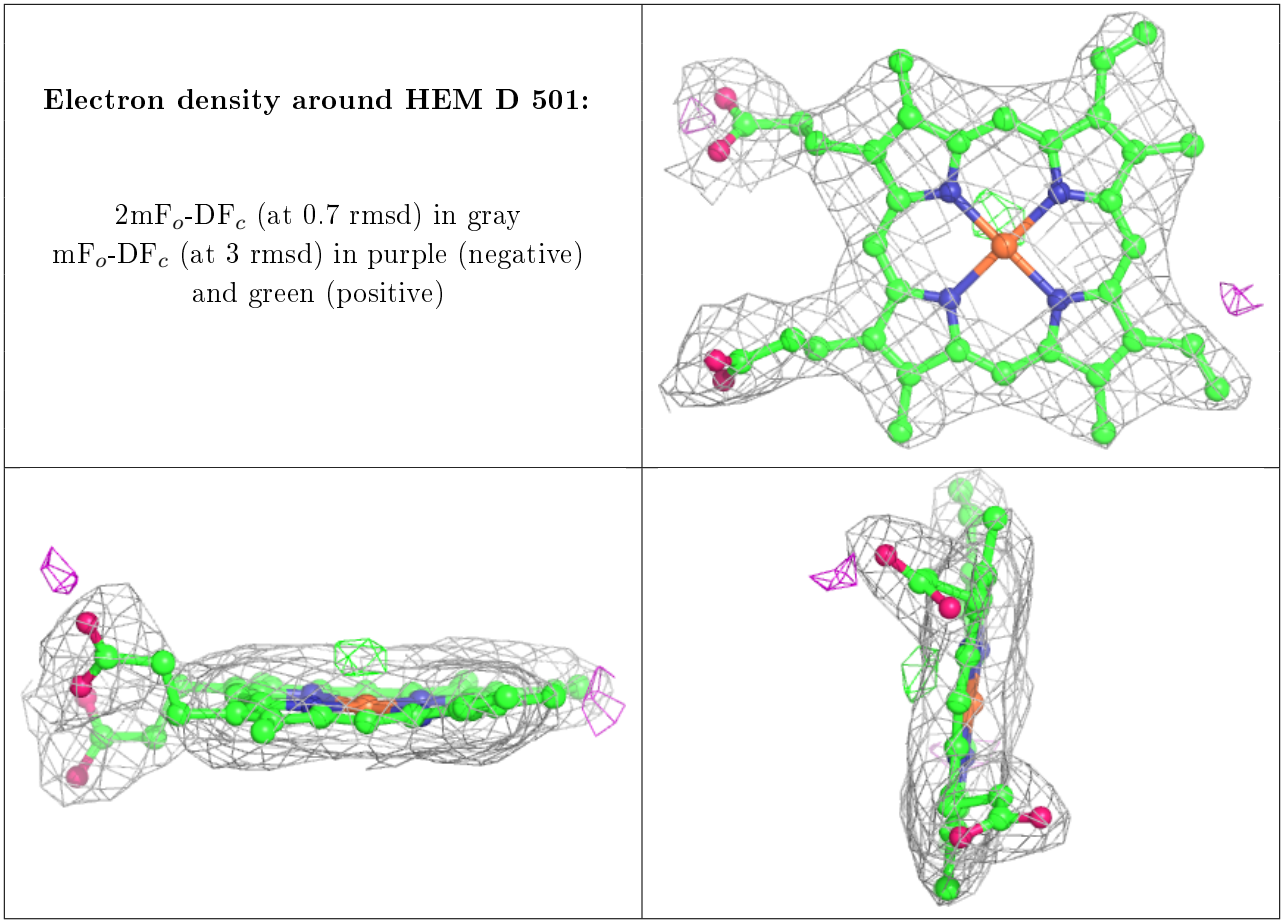






Electron density around HEM D 501:

$2mF_o$-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

There are no such residues in this entry.