Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 03:08 PM EDT

PDB ID	:	4FB2
Title	:	Crystal Structure of Substrate-Free P450cin
Authors	:	Madrona, Y.; Tripathi, S.M.; Li, H.; Poulos, T.L.
Deposited on	:	2012-05-22
Resolution	:	1.37 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:

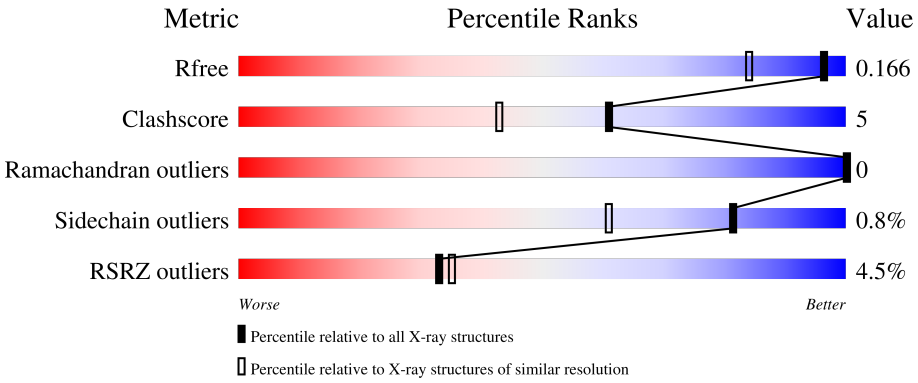
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 1.37 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	2907 (1.40-1.36)
Clashscore	141614	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)
RSRZ outliers	127900	2846 (1.40-1.36)

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	398	2% 90% 8%
1	B	398	8% 90% 8%
1	C	398	3% 93% 6%
1	D	398	5% 90% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27146 atoms, of which 12517 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.

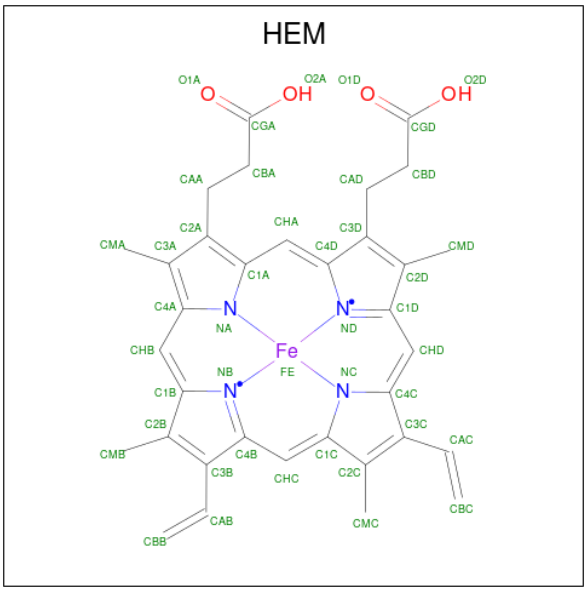
- Molecule 1 is a protein called P450cin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	H	N	O	S	0	7	0
			6269	2014	3120	548	574	13			
1	B	392	Total	C	H	N	O	S	0	2	0
			6200	1995	3079	545	570	11			
1	C	391	Total	C	H	N	O	S	0	12	0
			6301	2022	3140	551	575	13			
1	D	391	Total	C	H	N	O	S	0	7	0
			6263	2009	3123	547	573	11			

There are 4 discrepancies between the modelled and reference sequences:

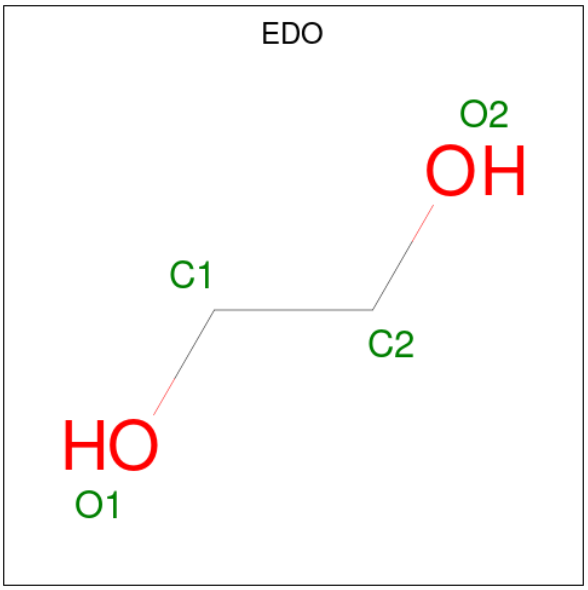
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q8VQF6
B	7	MET	-	expression tag	UNP Q8VQF6
C	7	MET	-	expression tag	UNP Q8VQF6
D	7	MET	-	expression tag	UNP Q8VQF6

- 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	H	N	O	0	0
			49	34	1	6	4	4		
2	B	1	Total	C	Fe	H	N	O	0	0
			49	34	1	6	4	4		
2	C	1	Total	C	Fe	H	N	O	0	0
			49	34	1	6	4	4		
2	D	1	Total	C	Fe	H	N	O	0	0
			49	34	1	6	4	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 12 2 7 3	0	1
3	C	1	Total C H O 10 2 6 2	0	0
3	C	1	Total C H O 10 2 6 2	0	0

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

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

- Molecule 5 is water.

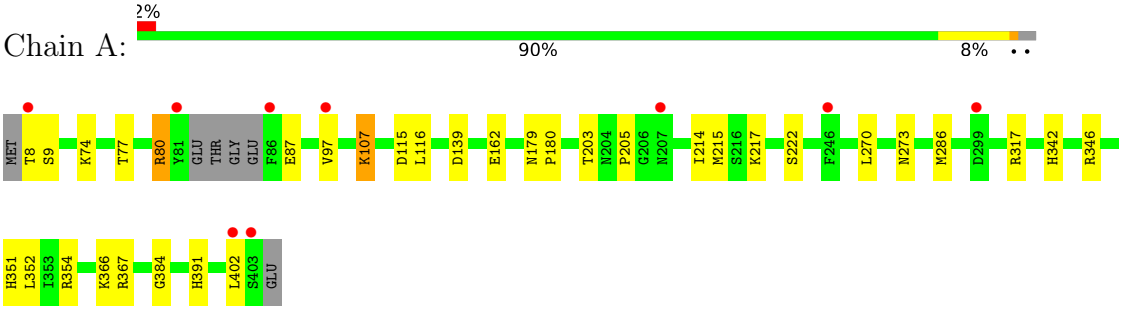
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	516	Total O 521 521	0	11
5	B	383	Total O 385 385	0	4
5	C	482	Total O 493 493	0	11
5	D	457	Total O 462 462	0	5

3 Residue-property plots

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.

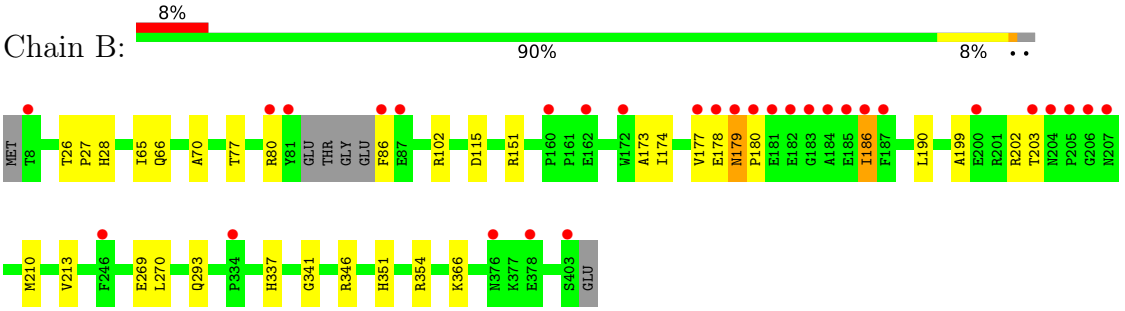
- Molecule 1: P450cin

Chain A:



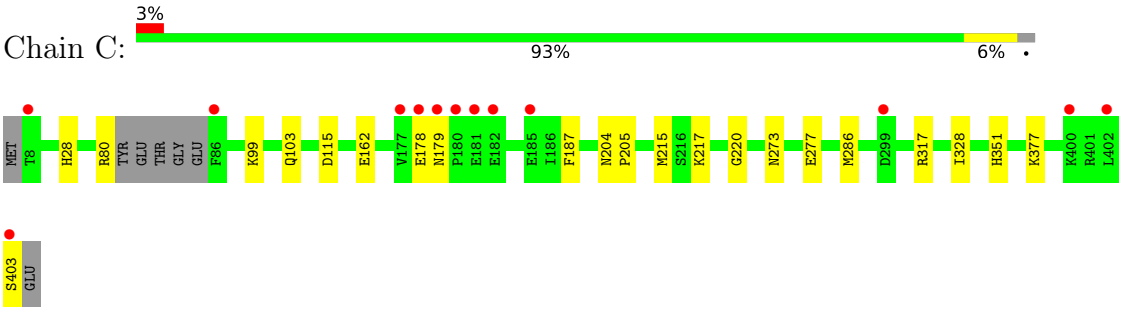
- Molecule 1: P450cin

Chain B:



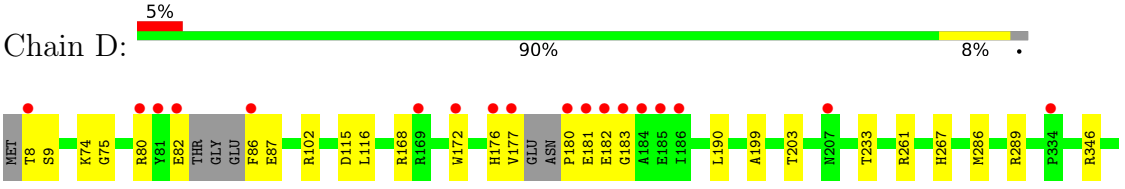
- Molecule 1: P450cin

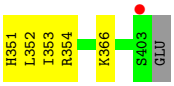
Chain C:



- Molecule 1: P450cin

Chain D:




H351
L352
I353
R354
K366
S403
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.38Å 83.91Å 88.19Å 96.81° 96.39° 89.94°	Depositor
Resolution (Å)	41.66 – 1.37 41.66 – 1.37	Depositor EDS
% Data completeness (in resolution range)	91.8 (41.66-1.37) 95.5 (41.66-1.37)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 1.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.136 , 0.167 0.137 , 0.166	Depositor DCC
R_{free} test set	17248 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.3	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	27146	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: HEM, EDO, 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	0.61	0/3246	0.71	1/4411 (0.0%)
1	B	0.58	0/3207	0.67	0/4360
1	C	0.61	0/3275	0.70	1/4449 (0.0%)
1	D	0.61	0/3237	0.70	2/4398 (0.0%)
All	All	0.60	0/12965	0.70	4/17618 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	261	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	317	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	317	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	289	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	3149	3120	3127	32	0
1	B	3121	3079	3074	24	0
1	C	3161	3140	3160	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3140	3123	3106	31	0
2	A	43	6	30	0	0
2	B	43	6	30	0	0
2	C	43	6	30	2	0
2	D	43	6	30	0	0
3	A	4	6	6	1	0
3	B	4	6	6	2	0
3	C	13	19	18	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	521	0	0	13	0
5	B	385	0	0	4	0
5	C	493	0	0	13	0
5	D	462	0	0	7	0
All	All	14629	12517	12617	115	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (115) 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:A:214:ILE:HG22	1:A:215[B]:MET:HE3	1.37	1.03
1:C:205:PRO:CB	1:C:215[B]:MET:HE3	2.00	0.91
1:C:205:PRO:CB	1:C:215[B]:MET:CE	2.56	0.83
1:C:205:PRO:HB2	1:C:215[B]:MET:HE3	1.62	0.80
1:A:214:ILE:HG22	1:A:215[B]:MET:CE	2.13	0.78
1:A:107:LYS:HD3	5:A:973:HOH:O	1.82	0.78
1:A:74:LYS:HE2	1:A:87:GLU:OE1	1.84	0.77
1:C:205:PRO:HB2	1:C:215[B]:MET:CE	2.14	0.75
1:D:182:GLU:N	1:D:183:GLY:HA3	2.01	0.75
1:A:286[B]:MET:HE1	5:A:818:HOH:O	1.85	0.74
3:C:505:EDO:H12	5:C:803:HOH:O	1.88	0.71
1:C:205:PRO:HB3	1:C:215[B]:MET:HE3	1.71	0.70
1:A:286[B]:MET:CE	5:A:818:HOH:O	2.43	0.66
1:C:286[B]:MET:HE2	5:C:695:HOH:O	1.94	0.65
1:A:217[B]:LYS:HE3	5:A:1030:HOH:O	1.97	0.64
1:B:341:GLY:O	3:B:502:EDO:H11	1.98	0.64
1:D:86:PHE:HZ	1:D:233:THR:HG21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:N	1:A:107:LYS:HD2	2.12	0.63
1:A:286[B]:MET:CE	5:A:1098:HOH:O	2.45	0.63
1:C:286[B]:MET:CE	5:C:695:HOH:O	2.46	0.62
1:B:173:ALA:HB1	1:B:186:ILE:HD13	1.82	0.62
1:D:80:ARG:NH2	5:D:839:HOH:O	2.34	0.61
1:D:80:ARG:O	1:D:80:ARG:HG3	2.02	0.60
1:A:203:THR:HG21	5:A:1090:HOH:O	2.03	0.59
1:B:346:ARG:HH22	1:B:354:ARG:HH12	1.50	0.59
1:D:75:GLY:HA2	1:D:80:ARG:NH2	2.16	0.59
1:A:115:ASP:OD1	1:A:351:HIS:HE1	1.85	0.59
1:D:115:ASP:OD1	1:D:351:HIS:HE1	1.86	0.58
1:D:286:MET:HE2	5:D:947:HOH:O	2.03	0.58
1:A:286[B]:MET:HE2	5:A:1098:HOH:O	2.02	0.57
1:D:176:HIS:O	1:D:177:VAL:CB	2.53	0.57
1:D:74:LYS:HE2	1:D:87:GLU:OE1	2.05	0.56
1:A:367:ARG:CZ	1:A:402:LEU:HD13	2.36	0.56
1:B:115:ASP:OD1	1:B:351:HIS:HE1	1.88	0.56
1:C:115:ASP:OD1	1:C:351:HIS:HE1	1.89	0.56
1:B:346:ARG:NH2	1:B:354:ARG:HH12	2.03	0.55
1:D:176:HIS:O	1:D:177:VAL:HB	2.06	0.55
1:D:346:ARG:NH2	1:D:354:ARG:HH12	2.05	0.55
1:A:116:LEU:HD12	5:A:810:HOH:O	2.07	0.54
1:C:217[B]:LYS:HE2	1:C:220:GLY:HA2	1.88	0.54
1:B:269:GLU:HG2	1:B:270:LEU:HD13	1.88	0.54
1:A:205:PRO:HB3	5:A:1114:HOH:O	2.06	0.54
1:D:176:HIS:O	1:D:177:VAL:HG23	2.08	0.53
1:B:151:ARG:NH1	5:B:871:HOH:O	2.41	0.53
1:A:205:PRO:HB2	1:A:215[A]:MET:HE1	1.90	0.53
1:A:162:GLU:H	1:A:162:GLU:CD	2.12	0.51
1:D:180:PRO:O	1:D:181:GLU:CB	2.58	0.51
1:D:80:ARG:NH1	5:D:735:HOH:O	2.38	0.51
1:D:176:HIS:C	1:D:177:VAL:HG23	2.31	0.51
1:D:8:THR:HG23	1:D:9:SER:N	2.28	0.49
1:D:116:LEU:HD12	5:D:876:HOH:O	2.11	0.49
1:B:66:GLN:NE2	5:B:717:HOH:O	2.44	0.49
1:C:403:SER:HB2	5:C:998:HOH:O	2.11	0.49
1:B:28:HIS:HD2	5:B:624:HOH:O	1.95	0.49
1:C:99[B]:LYS:HE2	1:C:103:GLN:NE2	2.28	0.48
1:D:80:ARG:HB2	1:D:82:GLU:HG3	1.96	0.48
1:C:205:PRO:CG	1:C:215[B]:MET:CE	2.91	0.47
1:D:75:GLY:HA2	1:D:80:ARG:HH22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217[B]:LYS:HG2	1:A:222:SER:OG	2.14	0.47
1:C:273[C]:ASN:HB3	5:C:748:HOH:O	2.15	0.47
1:C:286[B]:MET:HE2	5:C:958:HOH:O	2.15	0.47
1:A:352:LEU:HD12	5:A:813:HOH:O	2.16	0.46
1:C:99[A]:LYS:HE2	5:C:960[A]:HOH:O	2.15	0.46
5:C:750:HOH:O	1:D:267:HIS:HE1	1.99	0.46
1:B:366:LYS:HB2	1:B:366:LYS:NZ	2.31	0.45
1:A:286[B]:MET:HE3	1:A:384:GLY:O	2.16	0.45
1:B:337:HIS:O	3:B:502:EDO:H22	2.15	0.45
1:C:377:LYS:NZ	5:C:904:HOH:O	2.50	0.45
1:D:172:TRP:O	1:D:176:HIS:HD2	1.99	0.45
1:A:215[B]:MET:CE	1:A:215[B]:MET:HA	2.46	0.45
1:C:204[A]:ASN:OD1	5:C:843:HOH:O	2.20	0.45
1:B:174:ILE:O	1:B:177:VAL:HG23	2.18	0.44
1:A:342:HIS:HB2	3:A:502:EDO:H22	1.99	0.44
1:C:28:HIS:HD2	5:C:690:HOH:O	2.00	0.44
1:B:70:ALA:HA	1:B:293:GLN:HG2	2.00	0.43
1:A:346:ARG:HH22	1:A:354:ARG:HH12	1.65	0.43
1:D:176:HIS:O	1:D:177:VAL:CG2	2.66	0.43
1:B:199:ALA:O	1:B:203:THR:HG23	2.18	0.43
1:C:277[B]:GLU:HG3	1:C:328:ILE:HG23	1.99	0.43
1:A:77:THR:O	1:A:80:ARG:HG3	2.19	0.43
1:D:199:ALA:O	1:D:203:THR:HG23	2.19	0.43
1:A:139:ASP:OD2	1:A:391:HIS:HD2	2.00	0.43
1:B:190:LEU:C	1:B:190:LEU:HD23	2.40	0.42
1:A:366:LYS:HE3	1:A:366:LYS:HB2	1.75	0.42
1:C:286[B]:MET:CE	5:C:674:HOH:O	2.67	0.42
1:D:286:MET:CE	5:D:716:HOH:O	2.67	0.42
1:D:353:ILE:C	1:D:353:ILE:HD12	2.40	0.42
1:A:286[B]:MET:HE3	5:A:1098:HOH:O	2.11	0.42
1:B:269:GLU:HG2	1:B:270:LEU:CD1	2.50	0.42
1:D:366:LYS:NZ	1:D:366:LYS:HB2	2.34	0.42
1:C:162:GLU:CD	1:C:162:GLU:H	2.24	0.42
2:C:501:HEM:CMB	2:C:501:HEM:HBB2	2.50	0.42
1:B:28:HIS:HE1	5:B:761:HOH:O	2.02	0.41
1:B:179:ASN:HD22	1:B:179:ASN:HA	1.75	0.41
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	2.01	0.41
1:C:205:PRO:HG3	1:C:215[A]:MET:CE	2.51	0.41
1:D:352:LEU:HD12	5:D:826:HOH:O	2.20	0.41
1:A:273[A]:ASN:HB3	5:A:983:HOH:O	2.19	0.41
1:C:205:PRO:HB2	1:C:215[B]:MET:HE1	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:HD22	1:A:180:PRO:HD2	1.86	0.41
1:A:270:LEU:HD22	5:A:1061:HOH:O	2.19	0.41
1:B:210:MET:HA	1:B:213:VAL:HG22	2.02	0.41
1:C:178:GLU:O	1:C:179:ASN:HB2	2.21	0.41
1:C:286[A]:MET:HG3	5:C:695:HOH:O	2.21	0.41
1:B:173:ALA:HB1	1:B:186:ILE:CD1	2.49	0.41
1:D:190:LEU:HD23	1:D:190:LEU:C	2.41	0.41
1:A:8:THR:HG22	1:A:9:SER:N	2.36	0.40
1:B:179:ASN:CG	1:B:180:PRO:HD2	2.42	0.40
1:D:168:ARG:HG2	5:D:934:HOH:O	2.21	0.40
1:B:26:THR:HB	1:B:27:PRO:HD2	2.03	0.40
1:D:102:ARG:HD2	1:D:102:ARG:HA	1.92	0.40
1:A:346:ARG:NH2	1:A:354:ARG:HH12	2.19	0.40
1:B:77:THR:O	1:B:80:ARG:HG3	2.21	0.40
1:D:80:ARG:C	1:D:82:GLU:N	2.75	0.40
1:B:102:ARG:HD2	1:B:102:ARG:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	395/398 (99%)	389 (98%)	6 (2%)	0	100	100
1	B	390/398 (98%)	384 (98%)	6 (2%)	0	100	100
1	C	399/398 (100%)	389 (98%)	10 (2%)	0	100	100
1	D	392/398 (98%)	381 (97%)	11 (3%)	0	100	100
All	All	1576/1592 (99%)	1543 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	336/334 (101%)	333 (99%)	3 (1%)	78 56
1	B	331/334 (99%)	325 (98%)	6 (2%)	59 27
1	C	340/334 (102%)	338 (99%)	2 (1%)	86 70
1	D	335/334 (100%)	335 (100%)	0	100 100
All	All	1342/1336 (100%)	1331 (99%)	11 (1%)	81 61

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	97	VAL
1	A	107	LYS
1	B	65	ILE
1	B	86	PHE
1	B	178	GLU
1	B	179	ASN
1	B	186	ILE
1	B	202	ARG
1	C	80	ARG
1	C	187	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	179	ASN
1	A	327	ASN
1	A	351	HIS
1	A	391	HIS
1	B	28	HIS
1	B	66	GLN
1	B	176	HIS

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	267	HIS
1	B	351	HIS
1	B	391	HIS
1	C	28	HIS
1	C	66	GLN
1	C	176	HIS
1	C	267	HIS
1	C	327	ASN
1	C	351	HIS
1	C	391	HIS
1	D	66	GLN
1	D	103	GLN
1	D	176	HIS
1	D	267	HIS
1	D	273	ASN
1	D	327	ASN
1	D	351	HIS
1	D	391	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	EDO	C	502[B]	-	3,3,3	0.53	0	2,2,2	1.83	1 (50%)
3	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.32	0
3	EDO	C	502[A]	-	3,3,3	0.66	0	2,2,2	1.31	0
2	HEM	C	501	5,1	41,50,50	1.53	4 (9%)	45,82,82	1.73	11 (24%)
3	EDO	A	502	-	3,3,3	0.35	0	2,2,2	0.78	0
3	EDO	C	505	-	3,3,3	0.45	0	2,2,2	0.40	0
2	HEM	A	501	5,1	41,50,50	1.65	6 (14%)	45,82,82	1.69	9 (20%)
2	HEM	B	501	5,1	41,50,50	1.52	3 (7%)	45,82,82	1.47	5 (11%)
2	HEM	D	501	5,1	41,50,50	1.53	4 (9%)	45,82,82	1.40	4 (8%)
3	EDO	C	503	-	3,3,3	0.54	0	2,2,2	0.15	0

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	EDO	C	502[B]	-	-	1/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	C	502[A]	-	-	0/1/1/1	-
2	HEM	C	501	5,1	-	1/12/54/54	-
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	C	505	-	-	1/1/1/1	-
2	HEM	A	501	5,1	-	0/12/54/54	-
2	HEM	B	501	5,1	-	2/12/54/54	-
2	HEM	D	501	5,1	-	1/12/54/54	-
3	EDO	C	503	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-5.31	1.33	1.40
2	B	501	HEM	C3D-C2D	5.18	1.47	1.36
2	D	501	HEM	C3D-C2D	4.97	1.47	1.36
2	A	501	HEM	C3D-C2D	4.88	1.47	1.36
2	C	501	HEM	C3D-C2D	4.66	1.46	1.36
2	B	501	HEM	C3C-C2C	-4.59	1.34	1.40
2	D	501	HEM	C3C-C2C	-4.56	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C3C-C2C	-4.38	1.34	1.40
2	C	501	HEM	C3C-CAC	3.05	1.54	1.47
2	A	501	HEM	C3C-CAC	2.46	1.52	1.47
2	A	501	HEM	C2C-C1C	2.30	1.47	1.42
2	A	501	HEM	FE-NB	2.21	2.07	1.96
2	B	501	HEM	C3C-CAC	2.20	1.52	1.47
2	A	501	HEM	CAB-C3B	2.16	1.53	1.47
2	D	501	HEM	C3C-CAC	2.04	1.52	1.47
2	D	501	HEM	O2D-CGD	-2.01	1.24	1.30
2	C	501	HEM	FE-NB	2.00	2.06	1.96

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	C4D-ND-C1D	5.01	110.25	105.07
2	C	501	HEM	CMA-C3A-C4A	-4.59	121.41	128.46
2	A	501	HEM	C4D-ND-C1D	4.20	109.41	105.07
2	D	501	HEM	C4D-ND-C1D	4.11	109.32	105.07
2	A	501	HEM	C1B-NB-C4B	3.98	109.18	105.07
2	C	501	HEM	C4A-C3A-C2A	3.92	109.72	107.00
2	D	501	HEM	C4C-CHD-C1D	3.90	127.70	122.56
2	C	501	HEM	C1B-NB-C4B	3.28	108.46	105.07
2	A	501	HEM	CMA-C3A-C4A	-3.24	123.49	128.46
2	A	501	HEM	CMD-C2D-C1D	2.94	129.52	125.04
2	B	501	HEM	CHD-C1D-ND	2.89	127.57	124.43
2	D	501	HEM	CHC-C4B-NB	2.83	127.51	124.43
2	B	501	HEM	CAD-C3D-C4D	2.82	129.59	124.66
2	C	501	HEM	C4C-CHD-C1D	2.68	126.10	122.56
2	A	501	HEM	C4A-C3A-C2A	2.63	108.83	107.00
2	C	501	HEM	CAD-C3D-C4D	2.63	129.26	124.66
2	C	501	HEM	C4D-ND-C1D	2.60	107.76	105.07
3	C	502[B]	EDO	O2-C2-C1	-2.58	93.34	111.91
2	C	501	HEM	O1D-CGD-CBD	-2.54	114.93	123.08
2	A	501	HEM	CHD-C1D-ND	2.53	127.18	124.43
2	D	501	HEM	CMA-C3A-C4A	-2.38	124.81	128.46
2	C	501	HEM	C4B-CHC-C1C	2.36	125.67	122.56
2	C	501	HEM	C3B-C2B-C1B	2.29	108.19	106.49
2	C	501	HEM	CHC-C4B-NB	2.27	126.89	124.43
2	A	501	HEM	C4B-CHC-C1C	2.26	125.54	122.56
2	B	501	HEM	CHC-C4B-NB	2.21	126.83	124.43
2	A	501	HEM	C4C-CHD-C1D	2.21	125.47	122.56
2	A	501	HEM	CMB-C2B-C1B	-2.18	121.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	CMA-C3A-C2A	2.05	128.80	124.94
2	B	501	HEM	O2D-CGD-CBD	2.02	120.53	114.03

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502[B]	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
2	B	501	HEM	CAD-CBD-CGD-O2D
3	C	505	EDO	O1-C1-C2-O2
2	B	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D

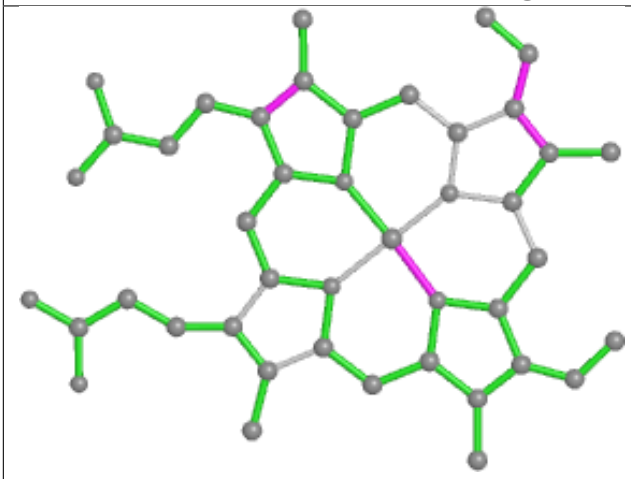
There are no ring outliers.

4 monomers are involved in 6 short contacts:

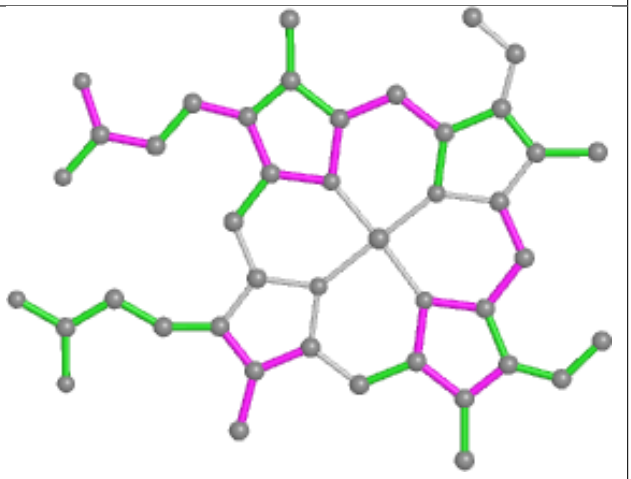
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	EDO	2	0
2	C	501	HEM	2	0
3	A	502	EDO	1	0
3	C	505	EDO	1	0

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.

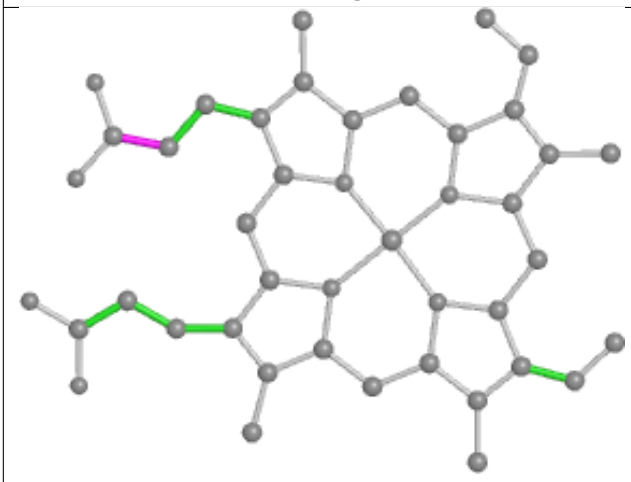
Ligand HEM C 501



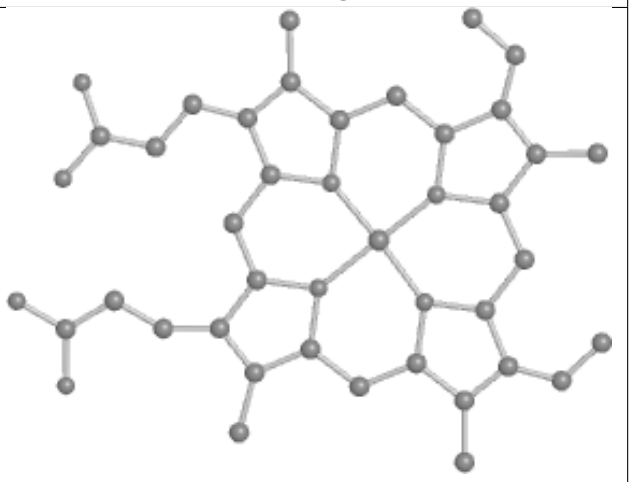
Bond lengths



Bond angles

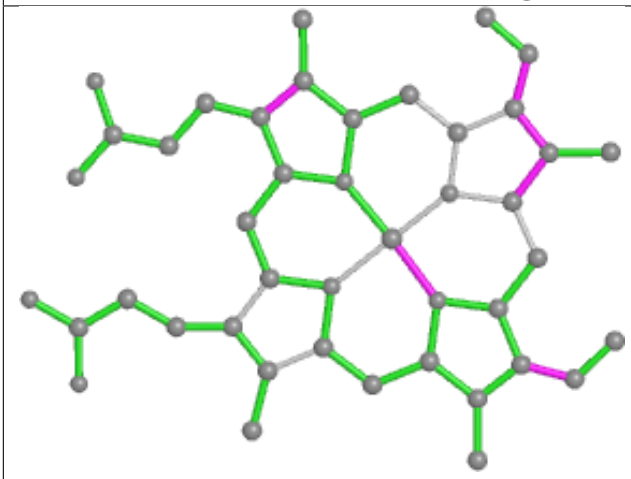


Torsions

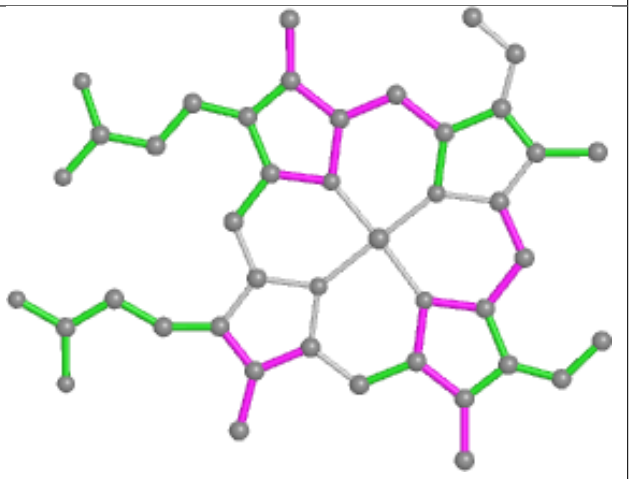


Rings

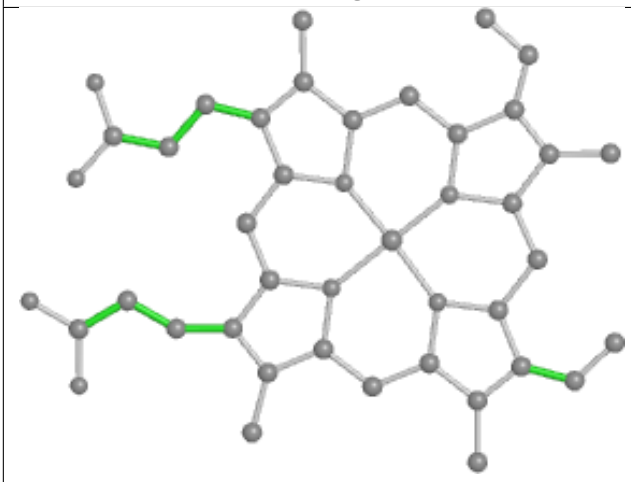
Ligand HEM A 501



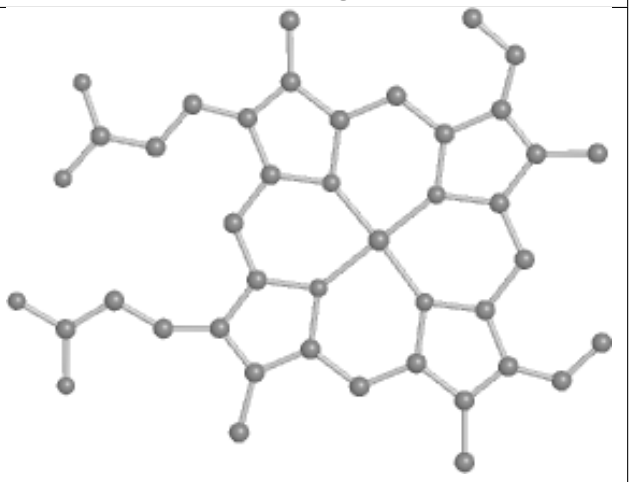
Bond lengths



Bond angles

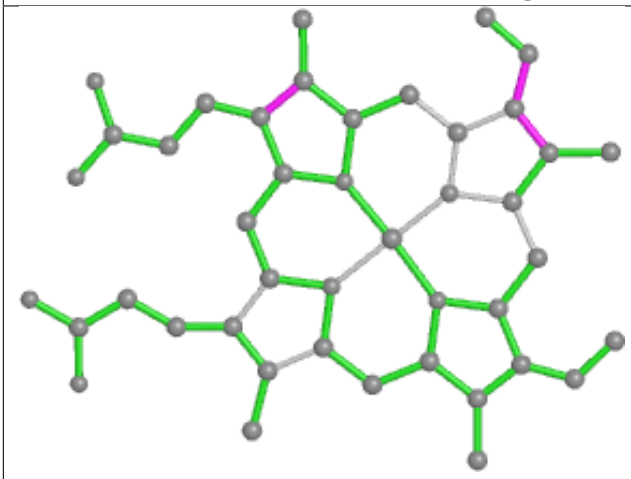


Torsions

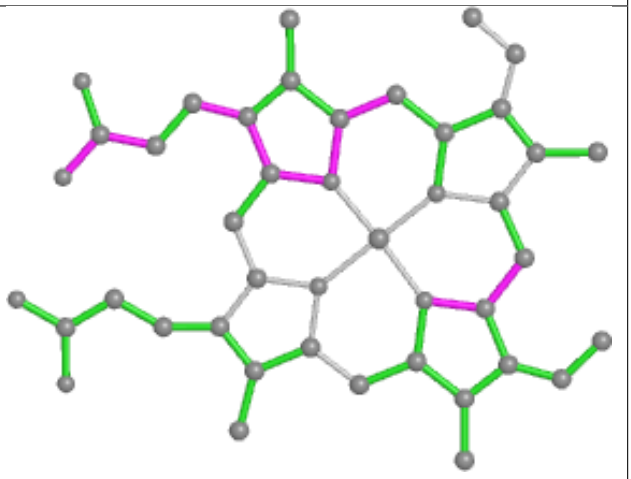


Rings

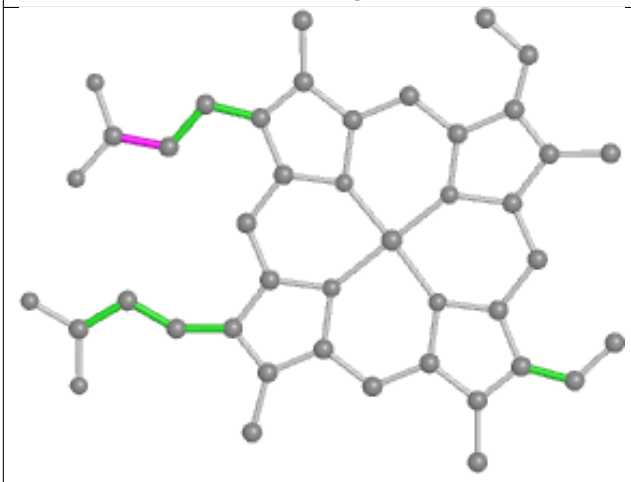
Ligand HEM B 501



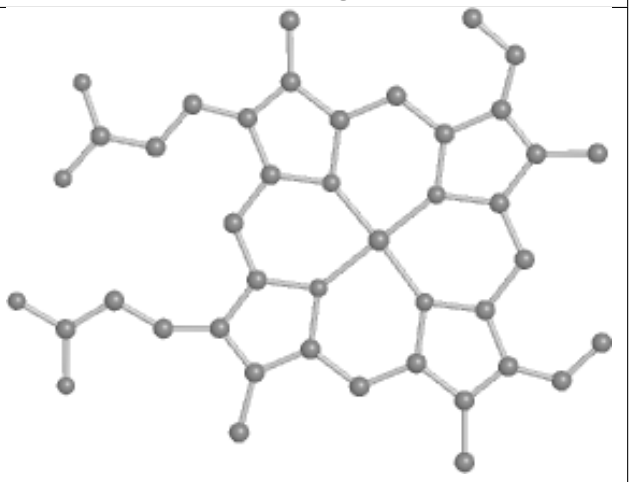
Bond lengths



Bond angles

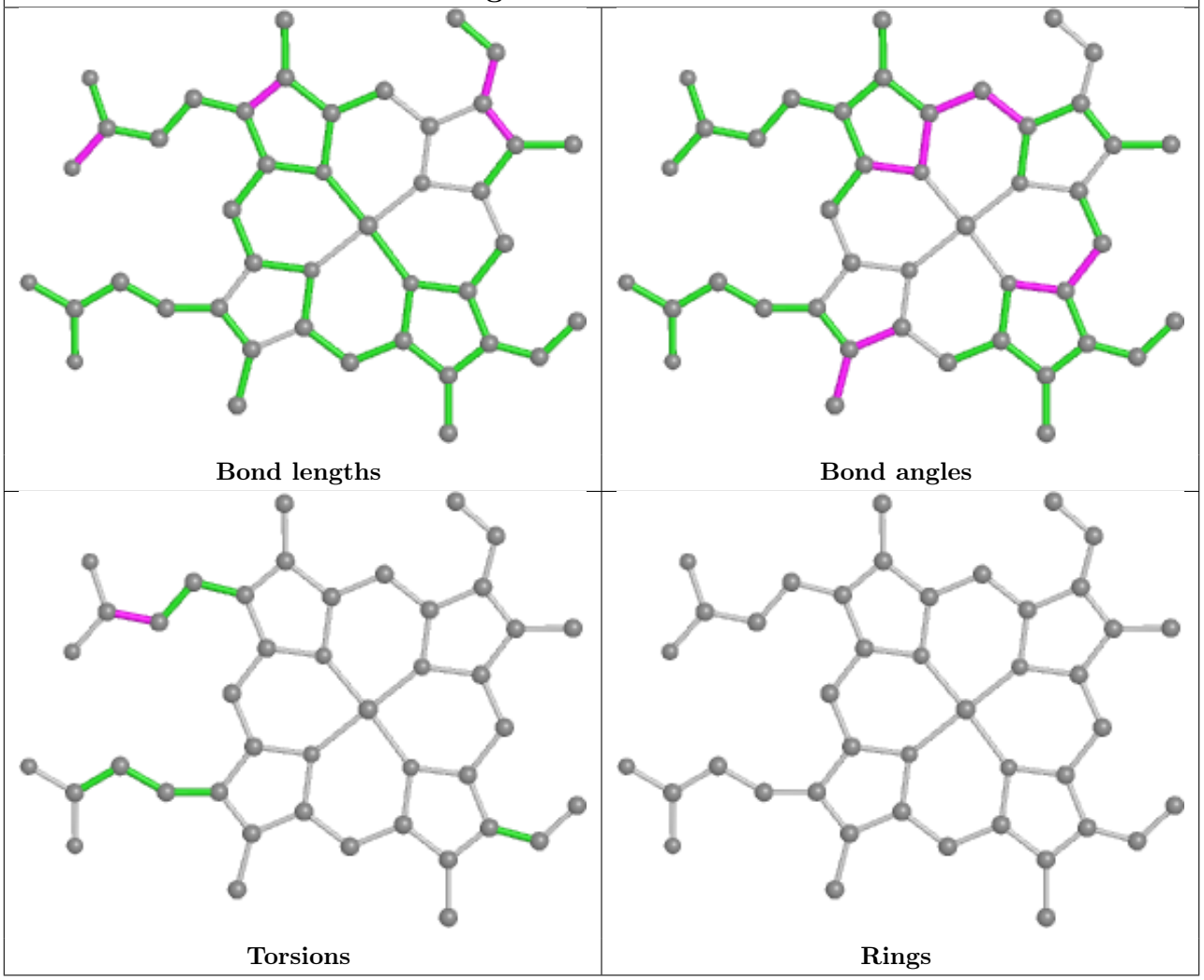


Torsions



Rings

Ligand HEM D 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	392/398 (98%)	-0.07	9 (2%)	60	63	9, 17, 33, 51	0
1	B	392/398 (98%)	0.30	30 (7%)	13	14	11, 22, 45, 67	0
1	C	391/398 (98%)	-0.01	13 (3%)	46	48	10, 17, 38, 66	0
1	D	391/398 (98%)	0.06	19 (4%)	29	30	11, 18, 43, 70	0
All	All	1566/1592 (98%)	0.07	71 (4%)	33	35	9, 18, 41, 70	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	VAL	10.7
1	A	81	TYR	10.2
1	B	177	VAL	9.8
1	B	81	TYR	9.1
1	B	180	PRO	8.3
1	D	180	PRO	8.2
1	C	177	VAL	7.7
1	B	8	THR	7.6
1	C	178	GLU	7.6
1	D	182	GLU	7.6
1	A	86	PHE	7.5
1	B	179	ASN	7.4
1	C	180	PRO	7.2
1	D	8	THR	7.1
1	D	181	GLU	6.1
1	B	403	SER	6.0
1	B	181	GLU	6.0
1	B	183	GLY	6.0
1	C	181	GLU	5.9
1	A	8	THR	5.7
1	C	86	PHE	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	187	PHE	5.5
1	B	186	ILE	5.5
1	B	178	GLU	5.2
1	A	403	SER	5.2
1	C	179	ASN	5.1
1	B	86	PHE	5.0
1	B	203	THR	4.9
1	D	86	PHE	4.8
1	D	81	TYR	4.8
1	B	182	GLU	4.8
1	B	184	ALA	4.8
1	B	172	TRP	4.5
1	D	172	TRP	4.4
1	B	204	ASN	4.2
1	D	186	ILE	4.2
1	C	403	SER	3.9
1	C	8	THR	3.8
1	D	183	GLY	3.5
1	D	185	GLU	3.5
1	A	97	VAL	3.5
1	D	184	ALA	3.3
1	B	160	PRO	3.2
1	C	402	LEU	3.1
1	B	185	GLU	3.1
1	D	169	ARG	3.0
1	A	402	LEU	3.0
1	D	82	GLU	2.9
1	D	403	SER	2.9
1	C	299	ASP	2.9
1	A	299	ASP	2.7
1	B	207	ASN	2.6
1	B	378	GLU	2.6
1	C	400	LYS	2.6
1	A	246	PHE	2.6
1	B	334	PRO	2.6
1	D	207	ASN	2.5
1	B	206	GLY	2.5
1	B	205	PRO	2.5
1	D	334	PRO	2.5
1	D	80	ARG	2.4
1	B	162	GLU	2.4
1	C	185	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	80	ARG	2.2
1	B	87	GLU	2.2
1	B	200	GLU	2.2
1	C	182	GLU	2.2
1	A	207	ASN	2.1
1	D	176	HIS	2.0
1	B	376	ASN	2.0
1	B	246	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

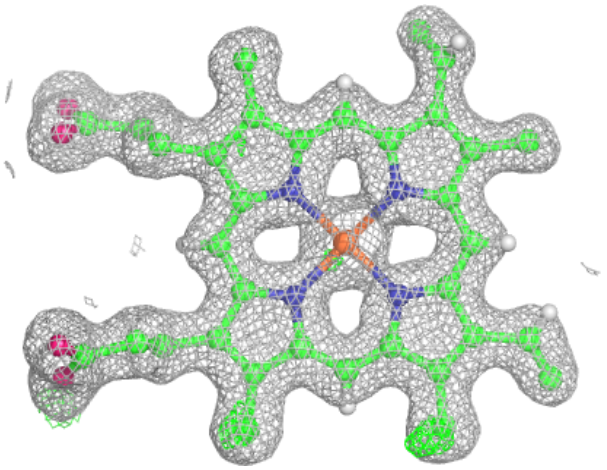
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

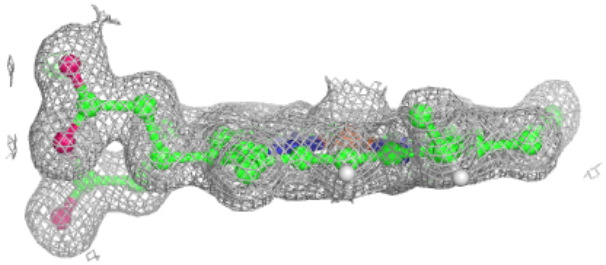
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	505	4/4	0.81	0.17	26,34,48,58	0
3	EDO	B	502	4/4	0.85	0.18	33,48,58,62	0
3	EDO	C	502[B]	4/4	0.91	0.16	26,34,40,40	2
3	EDO	C	502[A]	4/4	0.91	0.16	21,31,40,40	2
3	EDO	C	503	4/4	0.92	0.20	27,34,42,46	0
3	EDO	A	502	4/4	0.94	0.15	29,39,55,66	0
4	CL	B	503	1/1	0.97	0.07	29,29,29,29	0
4	CL	D	502	1/1	0.97	0.07	27,27,27,27	0
4	CL	C	504	1/1	0.98	0.04	25,25,25,25	0
2	HEM	B	501	43/43	0.99	0.13	11,14,20,26	0
4	CL	A	503	1/1	0.99	0.13	27,27,27,27	0
2	HEM	C	501	43/43	0.99	0.10	8,11,16,23	0
2	HEM	D	501	43/43	0.99	0.12	10,13,17,23	0
2	HEM	A	501	43/43	0.99	0.10	8,10,16,21	0

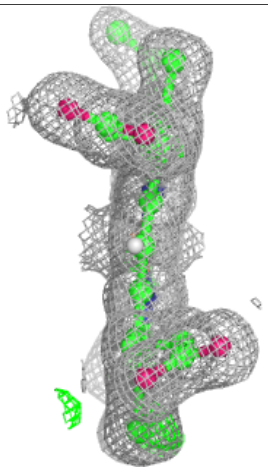
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM 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)

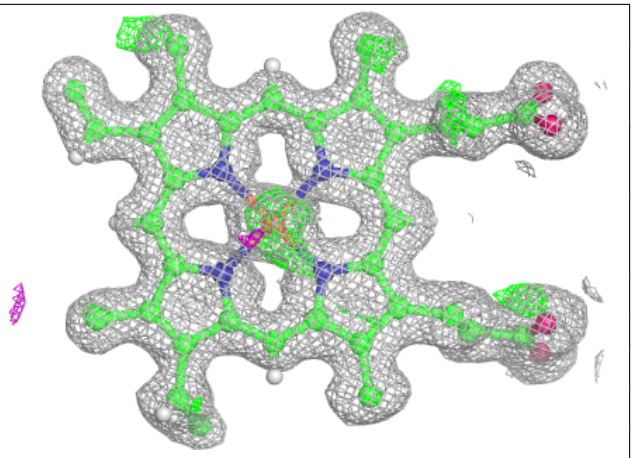


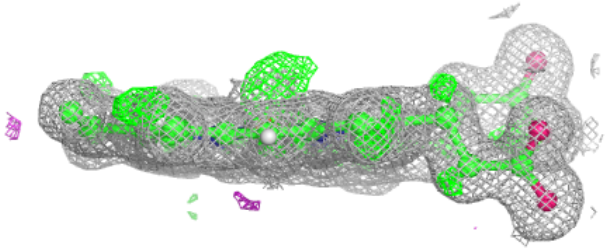


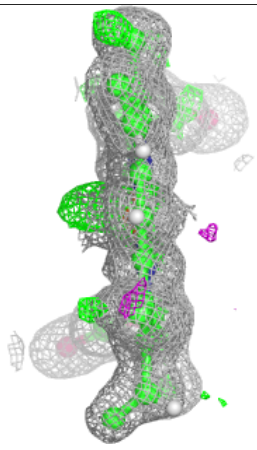


Electron density around HEM C 501:

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

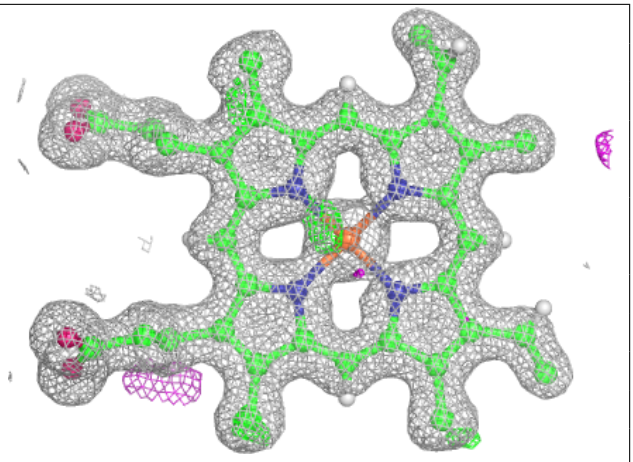


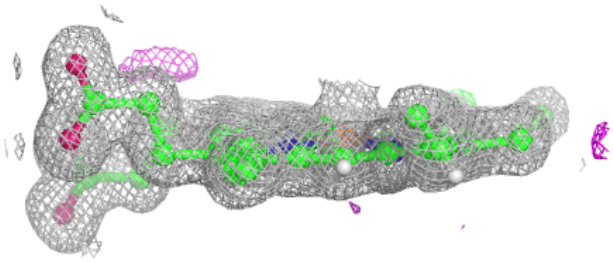


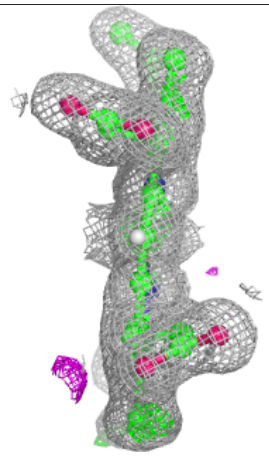


Electron density around HEM D 501:

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

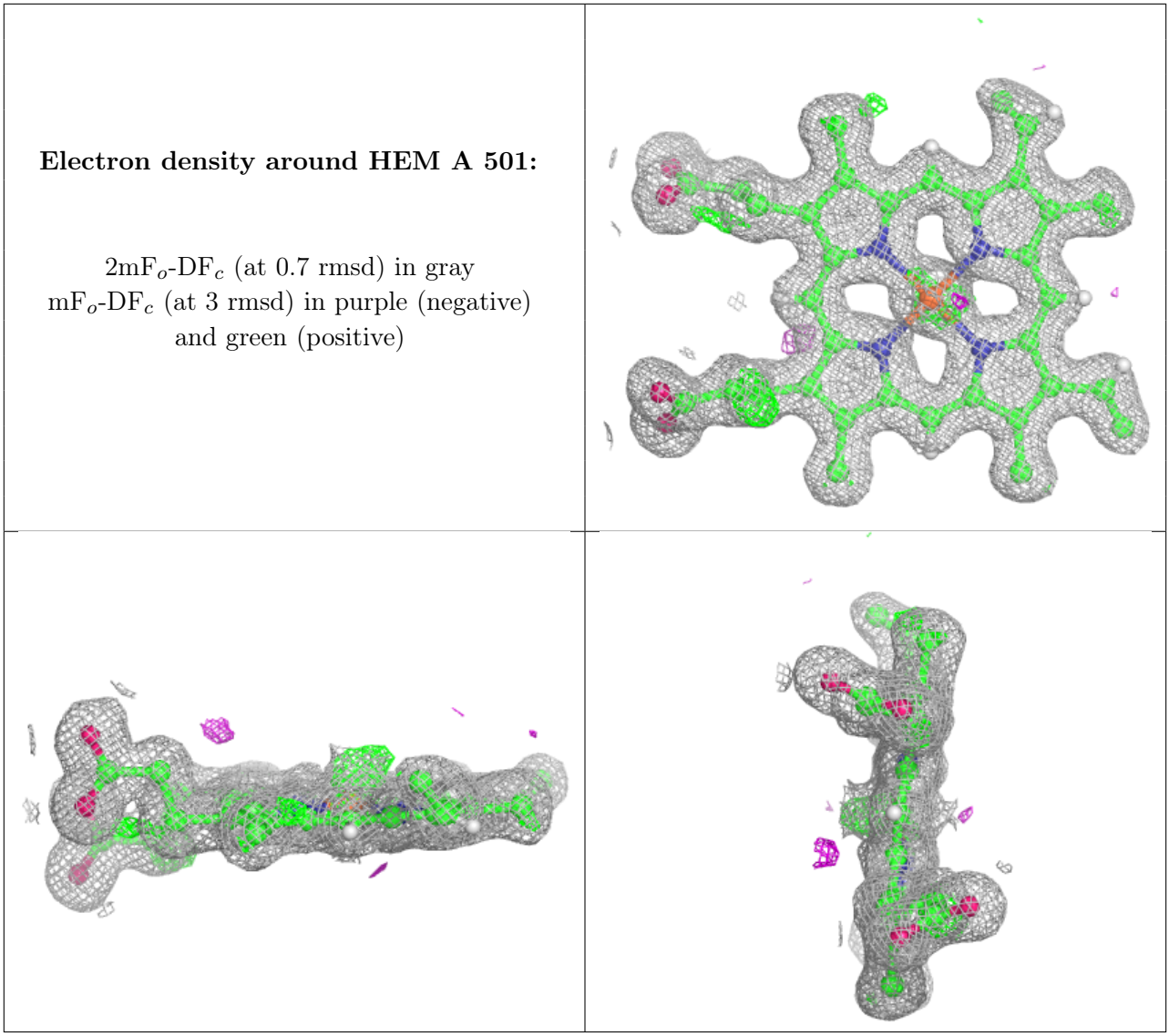






Electron density around HEM A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.