Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2022 – 03:14 pm GMT

PDB ID	:	7P6L
Title	:	Heme domain of CYP505A30, a fungal hydroxylase from Myceliophthora thermophila, bound to dodecanoic acid
Authors	:	Opperman, D.J.; Aschenbrenner, J.C.; Tolmie, C.; Ebrecht, A.C.
Deposited on	:	2021-07-16
Resolution	:	2.33 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:

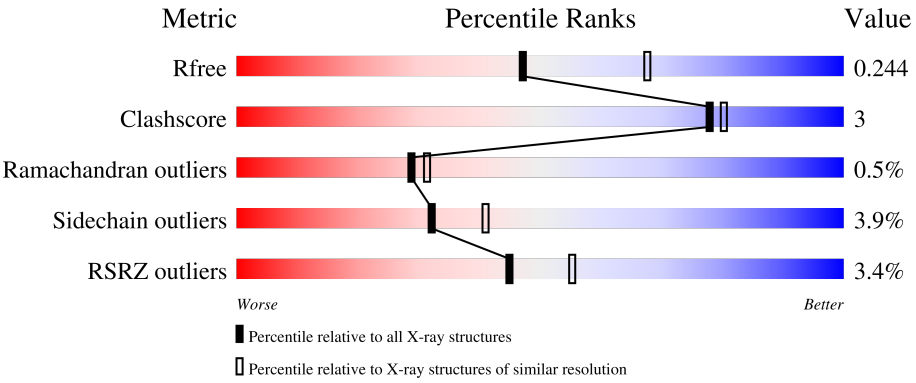
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	464	2% 88% 10% ·
1	B	464	2% 89% 9% ·
1	C	464	3% 86% 11% ••
1	D	464	7% 89% 9% ·

2 Entry composition

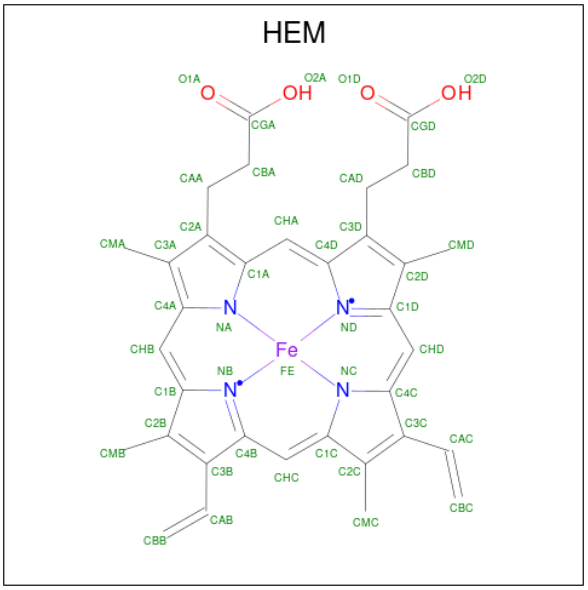
There are 4 unique types of molecules in this entry. The entry contains 14979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional cytochrome P450/NADPH–P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	458	Total	C	N	O	S	0	0	0
			3656	2343	633	663	17			
1	A	458	Total	C	N	O	S	0	0	0
			3656	2343	633	663	17			
1	C	458	Total	C	N	O	S	0	0	0
			3656	2343	633	663	17			
1	D	458	Total	C	N	O	S	0	0	0
			3656	2343	633	663	17			

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

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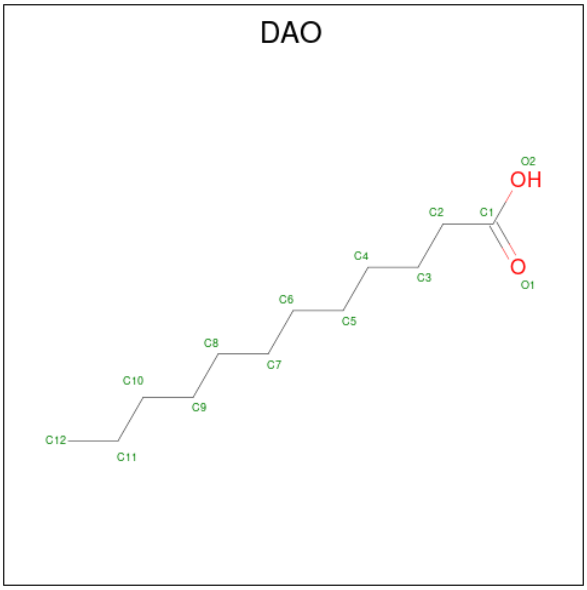
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C Fe N O 43 34 1 4 4	0	0
2	D	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 3 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 14 12 2	0	0
3	A	1	Total C O 14 12 2	0	0
3	C	1	Total C O 14 12 2	0	0
3	D	1	Total C O 14 12 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	32	Total O 32 32	0	0
4	A	38	Total O 38 38	0	0
4	C	32	Total O 32 32	0	0

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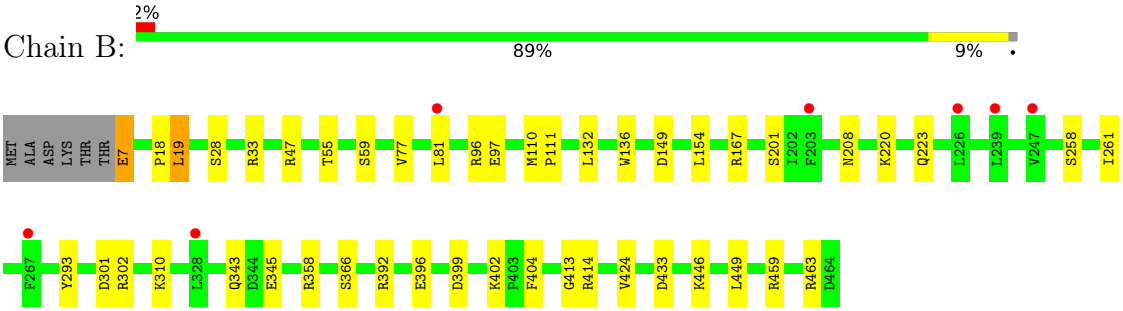
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	25	Total O 25 25	0	0

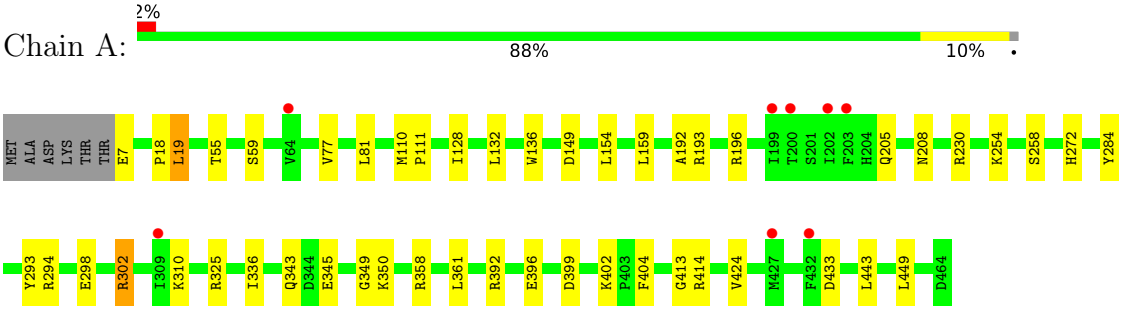
3 Residue-property plots (i)

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.

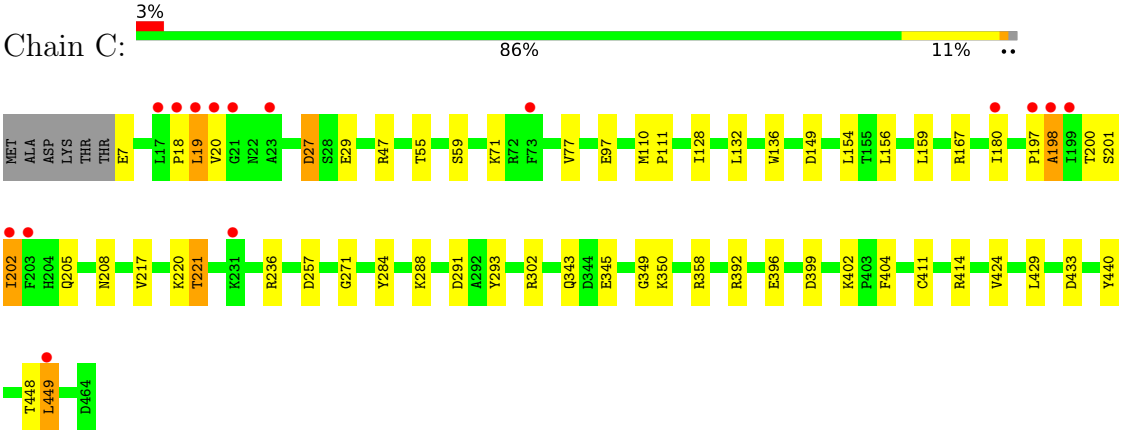
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase



• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

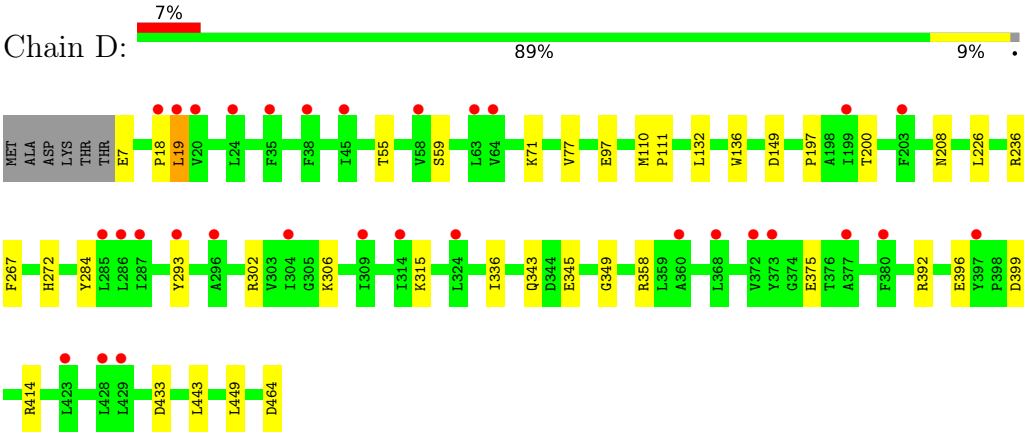


• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase



• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain D:


7%
89%
9%
MET ALA ASP LYS THR THR E7 P18 L19 V20 L24 F35 F38 I45 T55 V58 S59 L63 V64 K71 V77 E97 M110 P111 L132 W136 D149 P197 A198 I199 T200 F203 N208 L226 R236 L239 L244
F267 H272 Y284 L285 L286 I287 Y293 A296 R302 V303 I304 G305 K306 I309 I314 K315 L324 I336 Q343 D344 E345 G349 R358 L359 A360 L368 V372 Y373 G374 E375 T376 A377 F380 R392 E396 Y397 P398 D399 C400 W401 K402 P403 F404
R414 L423 L428 L429 D433 L443 L449 D464

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	171.49Å 171.49Å 175.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.43 – 2.33 61.35 – 2.33	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.43-2.33) 100.0 (61.35-2.33)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.203 , 0.234 0.215 , 0.244	Depositor DCC
R_{free} test set	5477 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	70.0	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14979	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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, DAO

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	0.72	0/3745	0.86	1/5080 (0.0%)
1	B	0.74	1/3745 (0.0%)	0.88	4/5080 (0.1%)
1	C	0.72	0/3745	0.90	1/5080 (0.0%)
1	D	0.73	0/3745	0.87	1/5080 (0.0%)
All	All	0.73	1/14980 (0.0%)	0.88	7/20320 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	366	SER	C-O	5.10	1.33	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	96	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	325	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	D	236	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	459	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	C	167	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	96	ARG	CG-CD-NE	-5.28	100.72	111.80
1	B	33	ARG	CG-CD-NE	5.20	122.72	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	201	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3656	0	3653	22	0
1	B	3656	0	3653	16	0
1	C	3656	0	3653	26	0
1	D	3656	0	3653	16	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	5	0
2	D	43	0	30	1	0
3	A	14	0	23	1	0
3	B	14	0	23	0	0
3	C	14	0	23	0	0
3	D	14	0	23	1	0
4	A	38	0	0	0	0
4	B	32	0	0	1	0
4	C	32	0	0	0	0
4	D	25	0	0	0	0
All	All	14979	0	14824	85	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 3.

All (85) 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:154:LEU:HD21	1:A:424:VAL:HG11	1.69	0.74
1:A:298:GLU:OE2	1:A:302:ARG:NH2	2.25	0.69
1:B:55:THR:HG23	1:B:358:ARG:HD3	1.76	0.67
1:C:217:VAL:O	1:C:221:THR:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HD21	1:C:424:VAL:HG21	1.79	0.64
1:B:7:GLU:N	1:B:7:GLU:OE2	2.34	0.61
1:A:55:THR:HG23	1:A:358:ARG:HD3	1.81	0.61
1:B:154:LEU:HD21	1:B:424:VAL:HG21	1.84	0.59
1:D:55:THR:HG23	1:D:358:ARG:HD3	1.85	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.87	0.57
1:A:413:GLY:HA3	2:A:501:HEM:C3C	2.40	0.56
1:C:19:LEU:HD23	1:C:20:VAL:HG13	1.87	0.56
1:C:197:PRO:C	1:C:198:ALA:O	2.44	0.55
1:C:55:THR:HG23	1:C:358:ARG:HD3	1.90	0.54
1:C:156:LEU:HD22	1:C:180:ILE:HD11	1.92	0.52
1:C:200:THR:O	1:C:200:THR:HG22	2.09	0.52
1:B:343:GLN:O	1:B:345:GLU:HG2	2.11	0.51
1:C:343:GLN:O	1:C:345:GLU:HG2	2.11	0.50
1:A:343:GLN:O	1:A:345:GLU:HG2	2.12	0.50
1:A:298:GLU:CD	1:A:302:ARG:HH21	2.15	0.49
1:D:343:GLN:O	1:D:345:GLU:HG2	2.13	0.49
1:C:159:LEU:C	1:C:159:LEU:HD13	2.33	0.49
1:D:306:LYS:HE3	1:D:464:ASP:OD1	2.13	0.48
1:B:293:TYR:OH	1:B:433:ASP:HA	2.13	0.48
1:A:336:ILE:HB	3:A:502:DAO:H21	1.96	0.47
2:A:501:HEM:HMC2	2:A:501:HEM:HBC2	1.98	0.46
1:C:271:GLY:HA2	2:C:501:HEM:C3C	2.51	0.46
1:C:399:ASP:HA	1:C:402:LYS:HD3	1.98	0.46
1:C:197:PRO:O	1:C:198:ALA:O	2.33	0.46
1:D:284:TYR:CE2	1:D:443:LEU:HB2	2.51	0.45
1:D:392:ARG:NH2	1:D:396:GLU:OE1	2.49	0.45
1:C:284:TYR:CZ	1:C:288:LYS:HG3	2.52	0.45
1:B:392:ARG:NH2	1:B:396:GLU:OE1	2.49	0.44
1:A:18:PRO:O	1:A:19:LEU:HB2	2.16	0.44
1:C:271:GLY:HA2	2:C:501:HEM:C2C	2.52	0.44
1:A:193:ARG:NH1	1:C:27:ASP:OD2	2.50	0.44
1:D:404:PHE:CG	1:D:414:ARG:HG3	2.53	0.44
1:D:399:ASP:HA	1:D:402:LYS:HD3	2.00	0.44
1:A:110:MET:N	1:A:111:PRO:CD	2.81	0.43
1:C:293:TYR:OH	1:C:433:ASP:HA	2.17	0.43
1:D:239:LEU:HD21	1:D:267:PHE:CD2	2.54	0.43
1:B:404:PHE:CG	1:B:414:ARG:HG3	2.53	0.43
1:C:404:PHE:CG	1:C:414:ARG:HG3	2.53	0.43
1:A:293:TYR:OH	1:A:433:ASP:HA	2.19	0.43
1:A:404:PHE:CG	1:A:414:ARG:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:C	1:A:159:LEU:HD13	2.39	0.43
1:D:110:MET:N	1:D:111:PRO:CD	2.82	0.42
1:B:110:MET:N	1:B:111:PRO:CD	2.82	0.42
1:A:128:ILE:HG22	1:A:154:LEU:HD12	2.02	0.42
1:A:284:TYR:CE2	1:A:443:LEU:HB2	2.55	0.42
1:A:392:ARG:NH2	1:A:396:GLU:OE1	2.53	0.42
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	2.01	0.42
1:B:18:PRO:O	1:B:19:LEU:HB2	2.19	0.42
1:C:411:CYS:HB2	2:C:501:HEM:NA	2.33	0.42
1:A:230:ARG:HG2	1:C:440:TYR:CZ	2.55	0.42
1:D:132:LEU:HD11	1:D:136:TRP:CE2	2.55	0.41
1:B:223:GLN:OE1	1:B:261:ILE:HD11	2.19	0.41
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.50	0.41
1:C:128:ILE:HG22	1:C:154:LEU:HD12	2.02	0.41
1:A:399:ASP:HA	1:A:402:LYS:HD3	2.03	0.41
1:C:18:PRO:O	1:C:19:LEU:HB3	2.19	0.41
1:D:336:ILE:HB	3:D:502:DAO:H21	2.01	0.41
1:C:110:MET:N	1:C:111:PRO:CD	2.84	0.41
1:C:448:THR:O	1:C:449:LEU:HB2	2.21	0.41
1:B:413:GLY:HA3	2:B:501:HEM:C3C	2.56	0.41
1:D:197:PRO:HG2	1:D:200:THR:HG23	2.03	0.41
1:B:399:ASP:HA	1:B:402:LYS:HD3	2.01	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.51	0.41
1:C:132:LEU:HD11	1:C:136:TRP:CE2	2.56	0.41
1:B:132:LEU:HD11	1:B:136:TRP:CE2	2.56	0.41
1:B:167:ARG:HA	4:B:623:HOH:O	2.21	0.41
1:A:132:LEU:HD11	1:A:136:TRP:CE2	2.55	0.41
1:D:18:PRO:O	1:D:19:LEU:HB2	2.21	0.41
1:D:239:LEU:HD21	1:D:267:PHE:CG	2.56	0.41
1:A:192:ALA:O	1:A:196:ARG:HB2	2.21	0.40
1:D:293:TYR:OH	1:D:433:ASP:HA	2.21	0.40
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.77	0.40
1:B:301:ASP:OD1	1:B:463:ARG:NH2	2.52	0.40
1:C:392:ARG:NH2	1:C:396:GLU:OE1	2.55	0.40
1:C:429:LEU:HD23	1:C:429:LEU:HA	1.98	0.40
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.81	0.40
1:A:361:LEU:N	1:A:361:LEU:HD12	2.36	0.40
2:C:501:HEM:HBC2	2:C:501:HEM:CMC	2.51	0.40
1:D:226:LEU:HD11	1:D:244:LEU:HD21	2.04	0.40
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.51	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	456/464 (98%)	436 (96%)	18 (4%)	2 (0%)	34	38
1	B	456/464 (98%)	440 (96%)	15 (3%)	1 (0%)	47	55
1	C	456/464 (98%)	437 (96%)	15 (3%)	4 (1%)	17	17
1	D	456/464 (98%)	439 (96%)	15 (3%)	2 (0%)	34	38
All	All	1824/1856 (98%)	1752 (96%)	63 (4%)	9 (0%)	29	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	ALA
1	C	202	ILE
1	A	349	GLY
1	D	77	VAL
1	A	77	VAL
1	C	77	VAL
1	B	77	VAL
1	D	349	GLY
1	C	349	GLY

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	388/393 (99%)	374 (96%)	14 (4%)	35	44
1	B	388/393 (99%)	373 (96%)	15 (4%)	32	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	388/393 (99%)	368 (95%)	20 (5%)	23 28
1	D	388/393 (99%)	376 (97%)	12 (3%)	40 49
All	All	1552/1572 (99%)	1491 (96%)	61 (4%)	32 41

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	GLU
1	B	19	LEU
1	B	28	SER
1	B	47	ARG
1	B	59	SER
1	B	97	GLU
1	B	149	ASP
1	B	201	SER
1	B	208	ASN
1	B	220	LYS
1	B	258	SER
1	B	302	ARG
1	B	310	LYS
1	B	446	LYS
1	B	449	LEU
1	A	7	GLU
1	A	19	LEU
1	A	59	SER
1	A	149	ASP
1	A	205	GLN
1	A	208	ASN
1	A	254	LYS
1	A	258	SER
1	A	272	HIS
1	A	294	ARG
1	A	302	ARG
1	A	310	LYS
1	A	350	LYS
1	A	449	LEU
1	C	7	GLU
1	C	19	LEU
1	C	27	ASP
1	C	29	GLU
1	C	47	ARG

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Mol	Chain	Res	Type
1	C	59	SER
1	C	71	LYS
1	C	97	GLU
1	C	149	ASP
1	C	202	ILE
1	C	205	GLN
1	C	208	ASN
1	C	220	LYS
1	C	221	THR
1	C	236	ARG
1	C	257	ASP
1	C	291	ASP
1	C	302	ARG
1	C	350	LYS
1	C	449	LEU
1	D	7	GLU
1	D	19	LEU
1	D	59	SER
1	D	71	LYS
1	D	97	GLU
1	D	149	ASP
1	D	208	ASN
1	D	272	HIS
1	D	302	ARG
1	D	315	LYS
1	D	375	GLU
1	D	449	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	D	365	GLN

5.3.3 RNA

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)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DAO	B	502	-	10,13,13	0.69	0	9,13,13	0.42	0
2	HEM	C	501	1	27,50,50	1.02	2 (7%)	17,82,82	1.38	4 (23%)
2	HEM	D	501	1	27,50,50	1.21	2 (7%)	17,82,82	1.67	5 (29%)
3	DAO	D	502	-	10,13,13	0.46	0	9,13,13	0.37	0
2	HEM	A	501	1	27,50,50	0.75	0	17,82,82	1.64	4 (23%)
3	DAO	A	502	-	10,13,13	0.31	0	9,13,13	0.38	0
3	DAO	C	502	-	10,13,13	0.37	0	9,13,13	0.40	0
2	HEM	B	501	1	27,50,50	1.27	3 (11%)	17,82,82	1.77	5 (29%)

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	DAO	B	502	-	-	5/9/11/11	-
2	HEM	C	501	1	-	0/6/54/54	-
2	HEM	D	501	1	-	0/6/54/54	-
3	DAO	D	502	-	-	5/9/11/11	-
2	HEM	A	501	1	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAO	A	502	-	-	3/9/11/11	-
3	DAO	C	502	-	-	4/9/11/11	-
2	HEM	B	501	1	-	0/6/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-C2C	-3.41	1.35	1.40
2	D	501	HEM	C3B-C2B	-3.36	1.35	1.40
2	D	501	HEM	C3D-C4D	3.15	1.49	1.42
2	B	501	HEM	C3D-C4D	2.25	1.47	1.42
2	C	501	HEM	C3D-C4D	2.19	1.47	1.42
2	B	501	HEM	C3B-CAB	2.19	1.52	1.47
2	C	501	HEM	C1A-NA	2.01	1.40	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	C4A-C3A-C2A	3.24	109.25	107.00
2	A	501	HEM	CMA-C3A-C4A	-3.15	123.63	128.46
2	D	501	HEM	CAD-CBD-CGD	2.99	117.68	112.67
2	D	501	HEM	CBA-CAA-C2A	-2.92	107.10	112.49
2	D	501	HEM	CBD-CAD-C3D	-2.77	107.37	112.48
2	A	501	HEM	CMB-C2B-C3B	2.76	129.84	124.68
2	B	501	HEM	C2C-C3C-C4C	-2.73	104.99	106.90
2	B	501	HEM	CMA-C3A-C2A	-2.67	119.91	124.94
2	B	501	HEM	C1D-C2D-C3D	-2.47	105.28	107.00
2	C	501	HEM	CMB-C2B-C3B	2.40	129.16	124.68
2	A	501	HEM	CMD-C2D-C1D	-2.34	124.87	128.46
2	D	501	HEM	CMC-C2C-C3C	2.22	128.84	124.68
2	C	501	HEM	C1D-C2D-C3D	-2.15	105.50	107.00
2	C	501	HEM	CMA-C3A-C4A	-2.10	125.23	128.46
2	B	501	HEM	CMD-C2D-C1D	2.06	131.63	128.46
2	A	501	HEM	CBD-CAD-C3D	-2.06	108.69	112.48
2	D	501	HEM	CMB-C2B-C3B	2.04	128.49	124.68
2	C	501	HEM	C2C-C3C-C4C	-2.02	105.49	106.90

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	DAO	C1-C2-C3-C4
3	D	502	DAO	C1-C2-C3-C4
3	D	502	DAO	C3-C4-C5-C6
3	A	502	DAO	C3-C4-C5-C6
3	C	502	DAO	C11-C10-C9-C8
3	B	502	DAO	C4-C5-C6-C7
3	C	502	DAO	C2-C3-C4-C5
3	B	502	DAO	C3-C4-C5-C6
3	D	502	DAO	C5-C6-C7-C8
3	D	502	DAO	C7-C8-C9-C10
3	A	502	DAO	C11-C10-C9-C8
3	B	502	DAO	C11-C10-C9-C8
3	A	502	DAO	C1-C2-C3-C4
3	C	502	DAO	C9-C10-C11-C12
3	B	502	DAO	C7-C8-C9-C10
3	D	502	DAO	C11-C10-C9-C8
3	C	502	DAO	C3-C4-C5-C6

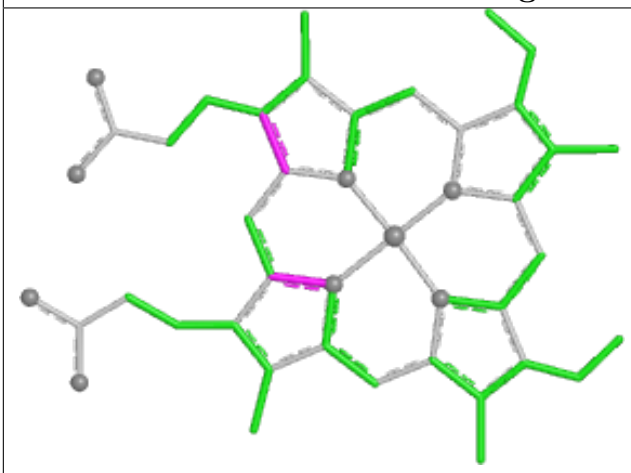
There are no ring outliers.

6 monomers are involved in 14 short contacts:

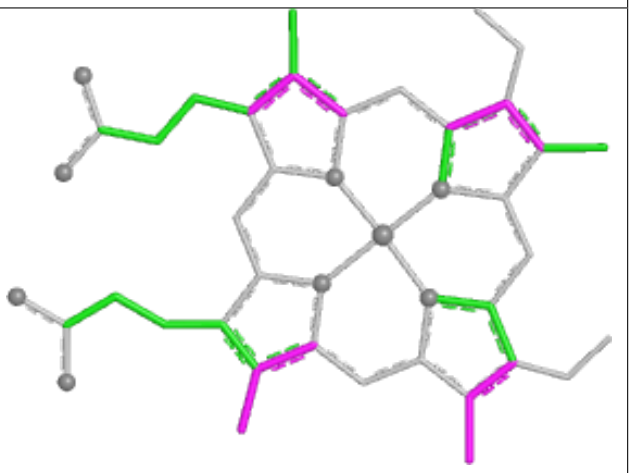
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	5	0
2	D	501	HEM	1	0
3	D	502	DAO	1	0
2	A	501	HEM	4	0
3	A	502	DAO	1	0
2	B	501	HEM	2	0

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.

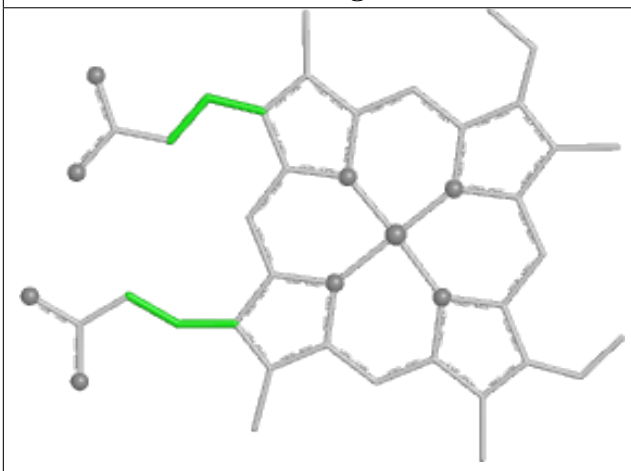
Ligand HEM C 501



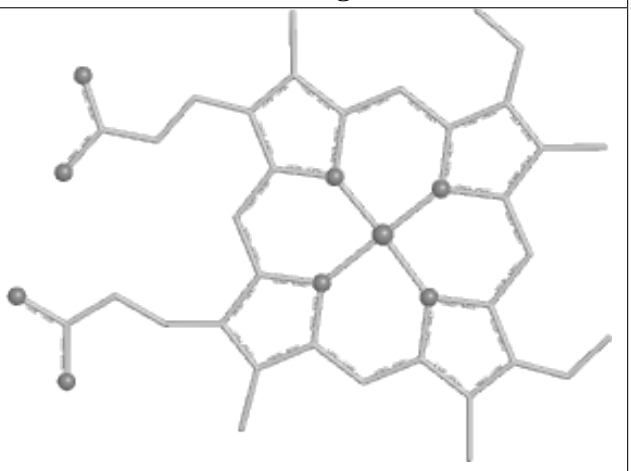
Bond lengths



Bond angles

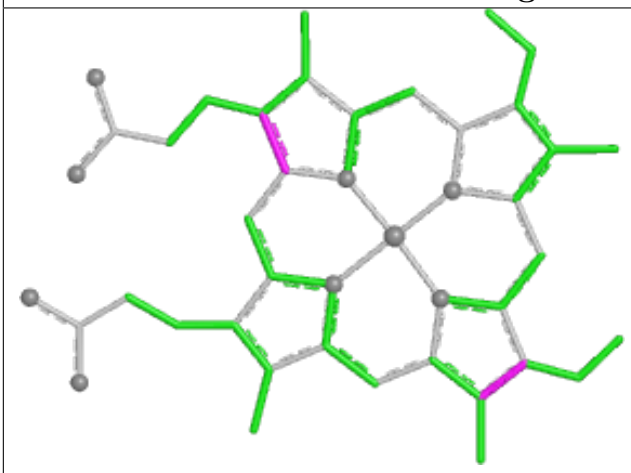


Torsions

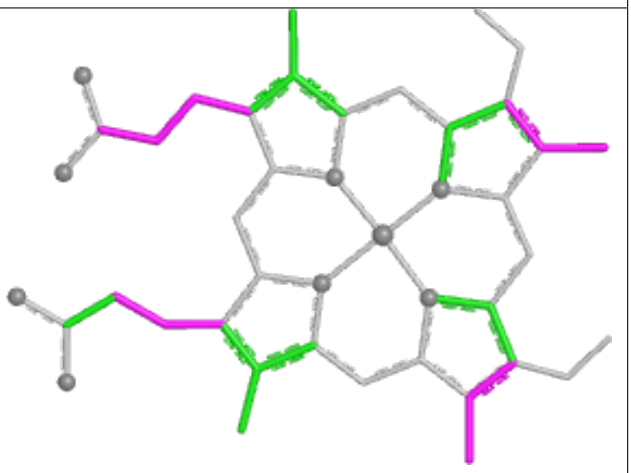


Rings

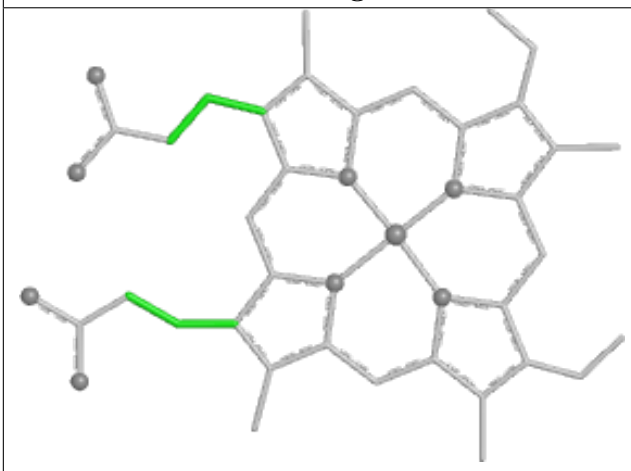
Ligand HEM D 501



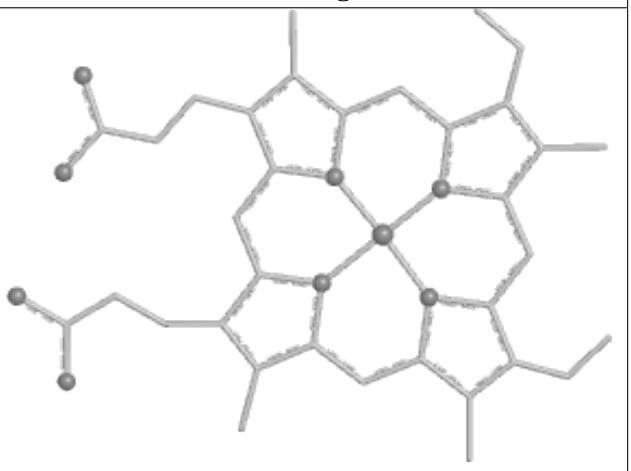
Bond lengths



Bond angles

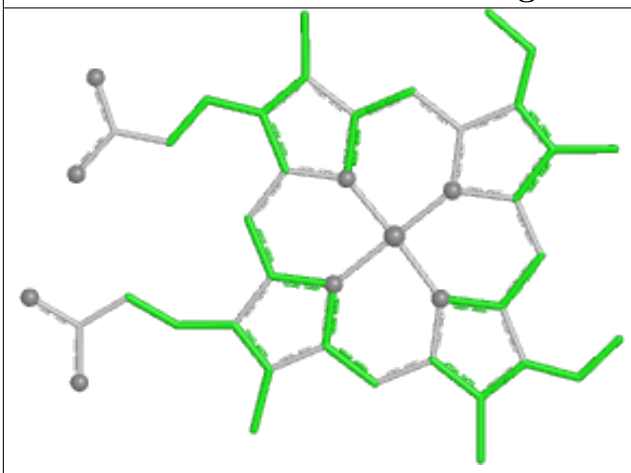


Torsions

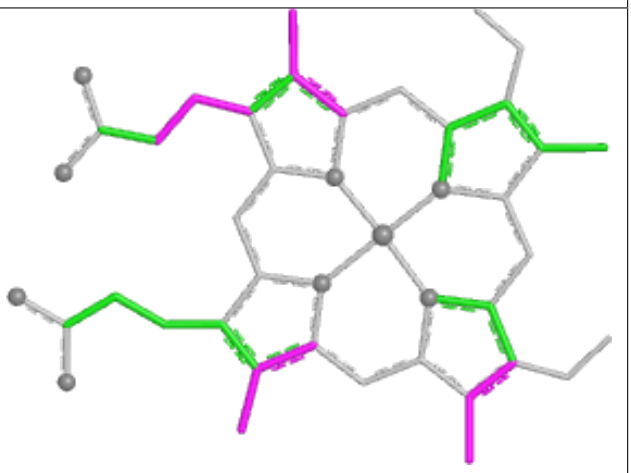


Rings

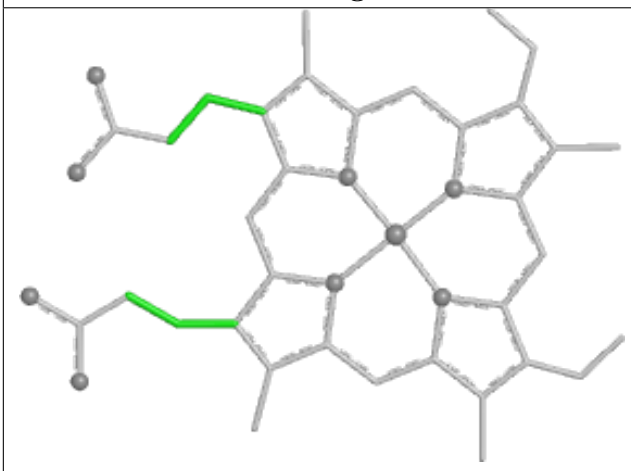
Ligand HEM A 501



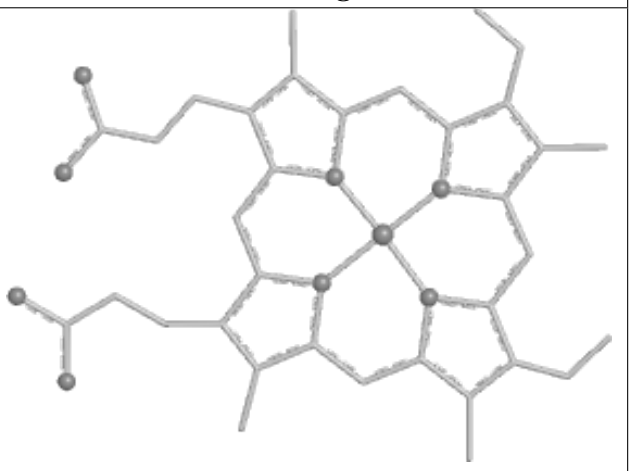
Bond lengths



Bond angles

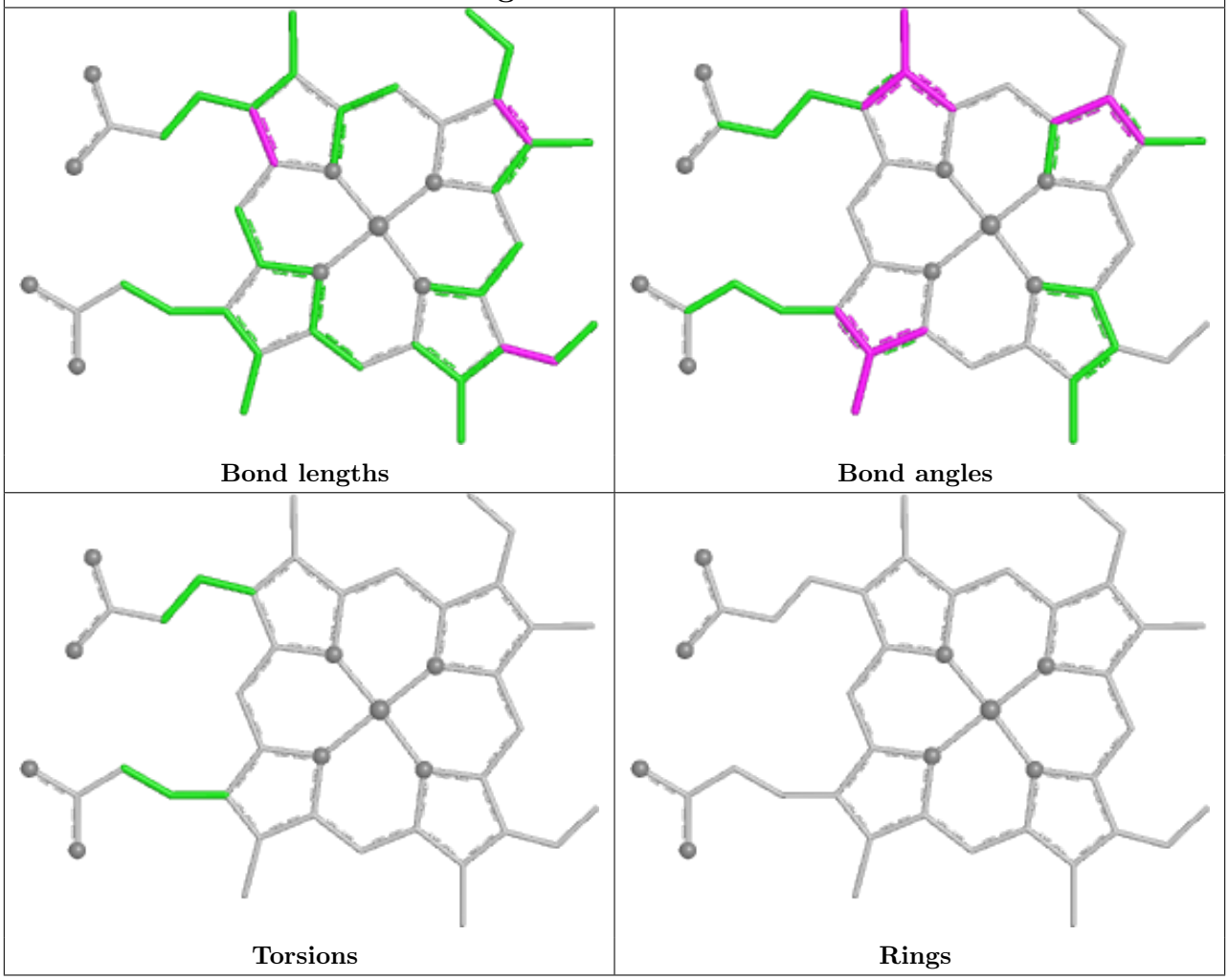


Torsions



Rings

Ligand HEM B 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	458/464 (98%)	0.36	8 (1%)	70	78	60, 80, 109, 145	0
1	B	458/464 (98%)	0.32	7 (1%)	73	81	60, 82, 107, 149	0
1	C	458/464 (98%)	0.38	15 (3%)	46	57	58, 88, 131, 193	0
1	D	458/464 (98%)	0.57	32 (6%)	16	24	60, 93, 132, 163	0
All	All	1832/1856 (98%)	0.40	62 (3%)	45	55	58, 84, 125, 193	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	LEU	7.3
1	C	199	ILE	7.0
1	C	202	ILE	5.3
1	C	197	PRO	5.0
1	C	21	GLY	4.8
1	D	377	ALA	4.7
1	A	203	PHE	4.6
1	D	373	TYR	4.1
1	A	202	ILE	3.7
1	C	18	PRO	3.6
1	A	199	ILE	3.5
1	D	35	PHE	3.5
1	C	203	PHE	3.4
1	B	247	VAL	3.4
1	D	285	LEU	3.2
1	D	19	LEU	3.2
1	D	314	ILE	3.2
1	D	20	VAL	3.2
1	D	63	LEU	3.2
1	C	180	ILE	3.1
1	D	380	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	45	ILE	3.1
1	A	200	THR	3.1
1	D	287	ILE	3.0
1	D	18	PRO	2.9
1	D	401	TRP	2.8
1	C	449	LEU	2.8
1	D	203	PHE	2.7
1	C	17	LEU	2.6
1	D	368	LEU	2.6
1	D	429	LEU	2.6
1	C	23	ALA	2.6
1	C	231	LYS	2.5
1	D	58	VAL	2.5
1	B	226	LEU	2.5
1	B	81	LEU	2.5
1	D	38	PHE	2.4
1	D	397	TYR	2.3
1	D	428	LEU	2.3
1	A	64	VAL	2.3
1	D	286	LEU	2.3
1	D	296	ALA	2.3
1	D	372	VAL	2.3
1	C	198	ALA	2.3
1	D	309	ILE	2.3
1	B	328	LEU	2.2
1	D	199	ILE	2.2
1	D	24	LEU	2.2
1	B	267	PHE	2.2
1	A	432	PHE	2.2
1	C	20	VAL	2.1
1	D	64	VAL	2.1
1	C	73	PHE	2.1
1	D	324	LEU	2.1
1	B	203	PHE	2.1
1	D	304	ILE	2.1
1	D	360	ALA	2.1
1	D	293	TYR	2.1
1	A	309	ILE	2.1
1	D	423	LEU	2.1
1	B	239	LEU	2.0
1	A	427	MET	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)

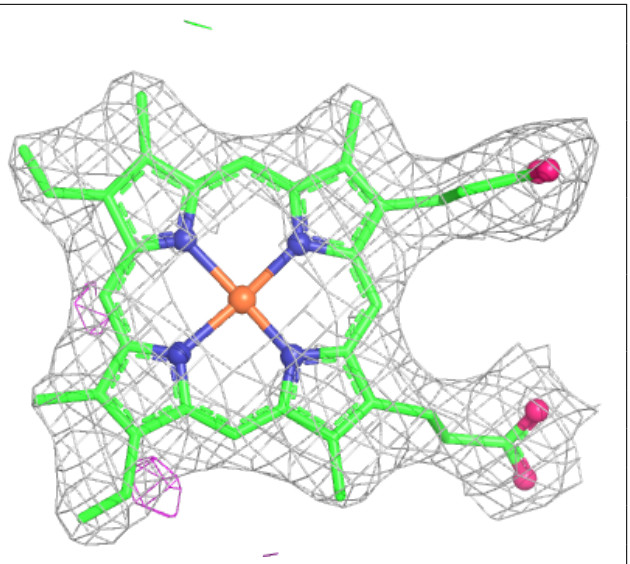
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

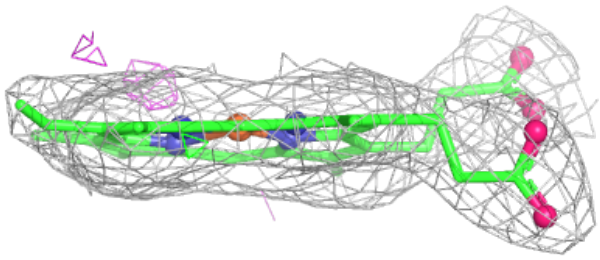
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DAO	C	502	14/14	0.82	0.25	89,96,110,113	0
3	DAO	D	502	14/14	0.82	0.42	79,91,115,116	0
3	DAO	A	502	14/14	0.84	0.27	67,70,98,99	0
3	DAO	B	502	14/14	0.86	0.21	79,84,98,100	0
2	HEM	C	501	43/43	0.97	0.15	66,70,74,79	0
2	HEM	D	501	43/43	0.97	0.16	73,81,86,87	0
2	HEM	B	501	43/43	0.98	0.16	66,79,84,87	0
2	HEM	A	501	43/43	0.98	0.16	62,66,72,75	0

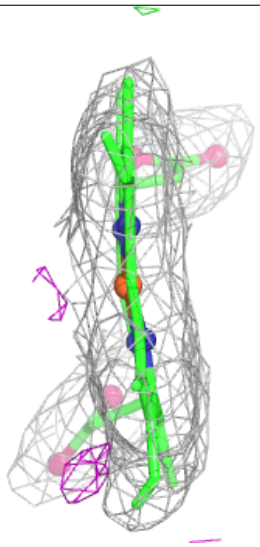
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM C 501:

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

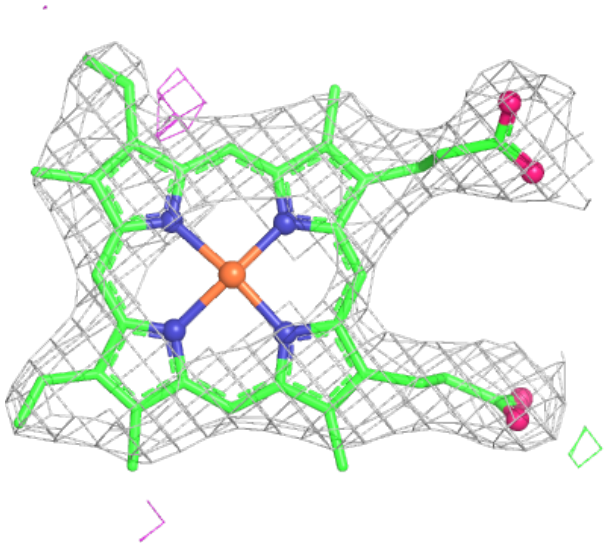


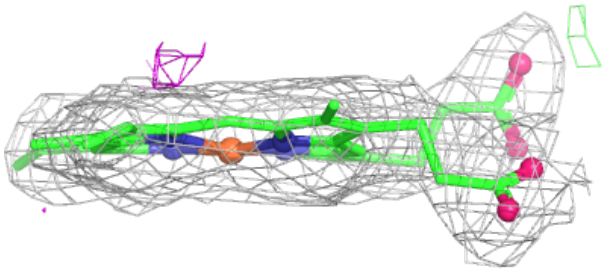


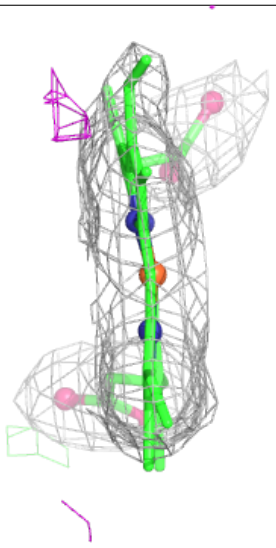


Electron density around HEM D 501:

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

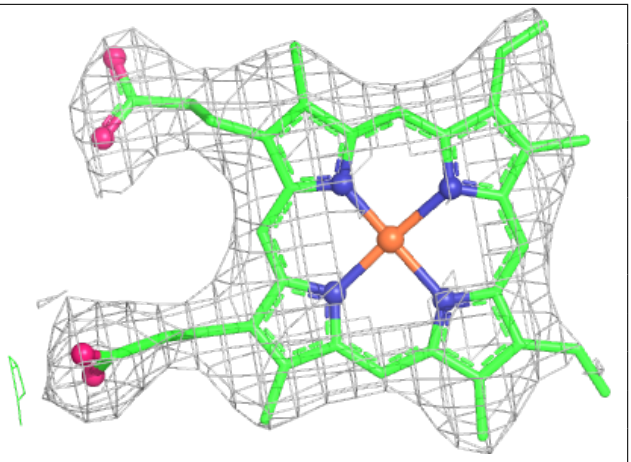


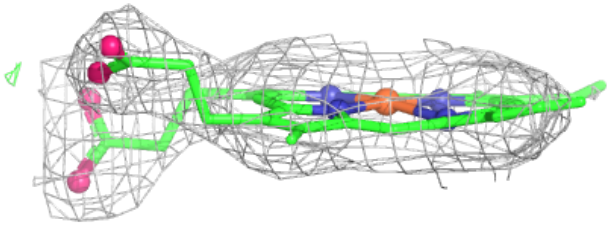


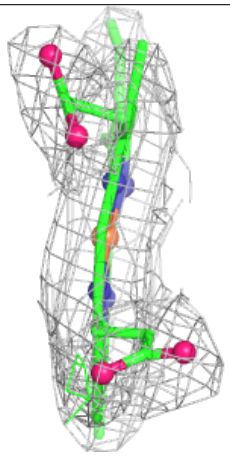


Electron density around HEM B 501:

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

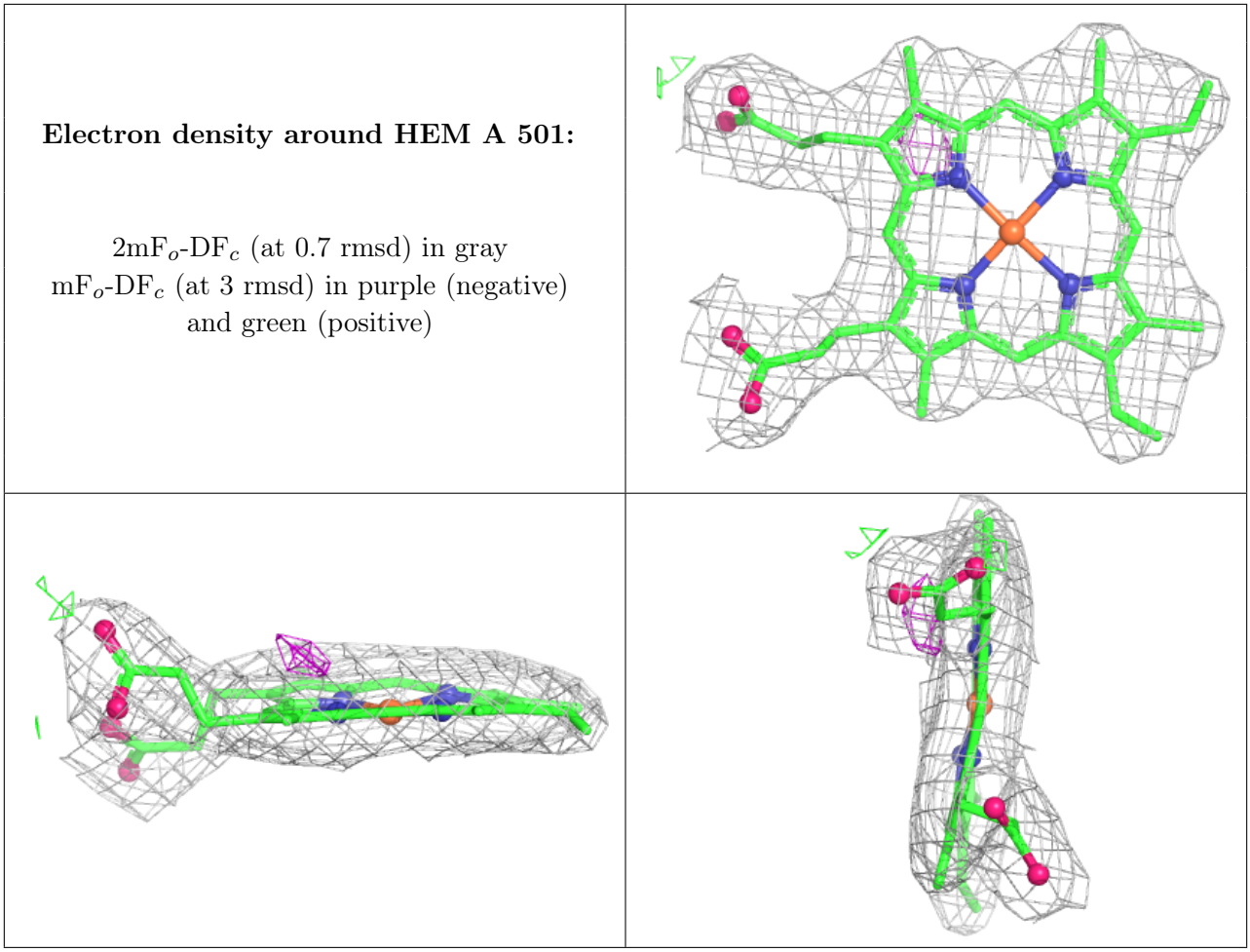






Electron density around HEM A 501:

$2mF_o$-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

There are no such residues in this entry.