



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:32 AM EDT

PDB ID : 1T88 / pdb_00001t88
Title : Crystal Structure of the Ferrous Cytochrome P450cam (C334A)
Authors : Nagano, S.; Tosha, T.; Ishimori, K.; Morishima, I.; Poulos, T.L.
Deposited on : 2004-05-11
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

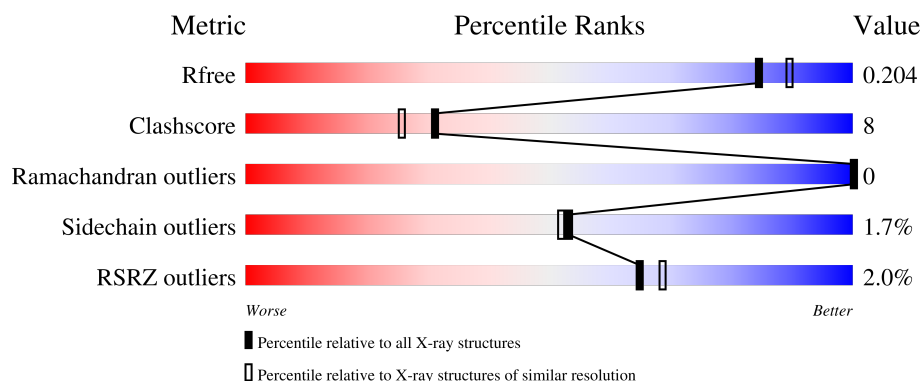
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

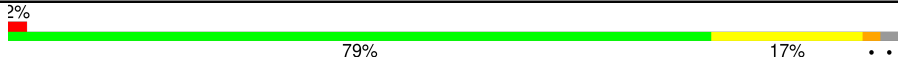
The reported resolution of this entry is 1.90 Å.

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	414	
1	B	414	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7056 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-cam.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3220	2040	563	600	17			
1	B	405	Total	C	N	O	S	0	0	0
			3207	2033	560	597	17			

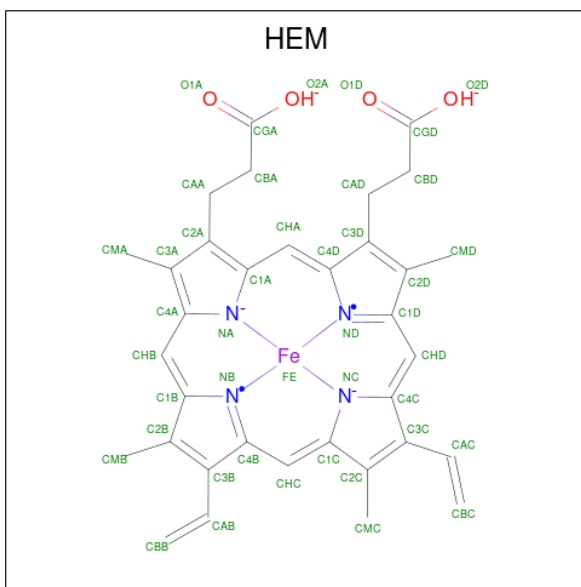
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	ALA	CYS	engineered mutation	UNP P00183
B	334	ALA	CYS	engineered mutation	UNP P00183

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

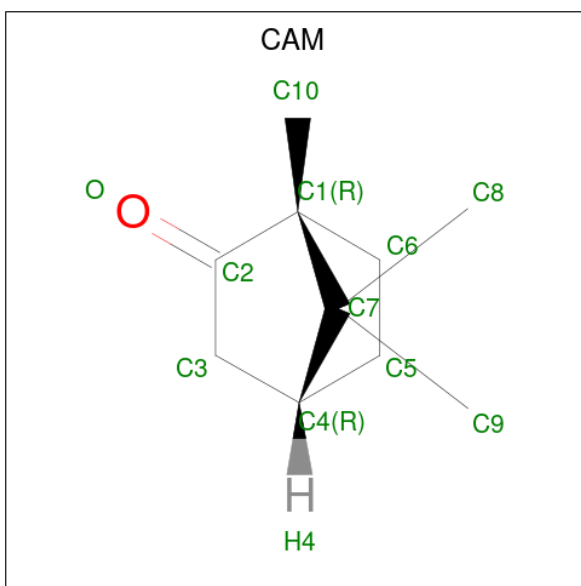
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is CAMPHOR (CCD ID: CAM) (formula: $C_{10}H_{16}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	10	1		
4	B	1	Total	C	O	0	0
			11	10	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).

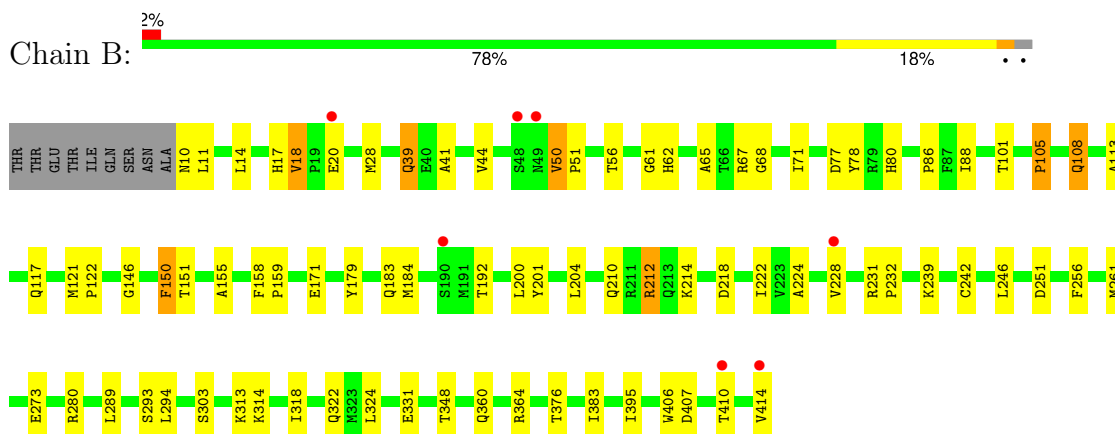


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	291	Total	O	0	0
			291	291		
6	B	219	Total	O	0	0
			219	219		

- Molecule 1: Cytochrome P450-cam



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.99Å 62.39Å 94.97Å 90.00° 89.57° 90.00°	Depositor
Resolution (Å)	45.66 – 1.90 45.66 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.66-1.90) 97.8 (45.66-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.187 , 0.212 0.179 , 0.204	Depositor DCC
R_{free} test set	3058 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7056	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: K, TRS, CAM, 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	0.38	0/3299	0.95	20/4482 (0.4%)
1	B	0.35	0/3286	0.91	12/4464 (0.3%)
All	All	0.37	0/6585	0.93	32/8946 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	PRO	N-CA-C	-8.52	100.30	110.70
1	A	109	ARG	N-CA-C	7.94	120.64	111.11
1	A	324	LEU	N-CA-C	7.59	120.63	111.82
1	B	101	THR	N-CA-C	7.08	119.85	111.71
1	A	204	LEU	N-CA-C	6.79	118.77	111.36
1	B	204	LEU	N-CA-C	6.70	118.66	111.36
1	B	212	ARG	N-CA-C	-6.61	104.24	112.90
1	A	18	VAL	N-CA-C	6.51	113.49	107.56
1	A	101	THR	N-CA-C	6.49	119.17	111.71
1	B	324	LEU	N-CA-C	6.42	119.27	111.82
1	B	18	VAL	N-CA-C	6.34	113.33	107.56
1	B	150	PHE	N-CA-C	6.31	118.69	111.11
1	B	251	ASP	N-CA-C	6.22	118.38	110.61
1	A	86	PRO	N-CA-C	5.97	122.33	114.27
1	A	150	PHE	N-CA-C	5.77	118.04	111.11
1	A	216	GLY	N-CA-C	-5.61	106.06	112.79
1	B	192	THR	N-CA-C	-5.56	103.36	110.53
1	A	9	ALA	N-CA-C	-5.53	106.30	113.16
1	B	383	ILE	N-CA-C	-5.53	102.44	109.58
1	A	343	GLN	N-CA-C	5.49	116.95	111.07
1	A	48	SER	N-CA-C	5.48	122.47	110.80
1	A	251	ASP	N-CA-C	5.43	117.40	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	SER	N-CA-C	-5.39	103.23	110.24
1	A	378	ILE	CA-C-N	5.38	125.19	119.28
1	A	378	ILE	C-N-CA	5.38	125.19	119.28
1	B	50	VAL	N-CA-C	5.38	113.75	107.89
1	B	105	PRO	N-CA-C	-5.34	104.19	110.70
1	A	214	LYS	CA-C-N	5.15	125.06	119.76
1	A	214	LYS	C-N-CA	5.15	125.06	119.76
1	A	212	ARG	N-CA-C	-5.13	106.52	112.89
1	A	85	CYS	CA-C-N	5.05	125.49	120.04
1	A	85	CYS	C-N-CA	5.05	125.49	120.04

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	3220	0	3167	49	0
1	B	3207	0	3156	56	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
4	A	11	0	16	0	0
4	B	11	0	16	0	0
5	A	8	0	12	0	0
6	A	291	0	0	1	0
6	B	219	0	0	3	0
All	All	7056	0	6427	106	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 8.

All (106) 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:327:LEU:HD22	1:A:336:MET:HE1	1.50	0.94
1:B:407:ASP:O	1:B:410:THR:HG22	1.73	0.88
1:B:360:GLN:HE21	1:B:364:ARG:HH22	1.23	0.85
1:A:360:GLN:HE21	1:A:364:ARG:HH22	1.21	0.85
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.62	0.80
1:B:218:ASP:O	1:B:222:ILE:HD13	1.85	0.76
1:B:376:THR:HG22	1:B:414:VAL:HG21	1.70	0.74
1:A:184:MET:HE1	1:A:200:LEU:HD22	1.71	0.73
1:B:158:PHE:HB3	1:B:159:PRO:HD3	1.69	0.72
1:A:121:MET:HE3	1:A:124:VAL:HB	1.75	0.69
1:A:163:PHE:HE2	1:A:246:LEU:HD23	1.61	0.66
1:B:67:ARG:O	1:B:71:ILE:HG12	1.97	0.65
1:B:210:GLN:HE22	1:B:214:LYS:HD2	1.62	0.64
1:A:294:LEU:HD23	1:A:294:LEU:H	1.62	0.64
1:A:376:THR:O	1:A:412:LYS:HE2	1.98	0.64
1:B:56:THR:O	1:B:61:GLY:HA2	1.98	0.64
1:A:69:GLN:O	1:A:73:GLU:HG3	1.98	0.63
1:B:294:LEU:H	1:B:294:LEU:HD23	1.65	0.61
1:A:73:GLU:OE2	1:A:308:HIS:HE1	1.84	0.61
1:A:181:THR:HA	1:A:184:MET:HE3	1.84	0.60
1:A:28:MET:HE1	1:A:395:ILE:HD13	1.84	0.60
1:B:28:MET:HE1	1:B:395:ILE:HD13	1.83	0.60
1:B:65:ALA:HB3	1:B:71:ILE:HD13	1.84	0.59
1:B:360:GLN:NE2	1:B:364:ARG:HH22	1.99	0.58
1:A:294:LEU:HD23	1:A:294:LEU:N	2.19	0.57
1:A:77:ASP:OD2	1:A:80:HIS:HD2	1.88	0.56
1:A:121:MET:HE2	1:A:125:ASP:OD2	2.06	0.56
1:A:68:GLY:O	1:A:72:ARG:HG3	2.07	0.54
1:B:20:GLU:H	1:B:20:GLU:CD	2.15	0.54
1:B:68:GLY:HA3	1:B:331:GLU:OE2	2.08	0.54
1:B:294:LEU:HD23	1:B:294:LEU:N	2.21	0.54
1:B:184:MET:HE1	1:B:200:LEU:HD22	1.90	0.53
1:B:410:THR:HG23	6:B:2537:HOH:O	2.07	0.53
1:A:327:LEU:HD22	1:A:336:MET:CE	2.31	0.53
1:A:51:PRO:HG2	1:A:54:VAL:HG12	1.91	0.52
1:B:303:SER:HA	1:B:314:LYS:HB2	1.92	0.52
1:B:41:ALA:O	1:B:44:VAL:HG22	2.10	0.52
1:B:414:VAL:O	1:B:414:VAL:HG12	2.09	0.52
1:A:201:TYR:HB3	1:A:239:LYS:HD2	1.92	0.51
1:A:210:GLN:CD	1:A:214:LYS:HE2	2.36	0.51
1:A:360:GLN:NE2	1:A:364:ARG:HH22	2.01	0.50
1:A:372:LYS:O	1:A:376:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLU:H	1:A:107:GLU:CD	2.20	0.50
1:A:118:VAL:HG23	1:A:119:VAL:HG13	1.93	0.50
1:B:376:THR:CG2	1:B:414:VAL:HG21	2.39	0.50
1:B:62:HIS:CD2	1:B:88:ILE:HD13	2.47	0.49
1:B:62:HIS:CG	1:B:88:ILE:HD13	2.46	0.49
1:A:163:PHE:CE2	1:A:246:LEU:HD23	2.44	0.49
1:B:113:ALA:O	1:B:117:GLN:HG3	2.13	0.49
1:B:318:ILE:HG23	1:B:318:ILE:O	2.13	0.49
1:B:39:GLN:NE2	1:B:39:GLN:H	2.11	0.48
1:B:231:ARG:HG2	1:B:232:PRO:HD2	1.94	0.48
1:B:17:HIS:CD2	1:B:313:LYS:HB2	2.49	0.48
1:A:41:ALA:O	1:A:44:VAL:HG22	2.14	0.48
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.93	0.48
1:A:212:ARG:HG3	1:A:224:ALA:HB1	1.94	0.48
1:B:322:GLN:HB3	1:B:348:THR:O	2.13	0.48
1:B:212:ARG:HG3	1:B:224:ALA:HB1	1.95	0.47
1:B:11:LEU:N	1:B:11:LEU:HD22	2.30	0.47
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.97	0.47
1:B:65:ALA:O	1:B:71:ILE:HD11	2.14	0.46
1:A:121:MET:HB3	1:A:122:PRO:HD3	1.98	0.46
1:A:294:LEU:N	1:A:294:LEU:CD2	2.79	0.46
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.50	0.45
1:B:201:TYR:HB3	1:B:239:LYS:HD2	1.99	0.45
1:A:146:GLY:HA2	1:A:406:TRP:CD1	2.51	0.45
1:A:155:ALA:O	1:A:159:PRO:HD2	2.17	0.45
1:A:165:LEU:C	1:A:165:LEU:HD13	2.41	0.45
1:B:77:ASP:OD2	1:B:80:HIS:HD2	1.99	0.45
1:A:18:VAL:HG11	1:A:55:TRP:CG	2.51	0.45
1:A:210:GLN:OE1	1:A:214:LYS:HE2	2.16	0.45
1:B:108:GLN:HE21	1:B:108:GLN:HB3	1.53	0.45
1:A:272:GLN:CD	1:A:276:GLU:OE2	2.60	0.45
1:A:179:TYR:O	1:A:183:GLN:HG2	2.18	0.44
1:B:171:GLU:HG3	6:B:2585:HOH:O	2.18	0.44
1:B:231:ARG:HD3	6:B:2666:HOH:O	2.16	0.44
1:A:115:ALA:O	1:A:118:VAL:HG22	2.18	0.43
1:A:121:MET:HE1	1:A:365:ARG:NH2	2.32	0.43
1:B:242:CYS:O	1:B:246:LEU:HD23	2.17	0.43
1:B:50:VAL:HA	1:B:51:PRO:HD3	1.82	0.43
1:B:121:MET:HB3	1:B:122:PRO:HD3	1.99	0.43
3:B:2417:HEM:HMC2	3:B:2417:HEM:HBC2	2.01	0.43
1:B:294:LEU:N	1:B:294:LEU:CD2	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLN:NE2	1:A:39:GLN:H	2.16	0.42
1:B:10:ASN:C	1:B:11:LEU:HD22	2.44	0.42
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.85	0.42
1:B:146:GLY:HA2	1:B:406:TRP:NE1	2.34	0.42
1:B:151:THR:HA	1:B:155:ALA:HB3	2.02	0.42
1:B:210:GLN:NE2	1:B:214:LYS:HD2	2.30	0.42
1:B:231:ARG:C	1:B:231:ARG:HD2	2.44	0.42
1:B:14:LEU:HD11	1:B:18:VAL:CG1	2.49	0.42
1:B:78:TYR:CE1	1:B:105:PRO:HG2	2.54	0.42
1:B:179:TYR:O	1:B:183:GLN:HG2	2.20	0.42
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.40	0.41
1:A:146:GLY:HA2	1:A:406:TRP:NE1	2.35	0.41
1:A:33:ASN:HB3	1:A:41:ALA:HA	2.03	0.41
1:B:20:GLU:CD	1:B:20:GLU:N	2.78	0.41
1:A:277:ARG:NE	1:A:279:GLU:OE1	2.54	0.41
1:B:273:GLU:OE1	1:B:280:ARG:NH2	2.54	0.41
1:A:83:SER:O	1:A:86:PRO:HD3	2.21	0.41
1:A:400:GLN:HG2	6:A:1938:HOH:O	2.20	0.41
1:B:77:ASP:OD2	1:B:80:HIS:CD2	2.74	0.41
1:B:256:PHE:CE2	1:B:289:LEU:HA	2.55	0.41
1:B:228:VAL:HG23	1:B:228:VAL:O	2.20	0.40
1:A:44:VAL:O	1:A:47:GLU:HG3	2.22	0.40
1:B:222:ILE:HD12	1:B:222:ILE:N	2.36	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	405/414 (98%)	393 (97%)	12 (3%)	0	100	100
1	B	403/414 (97%)	389 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	808/828 (98%)	782 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	350/357 (98%)	341 (97%)	9 (3%)	40	35
1	B	349/357 (98%)	346 (99%)	3 (1%)	70	73
All	All	699/714 (98%)	687 (98%)	12 (2%)	53	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	28	MET
1	A	39	GLN
1	A	107	GLU
1	A	198	GLU
1	A	210	GLN
1	A	272	GLN
1	A	362	LEU
1	A	412	LYS
1	B	39	GLN
1	B	86	PRO
1	B	108	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	30	ASN
1	A	33	ASN

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Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	69	GLN
1	A	80	HIS
1	A	117	GLN
1	A	129	ASN
1	A	132	GLN
1	A	210	GLN
1	A	308	HIS
1	A	360	GLN
1	A	388	GLN
1	B	39	GLN
1	B	46	GLN
1	B	69	GLN
1	B	80	HIS
1	B	108	GLN
1	B	110	GLN
1	B	117	GLN
1	B	129	ASN
1	B	132	GLN
1	B	210	GLN
1	B	213	GLN
1	B	308	HIS
1	B	317	GLN
1	B	360	GLN
1	B	390	GLN
1	B	400	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	HEM	B	2417	1	50,50,50	1.11	5 (10%)	67,82,82	1.00	3 (4%)
5	TRS	A	1430	-	7,7,7	2.12	3 (42%)	9,9,9	2.39	4 (44%)
3	HEM	A	1417	1	50,50,50	1.11	2 (4%)	67,82,82	0.88	1 (1%)
4	CAM	B	2422	-	12,12,12	2.17	4 (33%)	20,21,21	1.93	5 (25%)
4	CAM	A	1422	-	12,12,12	1.98	4 (33%)	20,21,21	1.95	5 (25%)

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	HEM	B	2417	1	-	0/14/54/54	-
5	TRS	A	1430	-	-	2/9/9/9	-
3	HEM	A	1417	1	-	2/14/54/54	-
4	CAM	B	2422	-	-	-	0/3/2/2
4	CAM	A	1422	-	-	-	0/3/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2422	CAM	C5-C4	3.47	1.63	1.53
4	B	2422	CAM	C1-C2	3.36	1.57	1.52
4	A	1422	CAM	C5-C4	3.34	1.62	1.53
4	B	2422	CAM	C3-C4	3.33	1.61	1.53
5	A	1430	TRS	O3-C3	3.30	1.52	1.42
4	A	1422	CAM	C3-C4	3.20	1.61	1.53
5	A	1430	TRS	O1-C1	3.06	1.52	1.42
5	A	1430	TRS	O2-C2	2.82	1.51	1.42
3	A	1417	HEM	CAC-C3C	-2.79	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1422	CAM	C8-C7	2.66	1.61	1.53
4	B	2422	CAM	C8-C7	2.64	1.61	1.53
3	B	2417	HEM	CAC-C3C	-2.47	1.40	1.47
3	A	1417	HEM	CAB-C3B	-2.38	1.41	1.47
3	B	2417	HEM	FE-NC	2.34	2.02	1.95
4	A	1422	CAM	C1-C2	2.30	1.55	1.52
3	B	2417	HEM	FE-NB	2.19	2.01	1.94
3	B	2417	HEM	CAB-C3B	-2.13	1.41	1.47
3	B	2417	HEM	CHD-C4C	2.13	1.42	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1422	CAM	C4-C3-C2	-4.64	93.90	102.05
4	B	2422	CAM	C4-C3-C2	-4.53	94.09	102.05
3	B	2417	HEM	C3B-C4B-NB	4.15	112.45	109.47
5	A	1430	TRS	C3-C-N	4.01	118.39	108.17
5	A	1430	TRS	C3-C-C2	-3.95	100.15	110.66
4	B	2422	CAM	C5-C6-C1	-3.36	97.97	104.73
4	A	1422	CAM	C5-C6-C1	-3.30	98.08	104.73
4	B	2422	CAM	C3-C4-C7	3.27	109.29	102.82
4	A	1422	CAM	C3-C4-C7	3.18	109.11	102.82
5	A	1430	TRS	C2-C-C1	-2.97	102.74	110.66
3	A	1417	HEM	C3B-C4B-NB	2.88	111.54	109.47
4	A	1422	CAM	C6-C1-C7	2.86	107.57	101.52
4	B	2422	CAM	C6-C1-C7	2.84	107.51	101.52
5	A	1430	TRS	C3-C-C1	2.77	118.03	110.66
4	A	1422	CAM	C9-C7-C1	2.43	118.46	113.05
4	B	2422	CAM	C9-C7-C1	2.34	118.26	113.05
3	B	2417	HEM	C4B-C3B-C2B	-2.20	105.26	107.28
3	B	2417	HEM	CAD-C3D-C4D	2.11	128.37	124.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

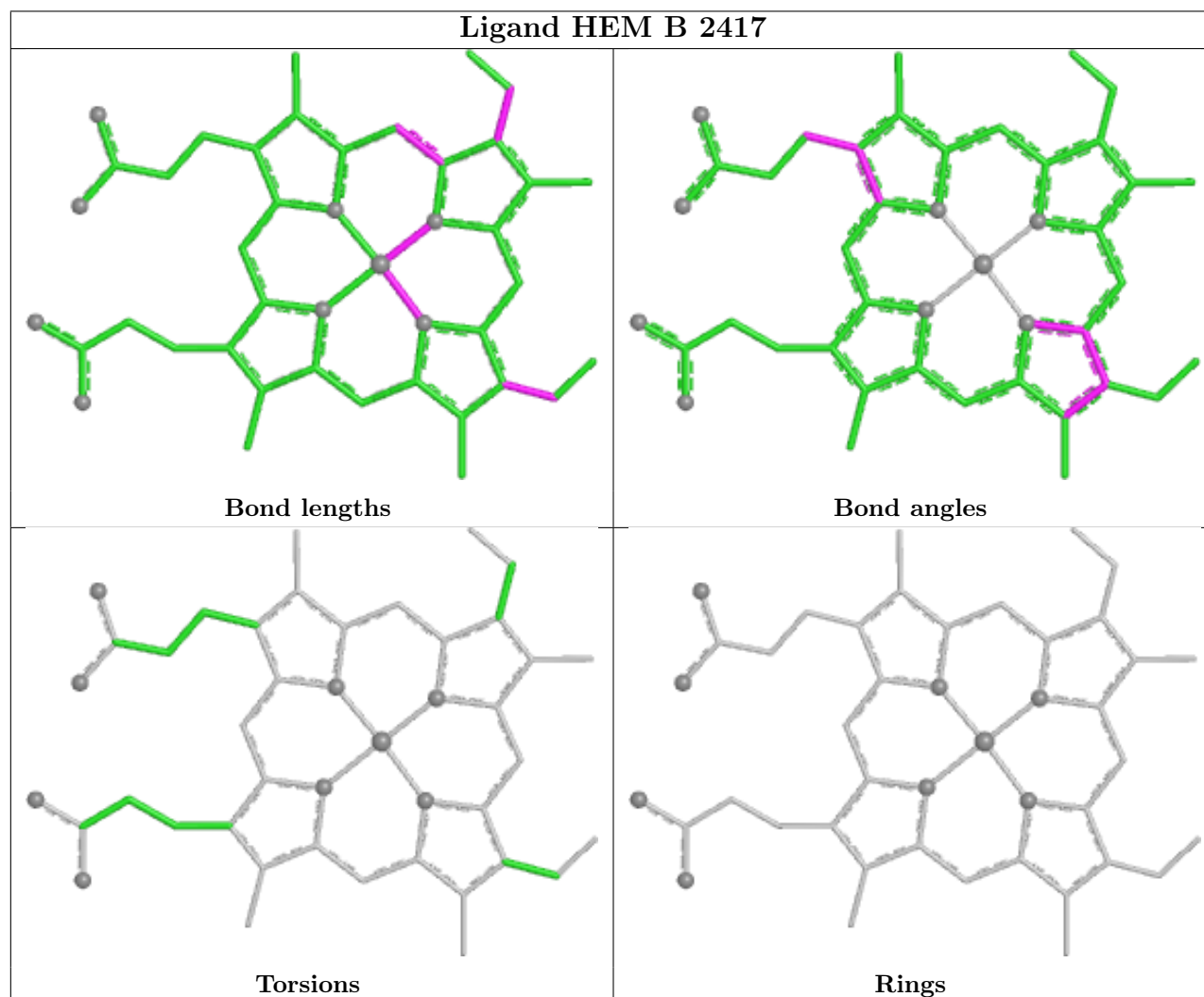
Mol	Chain	Res	Type	Atoms
3	A	1417	HEM	C2C-C3C-CAC-CBC
5	A	1430	TRS	C1-C-C3-O3
5	A	1430	TRS	N-C-C3-O3
3	A	1417	HEM	C4C-C3C-CAC-CBC

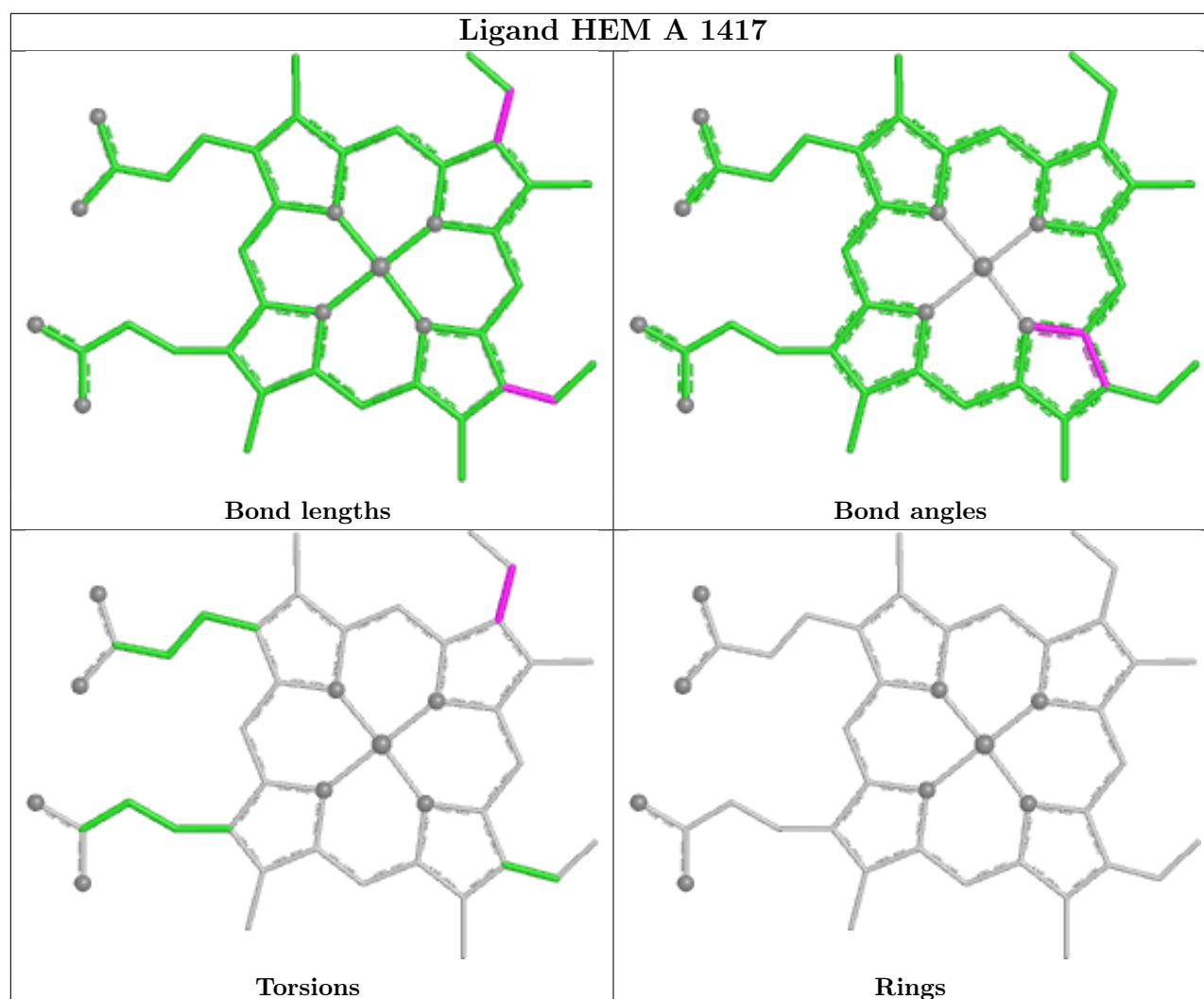
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2417	HEM	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	407/414 (98%)	-0.12	9 (2%) 62 66	10, 18, 33, 57	0
1	B	405/414 (97%)	0.11	7 (1%) 69 72	12, 22, 39, 51	0
All	All	812/828 (98%)	-0.01	16 (1%) 65 69	10, 20, 37, 57	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	3.5
1	A	272	GLN	3.0
1	B	414	VAL	2.8
1	B	49	ASN	2.7
1	A	236	ASP	2.6
1	A	376	THR	2.6
1	A	414	VAL	2.6
1	A	8	ASN	2.6
1	A	413	ALA	2.5
1	B	190	SER	2.4
1	A	48	SER	2.4
1	A	277	ARG	2.3
1	B	410	THR	2.2
1	B	48	SER	2.2
1	B	20	GLU	2.0
1	B	228	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

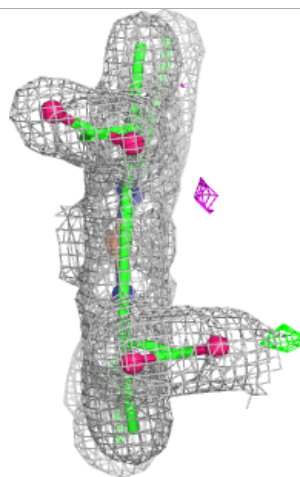
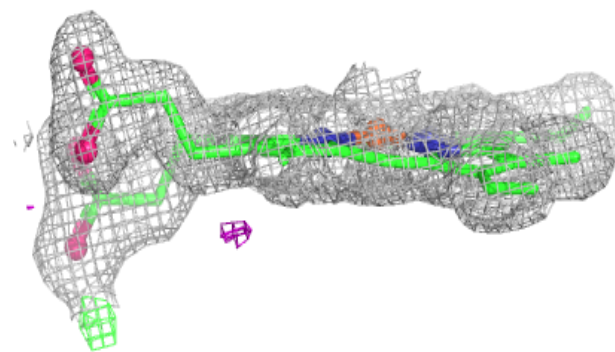
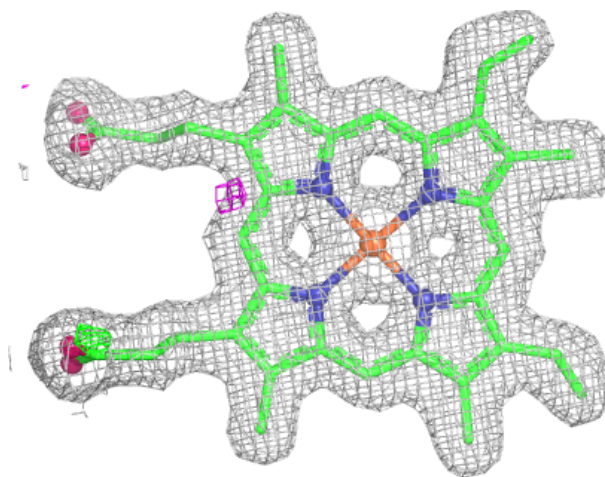
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TRS	A	1430	8/8	0.90	0.10	21,23,25,27	0
4	CAM	B	2422	11/11	0.94	0.07	14,16,19,19	0
4	CAM	A	1422	11/11	0.94	0.06	9,11,12,14	0
2	K	B	2515	1/1	0.95	0.07	22,22,22,22	0
3	HEM	B	2417	43/43	0.98	0.05	11,15,19,20	0
2	K	A	1715	1/1	0.98	0.05	19,19,19,19	0
2	K	A	1515	1/1	0.98	0.04	13,13,13,13	0
3	HEM	A	1417	43/43	0.98	0.05	8,11,16,25	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.

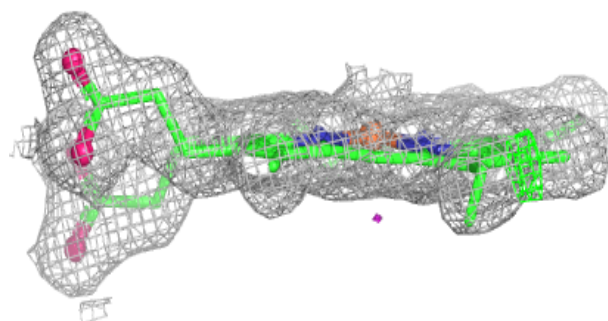
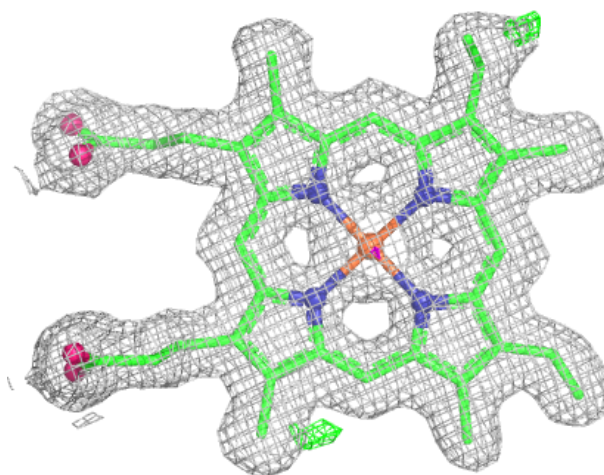
Electron density around HEM B 2417:

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



Electron density around HEM A 1417:

$2mF_o-DF_c$ (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.