



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:07 PM UTC

PDB ID : 1PHG / pdb_00001phg
Title : CRYSTAL STRUCTURES OF METYRAPONE-AND PHENYLIMIDAZOL
E-INHIBITED COMPLEXES OF CYTOCHROME P450-CAM
Authors : Poulos, T.L.
Deposited on : 1992-07-27
Resolution : 1.60 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

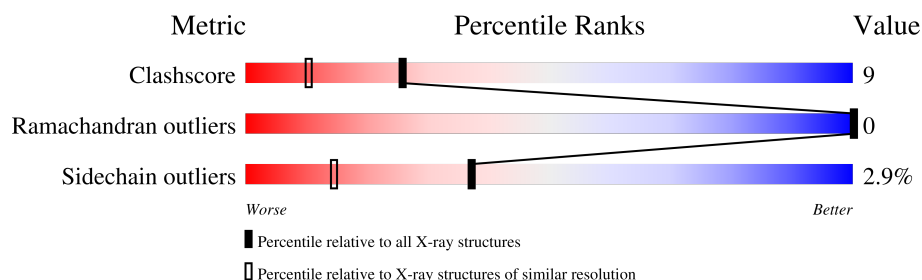
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	 58% 32% 7% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3468 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.

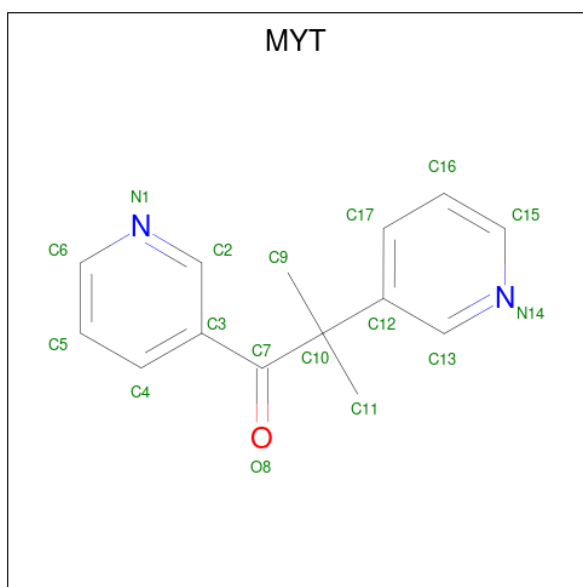
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3204	2030	559	597	18			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is METYRAPONE (CCD ID: MYT) (formula: $C_{14}H_{14}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	14	2	1		

- Molecule 4 is water.

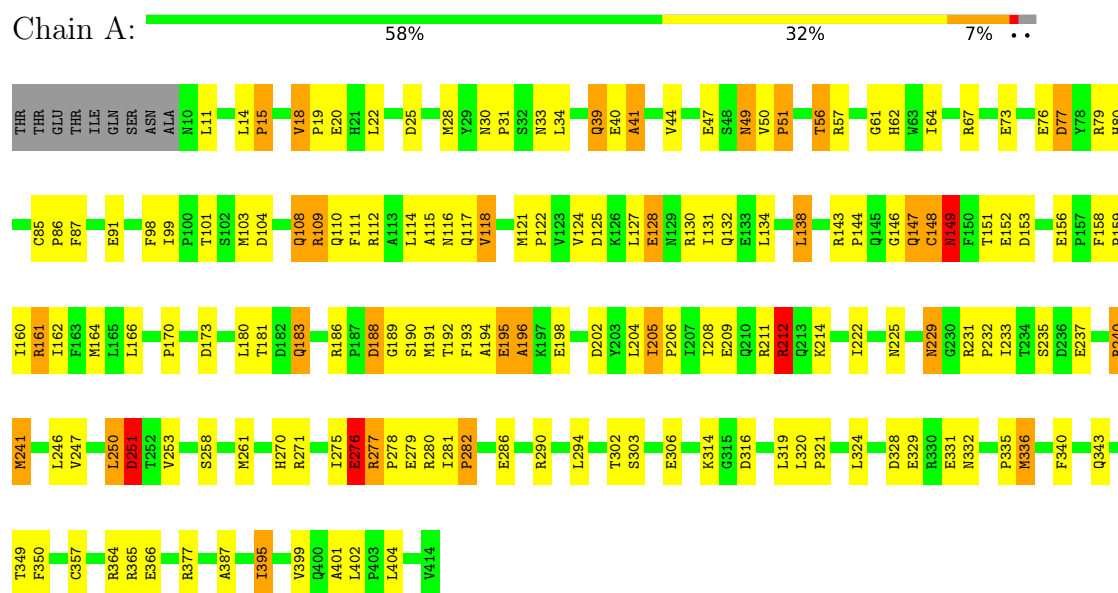
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: CYTOCHROME P450-CAM



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.67Å 103.90Å 36.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3468	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.37	6/3283 (0.2%)	2.25	142/4461 (3.2%)

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	A	0	13

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	ASP	C-O	6.79	1.33	1.24
1	A	149	ASN	C-O	6.44	1.32	1.24
1	A	33	ASN	N-CA	5.73	1.52	1.46
1	A	211	ARG	NE-CZ	-5.47	1.27	1.33
1	A	399	VAL	C-N	-5.32	1.26	1.33
1	A	276	GLU	CD-OE1	5.13	1.35	1.25

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	23.55	157.37	124.40
1	A	195	GLU	CA-CB-CG	11.30	136.70	114.10
1	A	67	ARG	NE-CZ-NH2	-10.67	109.60	119.20
1	A	33	ASN	OD1-CG-ND2	10.00	132.60	122.60
1	A	108	GLN	CB-CG-CD	9.25	128.33	112.60
1	A	33	ASN	CA-CB-CG	-9.25	103.35	112.60
1	A	20	GLU	CA-CB-CG	8.86	131.82	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	VAL	N-CA-C	8.78	120.57	111.00
1	A	87	PHE	CA-CB-CG	8.77	122.56	113.80
1	A	148	CYS	CA-C-N	8.62	138.01	121.54
1	A	148	CYS	C-N-CA	8.62	138.01	121.54
1	A	250	LEU	N-CA-C	8.45	122.08	111.69
1	A	251	ASP	O-C-N	-8.40	112.07	122.24
1	A	149	ASN	CA-C-O	-8.37	108.55	120.51
1	A	280	ARG	CD-NE-CZ	8.35	136.09	124.40
1	A	108	GLN	CA-CB-CG	8.23	130.55	114.10
1	A	365	ARG	CD-NE-CZ	8.21	135.89	124.40
1	A	125	ASP	CA-CB-CG	8.19	120.79	112.60
1	A	80	HIS	CA-CB-CG	-8.03	105.77	113.80
1	A	87	PHE	CA-C-N	8.00	132.23	123.43
1	A	87	PHE	C-N-CA	8.00	132.23	123.43
1	A	25	ASP	CA-C-N	7.87	132.76	121.50
1	A	25	ASP	C-N-CA	7.87	132.76	121.50
1	A	51	PRO	CA-C-N	7.87	131.87	120.38
1	A	51	PRO	C-N-CA	7.87	131.87	120.38
1	A	128	GLU	CB-CG-CD	7.70	125.69	112.60
1	A	124	VAL	O-C-N	7.24	129.00	121.91
1	A	395	ILE	O-C-N	7.16	128.93	121.91
1	A	98	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	209	GLU	CA-C-N	7.08	129.77	120.28
1	A	209	GLU	C-N-CA	7.08	129.77	120.28
1	A	62	HIS	CA-CB-CG	7.05	120.85	113.80
1	A	401	ALA	CA-C-O	-6.97	113.22	120.89
1	A	349	THR	CA-CB-OG1	-6.96	99.17	109.60
1	A	364	ARG	CD-NE-CZ	6.93	134.10	124.40
1	A	149	ASN	N-CA-CB	6.78	121.94	110.49
1	A	241	MET	N-CA-CB	6.74	119.85	110.07
1	A	33	ASN	N-CA-CB	-6.73	101.09	110.65
1	A	281	ILE	CA-C-N	6.73	125.97	118.97
1	A	281	ILE	C-N-CA	6.73	125.97	118.97
1	A	279	GLU	CB-CG-CD	6.67	123.94	112.60
1	A	204	LEU	N-CA-C	6.62	118.15	111.07
1	A	101	THR	N-CA-CB	6.57	120.33	110.22
1	A	258	SER	CA-C-O	-6.56	113.59	120.55
1	A	64	ILE	CA-C-O	-6.55	113.77	120.25
1	A	130	ARG	N-CA-CB	6.53	119.82	110.16
1	A	270	HIS	N-CA-CB	6.52	119.91	110.20
1	A	25	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	306	GLU	CB-CG-CD	6.50	123.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	LEU	CA-C-O	-6.48	113.68	120.55
1	A	161	ARG	CA-C-O	-6.48	113.68	120.55
1	A	67	ARG	NE-CZ-NH1	6.45	127.95	121.50
1	A	188	ASP	N-CA-CB	-6.43	100.68	110.26
1	A	211	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	A	153	ASP	CA-C-O	-6.35	112.66	119.97
1	A	290	ARG	CA-C-O	-6.30	114.21	120.82
1	A	195	GLU	CB-CG-CD	6.28	123.28	112.60
1	A	271	ARG	CD-NE-CZ	6.23	133.12	124.40
1	A	76	GLU	CB-CG-CD	6.23	123.19	112.60
1	A	85	CYS	N-CA-CB	-6.22	103.25	111.40
1	A	161	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	A	271	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	A	251	ASP	CA-C-O	-6.13	112.02	119.32
1	A	240	ARG	CA-C-O	-6.03	114.03	120.42
1	A	149	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	A	329	GLU	CA-CB-CG	6.01	126.13	114.10
1	A	286	GLU	N-CA-CB	6.01	118.95	110.12
1	A	152	GLU	N-CA-CB	5.99	119.53	110.30
1	A	153	ASP	N-CA-C	5.96	118.74	111.82
1	A	404	LEU	CA-C-O	-5.93	114.45	121.16
1	A	118	VAL	CA-C-N	5.92	129.62	122.16
1	A	118	VAL	C-N-CA	5.92	129.62	122.16
1	A	189	GLY	N-CA-C	-5.92	106.35	114.64
1	A	109	ARG	N-CA-C	5.92	118.21	111.11
1	A	118	VAL	CA-CB-CG2	5.90	120.43	110.40
1	A	229	ASN	CA-CB-CG	-5.89	106.71	112.60
1	A	180	LEU	O-C-N	5.87	128.34	122.12
1	A	34	LEU	CB-CA-C	5.87	120.66	110.68
1	A	101	THR	CA-CB-CG2	5.84	120.43	110.50
1	A	277	ARG	CA-C-N	5.84	125.51	119.56
1	A	277	ARG	C-N-CA	5.84	125.51	119.56
1	A	316	ASP	O-C-N	5.84	130.01	122.89
1	A	33	ASN	CA-C-O	-5.83	111.99	119.80
1	A	116	ASN	CA-CB-CG	-5.79	106.81	112.60
1	A	193	PHE	O-C-N	5.79	128.03	122.07
1	A	183	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	A	240	ARG	CD-NE-CZ	5.78	132.49	124.40
1	A	329	GLU	CB-CG-CD	5.76	122.40	112.60
1	A	73	GLU	N-CA-CB	5.76	118.36	110.01
1	A	209	GLU	CA-CB-CG	5.75	125.61	114.10
1	A	340	PHE	CA-CB-CG	5.75	119.55	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLU	CA-C-N	5.74	128.25	120.38
1	A	47	GLU	C-N-CA	5.74	128.25	120.38
1	A	41	ALA	CA-C-O	-5.74	114.80	120.82
1	A	196	ALA	O-C-N	5.73	127.97	122.07
1	A	138	LEU	CB-CA-C	5.64	120.44	110.85
1	A	30	ASN	CA-CB-CG	-5.63	106.97	112.60
1	A	104	ASP	O-C-N	5.63	126.27	121.20
1	A	131	ILE	CA-C-N	5.62	127.81	120.28
1	A	131	ILE	C-N-CA	5.62	127.81	120.28
1	A	324	LEU	N-CA-C	5.61	118.32	111.82
1	A	138	LEU	N-CA-CB	-5.59	101.89	110.16
1	A	253	VAL	O-C-N	5.58	127.29	121.87
1	A	212	ARG	N-CA-C	-5.58	104.70	112.45
1	A	343	GLN	N-CA-CB	5.57	118.31	110.12
1	A	336	MET	CA-CB-CG	5.54	125.18	114.10
1	A	11	LEU	CB-CA-C	5.49	118.80	109.75
1	A	151	THR	N-CA-CB	5.46	117.88	109.91
1	A	115	ALA	CB-CA-C	5.43	120.69	110.63
1	A	128	GLU	CG-CD-OE1	5.43	130.88	118.40
1	A	44	VAL	N-CA-CB	5.42	119.93	110.65
1	A	112	ARG	CA-C-N	5.39	127.77	120.38
1	A	112	ARG	C-N-CA	5.39	127.77	120.38
1	A	56	THR	CA-CB-OG1	-5.38	101.54	109.60
1	A	343	GLN	CB-CG-CD	5.37	121.73	112.60
1	A	316	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	320	LEU	N-CA-CB	-5.31	102.49	111.30
1	A	77	ASP	CA-C-O	-5.29	112.94	120.51
1	A	286	GLU	CA-C-O	-5.29	114.94	120.55
1	A	282	PRO	CA-C-N	5.28	127.30	120.44
1	A	282	PRO	C-N-CA	5.28	127.30	120.44
1	A	279	GLU	CA-CB-CG	5.26	124.62	114.10
1	A	15	PRO	CB-CA-C	-5.25	104.51	110.92
1	A	336	MET	CA-C-N	5.24	129.58	122.19
1	A	336	MET	C-N-CA	5.24	129.58	122.19
1	A	156	GLU	CB-CG-CD	5.21	121.45	112.60
1	A	387	ALA	N-CA-C	-5.17	100.87	109.46
1	A	366	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	205	ILE	CA-C-N	5.16	124.61	119.24
1	A	205	ILE	C-N-CA	5.16	124.61	119.24
1	A	132	GLN	N-CA-CB	-5.13	102.58	110.12
1	A	324	LEU	CA-C-O	-5.12	114.08	119.97
1	A	275	ILE	CA-C-O	-5.11	115.44	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ILE	O-C-N	5.08	127.06	121.83
1	A	47	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	130	ARG	O-C-N	5.05	127.91	122.15
1	A	214	LYS	CA-C-N	5.04	124.95	119.76
1	A	214	LYS	C-N-CA	5.04	124.95	119.76
1	A	76	GLU	CA-C-N	5.03	131.15	121.54
1	A	76	GLU	C-N-CA	5.03	131.15	121.54
1	A	202	ASP	CA-C-O	5.03	125.88	120.55
1	A	18	VAL	O-C-N	5.00	125.36	121.46

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	118	VAL	Mainchain
1	A	147	GLN	Mainchain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	161	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	377	ARG	Sidechain
1	A	77	ASP	Mainchain

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	3204	0	3145	58	0
2	A	43	0	30	5	0
3	A	17	0	14	4	0
4	A	204	0	0	2	0
All	All	3468	0	3189	61	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 9.

All (61) 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:191:MET:HE2	1:A:196:ALA:HA	1.55	0.86
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.71	0.73
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.73	0.70
1:A:111:PHE:HB3	1:A:241:MET:HE2	1.79	0.63
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.79	0.62
1:A:149:ASN:HD21	1:A:402:LEU:H	1.48	0.62
1:A:303:SER:HA	1:A:314:LYS:HG3	1.82	0.61
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.84	0.60
1:A:183:GLN:HE22	1:A:188:ASP:HB2	1.66	0.59
1:A:149:ASN:ND2	1:A:402:LEU:H	2.01	0.59
1:A:276:GLU:C	1:A:278:PRO:HD3	2.28	0.58
1:A:56:THR:O	1:A:61:GLY:HA2	2.03	0.58
1:A:191:MET:HE2	1:A:196:ALA:CA	2.32	0.57
1:A:208:ILE:O	1:A:212:ARG:HG3	2.06	0.56
1:A:49:ASN:HD22	1:A:49:ASN:H	1.54	0.56
1:A:247:VAL:HG11	3:A:422:MYT:C16	2.36	0.55
2:A:417:HEM:CHD	3:A:422:MYT:H6	2.37	0.55
1:A:91:GLU:H	1:A:91:GLU:CD	2.15	0.54
1:A:39:GLN:NE2	1:A:39:GLN:H	2.05	0.54
1:A:99:ILE:HG12	1:A:103:MET:HE3	1.89	0.54
1:A:19:PRO:HG2	1:A:22:LEU:HD12	1.90	0.52
1:A:282:PRO:HD2	4:A:661:HOH:O	2.09	0.52
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.25	0.51
1:A:170:PRO:HG2	1:A:173:ASP:OD2	2.11	0.50
2:A:417:HEM:C4C	3:A:422:MYT:H6	2.46	0.50
1:A:328:ASP:HB3	1:A:331:GLU:HG3	1.94	0.50
1:A:357:CYS:HB2	2:A:417:HEM:NA	2.27	0.50
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.12	0.49
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.93	0.49
1:A:134:LEU:O	1:A:138:LEU:HB2	2.13	0.49
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.43	0.48
1:A:31:PRO:HB2	1:A:41:ALA:HB1	1.96	0.48
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.44	0.47
1:A:233:ILE:HG13	1:A:237:GLU:HB2	1.97	0.46
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.97	0.46
2:A:417:HEM:C4A	3:A:422:MYT:H2	2.51	0.45
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HA	1:A:15:PRO:HD3	1.93	0.44
1:A:277:ARG:N	1:A:278:PRO:HD3	2.31	0.44
1:A:146:GLY:O	1:A:147:GLN:HB3	2.16	0.44
1:A:188:ASP:HB3	1:A:190:SER:H	1.83	0.44
1:A:57:ARG:HG2	4:A:508:HOH:O	2.17	0.44
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.48	0.43
1:A:181:THR:HG22	1:A:251:ASP:HB2	1.99	0.43
1:A:110:GLN:CD	1:A:229:ASN:H	2.26	0.43
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.99	0.43
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.49	0.42
1:A:28:MET:HE1	1:A:395:ILE:HD13	2.02	0.42
1:A:183:GLN:NE2	1:A:188:ASP:HB2	2.34	0.42
1:A:149:ASN:ND2	1:A:149:ASN:C	2.76	0.42
1:A:149:ASN:C	1:A:149:ASN:HD22	2.28	0.42
1:A:114:LEU:O	1:A:117:GLN:HB2	2.20	0.41
1:A:302:THR:C	1:A:314:LYS:HG3	2.46	0.41
1:A:160:ILE:O	1:A:164:MET:HG2	2.21	0.41
1:A:194:ALA:O	1:A:198:GLU:HG2	2.21	0.41
1:A:294:LEU:HD23	1:A:294:LEU:N	2.36	0.41
1:A:332:ASN:O	1:A:335:PRO:HD3	2.21	0.41
1:A:319:LEU:HG	1:A:321:PRO:HG3	2.03	0.40
1:A:357:CYS:HB2	2:A:417:HEM:C1A	2.57	0.40
1:A:134:LEU:HD23	1:A:162:ILE:HG13	2.03	0.40
1:A:212:ARG:HA	1:A:225:ASN:HD21	1.85	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	403/414 (97%)	386 (96%)	17 (4%)	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	349/358 (98%)	339 (97%)	10 (3%)	37	14

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	49	ASN
1	A	79	ARG
1	A	86	PRO
1	A	108	GLN
1	A	128	GLU
1	A	235	SER
1	A	246	LEU
1	A	261	MET
1	A	276	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	108	GLN
1	A	110	GLN
1	A	117	GLN
1	A	149	ASN
1	A	213	GLN
1	A	225	ASN
1	A	229	ASN
1	A	317	GLN
1	A	337	HIS

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Mol	Chain	Res	Type
1	A	388	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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HEM	A	417	1,3	50,50,50	1.39	7 (14%)	67,82,82	1.27	7 (10%)
3	MYT	A	422	2	18,18,18	3.41	10 (55%)	23,25,25	3.38	8 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	417	1,3	-	3/14/54/54	-
3	MYT	A	422	2	-	5/16/16/16	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	422	MYT	C10-C12	-9.93	1.44	1.53
3	A	422	MYT	C11-C10	4.53	1.61	1.54
3	A	422	MYT	C2-C3	-4.26	1.32	1.39
2	A	417	HEM	FE-NB	3.95	2.07	1.94
3	A	422	MYT	C3-C7	3.74	1.54	1.49
3	A	422	MYT	C5-C4	3.44	1.44	1.38
2	A	417	HEM	CAC-C3C	3.37	1.56	1.47
3	A	422	MYT	C6-N1	3.29	1.43	1.33
2	A	417	HEM	FE-NA	3.07	2.05	1.95
3	A	422	MYT	C9-C10	2.90	1.58	1.54
3	A	422	MYT	C2-N1	2.72	1.40	1.34
3	A	422	MYT	O8-C7	-2.40	1.18	1.21
2	A	417	HEM	FE-NC	2.33	2.02	1.95
3	A	422	MYT	C4-C3	-2.28	1.36	1.39
2	A	417	HEM	CAB-C3B	2.22	1.53	1.47
2	A	417	HEM	CMD-C2D	2.17	1.55	1.50
2	A	417	HEM	C2A-C3A	-2.04	1.33	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	422	MYT	O8-C7-C10	9.09	127.71	120.04
3	A	422	MYT	C11-C10-C9	-7.63	97.31	108.01
3	A	422	MYT	C4-C3-C2	6.21	124.54	117.61
2	A	417	HEM	O2A-CGA-O1A	4.05	133.75	123.33
3	A	422	MYT	C12-C10-C7	3.98	116.14	108.28
3	A	422	MYT	C16-C17-C12	3.89	124.71	120.75
3	A	422	MYT	C9-C10-C12	3.88	119.19	110.51
3	A	422	MYT	C4-C5-C6	-3.12	114.41	118.92
2	A	417	HEM	O1D-CGD-CBD	-3.02	113.51	123.09
2	A	417	HEM	C3B-C4B-NB	2.61	111.34	109.47
3	A	422	MYT	C17-C12-C13	-2.60	114.90	117.73
2	A	417	HEM	O2A-CGA-CBA	-2.38	106.47	114.00
2	A	417	HEM	CBD-CAD-C3D	2.25	118.75	112.53
2	A	417	HEM	CAA-C2A-C1A	-2.18	120.68	124.94
2	A	417	HEM	C4C-C3C-C2C	2.10	108.63	106.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

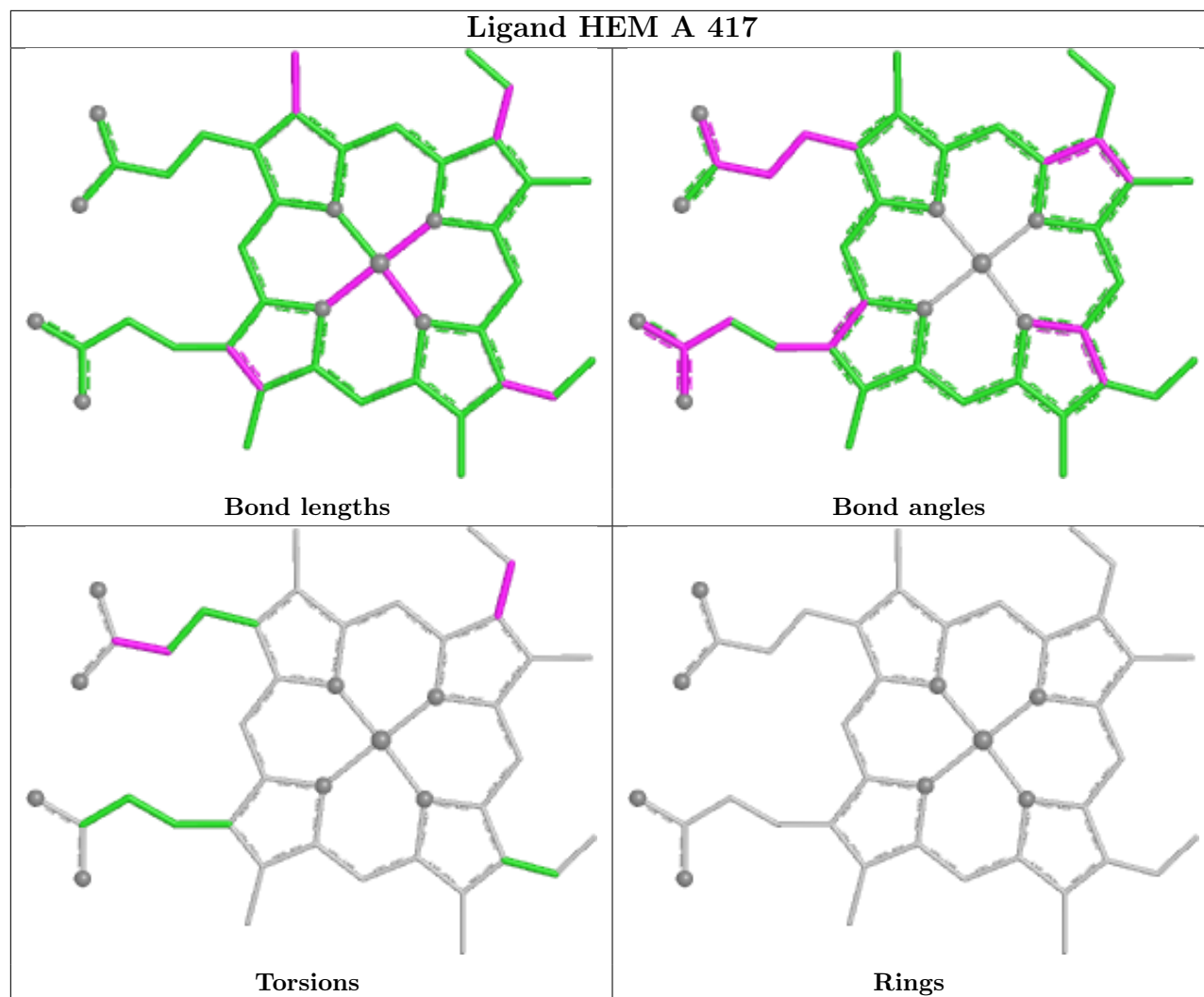
Mol	Chain	Res	Type	Atoms
2	A	417	HEM	C2C-C3C-CAC-CBC
3	A	422	MYT	C2-C3-C7-O8
2	A	417	HEM	C4C-C3C-CAC-CBC
3	A	422	MYT	C4-C3-C7-O8
3	A	422	MYT	C2-C3-C7-C10
3	A	422	MYT	C9-C10-C7-O8
3	A	422	MYT	C4-C3-C7-C10
2	A	417	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	417	HEM	5	0
3	A	422	MYT	4	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.