



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:19 AM UTC

PDB ID : 1PHF / pdb\_00001phf  
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](mailto: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>.

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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)  
Xtrriage (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

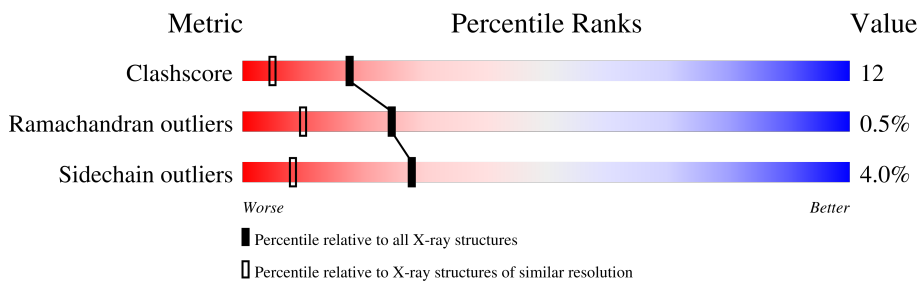
# 1 Overall quality at a glance

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  $\geq 3$ , 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PIM	A	422	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3469 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.

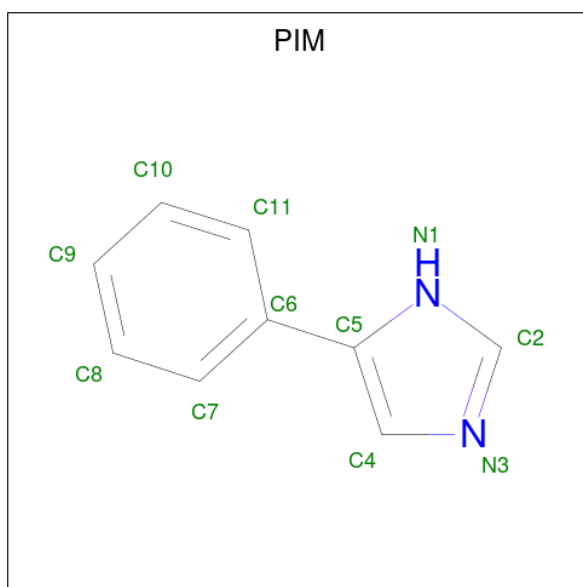
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3209	2033	559	599	18	0	1	0

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



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

- Molecule 3 is 4-PHENYL-1H-IMIDAZOLE (CCD ID: PIM) (formula:  $C_9H_8N_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 11 9 2	0	0

- Molecule 4 is water.

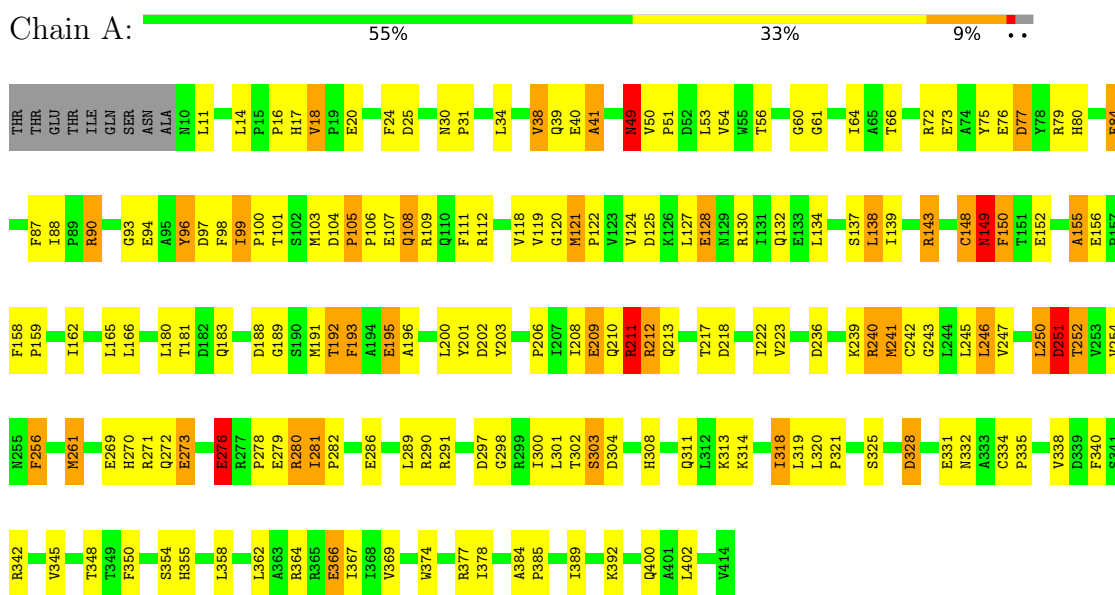
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	206	Total O 206 206	0	0

### 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. 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

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	3469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PIM, 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	1.41	12/3292 (0.4%)	2.16	134/4473 (3.0%)

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	A	0	12

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	ASP	N-CA	7.28	1.55	1.46
1	A	156	GLU	C-O	6.02	1.30	1.24
1	A	251	ASP	C-O	5.92	1.31	1.24
1	A	149	ASN	N-CA	-5.90	1.38	1.46
1	A	149	ASN	C-O	5.84	1.31	1.24
1	A	99	ILE	CA-CB	5.80	1.61	1.54
1	A	77	ASP	C-O	5.67	1.31	1.24
1	A	192	THR	CA-CB	5.41	1.61	1.53
1	A	400	GLN	N-CA	5.38	1.52	1.46
1	A	88	ILE	CA-CB	5.08	1.60	1.54
1	A	112	ARG	NE-CZ	5.02	1.38	1.33
1	A	389	ILE	CA-CB	5.01	1.59	1.54

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	18.30	150.02	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	CYS	CA-C-N	13.51	147.34	121.54
1	A	148	CYS	C-N-CA	13.51	147.34	121.54
1	A	195	GLU	CA-CB-CG	10.32	134.74	114.10
1	A	195	GLU	CB-CG-CD	8.94	127.80	112.60
1	A	80	HIS	CA-CB-CG	-8.94	104.86	113.80
1	A	209	GLU	CA-C-N	8.89	132.19	120.28
1	A	209	GLU	C-N-CA	8.89	132.19	120.28
1	A	241	MET	N-CA-CB	8.72	122.71	110.07
1	A	156	GLU	CB-CG-CD	8.57	127.16	112.60
1	A	328	ASP	CA-CB-CG	8.35	120.95	112.60
1	A	149	ASN	CA-C-O	-8.02	109.04	120.51
1	A	118	VAL	N-CA-C	7.99	118.78	110.72
1	A	251	ASP	O-C-N	-7.86	112.12	122.42
1	A	20	GLU	CA-CB-CG	7.79	129.68	114.10
1	A	149	ASN	N-CA-CB	7.77	123.62	110.49
1	A	38	VAL	CA-C-N	7.75	130.67	120.28
1	A	38	VAL	C-N-CA	7.75	130.67	120.28
1	A	252	THR	N-CA-C	7.53	122.58	111.96
1	A	212	ARG	N-CA-C	-7.34	102.66	111.69
1	A	64	ILE	CA-C-O	-7.23	112.55	120.43
1	A	211	ARG	NE-CZ-NH2	7.22	125.69	119.20
1	A	148	CYS	O-C-N	-7.17	113.06	122.59
1	A	202	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	109	ARG	N-CA-C	6.75	119.50	111.33
1	A	250	LEU	N-CA-C	6.71	119.95	111.69
1	A	124	VAL	O-C-N	6.51	128.67	121.90
1	A	297	ASP	CB-CA-C	6.46	123.28	110.42
1	A	239	LYS	CA-C-N	6.37	128.82	120.28
1	A	239	LYS	C-N-CA	6.37	128.82	120.28
1	A	11	LEU	CB-CA-C	6.37	120.74	109.72
1	A	108	GLN	CB-CG-CD	6.37	123.42	112.60
1	A	152	GLU	CA-CB-CG	6.33	126.75	114.10
1	A	289	LEU	O-C-N	6.28	128.78	122.12
1	A	350	PHE	CA-CB-CG	6.25	120.06	113.80
1	A	108	GLN	CA-CB-CG	6.23	126.55	114.10
1	A	270	HIS	N-CA-CB	6.21	119.36	110.16
1	A	130	ARG	CD-NE-CZ	6.20	133.08	124.40
1	A	25	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	254	VAL	N-CA-CB	-6.13	103.38	110.55
1	A	105	PRO	N-CA-C	-6.11	104.60	110.47
1	A	53	LEU	CA-C-O	-6.08	112.79	120.20
1	A	96	TYR	CA-CB-CG	6.06	124.81	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	PHE	N-CA-CB	6.06	118.85	110.07
1	A	119	VAL	CB-CA-C	6.04	116.57	110.65
1	A	51	PRO	CA-C-N	6.04	128.97	120.28
1	A	51	PRO	C-N-CA	6.04	128.97	120.28
1	A	246	LEU	CA-C-N	6.03	128.16	120.56
1	A	246	LEU	C-N-CA	6.03	128.16	120.56
1	A	138	LEU	N-CA-CB	-6.02	101.26	110.16
1	A	18	VAL	N-CA-C	5.92	114.41	107.77
1	A	251	ASP	CA-C-O	-5.92	112.41	119.15
1	A	98	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	211	ARG	CG-CD-NE	5.89	124.95	112.00
1	A	340	PHE	CA-CB-CG	5.88	119.68	113.80
1	A	270	HIS	CA-CB-CG	-5.87	107.93	113.80
1	A	279	GLU	CB-CG-CD	5.86	122.56	112.60
1	A	53	LEU	N-CA-CB	-5.85	101.24	110.77
1	A	66	THR	CA-CB-OG1	-5.82	100.88	109.60
1	A	108	GLN	CA-C-N	5.79	128.31	120.38
1	A	108	GLN	C-N-CA	5.79	128.31	120.38
1	A	211	ARG	CA-CB-CG	5.79	125.67	114.10
1	A	212	ARG	CD-NE-CZ	5.78	132.49	124.40
1	A	106	PRO	N-CD-CG	-5.76	96.89	103.80
1	A	281	ILE	CA-C-N	5.75	124.95	118.97
1	A	281	ILE	C-N-CA	5.75	124.95	118.97
1	A	121	MET	O-C-N	5.74	127.92	121.32
1	A	75	TYR	N-CA-CB	5.73	118.54	110.12
1	A	272	GLN	N-CA-CB	5.70	118.49	110.12
1	A	143	ARG	CA-C-N	5.69	125.31	119.56
1	A	143	ARG	C-N-CA	5.69	125.31	119.56
1	A	125	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	286	GLU	N-CA-CB	5.67	118.46	110.12
1	A	107	GLU	CA-C-N	5.67	129.32	120.82
1	A	107	GLU	C-N-CA	5.67	129.32	120.82
1	A	49	ASN	CA-CB-CG	5.66	118.25	112.60
1	A	101	THR	N-CA-CB	5.61	118.86	110.22
1	A	301	LEU	O-C-N	5.61	129.62	123.01
1	A	334	CYS	O-C-N	5.60	124.11	121.53
1	A	49	ASN	CA-C-N	-5.60	117.27	123.43
1	A	49	ASN	C-N-CA	-5.60	117.27	123.43
1	A	76	GLU	CB-CG-CD	5.58	122.09	112.60
1	A	156	GLU	N-CA-CB	5.54	115.65	110.39
1	A	212	ARG	N-CA-CB	5.53	118.44	110.20
1	A	192	THR	CA-C-O	-5.51	115.71	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	VAL	CA-C-N	5.50	128.20	120.28
1	A	223	VAL	C-N-CA	5.50	128.20	120.28
1	A	251	ASP	N-CA-C	5.45	120.09	113.38
1	A	193	PHE	CA-C-O	-5.44	115.09	120.70
1	A	366	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	137	SER	CA-C-N	5.40	127.96	120.29
1	A	137	SER	C-N-CA	5.40	127.96	120.29
1	A	201	TYR	CA-CB-CG	5.40	123.61	113.90
1	A	348	THR	CA-CB-CG2	5.39	119.67	110.50
1	A	40	GLU	CB-CG-CD	5.38	121.74	112.60
1	A	364	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	189	GLY	N-CA-C	-5.36	107.14	114.64
1	A	152	GLU	N-CA-CB	5.36	118.18	110.20
1	A	304	ASP	N-CA-C	-5.36	101.93	109.96
1	A	24	PHE	CB-CA-C	5.35	118.06	111.43
1	A	41	ALA	CA-C-N	5.35	127.44	120.28
1	A	41	ALA	C-N-CA	5.35	127.44	120.28
1	A	90	ARG	CA-C-O	-5.35	115.19	121.07
1	A	155	ALA	CA-C-N	5.34	125.75	119.83
1	A	155	ALA	C-N-CA	5.34	125.75	119.83
1	A	298	GLY	CA-C-O	-5.32	116.38	121.38
1	A	213	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	303	SER	O-C-N	5.27	128.63	122.99
1	A	342	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	A	77	ASP	CA-C-O	-5.25	113.00	120.51
1	A	34	LEU	N-CA-CB	5.25	117.76	109.94
1	A	279	GLU	CA-CB-CG	5.24	124.59	114.10
1	A	76	GLU	CA-C-N	5.23	131.52	121.54
1	A	76	GLU	C-N-CA	5.23	131.52	121.54
1	A	273	GLU	CA-C-N	5.21	128.23	120.31
1	A	273	GLU	C-N-CA	5.21	128.23	120.31
1	A	180	LEU	O-C-N	5.20	127.64	122.12
1	A	256	PHE	CA-C-N	5.18	127.64	120.29
1	A	256	PHE	C-N-CA	5.18	127.64	120.29
1	A	245	LEU	O-C-N	5.17	127.60	122.12
1	A	128	GLU	CG-CD-OE2	-5.17	106.52	118.40
1	A	276	GLU	N-CA-C	5.16	118.73	112.23
1	A	132	GLN	CA-CB-CG	5.13	124.36	114.10
1	A	213	GLN	CB-CG-CD	5.12	121.31	112.60
1	A	105	PRO	N-CA-CB	5.11	106.05	103.19
1	A	165	LEU	CA-C-N	5.10	127.11	120.28
1	A	165	LEU	C-N-CA	5.10	127.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	MET	O-C-N	5.09	127.59	122.09
1	A	369	VAL	CB-CA-C	5.08	118.68	112.02
1	A	240	ARG	N-CA-C	5.08	116.82	111.28
1	A	60	GLY	N-CA-C	5.07	122.34	115.30
1	A	77	ASP	N-CA-C	5.06	121.58	110.80
1	A	392	LYS	O-C-N	5.02	129.09	123.27
1	A	289	LEU	CA-C-O	-5.01	115.24	120.55

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ARG	Sidechain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	211	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	271	ARG	Sidechain
1	A	280	ARG	Sidechain
1	A	377	ARG	Sidechain
1	A	77	ASP	Mainchain
1	A	84[A]	GLU	Sidechain
1	A	84[B]	GLU	Sidechain

## 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	3209	0	3146	78	0
2	A	43	0	30	3	0
3	A	11	0	8	4	0
4	A	206	0	0	4	0
All	All	3469	0	3184	80	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 12.

All (80) 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:181:THR:HG23	1:A:247:VAL:HG13	1.63	0.80
1:A:183:GLN:HE22	1:A:188:ASP:HB2	1.54	0.72
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.77	0.66
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.78	0.65
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.61	0.64
1:A:134:LEU:HD23	1:A:162:ILE:HG13	1.82	0.62
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.01	0.60
1:A:111:PHE:HB3	1:A:241:MET:HE2	1.83	0.59
1:A:97:ASP:O	1:A:240:ARG:HD2	2.04	0.58
1:A:358:LEU:HD12	2:A:417:HEM:HMD3	1.85	0.57
1:A:240:ARG:HD3	4:A:675:HOH:O	2.06	0.56
1:A:127:LEU:CD1	1:A:166:LEU:HD13	2.37	0.55
1:A:191:MET:HE2	1:A:196:ALA:HA	1.87	0.55
1:A:332:ASN:O	1:A:335:PRO:HD3	2.07	0.55
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.90	0.54
1:A:50:VAL:HG12	1:A:54:VAL:HG11	1.91	0.53
1:A:325:SER:O	1:A:331:GLU:HG3	2.08	0.53
1:A:99:ILE:HG12	1:A:103:MET:HE3	1.90	0.53
1:A:319:LEU:C	1:A:321:PRO:HD3	2.34	0.52
1:A:183:GLN:HE22	1:A:188:ASP:CB	2.20	0.52
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.39	0.52
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.41	0.51
1:A:252:THR:HG21	3:A:422:PIM:HN1	1.74	0.51
2:A:417:HEM:C4B	3:A:422:PIM:H2	2.45	0.50
2:A:417:HEM:NB	3:A:422:PIM:H2	2.25	0.50
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.42	0.50
1:A:87:PHE:HB2	1:A:93:GLY:HA2	1.94	0.50
1:A:149:ASN:C	1:A:149:ASN:HD22	2.20	0.50
1:A:31:PRO:HB2	1:A:41:ALA:HB1	1.94	0.50
1:A:362:LEU:O	1:A:366:GLU:HG3	2.12	0.49
1:A:252:THR:HG21	3:A:422:PIM:N1	2.28	0.49
1:A:302:THR:C	1:A:314:LYS:HG3	2.37	0.49
1:A:56:THR:O	1:A:61:GLY:HA2	2.12	0.48
1:A:236:ASP:O	1:A:240:ARG:HG3	2.13	0.48
1:A:149:ASN:ND2	1:A:402:LEU:H	2.12	0.48
1:A:302:THR:O	1:A:314:LYS:HG3	2.14	0.48
1:A:39:GLN:NE2	1:A:39:GLN:H	2.11	0.48
1:A:290:ARG:HD3	1:A:345:VAL:HG13	1.95	0.47
1:A:72:ARG:NH1	1:A:331:GLU:OE1	2.45	0.47
1:A:50:VAL:CG1	1:A:54:VAL:HG11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:O	1:A:321:PRO:HD3	2.14	0.46
1:A:193:PHE:HB2	4:A:689:HOH:O	2.15	0.46
1:A:30:ASN:ND2	4:A:555:HOH:O	2.48	0.46
1:A:104:ASP:HB3	1:A:105:PRO:HD2	1.98	0.46
1:A:261:MET:HA	1:A:261:MET:HE2	1.97	0.46
1:A:49:ASN:HD22	1:A:49:ASN:H	1.64	0.45
1:A:150:PHE:CE2	1:A:155:ALA:HB2	2.50	0.45
1:A:303:SER:HA	1:A:314:LYS:HG3	1.99	0.45
1:A:243:GLY:O	1:A:247:VAL:HG23	2.17	0.45
1:A:183:GLN:NE2	1:A:188:ASP:HB2	2.27	0.45
1:A:99:ILE:HD12	1:A:240:ARG:HB2	1.99	0.45
1:A:84[B]:GLU:CD	1:A:300:ILE:HG21	2.42	0.44
1:A:276:GLU:C	1:A:278:PRO:HD3	2.42	0.44
1:A:200:LEU:O	1:A:203:TYR:HB3	2.17	0.44
1:A:318:ILE:HD13	1:A:320:LEU:HD21	1.99	0.44
1:A:208:ILE:O	1:A:212:ARG:HG3	2.18	0.44
1:A:100:PRO:O	1:A:355:HIS:HE1	2.01	0.44
1:A:191:MET:HE2	1:A:196:ALA:CA	2.48	0.44
1:A:218:ASP:O	1:A:222:ILE:HG12	2.18	0.44
1:A:181:THR:HG21	1:A:251:ASP:HB2	2.00	0.44
1:A:211:ARG:NH1	1:A:218:ASP:OD2	2.51	0.43
1:A:108:GLN:NE2	1:A:354:SER:HB2	2.30	0.43
1:A:203:TYR:O	1:A:206:PRO:HD2	2.17	0.43
1:A:17:HIS:CD2	1:A:313:LYS:HG3	2.54	0.43
1:A:273:GLU:OE2	1:A:280:ARG:NH1	2.47	0.43
1:A:209:GLU:HG2	4:A:603:HOH:O	2.19	0.43
1:A:73:GLU:OE1	1:A:308:HIS:NE2	2.44	0.43
1:A:90:ARG:O	1:A:94:GLU:HG3	2.19	0.42
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.90	0.42
1:A:328:ASP:HB3	1:A:331:GLU:HG3	2.02	0.42
1:A:134:LEU:O	1:A:138:LEU:HB2	2.19	0.42
1:A:139:ILE:HG12	1:A:374:TRP:CE3	2.55	0.41
1:A:14:LEU:HD11	1:A:18:VAL:HG11	2.01	0.41
1:A:291:ARG:HG2	1:A:338:VAL:HG22	2.03	0.41
1:A:313:LYS:O	1:A:314:LYS:C	2.64	0.41
1:A:256:PHE:CE2	1:A:367:ILE:HD13	2.56	0.41
1:A:242:CYS:O	1:A:246:LEU:HD23	2.21	0.40
1:A:319:LEU:HG	1:A:321:PRO:HG3	2.02	0.40
1:A:269:GLU:CD	1:A:269:GLU:H	2.30	0.40
1:A:281:ILE:N	1:A:282:PRO:CD	2.85	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	404/414 (98%)	380 (94%)	22 (5%)	2 (0%)	24 10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLY
1	A	150	PHE

### 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	350/358 (98%)	336 (96%)	14 (4%)	28 8

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PRO
1	A	38	VAL
1	A	49	ASN
1	A	79	ARG
1	A	96	TYR
1	A	128	GLU
1	A	210	GLN
1	A	211	ARG
1	A	217	THR

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Mol	Chain	Res	Type
1	A	261	MET
1	A	276	GLU
1	A	311	GLN
1	A	318	ILE
1	A	378	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	59	ASN
1	A	108	GLN
1	A	110	GLN
1	A	149	ASN
1	A	213	GLN
1	A	225	ASN
1	A	388	GLN

### 5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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
3	PIM	A	422	2	11,12,12	2.16	6 (54%)	14,15,15	1.61	3 (21%)
2	HEM	A	417	1,3	50,50,50	1.41	8 (16%)	67,82,82	1.34	10 (14%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PIM	A	422	2	-	4/4/4/4	0/2/2/2
2	HEM	A	417	1,3	-	5/14/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	417	HEM	FE-NB	3.41	2.05	1.94
3	A	422	PIM	C5-N1	-3.07	1.34	1.38
3	A	422	PIM	C2-N1	3.07	1.40	1.35
2	A	417	HEM	FE-NC	3.05	2.05	1.95
2	A	417	HEM	FE-NA	2.96	2.04	1.95
3	A	422	PIM	C6-C5	2.74	1.51	1.47
3	A	422	PIM	C4-N3	-2.71	1.32	1.37
3	A	422	PIM	C11-C6	-2.59	1.35	1.39
2	A	417	HEM	CAC-C3C	2.48	1.54	1.47
2	A	417	HEM	C2A-C3A	-2.44	1.32	1.38
2	A	417	HEM	CMD-C2D	2.43	1.55	1.50
3	A	422	PIM	C8-C7	2.14	1.42	1.38
2	A	417	HEM	C4A-C3A	2.11	1.48	1.43
2	A	417	HEM	CMA-C3A	2.09	1.55	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	O2A-CGA-O1A	3.23	131.64	123.33
2	A	417	HEM	CMA-C3A-C4A	-2.73	121.26	125.42
2	A	417	HEM	CMA-C3A-C2A	2.66	131.27	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	417	HEM	O1D-CGD-CBD	-2.46	115.29	123.09
2	A	417	HEM	CHB-C4A-NA	2.45	128.31	123.86
2	A	417	HEM	C3B-C2B-C1B	2.45	108.25	106.41
3	A	422	PIM	C9-C10-C11	-2.43	117.24	120.24
2	A	417	HEM	CAA-C2A-C1A	-2.40	120.26	124.94
3	A	422	PIM	C4-N3-C2	2.35	110.55	105.94
2	A	417	HEM	O1A-CGA-CBA	-2.17	116.22	123.09
2	A	417	HEM	CHB-C1B-NB	2.07	126.93	124.37
3	A	422	PIM	C2-N1-C5	-2.07	106.47	107.53
2	A	417	HEM	CHA-C1A-NA	2.02	127.52	123.86

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	417	HEM	C2C-C3C-CAC-CBC
2	A	417	HEM	C4C-C3C-CAC-CBC
3	A	422	PIM	N1-C5-C6-C11
3	A	422	PIM	C4-C5-C6-C11
3	A	422	PIM	N1-C5-C6-C7
3	A	422	PIM	C4-C5-C6-C7
2	A	417	HEM	C2B-C3B-CAB-CBB
2	A	417	HEM	CAD-CBD-CGD-O2D
2	A	417	HEM	CAD-CBD-CGD-O1D

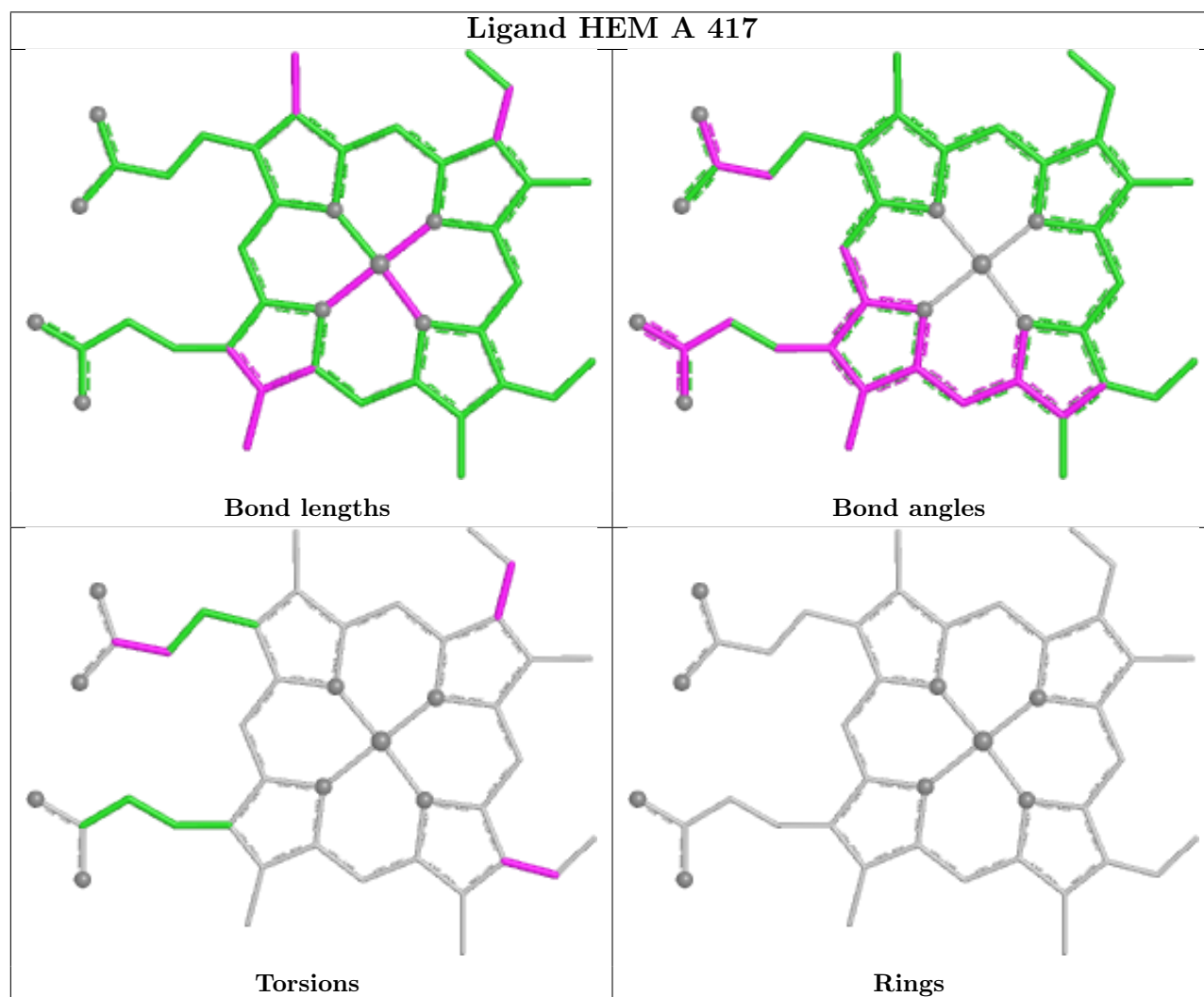
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	422	PIM	4	0
2	A	417	HEM	3	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](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.