



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:55 PM UTC

PDB ID : 1PHE / pdb_00001phe
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

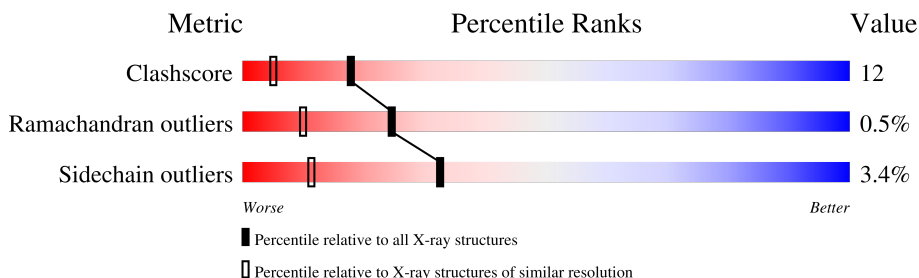
1 Overall quality at a glance

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	 51% 36% 10% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3464 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	3204	2030	559	597	18	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



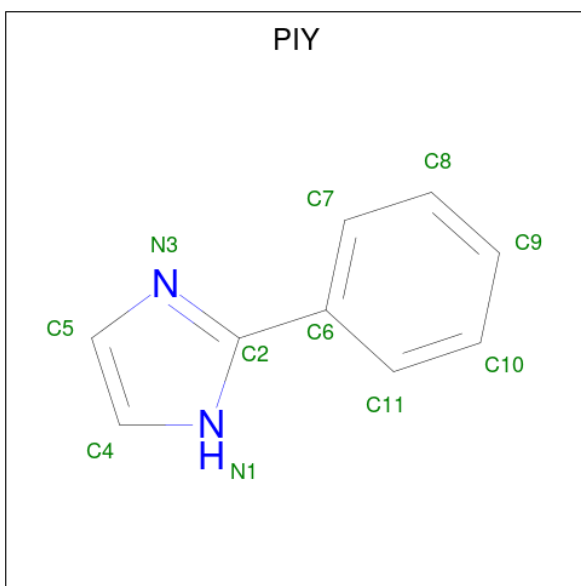
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	S	0	0
			1	1		

- 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		

- Molecule 4 is 2-phenyl-1H-imidazole (CCD ID: PIY) (formula: $\text{C}_9\text{H}_8\text{N}_2$).



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

- Molecule 5 is water.

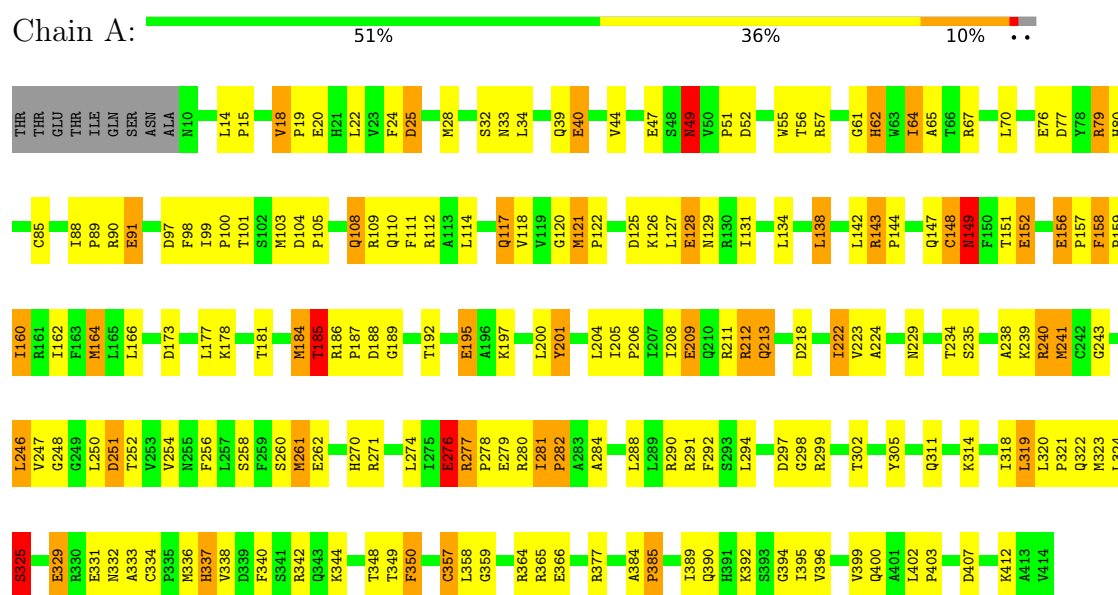
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	205	Total 205	O 205	0	0

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. 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	3464	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: HEM, SO4, PIY

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	1.49	12/3283 (0.4%)	2.36	187/4461 (4.2%)

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	8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	CYS	C-N	-7.21	1.25	1.33
1	A	85	CYS	N-CA	7.08	1.54	1.46
1	A	77	ASP	C-O	5.98	1.30	1.23
1	A	131	ILE	C-N	-5.70	1.26	1.33
1	A	392	LYS	N-CA	5.58	1.52	1.45
1	A	276	GLU	CD-OE1	5.47	1.35	1.25
1	A	412	LYS	CA-CB	-5.30	1.45	1.53
1	A	52	ASP	N-CA	-5.29	1.40	1.46
1	A	399	VAL	C-N	-5.24	1.26	1.33
1	A	262	GLU	N-CA	5.06	1.52	1.46
1	A	319	LEU	C-N	-5.06	1.26	1.34
1	A	395	ILE	CA-CB	5.03	1.60	1.54

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	13.80	143.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	CYS	CA-C-N	12.32	139.29	122.79
1	A	148	CYS	C-N-CA	12.32	139.29	122.79
1	A	51	PRO	CA-C-N	11.84	136.14	120.28
1	A	51	PRO	C-N-CA	11.84	136.14	120.28
1	A	195	GLU	CA-CB-CG	11.03	136.16	114.10
1	A	67	ARG	NE-CZ-NH2	-9.78	110.40	119.20
1	A	80	HIS	CA-CB-CG	-9.28	104.52	113.80
1	A	209	GLU	CA-C-N	9.27	133.08	120.38
1	A	209	GLU	C-N-CA	9.27	133.08	120.38
1	A	131	ILE	CA-C-N	8.80	132.07	120.28
1	A	131	ILE	C-N-CA	8.80	132.07	120.28
1	A	412	LYS	CA-CB-CG	8.76	131.61	114.10
1	A	365	ARG	CD-NE-CZ	8.59	136.43	124.40
1	A	364	ARG	CD-NE-CZ	8.56	136.39	124.40
1	A	20	GLU	CA-CB-CG	8.49	131.08	114.10
1	A	25	ASP	CA-CB-CG	8.21	120.81	112.60
1	A	125	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	52	ASP	CA-CB-CG	8.05	120.65	112.60
1	A	40	GLU	CA-C-N	7.82	130.76	120.28
1	A	40	GLU	C-N-CA	7.82	130.76	120.28
1	A	32	SER	N-CA-C	7.78	119.39	111.07
1	A	241	MET	N-CA-CB	7.71	121.25	110.07
1	A	322	GLN	OE1-CD-NE2	-7.68	114.92	122.60
1	A	270	HIS	N-CA-CB	7.65	121.60	110.20
1	A	118	VAL	CA-C-N	7.60	130.58	122.14
1	A	118	VAL	C-N-CA	7.60	130.58	122.14
1	A	76	GLU	CA-C-N	7.55	133.38	122.21
1	A	76	GLU	C-N-CA	7.55	133.38	122.21
1	A	67	ARG	NE-CZ-NH1	7.53	129.03	121.50
1	A	108	GLN	CA-CB-CG	7.49	129.08	114.10
1	A	49	ASN	CA-CB-CG	7.48	120.08	112.60
1	A	340	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	240	ARG	CA-C-O	-7.40	112.58	120.42
1	A	164	MET	CB-CA-C	7.31	122.51	110.81
1	A	44	VAL	CA-C-O	-7.26	113.39	120.95
1	A	204	LEU	N-CA-C	7.23	119.24	111.36
1	A	118	VAL	N-CA-C	7.13	120.01	111.09
1	A	149	ASN	CB-CA-C	7.10	122.58	111.72
1	A	44	VAL	N-CA-CB	7.07	120.15	110.54
1	A	235	SER	CA-C-N	7.04	129.60	120.44
1	A	235	SER	C-N-CA	7.04	129.60	120.44
1	A	149	ASN	CA-C-O	-7.00	112.13	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	HIS	CA-CB-CG	6.92	120.72	113.80
1	A	55	TRP	O-C-N	6.89	131.50	123.30
1	A	396	VAL	CB-CA-C	6.72	120.32	110.77
1	A	90	ARG	CA-C-N	6.72	129.58	120.38
1	A	90	ARG	C-N-CA	6.72	129.58	120.38
1	A	152	GLU	N-CA-CB	6.71	120.63	110.30
1	A	280	ARG	CD-NE-CZ	6.67	133.74	124.40
1	A	212	ARG	N-CA-C	-6.67	103.49	111.69
1	A	322	GLN	CB-CG-CD	6.65	123.91	112.60
1	A	105	PRO	N-CA-C	-6.58	104.15	110.47
1	A	200	LEU	N-CA-C	-6.57	104.20	111.82
1	A	256	PHE	CA-CB-CG	-6.54	107.27	113.80
1	A	64	ILE	CA-C-O	-6.51	113.80	120.25
1	A	91	GLU	CB-CG-CD	6.42	123.52	112.60
1	A	195	GLU	CB-CA-C	-6.42	100.80	110.88
1	A	89	PRO	CA-C-N	6.41	128.77	120.44
1	A	89	PRO	C-N-CA	6.41	128.77	120.44
1	A	195	GLU	CB-CG-CD	6.41	123.50	112.60
1	A	18	VAL	N-CA-C	6.39	114.22	107.76
1	A	184	MET	CA-C-N	6.32	135.10	121.64
1	A	184	MET	C-N-CA	6.32	135.10	121.64
1	A	277	ARG	N-CA-CB	-6.31	100.85	110.75
1	A	128	GLU	N-CA-C	6.30	118.67	111.11
1	A	282	PRO	CA-C-N	6.29	128.62	120.44
1	A	282	PRO	C-N-CA	6.29	128.62	120.44
1	A	18	VAL	O-C-N	6.28	127.03	121.57
1	A	104	ASP	O-C-N	6.28	126.85	121.20
1	A	324	LEU	CA-C-O	-6.27	112.39	119.79
1	A	91	GLU	CB-CA-C	-6.27	100.02	110.68
1	A	392	LYS	CA-CB-CG	6.24	126.57	114.10
1	A	395	ILE	O-C-N	6.22	128.01	121.91
1	A	178	LYS	CB-CA-C	6.20	120.69	110.90
1	A	279	GLU	CA-CB-CG	6.20	126.49	114.10
1	A	129	ASN	CA-CB-CG	6.19	118.79	112.60
1	A	334	CYS	N-CA-CB	-6.17	104.81	111.66
1	A	332	ASN	OD1-CG-ND2	6.14	128.74	122.60
1	A	108	GLN	CB-CG-CD	6.05	122.89	112.60
1	A	305	TYR	O-C-N	6.04	130.37	123.48
1	A	149	ASN	N-CA-CB	6.04	119.60	110.11
1	A	350	PHE	CA-CB-CG	6.00	119.81	113.80
1	A	109	ARG	N-CA-C	5.97	118.56	111.33
1	A	151	THR	N-CA-CB	5.94	118.58	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	GLU	CB-CG-CD	5.94	122.70	112.60
1	A	201	TYR	CA-C-O	-5.94	114.13	120.42
1	A	281	ILE	CA-C-N	5.93	125.14	118.97
1	A	281	ILE	C-N-CA	5.93	125.14	118.97
1	A	201	TYR	CA-CB-CG	5.89	124.51	113.90
1	A	77	ASP	CA-C-O	-5.88	114.56	122.44
1	A	407	ASP	O-C-N	5.88	126.75	121.35
1	A	260	SER	O-C-N	5.85	128.82	122.15
1	A	34	LEU	CB-CA-C	5.84	120.16	110.81
1	A	222	ILE	CA-C-O	-5.78	114.72	120.85
1	A	251	ASP	N-CA-C	5.78	120.71	113.43
1	A	76	GLU	CB-CG-CD	5.77	122.41	112.60
1	A	85	CYS	N-CA-CB	-5.76	103.94	111.09
1	A	258	SER	CA-C-O	-5.73	114.34	120.42
1	A	311	GLN	N-CA-CB	5.72	119.78	110.17
1	A	349	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	234	THR	CA-C-N	5.68	128.16	120.44
1	A	234	THR	C-N-CA	5.68	128.16	120.44
1	A	100	PRO	CA-C-N	5.67	128.66	120.38
1	A	100	PRO	C-N-CA	5.67	128.66	120.38
1	A	156	GLU	CB-CG-CD	5.65	122.20	112.60
1	A	322	GLN	CG-CD-OE1	5.65	132.10	120.80
1	A	104	ASP	CA-C-O	-5.61	114.64	120.87
1	A	276	GLU	N-CA-CB	5.59	118.91	110.30
1	A	224	ALA	N-CA-C	5.59	118.90	111.75
1	A	238	ALA	CA-C-O	5.57	126.32	120.42
1	A	323	MET	N-CA-C	5.57	117.35	111.28
1	A	33	ASN	N-CA-CB	-5.55	102.77	110.65
1	A	366	GLU	O-C-N	-5.55	116.24	122.12
1	A	222	ILE	O-C-N	5.54	127.54	121.83
1	A	234	THR	N-CA-C	-5.53	103.39	110.53
1	A	187	PRO	CA-C-N	5.53	130.03	120.58
1	A	187	PRO	C-N-CA	5.53	130.03	120.58
1	A	138	LEU	CB-CA-C	5.51	119.94	110.79
1	A	55	TRP	CA-C-O	-5.50	114.42	120.36
1	A	294	LEU	N-CA-C	5.49	122.60	114.09
1	A	173	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	47	GLU	CA-C-N	5.46	127.86	120.38
1	A	47	GLU	C-N-CA	5.46	127.86	120.38
1	A	292	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	160	ILE	N-CA-C	5.38	115.58	110.42
1	A	395	ILE	CA-C-O	-5.36	115.48	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ASP	CA-C-N	5.36	129.74	122.19
1	A	25	ASP	C-N-CA	5.36	129.74	122.19
1	A	358	LEU	O-C-N	5.36	128.26	122.15
1	A	329	GLU	CA-CB-CG	5.35	124.79	114.10
1	A	185	THR	OG1-CB-CG2	5.34	119.98	109.30
1	A	276	GLU	N-CA-C	5.33	118.95	112.23
1	A	365	ARG	O-C-N	-5.33	116.58	122.07
1	A	344	LYS	CA-CB-CG	5.32	124.75	114.10
1	A	138	LEU	N-CA-CB	-5.32	102.30	110.12
1	A	117	GLN	CA-C-N	5.32	129.02	120.30
1	A	117	GLN	C-N-CA	5.32	129.02	120.30
1	A	252	THR	CA-CB-OG1	-5.31	101.64	109.60
1	A	147	GLN	CA-CB-CG	5.31	124.71	114.10
1	A	403	PRO	CA-C-O	-5.30	114.72	120.92
1	A	70	LEU	CA-C-O	-5.30	114.80	120.42
1	A	65	ALA	N-CA-C	-5.30	101.83	110.20
1	A	185	THR	N-CA-CB	-5.30	102.37	110.26
1	A	125	ASP	CA-C-N	5.29	127.81	120.29
1	A	125	ASP	C-N-CA	5.29	127.81	120.29
1	A	223	VAL	CA-C-N	5.29	128.11	120.38
1	A	223	VAL	C-N-CA	5.29	128.11	120.38
1	A	365	ARG	CA-C-N	5.29	127.36	120.28
1	A	365	ARG	C-N-CA	5.29	127.36	120.28
1	A	100	PRO	N-CD-CG	-5.26	97.49	103.80
1	A	344	LYS	CA-C-N	5.25	129.81	122.93
1	A	344	LYS	C-N-CA	5.25	129.81	122.93
1	A	325	SER	N-CA-C	5.24	117.67	111.33
1	A	77	ASP	N-CA-C	5.22	118.79	110.70
1	A	348	THR	OG1-CB-CG2	5.21	119.71	109.30
1	A	126	LYS	CA-CB-CG	5.20	124.50	114.10
1	A	329	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	101	THR	N-CA-CB	5.19	118.34	110.14
1	A	394	GLY	CA-C-O	-5.18	117.33	120.91
1	A	390	GLN	CA-CB-CG	-5.17	103.76	114.10
1	A	357	CYS	CA-C-N	5.14	127.59	120.29
1	A	357	CYS	C-N-CA	5.14	127.59	120.29
1	A	333	ALA	CA-C-O	-5.13	116.12	121.55
1	A	55	TRP	N-CA-CB	5.12	119.28	110.68
1	A	366	GLU	CA-C-N	5.11	127.09	120.56
1	A	366	GLU	C-N-CA	5.11	127.09	120.56
1	A	248	GLY	CA-C-N	5.10	131.41	121.41
1	A	248	GLY	C-N-CA	5.10	131.41	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	PRO	CB-CA-C	-5.10	106.00	111.56
1	A	277	ARG	CA-C-N	5.10	126.21	119.84
1	A	277	ARG	C-N-CA	5.10	126.21	119.84
1	A	33	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	A	241	MET	CB-CA-C	-5.09	102.86	110.90
1	A	24	PHE	CB-CA-C	5.08	118.08	111.42
1	A	297	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	121	MET	CA-C-N	5.08	125.11	119.32
1	A	121	MET	C-N-CA	5.08	125.11	119.32
1	A	290	ARG	CB-CA-C	-5.08	102.88	110.90
1	A	323	MET	CA-C-N	5.08	129.31	120.68
1	A	323	MET	C-N-CA	5.08	129.31	120.68
1	A	213	GLN	CB-CG-CD	5.06	121.21	112.60
1	A	337	HIS	CB-CA-C	5.04	117.84	109.53
1	A	188	ASP	N-CA-CB	-5.02	102.72	110.20
1	A	325	SER	CA-C-O	-5.01	115.22	120.63
1	A	395	ILE	N-CA-CB	5.00	116.41	110.55
1	A	189	GLY	N-CA-C	-5.00	108.10	114.85

There are no chirality outliers.

All (8) 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	271	ARG	Sidechain
1	A	325	SER	Mainchain
1	A	342	ARG	Sidechain
1	A	377	ARG	Sidechain
1	A	79	ARG	Sidechain

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	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	43	0	30	3	0
4	A	11	0	8	2	0
5	A	205	0	0	8	0
All	All	3464	0	3183	79	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 (79) 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:185:THR:HG21	1:A:251:ASP:OD2	1.89	0.72
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.76	0.67
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.77	0.66
1:A:149:ASN:ND2	1:A:402:LEU:H	1.96	0.64
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.80	0.64
1:A:177:LEU:HD13	1:A:246:LEU:HD11	1.80	0.63
1:A:111:PHE:HB3	1:A:241:MET:HE2	1.82	0.61
1:A:56:THR:O	1:A:61:GLY:HA2	2.03	0.59
1:A:254:VAL:HG23	5:A:687:HOH:O	2.03	0.57
1:A:25:ASP:OD1	1:A:57:ARG:HB2	2.05	0.57
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.87	0.56
1:A:181:THR:HG21	1:A:251:ASP:HB2	1.86	0.56
1:A:39:GLN:NE2	1:A:39:GLN:H	2.04	0.55
1:A:325:SER:O	1:A:331:GLU:HG3	2.07	0.55
1:A:201:TYR:OH	1:A:240:ARG:HG2	2.06	0.55
1:A:243:GLY:O	1:A:247:VAL:HG22	2.07	0.55
1:A:122:PRO:HD2	5:A:701:HOH:O	2.07	0.54
1:A:337:HIS:HB2	5:A:694:HOH:O	2.09	0.53
1:A:15:PRO:HG2	1:A:18:VAL:CG2	2.38	0.53
1:A:318:ILE:HD13	1:A:320:LEU:HD21	1.91	0.53
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.90	0.52
1:A:57:ARG:HG2	5:A:508:HOH:O	2.09	0.52
1:A:134:LEU:HB2	5:A:590:HOH:O	2.10	0.52
1:A:160:ILE:O	1:A:164:MET:HG2	2.10	0.51
1:A:277:ARG:N	1:A:278:PRO:HD3	2.25	0.51
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.41	0.51
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.26	0.51
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.47	0.50
1:A:149:ASN:HD21	1:A:402:LEU:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE2	1:A:197:LYS:HA	1.93	0.50
1:A:302:THR:C	1:A:314:LYS:HG3	2.37	0.49
1:A:156:GLU:HB2	1:A:157:PRO:HD3	1.94	0.49
1:A:114:LEU:O	1:A:117:GLN:HB2	2.12	0.49
1:A:164:MET:HB2	5:A:525:HOH:O	2.12	0.49
1:A:14:LEU:HD11	1:A:18:VAL:HG11	1.95	0.48
1:A:19:PRO:HG2	1:A:22:LEU:HD12	1.96	0.48
1:A:121:MET:N	1:A:122:PRO:CD	2.77	0.48
1:A:281:ILE:N	1:A:282:PRO:HD3	2.28	0.48
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.15	0.47
1:A:185:THR:CG2	1:A:186:ARG:NH1	2.77	0.47
1:A:389:ILE:HA	5:A:659:HOH:O	2.14	0.47
1:A:99:ILE:HG13	1:A:240:ARG:HB3	1.97	0.47
1:A:261:MET:HA	1:A:261:MET:HE2	1.96	0.47
1:A:201:TYR:HB3	1:A:239:LYS:HD2	1.97	0.47
1:A:281:ILE:N	1:A:282:PRO:CD	2.77	0.46
1:A:291:ARG:HG2	1:A:338:VAL:HG22	1.96	0.46
1:A:15:PRO:HG2	1:A:18:VAL:HG23	1.97	0.46
1:A:98:PHE:CE2	4:A:422:PIY:H4	2.50	0.46
1:A:276:GLU:C	1:A:278:PRO:HD3	2.42	0.45
1:A:99:ILE:HG23	1:A:103:MET:SD	2.56	0.45
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.98	0.45
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.85	0.44
1:A:97:ASP:OD2	1:A:197:LYS:NZ	2.47	0.44
1:A:158:PHE:CE1	1:A:162:ILE:HD11	2.54	0.43
1:A:209:GLU:O	1:A:213:GLN:HG3	2.18	0.43
1:A:298:GLY:C	1:A:299:ARG:HG2	2.43	0.43
1:A:91:GLU:H	1:A:91:GLU:CD	2.25	0.42
1:A:319:LEU:O	1:A:321:PRO:HD3	2.19	0.42
1:A:98:PHE:HE2	4:A:422:PIY:H4	1.84	0.42
1:A:143:ARG:HB3	1:A:144:PRO:HD3	2.00	0.42
1:A:319:LEU:C	1:A:321:PRO:HD3	2.45	0.42
1:A:208:ILE:O	1:A:212:ARG:HG3	2.20	0.42
3:A:417:HEM:HMB2	3:A:417:HEM:HBB2	2.00	0.42
1:A:110:GLN:NE2	1:A:229:ASN:HD22	2.18	0.42
1:A:138:LEU:O	1:A:142:LEU:HG	2.20	0.42
1:A:15:PRO:HG2	1:A:18:VAL:HG21	2.02	0.42
1:A:49:ASN:HD22	1:A:49:ASN:H	1.66	0.42
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.49	0.42
1:A:284:ALA:O	1:A:288:LEU:HG	2.20	0.41
1:A:274:LEU:HD21	1:A:284:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PRO:O	1:A:209:GLU:HB2	2.19	0.41
1:A:359:GLY:HA3	3:A:417:HEM:C3C	2.55	0.41
1:A:112:ARG:NH1	3:A:417:HEM:O1D	2.47	0.41
1:A:152:GLU:HB3	5:A:563:HOH:O	2.20	0.41
1:A:56:THR:HG21	1:A:64:ILE:HD11	2.03	0.41
1:A:28:MET:HE3	1:A:28:MET:HB2	1.87	0.40
1:A:110:GLN:HE21	1:A:229:ASN:HD22	1.67	0.40
1:A:149:ASN:ND2	1:A:149:ASN:C	2.79	0.40
1:A:218:ASP:O	1:A:222:ILE:HG12	2.21	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%)	384 (95%)	17 (4%)	2 (0%)	24 10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	GLY
1	A	158	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	349/358 (98%)	337 (97%)	12 (3%)	32	11

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

Mol	Chain	Res	Type
1	A	49	ASN
1	A	79	ARG
1	A	108	GLN
1	A	128	GLU
1	A	185	THR
1	A	246	LEU
1	A	250	LEU
1	A	261	MET
1	A	276	GLU
1	A	329	GLU
1	A	385	PRO
1	A	400	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	30	ASN
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	59	ASN
1	A	69	GLN
1	A	108	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
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 [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](#)

Of 3 ligands modelled in this entry, 1 is modelled with single atom - leaving 2 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$
4	PIY	A	422	-	12,12,12	1.48	3 (25%)	15,15,15	2.54	4 (26%)
3	HEM	A	417	2,1	50,50,50	1.54	7 (14%)	67,82,82	1.23	7 (10%)

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
4	PIY	A	422	-	-	0/4/4/4	0/2/2/2
3	HEM	A	417	2,1	-	2/14/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	417	HEM	FE-NA	4.38	2.09	1.95
3	A	417	HEM	FE-NC	3.82	2.07	1.95
3	A	417	HEM	CAC-C3C	3.67	1.57	1.47
3	A	417	HEM	FE-NB	3.50	2.05	1.94
4	A	422	PIY	C5-N3	-3.02	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	417	HEM	CMD-C2D	2.47	1.55	1.50
3	A	417	HEM	O1A-CGA	2.47	1.30	1.22
4	A	422	PIY	C6-C2	2.19	1.51	1.47
4	A	422	PIY	C2-N3	2.18	1.38	1.33
3	A	417	HEM	O2D-CGD	-2.08	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	422	PIY	C6-C2-N1	6.23	130.29	124.29
4	A	422	PIY	C5-N3-C2	5.18	111.11	105.60
3	A	417	HEM	C3B-C4B-NB	4.18	112.47	109.47
4	A	422	PIY	N1-C2-N3	-3.70	105.20	110.83
3	A	417	HEM	CBD-CAD-C3D	2.88	120.49	112.53
3	A	417	HEM	C4C-C3C-C2C	2.65	109.11	106.81
3	A	417	HEM	CHA-C4D-ND	-2.42	121.38	124.37
4	A	422	PIY	C5-C4-N1	2.14	109.63	106.35
3	A	417	HEM	CBC-CAC-C3C	-2.10	117.06	127.53
3	A	417	HEM	O2A-CGA-O1A	2.05	128.61	123.33
3	A	417	HEM	O1D-CGD-CBD	-2.05	116.60	123.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	417	HEM	C2C-C3C-CAC-CBC
3	A	417	HEM	C4C-C3C-CAC-CBC

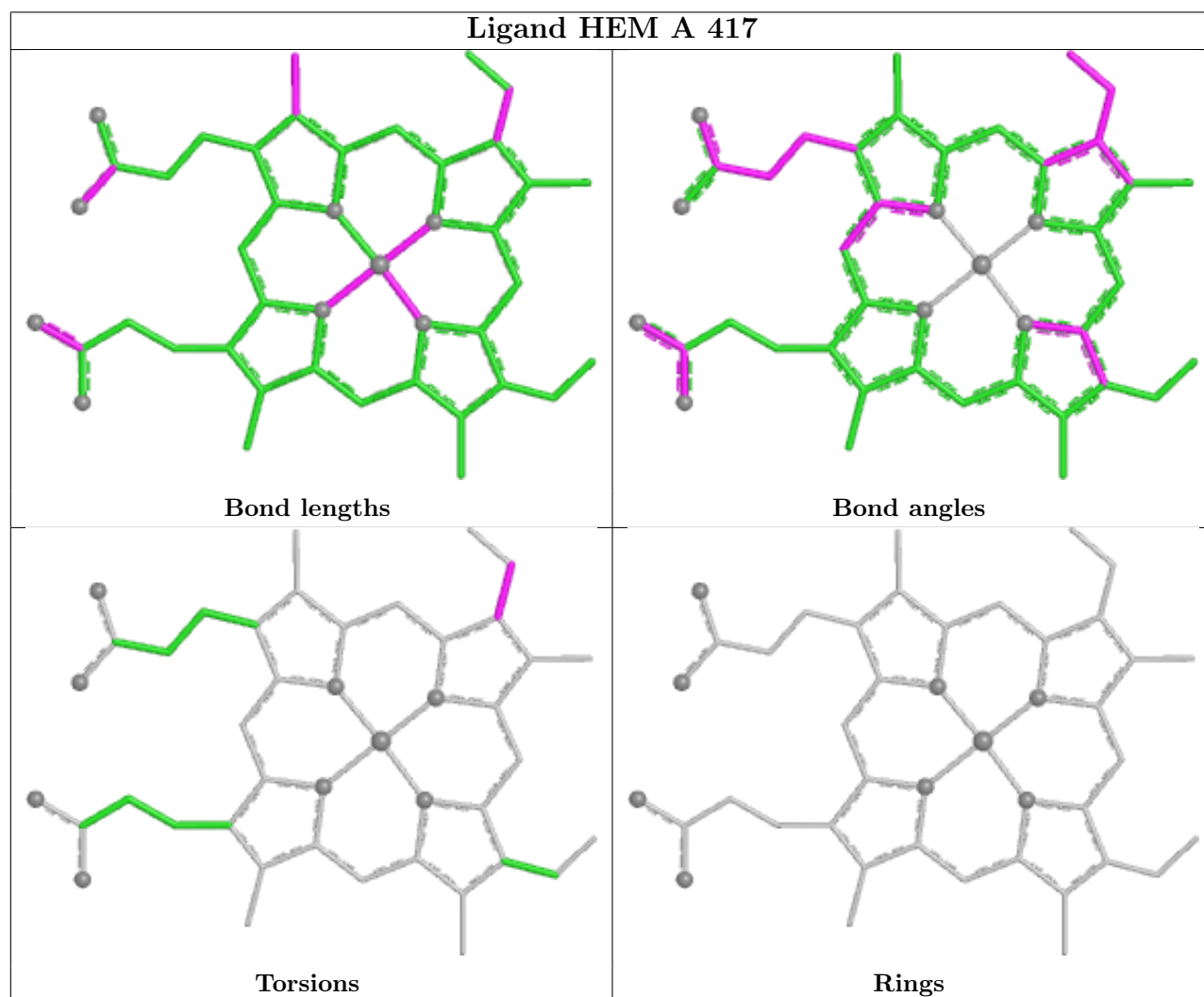
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	422	PIY	2	0
3	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

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.