



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:19 AM UTC

PDB ID : 1PHD / pdb_00001phd
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

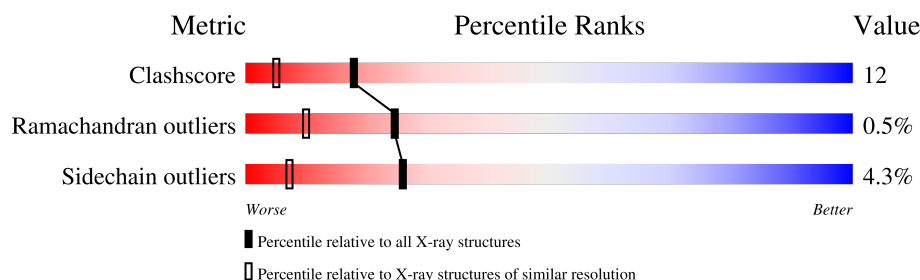
1 Overall quality at a glance

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% 8% ..

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	PIW	A	422	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3462 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.

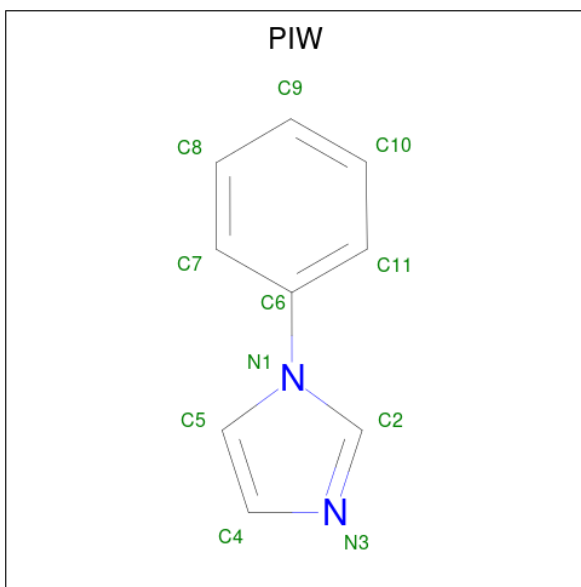
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3204	2030	559	597	18			

- 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 1-phenyl-1H-imidazole (CCD ID: PIW) (formula: $C_9H_8N_2$).



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

- Molecule 4 is water.

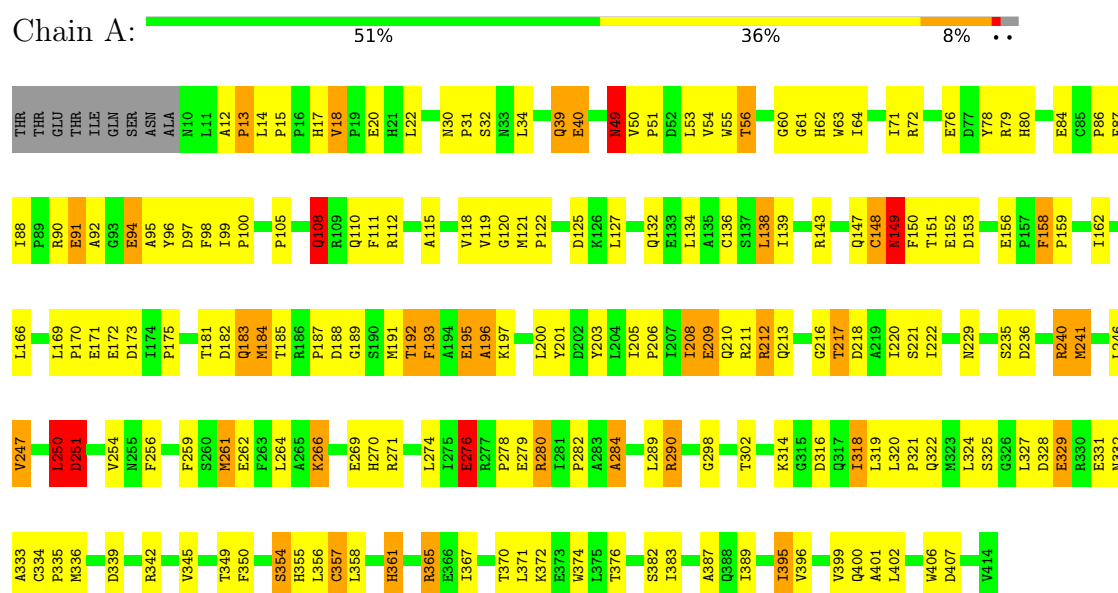
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		

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	3462	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: PIW, 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	1.65	29/3283 (0.9%)	2.21	132/4461 (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 (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	GLU	C-O	9.12	1.33	1.24
1	A	251	ASP	C-O	8.53	1.35	1.23
1	A	96	TYR	N-CA	7.36	1.54	1.46
1	A	370	THR	CA-CB	7.16	1.64	1.53
1	A	266	LYS	C-O	6.86	1.33	1.24
1	A	149	ASN	N-CA	-6.79	1.37	1.46
1	A	349	THR	CB-OG1	6.55	1.54	1.43
1	A	259	PHE	N-CA	6.42	1.54	1.46
1	A	334	CYS	C-O	-6.32	1.20	1.23
1	A	361	HIS	N-CA	6.25	1.53	1.46
1	A	354	SER	C-O	6.14	1.31	1.24
1	A	276	GLU	CD-OE1	6.10	1.36	1.25
1	A	71	ILE	CA-CB	6.08	1.61	1.54
1	A	367	ILE	CA-CB	5.99	1.61	1.54
1	A	136	CYS	N-CA	5.77	1.53	1.46
1	A	266	LYS	N-CA	5.57	1.53	1.46
1	A	192	THR	CA-CB	5.51	1.62	1.53
1	A	399	VAL	C-O	5.48	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	CYS	N-CA	-5.37	1.39	1.46
1	A	264	LEU	C-O	5.32	1.30	1.24
1	A	251	ASP	CA-C	-5.28	1.45	1.52
1	A	18	VAL	N-CA	5.28	1.50	1.46
1	A	53	LEU	C-N	-5.26	1.27	1.33
1	A	88	ILE	CA-CB	5.23	1.60	1.54
1	A	290	ARG	NE-CZ	5.18	1.38	1.33
1	A	354	SER	N-CA	5.05	1.52	1.46
1	A	87	PHE	C-N	-5.03	1.27	1.33
1	A	266	LYS	CA-C	-5.01	1.46	1.52
1	A	324	LEU	C-O	5.00	1.30	1.24

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	13.36	143.10	124.40
1	A	365	ARG	CD-NE-CZ	13.33	143.07	124.40
1	A	118	VAL	N-CA-C	11.36	122.19	110.72
1	A	148	CYS	CA-C-N	10.73	142.04	121.54
1	A	148	CYS	C-N-CA	10.73	142.04	121.54
1	A	195	GLU	CA-CB-CG	10.33	134.76	114.10
1	A	209	GLU	CA-C-N	9.08	132.45	120.28
1	A	209	GLU	C-N-CA	9.08	132.45	120.28
1	A	125	ASP	CA-CB-CG	8.68	121.28	112.60
1	A	365	ARG	NE-CZ-NH2	8.51	126.86	119.20
1	A	118	VAL	CA-C-N	8.48	131.56	122.14
1	A	118	VAL	C-N-CA	8.48	131.56	122.14
1	A	279	GLU	CB-CG-CD	8.34	126.78	112.60
1	A	329	GLU	CB-CG-CD	8.11	126.38	112.60
1	A	20	GLU	CA-CB-CG	8.02	130.14	114.10
1	A	51	PRO	CA-C-N	8.00	131.00	120.28
1	A	51	PRO	C-N-CA	8.00	131.00	120.28
1	A	259	PHE	CA-CB-CG	7.89	121.69	113.80
1	A	241	MET	N-CA-CB	7.76	121.32	110.07
1	A	32	SER	N-CA-C	7.52	119.26	111.14
1	A	327	LEU	CA-C-N	7.51	132.05	121.24
1	A	327	LEU	C-N-CA	7.51	132.05	121.24
1	A	149	ASN	N-CA-CB	7.47	123.11	110.49
1	A	153	ASP	CA-C-O	-7.23	111.65	119.97
1	A	108	GLN	CB-CG-CD	7.22	124.87	112.60
1	A	280	ARG	NE-CZ-NH2	-7.22	112.70	119.20
1	A	395	ILE	O-C-N	7.18	128.83	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ASP	CA-C-O	-7.16	110.97	119.35
1	A	49	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	80	HIS	CA-CB-CG	-7.01	106.79	113.80
1	A	98	PHE	CA-CB-CG	6.99	120.79	113.80
1	A	289	LEU	O-C-N	6.97	129.51	122.12
1	A	251	ASP	CB-CA-C	6.71	121.29	110.09
1	A	407	ASP	CB-CA-C	6.69	119.05	109.08
1	A	279	GLU	CA-CB-CG	6.65	127.41	114.10
1	A	216	GLY	N-CA-C	-6.65	104.81	112.79
1	A	149	ASN	CA-C-O	-6.56	111.12	120.51
1	A	401	ALA	CA-C-O	-6.52	113.72	120.89
1	A	138	LEU	N-CA-CB	-6.50	100.57	110.12
1	A	189	GLY	N-CA-C	-6.46	106.12	114.85
1	A	211	ARG	CB-CG-CD	6.46	126.17	111.30
1	A	211	ARG	NE-CZ-NH1	6.45	127.95	121.50
1	A	334	CYS	O-C-N	6.41	124.48	121.53
1	A	143	ARG	NE-CZ-NH1	6.33	127.83	121.50
1	A	156	GLU	CB-CG-CD	6.27	123.25	112.60
1	A	266	LYS	CG-CD-CE	6.12	125.38	111.30
1	A	250	LEU	N-CA-C	6.10	119.20	111.69
1	A	251	ASP	O-C-N	-6.07	114.76	122.34
1	A	148	CYS	O-C-N	-6.03	114.57	122.59
1	A	196	ALA	O-C-N	6.02	128.27	122.07
1	A	195	GLU	N-CA-C	-6.02	104.63	111.07
1	A	108	GLN	CA-CB-CG	6.02	126.13	114.10
1	A	53	LEU	CA-C-O	-5.95	113.93	120.24
1	A	322	GLN	CA-C-N	5.95	128.57	120.54
1	A	322	GLN	C-N-CA	5.95	128.57	120.54
1	A	211	ARG	CA-CB-CG	5.93	125.97	114.10
1	A	371	LEU	O-C-N	5.92	128.17	122.07
1	A	183	GLN	O-C-N	5.86	129.07	122.22
1	A	318	ILE	CA-C-N	5.82	129.83	121.50
1	A	318	ILE	C-N-CA	5.82	129.83	121.50
1	A	152	GLU	N-CA-CB	5.82	118.87	110.20
1	A	218	ASP	CA-CB-CG	-5.81	106.79	112.60
1	A	289	LEU	CA-C-O	-5.81	114.40	120.55
1	A	96	TYR	N-CA-CB	-5.80	101.44	109.97
1	A	91	GLU	CB-CA-C	-5.79	100.83	110.68
1	A	325	SER	CA-C-N	5.78	131.08	120.79
1	A	325	SER	C-N-CA	5.78	131.08	120.79
1	A	247	VAL	CA-C-N	5.74	126.31	119.94
1	A	247	VAL	C-N-CA	5.74	126.31	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	HIS	O-C-N	5.71	130.02	122.30
1	A	193	PHE	O-C-N	5.70	127.94	122.07
1	A	62	HIS	CA-CB-CG	5.70	119.50	113.80
1	A	251	ASP	N-CA-C	5.68	120.32	113.17
1	A	356	LEU	CA-C-N	5.65	132.34	121.54
1	A	356	LEU	C-N-CA	5.65	132.34	121.54
1	A	96	TYR	CA-C-O	-5.62	114.86	121.16
1	A	175	PRO	CA-C-N	5.61	128.07	120.44
1	A	175	PRO	C-N-CA	5.61	128.07	120.44
1	A	280	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	A	210	GLN	CA-CB-CG	5.59	125.28	114.10
1	A	97	ASP	O-C-N	5.57	127.70	122.18
1	A	193	PHE	CA-C-O	-5.57	114.97	120.82
1	A	94	GLU	N-CA-CB	5.54	118.10	110.07
1	A	217	THR	CA-CB-OG1	-5.53	101.30	109.60
1	A	387	ALA	O-C-N	5.52	129.51	123.22
1	A	256	PHE	CA-C-N	5.51	128.11	120.29
1	A	256	PHE	C-N-CA	5.51	128.11	120.29
1	A	158	PHE	CB-CA-C	5.48	120.97	110.17
1	A	13	PRO	CA-C-N	5.48	128.01	120.67
1	A	13	PRO	C-N-CA	5.48	128.01	120.67
1	A	400	GLN	CA-CB-CG	5.45	125.01	114.10
1	A	270	HIS	N-CA-CB	5.45	118.22	110.16
1	A	193	PHE	N-CA-CB	5.45	117.91	110.01
1	A	64	ILE	CA-C-O	-5.42	114.88	120.25
1	A	184	MET	CA-C-O	-5.40	114.69	120.42
1	A	376	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	55	TRP	CA-C-O	-5.36	114.91	120.70
1	A	151	THR	N-CA-CB	5.36	117.73	109.91
1	A	158	PHE	CA-C-N	5.34	124.97	119.05
1	A	158	PHE	C-N-CA	5.34	124.97	119.05
1	A	34	LEU	CB-CA-C	5.32	119.32	110.81
1	A	209	GLU	CA-CB-CG	5.30	124.71	114.10
1	A	96	TYR	N-CA-C	-5.29	102.46	110.28
1	A	256	PHE	O-C-N	-5.28	116.60	122.09
1	A	329	GLU	CA-CB-CG	5.27	124.64	114.10
1	A	171	GLU	CA-C-O	5.25	126.03	120.10
1	A	62	HIS	CA-C-O	-5.23	115.35	121.10
1	A	60	GLY	N-CA-C	5.22	122.53	115.32
1	A	92	ALA	O-C-N	5.22	127.72	122.09
1	A	196	ALA	N-CA-CB	5.20	117.55	110.01
1	A	372	LYS	N-CA-CB	5.19	117.54	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	LEU	CB-CA-C	5.19	117.63	109.84
1	A	132	GLN	CA-C-O	5.17	125.90	120.42
1	A	22	LEU	CA-C-O	-5.17	113.31	119.35
1	A	396	VAL	CB-CA-C	5.16	117.86	110.33
1	A	172	GLU	CG-CD-OE2	5.16	130.26	118.40
1	A	17	HIS	CA-C-N	-5.16	118.88	122.59
1	A	17	HIS	C-N-CA	-5.16	118.88	122.59
1	A	208	ILE	CA-C-O	-5.15	115.71	121.17
1	A	333	ALA	CA-C-O	-5.13	115.55	121.19
1	A	221	SER	CA-C-O	-5.12	115.13	120.55
1	A	316	ASP	O-C-N	5.11	129.13	122.89
1	A	406	TRP	O-C-N	5.06	128.84	123.42
1	A	298	GLY	CA-C-N	5.05	130.44	122.36
1	A	298	GLY	C-N-CA	5.05	130.44	122.36
1	A	395	ILE	N-CA-CB	5.04	117.39	110.54
1	A	182	ASP	O-C-N	5.03	127.45	122.12
1	A	40	GLU	CB-CG-CD	5.02	121.14	112.60
1	A	269	GLU	CG-CD-OE2	-5.02	106.86	118.40
1	A	339	ASP	N-CA-CB	-5.02	103.21	110.84
1	A	156	GLU	CA-C-N	5.02	124.19	118.97
1	A	156	GLU	C-N-CA	5.02	124.19	118.97

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	GLN	Mainchain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	212	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	271	ARG	Sidechain
1	A	280	ARG	Sidechain
1	A	284	ALA	Mainchain
1	A	342	ARG	Sidechain
1	A	95	ALA	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	78	0
2	A	43	0	30	3	0
3	A	11	0	8	4	0
4	A	204	0	0	7	0
All	All	3462	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:183:GLN:HE22	1:A:188:ASP:HB2	1.54	0.71
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.56	0.70
1:A:56:THR:O	1:A:61:GLY:HA2	1.94	0.67
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.77	0.67
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.78	0.66
1:A:15:PRO:HG2	1:A:18:VAL:HG23	1.76	0.66
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.79	0.65
1:A:328:ASP:HB3	1:A:331:GLU:HG3	1.79	0.65
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.28	0.64
1:A:14:LEU:HD11	1:A:18:VAL:HG11	1.79	0.62
1:A:15:PRO:HG2	1:A:18:VAL:CG2	2.32	0.59
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.32	0.59
1:A:203:TYR:O	1:A:206:PRO:HD2	2.01	0.59
1:A:276:GLU:C	1:A:278:PRO:HD3	2.29	0.58
1:A:40:GLU:HG3	1:A:336:MET:HE2	1.88	0.55
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.88	0.55
1:A:134:LEU:HD23	1:A:162:ILE:HG13	1.90	0.54
1:A:395:ILE:HG21	3:A:422:PIW:H9	1.90	0.53
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.38	0.53
1:A:115:ALA:O	1:A:119:VAL:HG22	2.10	0.52
1:A:158:PHE:CE1	1:A:162:ILE:HD11	2.44	0.51
1:A:185:THR:C	1:A:187:PRO:HD3	2.35	0.51
1:A:201:TYR:O	1:A:205:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PRO:HD2	4:A:661:HOH:O	2.11	0.51
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.93	0.51
1:A:181:THR:HG21	1:A:251:ASP:HB2	1.92	0.50
1:A:39:GLN:NE2	1:A:39:GLN:H	2.10	0.50
1:A:266:LYS:HD2	1:A:383:ILE:CD1	2.41	0.50
1:A:208:ILE:O	1:A:212:ARG:HG3	2.12	0.50
1:A:30:ASN:ND2	4:A:555:HOH:O	2.44	0.49
1:A:209:GLU:O	1:A:213:GLN:HG3	2.11	0.49
1:A:90:ARG:O	1:A:94:GLU:HG3	2.13	0.49
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.28	0.49
1:A:247:VAL:HG12	3:A:422:PIW:H7	1.95	0.49
1:A:183:GLN:NE2	1:A:188:ASP:HB2	2.25	0.49
1:A:358:LEU:HD12	2:A:417:HEM:HMD3	1.95	0.49
1:A:274:LEU:HD21	1:A:284:ALA:HB2	1.94	0.48
1:A:266:LYS:HD2	1:A:383:ILE:HD11	1.96	0.47
1:A:200:LEU:O	1:A:203:TYR:HB3	2.14	0.47
1:A:149:ASN:ND2	1:A:402:LEU:H	2.12	0.47
1:A:250:LEU:O	1:A:254:VAL:HG21	2.15	0.47
1:A:138:LEU:HD23	1:A:158:PHE:HB2	1.97	0.47
1:A:328:ASP:HB3	1:A:331:GLU:CG	2.43	0.46
1:A:191:MET:HE2	1:A:196:ALA:HA	1.97	0.46
1:A:319:LEU:O	1:A:321:PRO:HD3	2.16	0.46
1:A:100:PRO:O	1:A:355:HIS:HE1	1.99	0.46
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.16	0.45
2:A:417:HEM:C4C	3:A:422:PIW:H4	2.51	0.45
1:A:111:PHE:HB3	1:A:241:MET:HE2	1.98	0.45
1:A:169:LEU:HD21	1:A:220:ILE:CD1	2.48	0.44
1:A:184:MET:HE2	1:A:197:LYS:HA	1.98	0.44
1:A:319:LEU:C	1:A:321:PRO:HD3	2.43	0.44
1:A:193:PHE:HB3	4:A:690:HOH:O	2.16	0.44
1:A:236:ASP:O	1:A:240:ARG:HG3	2.18	0.44
1:A:332:ASN:O	1:A:335:PRO:HD3	2.17	0.44
1:A:261:MET:HA	1:A:261:MET:HE2	1.98	0.44
1:A:99:ILE:HD12	1:A:240:ARG:HB2	1.99	0.44
1:A:31:PRO:HA	4:A:502:HOH:O	2.17	0.43
1:A:91:GLU:H	1:A:91:GLU:CD	2.25	0.43
1:A:169:LEU:HD21	1:A:220:ILE:HD12	1.99	0.43
1:A:302:THR:C	1:A:314:LYS:HG3	2.44	0.43
1:A:170:PRO:HG2	1:A:173:ASP:OD2	2.19	0.43
1:A:50:VAL:CG1	1:A:54:VAL:HG11	2.48	0.43
1:A:49:ASN:HD22	1:A:49:ASN:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:HD13	1:A:320:LEU:HD21	2.00	0.42
1:A:382:SER:HB2	4:A:608:HOH:O	2.19	0.42
1:A:78:TYR:CD1	1:A:105:PRO:HD2	2.55	0.42
1:A:112:ARG:NH1	2:A:417:HEM:O1D	2.44	0.42
1:A:247:VAL:CG1	3:A:422:PIW:H7	2.50	0.42
1:A:63:TRP:O	1:A:318:ILE:HA	2.19	0.42
1:A:262:GLU:OE2	1:A:389:ILE:HG21	2.20	0.42
1:A:12:ALA:HB1	1:A:13:PRO:HD2	2.02	0.41
1:A:139:ILE:HG12	1:A:374:TRP:CE3	2.55	0.41
1:A:72:ARG:O	1:A:76:GLU:HG3	2.21	0.41
1:A:122:PRO:HD2	4:A:701:HOH:O	2.21	0.41
1:A:290:ARG:HD3	1:A:345:VAL:HG13	2.03	0.41
1:A:72:ARG:NH1	1:A:331:GLU:OE1	2.42	0.40
1:A:181:THR:HG22	1:A:251:ASP:HB2	2.00	0.40
1:A:361:HIS:HB2	4:A:560:HOH:O	2.22	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%)	382 (95%)	19 (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 ⓘ

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%)	334 (96%)	15 (4%)	26 7

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	49	ASN
1	A	56	THR
1	A	79	ARG
1	A	84	GLU
1	A	86	PRO
1	A	108	GLN
1	A	217	THR
1	A	222	ILE
1	A	235	SER
1	A	246	LEU
1	A	261	MET
1	A	276	GLU
1	A	329	GLU
1	A	365	ARG

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	110	GLN
1	A	116	ASN

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Mol	Chain	Res	Type
1	A	117	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	PIW	A	422	2	12,12,12	1.77	4 (33%)	15,15,15	2.21	6 (40%)
2	HEM	A	417	1,3	50,50,50	1.46	9 (18%)	67,82,82	1.28	11 (16%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	422	PIW	C6-N1	4.43	1.51	1.43
2	A	417	HEM	FE-NB	3.33	2.05	1.94
2	A	417	HEM	C4A-C3A	3.17	1.50	1.43
2	A	417	HEM	FE-NA	2.94	2.04	1.95
2	A	417	HEM	CMD-C2D	2.88	1.56	1.50
2	A	417	HEM	CMB-C2B	2.56	1.56	1.50
3	A	422	PIW	C8-C7	2.43	1.43	1.38
2	A	417	HEM	FE-NC	2.43	2.03	1.95
2	A	417	HEM	CAC-C3C	2.40	1.53	1.47
3	A	422	PIW	C4-N3	-2.17	1.29	1.37
2	A	417	HEM	CHB-C4A	-2.06	1.34	1.39
2	A	417	HEM	C3B-C2B	-2.01	1.33	1.37
3	A	422	PIW	C2-N3	-2.01	1.27	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	422	PIW	C10-C9-C8	4.42	125.93	119.87
3	A	422	PIW	C9-C10-C11	-3.83	115.51	120.24
2	A	417	HEM	C3B-C2B-C1B	3.57	109.09	106.41
3	A	422	PIW	C9-C8-C7	-3.16	116.34	120.24
2	A	417	HEM	CHC-C4B-NB	-2.70	121.52	124.42
2	A	417	HEM	O2A-CGA-O1A	2.66	130.16	123.33
2	A	417	HEM	CHB-C4A-NA	2.63	128.63	123.86
3	A	422	PIW	C4-N3-C2	2.48	110.22	105.47
2	A	417	HEM	CBD-CAD-C3D	2.35	119.04	112.53
3	A	422	PIW	C11-C6-C7	2.28	123.53	119.18
2	A	417	HEM	CMA-C3A-C2A	2.27	130.43	125.62
3	A	422	PIW	C6-N1-C2	-2.24	123.54	127.20
2	A	417	HEM	CBB-CAB-C3B	2.23	138.65	127.53
2	A	417	HEM	C3B-C4B-NB	2.21	111.06	109.47
2	A	417	HEM	CHA-C1A-NA	2.18	127.81	123.86
2	A	417	HEM	C4A-NA-C1A	2.10	109.24	105.82
2	A	417	HEM	CMA-C3A-C4A	-2.01	122.37	125.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

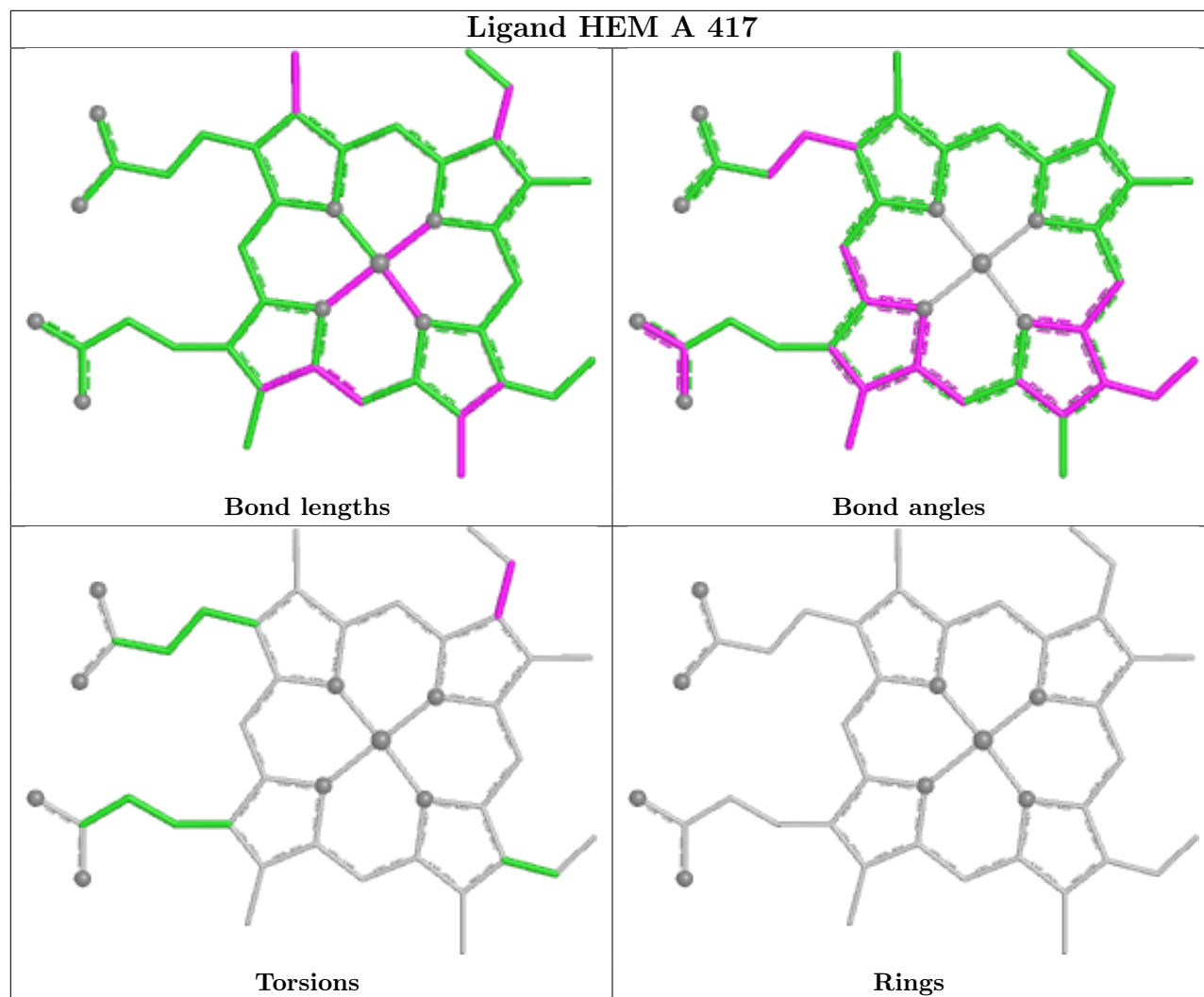
Mol	Chain	Res	Type	Atoms
2	A	417	HEM	C2C-C3C-CAC-CBC
2	A	417	HEM	C4C-C3C-CAC-CBC
3	A	422	PIW	C11-C6-N1-C5
3	A	422	PIW	C7-C6-N1-C5

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	422	PIW	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

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.