Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:32 PM GMT

PDB ID	:	1PHE
Title	:	CRYSTAL STRUCTURES OF METYRAPONE-AND PHENYLIMIDAZOLE-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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

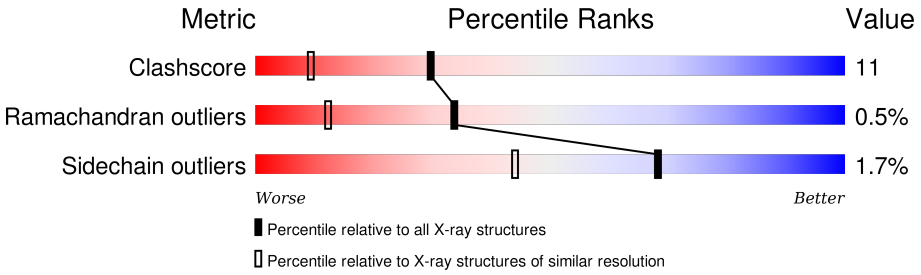
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	63% 29% 5%

2 Entry composition

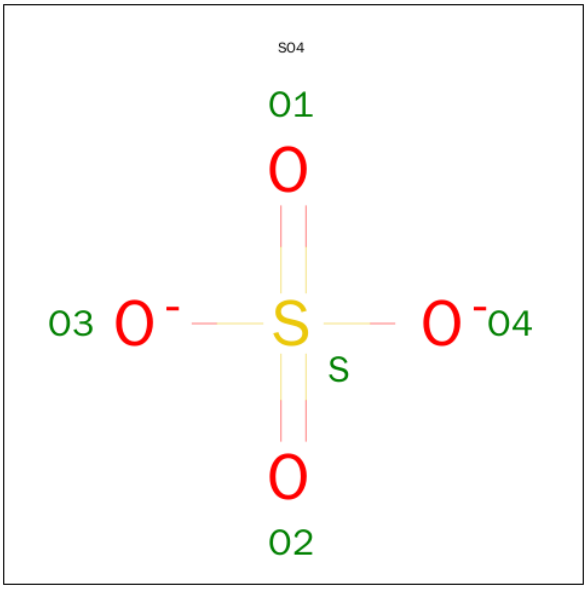
There are 5 unique types of molecules in this entry. The entry contains 3464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

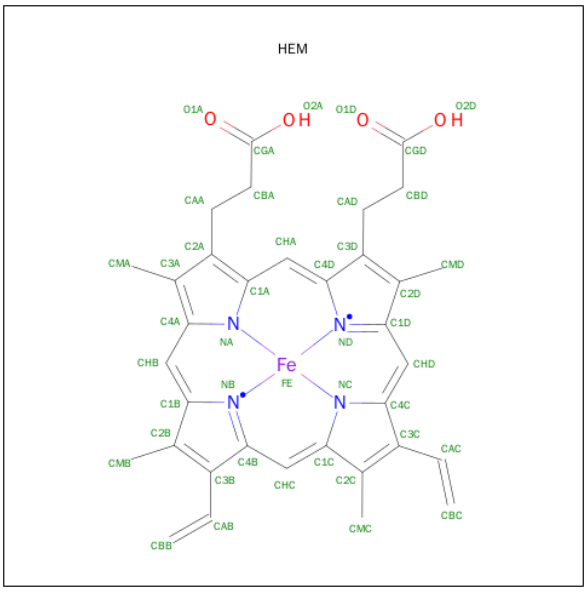
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3204	2030	559	597	18	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



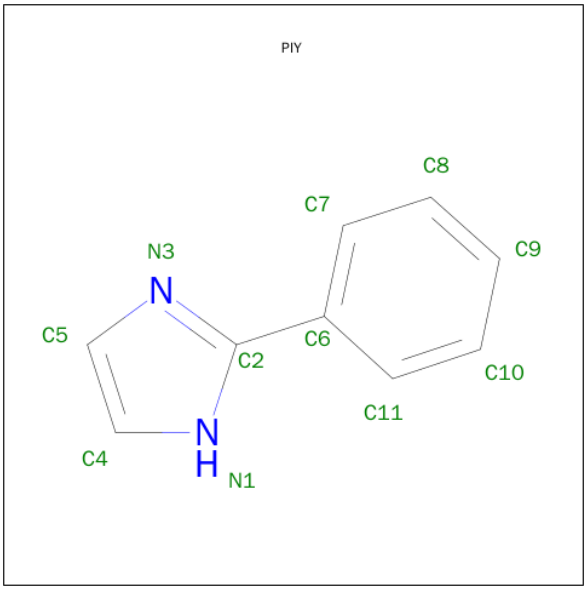
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	S		
2	A	1	1	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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 (three-letter code: PIY) (formula: $C_9H_8N_2$).



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	O	0	0
			205	205		

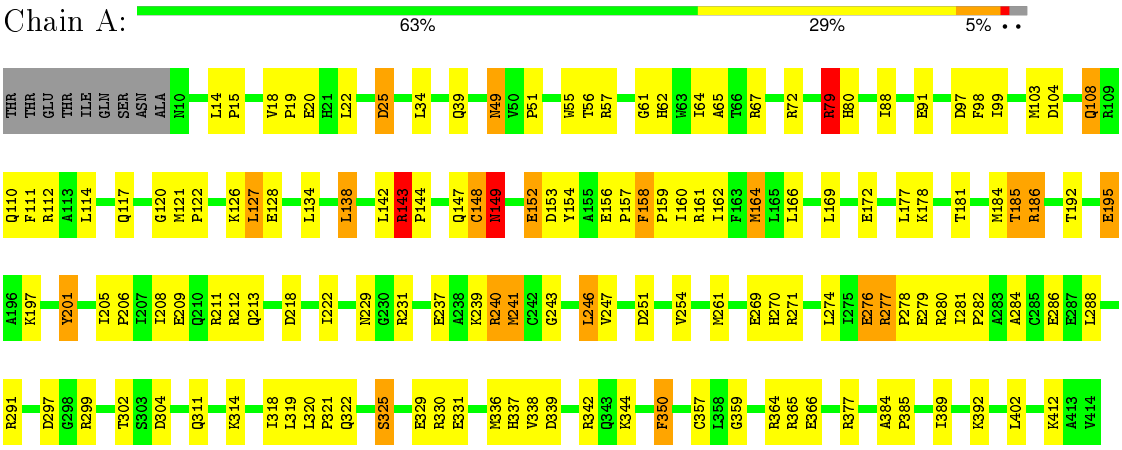
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

5.1 Standard geometry

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	1.16	3/3283 (0.1%)	1.87	75/4461 (1.7%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLU	CD-OE1	9.18	1.35	1.25
1	A	237	GLU	CD-OE1	6.83	1.33	1.25
1	A	286	GLU	CD-OE1	-5.88	1.19	1.25

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ARG	NE-CZ-NH2	-19.80	110.40	120.30
1	A	67	ARG	NE-CZ-NH1	17.46	129.03	120.30
1	A	211	ARG	CD-NE-CZ	14.37	143.72	123.60
1	A	211	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	143	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	280	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	A	240	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	A	299	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	A	195	GLU	CA-CB-CG	10.34	136.16	113.40
1	A	280	ARG	NE-CZ-NH2	-9.79	115.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	A	365	ARG	CD-NE-CZ	9.16	136.43	123.60
1	A	364	ARG	CD-NE-CZ	9.14	136.39	123.60
1	A	231	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	366	GLU	OE1-CD-OE2	-8.78	112.76	123.30
1	A	161	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	104	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	A	79	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	412	LYS	CA-CB-CG	8.28	131.61	113.40
1	A	365	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	20	GLU	CA-CB-CG	8.04	131.08	113.40
1	A	339	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	25	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	A	138	LEU	CA-CB-CG	7.25	131.99	115.30
1	A	280	ARG	CD-NE-CZ	7.25	133.74	123.60
1	A	72	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	A	108	GLN	CA-CB-CG	7.13	129.08	113.40
1	A	330	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	154	TYR	CB-CG-CD1	7.08	125.25	121.00
1	A	148	CYS	C-N-CA	7.04	139.29	121.70
1	A	161	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	A	79	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	A	127	LEU	CA-CB-CG	6.56	130.38	115.30
1	A	154	TYR	CB-CG-CD2	-6.40	117.16	121.00
1	A	25	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	186	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	270	HIS	N-CA-CB	6.11	121.60	110.60
1	A	149	ASN	CB-CA-C	6.09	122.58	110.40
1	A	164	MET	CB-CA-C	6.05	122.51	110.40
1	A	392	LYS	CA-CB-CG	5.99	126.57	113.40
1	A	304	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	279	GLU	CA-CB-CG	5.95	126.49	113.40
1	A	241	MET	N-CA-CB	5.92	121.25	110.60
1	A	201	TYR	CB-CG-CD1	5.90	124.54	121.00
1	A	201	TYR	CA-CB-CG	5.85	124.51	113.40
1	A	51	PRO	C-N-CA	5.78	136.14	121.70
1	A	240	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	152	GLU	N-CA-CB	5.57	120.63	110.60
1	A	336	MET	CA-CB-CG	5.55	122.73	113.30
1	A	55	TRP	O-C-N	5.50	131.50	122.70
1	A	350	PHE	CB-CG-CD2	5.50	124.65	120.80
1	A	277	ARG	N-CA-CB	-5.42	100.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	164	MET	CG-SD-CE	5.37	108.78	100.20
1	A	184	MET	C-N-CA	5.36	135.10	121.70
1	A	80	HIS	CA-CB-CG	-5.34	104.52	113.60
1	A	172	GLU	CG-CD-OE2	5.31	128.93	118.30
1	A	269	GLU	CG-CD-OE1	5.25	128.80	118.30
1	A	322	GLN	CG-CD-OE1	5.25	132.10	121.60
1	A	34	LEU	CB-CA-C	5.24	120.16	110.20
1	A	91	GLU	CB-CA-C	-5.19	100.02	110.40
1	A	329	GLU	CA-CB-CG	5.18	124.79	113.40
1	A	299	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	344	LYS	CA-CB-CG	5.16	124.75	113.40
1	A	178	LYS	CB-CA-C	5.14	120.69	110.40
1	A	147	GLN	CA-CB-CG	5.14	124.71	113.40
1	A	169	LEU	CA-CB-CG	5.14	127.13	115.30
1	A	138	LEU	CB-CA-C	5.12	119.94	110.20
1	A	311	GLN	N-CA-CB	5.10	119.78	110.60
1	A	297	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	153	ASP	CB-CG-OD1	5.07	122.87	118.30
1	A	126	LYS	CA-CB-CG	5.04	124.50	113.40
1	A	364	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	237	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	A	65	ALA	CB-CA-C	5.01	117.62	110.10

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 (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	3204	0	3144	71	0
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	3182	72	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 11.

All (72) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:HD21	1:A:402:LEU:H	1.60	0.50
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.47	0.50
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:261:MET:HA	1:A:261:MET:HE2	1.94	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: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: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:302:THR:C	1:A:314:LYS:HG3	2.37	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:209:GLU:O	1:A:213:GLN:HG3	2.18	0.43
1:A:158:PHE:CE1	1:A:162:ILE:HD11	2.54	0.43
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: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:181:THR:CG2	1:A:251:ASP:HB2	2.49	0.42
1:A:15:PRO:HG2	1:A:18:VAL:HG21	2.02	0.42
1:A:49:ASN:H	1:A:49:ASN:HD22	1.66	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:110:GLN:HE21	1:A:229:ASN:HD22	1.67	0.40
1:A:218:ASP:O	1:A:222:ILE:HG12	2.21	0.40
1:A:276:GLU:C	1:A:278:PRO:HD3	2.42	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%)	34 12

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%)	343 (98%)	6 (2%)	68 44

All (6) 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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	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 carbohydrates 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	$\#\|Z\| > 2$
3	HEM	A	417	1,2	30,50,50	2.89	8 (26%)	24,82,82	2.80	11 (45%)
4	PIY	A	422	-	12,12,12	0.99	0	14,15,15	1.75	2 (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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	417	1,2	-	0/10/54/54	0/0/8/8
4	PIY	A	422	-	-	0/4/4/4	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	417	HEM	C3B-C4B	-10.15	1.42	1.51
3	A	417	HEM	C2D-C3D	-6.62	1.34	1.54
3	A	417	HEM	C3D-C4D	-6.31	1.43	1.51
3	A	417	HEM	C2C-C1C	-3.94	1.45	1.52
3	A	417	HEM	C2D-C1D	-2.53	1.43	1.51
3	A	417	HEM	C4C-NC	2.58	1.39	1.36
3	A	417	HEM	FE-NC	3.04	2.07	1.95
3	A	417	HEM	C3C-CAC	3.13	1.57	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	417	HEM	C3C-CAC-CBC	-4.83	117.06	124.46
3	A	417	HEM	CAA-C2A-C1A	-3.17	123.57	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	417	HEM	CMA-C3A-C4A	-2.18	124.76	128.36
3	A	417	HEM	CBD-CAD-C3D	2.38	120.49	113.55
4	A	422	PIY	C5-N3-C2	2.58	111.11	104.33
3	A	417	HEM	CAD-C3D-C4D	3.32	124.17	112.47
3	A	417	HEM	CMD-C2D-C3D	3.42	129.46	114.35
3	A	417	HEM	C2D-C3D-C4D	3.52	107.46	101.50
3	A	417	HEM	C3B-CAB-CBB	4.50	131.36	124.46
3	A	417	HEM	CMB-C2B-C3B	4.55	127.90	116.53
3	A	417	HEM	CAD-C3D-C2D	5.25	128.31	113.22
4	A	422	PIY	C6-C2-N1	5.43	130.29	123.83
3	A	417	HEM	CMC-C2C-C3C	5.48	130.21	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.