



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:05 AM GMT

PDB ID : 3OZU  
Title : The Crystal Structure of flavohemoglobin from *R. eutrophus* in complex with miconazole  
Authors : El Hammi, E.; Warkentin, E.; Demmer, U.; Ermler, U.; Baciou, L.  
Deposited on : 2010-09-27  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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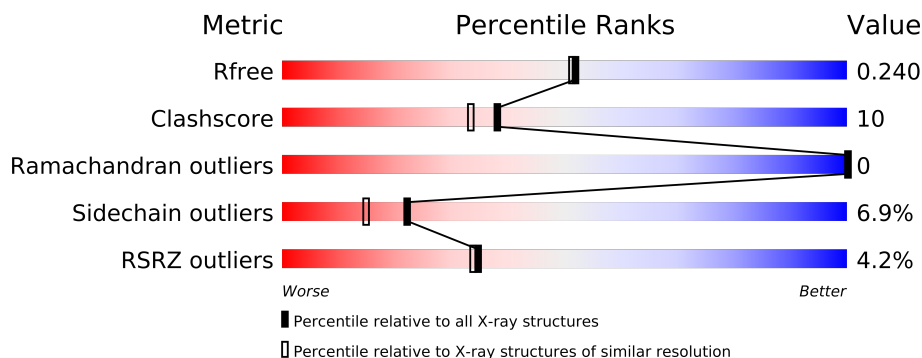
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	403	

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3666 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Flavohemoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	6	0
			3204	2044	552	593	15			

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



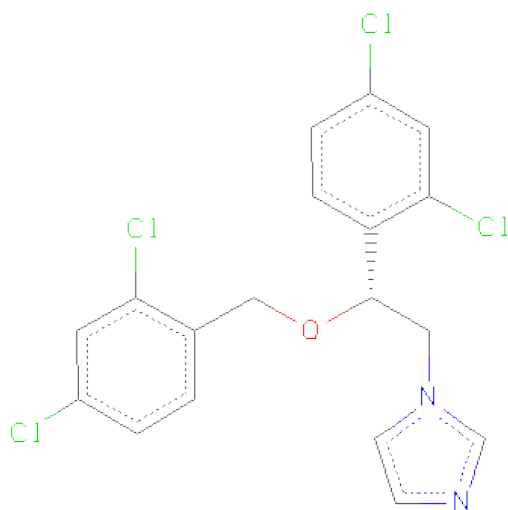
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 1-[(2R)-2-[(2,4-DICHLOROBENZYL)OXY]-2-(2,4-DICHLOROPHENYL)ETHYL]-1H-IMIDAZOLE (three-letter code: X89) (formula:  $C_{18}H_{14}Cl_4N_2O$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			25	18	4	2	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		

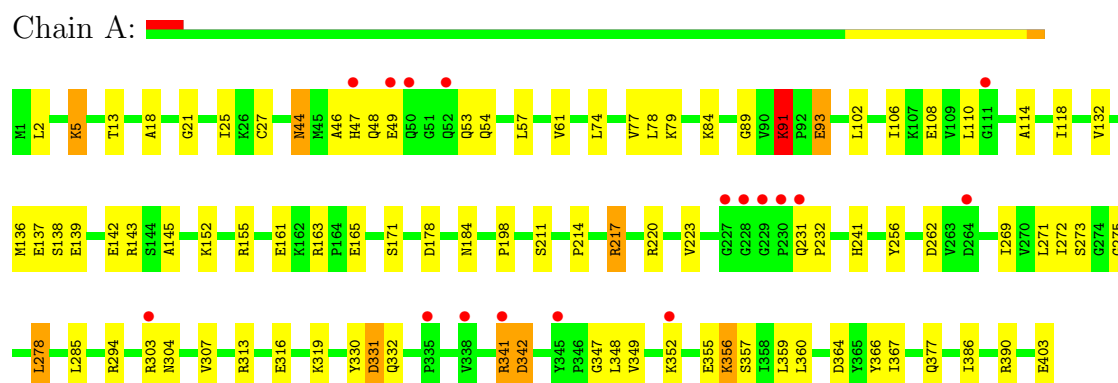
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	336	Total	O	0	0
			336	336		

### 3 Residue-property plots

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.

#### • Molecule 1: Flavohemoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.34Å 105.28Å 46.45Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.00) 98.3 (29.68-2.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.56 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, $R_{free}$	0.185 , 0.233 0.201 , 0.240	Depositor DCC
$R_{free}$ test set	1892 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 37583 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PO4, X89, FAD

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	1.09	6/3294 (0.2%)	0.94	3/4472 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	GLU	CB-CG	-6.79	1.39	1.52
1	A	89	GLY	N-CA	5.81	1.54	1.46
1	A	61	VAL	CB-CG2	5.74	1.65	1.52
1	A	137	GLU	CD-OE2	5.73	1.31	1.25
1	A	256	TYR	CD2-CE2	5.59	1.47	1.39
1	A	93	GLU	CD-OE1	5.08	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	LYS	CD-CE-NZ	-8.97	91.07	111.70
1	A	178	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	155	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3204	0	3173	64	0
2	A	43	0	30	1	0
3	A	53	0	31	2	0
4	A	25	0	14	3	0
5	A	5	0	0	1	0
6	A	336	0	0	11	0
All	All	3666	0	3248	65	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (65) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:356:LYS:HD2	6:A:729:HOH:O	1.49	1.10
1:A:25[A]:ILE:HD12	4:A:411:X89:CL2A	1.93	1.06
1:A:25[A]:ILE:CD1	4:A:411:X89:CL2A	2.56	0.91
2:A:404:HEM:HMB1	5:A:406:PO4:O3	1.84	0.78
1:A:341:ARG:HG2	1:A:342:ASP:OD1	1.86	0.75
1:A:21:GLY:H	1:A:54[A]:GLN:HE22	1.39	0.70
1:A:18:ALA:O	1:A:54[A]:GLN:NE2	2.26	0.69
1:A:44:ASN:ND2	1:A:46:ALA:H	1.91	0.68
1:A:25[A]:ILE:HD11	1:A:57:LEU:HD22	1.74	0.68
1:A:217[A]:ARG:NH1	6:A:545:HOH:O	2.29	0.65
1:A:47:HIS:HB3	6:A:668:HOH:O	1.97	0.64
1:A:110:LEU:HB3	1:A:114:ALA:HB2	1.81	0.61
1:A:47:HIS:CB	6:A:668:HOH:O	2.49	0.60
1:A:364:ASP:OD1	1:A:390[B]:ARG:HD3	2.02	0.60
1:A:356:LYS:HD3	1:A:357:SER:H	1.69	0.57
1:A:44:ASN:C	1:A:44:ASN:HD22	2.08	0.56
1:A:44:ASN:HD22	1:A:46:ALA:H	1.53	0.54
1:A:79:LYS:HB3	1:A:136:MET:HE1	1.88	0.54
1:A:79:LYS:HA	1:A:136:MET:HE2	1.89	0.53
1:A:25[B]:ILE:HD13	1:A:53:GLN:HB3	1.92	0.52
1:A:21:GLY:N	1:A:54[A]:GLN:HE22	2.06	0.51
1:A:171:SER:OG	1:A:220:ARG:NH2	2.41	0.50
1:A:269:ILE:HD11	1:A:294:ARG:CZ	2.41	0.50
1:A:110:LEU:CB	1:A:114:ALA:HB2	2.41	0.50
1:A:138:SER:O	1:A:142:GLU:HG3	2.11	0.49
1:A:348:LEU:O	1:A:349:VAL:C	2.51	0.48
1:A:377:GLN:HA	1:A:377:GLN:NE2	2.29	0.48
1:A:331:ASP:HA	1:A:347:GLY:H	1.78	0.48
1:A:359:LEU:CD1	1:A:386:ILE:HD11	2.43	0.48
1:A:304:ASN:HA	1:A:330:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:13:THR:HG21	1:A:118:ILE:HG12	1.97	0.47
1:A:184:ASN:HD22	1:A:214:PRO:HB2	1.79	0.47
1:A:79:LYS:CB	1:A:136:MET:HE1	2.45	0.47
1:A:359:LEU:HD13	1:A:386:ILE:HD11	1.96	0.47
1:A:48:GLN:HB3	6:A:589:HOH:O	2.16	0.46
1:A:355:GLU:HG3	6:A:615:HOH:O	2.16	0.46
1:A:223:VAL:O	1:A:241:HIS:HE1	1.98	0.46
1:A:275:GLY:HA2	1:A:403:GLU:O	2.15	0.46
1:A:78:LEU:HD13	1:A:132:VAL:HG11	1.98	0.45
1:A:48:GLN:CB	6:A:589:HOH:O	2.65	0.44
1:A:262:ASP:HA	6:A:590:HOH:O	2.16	0.44
1:A:303:ARG:HE	1:A:332:GLN:HG2	1.82	0.44
1:A:232:PRO:O	3:A:405:FAD:H8A	2.18	0.44
1:A:21:GLY:O	1:A:25[A]:ILE:HG12	2.17	0.44
1:A:390[B]:ARG:NH2	6:A:731:HOH:O	2.40	0.44
1:A:184:ASN:ND2	1:A:214:PRO:HB2	2.32	0.44
1:A:5:LYS:HB3	1:A:5:LYS:HE3	1.24	0.44
1:A:307:VAL:HG12	1:A:403:GLU:HG3	1.99	0.43
1:A:74:LEU:O	1:A:77:VAL:HG22	2.18	0.43
1:A:27:CYS:SG	1:A:108:GLU:OE2	2.76	0.43
1:A:271:LEU:HD23	1:A:366:TYR:HB2	2.00	0.43
1:A:91:LYS:NZ	1:A:93:GLU:OE2	2.52	0.43
1:A:145:ALA:HB2	1:A:152:LYS:HG3	2.01	0.43
1:A:217[A]:ARG:CZ	6:A:545:HOH:O	2.65	0.42
1:A:106:ILE:O	1:A:110:LEU:HB2	2.19	0.42
1:A:79:LYS:HA	1:A:136:MET:CE	2.50	0.42
1:A:272:ILE:O	1:A:367:ILE:HA	2.20	0.42
1:A:278:LEU:HD21	1:A:313:ARG:HB2	2.02	0.41
1:A:231:GLN:HB3	1:A:231:GLN:HE21	1.68	0.41
1:A:232:PRO:HG2	3:A:405:FAD:N7A	2.36	0.41
1:A:331:ASP:HA	1:A:347:GLY:CA	2.51	0.41
1:A:47:HIS:HB2	6:A:668:HOH:O	2.18	0.41
1:A:2:LEU:HD12	1:A:2:LEU:N	2.36	0.41
1:A:102:LEU:HD21	4:A:411:X89:C1B	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	407/403 (101%)	395 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	340/334 (102%)	316 (93%)	24 (7%)	21	14

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	44	ASN
1	A	49	GLU
1	A	84	LYS
1	A	91	LYS
1	A	143	ARG
1	A	161	GLU
1	A	163	ARG
1	A	165	GLU
1	A	198	PRO
1	A	211	SER
1	A	217[A]	ARG
1	A	217[B]	ARG
1	A	273	SER
1	A	278	LEU
1	A	285	LEU

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Mol	Chain	Res	Type
1	A	316	GLU
1	A	319	LYS
1	A	331	ASP
1	A	341	ARG
1	A	342	ASP
1	A	352	LYS
1	A	356	LYS
1	A	360	LEU

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

Mol	Chain	Res	Type
1	A	44	ASN
1	A	48	GLN
1	A	52	GLN
1	A	55	GLN
1	A	184	ASN
1	A	231	GLN
1	A	241	HIS
1	A	249	GLN
1	A	290	GLN
1	A	377	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	HEM	A	404	1,4	49,50,50	2.82	17 (34%)	46,82,82	2.71	16 (34%)
3	FAD	A	405	-	58,58,58	1.63	6 (10%)	85,89,89	2.28	20 (23%)
5	PO4	A	406	-	4,4,4	0.53	0	6,6,6	0.34	0
4	X89	A	411	2	27,27,27	1.49	3 (11%)	37,37,37	1.76	9 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	404	1,4	-	0/14/114/114	0/0/8/8
3	FAD	A	405	-	-	1/34/50/50	0/1/6/6
5	PO4	A	406	-	-	0/0/0/0	0/0/0/0
4	X89	A	411	2	-	0/13/13/13	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	404	HEM	C3D-C4D	10.57	1.47	1.44
3	A	405	FAD	C1'-C2'	5.42	1.56	1.51
3	A	405	FAD	C5X-N5	5.32	1.43	1.35
4	A	411	X89	C1-N1	5.23	1.53	1.48
2	A	404	HEM	C3B-CAB	5.15	1.56	1.40
2	A	404	HEM	C3C-C2C	-5.15	1.34	1.43
2	A	404	HEM	C2D-C1D	5.02	1.45	1.44
2	A	404	HEM	C3D-C2D	4.92	1.52	1.43
2	A	404	HEM	FE-NC	4.84	2.16	1.97
2	A	404	HEM	FE-NA	4.83	2.13	1.92
3	A	405	FAD	C1'-N10	4.74	1.53	1.48
2	A	404	HEM	C4A-C3A	4.13	1.45	1.40
3	A	405	FAD	PA-O3P	4.00	1.67	1.59
2	A	404	HEM	C3B-C2B	-3.93	1.36	1.43
2	A	404	HEM	C3C-CAC	3.67	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	405	FAD	C2A-N3A	3.61	1.39	1.32
2	A	404	HEM	CMD-C2D	3.54	1.58	1.47
4	A	411	X89	C2B-CL2B	3.18	1.81	1.73
2	A	404	HEM	FE-ND	3.09	2.09	1.97
2	A	404	HEM	CMC-C2C	2.82	1.56	1.47
3	A	405	FAD	C2A-N1A	2.72	1.39	1.33
4	A	411	X89	C4A-CL4A	2.51	1.80	1.74
2	A	404	HEM	CHA-C4D	2.32	1.39	1.35
2	A	404	HEM	FE-NB	2.28	2.06	1.97
2	A	404	HEM	CMB-C2B	2.28	1.54	1.47
2	A	404	HEM	C2B-C1B	-2.17	1.44	1.44

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	FAD	N3A-C2A-N1A	-13.34	117.56	128.71
2	A	404	HEM	C3B-C4B-NB	-8.39	108.00	114.00
3	A	405	FAD	C2'-C1'-N10	-6.67	103.59	112.45
2	A	404	HEM	C4D-ND-C1D	6.41	111.72	105.16
2	A	404	HEM	C4C-NC-C1C	6.25	112.03	105.53
2	A	404	HEM	CBA-CAA-C2A	-6.08	101.97	112.69
3	A	405	FAD	C1'-N10-C9A	5.30	124.03	118.87
2	A	404	HEM	C3A-C4A-NA	-4.96	105.66	109.41
3	A	405	FAD	C2-N1-C10	4.66	119.68	114.98
4	A	411	X89	O-CBA-C1A	-4.35	106.09	112.42
4	A	411	X89	C3B-C2B-C1B	-4.16	118.54	122.54
2	A	404	HEM	C4A-NA-C1A	4.16	112.24	106.76
3	A	405	FAD	N3A-C4A-N9A	4.06	132.77	125.43
2	A	404	HEM	C1B-NB-C4B	3.91	109.16	105.16
3	A	405	FAD	C4X-C10-N10	3.85	122.43	120.51
2	A	404	HEM	C2D-C1D-ND	-3.37	108.95	112.93
2	A	404	HEM	CMA-C3A-C4A	-3.07	123.90	128.62
4	A	411	X89	O-CBA-C1	3.06	110.93	105.85
4	A	411	X89	C6A-C1A-C2A	2.90	119.98	116.81
3	A	405	FAD	C9A-N10-C10	-2.89	118.93	121.77
3	A	405	FAD	C4X-N5-C5X	2.86	119.91	116.69
3	A	405	FAD	C2A-N3A-C4A	2.86	122.15	114.01
2	A	404	HEM	C2A-C1A-NA	-2.73	105.94	109.73
3	A	405	FAD	C4X-C10-N1	-2.72	120.02	122.73
4	A	411	X89	CBB-C1B-C2B	-2.67	117.52	121.51
3	A	405	FAD	C5X-C9A-N10	2.58	119.35	116.80
3	A	405	FAD	C1B-N9A-C4A	-2.58	122.18	126.64

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	405	FAD	C5A-C4A-N3A	-2.49	120.28	125.70
3	A	405	FAD	C4-C4X-C10	2.48	120.95	116.95
3	A	405	FAD	O4B-C1B-N9A	-2.47	106.14	108.44
4	A	411	X89	CBB-O-CBA	-2.46	110.52	113.91
4	A	411	X89	C3B-C4B-CL4B	-2.46	116.11	119.14
2	A	404	HEM	CMB-C2B-C3B	2.38	131.77	126.16
4	A	411	X89	C2A-C1A-CBA	-2.35	118.91	122.23
2	A	404	HEM	CHD-C1D-ND	2.32	126.51	124.58
3	A	405	FAD	C2B-C1B-N9A	2.29	119.15	113.27
3	A	405	FAD	C6-C5X-C9A	2.27	122.16	119.02
2	A	404	HEM	O2D-CGD-CBD	2.27	122.23	114.22
4	A	411	X89	C2A-C3A-C4A	-2.23	116.08	118.67
3	A	405	FAD	C5A-C6A-N6A	-2.17	115.80	120.72
2	A	404	HEM	O2D-CGD-O1D	-2.16	117.79	123.30
2	A	404	HEM	CHB-C1B-NB	2.06	127.14	124.31
3	A	405	FAD	C8A-N9A-C1B	2.04	130.40	126.38
2	A	404	HEM	CMA-C3A-C2A	2.03	128.78	124.94
3	A	405	FAD	O2B-C2B-C1B	2.03	117.36	111.23

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	FAD	C2B-C1B-N9A-C8A

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	403/403 (100%)	0.03	17 (4%) 35 34	11, 29, 61, 88	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	GLY	7.9
1	A	229	GLY	5.0
1	A	345	TYR	4.7
1	A	230	PRO	4.3
1	A	335	PRO	3.7
1	A	231	GLN	3.1
1	A	47	HIS	3.1
1	A	352	LYS	3.0
1	A	227	GLY	2.8
1	A	50	GLN	2.8
1	A	341	ARG	2.7
1	A	49	GLU	2.6
1	A	111	GLY	2.6
1	A	303	ARG	2.3
1	A	264	ASP	2.3
1	A	338	VAL	2.2
1	A	52	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	404	43/43	0.15	1.17	17,18,34,44	0
4	X89	A	411	25/25	0.13	0.18	26,33,41,55	0
3	FAD	A	405	53/53	0.12	-0.31	15,22,74,81	0
5	PO4	A	406	5/5	0.10	-2.55	46,47,52,57	0

## 6.5 Other polymers

There are no such residues in this entry.