



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:40 PM GMT

PDB ID : 1Q5D
Title : Epothilone B-bound Cytochrome P450epoK
Authors : Nagano, S.; Li, H.; Shimizu, H.; Nishida, C.; Ogura, H.; Ortiz de Montellano, P.R.; Poulos, T.L.
Deposited on : 2003-08-06
Resolution : 1.93 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

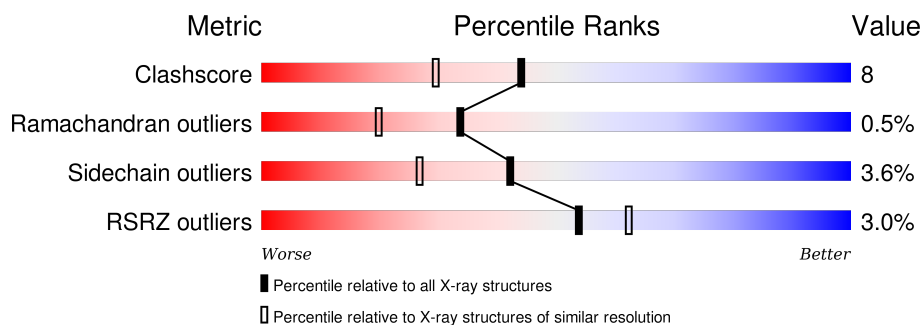
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	419	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3485 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 P 450 epoxidase.

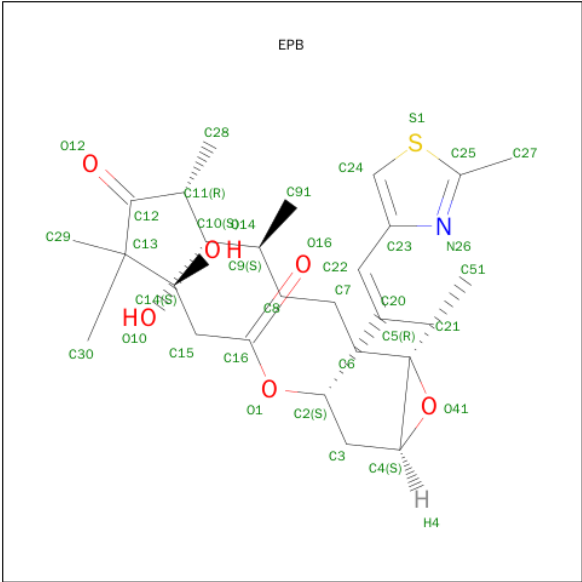
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3159	2008	555	587	9			

- 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 7,11-DIHYDROXY-8,8,10,12,16-PENTAMETHYL-3-[1-METHYL-2-(2-METHYL-THIAZOL-4-YL)VINYL]-4,17-DIOXABICYCLO[14.1.0]HEPTADECANE-5,9-DIONE (three-letter code: EPB) (formula: $C_{27}H_{41}NO_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	27	1	6	1		

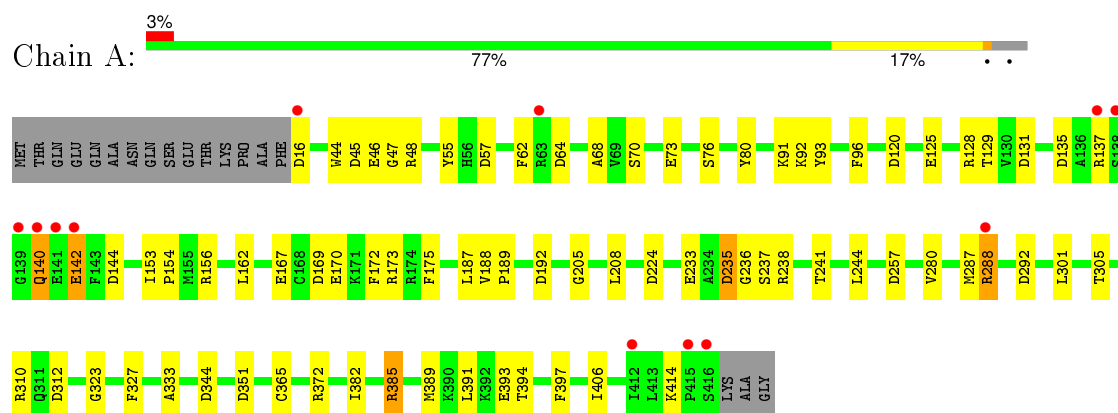
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		

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.

- Molecule 1: P450 epoxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	60.43 Å 60.43 Å 252.84 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.93 49.11 – 1.93	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-1.93) 93.9 (49.11-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 1.94 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.218 , 0.260 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 34134 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3485	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/3223	0.71	16/4368 (0.4%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ASP	CB-CG-OD2	7.17	124.76	118.30
1	A	312	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	192	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	57	ASP	CB-CG-OD2	6.15	123.83	118.30
1	A	169	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	257	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	64	ASP	CB-CG-OD2	5.93	123.63	118.30
1	A	144	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	16	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	135	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	344	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	292	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	235	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	351	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	224	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	120	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3159	0	3177	46	0
2	A	43	0	30	4	0
3	A	35	0	40	6	0
4	A	248	0	0	6	0
All	All	3485	0	3247	52	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 8.

All (52) 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:187:LEU:HD12	1:A:188:VAL:HG13	1.54	0.90
1:A:131:ASP:OD1	1:A:385:ARG:NH2	2.22	0.73
1:A:172:PHE:CZ	1:A:208:LEU:HD22	2.24	0.72
1:A:288:ARG:HE	1:A:372:ARG:HD3	1.55	0.72
3:A:450:EPB:O41	4:A:451:HOH:O	2.09	0.70
1:A:125:GLU:OE2	1:A:128:ARG:NH1	2.28	0.67
1:A:137:ARG:O	1:A:140:GLN:HG2	1.96	0.64
1:A:382:ILE:HG12	1:A:389:MET:HE1	1.80	0.63
1:A:301:LEU:HD21	3:A:450:EPB:C51	2.30	0.61
1:A:288:ARG:NE	1:A:372:ARG:HD3	2.17	0.60
1:A:244:LEU:HD23	1:A:244:LEU:C	2.24	0.58
1:A:129:THR:OG1	1:A:156:ARG:HG2	2.05	0.57
2:A:440:HEM:HBB2	2:A:440:HEM:HHC	1.85	0.56
1:A:70:SER:HA	1:A:96:PHE:O	2.05	0.56
1:A:137:ARG:HG3	4:A:591:HOH:O	2.06	0.55
1:A:62:PHE:O	4:A:493:HOH:O	2.18	0.55
1:A:92:LYS:HG3	1:A:93:TYR:CD1	2.42	0.55
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.90	0.53
2:A:440:HEM:HBC2	2:A:440:HEM:HMC2	1.92	0.51
1:A:187:LEU:C	1:A:187:LEU:HD13	2.31	0.50
1:A:48:ARG:NH2	1:A:76:SER:OG	2.44	0.50
1:A:137:ARG:NH1	1:A:140:GLN:HG3	2.28	0.49
1:A:140:GLN:NE2	4:A:636:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:VAL:HG11	1:A:287:MET:CE	2.43	0.48
1:A:173:ARG:HG2	1:A:173:ARG:HH11	1.79	0.48
1:A:187:LEU:HD12	1:A:188:VAL:CG1	2.37	0.48
1:A:397:PHE:CE1	1:A:406:ILE:HG12	2.49	0.47
1:A:382:ILE:HG12	1:A:389:MET:CE	2.45	0.47
1:A:80:TYR:CZ	1:A:91:LYS:HE2	2.50	0.47
1:A:305:THR:HA	3:A:450:EPB:H9	1.98	0.46
2:A:440:HEM:HBC2	2:A:440:HEM:CMC	2.46	0.46
3:A:450:EPB:H1	3:A:450:EPB:H152	1.97	0.46
1:A:170:GLU:OE1	1:A:173:ARG:NH2	2.49	0.46
1:A:92:LYS:HG3	1:A:93:TYR:CE1	2.51	0.45
1:A:172:PHE:CE1	1:A:208:LEU:HD22	2.51	0.45
1:A:167:GLU:HB2	4:A:482:HOH:O	2.17	0.45
1:A:188:VAL:HB	4:A:658:HOH:O	2.17	0.44
1:A:44:TRP:CE3	1:A:47:GLY:HA3	2.53	0.44
1:A:68:ALA:HB2	1:A:310:ARG:HD2	2.00	0.44
1:A:175:PHE:CD1	1:A:205:GLY:HA3	2.52	0.44
3:A:450:EPB:H62	3:A:450:EPB:H31	1.20	0.43
1:A:55:TYR:HA	1:A:333:ALA:HB1	2.02	0.42
1:A:80:TYR:CE1	1:A:187:LEU:HB2	2.55	0.42
1:A:187:LEU:O	1:A:187:LEU:HD13	2.19	0.42
1:A:46:GLU:HG2	1:A:189:PRO:HB3	2.01	0.41
1:A:305:THR:HB	3:A:450:EPB:H82	2.03	0.41
1:A:233:GLU:OE1	1:A:241:THR:OG1	2.21	0.41
1:A:365:CYS:HB2	2:A:440:HEM:NA	2.36	0.41
1:A:73:GLU:O	1:A:323:GLY:HA2	2.21	0.41
1:A:187:LEU:CD1	1:A:188:VAL:HG13	2.37	0.40
1:A:288:ARG:HH11	1:A:288:ARG:HG3	1.85	0.40
1:A:142:GLU:CD	1:A:142:GLU:H	2.24	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	399/419 (95%)	386 (97%)	11 (3%)	2 (0%)	34 20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	A	236	GLY

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	336/350 (96%)	324 (96%)	12 (4%)	42 27

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

Mol	Chain	Res	Type
1	A	140	GLN
1	A	142	GLU
1	A	162	LEU
1	A	237	SER
1	A	238	ARG
1	A	288	ARG
1	A	327	PHE
1	A	385	ARG
1	A	391	LEU
1	A	393	GLU
1	A	394	THR
1	A	414	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	231	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 ⓘ

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	$\# Z > 2$
2	HEM	A	440	1,4	30,50,50	2.22	7 (23%)	24,82,82	2.35	8 (33%)
3	EPB	A	450	-	33,37,37	3.19	14 (42%)	39,56,56	4.69	17 (43%)

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	440	1,4	-	0/10/54/54	0/0/8/8
3	EPB	A	450	-	-	0/50/59/59	0/1/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	440	HEM	C3B-C4B	-7.38	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	440	HEM	C3D-C4D	-5.76	1.44	1.51
2	A	440	HEM	C2C-C1C	-3.94	1.45	1.52
3	A	450	EPB	C3-C4	-3.48	1.44	1.52
3	A	450	EPB	C91-C9	-2.76	1.46	1.53
2	A	440	HEM	C2D-C1D	-2.46	1.43	1.51
3	A	450	EPB	O41-C5	-2.28	1.42	1.46
2	A	440	HEM	C2B-C1B	-2.19	1.44	1.51
2	A	440	HEM	CMA-C3A	2.02	1.55	1.51
3	A	450	EPB	C15-C16	2.22	1.55	1.50
3	A	450	EPB	C22-C20	2.36	1.36	1.33
3	A	450	EPB	C6-C7	2.65	1.62	1.52
3	A	450	EPB	C2-C20	2.68	1.58	1.51
3	A	450	EPB	C3-C2	2.71	1.58	1.53
2	A	440	HEM	FE-NC	2.82	2.06	1.95
3	A	450	EPB	O12-C12	2.91	1.27	1.21
3	A	450	EPB	O1-C2	4.36	1.55	1.45
3	A	450	EPB	C6-C5	5.45	1.68	1.51
3	A	450	EPB	C13-C12	5.85	1.63	1.54
3	A	450	EPB	C15-C14	6.00	1.59	1.52
3	A	450	EPB	C5-C4	11.10	1.62	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	450	EPB	C6-C5-C4	-13.42	94.64	119.01
3	A	450	EPB	O41-C4-C5	-7.65	55.04	59.92
3	A	450	EPB	C6-C7-C8	-6.21	99.23	112.69
3	A	450	EPB	C51-C5-C6	-6.04	107.48	116.14
3	A	450	EPB	C91-C9-C8	-5.80	100.67	110.35
3	A	450	EPB	C11-C10-C9	-5.12	106.45	114.75
3	A	450	EPB	O41-C5-C4	-4.62	55.68	59.23
2	A	440	HEM	CBD-CAD-C3D	-2.83	105.30	113.55
3	A	450	EPB	O1-C2-C20	-2.61	101.82	109.44
3	A	450	EPB	C3-C4-C5	-2.34	121.14	125.69
3	A	450	EPB	O14-C14-C15	-2.34	103.23	109.10
2	A	440	HEM	C3C-CAC-CBC	-2.29	120.95	124.46
3	A	450	EPB	C30-C13-C29	-2.21	105.33	108.94
3	A	450	EPB	C8-C9-C10	2.16	115.40	111.29
2	A	440	HEM	C2D-C3D-C4D	2.35	105.48	101.50
2	A	440	HEM	CMD-C2D-C3D	3.03	127.73	114.35
2	A	440	HEM	CMB-C2B-C3B	3.41	125.05	116.53
3	A	450	EPB	C2-O1-C16	4.10	122.76	116.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	440	HEM	CAD-C3D-C4D	4.18	127.21	112.47
3	A	450	EPB	C51-C5-C4	4.26	130.20	121.62
2	A	440	HEM	CAD-C3D-C2D	4.90	127.30	113.22
2	A	440	HEM	CMC-C2C-C3C	5.07	129.20	116.53
3	A	450	EPB	C28-C11-C10	8.74	127.75	112.37
3	A	450	EPB	C5-O41-C4	10.62	69.28	60.86
3	A	450	EPB	O41-C5-C51	13.47	135.00	113.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	440	HEM	4	0
3	A	450	EPB	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	401/419 (95%)	0.40	12 (2%) 54 62	25, 36, 55, 69	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	GLY	6.4
1	A	141	GLU	5.0
1	A	140	GLN	4.2
1	A	416	SER	3.1
1	A	288	ARG	3.0
1	A	137	ARG	2.9
1	A	142	GLU	2.8
1	A	415	PRO	2.7
1	A	412	ILE	2.4
1	A	138	SER	2.3
1	A	16	ASP	2.2
1	A	63	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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, 95th 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	HEM	A	440	43/43	0.98	0.13	1.30	24,26,30,31	0
3	EPB	A	450	35/35	0.91	0.15	1.04	33,39,45,47	0

6.5 Other polymers

There are no such residues in this entry.