



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2016 – 02:41 PM EST

PDB ID : 5L94  
Title : The 2.25 Å crystal structure of CYP109E1 from *Bacillus megaterium* in complex with testosterone  
Authors : Jozwik, I.K.; Thunnissen, A.M.W.H.  
Deposited on : 2016-06-09  
Resolution : 2.25 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](mailto: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.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028320  
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) : rb-20028320

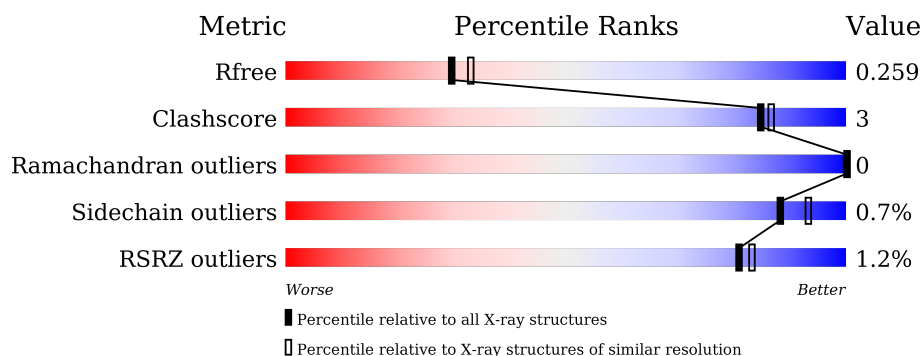
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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. 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	410	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	B	410	<div> <div>82%</div> <div>5%</div> <div>12%</div> </div>

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	TES	A	502	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6444 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.

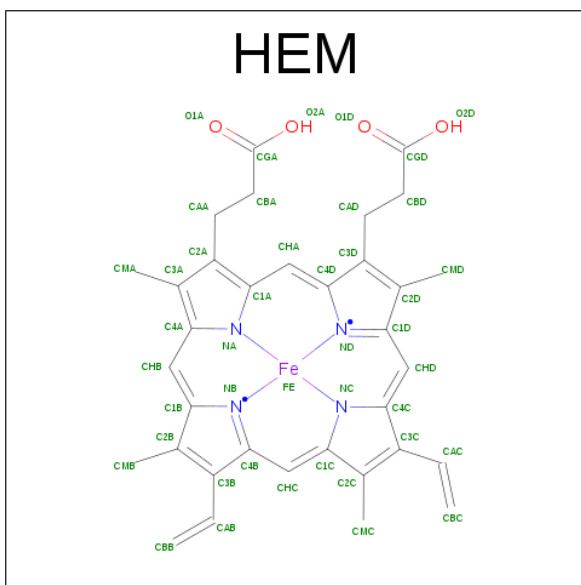
- Molecule 1 is a protein called Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3150	2008	539	591	12			
1	B	360	Total	C	N	O	S	0	0	0
			2944	1890	493	549	12			

There are 12 discrepancies between the modelled and reference sequences:

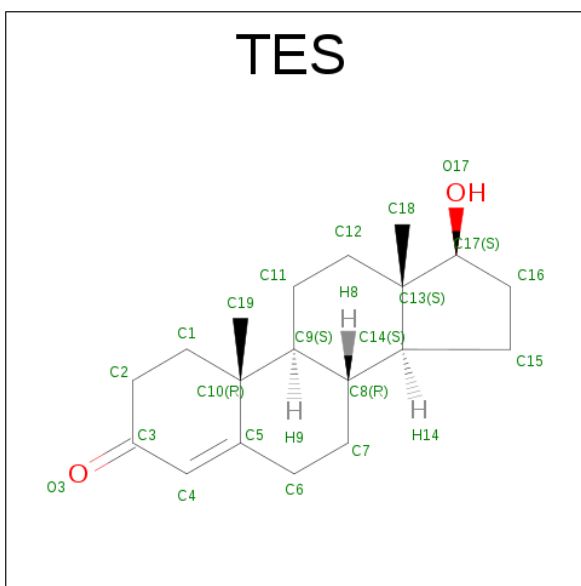
Chain	Residue	Modelled	Actual	Comment	Reference
A	405	HIS	-	expression tag	UNP D5DKI8
A	406	HIS	-	expression tag	UNP D5DKI8
A	407	HIS	-	expression tag	UNP D5DKI8
A	408	HIS	-	expression tag	UNP D5DKI8
A	409	HIS	-	expression tag	UNP D5DKI8
A	410	HIS	-	expression tag	UNP D5DKI8
B	405	HIS	-	expression tag	UNP D5DKI8
B	406	HIS	-	expression tag	UNP D5DKI8
B	407	HIS	-	expression tag	UNP D5DKI8
B	408	HIS	-	expression tag	UNP D5DKI8
B	409	HIS	-	expression tag	UNP D5DKI8
B	410	HIS	-	expression tag	UNP D5DKI8

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is TESTOSTERONE (three-letter code: TES) (formula:  $\text{C}_{19}\text{H}_{28}\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		

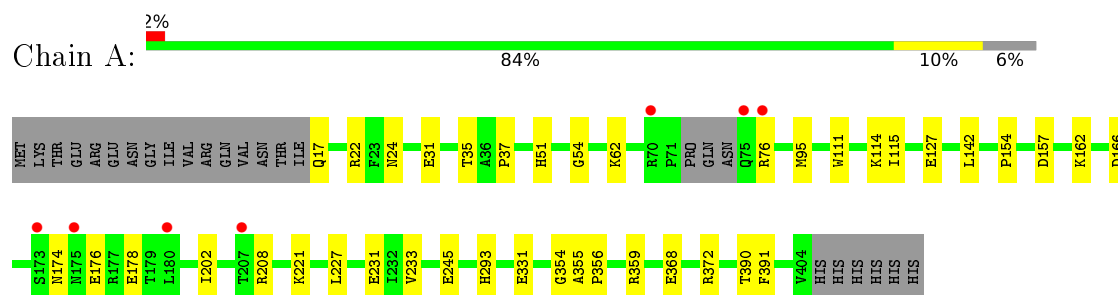
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	108	Total 108	O 108	0	0

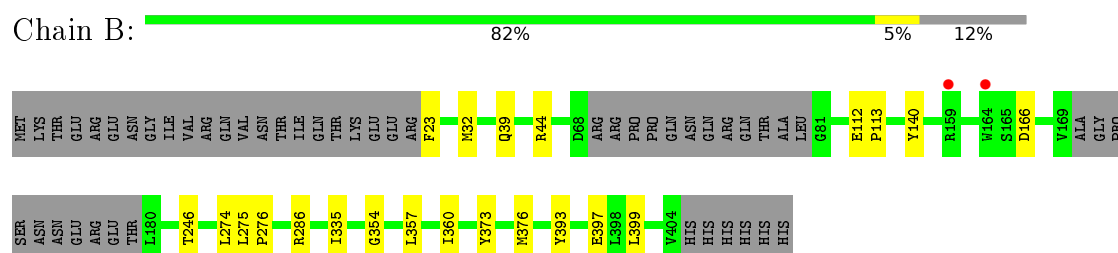
### 3 Residue-property plots [i](#)

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: Cytochrome P450



#### • Molecule 1: Cytochrome P450



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.36Å 134.92Å 61.87Å 90.00° 113.83° 90.00°	Depositor
Resolution (Å)	56.59 – 2.25 56.60 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (56.59-2.25) 99.7 (56.60-2.25)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.69 (at 2.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.219 , 0.263 0.216 , 0.259	Depositor DCC
$R_{free}$ test set	2171 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 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, TES

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	0.66	1/3217 (0.0%)	0.70	2/4348 (0.0%)
1	B	0.63	0/3008	0.69	1/4066 (0.0%)
All	All	0.64	1/6225 (0.0%)	0.70	3/8414 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	GLU	CB-CG	5.00	1.61	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	B	44	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	359	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3150	0	3147	22	0
1	B	2944	0	2944	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	1	0
2	B	43	0	30	2	0
3	A	21	0	27	0	0
4	A	135	0	0	1	0
4	B	108	0	0	0	0
All	All	6444	0	6178	36	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 3.

All (36) 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:B:140:TYR:OH	1:B:166:ASP:OD1	1.94	0.86
1:A:390:THR:OG1	1:A:391:PHE:CE2	2.57	0.58
1:B:373:TYR:O	1:B:376:MET:HG3	2.04	0.57
1:A:166:ASP:OD1	1:A:245:GLU:OE2	2.26	0.54
1:A:24:ASN:O	1:A:24:ASN:CG	2.48	0.51
1:A:293:HIS:CE1	1:A:391:PHE:CZ	2.98	0.51
1:A:202:ILE:CD1	1:A:233:VAL:HG23	2.41	0.51
1:A:355:ALA:HB3	1:A:356:PRO:HD3	1.93	0.50
1:A:368:GLU:OE2	1:A:372:ARG:HD2	2.11	0.49
1:A:115:ILE:HG23	1:A:142:LEU:HD11	1.94	0.48
1:A:51:HIS:CE1	1:A:54:GLY:HA3	2.49	0.48
1:A:95:MET:HE1	1:A:231:GLU:HB3	1.97	0.47
1:A:293:HIS:NE2	1:A:391:PHE:CZ	2.83	0.47
1:B:376:MET:HB3	1:B:376:MET:HE2	1.59	0.47
1:A:162:LYS:HE2	4:A:703:HOH:O	2.15	0.47
1:A:390:THR:OG1	1:A:391:PHE:CD2	2.68	0.46
1:B:357:LEU:O	1:B:360:ILE:HG22	2.15	0.46
1:B:275:LEU:HB3	1:B:276:PRO:HD3	1.98	0.45
1:B:286:ARG:HD3	1:B:393:TYR:HE2	1.83	0.44
1:A:221:LYS:HD2	1:A:227:LEU:O	2.18	0.44
1:A:154:PRO:HG2	1:A:157:ASP:OD2	2.18	0.43
1:B:274:LEU:HD13	1:B:335:ILE:CD1	2.48	0.43
1:B:112:GLU:HB2	1:B:113:PRO:CD	2.50	0.42
1:A:354:GLY:HA3	2:A:501:HEM:C3C	2.55	0.42
1:A:17:GLN:HG3	1:A:22:ARG:HG3	2.02	0.42
1:B:32:MET:SD	1:B:39:GLN:OE1	2.78	0.42
1:B:354:GLY:HA3	2:B:501:HEM:C3C	2.54	0.42
1:A:31:GLU:O	1:A:35:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:THR:HB	2:B:501:HEM:C3B	2.55	0.41
1:B:360:ILE:HD12	1:B:360:ILE:HA	1.84	0.41
1:B:357:LEU:HA	1:B:360:ILE:HG22	2.02	0.41
1:B:397:GLU:OE2	1:B:399:LEU:HG	2.21	0.41
1:A:37:PRO:HB2	1:A:51:HIS:ND1	2.36	0.40
1:A:111:TRP:CE3	1:A:114:LYS:HD2	2.56	0.40
1:A:176:GLU:HG2	1:A:178:GLU:H	1.87	0.40
1:A:174:ASN:OD1	1:A:176:GLU:HB3	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	381/410 (93%)	365 (96%)	16 (4%)	0	100	100
1	B	354/410 (86%)	341 (96%)	13 (4%)	0	100	100
All	All	735/820 (90%)	706 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	345/369 (94%)	341 (99%)	4 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	323/369 (88%)	322 (100%)	1 (0%)	94	97
All	All	668/738 (90%)	663 (99%)	5 (1%)	88	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LYS
1	A	76	ARG
1	A	127	GLU
1	A	208	ARG
1	B	23	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

3 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	501	1,3	24,50,50	1.96	7 (29%)	16,82,82	1.50	4 (25%)
3	TES	A	502	2	24,24,24	5.26	14 (58%)	39,39,39	2.26	14 (35%)
2	HEM	B	501	1	24,50,50	1.93	7 (29%)	16,82,82	1.38	2 (12%)

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	501	1,3	-	0/6/54/54	0/0/8/8
3	TES	A	502	2	-	0/0/58/58	0/4/4/4
2	HEM	B	501	1	-	0/6/54/54	0/0/8/8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	TES	O17-C17	-11.46	1.23	1.43
2	A	501	HEM	C3C-C2C	-5.02	1.34	1.40
2	A	501	HEM	C3B-C2B	-4.42	1.34	1.40
2	B	501	HEM	C3B-C2B	-4.23	1.35	1.40
2	B	501	HEM	C3C-C2C	-4.22	1.35	1.40
3	A	502	TES	O3-C3	-2.42	1.19	1.23
2	A	501	HEM	CAD-C3D	2.05	1.54	1.52
2	A	501	HEM	CMD-C2D	2.05	1.55	1.51
2	A	501	HEM	CMA-C3A	2.21	1.56	1.51
2	A	501	HEM	CMC-C2C	2.22	1.56	1.51
2	B	501	HEM	CAD-C3D	2.25	1.55	1.52
2	B	501	HEM	CMC-C2C	2.28	1.56	1.51
3	A	502	TES	C2-C3	2.33	1.55	1.49
2	B	501	HEM	CMB-C2B	2.41	1.56	1.51
3	A	502	TES	C13-C14	2.45	1.59	1.55
3	A	502	TES	C16-C15	2.45	1.60	1.54
2	B	501	HEM	C3C-CAC	2.53	1.53	1.47
2	A	501	HEM	C3C-CAC	2.78	1.53	1.47
3	A	502	TES	C7-C6	2.83	1.59	1.52
3	A	502	TES	C15-C14	3.08	1.60	1.54
2	B	501	HEM	C3B-CAB	3.57	1.55	1.47
3	A	502	TES	C4-C3	4.58	1.55	1.45
3	A	502	TES	C8-C9	5.91	1.65	1.53
3	A	502	TES	C13-C17	6.87	1.65	1.54
3	A	502	TES	C12-C11	6.89	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	TES	C6-C5	7.65	1.62	1.50
3	A	502	TES	C16-C17	10.45	1.70	1.53
3	A	502	TES	C4-C5	12.96	1.53	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	TES	C5-C4-C3	-6.11	113.94	123.72
3	A	502	TES	C18-C13-C12	-3.49	104.53	110.53
3	A	502	TES	C19-C10-C1	-3.48	103.80	109.39
3	A	502	TES	O17-C17-C13	-3.08	108.25	114.74
2	B	501	HEM	CMA-C3A-C4A	-3.02	123.18	128.31
3	A	502	TES	C18-C13-C17	-2.87	104.73	109.50
2	A	501	HEM	CBA-CAA-C2A	-2.37	108.32	112.49
3	A	502	TES	C6-C7-C8	-2.30	107.33	111.71
2	A	501	HEM	CMD-C2D-C1D	-2.23	124.52	128.31
3	A	502	TES	C11-C12-C13	-2.10	109.03	112.81
3	A	502	TES	C10-C9-C8	-2.05	109.47	112.72
2	B	501	HEM	CMB-C2B-C3B	2.23	129.45	125.09
3	A	502	TES	C14-C8-C9	2.35	112.42	109.09
2	A	501	HEM	CMB-C2B-C3B	2.61	130.19	125.09
2	A	501	HEM	CMC-C2C-C3C	2.77	130.50	125.09
3	A	502	TES	C12-C13-C17	3.29	120.12	115.32
3	A	502	TES	C1-C10-C5	3.42	115.94	108.83
3	A	502	TES	C12-C13-C14	3.42	112.91	107.33
3	A	502	TES	C7-C8-C9	3.43	114.93	110.47
3	A	502	TES	C14-C13-C17	5.35	105.09	99.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	1	0
2	B	501	HEM	2	0

## 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 [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, 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	385/410 (93%)	-0.14	7 (1%) 71 75	20, 33, 58, 81	0
1	B	360/410 (87%)	-0.02	2 (0%) 90 91	21, 35, 60, 81	0
All	All	745/820 (90%)	-0.08	9 (1%) 81 83	20, 34, 58, 81	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	GLN	2.9
1	A	70	ARG	2.6
1	A	76	ARG	2.6
1	B	159	ARG	2.3
1	A	207	THR	2.3
1	A	180	LEU	2.3
1	B	164	TRP	2.2
1	A	175	ASN	2.1
1	A	173	SER	2.0

### 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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TES	A	502	21/21	0.85	0.20	5.17	26,30,36,39	0
2	HEM	A	501	43/43	0.97	0.13	0.18	21,24,28,31	0
2	HEM	B	501	43/43	0.98	0.13	0.06	21,24,27,33	0

## 6.5 Other polymers

There are no such residues in this entry.