



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:40 am GMT

PDB ID : 3IVY  
Title : Crystal structure of Mycobacterium tuberculosis cytochrome P450 CYP125, p212121 crystal form  
Authors : McLean, K.J.; Levy, C.; Munro, A.W.; Leys, D.  
Deposited on : 2009-09-02  
Resolution : 1.35 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

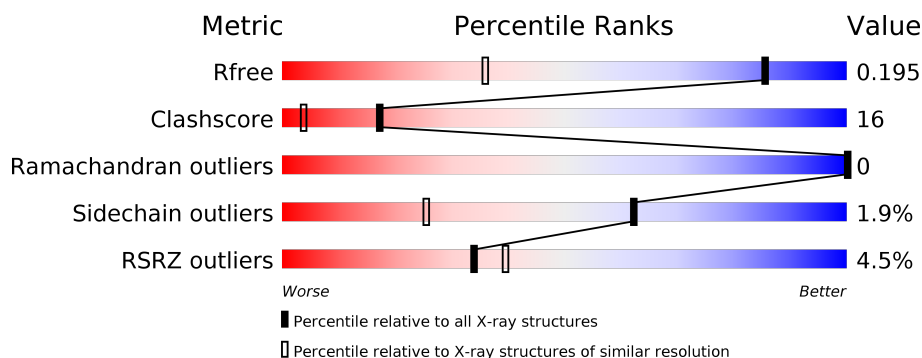
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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))
$R_{free}$	100719	1024 (1.38-1.34)
Clashscore	112137	1063 (1.38-1.34)
Ramachandran outliers	110173	1048 (1.38-1.34)
Sidechain outliers	110143	1048 (1.38-1.34)
RSRZ outliers	101464	1025 (1.38-1.34)

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	433	<div> <div>4%</div> <div>70%</div> <div>17%</div> <div>8%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4002 atoms, of which 13 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 CYP125.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	H	N	O	S	0	12	0
			3251	2052	13	568	602	16			

- 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		

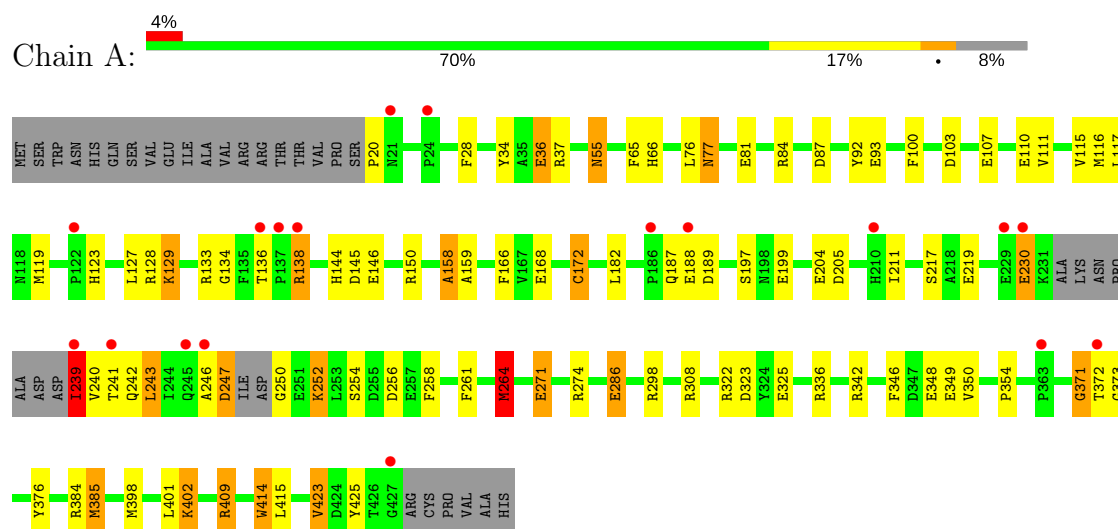
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	708	Total	O	0	0
			708	708		

### 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 the various outlier classes 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 CYP125



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.03Å 86.02Å 89.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.22 – 1.35 28.22 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (28.22-1.35) 97.9 (28.22-1.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.35Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.159 , 0.204 0.151 , 0.195	Depositor DCC
$R_{free}$ test set	5009 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.61	40/3322 (1.2%)	1.41	33/4501 (0.7%)

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	3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLU	CD-OE1	14.13	1.41	1.25
1	A	129	LYS	CD-CE	10.96	1.78	1.51
1	A	271	GLU	CD-OE2	10.22	1.36	1.25
1	A	129	LYS	CE-NZ	9.44	1.72	1.49
1	A	252	LYS	CE-NZ	9.16	1.72	1.49
1	A	168	GLU	CD-OE1	8.98	1.35	1.25
1	A	286	GLU	CD-OE1	8.20	1.34	1.25
1	A	168	GLU	CG-CD	8.09	1.64	1.51
1	A	219	GLU	CD-OE1	7.83	1.34	1.25
1	A	322	ARG	CZ-NH1	7.51	1.42	1.33
1	A	239	ILE	N-CA	-7.22	1.31	1.46
1	A	36	GLU	CD-OE1	7.11	1.33	1.25
1	A	92	TYR	CE2-CZ	7.04	1.47	1.38
1	A	107	GLU	CG-CD	6.98	1.62	1.51
1	A	204	GLU	CD-OE2	-6.45	1.18	1.25
1	A	348	GLU	CD-OE2	6.42	1.32	1.25
1	A	371	GLY	C-O	-6.32	1.13	1.23
1	A	286	GLU	CG-CD	6.25	1.61	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	GLU	CD-OE1	6.25	1.32	1.25
1	A	168	GLU	CD-OE2	6.17	1.32	1.25
1	A	197	SER	CB-OG	5.82	1.49	1.42
1	A	172	CYS	CB-SG	5.79	1.92	1.82
1	A	414	TRP	CG-CD1	5.71	1.44	1.36
1	A	219	GLU	CD-OE2	5.70	1.31	1.25
1	A	336	ARG	NE-CZ	5.64	1.40	1.33
1	A	128	ARG	CG-CD	-5.55	1.38	1.51
1	A	81	GLU	CD-OE1	-5.54	1.19	1.25
1	A	346	PHE	CG-CD1	5.53	1.47	1.38
1	A	158	ALA	CA-CB	5.39	1.63	1.52
1	A	77	ASN	CG-OD1	5.38	1.35	1.24
1	A	371	GLY	CA-C	5.36	1.60	1.51
1	A	36	GLU	CD-OE2	5.34	1.31	1.25
1	A	115	VAL	CB-CG1	5.33	1.64	1.52
1	A	150	ARG	CG-CD	5.20	1.65	1.51
1	A	110	GLU	CB-CG	5.15	1.61	1.52
1	A	423[A]	VAL	CB-CG2	-5.14	1.42	1.52
1	A	423[B]	VAL	CB-CG2	-5.14	1.42	1.52
1	A	65	PHE	CE2-CZ	5.12	1.47	1.37
1	A	230	GLU	CG-CD	5.06	1.59	1.51
1	A	217	SER	CB-OG	-5.01	1.35	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ARG	NE-CZ-NH2	-11.43	114.59	120.30
1	A	298	ARG	NE-CZ-NH2	-10.97	114.82	120.30
1	A	308	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	A	37	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	A	129	LYS	CD-CE-NZ	9.14	132.72	111.70
1	A	342	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	A	145	ASP	CB-CG-OD1	8.94	126.34	118.30
1	A	111	VAL	CG1-CB-CG2	-8.66	97.05	110.90
1	A	87	ASP	CB-CG-OD1	8.61	126.05	118.30
1	A	264[A]	MET	CG-SD-CE	-8.42	86.72	100.20
1	A	264[B]	MET	CG-SD-CE	-8.42	86.72	100.20
1	A	322	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	322	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	205	ASP	CB-CG-OD2	7.35	124.92	118.30
1	A	409	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	384	ARG	NH1-CZ-NH2	6.51	126.56	119.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	133	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	371	GLY	O-C-N	-6.30	112.61	122.70
1	A	271	GLU	CG-CD-OE2	-6.03	106.25	118.30
1	A	323	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	100	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	A	402	LYS	CD-CE-NZ	5.70	124.82	111.70
1	A	409	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	242	GLN	CB-CA-C	-5.56	99.27	110.40
1	A	146	GLU	OE1-CD-OE2	5.49	129.88	123.30
1	A	128	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	189	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	247	ASP	N-CA-C	-5.29	96.71	111.00
1	A	103	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	243	LEU	CB-CG-CD1	5.26	119.94	111.00
1	A	37	ARG	NH1-CZ-NH2	5.16	125.07	119.40
1	A	34	TYR	CB-CG-CD2	-5.04	117.98	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	GLU	Sidechain
1	A	409	ARG	Sidechain
1	A	55[A]	ASN	Sidechain

## 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	3238	13	3110	100	0
2	A	43	0	30	0	0
3	A	708	0	0	43	7
All	All	3989	13	3140	100	7

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 16.



All (100) 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:129:LYS:CE	1:A:129:LYS:CD	1.78	1.56
1:A:252:LYS:NZ	1:A:252:LYS:CE	1.72	1.51
1:A:129:LYS:CE	1:A:129:LYS:NZ	1.72	1.49
1:A:36:GLU:HG2	3:A:615:HOH:O	1.26	1.34
1:A:129:LYS:HE3	3:A:1083:HOH:O	1.41	1.18
1:A:84[B]:ARG:HD2	3:A:655:HOH:O	1.54	1.08
1:A:371:GLY:CA	3:A:650:HOH:O	2.00	1.07
1:A:239:ILE:HD11	1:A:243:LEU:HD11	1.39	1.02
1:A:371:GLY:HA3	3:A:650:HOH:O	1.59	0.97
1:A:247:ASP:O	3:A:617:HOH:O	1.81	0.96
1:A:372:THR:C	3:A:613:HOH:O	2.05	0.95
1:A:385[A]:MET:HE3	3:A:951:HOH:O	1.70	0.91
1:A:239:ILE:HD11	1:A:243:LEU:CD1	2.01	0.91
1:A:250:GLY:N	3:A:461:HOH:O	2.06	0.86
1:A:84[A]:ARG:HD3	3:A:1053:HOH:O	1.75	0.86
1:A:84[B]:ARG:HD3	3:A:1053:HOH:O	1.76	0.86
1:A:116:MET:HE2	1:A:264[B]:MET:HE1	1.57	0.84
1:A:123[A]:HIS:ND1	3:A:451:HOH:O	1.97	0.84
1:A:116:MET:HE2	1:A:264[B]:MET:CE	2.09	0.81
1:A:138:ARG:HB3	3:A:695:HOH:O	1.83	0.79
1:A:401:LEU:HG	3:A:580:HOH:O	1.82	0.79
1:A:84[B]:ARG:CD	3:A:655:HOH:O	2.20	0.78
1:A:247:ASP:OD1	1:A:247:ASP:C	2.19	0.78
1:A:116:MET:CE	1:A:264[B]:MET:CE	2.62	0.77
1:A:77:ASN:HB2	3:A:966:HOH:O	1.83	0.77
1:A:20:PRO:N	3:A:622:HOH:O	2.19	0.76
1:A:325:GLU:HG2	3:A:1045:HOH:O	1.87	0.74
1:A:372:THR:O	3:A:613:HOH:O	2.04	0.71
1:A:129:LYS:CE	1:A:129:LYS:CG	2.68	0.69
1:A:158:ALA:HB3	1:A:398[B]:MET:HE1	1.75	0.68
1:A:371:GLY:O	3:A:613:HOH:O	2.11	0.68
1:A:402:LYS:HE3	3:A:660:HOH:O	1.94	0.67
1:A:116:MET:CE	1:A:264[B]:MET:HE3	2.24	0.66
1:A:376:TYR:HA	3:A:943:HOH:O	1.94	0.66
1:A:371:GLY:C	3:A:650:HOH:O	2.24	0.65
1:A:84[A]:ARG:HD2	3:A:655:HOH:O	1.97	0.64
1:A:84[B]:ARG:NH2	1:A:84[B]:ARG:HB3	2.11	0.64
1:A:230:GLU:HG3	3:A:1096:HOH:O	1.97	0.64
1:A:123[B]:HIS:ND1	3:A:787:HOH:O	2.29	0.64
1:A:119:MET:SD	1:A:123[B]:HIS:CD2	2.91	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84[B]:ARG:HG3	3:A:928:HOH:O	1.98	0.63
1:A:401:LEU:CG	3:A:580:HOH:O	2.44	0.62
1:A:138:ARG:HB2	1:A:138:ARG:NH1	2.17	0.59
1:A:398[A]:MET:O	1:A:401:LEU:HD22	2.01	0.59
1:A:239:ILE:HD12	1:A:243:LEU:HG	1.84	0.59
1:A:116:MET:HB3	1:A:264[A]:MET:HE2	1.86	0.58
1:A:144:HIS:HD2	1:A:385[A]:MET:SD	2.27	0.58
1:A:166:PHE:HB2	1:A:423[B]:VAL:HG11	1.86	0.57
1:A:76:LEU:CD2	1:A:350:VAL:HG11	2.35	0.57
1:A:136:THR:OG1	1:A:138:ARG:HG3	2.06	0.56
1:A:93[A]:GLU:HG3	3:A:509:HOH:O	2.06	0.56
1:A:239:ILE:CD1	1:A:243:LEU:CD1	2.82	0.55
1:A:354:PRO:HD2	3:A:847:HOH:O	2.08	0.54
1:A:398[B]:MET:O	1:A:401:LEU:HD22	2.06	0.54
1:A:76:LEU:HD22	1:A:350:VAL:HG11	1.89	0.53
1:A:84[A]:ARG:HG3	3:A:928:HOH:O	2.10	0.52
1:A:373:GLY:N	3:A:613:HOH:O	2.31	0.51
1:A:76:LEU:HD23	1:A:350:VAL:HG21	1.91	0.51
1:A:158:ALA:HB3	1:A:398[B]:MET:CE	2.41	0.50
1:A:117:LEU:H	1:A:264[A]:MET:CE	2.24	0.50
1:A:28:PHE:H	1:A:55[B]:ASN:HD21	1.58	0.50
1:A:239:ILE:CG1	1:A:239:ILE:O	2.55	0.49
1:A:373:GLY:HA3	3:A:613:HOH:O	2.12	0.49
1:A:117:LEU:HB2	1:A:264[A]:MET:HE1	1.93	0.49
1:A:372:THR:N	3:A:650:HOH:O	2.43	0.49
1:A:373:GLY:CA	3:A:613:HOH:O	2.61	0.49
1:A:401:LEU:CD1	3:A:580:HOH:O	2.61	0.49
1:A:261:PHE:O	1:A:264[A]:MET:HB3	2.13	0.48
1:A:199:GLU:HB3	1:A:211:ILE:CG2	2.43	0.48
1:A:28:PHE:H	1:A:55[B]:ASN:ND2	2.10	0.48
1:A:239:ILE:CD1	1:A:243:LEU:HD11	2.27	0.47
1:A:84[B]:ARG:CZ	1:A:84[B]:ARG:CB	2.92	0.47
1:A:239:ILE:N	3:A:529:HOH:O	2.48	0.47
1:A:66:HIS:HE1	3:A:597:HOH:O	1.97	0.46
1:A:166:PHE:HB2	1:A:423[B]:VAL:CG1	2.44	0.46
1:A:239:ILE:HG13	1:A:239:ILE:O	1.93	0.46
1:A:398[B]:MET:HE3	1:A:425:TYR:HB3	1.96	0.46
1:A:84[B]:ARG:CZ	1:A:84[B]:ARG:HB3	2.45	0.46
1:A:158:ALA:CB	1:A:398[B]:MET:HE1	2.46	0.45
1:A:246:ALA:HB1	1:A:250:GLY:HA2	1.98	0.45
1:A:172:CYS:SG	3:A:562:HOH:O	2.00	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:N	1:A:398[B]:MET:HE1	2.33	0.44
1:A:286:GLU:HG2	3:A:441:HOH:O	2.16	0.44
1:A:55[B]:ASN:OD1	3:A:612:HOH:O	2.19	0.43
1:A:117:LEU:H	1:A:264[A]:MET:HE2	1.84	0.43
1:A:264[B]:MET:HB3	1:A:264[B]:MET:HE2	1.73	0.42
1:A:414:TRP:CZ3	1:A:415[B]:LEU:HG	2.54	0.42
1:A:119:MET:SD	1:A:127:LEU:HD12	2.59	0.42
1:A:211:ILE:HD11	3:A:1039:HOH:O	2.20	0.42
1:A:199:GLU:HG2	1:A:211:ILE:HD13	2.01	0.41
1:A:254:SER:OG	1:A:256:ASP:OD1	2.23	0.41
1:A:138:ARG:HB2	1:A:138:ARG:HH11	1.84	0.41
1:A:239:ILE:CD1	1:A:243:LEU:HG	2.48	0.41
1:A:239:ILE:HG13	1:A:240:VAL:N	2.17	0.41
1:A:20:PRO:CA	3:A:622:HOH:O	2.64	0.41
1:A:134:GLY:O	1:A:182:LEU:HD11	2.20	0.41
1:A:117:LEU:N	1:A:264[A]:MET:CE	2.84	0.40
1:A:240:VAL:HG22	1:A:258:PHE:CZ	2.56	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:462:HOH:O	3:A:902:HOH:O[2_564]	2.01	0.19
3:A:462:HOH:O	3:A:990:HOH:O[2_564]	2.06	0.14
3:A:462:HOH:O	3:A:878:HOH:O[2_564]	2.06	0.14
3:A:462:HOH:O	3:A:919:HOH:O[2_564]	2.07	0.13
3:A:590:HOH:O	3:A:1001:HOH:O[2_564]	2.11	0.09
3:A:583:HOH:O	3:A:602:HOH:O[4_455]	2.13	0.07
3:A:654:HOH:O	3:A:669:HOH:O[4_555]	2.17	0.03

## 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	405/433 (94%)	400 (99%)	5 (1%)	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	336/356 (94%)	327 (97%)	9 (3%)	50	15

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ARG
1	A	187[A]	GLN
1	A	187[B]	GLN
1	A	239	ILE
1	A	241	THR
1	A	264[A]	MET
1	A	264[B]	MET
1	A	385[A]	MET
1	A	385[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	HIS

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	28,50,50	2.16	9 (32%)	17,82,82	2.79	8 (47%)

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3C-C2C	-4.71	1.34	1.40
2	A	501	HEM	C3B-C2B	-3.91	1.35	1.40
2	A	501	HEM	C3D-C2D	2.14	1.44	1.37
2	A	501	HEM	C1A-NA	2.70	1.41	1.36
2	A	501	HEM	CAA-C2A	2.73	1.56	1.52
2	A	501	HEM	CAD-C3D	3.26	1.58	1.52
2	A	501	HEM	C1D-ND	3.33	1.43	1.36
2	A	501	HEM	C4D-ND	3.34	1.40	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-CAB	4.32	1.56	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C4A-C3A-C2A	-5.48	103.18	107.00
2	A	501	HEM	C1D-C2D-C3D	-4.55	103.83	107.00
2	A	501	HEM	CBA-CAA-C2A	-2.92	106.89	112.48
2	A	501	HEM	CMD-C2D-C3D	2.08	128.85	124.94
2	A	501	HEM	CMA-C3A-C2A	3.09	130.76	124.94
2	A	501	HEM	CMB-C2B-C3B	3.68	131.72	124.89
2	A	501	HEM	C4C-C3C-C2C	3.75	109.52	106.90
2	A	501	HEM	CMC-C2C-C3C	3.81	131.96	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	399/433 (92%)	0.22	18 (4%) 34 39	10, 20, 38, 58	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	PRO	5.4
1	A	239	ILE	4.6
1	A	138	ARG	4.0
1	A	230	GLU	3.5
1	A	372	THR	3.5
1	A	245	GLN	3.4
1	A	241	THR	3.3
1	A	24	PRO	3.3
1	A	229	GLU	2.6
1	A	427	GLY	2.6
1	A	21	ASN	2.4
1	A	210	HIS	2.3
1	A	136	THR	2.3
1	A	188	GLU	2.3
1	A	246	ALA	2.1
1	A	122	PRO	2.1
1	A	186	PRO	2.1
1	A	363	PRO	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( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	501	43/43	0.98	0.08	-0.29	11,13,17,18	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.