



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:47 am GMT

PDB ID : 2CCD  
Title : CRYSTAL STRUCTURE OF THE CATALASE-PEROXIDASE (KATG)  
AND S315T MUTANT FROM MYCOBACTERIUM TUBERCULOSIS  
Authors : Yu, H.; Sacchettini, J.C.  
Deposited on : 2006-01-16  
Resolution : 2.10 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 : 1.7.2 (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

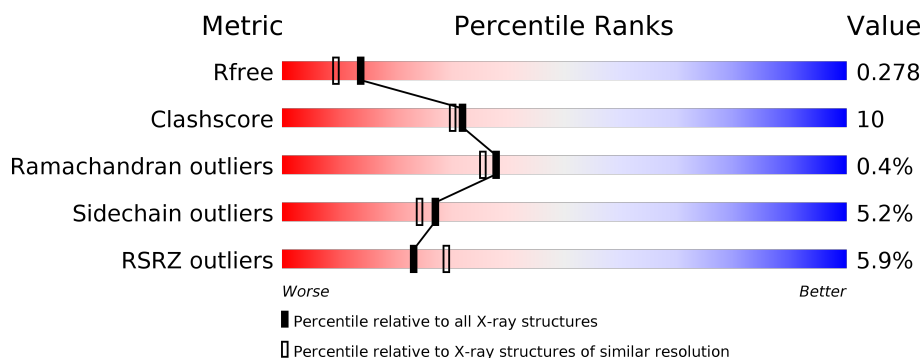
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	740	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	740	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11715 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.

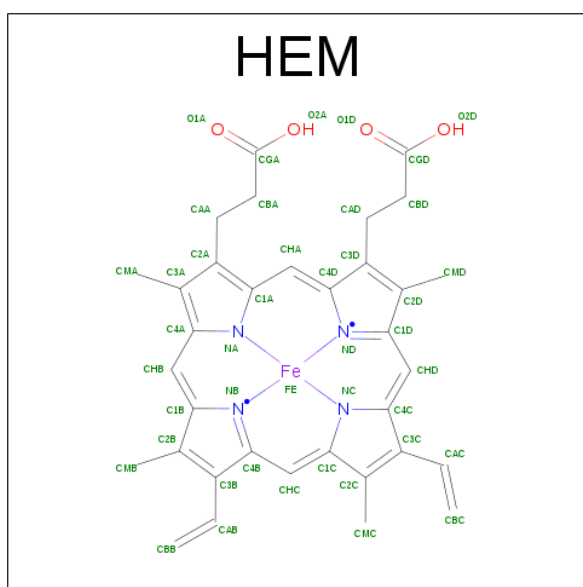
- Molecule 1 is a protein called PEROXIDASE/CATALASE T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5517	3508	949	1041	19			
1	B	715	Total	C	N	O	S	0	0	0
			5517	3508	949	1041	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	THR	SER	ENGINEERED MUTATION	UNP Q08129
B	315	THR	SER	ENGINEERED MUTATION	UNP Q08129

- 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		

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

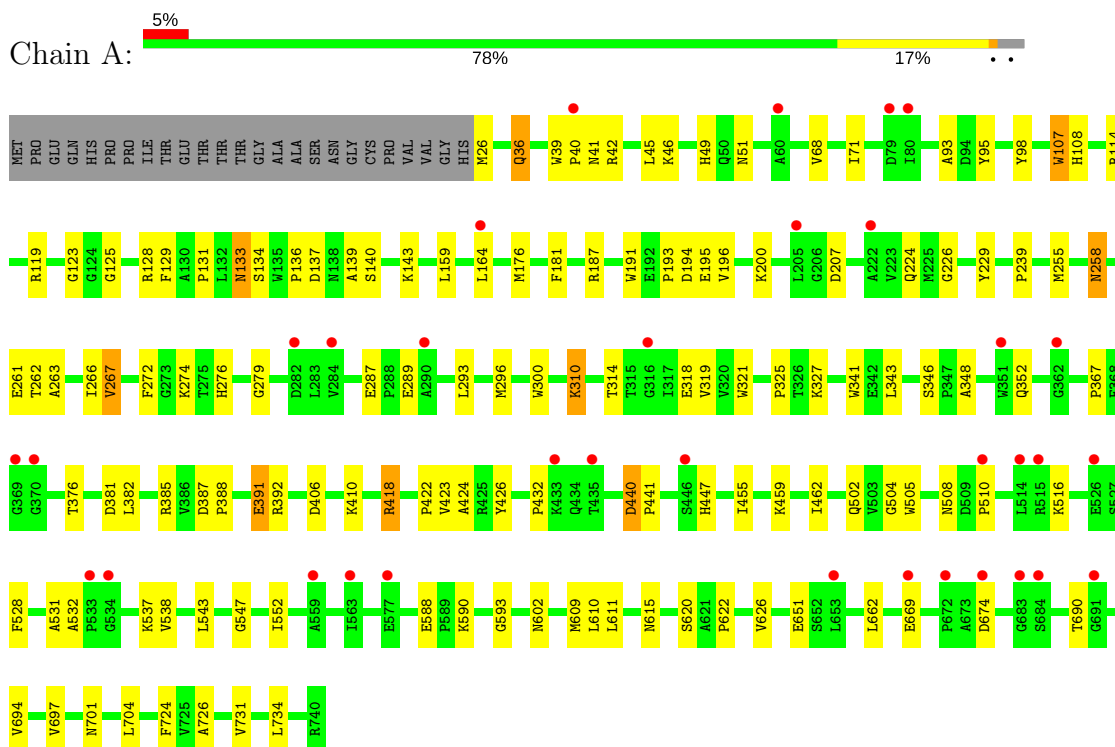
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	340	Total	O	0	0
			340	340		
3	B	255	Total	O	0	0
			255	255		

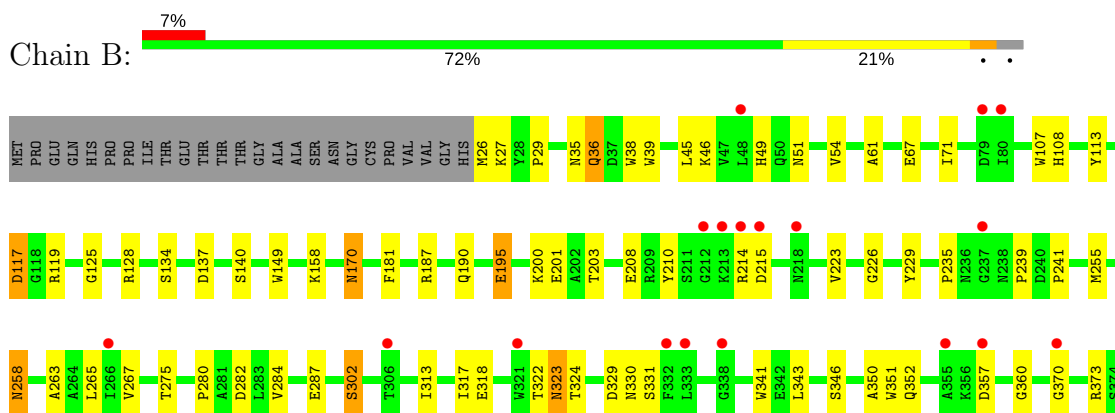
### 3 Residue-property plots [i](#)

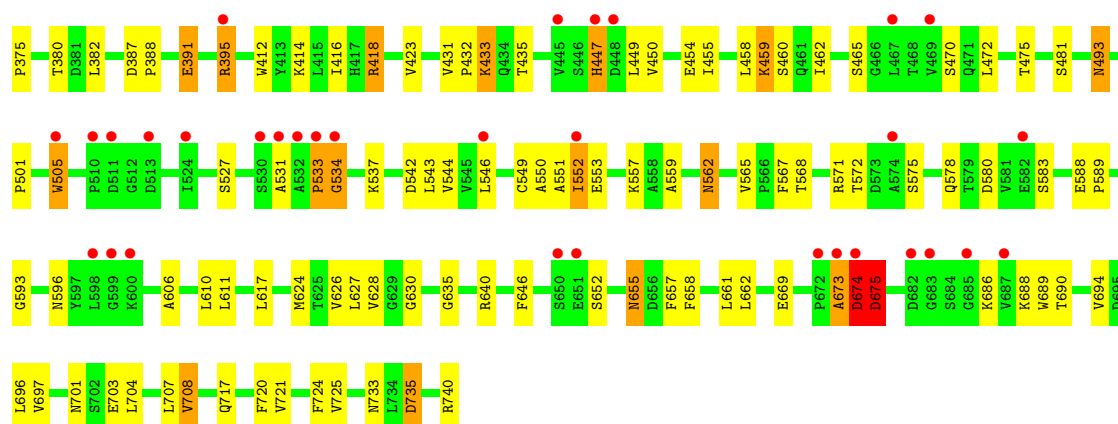
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PEROXIDASE/CATALASE T



#### • Molecule 1: PEROXIDASE/CATALASE T





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.81Å 149.81Å 154.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	78.5 (20.00-2.10) 78.5 (20.01-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.230 , 0.276 0.237 , 0.278	Depositor DCC
$R_{free}$ test set	3987 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k 0.026 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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	0.60	2/5667 (0.0%)	0.66	1/7714 (0.0%)
1	B	0.54	0/5667	0.69	5/7714 (0.1%)
All	All	0.57	2/11334 (0.0%)	0.68	6/15428 (0.0%)

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	1
1	B	0	6
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	ASP	C-N	19.62	1.71	1.34
1	A	440	ASP	CA-C	9.06	1.76	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	674	ASP	CB-CG-OD2	7.15	124.73	118.30
1	B	675	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	673	ALA	CB-CA-C	5.90	118.95	110.10
1	A	440	ASP	CA-C-N	-5.79	100.89	117.10
1	B	673	ALA	O-C-N	-5.53	113.85	122.70
1	B	735	ASP	CB-CA-C	-5.51	99.37	110.40



There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	SER	Mainchain
1	B	140	SER	Mainchain
1	B	673	ALA	Mainchain,Peptide
1	B	674	ASP	Mainchain
1	B	675	ASP	Mainchain
1	B	735	ASP	Peptide

## 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	5517	0	5347	93	0
1	B	5517	0	5347	133	0
2	A	43	0	30	0	0
2	B	43	0	30	5	0
3	A	340	0	0	9	0
3	B	255	0	0	14	0
All	All	11715	0	10754	221	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 10.

All (221) 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:440:ASP:CA	1:A:440:ASP:C	1.76	1.49
1:A:440:ASP:C	1:A:441:PRO:N	1.71	1.41
1:B:107:TRP:CH2	1:B:229:TYR:CE1	2.17	1.31
1:A:229:TYR:CE2	1:A:255:MET:SD	2.25	1.30
1:B:107:TRP:HH2	1:B:229:TYR:CE1	1.50	1.28
1:B:107:TRP:CH2	1:B:229:TYR:HE1	1.50	1.27
1:B:350:ALA:HB1	3:B:2106:HOH:O	1.21	1.25
1:B:229:TYR:CE2	1:B:255:MET:SD	2.39	1.16
1:B:447:HIS:HB2	1:B:537:LYS:HE2	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD23	1:B:611:LEU:HD21	1.40	1.02
1:B:447:HIS:CB	1:B:537:LYS:HE2	1.90	1.01
1:A:229:TYR:HE2	1:A:255:MET:SD	1.76	0.95
1:A:516:LYS:NZ	3:A:2240:HOH:O	1.86	0.92
1:B:552:ILE:HG23	1:B:565:VAL:HG21	1.56	0.86
1:B:229:TYR:CZ	1:B:255:MET:SD	2.70	0.85
1:A:229:TYR:HE2	1:A:255:MET:CG	1.91	0.82
1:B:51:ASN:HD21	1:B:190:GLN:HB3	1.44	0.80
1:B:533:PRO:O	1:B:534:GLY:O	2.00	0.79
1:B:117:ASP:OD1	1:B:119:ARG:NH1	2.18	0.77
1:B:701:ASN:HD22	1:B:704:LEU:H	1.32	0.77
1:B:229:TYR:HE2	1:B:255:MET:SD	2.07	0.77
1:B:542:ASP:HB2	1:B:567:PHE:HZ	1.47	0.77
1:B:107:TRP:HH2	1:B:229:TYR:CD1	2.02	0.77
1:B:107:TRP:CH2	1:B:229:TYR:CD1	2.74	0.75
1:B:527:SER:O	1:B:531:ALA:HB2	1.86	0.75
1:B:433:LYS:HD2	1:B:433:LYS:H	1.51	0.74
1:A:440:ASP:C	1:A:440:ASP:CB	2.56	0.73
1:A:505:TRP:HB2	1:A:508:ASN:HD22	1.54	0.72
1:A:51:ASN:HD21	1:A:191:TRP:H	1.35	0.72
1:B:450:VAL:HG12	1:B:455:ILE:HG13	1.72	0.71
1:B:258:ASN:HD22	1:B:258:ASN:C	1.93	0.70
1:A:229:TYR:CZ	1:A:255:MET:SD	2.84	0.70
1:A:406:ASP:O	1:A:410:LYS:HG3	1.91	0.70
1:B:210:TYR:HD2	1:B:214:ARG:O	1.75	0.69
1:B:447:HIS:HB2	1:B:537:LYS:CE	2.18	0.69
1:B:395:ARG:NH2	3:B:2166:HOH:O	2.24	0.69
1:B:447:HIS:HB3	1:B:537:LYS:HE2	1.74	0.68
1:B:553:GLU:HG3	1:B:565:VAL:HG23	1.76	0.67
1:B:210:TYR:CD2	1:B:214:ARG:O	2.48	0.67
1:B:357:ASP:HB3	3:B:2153:HOH:O	1.95	0.66
1:B:610:LEU:HD22	1:B:694:VAL:HG13	1.77	0.65
1:A:318:GLU:H	1:A:352:GLN:HE22	1.43	0.64
1:A:45:LEU:HD23	1:A:611:LEU:HD21	1.79	0.63
1:B:107:TRP:CZ3	1:B:229:TYR:HE1	2.14	0.63
1:B:195:GLU:HB2	3:B:2085:HOH:O	1.99	0.62
1:B:170:ASN:HD22	1:B:412:TRP:HE1	1.46	0.62
1:B:655:ASN:ND2	1:B:717:GLN:HE21	1.96	0.62
1:B:239:PRO:HG3	1:B:351:TRP:CG	2.35	0.61
1:A:133:ASN:HD22	1:A:134:SER:N	1.98	0.60
1:A:505:TRP:HB2	1:A:508:ASN:ND2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:LYS:HD3	1:B:546:LEU:HD11	1.83	0.60
1:B:26:MET:N	3:B:2002:HOH:O	2.35	0.60
1:A:258:ASN:ND2	1:A:261:GLU:H	2.00	0.59
1:B:542:ASP:HB2	1:B:567:PHE:CZ	2.34	0.58
1:B:125:GLY:O	1:B:128:ARG:HG2	2.02	0.58
1:A:531:ALA:HB2	3:A:2243:HOH:O	2.03	0.58
2:B:1741:HEM:HMB2	2:B:1741:HEM:HBB2	1.86	0.58
1:A:440:ASP:C	1:A:441:PRO:CA	2.68	0.57
1:A:609:MET:HA	1:A:609:MET:HE2	1.86	0.57
1:B:318:GLU:H	1:B:352:GLN:HE22	1.53	0.57
1:B:433:LYS:N	1:B:433:LYS:HD2	2.17	0.57
1:B:239:PRO:O	1:B:241:PRO:HD3	2.05	0.57
1:A:440:ASP:CA	1:A:441:PRO:N	2.68	0.56
1:B:275:THR:HG22	2:B:1741:HEM:CAA	2.35	0.56
1:A:41:ASN:OD1	1:B:27:LYS:NZ	2.36	0.56
1:A:181:PHE:CE2	1:A:432:PRO:HG3	2.41	0.56
1:A:258:ASN:HD22	1:A:258:ASN:C	2.09	0.56
1:B:113:TYR:HB3	1:B:418:ARG:HH11	1.72	0.55
1:B:187:ARG:HA	3:B:2075:HOH:O	2.06	0.55
1:B:658:PHE:HD2	1:B:708:VAL:HB	1.73	0.54
1:B:472:LEU:HB2	1:B:551:ALA:HB2	1.90	0.54
1:B:210:TYR:OH	1:B:223:VAL:HG12	2.08	0.54
1:B:357:ASP:CB	3:B:2153:HOH:O	2.54	0.54
1:B:323:ASN:H	1:B:323:ASN:HD22	1.55	0.54
1:B:350:ALA:CB	3:B:2106:HOH:O	2.02	0.53
1:B:733:ASN:O	1:B:740:ARG:NH1	2.41	0.53
1:B:459:LYS:HG3	1:B:550:ALA:HB2	1.90	0.53
1:A:159:LEU:HD21	1:A:164:LEU:HD13	1.91	0.52
1:A:143:LYS:NZ	3:A:2058:HOH:O	2.42	0.52
1:A:731:VAL:HA	1:A:734:LEU:HG	1.92	0.52
1:A:620:SER:HB2	1:A:622:PRO:HD2	1.92	0.52
1:A:133:ASN:HD22	1:A:133:ASN:C	2.12	0.51
1:B:107:TRP:CD1	1:B:108:HIS:HD2	2.28	0.51
1:B:470:SER:OG	1:B:635:GLY:HA3	2.10	0.51
1:A:125:GLY:O	1:A:128:ARG:HG2	2.09	0.51
1:A:609:MET:CE	1:A:609:MET:HA	2.41	0.51
1:B:626:VAL:HG23	1:B:720:PHE:CD1	2.46	0.51
1:A:143:LYS:HD2	1:A:143:LYS:H	1.76	0.51
1:B:284:VAL:HG22	1:B:302:SER:HB2	1.93	0.51
1:A:341:TRP:HB2	1:A:382:LEU:HD21	1.92	0.50
1:B:170:ASN:ND2	1:B:412:TRP:HE1	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:O	1:A:267:VAL:CG1	2.59	0.50
1:B:493:ASN:HD21	1:B:572:THR:H	1.59	0.50
1:B:36:GLN:NE2	1:B:36:GLN:H	2.09	0.50
1:A:26:MET:HA	1:B:200:LYS:O	2.12	0.50
1:B:113:TYR:HB3	1:B:418:ARG:NH1	2.27	0.50
1:A:107:TRP:CD1	1:A:108:HIS:HD2	2.30	0.49
1:A:694:VAL:O	1:A:697:VAL:HG12	2.11	0.49
1:A:263:ALA:O	1:A:267:VAL:HG13	2.13	0.49
1:B:416:ILE:HG22	1:B:416:ILE:O	2.13	0.49
1:A:128:ARG:NH1	3:B:2240:HOH:O	2.45	0.49
1:A:195:GLU:HB3	1:B:29:PRO:HB3	1.95	0.49
1:B:134:SER:HB3	1:B:287:GLU:HG3	1.94	0.49
1:B:67:GLU:HB3	1:B:158:LYS:HA	1.94	0.49
1:B:662:LEU:HD21	1:B:708:VAL:HG22	1.94	0.49
1:B:258:ASN:ND2	1:B:258:ASN:C	2.65	0.49
1:B:701:ASN:ND2	1:B:703:GLU:H	2.10	0.49
1:B:181:PHE:CE2	1:B:432:PRO:HG2	2.48	0.48
1:B:542:ASP:HB3	1:B:571:ARG:HH11	1.78	0.48
1:B:694:VAL:O	1:B:697:VAL:HG12	2.13	0.48
1:B:137:ASP:HB2	1:B:226:GLY:O	2.13	0.48
1:A:136:PRO:HD2	1:A:226:GLY:HA3	1.95	0.48
1:A:620:SER:HB3	1:B:54:VAL:HG22	1.95	0.48
1:A:662:LEU:HD13	1:B:149:TRP:CZ2	2.48	0.48
1:A:129:PHE:HB3	1:A:193:PRO:HG3	1.95	0.48
1:B:701:ASN:ND2	1:B:704:LEU:H	2.05	0.48
1:B:552:ILE:HG13	1:B:724:PHE:HE2	1.78	0.48
1:B:265:LEU:O	2:B:1741:HEM:HBC2	2.13	0.47
1:A:310:LYS:HB2	3:A:2151:HOH:O	2.13	0.47
1:B:565:VAL:HG13	1:B:725:VAL:HG13	1.96	0.47
1:B:721:VAL:O	1:B:725:VAL:HG23	2.15	0.47
1:A:462:ILE:HG21	1:A:547:GLY:HA2	1.96	0.47
1:A:459:LYS:NZ	3:A:2210:HOH:O	2.43	0.47
1:A:590:LYS:HB2	1:A:602:ASN:HD21	1.80	0.47
1:A:701:ASN:HD22	1:A:704:LEU:H	1.63	0.47
1:A:385:ARG:O	1:A:391:GLU:HG2	2.15	0.47
1:A:262:THR:O	1:A:266:ILE:HG13	2.15	0.47
1:A:423:VAL:HA	1:A:426:TYR:CD2	2.50	0.47
1:A:68:VAL:O	1:A:71:ILE:HG22	2.15	0.47
1:B:450:VAL:HG13	1:B:454:GLU:HB2	1.97	0.47
1:A:229:TYR:HE2	1:A:255:MET:HG3	1.75	0.46
1:A:134:SER:HB3	1:A:287:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLN:O	1:A:40:PRO:HA	2.15	0.46
1:A:455:ILE:HG22	1:A:459:LYS:HE2	1.98	0.46
1:B:201:GLU:OE2	1:B:208:GLU:N	2.46	0.46
1:A:239:PRO:HG2	1:A:343:LEU:HD11	1.98	0.46
1:A:504:GLY:HA2	1:A:510:PRO:HB3	1.97	0.46
1:B:462:ILE:HA	1:B:465:SER:OG	2.15	0.46
1:A:139:ALA:O	1:A:314:THR:HG23	2.15	0.46
1:A:95:TYR:CZ	1:A:325:PRO:HG2	2.51	0.46
1:A:26:MET:N	3:A:2001:HOH:O	2.50	0.45
3:A:2014:HOH:O	1:B:707:LEU:HD11	2.15	0.45
1:B:630:GLY:HA3	1:B:724:PHE:CE1	2.52	0.45
1:B:575:SER:OG	1:B:578:GLN:HG3	2.16	0.45
1:B:593:GLY:HA3	1:B:610:LEU:HD13	1.97	0.45
1:B:229:TYR:HE2	1:B:255:MET:CG	2.30	0.45
1:A:276:HIS:HB2	1:A:314:THR:HB	1.99	0.45
1:A:321:TRP:NE1	1:A:381:ASP:OD2	2.50	0.44
1:A:119:ARG:HH21	1:A:615:ASN:ND2	2.16	0.44
1:A:133:ASN:HD21	1:A:289:GLU:HG2	1.83	0.44
1:B:501:PRO:HB2	1:B:505:TRP:CZ3	2.52	0.44
1:B:258:ASN:HB2	3:B:2119:HOH:O	2.18	0.44
1:B:214:ARG:O	1:B:215:ASP:C	2.56	0.44
1:B:107:TRP:CZ3	1:B:229:TYR:CE1	2.94	0.44
1:B:414:LYS:O	1:B:418:ARG:HG2	2.18	0.44
1:B:559:ALA:HB2	1:B:652:SER:OG	2.18	0.43
1:B:688:LYS:HG3	1:B:689:TRP:CE2	2.53	0.43
1:A:319:VAL:HG22	1:A:376:THR:HB	2.00	0.43
1:B:324:THR:O	3:B:2142:HOH:O	2.20	0.43
1:B:275:THR:HG22	2:B:1741:HEM:HAA2	2.01	0.43
1:A:181:PHE:CE2	1:A:432:PRO:CG	3.01	0.43
1:A:502:GLN:HG2	1:A:505:TRP:CZ3	2.54	0.43
1:A:418:ARG:CA	1:A:418:ARG:HE	2.32	0.43
1:A:46:LYS:HG2	1:A:49:HIS:CE1	2.53	0.43
1:B:280:PRO:HB2	1:B:282:ASP:OD2	2.19	0.43
1:A:388:PRO:O	1:A:392:ARG:HG3	2.18	0.43
1:A:274:LYS:HE3	1:A:367:PRO:HG3	2.01	0.43
1:A:279:GLY:O	1:A:348:ALA:HB2	2.18	0.43
1:B:341:TRP:HB2	1:B:382:LEU:HD21	2.01	0.43
1:B:493:ASN:ND2	1:B:572:THR:H	2.16	0.43
1:B:229:TYR:OH	1:B:255:MET:SD	2.74	0.42
1:B:235:PRO:HB3	3:B:2094:HOH:O	2.19	0.42
1:A:528:PHE:O	1:A:532:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:HH21	1:A:615:ASN:HD22	1.66	0.42
1:B:624:MET:O	1:B:628:VAL:HG23	2.19	0.42
1:B:387:ASP:O	1:B:391:GLU:HB2	2.19	0.42
1:B:505:TRP:CE3	1:B:505:TRP:HA	2.54	0.42
1:B:505:TRP:HE3	1:B:505:TRP:HA	1.85	0.42
1:A:207:ASP:HB2	1:A:224:GLN:HG2	2.02	0.42
1:A:552:ILE:HD13	1:A:724:PHE:HE2	1.85	0.42
1:B:263:ALA:O	1:B:267:VAL:HG23	2.20	0.42
1:B:343:LEU:HD11	1:B:351:TRP:CE3	2.54	0.42
1:B:317:ILE:HG23	1:B:352:GLN:HE21	1.84	0.42
1:B:431:VAL:HA	1:B:432:PRO:HD3	1.91	0.42
1:B:458:LEU:HD22	1:B:543:LEU:HD11	2.01	0.41
1:A:593:GLY:HA3	1:A:610:LEU:HD13	2.00	0.41
1:A:610:LEU:HD22	1:A:694:VAL:HG13	2.02	0.41
1:B:606:ALA:HB1	1:B:694:VAL:HG23	2.02	0.41
1:A:296:MET:HE1	1:B:696:LEU:HB3	2.02	0.41
1:A:387:ASP:HA	1:A:388:PRO:HD2	1.82	0.41
1:B:646:PHE:HE2	1:B:661:LEU:HD13	1.85	0.41
1:A:139:ALA:HA	1:A:300:TRP:CZ3	2.55	0.41
1:A:505:TRP:CE2	1:A:588:GLU:HB2	2.56	0.41
1:A:123:GLY:O	1:A:187:ARG:HB3	2.21	0.41
1:A:422:PRO:HG3	3:A:2220:HOH:O	2.20	0.41
1:A:726:ALA:HB1	3:A:2324:HOH:O	2.20	0.41
1:A:447:HIS:CD2	1:A:537:LYS:HG3	2.55	0.41
1:A:346:SER:HB3	1:A:352:GLN:NE2	2.35	0.41
1:B:475:THR:HG22	1:B:544:VAL:HG13	2.02	0.41
1:B:580:ASP:HB3	1:B:583:SER:HB3	2.03	0.41
1:A:176:MET:HB2	1:A:176:MET:HE3	1.86	0.41
1:B:646:PHE:HB2	1:B:657:PHE:HA	2.02	0.41
1:B:322:THR:HB	1:B:331:SER:OG	2.21	0.41
1:A:131:PRO:HD3	1:B:35:ASN:HD21	1.86	0.41
1:B:360:GLY:O	1:B:375:PRO:HD3	2.21	0.41
1:B:588:GLU:HA	1:B:589:PRO:HD3	1.94	0.41
1:B:61:ALA:HB3	3:B:2019:HOH:O	2.21	0.41
1:A:119:ARG:HD3	1:A:196:VAL:HG22	2.02	0.41
1:B:239:PRO:HG3	1:B:351:TRP:CD1	2.56	0.41
1:B:346:SER:OG	1:B:350:ALA:HB3	2.20	0.41
1:B:549:CYS:HA	1:B:552:ILE:HG22	2.02	0.41
1:B:562:ASN:HD22	1:B:562:ASN:HA	1.66	0.41
1:B:388:PRO:HG2	3:B:2161:HOH:O	2.20	0.40
1:B:38:TRP:HB2	1:B:39:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:HG2	1:B:49:HIS:CE1	2.56	0.40
1:B:626:VAL:HG23	1:B:720:PHE:HD1	1.86	0.40
1:B:71:ILE:HG21	1:B:71:ILE:HD13	1.88	0.40
1:A:39:TRP:HB2	1:A:42:ARG:HD2	2.04	0.40
1:A:93:ALA:HB2	1:A:98:TYR:CZ	2.57	0.40
2:B:1741:HEM:HBB2	2:B:1741:HEM:CMB	2.52	0.40
1:B:481:SER:HA	1:B:617:LEU:HD21	2.03	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	713/740 (96%)	681 (96%)	30 (4%)	2 (0%)	44	44
1	B	713/740 (96%)	684 (96%)	25 (4%)	4 (1%)	28	24
All	All	1426/1480 (96%)	1365 (96%)	55 (4%)	6 (0%)	38	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	534	GLY
1	A	674	ASP
1	B	370	GLY
1	A	424	ALA
1	B	674	ASP
1	B	533	PRO

### 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	564/584 (97%)	543 (96%)	21 (4%)	39	39
1	B	564/584 (97%)	526 (93%)	38 (7%)	19	15
All	All	1128/1168 (97%)	1069 (95%)	59 (5%)	27	24

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	107	TRP
1	A	114	ARG
1	A	133	ASN
1	A	137	ASP
1	A	194	ASP
1	A	200	LYS
1	A	258	ASN
1	A	267	VAL
1	A	272	PHE
1	A	293	LEU
1	A	310	LYS
1	A	327	LYS
1	A	391	GLU
1	A	418	ARG
1	A	538	VAL
1	A	543	LEU
1	A	626	VAL
1	A	651	GLU
1	A	669	GLU
1	A	690	THR
1	B	36	GLN
1	B	117	ASP
1	B	170	ASN
1	B	195	GLU
1	B	203	THR
1	B	258	ASN

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Mol	Chain	Res	Type
1	B	302	SER
1	B	313	ILE
1	B	323	ASN
1	B	329	ASP
1	B	330	ASN
1	B	373	ARG
1	B	380	THR
1	B	391	GLU
1	B	395	ARG
1	B	418	ARG
1	B	423	VAL
1	B	433	LYS
1	B	435	THR
1	B	447	HIS
1	B	449	LEU
1	B	459	LYS
1	B	460	SER
1	B	493	ASN
1	B	505	TRP
1	B	552	ILE
1	B	557	LYS
1	B	562	ASN
1	B	568	THR
1	B	596	ASN
1	B	627	LEU
1	B	640	ARG
1	B	655	ASN
1	B	669	GLU
1	B	675	ASP
1	B	686	LYS
1	B	690	THR
1	B	708	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	51	ASN
1	A	133	ASN
1	A	218	ASN
1	A	258	ASN
1	A	330	ASN

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Mol	Chain	Res	Type
1	A	352	GLN
1	A	434	GLN
1	A	508	ASN
1	A	535	ASN
1	A	561	HIS
1	A	562	ASN
1	A	602	ASN
1	A	615	ASN
1	A	701	ASN
1	A	722	GLN
1	B	35	ASN
1	B	36	GLN
1	B	50	GLN
1	B	51	ASN
1	B	116	HIS
1	B	170	ASN
1	B	258	ASN
1	B	323	ASN
1	B	330	ASN
1	B	352	GLN
1	B	434	GLN
1	B	439	GLN
1	B	493	ASN
1	B	500	GLN
1	B	525	GLN
1	B	562	ASN
1	B	596	ASN
1	B	655	ASN
1	B	701	ASN

### 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	1741	1	28,50,50	2.27	8 (28%)	17,82,82	1.34	3 (17%)
2	HEM	B	1741	1	28,50,50	2.11	6 (21%)	17,82,82	2.01	4 (23%)

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	1741	1	-	0/6/54/54	0/0/8/8
2	HEM	B	1741	1	-	0/6/54/54	0/0/8/8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1741	HEM	C3C-C2C	-4.34	1.34	1.40
2	A	1741	HEM	C3B-C2B	-4.29	1.34	1.40
2	B	1741	HEM	C3C-C2C	-3.51	1.35	1.40
2	B	1741	HEM	C3B-C2B	-3.17	1.36	1.40
2	A	1741	HEM	CAD-C3D	2.13	1.56	1.52
2	A	1741	HEM	CMC-C2C	2.26	1.56	1.51
2	A	1741	HEM	C4D-ND	2.51	1.39	1.36
2	B	1741	HEM	C1C-NC	3.14	1.40	1.36
2	B	1741	HEM	C3B-CAB	3.78	1.55	1.47
2	A	1741	HEM	C3B-CAB	3.89	1.55	1.47
2	B	1741	HEM	C3C-CAC	4.02	1.55	1.47
2	A	1741	HEM	C3C-CAC	4.42	1.56	1.47
2	A	1741	HEM	C3D-C2D	5.05	1.52	1.37
2	B	1741	HEM	C3D-C2D	5.40	1.53	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1741	HEM	CAA-CBA-CGA	-4.39	105.16	112.66
2	B	1741	HEM	CMA-C3A-C4A	-3.08	123.72	128.46
2	A	1741	HEM	CAA-CBA-CGA	-2.65	108.13	112.66
2	A	1741	HEM	CMA-C3A-C4A	-2.22	125.05	128.46
2	A	1741	HEM	CMC-C2C-C3C	2.50	129.52	124.89
2	B	1741	HEM	CMB-C2B-C3B	3.03	130.52	124.89
2	B	1741	HEM	CMC-C2C-C3C	3.31	131.04	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1741	HEM	5	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

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	715/740 (96%)	0.66	34 (4%) 31 37	7, 19, 31, 38	0
1	B	715/740 (96%)	0.81	50 (6%) 17 22	8, 20, 34, 40	0
All	All	1430/1480 (96%)	0.73	84 (5%) 23 29	7, 20, 33, 40	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	531	ALA	7.4
1	B	533	PRO	6.9
1	B	532	ALA	5.3
1	A	369	GLY	4.5
1	B	673	ALA	4.4
1	A	510	PRO	3.8
1	B	212	GLY	3.7
1	B	505	TRP	3.7
1	B	582	GLU	3.6
1	B	650	SER	3.5
1	A	533	PRO	3.3
1	A	684	SER	3.2
1	B	79	ASP	3.2
1	B	672	PRO	3.2
1	A	79	ASP	3.2
1	A	534	GLY	3.2
1	B	511	ASP	3.1
1	A	370	GLY	2.9
1	B	598	LEU	2.9
1	A	433	LYS	2.9
1	B	48	LEU	2.9
1	B	306	THR	2.8
1	A	674	ASP	2.8
1	A	683	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	515	ARG	2.8
1	B	447	HIS	2.8
1	A	351	TRP	2.7
1	A	80	ILE	2.7
1	B	237	GLY	2.7
1	B	674	ASP	2.7
1	B	213	LYS	2.7
1	B	685	GLY	2.7
1	A	205	LEU	2.6
1	B	469	VAL	2.6
1	B	448	ASP	2.6
1	A	282	ASP	2.5
1	B	513	ASP	2.5
1	B	530	SER	2.5
1	A	435	THR	2.5
1	B	355	ALA	2.5
1	B	682	ASP	2.5
1	B	370	GLY	2.5
1	A	559	ALA	2.5
1	B	215	ASP	2.4
1	A	222	ALA	2.4
1	B	534	GLY	2.4
1	B	599	GLY	2.4
1	B	214	ARG	2.4
1	B	467	LEU	2.4
1	A	672	PRO	2.4
1	A	60	ALA	2.4
1	B	552	ILE	2.4
1	B	395	ARG	2.3
1	B	574	ALA	2.3
1	B	333	LEU	2.3
1	B	651	GLU	2.3
1	B	357	ASP	2.3
1	A	446	SER	2.3
1	A	284	VAL	2.3
1	B	600	LYS	2.3
1	A	362	GLY	2.3
1	A	164	LEU	2.3
1	A	653	LEU	2.2
1	B	332	PHE	2.2
1	B	510	PRO	2.2
1	A	526	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	669	GLU	2.2
1	A	514	LEU	2.2
1	A	40	PRO	2.2
1	A	691	GLY	2.1
1	B	266	ILE	2.1
1	B	338	GLY	2.1
1	A	290	ALA	2.1
1	A	577	GLU	2.1
1	B	445	VAL	2.1
1	B	321	TRP	2.1
1	B	80	ILE	2.1
1	B	546	LEU	2.0
1	B	687	VAL	2.0
1	B	218	ASN	2.0
1	B	524	ILE	2.0
1	A	563	ILE	2.0
1	A	316	GLY	2.0
1	B	683	GLY	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
2	HEM	B	1741	43/43	0.95	0.14	-0.70	3,7,10,15	0
2	HEM	A	1741	43/43	0.96	0.14	-1.05	2,7,10,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.