



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:44 am GMT

PDB ID : 4BFL  
Title : Structure of natively expressed catalase HPII  
Authors : Gabrielsen, M.; Schuttelkopf, A.W.  
Deposited on : 2013-03-19  
Resolution : 1.64 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

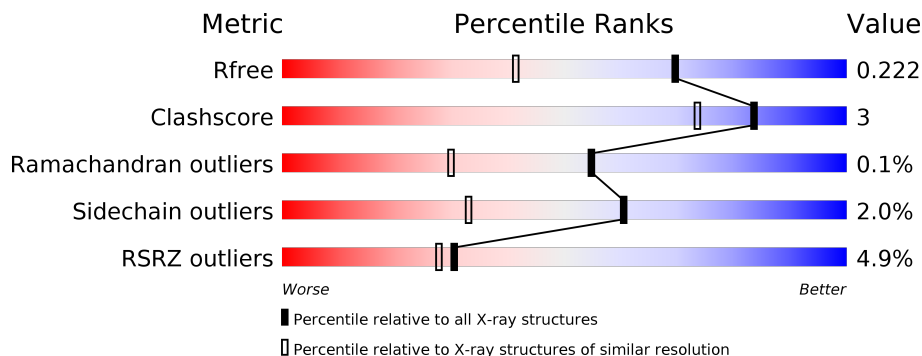
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.64 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	2211 (1.66-1.62)
Clashscore	112137	2356 (1.66-1.62)
Ramachandran outliers	110173	2315 (1.66-1.62)
Sidechain outliers	110143	2315 (1.66-1.62)
RSRZ outliers	101464	2219 (1.66-1.62)

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	753	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> <div>•</div> </div>
1	B	753	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> <div>•</div> </div>
1	C	753	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> <div>••</div> </div>
1	D	753	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>8%</div> </div> <div>•</div> </div>

## 2 Entry composition [i](#)

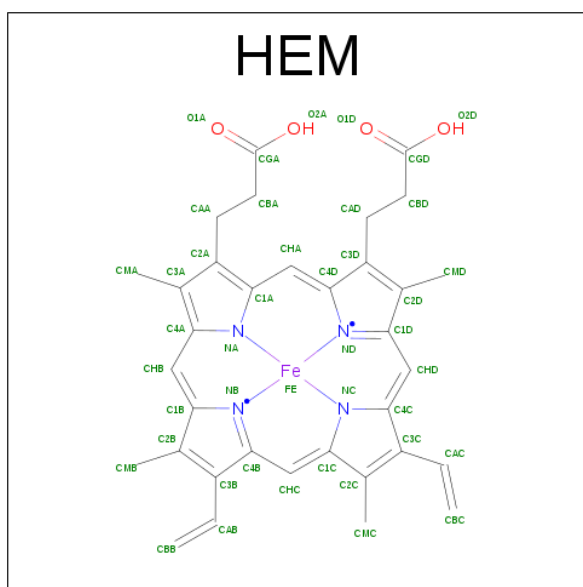
There are 4 unique types of molecules in this entry. The entry contains 25666 atoms, of which 18 are hydrogens and 0 are deuteriums.

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 CATALASE HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	744	Total	C	N	O	S	0	3	0
			5889	3733	1033	1110	13			
1	B	745	Total	C	N	O	S	0	3	0
			5899	3741	1036	1109	13			
1	C	743	Total	C	N	O	S	0	4	0
			5895	3736	1034	1112	13			
1	D	735	Total	C	N	O	S	0	1	0
			5807	3683	1016	1095	13			

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



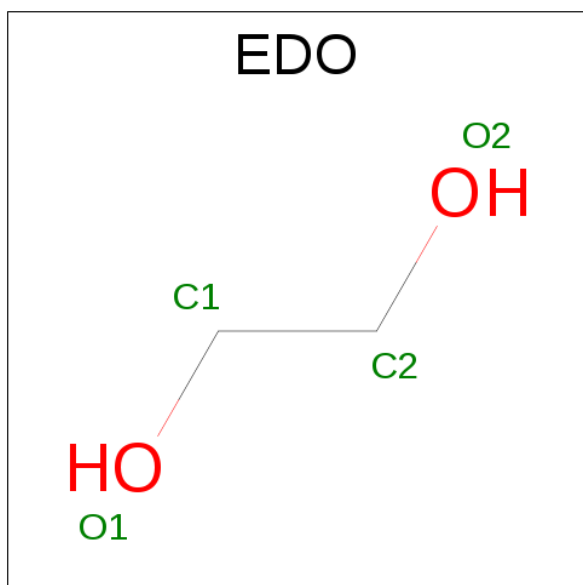
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		

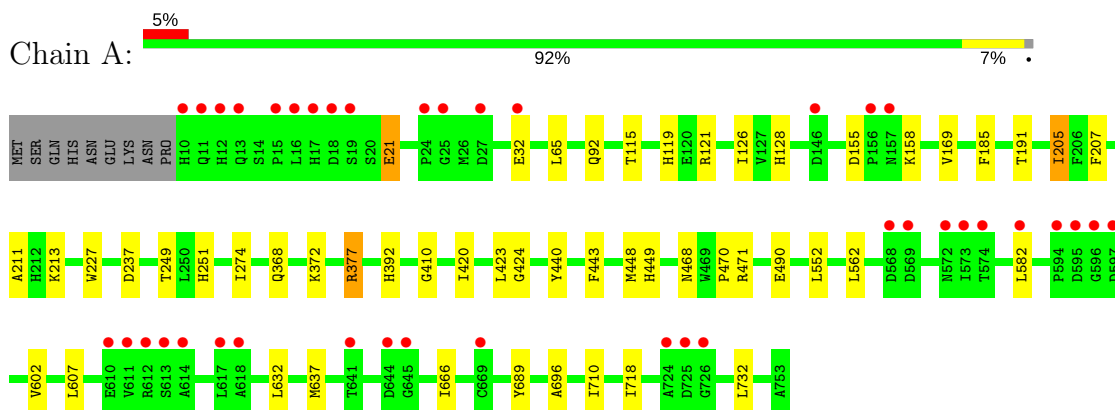
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	588	Total	O	0	0
			588	588		
4	B	572	Total	O	0	0
			572	572		
4	C	437	Total	O	0	0
			437	437		
4	D	377	Total	O	0	0
			377	377		

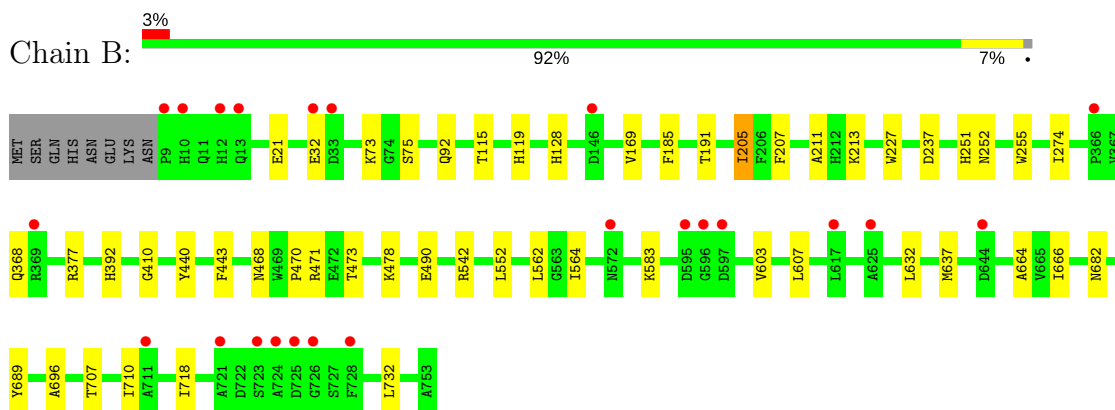
### 3 Residue-property plots [i](#)

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.

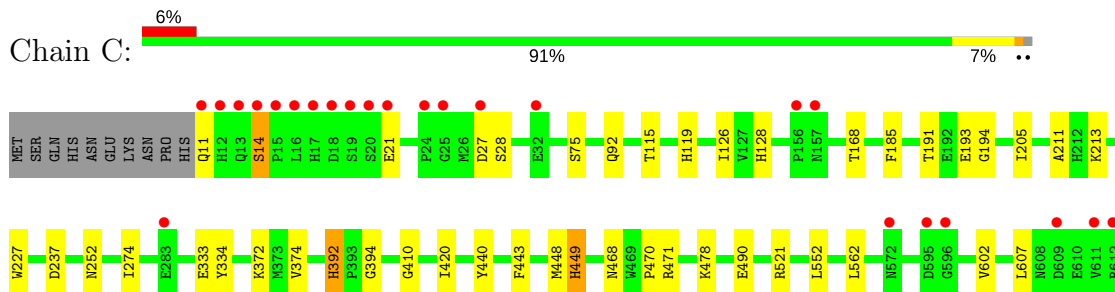
#### • Molecule 1: CATALASE HP11

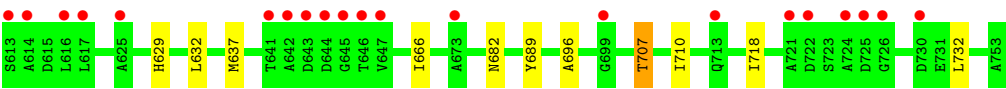


#### • Molecule 1: CATALASE HP11

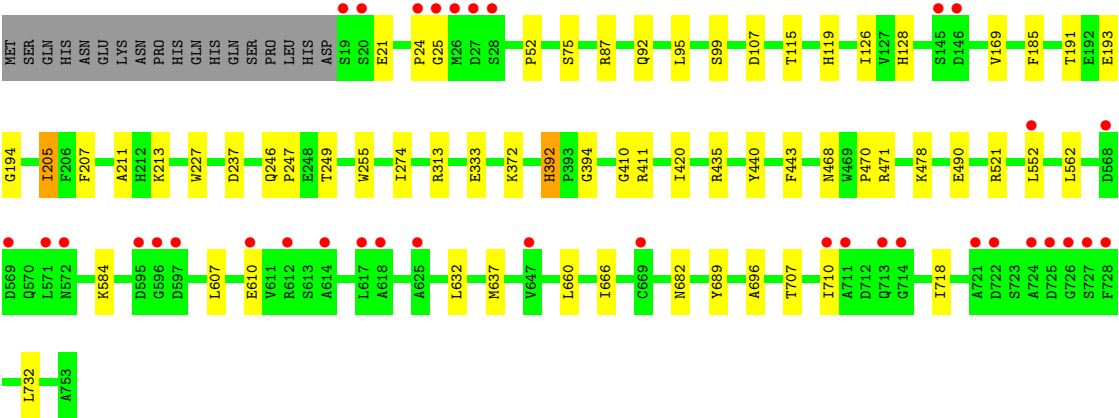
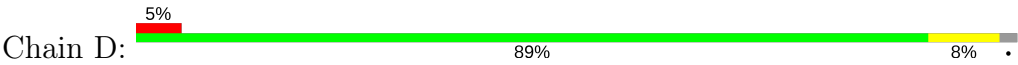


#### • Molecule 1: CATALASE HP11





● Molecule 1: CATALASE HP11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.40Å 171.67Å 123.21Å 90.00° 104.67° 90.00°	Depositor
Resolution (Å)	48.95 – 1.64 48.95 – 1.64	Depositor EDS
% Data completeness (in resolution range)	80.8 (48.95-1.64) 81.0 (48.95-1.64)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.64Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.174 , 0.202 0.192 , 0.222	Depositor DCC
$R_{free}$ test set	14725 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtriage
Anisotropy	1.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	25666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, EDO

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	0.46	0/6054	0.62	0/8231
1	B	0.46	0/6065	0.61	0/8247
1	C	0.47	0/6056	0.62	0/8232
1	D	0.46	0/5965	0.62	0/8109
All	All	0.46	0/24140	0.62	0/32819

There are no bond length outliers.

There are no bond angle outliers.

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	5889	0	5694	42	0
1	B	5899	0	5718	27	0
1	C	5895	0	5704	45	0
1	D	5807	0	5627	41	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	B	8	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4	6	6	0	0
4	A	588	0	0	2	0
4	B	572	0	0	0	0
4	C	437	0	0	2	0
4	D	377	0	0	4	0
All	All	25648	18	22881	130	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 (130) 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:449[B]:HIS:CE1	1:C:449[B]:HIS:CE1	2.39	1.10
1:A:21:GLU:HG3	1:D:247:PRO:HD2	1.57	0.86
1:C:448:MET:HG3	1:C:449[B]:HIS:ND1	1.91	0.86
1:B:682:ASN:OD1	1:B:707:THR:HG21	1.79	0.83
1:D:682:ASN:OD1	1:D:707:THR:HG21	1.79	0.80
1:D:191:THR:HB	1:D:194:GLY:O	1.80	0.80
1:D:191:THR:HG21	4:D:2095:HOH:O	1.82	0.78
1:C:448:MET:HG3	1:C:449[B]:HIS:CE1	2.18	0.78
1:D:191:THR:HG22	1:D:193:GLU:H	1.49	0.77
1:A:449[B]:HIS:CE1	1:C:449[B]:HIS:ND1	2.52	0.76
1:A:65:LEU:HD21	1:A:377[A]:ARG:NH1	2.04	0.73
1:C:191:THR:HB	1:C:194:GLY:O	1.89	0.73
1:A:65:LEU:CD2	1:A:377[A]:ARG:NH1	2.55	0.70
1:A:65:LEU:HD21	1:A:377[A]:ARG:HH12	1.59	0.67
1:C:710:ILE:HD13	1:C:718:ILE:HG13	1.77	0.66
1:C:27:ASP:CG	1:C:28:SER:H	1.99	0.66
1:A:710:ILE:HD13	1:A:718:ILE:HG13	1.77	0.66
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.78	0.66
1:D:710:ILE:HD13	1:D:718:ILE:HG13	1.78	0.66
1:A:424:GLY:HA3	1:C:449[B]:HIS:HE1	1.64	0.62
1:A:274:ILE:HD12	2:A:1754:HEM:HMB1	1.82	0.62
1:B:542:ARG:HG2	1:C:14:SER:H	1.68	0.58
1:A:213:LYS:HD3	1:D:92:GLN:HA	1.85	0.58
1:C:666:ILE:HD11	1:C:732:LEU:HD22	1.87	0.57
1:A:92:GLN:HA	1:D:213:LYS:HD3	1.86	0.57
1:A:449[B]:HIS:ND1	1:C:449[B]:HIS:CE1	2.72	0.57
1:B:666:ILE:HD11	1:B:732:LEU:HD22	1.87	0.56
1:B:92:GLN:HA	1:C:213:LYS:HD3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ILE:HD12	2:C:1754:HEM:HMB1	1.88	0.56
1:B:689:TYR:CE1	1:B:710:ILE:HD11	2.41	0.56
1:D:666:ILE:HD11	1:D:732:LEU:HD22	1.88	0.56
1:A:423:LEU:O	1:C:449[B]:HIS:NE2	2.38	0.56
1:D:205:ILE:HD11	1:D:255:TRP:CD1	2.41	0.56
1:A:666:ILE:HD11	1:A:732:LEU:HD22	1.89	0.55
1:A:689:TYR:CE1	1:A:710:ILE:HD11	2.41	0.55
1:D:392:HIS:HD1	1:D:394:GLY:H	1.55	0.55
1:D:689:TYR:CE1	1:D:710:ILE:HD11	2.42	0.55
1:C:689:TYR:CE1	1:C:710:ILE:HD11	2.42	0.55
1:B:213:LYS:HD3	1:C:92:GLN:HA	1.88	0.55
1:C:126:ILE:CG2	2:C:1754:HEM:HMD1	2.37	0.54
1:A:65:LEU:CD2	1:A:377[A]:ARG:HH12	2.19	0.53
1:C:490:GLU:HG2	1:D:490:GLU:HG2	1.90	0.53
1:B:603[B]:VAL:HG12	1:B:664:ALA:HB3	1.91	0.53
1:A:710:ILE:CD1	1:A:718:ILE:HG13	2.40	0.52
1:A:562:LEU:HA	1:D:637:MET:HB2	1.92	0.52
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.44	0.52
1:A:448:MET:HG3	1:A:449[B]:HIS:CE1	2.45	0.52
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.92	0.51
1:C:710:ILE:CD1	1:C:718:ILE:HG13	2.40	0.51
1:C:602:VAL:HG22	1:C:629:HIS:HB2	1.91	0.51
1:D:126:ILE:CG2	2:D:1754:HEM:HMD1	2.41	0.51
1:D:710:ILE:CD1	1:D:718:ILE:HG13	2.40	0.51
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.41	0.50
1:C:128:HIS:HA	1:C:168:THR:O	2.11	0.50
1:A:423:LEU:O	1:C:449[B]:HIS:CE1	2.64	0.50
1:A:65:LEU:HD22	1:A:377[A]:ARG:NH1	2.26	0.50
1:D:607:LEU:HD11	1:D:632:LEU:HB3	1.94	0.50
1:B:607:LEU:HD11	1:B:632:LEU:HB3	1.94	0.50
1:A:449[B]:HIS:HE1	1:C:449[B]:HIS:CE1	2.21	0.49
1:C:191:THR:HG22	1:C:193:GLU:H	1.78	0.49
1:A:637:MET:HB2	1:D:562:LEU:HA	1.96	0.48
1:B:689:TYR:HE1	1:B:710:ILE:HD11	1.78	0.48
1:C:372[B]:LYS:HE2	1:C:374:VAL:CG2	2.44	0.48
1:A:696:ALA:HB2	1:A:732:LEU:HD13	1.96	0.48
1:C:392:HIS:HD1	1:C:394:GLY:H	1.61	0.48
1:B:637:MET:HB2	1:C:562:LEU:HA	1.95	0.47
1:B:473:THR:HG21	1:D:87:ARG:HH11	1.79	0.47
1:D:696:ALA:HB2	1:D:732:LEU:HD13	1.97	0.47
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.96	0.47
2:C:1754:HEM:CMC	2:C:1754:HEM:HBC2	2.46	0.46
1:D:191:THR:CG2	4:D:2095:HOH:O	2.53	0.46
1:B:468:ASN:O	1:B:471:ARG:HG3	2.16	0.46
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.98	0.46
1:C:468:ASN:O	1:C:471:ARG:HG3	2.16	0.46
1:C:696:ALA:HB2	1:C:732:LEU:HD13	1.98	0.46
1:B:115:THR:O	1:B:119:HIS:HD2	1.99	0.45
1:B:696:ALA:HB2	1:B:732:LEU:HD13	1.97	0.45
1:C:191:THR:HG21	4:C:2107:HOH:O	2.16	0.45
1:C:689:TYR:HE1	1:C:710:ILE:HD11	1.81	0.45
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.47	0.45
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.47	0.45
1:B:562:LEU:HA	1:C:637:MET:HB2	1.98	0.45
1:D:115:THR:O	1:D:119:HIS:HD2	1.99	0.45
1:C:115:THR:O	1:C:119:HIS:HD2	2.00	0.45
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.52	0.45
1:D:24:PRO:HA	1:D:25:GLY:HA2	1.85	0.45
1:D:468:ASN:O	1:D:471:ARG:HG3	2.16	0.45
1:C:607:LEU:HD11	1:C:632:LEU:HB3	1.99	0.44
1:D:274:ILE:HD12	2:D:1754:HEM:HMB1	1.99	0.44
1:A:155:ASP:HB3	1:A:158:LYS:HG3	1.98	0.44
1:A:689:TYR:HE1	1:A:710:ILE:HD11	1.79	0.44
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.52	0.44
1:C:682:ASN:HB3	1:C:707:THR:HG21	1.98	0.44
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.53	0.44
1:A:115:THR:O	1:A:119:HIS:HD2	2.01	0.44
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.48	0.43
1:C:205:ILE:HD11	1:C:252:ASN:N	2.32	0.43
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.53	0.43
1:A:468:ASN:O	1:A:471:ARG:HG3	2.18	0.43
1:B:274:ILE:HD12	2:B:1754:HEM:HMB1	1.99	0.43
1:C:191:THR:CG2	4:C:2107:HOH:O	2.66	0.43
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.43
1:A:420:ILE:HG21	1:C:119:HIS:CE1	2.54	0.42
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.54	0.42
4:A:2253:HOH:O	1:D:52:PRO:HG3	2.20	0.42
1:A:121:ARG:CZ	1:D:126:ILE:HD12	2.49	0.42
1:D:689:TYR:HE1	1:D:710:ILE:HD11	1.81	0.42
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.50	0.42
1:B:205:ILE:HD13	1:B:251:HIS:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:GLU:HB3	1:D:372:LYS:CE	2.50	0.41
1:C:334:TYR:N	1:C:372[A]:LYS:HZ1	2.19	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.41
1:D:435:ARG:HD3	4:D:2231:HOH:O	2.18	0.41
1:D:584:LYS:HD2	4:D:2315:HOH:O	2.21	0.41
1:A:602:VAL:HG21	4:A:2127:HOH:O	2.21	0.41
1:C:333:GLU:HB3	1:C:372[A]:LYS:NZ	2.35	0.41
1:D:333:GLU:HB3	1:D:372:LYS:HE3	2.02	0.41
1:A:205:ILE:HD13	1:A:251:HIS:CG	2.55	0.41
1:B:564:ILE:HG23	1:C:11:GLN:HG3	2.01	0.41
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.55	0.41
1:B:207:PHE:CD1	1:B:252:ASN:HB3	2.56	0.41
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.56	0.41
1:D:95:LEU:HB3	1:D:107:ASP:HB2	2.03	0.41
1:C:372[B]:LYS:HE2	1:C:374:VAL:HG23	2.03	0.41
1:A:126:ILE:CG2	2:A:1754:HEM:HMD1	2.51	0.40
1:A:21:GLU:HG3	1:D:246:GLN:HA	2.03	0.40
1:A:372:LYS:HE2	1:A:372:LYS:HB3	1.97	0.40
1:B:205:ILE:HD11	1:B:255:TRP:CD1	2.57	0.40
1:D:411:ARG:HG2	2:D:1754:HEM:C2C	2.56	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	745/753 (99%)	725 (97%)	20 (3%)	0	100	100
1	B	746/753 (99%)	724 (97%)	21 (3%)	1 (0%)	55	30
1	C	745/753 (99%)	725 (97%)	18 (2%)	2 (0%)	44	22
1	D	734/753 (98%)	717 (98%)	16 (2%)	1 (0%)	55	30
All	All	2970/3012 (99%)	2891 (97%)	75 (2%)	4 (0%)	55	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	SER
1	B	75	SER
1	C	75	SER
1	D	75	SER

### 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	627/636 (99%)	613 (98%)	14 (2%)	57	28
1	B	630/636 (99%)	615 (98%)	15 (2%)	54	24
1	C	628/636 (99%)	616 (98%)	12 (2%)	62	36
1	D	618/636 (97%)	606 (98%)	12 (2%)	62	36
All	All	2503/2544 (98%)	2450 (98%)	53 (2%)	60	30

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	A	32	GLU
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	368	GLN
1	A	377[A]	ARG
1	A	377[B]	ARG
1	A	392	HIS
1	A	440	TYR
1	A	552	LEU
1	A	582	LEU
1	B	21	GLU
1	B	32	GLU

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Mol	Chain	Res	Type
1	B	73	LYS
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	368	GLN
1	B	377	ARG
1	B	392	HIS
1	B	440	TYR
1	B	478	LYS
1	B	552	LEU
1	B	583	LYS
1	C	21	GLU
1	C	185	PHE
1	C	227	TRP
1	C	237	ASP
1	C	392	HIS
1	C	440	TYR
1	C	449[A]	HIS
1	C	449[B]	HIS
1	C	478	LYS
1	C	521	ARG
1	C	552	LEU
1	C	707	THR
1	D	21	GLU
1	D	99	SER
1	D	185	PHE
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	392	HIS
1	D	440	TYR
1	D	478	LYS
1	D	521	ARG
1	D	552	LEU
1	D	610	GLU

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

### 5.3.3 RNA [i](#)

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](#)

7 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	1754	1	28,50,50	2.09	6 (21%)	17,82,82	2.36	6 (35%)
2	HEM	B	1754	1	28,50,50	1.52	4 (14%)	17,82,82	2.38	7 (41%)
3	EDO	B	1755	-	3,3,3	0.87	0	2,2,2	0.36	0
3	EDO	B	1756	-	3,3,3	0.48	0	2,2,2	0.06	0
2	HEM	C	1754	1	28,50,50	1.75	6 (21%)	17,82,82	2.47	6 (35%)
3	EDO	C	1755	-	3,3,3	0.60	0	2,2,2	0.49	0
2	HEM	D	1754	1	28,50,50	1.85	5 (17%)	17,82,82	2.25	6 (35%)

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	1754	1	-	0/6/54/54	0/0/8/8
2	HEM	B	1754	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1755	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1756	-	-	0/1/1/1	0/0/0/0
2	HEM	C	1754	1	-	0/6/54/54	0/0/8/8
3	EDO	C	1755	-	-	0/1/1/1	0/0/0/0
2	HEM	D	1754	1	-	0/6/54/54	0/0/8/8

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1754	HEM	C3B-C2B	-5.34	1.33	1.40
2	D	1754	HEM	CAA-C2A	-3.89	1.45	1.52
2	C	1754	HEM	C3B-C2B	-2.93	1.36	1.40
2	B	1754	HEM	C4D-ND	-2.52	1.33	1.36
2	A	1754	HEM	C1B-NB	-2.46	1.33	1.36
2	A	1754	HEM	C4D-ND	-2.10	1.34	1.36
2	C	1754	HEM	C1B-NB	-2.07	1.34	1.36
2	D	1754	HEM	C1D-ND	2.04	1.40	1.36
2	C	1754	HEM	C1A-NA	2.58	1.41	1.36
2	C	1754	HEM	C3B-CAB	2.85	1.53	1.47
2	A	1754	HEM	C1A-NA	2.86	1.42	1.36
2	C	1754	HEM	C4A-NA	2.86	1.42	1.36
2	D	1754	HEM	C4C-NC	2.89	1.40	1.36
2	B	1754	HEM	C4A-NA	2.97	1.42	1.36
2	A	1754	HEM	C4C-NC	3.16	1.40	1.36
2	B	1754	HEM	C1A-NA	3.24	1.43	1.36
2	D	1754	HEM	C4A-NA	3.30	1.43	1.36
2	B	1754	HEM	C4C-NC	4.02	1.41	1.36
2	C	1754	HEM	C1C-NC	6.01	1.43	1.36
2	D	1754	HEM	C1C-NC	6.15	1.44	1.36
2	A	1754	HEM	C1C-NC	6.64	1.44	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1754	HEM	CAA-CBA-CGA	-4.84	104.39	112.66
2	C	1754	HEM	CBD-CAD-C3D	-4.83	103.26	112.47
2	B	1754	HEM	C1D-C2D-C3D	-4.67	103.75	107.00
2	C	1754	HEM	CMD-C2D-C1D	-4.59	121.41	128.46
2	A	1754	HEM	CBD-CAD-C3D	-4.56	103.78	112.47
2	D	1754	HEM	CAA-CBA-CGA	-4.45	105.05	112.66
2	D	1754	HEM	CBD-CAD-C3D	-4.27	104.32	112.47
2	A	1754	HEM	CMD-C2D-C1D	-3.93	122.43	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1754	HEM	C4A-C3A-C2A	-3.82	104.34	107.00
2	B	1754	HEM	CAA-CBA-CGA	-3.78	106.20	112.66
2	C	1754	HEM	CAA-CBA-CGA	-3.50	106.69	112.66
2	B	1754	HEM	CBD-CAD-C3D	-2.82	107.08	112.47
2	C	1754	HEM	CAD-CBD-CGD	-2.26	108.81	112.66
2	B	1754	HEM	CMD-C2D-C1D	-2.18	125.12	128.46
2	D	1754	HEM	C3B-C4B-NB	2.02	111.82	109.21
2	A	1754	HEM	CMC-C2C-C3C	2.11	128.81	124.89
2	D	1754	HEM	CBA-CAA-C2A	2.28	116.84	112.48
2	A	1754	HEM	CMD-C2D-C3D	2.77	130.17	124.94
2	A	1754	HEM	CMB-C2B-C3B	3.21	130.85	124.89
2	B	1754	HEM	CMD-C2D-C3D	3.28	131.12	124.94
2	B	1754	HEM	C3B-C4B-NB	3.33	113.51	109.21
2	D	1754	HEM	CMB-C2B-C3B	3.39	131.18	124.89
2	B	1754	HEM	CMB-C2B-C3B	3.73	131.81	124.89
2	C	1754	HEM	CMD-C2D-C3D	3.88	132.25	124.94
2	C	1754	HEM	CMB-C2B-C3B	4.17	132.63	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1754	HEM	2	0
2	B	1754	HEM	1	0
2	C	1754	HEM	3	0
2	D	1754	HEM	3	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 ⓘ

### 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	744/753 (98%)	0.14	40 (5%)	26	24	13, 27, 50, 70	0
1	B	745/753 (98%)	0.10	23 (3%)	49	49	12, 26, 48, 65	0
1	C	743/753 (98%)	0.14	45 (6%)	22	19	12, 24, 48, 72	0
1	D	735/753 (97%)	0.17	36 (4%)	30	28	13, 26, 50, 68	0
All	All	2967/3012 (98%)	0.14	144 (4%)	30	28	12, 26, 49, 72	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	7.9
1	C	25	GLY	6.1
1	D	726	GLY	6.1
1	B	726	GLY	5.9
1	A	726	GLY	5.8
1	A	596	GLY	5.7
1	D	724	ALA	5.2
1	A	10	HIS	4.9
1	D	27	ASP	4.8
1	D	725	ASP	4.8
1	C	24	PRO	4.7
1	C	724	ALA	4.5
1	C	15	PRO	4.5
1	D	625	ALA	4.4
1	C	27	ASP	4.4
1	C	13	GLN	4.4
1	C	17	HIS	4.3
1	C	11	GLN	4.3
1	B	595	ASP	4.3
1	A	11	GLN	4.3
1	A	12	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	18	ASP	4.2
1	C	614	ALA	4.1
1	A	595	ASP	3.9
1	B	10	HIS	3.8
1	D	571	LEU	3.8
1	A	15	PRO	3.8
1	D	24	PRO	3.8
1	A	582	LEU	3.7
1	C	14	SER	3.7
1	C	611	VAL	3.7
1	B	721	ALA	3.5
1	D	617	LEU	3.5
1	C	595	ASP	3.5
1	C	19	SER	3.5
1	C	20	SER	3.4
1	A	611	VAL	3.3
1	D	569	ASP	3.3
1	B	723	SER	3.3
1	C	596	GLY	3.3
1	C	645	GLY	3.3
1	A	569	ASP	3.2
1	B	725	ASP	3.2
1	C	612	ARG	3.2
1	A	16	LEU	3.2
1	D	618	ALA	3.1
1	D	722	ASP	3.1
1	D	25	GLY	3.1
1	C	647	VAL	3.0
1	B	572	ASN	3.0
1	D	146	ASP	3.0
1	D	721	ALA	3.0
1	B	13	GLN	3.0
1	A	669	CYS	3.0
1	D	647	VAL	2.9
1	A	17	HIS	2.9
1	C	646	THR	2.9
1	D	568	ASP	2.9
1	B	596	GLY	2.9
1	D	595	ASP	2.9
1	B	625	ALA	2.9
1	B	146	ASP	2.8
1	A	13	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	613	SER	2.8
1	D	552	LEU	2.8
1	A	614	ALA	2.8
1	B	711	ALA	2.8
1	B	9	PRO	2.8
1	C	644	ASP	2.8
1	C	572	ASN	2.8
1	A	645	GLY	2.7
1	B	728	PHE	2.7
1	A	27	ASP	2.7
1	C	625	ALA	2.7
1	C	642	ALA	2.7
1	D	596	GLY	2.7
1	A	19	SER	2.7
1	A	612	ARG	2.7
1	C	643	ASP	2.7
1	A	156	PRO	2.7
1	A	574	THR	2.6
1	C	699	GLY	2.6
1	A	725	ASP	2.6
1	D	610	GLU	2.6
1	C	16	LEU	2.6
1	A	146	ASP	2.6
1	C	283	GLU	2.6
1	A	572	ASN	2.6
1	C	12	HIS	2.6
1	D	614	ALA	2.5
1	C	613	SER	2.5
1	D	145	SER	2.5
1	D	713	GLN	2.5
1	B	617	LEU	2.5
1	D	20	SER	2.5
1	D	597	ASP	2.5
1	C	21	GLU	2.5
1	B	366	PRO	2.5
1	A	157	ASN	2.5
1	C	641	THR	2.5
1	D	26	MET	2.4
1	A	597	ASP	2.4
1	C	713	GLN	2.4
1	C	725	ASP	2.4
1	A	617	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	711	ALA	2.4
1	A	594	PRO	2.4
1	D	19	SER	2.4
1	C	673	ALA	2.4
1	A	24	PRO	2.3
1	D	28	SER	2.3
1	A	618	ALA	2.3
1	A	610	GLU	2.3
1	A	25	GLY	2.3
1	C	722	ASP	2.3
1	C	609	ASP	2.2
1	A	641	THR	2.2
1	D	727	SER	2.2
1	D	612	ARG	2.2
1	A	32	GLU	2.2
1	C	156	PRO	2.2
1	A	568	ASP	2.2
1	D	728	PHE	2.1
1	D	572	ASN	2.1
1	D	669	CYS	2.1
1	A	18	ASP	2.1
1	A	644	ASP	2.1
1	B	33	ASP	2.1
1	A	573	ILE	2.1
1	D	710	ILE	2.1
1	B	369	ARG	2.1
1	C	157	ASN	2.1
1	B	32	GLU	2.1
1	B	644	ASP	2.1
1	A	724	ALA	2.1
1	C	616	LEU	2.1
1	C	617	LEU	2.1
1	C	721	ALA	2.1
1	B	597	ASP	2.1
1	C	32	GLU	2.1
1	B	12	HIS	2.1
1	B	724	ALA	2.1
1	C	730	ASP	2.1
1	D	714	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( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	1756	4/4	0.81	0.10	0.31	39,41,42,42	0
2	HEM	D	1754	43/43	0.97	0.11	0.20	11,12,15,16	0
3	EDO	C	1755	4/4	0.92	0.08	-0.23	33,34,35,35	0
2	HEM	B	1754	43/43	0.97	0.10	-0.24	11,12,15,17	0
2	HEM	C	1754	43/43	0.97	0.09	-0.42	12,13,15,16	0
3	EDO	B	1755	4/4	0.91	0.08	-0.53	19,19,20,20	0
2	HEM	A	1754	43/43	0.97	0.09	-0.78	12,13,15,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.