



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2019 – 09:45 PM EDT

PDB ID : 6HQQ  
Title : Cytochrome P450-153 from Phenyllobacterium zucineum  
Authors : Fiorentini, F.; Mattevi, A.  
Deposited on : 2018-09-25  
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

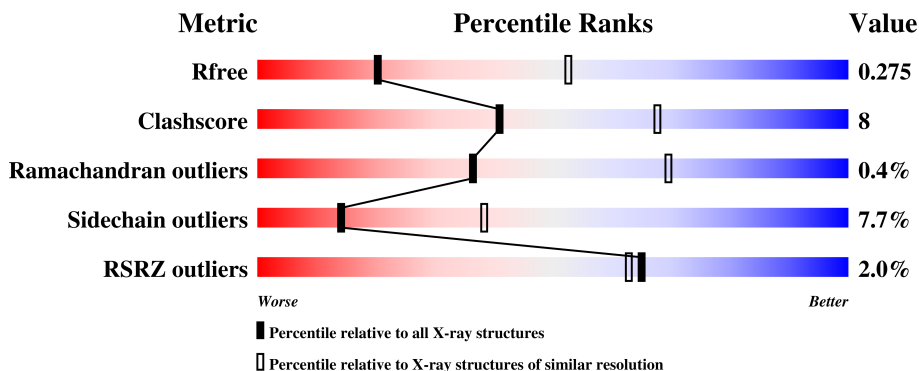
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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	425	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	425	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	425	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>17%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	425	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>15%</div> <div>••</div> <div>15%</div> </div> </div>

## 2 Entry composition [i](#)

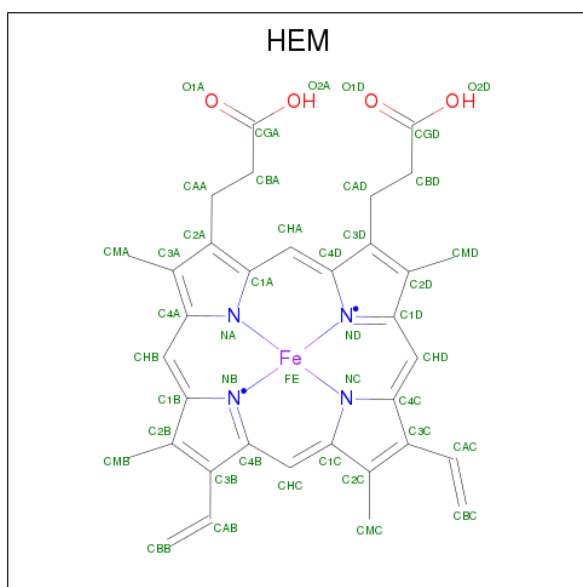
There are 3 unique types of molecules in this entry. The entry contains 12087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	363	Total	C	N	O	S	0	0	0
			2978	1901	522	542	13			
1	B	364	Total	C	N	O	S	0	0	0
			2987	1906	523	545	13			
1	C	362	Total	C	N	O	S	0	0	0
			2962	1890	518	541	13			
1	D	362	Total	C	N	O	S	0	0	0
			2959	1888	518	540	13			

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



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

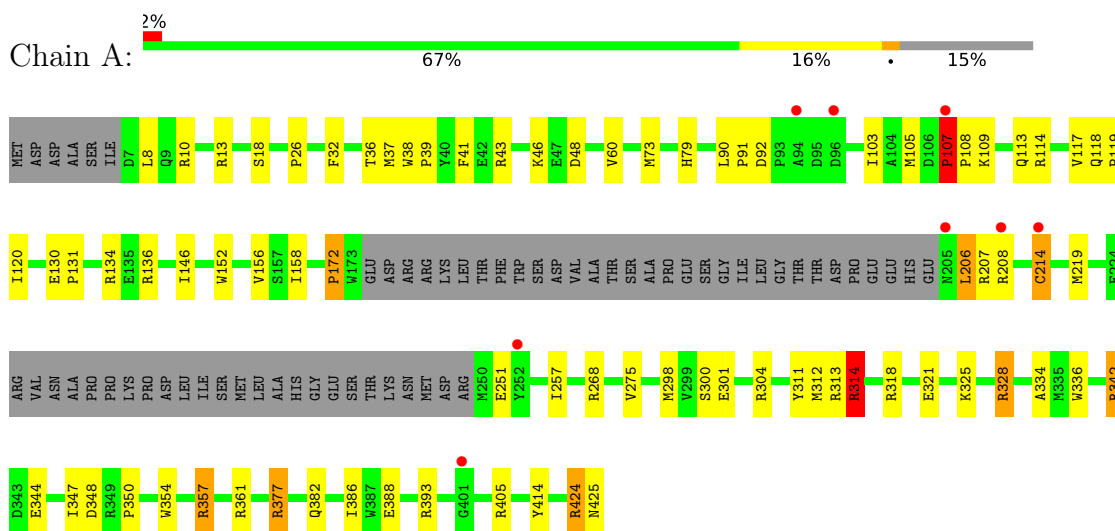
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	9	Total	O	0	0
			9	9		
3	C	7	Total	O	0	0
			7	7		
3	D	5	Total	O	0	0
			5	5		

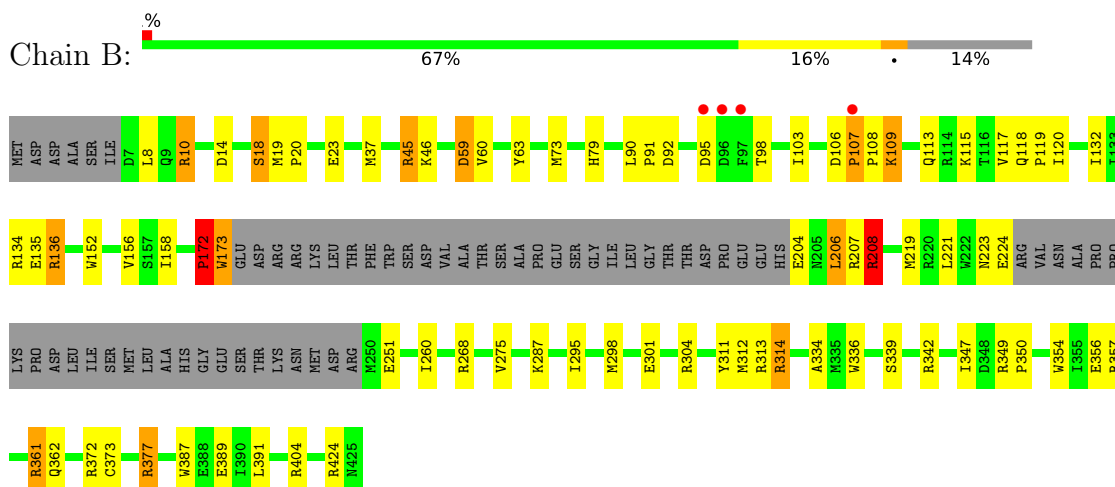
### 3 Residue-property plots [i](#)

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

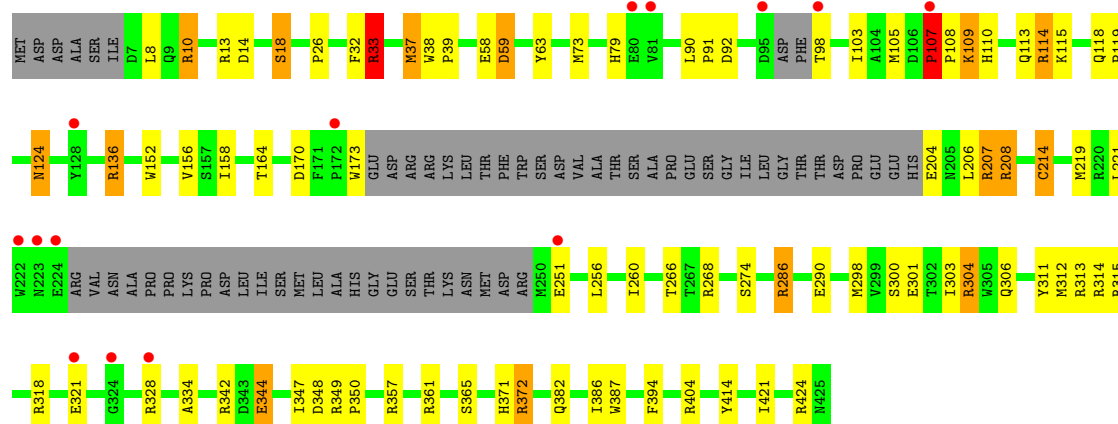


#### • Molecule 1: Cytochrome P450

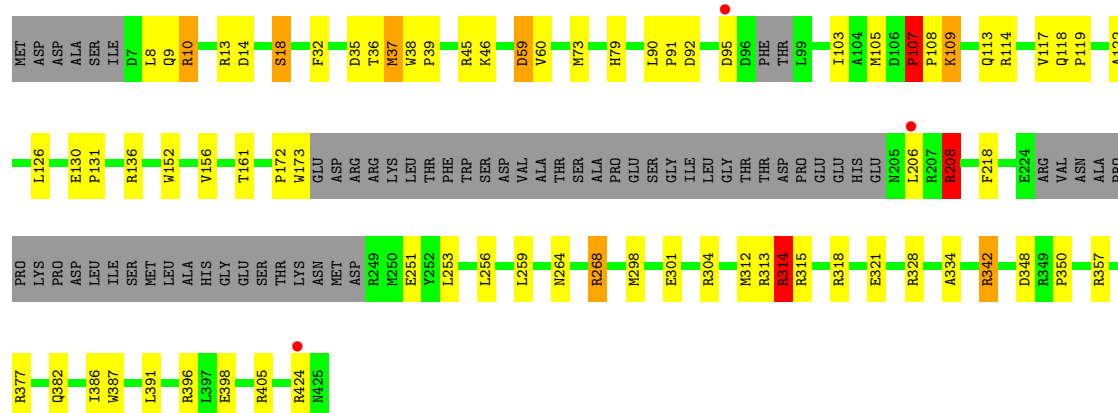


#### • Molecule 1: Cytochrome P450





- Molecule 1: Cytochrome P450



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.46Å 89.21Å 201.82Å 90.00° 96.60° 90.00°	Depositor
Resolution (Å)	49.31 – 2.90 49.31 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.31-2.90) 97.3 (49.31-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.212 , 0.272 0.216 , 0.275	Depositor DCC
$R_{free}$ test set	2007 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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

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	0.53	0/3057	0.73	0/4159
1	B	0.53	0/3066	0.75	0/4171
1	C	0.49	0/3039	0.73	3/4134 (0.1%)
1	D	0.51	0/3036	0.73	1/4130 (0.0%)
All	All	0.52	0/12198	0.73	4/16594 (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	10
1	B	0	9
1	C	0	13
1	D	0	10
All	All	0	42

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	107	PRO	N-CA-C	6.06	127.86	112.10
1	C	33	ARG	CB-CG-CD	-5.61	97.01	111.60
1	C	107	PRO	N-CA-C	5.53	126.47	112.10
1	C	58	GLU	CB-CA-C	-5.03	100.34	110.40

There are no chirality outliers.

All (42) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	13	ARG	Sidechain
1	A	136	ARG	Sidechain
1	A	207	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	314	ARG	Sidechain
1	A	328	ARG	Sidechain
1	A	342	ARG	Sidechain
1	A	377	ARG	Sidechain
1	A	43	ARG	Sidechain
1	B	10	ARG	Sidechain
1	B	136	ARG	Sidechain
1	B	208	ARG	Sidechain
1	B	314	ARG	Sidechain
1	B	342	ARG	Sidechain
1	B	372	ARG	Sidechain
1	B	377	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	45	ARG	Sidechain
1	C	10	ARG	Sidechain
1	C	114	ARG	Sidechain
1	C	136	ARG	Sidechain
1	C	207	ARG	Sidechain
1	C	208	ARG	Sidechain
1	C	286	ARG	Sidechain
1	C	304	ARG	Sidechain
1	C	328	ARG	Sidechain
1	C	33	ARG	Sidechain
1	C	349	ARG	Sidechain
1	C	372	ARG	Sidechain
1	C	404	ARG	Sidechain
1	C	424	ARG	Sidechain
1	D	114	ARG	Sidechain
1	D	136	ARG	Sidechain
1	D	208	ARG	Sidechain
1	D	268	ARG	Sidechain
1	D	314	ARG	Sidechain
1	D	315	ARG	Sidechain
1	D	328	ARG	Sidechain
1	D	342	ARG	Sidechain
1	D	405	ARG	Sidechain
1	D	45	ARG	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	2978	0	2927	40	2
1	B	2987	0	2934	50	0
1	C	2962	0	2908	52	2
1	D	2959	0	2901	39	0
2	A	43	0	30	2	0
2	B	43	0	30	6	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
3	A	8	0	0	1	0
3	B	9	0	0	0	0
3	C	7	0	0	3	0
3	D	5	0	0	1	0
All	All	12087	0	11790	183	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (183) 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:C:304:ARG:NH2	1:C:350:PRO:O	1.97	0.98
1:D:304:ARG:NH2	1:D:350:PRO:O	2.01	0.93
1:B:304:ARG:NH2	1:B:350:PRO:O	2.08	0.86
1:A:301:GLU:OE2	1:A:304:ARG:NH1	2.08	0.85
1:D:79:HIS:ND1	1:D:107:PRO:HG2	1.91	0.85
1:B:79:HIS:ND1	1:B:107:PRO:HG3	1.93	0.83
1:B:107:PRO:HB2	1:B:108:PRO:HD3	1.62	0.82
1:D:314:ARG:NH2	3:D:601:HOH:O	2.15	0.79
1:B:373:CYS:SG	2:B:501:HEM:NB	2.55	0.78
1:B:373:CYS:SG	2:B:501:HEM:NC	2.56	0.78
1:D:382:GLN:O	1:D:386:ILE:HG12	1.83	0.78
1:B:208:ARG:HH21	1:B:208:ARG:HG2	1.48	0.77
1:C:33:ARG:NE	3:C:601:HOH:O	2.17	0.75
1:B:107:PRO:HB2	1:B:108:PRO:CD	2.16	0.75
1:A:304:ARG:NH2	1:A:350:PRO:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ILE:HG12	1:B:268:ARG:HD3	1.69	0.74
1:A:46:LYS:HZ3	1:D:348:ASP:HA	1.52	0.74
1:A:46:LYS:NZ	1:D:348:ASP:HA	2.02	0.74
1:C:114:ARG:NH1	1:C:372:ARG:O	2.22	0.73
1:D:208:ARG:HH21	1:D:208:ARG:HG2	1.54	0.72
1:D:103:ILE:HD11	1:D:312:MET:HE1	1.70	0.72
1:A:103:ILE:HD11	1:A:312:MET:HE1	1.72	0.71
1:C:103:ILE:HD11	1:C:312:MET:HE1	1.72	0.71
1:D:113:GLN:OE1	1:D:251:GLU:HG3	1.90	0.71
1:D:32:PHE:HA	1:D:37:MET:HE2	1.76	0.68
1:B:103:ILE:HD11	1:B:312:MET:HE1	1.76	0.67
1:B:361:ARG:HH11	1:B:361:ARG:HB3	1.59	0.67
1:C:90:LEU:HD11	1:C:334:ALA:HB2	1.78	0.66
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.78	0.65
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.78	0.65
1:A:107:PRO:HB2	1:A:108:PRO:HD3	1.78	0.64
1:B:347:ILE:O	1:B:350:PRO:HD3	1.97	0.64
1:B:295:ILE:HD11	1:B:391:LEU:HD12	1.81	0.63
2:C:501:HEM:HMB2	2:C:501:HEM:HBB2	1.82	0.62
1:D:14:ASP:O	1:D:18:SER:HB3	2.00	0.61
1:A:382:GLN:O	1:A:386:ILE:HG12	2.00	0.61
1:C:79:HIS:ND1	1:C:107:PRO:HG2	2.16	0.60
1:D:90:LEU:HD11	1:D:334:ALA:HB2	1.84	0.59
1:D:105:MET:HE1	1:D:113:GLN:HG3	1.83	0.59
1:B:158:ILE:CG1	1:B:268:ARG:HD3	2.31	0.58
1:B:90:LEU:HD11	1:B:334:ALA:HB2	1.84	0.58
1:A:158:ILE:HG12	1:A:268:ARG:HD3	1.84	0.58
1:D:38:TRP:HB2	1:D:39:PRO:HD3	1.86	0.58
1:C:382:GLN:O	1:C:386:ILE:HG12	2.03	0.57
1:C:204:GLU:HG3	1:C:204:GLU:O	2.03	0.57
1:C:33:ARG:NH1	3:C:601:HOH:O	2.31	0.57
1:A:158:ILE:HG12	1:A:268:ARG:CD	2.34	0.57
1:B:118:GLN:N	1:B:119:PRO:CD	2.68	0.57
1:A:348:ASP:HA	1:D:46:LYS:NZ	2.21	0.56
1:C:152:TRP:CZ2	1:C:156:VAL:HG11	2.41	0.56
1:A:32:PHE:HA	1:A:37:MET:CE	2.36	0.56
1:C:26:PRO:HD2	1:C:63:TYR:OH	2.05	0.56
1:D:122:ALA:O	1:D:126:LEU:HG	2.06	0.56
1:A:152:TRP:CE2	1:A:275:VAL:HG21	2.41	0.55
1:D:268:ARG:HG3	1:D:268:ARG:HH11	1.70	0.55
1:D:32:PHE:HA	1:D:37:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:NH1	1:A:388:GLU:OE1	2.37	0.55
1:A:60:VAL:HG13	1:A:90:LEU:HD23	1.87	0.55
1:C:113:GLN:HE22	1:C:251:GLU:HG3	1.71	0.55
1:B:152:TRP:CE2	1:B:275:VAL:HG21	2.41	0.54
1:A:314:ARG:NH2	3:A:601:HOH:O	2.40	0.54
1:A:90:LEU:HD11	1:A:334:ALA:HB2	1.88	0.54
1:B:172:PRO:O	1:B:173:TRP:HB2	2.08	0.54
1:C:118:GLN:N	1:C:119:PRO:CD	2.70	0.53
1:C:113:GLN:HE22	1:C:251:GLU:CG	2.22	0.53
1:C:14:ASP:O	1:C:18:SER:HB3	2.07	0.53
1:D:152:TRP:CZ2	1:D:156:VAL:HG11	2.44	0.53
1:A:32:PHE:HA	1:A:37:MET:HE2	1.91	0.53
1:B:60:VAL:HG13	1:B:90:LEU:HD23	1.90	0.53
1:C:274:SER:HB3	1:C:387:TRP:CZ2	2.44	0.53
1:A:117:VAL:O	1:A:120:ILE:HG22	2.09	0.52
1:C:109:LYS:HD3	1:C:109:LYS:H	1.73	0.52
1:B:108:PRO:HG2	1:B:109:LYS:HE2	1.92	0.52
1:B:287:LYS:HD2	1:B:356:GLU:OE1	2.10	0.52
1:A:90:LEU:N	1:A:91:PRO:HD2	2.25	0.52
1:A:311:TYR:HB3	1:A:336:TRP:CE3	2.44	0.51
1:B:219:MET:HE3	1:B:260:ILE:HG21	1.92	0.51
1:D:9:GLN:NE2	1:D:35:ASP:O	2.43	0.51
1:B:373:CYS:SG	2:B:501:HEM:ND	2.83	0.51
1:C:301:GLU:HA	1:C:301:GLU:OE1	2.10	0.51
1:B:63:TYR:CD2	1:B:90:LEU:HD21	2.46	0.51
1:C:219:MET:HE3	1:C:260:ILE:HG21	1.92	0.51
1:A:393:ARG:O	1:A:425:ASN:N	2.42	0.50
1:A:79:HIS:ND1	1:A:107:PRO:HG2	2.26	0.50
1:B:134:ARG:NH1	1:B:389:GLU:OE2	2.35	0.50
1:D:60:VAL:HG13	1:D:90:LEU:HD23	1.94	0.50
1:C:59:ASP:O	1:C:91:PRO:HA	2.12	0.50
1:C:107:PRO:HA	1:C:110:HIS:HB3	1.92	0.50
1:D:218:PHE:CE2	1:D:253:LEU:HD21	2.47	0.50
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.92	0.49
1:B:362:GLN:O	1:B:362:GLN:HG2	2.13	0.49
1:C:63:TYR:CD2	1:C:90:LEU:HD21	2.47	0.49
1:B:14:ASP:O	1:B:18:SER:HB3	2.13	0.49
1:A:105:MET:HE1	1:A:113:GLN:HG3	1.95	0.48
1:C:90:LEU:CD1	1:C:311:TYR:CE2	2.96	0.48
1:D:387:TRP:O	1:D:391:LEU:HG	2.13	0.48
1:D:208:ARG:NH2	1:D:208:ARG:HG2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:N	1:A:119:PRO:CD	2.77	0.48
1:B:206:LEU:HD22	1:B:206:LEU:O	2.12	0.48
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.95	0.48
1:C:342:ARG:HA	1:C:350:PRO:HB2	1.95	0.48
1:A:206:LEU:O	1:A:206:LEU:HD22	2.14	0.48
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	1.96	0.47
1:B:113:GLN:OE1	1:B:251:GLU:HG3	2.14	0.47
1:B:354:TRP:CH2	1:C:13:ARG:HD3	2.49	0.47
1:C:38:TRP:HB2	1:C:39:PRO:HD3	1.96	0.47
1:A:405:ARG:NH1	1:A:414:TYR:HE1	2.13	0.47
1:B:59:ASP:OD1	1:B:59:ASP:N	2.47	0.47
1:B:301:GLU:CD	1:B:304:ARG:HH11	2.17	0.47
1:A:152:TRP:CZ2	1:A:156:VAL:HG11	2.49	0.47
1:A:146:ILE:HD11	1:A:424:ARG:HD3	1.96	0.47
1:C:394:PHE:CD1	1:C:421:ILE:HG21	2.50	0.46
1:C:124:ASN:H	1:C:124:ASN:HD22	1.63	0.46
1:D:117:VAL:HB	1:D:259:LEU:HD11	1.97	0.46
1:C:301:GLU:OE2	1:C:304:ARG:NH1	2.49	0.46
1:A:26:PRO:HB3	1:A:41:PHE:CZ	2.51	0.46
1:B:301:GLU:OE1	1:B:304:ARG:HD3	2.15	0.46
1:C:170:ASP:O	1:C:208:ARG:HD2	2.15	0.46
1:C:158:ILE:HG12	1:C:268:ARG:CD	2.45	0.46
1:B:152:TRP:CZ2	1:B:156:VAL:HG11	2.51	0.46
1:B:223:ASN:O	1:B:224:GLU:C	2.54	0.46
1:C:90:LEU:HD12	1:C:311:TYR:CE2	2.51	0.45
1:B:387:TRP:O	1:B:391:LEU:HG	2.16	0.45
1:C:108:PRO:HB2	1:C:109:LYS:HD3	1.98	0.45
1:D:118:GLN:N	1:D:119:PRO:CD	2.79	0.45
1:C:301:GLU:CD	1:C:304:ARG:HH11	2.20	0.45
1:A:348:ASP:HA	1:D:46:LYS:HZ3	1.82	0.45
1:C:158:ILE:HG12	1:C:268:ARG:HD3	1.98	0.45
1:B:19:MET:HB2	1:B:20:PRO:HD2	1.99	0.45
1:B:349:ARG:N	1:B:350:PRO:CD	2.80	0.45
1:A:219:MET:HE2	1:A:257:ILE:CD1	2.47	0.44
1:B:117:VAL:O	1:B:120:ILE:HG22	2.18	0.44
1:B:20:PRO:HG2	1:B:23:GLU:HG3	1.99	0.44
1:B:59:ASP:O	1:B:91:PRO:HA	2.18	0.44
1:C:109:LYS:HD3	1:C:109:LYS:N	2.31	0.44
1:D:90:LEU:N	1:D:91:PRO:HD2	2.33	0.44
1:C:90:LEU:N	1:C:91:PRO:HD2	2.32	0.44
1:D:38:TRP:CZ3	1:D:342:ARG:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ILE:HD12	2:D:501:HEM:HAD2	1.99	0.44
2:D:501:HEM:HBB2	2:D:501:HEM:HMB2	2.01	0.43
1:B:373:CYS:SG	2:B:501:HEM:NA	2.91	0.43
1:A:130:GLU:HB3	1:A:131:PRO:HD3	2.01	0.43
1:B:90:LEU:N	1:B:91:PRO:HD2	2.33	0.43
1:A:38:TRP:CZ3	1:A:342:ARG:HD3	2.53	0.43
1:D:301:GLU:OE2	1:D:304:ARG:NH1	2.52	0.43
1:C:136:ARG:NH1	3:C:603:HOH:O	2.52	0.43
1:B:301:GLU:OE1	1:B:301:GLU:HA	2.19	0.42
1:D:36:THR:O	1:D:39:PRO:HD2	2.19	0.42
1:B:132:ILE:HG22	1:B:136:ARG:HE	1.85	0.42
1:A:301:GLU:OE1	1:A:357:ARG:HD2	2.20	0.42
1:A:48:ASP:OD1	1:A:325:LYS:NZ	2.48	0.42
1:B:207:ARG:O	1:B:208:ARG:C	2.58	0.42
1:B:311:TYR:HB3	1:B:336:TRP:CE3	2.55	0.42
1:C:79:HIS:CG	1:C:107:PRO:HG2	2.55	0.42
1:D:396:ARG:NH2	1:D:398:GLU:OE2	2.53	0.42
1:A:36:THR:O	1:A:39:PRO:HD2	2.20	0.42
1:C:105:MET:HE1	1:C:113:GLN:HG3	2.02	0.42
1:D:130:GLU:HB3	1:D:131:PRO:HD3	2.02	0.42
1:A:354:TRP:CZ2	1:D:13:ARG:HD3	2.55	0.41
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	2.02	0.41
1:D:161:THR:HG21	1:D:264:ASN:O	2.20	0.41
1:B:46:LYS:HE3	1:C:344:GLU:O	2.20	0.41
1:D:108:PRO:HB2	1:D:109:LYS:HD3	2.02	0.41
1:B:46:LYS:NZ	1:C:348:ASP:HA	2.36	0.41
1:C:32:PHE:CD2	1:C:37:MET:HE2	2.56	0.41
1:B:132:ILE:CG2	1:B:136:ARG:HE	2.34	0.41
1:C:113:GLN:NE2	1:C:251:GLU:HG3	2.36	0.41
1:C:79:HIS:CE1	1:C:107:PRO:HG2	2.55	0.41
1:A:134:ARG:NH2	1:A:388:GLU:OE1	2.53	0.41
1:D:59:ASP:OD1	1:D:59:ASP:N	2.54	0.41
1:C:164:THR:HB	1:C:382:GLN:NE2	2.36	0.41
1:C:286:ARG:HD3	1:C:290:GLU:OE2	2.20	0.41
1:C:371:HIS:O	1:C:372:ARG:C	2.59	0.41
1:A:113:GLN:HE22	1:A:251:GLU:CG	2.34	0.41
1:C:347:ILE:O	1:C:350:PRO:HD3	2.21	0.41
1:C:303:ILE:O	1:C:365:SER:OG	2.20	0.40
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.52	0.40
1:C:306:GLN:OE1	1:C:414:TYR:CE2	2.73	0.40
1:D:10:ARG:HD2	1:D:10:ARG:HA	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:NH1	1:B:339:SER:OG	2.50	0.40
1:C:118:GLN:N	1:C:119:PRO:HD2	2.36	0.40
1:A:38:TRP:N	1:A:39:PRO:CD	2.84	0.40
2:C:501:HEM:CMB	2:C:501:HEM:HBB2	2.48	0.40

All (2) 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)
1:A:214:CYS:SG	1:C:214:CYS:SG[4_547]	1.78	0.42
1:A:214:CYS:SG	1:C:214:CYS:CB[4_547]	2.13	0.07

## 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	357/425 (84%)	339 (95%)	16 (4%)	2 (1%)	27	61
1	B	358/425 (84%)	340 (95%)	16 (4%)	2 (1%)	27	61
1	C	354/425 (83%)	337 (95%)	17 (5%)	0	100	100
1	D	354/425 (83%)	336 (95%)	16 (4%)	2 (1%)	27	61
All	All	1423/1700 (84%)	1352 (95%)	65 (5%)	6 (0%)	36	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	PRO
1	B	107	PRO
1	B	172	PRO
1	A	107	PRO
1	D	107	PRO

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Mol	Chain	Res	Type
1	D	172	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	325/379 (86%)	302 (93%)	23 (7%)	16	43
1	B	326/379 (86%)	300 (92%)	26 (8%)	13	36
1	C	323/379 (85%)	294 (91%)	29 (9%)	10	31
1	D	322/379 (85%)	300 (93%)	22 (7%)	17	45
All	All	1296/1516 (86%)	1196 (92%)	100 (8%)	14	38

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	10	ARG
1	A	18	SER
1	A	73	MET
1	A	92	ASP
1	A	107	PRO
1	A	109	LYS
1	A	172	PRO
1	A	206	LEU
1	A	214	CYS
1	A	298	MET
1	A	300	SER
1	A	313	ARG
1	A	314	ARG
1	A	318	ARG
1	A	321	GLU
1	A	328	ARG
1	A	344	GLU
1	A	347	ILE
1	A	357	ARG

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Mol	Chain	Res	Type
1	A	361	ARG
1	A	377	ARG
1	A	424	ARG
1	B	8	LEU
1	B	10	ARG
1	B	18	SER
1	B	37	MET
1	B	59	ASP
1	B	73	MET
1	B	92	ASP
1	B	95	ASP
1	B	98	THR
1	B	106	ASP
1	B	109	LYS
1	B	115	LYS
1	B	135	GLU
1	B	172	PRO
1	B	173	TRP
1	B	204	GLU
1	B	206	LEU
1	B	208	ARG
1	B	221	LEU
1	B	298	MET
1	B	313	ARG
1	B	314	ARG
1	B	357	ARG
1	B	361	ARG
1	B	377	ARG
1	B	424	ARG
1	C	8	LEU
1	C	10	ARG
1	C	18	SER
1	C	37	MET
1	C	59	ASP
1	C	73	MET
1	C	92	ASP
1	C	98	THR
1	C	107	PRO
1	C	109	LYS
1	C	115	LYS
1	C	124	ASN
1	C	173	TRP

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Mol	Chain	Res	Type
1	C	206	LEU
1	C	207	ARG
1	C	214	CYS
1	C	221	LEU
1	C	256	LEU
1	C	266	THR
1	C	298	MET
1	C	300	SER
1	C	313	ARG
1	C	314	ARG
1	C	315	ARG
1	C	318	ARG
1	C	321	GLU
1	C	344	GLU
1	C	357	ARG
1	C	361	ARG
1	D	8	LEU
1	D	10	ARG
1	D	18	SER
1	D	37	MET
1	D	59	ASP
1	D	73	MET
1	D	92	ASP
1	D	95	ASP
1	D	107	PRO
1	D	109	LYS
1	D	173	TRP
1	D	206	LEU
1	D	208	ARG
1	D	256	LEU
1	D	298	MET
1	D	313	ARG
1	D	314	ARG
1	D	318	ARG
1	D	321	GLU
1	D	357	ARG
1	D	377	ARG
1	D	424	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	C	113	GLN
1	C	124	ASN
1	C	371	HIS
1	D	371	HIS

### 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](#)

4 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	27,50,50	0.93	1 (3%)	17,82,82	1.30	3 (17%)
2	HEM	B	501	1	27,50,50	0.94	1 (3%)	17,82,82	1.10	1 (5%)
2	HEM	C	501	1	27,50,50	0.97	2 (7%)	17,82,82	1.55	3 (17%)
2	HEM	D	501	1	27,50,50	0.85	0	17,82,82	1.33	2 (11%)

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	-	0/6/54/54	0/0/8/8
2	HEM	B	501	1	-	0/6/54/54	0/0/8/8
2	HEM	C	501	1	-	0/6/54/54	0/0/8/8
2	HEM	D	501	1	-	0/6/54/54	0/0/8/8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3B-C2B	-2.81	1.36	1.40
2	C	501	HEM	C3B-C2B	-2.63	1.36	1.40
2	C	501	HEM	C4D-C3D	2.19	1.47	1.42
2	A	501	HEM	C4D-C3D	2.78	1.48	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	HEM	CBD-CAD-C3D	-2.46	107.77	112.47
2	A	501	HEM	CBD-CAD-C3D	-2.33	108.02	112.47
2	B	501	HEM	CMA-C3A-C4A	-2.27	124.97	128.46
2	A	501	HEM	C1D-C2D-C3D	-2.17	105.49	107.00
2	A	501	HEM	C4A-C3A-C2A	2.30	108.60	107.00
2	D	501	HEM	C4A-C3A-C2A	2.75	108.91	107.00
2	C	501	HEM	CMC-C2C-C3C	2.81	130.07	124.80
2	C	501	HEM	C4A-C3A-C2A	3.12	109.17	107.00
2	C	501	HEM	CAA-CBA-CGA	3.89	119.31	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
2	B	501	HEM	6	0
2	C	501	HEM	3	0
2	D	501	HEM	4	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	363/425 (85%)	-0.11	8 (2%) 62 59	23, 40, 71, 100	0
1	B	364/425 (85%)	-0.29	4 (1%) 80 80	18, 35, 67, 107	0
1	C	362/425 (85%)	0.07	14 (3%) 39 35	26, 46, 77, 112	0
1	D	362/425 (85%)	-0.08	3 (0%) 86 85	20, 38, 65, 96	0
All	All	1451/1700 (85%)	-0.10	29 (1%) 65 63	18, 40, 71, 112	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	ASP	4.6
1	A	96	ASP	4.0
1	B	95	ASP	3.9
1	C	95	ASP	3.5
1	D	206	LEU	3.1
1	C	223	ASN	2.9
1	C	324	GLY	2.9
1	A	401	GLY	2.9
1	C	222	TRP	2.7
1	C	81	VAL	2.7
1	A	205	ASN	2.6
1	B	97	PHE	2.6
1	C	80	GLU	2.6
1	C	321	GLU	2.4
1	A	94	ALA	2.4
1	A	214	CYS	2.3
1	C	98	THR	2.3
1	C	251	GLU	2.3
1	C	328	ARG	2.3
1	A	252	TYR	2.3
1	B	107	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	224	GLU	2.2
1	D	95	ASP	2.1
1	A	208	ARG	2.1
1	C	128	TYR	2.1
1	D	424	ARG	2.0
1	C	107	PRO	2.0
1	A	107	PRO	2.0
1	C	172	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	C	501	43/43	0.97	0.15	31,34,38,41	0
2	HEM	D	501	43/43	0.97	0.14	24,26,27,29	0
2	HEM	B	501	43/43	0.98	0.14	22,27,30,38	0
2	HEM	A	501	43/43	0.98	0.15	29,32,34,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.