



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:09 AM GMT

PDB ID : 3O5C  
Title : Cytochrome c Peroxidase BccP of Shewanella oneidensis  
Authors : Seidel, J.; Einsle, O.  
Deposited on : 2010-07-28  
Resolution : 1.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



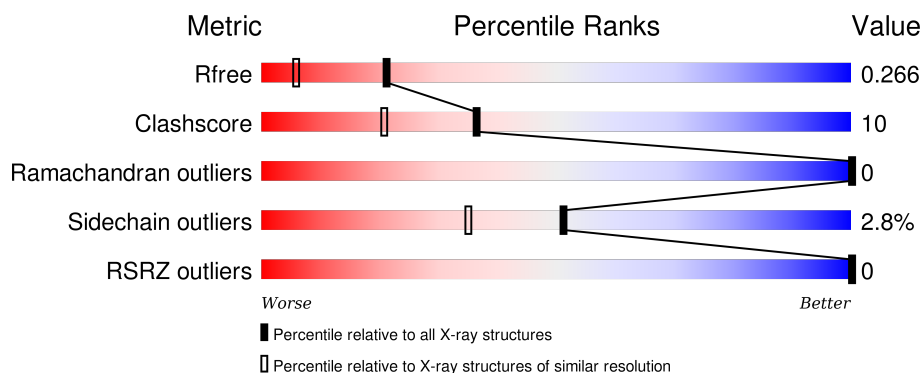
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




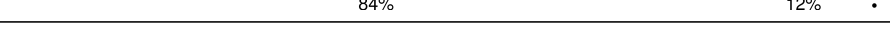
The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	320	
1	B	320	
1	C	320	
1	D	320	



## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11114 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 c551 peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	2	0
			2380	1514	397	456	13			
1	B	307	Total	C	N	O	S	0	1	0
			2356	1501	393	449	13			
1	C	304	Total	C	N	O	S	0	3	0
			2355	1500	391	451	13			
1	D	307	Total	C	N	O	S	0	0	0
			2361	1504	394	450	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	ALA	-	EXPRESSION TAG	UNP Q8EF24
A	15	HIS	-	EXPRESSION TAG	UNP Q8EF24
A	16	HIS	-	EXPRESSION TAG	UNP Q8EF24
A	17	HIS	-	EXPRESSION TAG	UNP Q8EF24
A	18	HIS	-	EXPRESSION TAG	UNP Q8EF24
A	19	HIS	-	EXPRESSION TAG	UNP Q8EF24
A	20	HIS	-	EXPRESSION TAG	UNP Q8EF24
A	21	GLY	-	EXPRESSION TAG	UNP Q8EF24
A	22	GLY	-	EXPRESSION TAG	UNP Q8EF24
B	14	ALA	-	EXPRESSION TAG	UNP Q8EF24
B	15	HIS	-	EXPRESSION TAG	UNP Q8EF24
B	16	HIS	-	EXPRESSION TAG	UNP Q8EF24
B	17	HIS	-	EXPRESSION TAG	UNP Q8EF24
B	18	HIS	-	EXPRESSION TAG	UNP Q8EF24
B	19	HIS	-	EXPRESSION TAG	UNP Q8EF24
B	20	HIS	-	EXPRESSION TAG	UNP Q8EF24
B	21	GLY	-	EXPRESSION TAG	UNP Q8EF24
B	22	GLY	-	EXPRESSION TAG	UNP Q8EF24
C	14	ALA	-	EXPRESSION TAG	UNP Q8EF24
C	15	HIS	-	EXPRESSION TAG	UNP Q8EF24
C	16	HIS	-	EXPRESSION TAG	UNP Q8EF24

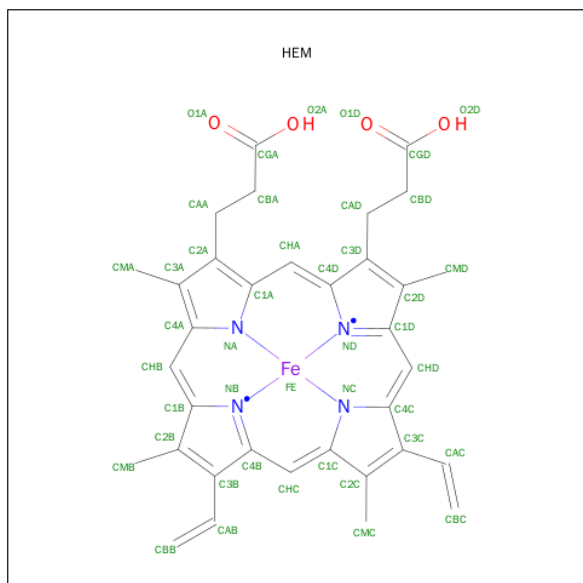
*Continued on next page...*



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	HIS	-	EXPRESSION TAG	UNP Q8EF24
C	18	HIS	-	EXPRESSION TAG	UNP Q8EF24
C	19	HIS	-	EXPRESSION TAG	UNP Q8EF24
C	20	HIS	-	EXPRESSION TAG	UNP Q8EF24
C	21	GLY	-	EXPRESSION TAG	UNP Q8EF24
C	22	GLY	-	EXPRESSION TAG	UNP Q8EF24
D	14	ALA	-	EXPRESSION TAG	UNP Q8EF24
D	15	HIS	-	EXPRESSION TAG	UNP Q8EF24
D	16	HIS	-	EXPRESSION TAG	UNP Q8EF24
D	17	HIS	-	EXPRESSION TAG	UNP Q8EF24
D	18	HIS	-	EXPRESSION TAG	UNP Q8EF24
D	19	HIS	-	EXPRESSION TAG	UNP Q8EF24
D	20	HIS	-	EXPRESSION TAG	UNP Q8EF24
D	21	GLY	-	EXPRESSION TAG	UNP Q8EF24
D	22	GLY	-	EXPRESSION TAG	UNP Q8EF24

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



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

Continued on next page...



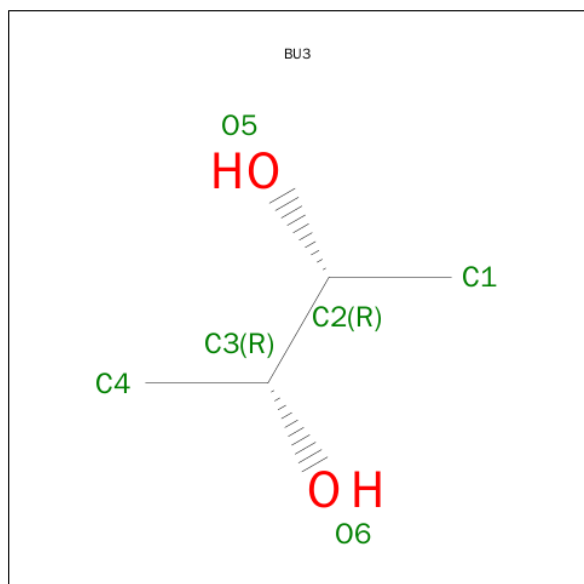
Continued from previous page...

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is water.

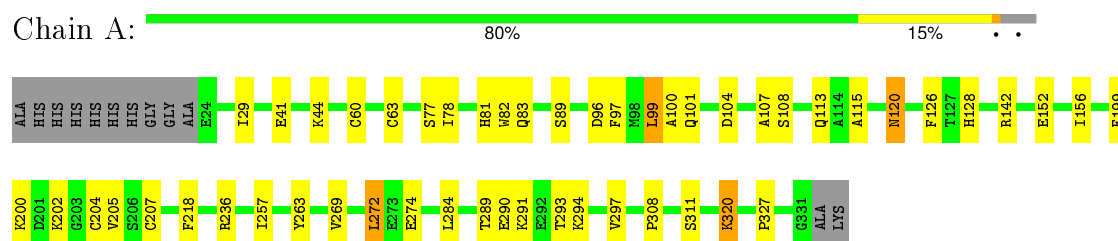
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	331	Total	O	0	0
			331	331		
5	B	320	Total	O	0	0
			320	320		
5	C	314	Total	O	0	0
			314	314		
5	D	343	Total	O	0	0
			343	343		



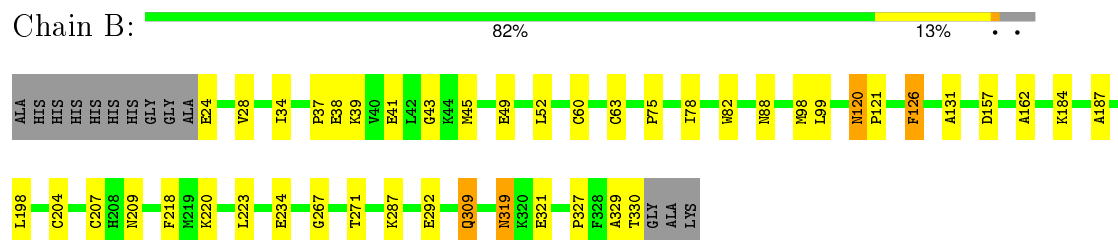
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

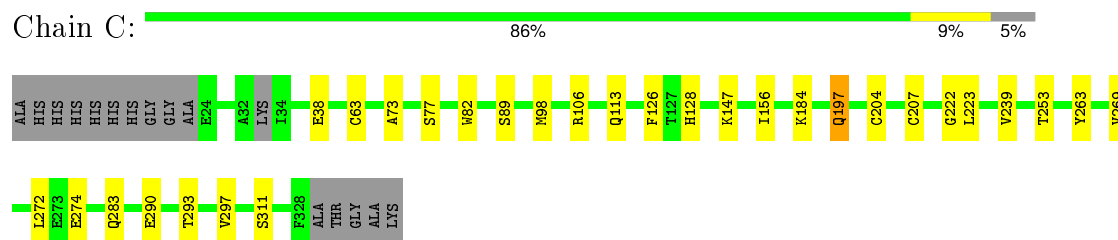
- Molecule 1: Cytochrome c551 peroxidase



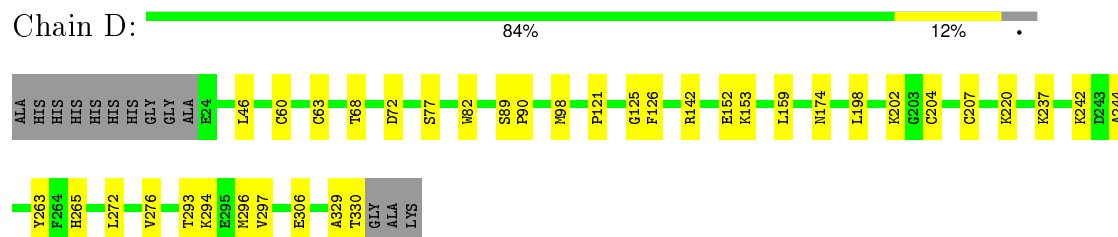
- Molecule 1: Cytochrome c551 peroxidase



- Molecule 1: Cytochrome c551 peroxidase



- Molecule 1: Cytochrome c551 peroxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.84Å 81.22Å 85.92Å 113.96° 102.10° 90.01°	Depositor
Resolution (Å)	40.50 – 1.80 40.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.7 (40.50-1.80) 80.5 (40.50-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.198 , 0.257 0.209 , 0.266	Depositor DCC
$R_{free}$ test set	5345 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 23.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 106124 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BU3, CA, 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	0.48	0/2439	0.59	0/3311
1	B	0.45	0/2418	0.59	0/3285
1	C	0.48	0/2419	0.56	0/3283
1	D	0.47	0/2420	0.56	0/3285
All	All	0.47	0/9696	0.58	0/13164

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	329	ALA	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	2380	0	2342	58	0
1	B	2356	0	2319	61	0
1	C	2355	0	2317	30	0
1	D	2361	0	2327	41	0
2	A	86	0	60	22	0
2	B	86	0	60	19	0
2	C	86	0	60	13	0
2	D	86	0	60	20	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	6	0	10	0	0
5	A	331	0	0	3	1
5	B	320	0	0	20	2
5	C	314	0	0	7	0
5	D	343	0	0	7	1
All	All	11114	0	9555	184	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 10.

All (184) 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:D:60:CYS:SG	2:D:404:HEM:CAB	2.03	1.47
1:D:204:CYS:SG	2:D:504:HEM:CAB	2.06	1.42
1:A:204:CYS:SG	2:A:501:HEM:CAB	2.09	1.39
1:A:204:CYS:SG	2:A:501:HEM:HAB	1.62	1.38
1:A:60:CYS:SG	2:A:401:HEM:CAB	2.10	1.38
1:B:60:CYS:SG	2:B:402:HEM:CAB	2.11	1.37
1:A:63:CYS:SG	2:A:401:HEM:CAC	2.17	1.32
1:C:63:CYS:SG	2:C:403:HEM:CAC	2.19	1.29
1:B:204:CYS:SG	2:B:502:HEM:HAB	1.72	1.28
1:D:63:CYS:SG	2:D:404:HEM:CAC	2.22	1.27
1:C:204:CYS:SG	2:C:503:HEM:HAB	1.74	1.26
1:D:204:CYS:SG	2:D:504:HEM:HAB	1.72	1.24
1:A:60:CYS:SG	2:A:401:HEM:HAB	1.71	1.23
1:A:207:CYS:SG	2:A:501:HEM:CAC	2.26	1.23
1:B:204:CYS:SG	2:B:502:HEM:CAB	2.26	1.22
1:C:204:CYS:SG	2:C:503:HEM:CAB	2.28	1.22
1:A:63:CYS:HG	2:A:401:HEM:CAC	1.53	1.17

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:CYS:SG	2:D:404:HEM:HAB	1.74	1.14
1:B:63:CYS:SG	2:B:402:HEM:CAC	2.36	1.14
1:A:207:CYS:HG	2:A:501:HEM:CAC	1.60	1.12
1:D:207:CYS:SG	2:D:504:HEM:CAC	2.38	1.12
1:B:162:ALA:HB1	5:B:1290:HOH:O	1.50	1.10
1:C:207:CYS:SG	2:C:503:HEM:CAC	2.42	1.08
1:B:207:CYS:SG	2:B:502:HEM:CAC	2.43	1.06
1:B:60:CYS:SG	2:B:402:HEM:HAB	1.93	1.04
1:B:60:CYS:HG	2:B:402:HEM:CAB	1.58	1.03
1:B:75:PRO:O	5:B:1265:HOH:O	1.75	1.02
1:A:63:CYS:SG	2:A:401:HEM:HAC	1.93	1.01
1:A:204:CYS:HG	2:A:501:HEM:HAB	1.15	0.97
1:A:83:GLN:OE1	5:A:1317:HOH:O	1.87	0.92
1:C:63:CYS:SG	2:C:403:HEM:HAC	2.10	0.90
1:C:204:CYS:HG	2:C:503:HEM:HAB	1.33	0.87
1:B:60:CYS:SG	2:B:402:HEM:CBB	2.65	0.85
1:B:34:ILE:HD11	1:B:37:PRO:HA	1.58	0.85
1:A:207:CYS:SG	2:A:501:HEM:HAC	2.17	0.84
1:C:207:CYS:HG	2:C:503:HEM:CAC	1.92	0.81
1:B:39:LYS:O	5:B:1290:HOH:O	2.01	0.79
1:C:77[A]:SER:HG	1:C:89[A]:SER:HG	1.23	0.79
1:B:267:GLY:HA3	5:B:1265:HOH:O	1.81	0.79
1:D:60:CYS:SG	2:D:404:HEM:CBB	2.71	0.78
1:D:63:CYS:SG	2:D:404:HEM:HAC	2.22	0.78
1:D:207:CYS:SG	2:D:504:HEM:HAC	2.24	0.77
1:D:276:VAL:HG13	2:D:504:HEM:HMB3	1.66	0.77
1:A:63:CYS:SG	2:A:401:HEM:C3C	2.76	0.77
1:C:98:MET:HE3	5:C:1119:HOH:O	1.83	0.76
1:D:77:SER:OG	1:D:89:SER:OG	2.04	0.76
1:B:204:CYS:HG	2:B:502:HEM:HAB	1.48	0.76
1:D:63:CYS:SG	2:D:404:HEM:C3C	2.80	0.75
1:B:88:ASN:ND2	5:B:1265:HOH:O	2.21	0.74
1:B:43:GLY:N	5:B:1290:HOH:O	2.20	0.74
1:B:63:CYS:SG	2:B:402:HEM:HAC	2.26	0.74
1:C:63:CYS:SG	2:C:403:HEM:C3C	2.80	0.74
1:B:319:ASN:HD22	1:B:321:GLU:H	1.34	0.74
1:A:320:LYS:HE3	1:B:271:THR:HG22	1.68	0.73
1:D:63:CYS:SG	2:D:404:HEM:CBC	2.77	0.73
1:B:60:CYS:HG	2:B:402:HEM:CBB	2.01	0.72
1:D:244:ALA:HB1	5:D:1293:HOH:O	1.88	0.72
1:B:309:GLN:OE1	5:B:1210:HOH:O	2.09	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:CYS:SG	2:C:403:HEM:CBC	2.80	0.70
1:A:207:CYS:SG	2:A:501:HEM:C3C	2.84	0.69
1:D:98:MET:HE2	5:D:1168:HOH:O	1.92	0.69
1:A:293:THR:HG23	1:A:294:LYS:HD2	1.76	0.68
1:D:204:CYS:SG	2:D:504:HEM:CBB	2.78	0.68
1:C:207:CYS:SG	2:C:503:HEM:HAC	2.33	0.67
1:C:311:SER:OG	5:C:1033:HOH:O	2.11	0.67
1:D:46:LEU:HD13	1:D:159:LEU:HD22	1.77	0.67
1:D:204:CYS:SG	2:D:504:HEM:C3B	2.89	0.65
1:A:199:PHE:CD2	1:A:205:VAL:HG22	2.32	0.65
1:C:147:LYS:NZ	5:C:1220:HOH:O	2.28	0.64
1:B:52:LEU:HA	5:B:1283:HOH:O	1.98	0.64
1:A:99:LEU:HD12	1:A:100:ALA:N	2.13	0.63
1:B:207:CYS:SG	2:B:502:HEM:HAC	2.35	0.63
1:B:88:ASN:HB2	5:B:1265:HOH:O	1.98	0.63
1:D:60:CYS:SG	2:D:404:HEM:C3B	2.89	0.63
1:C:207:CYS:SG	2:C:503:HEM:C3C	2.92	0.62
1:A:207:CYS:HG	2:A:501:HEM:CBC	2.10	0.62
1:C:128:HIS:HB3	1:C:156:ILE:HG13	1.82	0.62
1:B:120:ASN:HD22	1:B:120:ASN:C	2.04	0.61
1:A:82:TRP:HB2	1:B:82:TRP:HB2	1.82	0.61
1:A:60:CYS:SG	2:A:401:HEM:CBB	2.84	0.60
1:A:207:CYS:SG	2:A:501:HEM:CBC	2.89	0.60
1:B:63:CYS:SG	2:B:402:HEM:C3C	2.94	0.60
1:B:98:MET:HE1	5:B:1124:HOH:O	2.01	0.60
1:A:204:CYS:SG	2:A:501:HEM:CBB	2.84	0.59
1:A:142:ARG:HB3	1:A:152:GLU:HB2	1.86	0.58
1:C:222:GLY:H	1:C:283:GLN:HE22	1.52	0.58
1:C:293:THR:O	1:C:297:VAL:HG23	2.04	0.57
1:C:98:MET:CE	5:C:1119:HOH:O	2.46	0.57
1:A:200:LYS:HG2	1:A:205:VAL:HG21	1.86	0.57
1:A:99:LEU:HD11	1:A:218:PHE:CE2	2.40	0.56
1:A:60:CYS:SG	2:A:401:HEM:C3B	2.94	0.56
1:B:267:GLY:CA	5:B:1265:HOH:O	2.45	0.56
1:A:99:LEU:C	1:A:99:LEU:HD12	2.25	0.56
1:B:131:ALA:HA	5:B:1283:HOH:O	2.04	0.56
1:D:207:CYS:SG	2:D:504:HEM:C3C	2.99	0.56
1:D:276:VAL:HG13	2:D:504:HEM:CMB	2.35	0.56
1:B:60:CYS:SG	2:B:402:HEM:C3B	2.95	0.56
1:B:63:CYS:SG	2:B:402:HEM:CBC	2.94	0.55
1:C:222:GLY:H	1:C:283:GLN:NE2	2.05	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ASN:CB	5:B:1265:HOH:O	2.55	0.55
1:B:234:GLU:OE1	5:B:1274:HOH:O	2.18	0.55
1:B:198:LEU:HD11	1:B:292:GLU:HG2	1.87	0.54
1:A:77:SER:HG	1:A:89[B]:SER:HG	1.50	0.54
1:A:269:VAL:CG1	1:A:274[A]:GLU:HB2	2.37	0.54
1:B:34:ILE:HD11	1:B:37:PRO:CA	2.35	0.53
1:B:49:GLU:HB3	1:B:52:LEU:HD13	1.90	0.53
1:C:82:TRP:HB2	1:D:82:TRP:HB2	1.89	0.53
1:A:327:PRO:HB3	1:B:78:ILE:HD11	1.91	0.53
1:D:46:LEU:CD1	1:D:159:LEU:HD22	2.39	0.53
1:C:38:GLU:HG3	5:C:1300:HOH:O	2.08	0.53
1:D:46:LEU:HD22	1:D:159:LEU:HD21	1.90	0.53
1:B:223:LEU:HD22	2:B:502:HEM:HBC1	1.90	0.52
1:B:207:CYS:SG	2:B:502:HEM:C3C	3.02	0.52
1:A:320:LYS:HE3	1:B:271:THR:CG2	2.40	0.52
1:A:263:TYR:CZ	1:A:272:LEU:HD13	2.44	0.52
1:B:207:CYS:SG	2:B:502:HEM:CBC	2.98	0.52
1:D:293:THR:O	1:D:297:VAL:HG23	2.11	0.51
1:B:99:LEU:HD11	1:B:218:PHE:CE2	2.46	0.50
1:A:290:GLU:O	1:A:293:THR:HG22	2.11	0.50
1:D:207:CYS:SG	2:D:504:HEM:CBC	2.98	0.50
1:A:77:SER:OG	1:A:89[B]:SER:OG	2.24	0.50
1:A:99:LEU:HD11	1:A:218:PHE:CZ	2.47	0.49
1:A:78:ILE:HD11	1:B:327:PRO:HB3	1.94	0.49
2:C:503:HEM:HMC1	2:C:503:HEM:HBC2	1.96	0.48
1:B:49:GLU:HG3	1:B:52:LEU:CD1	2.43	0.47
1:A:320:LYS:CE	1:B:271:THR:HG22	2.42	0.47
5:C:1054:HOH:O	1:D:68:THR:HG22	2.14	0.47
1:B:319:ASN:ND2	1:B:321:GLU:H	2.06	0.47
1:A:29:ILE:HD12	1:A:97:PHE:CZ	2.50	0.47
1:B:28:VAL:HG13	5:B:1035:HOH:O	2.13	0.47
1:A:257:ILE:HG23	1:A:272:LEU:HD21	1.97	0.47
1:C:269:VAL:HG13	1:C:274:GLU:HB2	1.97	0.47
1:C:197:GLN:HE21	1:C:197:GLN:HA	1.80	0.47
1:A:99:LEU:C	1:A:99:LEU:CD1	2.83	0.46
1:A:269:VAL:HG13	1:A:274[A]:GLU:HB2	1.96	0.46
1:D:329:ALA:O	1:D:330:THR:HB	2.16	0.46
1:A:101:GLN:HB2	1:A:107:ALA:HB3	1.97	0.46
1:D:98:MET:HE3	5:D:1101:HOH:O	2.16	0.46
1:B:98:MET:CE	5:B:1293:HOH:O	2.62	0.46
1:A:293:THR:O	1:A:297:VAL:HG23	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:MET:HE3	5:B:1069:HOH:O	2.14	0.46
1:D:220:LYS:NZ	5:D:1122:HOH:O	2.48	0.46
1:D:90:PRO:HG2	2:D:404:HEM:HBA1	1.99	0.45
1:A:200:LYS:HA	1:A:205:VAL:HG23	1.99	0.45
1:D:237:LYS:NZ	5:D:1153:HOH:O	2.48	0.45
1:B:49:GLU:CG	1:B:52:LEU:CD1	2.94	0.45
1:A:120:ASN:HD22	1:A:120:ASN:C	2.19	0.45
1:A:204:CYS:SG	2:A:501:HEM:C3B	3.02	0.45
1:C:106:ARG:HB3	1:C:239:VAL:HG21	1.98	0.45
1:D:98:MET:HE1	5:D:1300:HOH:O	2.17	0.44
1:A:128:HIS:HB3	1:A:156:ILE:HG13	1.99	0.44
1:A:115:ALA:O	1:A:128:HIS:HE1	2.01	0.44
1:B:98:MET:HE2	5:B:1293:HOH:O	2.17	0.44
1:B:24:GLU:N	5:B:1036:HOH:O	2.51	0.44
1:D:263:TYR:CZ	1:D:272:LEU:HD13	2.52	0.44
1:A:63:CYS:SG	2:A:401:HEM:CBC	2.96	0.44
1:B:309:GLN:NE2	5:B:1184:HOH:O	2.51	0.44
1:A:202:LYS:O	1:A:284:LEU:HD13	2.18	0.43
1:A:289:THR:HG22	1:A:291:LYS:H	1.83	0.43
1:D:121:PRO:HA	1:D:125:GLY:HA2	2.01	0.43
1:A:104:ASP:O	1:A:236:ARG:HD2	2.18	0.42
1:D:265:HIS:ND1	2:D:504:HEM:O2D	2.50	0.42
1:A:96:ASP:OD2	5:A:1071:HOH:O	2.21	0.42
1:A:63:CYS:HG	2:A:401:HEM:CBC	2.18	0.42
1:D:242:LYS:NZ	5:D:1337:HOH:O	2.46	0.42
1:B:120:ASN:HD22	1:B:121:PRO:N	2.16	0.42
1:B:184:LYS:HD3	1:B:187:ALA:HB2	2.02	0.41
1:D:142:ARG:HB3	1:D:152:GLU:HB3	2.02	0.41
1:B:126:PHE:HD1	1:B:126:PHE:HA	1.81	0.41
1:C:207:CYS:SG	2:C:503:HEM:CBC	3.04	0.41
1:B:49:GLU:CG	1:B:52:LEU:HD13	2.50	0.41
1:A:44:LYS:NZ	1:A:311:SER:OG	2.53	0.41
1:B:49:GLU:HG3	1:B:52:LEU:HD13	2.03	0.41
1:B:41:GLU:O	1:B:45:MET:HG3	2.21	0.41
1:C:98:MET:HE1	1:C:253:THR:HB	2.02	0.41
1:A:152:GLU:HG2	5:A:1306:HOH:O	2.21	0.41
1:C:223:LEU:H	1:C:283:GLN:NE2	2.19	0.41
1:C:73:ALA:HB2	5:C:1121:HOH:O	2.20	0.41
1:C:263:TYR:CZ	1:C:272:LEU:HD13	2.56	0.40
1:D:63:CYS:HA	1:D:72:ASP:HB3	2.02	0.40
1:D:198:LEU:HD22	1:D:202:LYS:CE	2.51	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:ASN:HB3	1:D:306:GLU:HG3	2.03	0.40
1:B:204:CYS:SG	2:B:502:HEM:C3B	3.10	0.40
1:A:63:CYS:CB	2:A:401:HEM:C3C	3.04	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)
5:A:1320:HOH:O	5:B:1284:HOH:O[1_655]	2.18	0.02
5:B:1295:HOH:O	5:D:1318:HOH:O[1_465]	2.19	0.01

## 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	308/320 (96%)	297 (96%)	11 (4%)	0	100	100
1	B	306/320 (96%)	297 (97%)	9 (3%)	0	100	100
1	C	303/320 (95%)	292 (96%)	11 (4%)	0	100	100
1	D	305/320 (95%)	296 (97%)	9 (3%)	0	100	100
All	All	1222/1280 (96%)	1182 (97%)	40 (3%)	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	258/264 (98%)	248 (96%)	10 (4%)	39	21
1	B	255/264 (97%)	245 (96%)	10 (4%)	39	21
1	C	257/264 (97%)	252 (98%)	5 (2%)	65	52
1	D	256/264 (97%)	252 (98%)	4 (2%)	70	59
All	All	1026/1056 (97%)	997 (97%)	29 (3%)	51	35

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	81	HIS
1	A	99	LEU
1	A	108	SER
1	A	113	GLN
1	A	120	ASN
1	A	126	PHE
1	A	272	LEU
1	A	308	PRO
1	A	320	LYS
1	B	38	GLU
1	B	120	ASN
1	B	126	PHE
1	B	157	ASP
1	B	209	ASN
1	B	220	LYS
1	B	287	LYS
1	B	309	GLN
1	B	319	ASN
1	B	330	THR
1	C	113	GLN
1	C	126	PHE
1	C	184	LYS
1	C	197	GLN
1	C	290	GLU
1	D	126	PHE
1	D	153	LYS
1	D	294	LYS
1	D	296	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	81	HIS
1	A	113	GLN
1	A	120	ASN
1	A	128	HIS
1	B	120	ASN
1	B	197	GLN
1	B	209	ASN
1	B	286	GLN
1	B	309	GLN
1	B	319	ASN
1	C	83	GLN
1	C	101	GLN
1	C	113	GLN
1	C	197	GLN
1	C	277	ASN
1	C	283	GLN
1	D	228	HIS
1	D	277	ASN

### 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](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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	401	1,5	30,50,50	2.28	7 (23%)	24,82,82	2.60	13 (54%)
2	HEM	A	501	1	30,50,50	2.24	9 (30%)	24,82,82	2.80	13 (54%)
2	HEM	B	402	1	30,50,50	2.15	5 (16%)	24,82,82	2.59	13 (54%)
2	HEM	B	502	1	30,50,50	2.18	9 (30%)	24,82,82	2.73	14 (58%)
2	HEM	C	403	1,5	30,50,50	2.35	6 (20%)	24,82,82	2.74	11 (45%)
2	HEM	C	503	1	30,50,50	2.28	7 (23%)	24,82,82	2.77	11 (45%)
4	BU3	C	701	-	4,5,5	0.45	0	6,6,6	0.29	0
2	HEM	D	404	1,5	30,50,50	2.20	9 (30%)	24,82,82	2.65	13 (54%)
2	HEM	D	504	1	30,50,50	2.29	6 (20%)	24,82,82	2.78	12 (50%)

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	401	1,5	-	0/10/54/54	0/0/8/8
2	HEM	A	501	1	-	0/10/54/54	0/0/8/8
2	HEM	B	402	1	-	0/10/54/54	0/0/8/8
2	HEM	B	502	1	-	0/10/54/54	0/0/8/8
2	HEM	C	403	1,5	-	0/10/54/54	0/0/8/8
2	HEM	C	503	1	-	0/10/54/54	0/0/8/8
4	BU3	C	701	-	-	0/4/4/4	0/0/0/0
2	HEM	D	404	1,5	-	0/10/54/54	0/0/8/8
2	HEM	D	504	1	-	0/10/54/54	0/0/8/8

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	403	HEM	C3B-C4B	-8.90	1.43	1.51
2	C	503	HEM	C3B-C4B	-8.20	1.44	1.51
2	B	402	HEM	C3B-C4B	-7.87	1.44	1.51
2	D	504	HEM	C3B-C4B	-7.81	1.44	1.51
2	D	404	HEM	C3B-C4B	-7.65	1.45	1.51
2	A	401	HEM	C3B-C4B	-7.50	1.45	1.51
2	A	501	HEM	C3B-C4B	-7.15	1.45	1.51
2	B	502	HEM	C3B-C4B	-6.44	1.46	1.51
2	A	401	HEM	C3D-C4D	-6.03	1.43	1.51
2	C	403	HEM	C3D-C4D	-5.70	1.44	1.51
2	B	502	HEM	C3D-C4D	-5.67	1.44	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C4D	-5.53	1.44	1.51
2	D	504	HEM	C3D-C4D	-5.45	1.44	1.51
2	B	402	HEM	C3D-C4D	-5.45	1.44	1.51
2	C	503	HEM	C3D-C4D	-5.17	1.44	1.51
2	D	404	HEM	C3D-C4D	-4.75	1.45	1.51
2	D	504	HEM	C2C-C1C	-4.17	1.44	1.52
2	A	401	HEM	C2C-C1C	-3.88	1.45	1.52
2	B	502	HEM	C2C-C1C	-3.87	1.45	1.52
2	A	501	HEM	C2C-C1C	-3.79	1.45	1.52
2	D	404	HEM	C2C-C1C	-3.72	1.45	1.52
2	C	503	HEM	C2C-C1C	-3.59	1.45	1.52
2	B	402	HEM	C2C-C1C	-3.51	1.45	1.52
2	C	403	HEM	C2C-C1C	-3.23	1.46	1.52
2	A	501	HEM	C2D-C1D	-2.33	1.44	1.51
2	D	504	HEM	C2D-C1D	-2.29	1.44	1.51
2	A	501	HEM	C2B-C1B	-2.25	1.44	1.51
2	B	402	HEM	C2D-C1D	-2.22	1.44	1.51
2	A	401	HEM	C2D-C1D	-2.21	1.44	1.51
2	D	504	HEM	C2B-C1B	-2.18	1.44	1.51
2	C	503	HEM	C2B-C1B	-2.18	1.44	1.51
2	C	503	HEM	C2D-C1D	-2.17	1.44	1.51
2	C	403	HEM	C2B-C1B	-2.15	1.44	1.51
2	B	502	HEM	C2D-C1D	-2.14	1.44	1.51
2	D	404	HEM	C2D-C1D	-2.07	1.45	1.51
2	B	502	HEM	C2B-C1B	-2.06	1.45	1.51
2	A	501	HEM	C3B-CAB	2.00	1.55	1.51
2	B	402	HEM	C3B-CAB	2.04	1.55	1.51
2	A	401	HEM	C3C-CAC	2.09	1.55	1.51
2	D	404	HEM	CAA-C2A	2.11	1.55	1.52
2	B	502	HEM	C1C-NC	2.14	1.38	1.36
2	A	501	HEM	C3C-CAC	2.15	1.55	1.51
2	D	404	HEM	FE-ND	2.19	2.09	1.97
2	D	404	HEM	FE-NC	2.20	2.04	1.95
2	D	504	HEM	FE-NC	2.24	2.04	1.95
2	B	502	HEM	C3B-CAB	2.25	1.55	1.51
2	A	401	HEM	C3B-CAB	2.27	1.55	1.51
2	B	502	HEM	FE-ND	2.30	2.09	1.97
2	A	501	HEM	FE-NC	2.33	2.05	1.95
2	A	501	HEM	C1C-NC	2.41	1.39	1.36
2	C	503	HEM	C3C-CAC	2.44	1.55	1.51
2	C	403	HEM	C3C-CAC	2.50	1.56	1.51
2	D	404	HEM	C3C-CAC	2.70	1.56	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	HEM	FE-NC	2.77	2.06	1.95
2	D	404	HEM	C3B-CAB	2.81	1.56	1.51
2	A	401	HEM	FE-NC	3.11	2.08	1.95
2	C	403	HEM	FE-NC	3.24	2.08	1.95
2	B	502	HEM	FE-NC	3.32	2.08	1.95

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	403	HEM	C3B-CAB-CBB	-5.71	115.69	124.46
2	D	404	HEM	C3B-CAB-CBB	-5.56	115.93	124.46
2	C	503	HEM	C3B-CAB-CBB	-5.32	116.30	124.46
2	D	504	HEM	C3B-CAB-CBB	-5.05	116.72	124.46
2	A	501	HEM	C3B-CAB-CBB	-5.04	116.72	124.46
2	A	401	HEM	C3B-CAB-CBB	-4.33	117.82	124.46
2	B	402	HEM	C3B-CAB-CBB	-4.25	117.94	124.46
2	B	502	HEM	C3B-CAB-CBB	-4.20	118.02	124.46
2	B	502	HEM	CBD-CAD-C3D	-4.04	101.81	113.55
2	D	504	HEM	CAA-C2A-C1A	-3.78	122.90	127.01
2	C	503	HEM	CBD-CAD-C3D	-3.76	102.61	113.55
2	C	503	HEM	CAA-C2A-C1A	-3.76	122.92	127.01
2	C	403	HEM	CBD-CAD-C3D	-3.64	102.96	113.55
2	D	504	HEM	CBD-CAD-C3D	-3.59	103.09	113.55
2	B	502	HEM	C3C-CAC-CBC	-3.42	119.22	124.46
2	A	501	HEM	C3C-CAC-CBC	-3.33	119.36	124.46
2	B	402	HEM	CBD-CAD-C3D	-3.32	103.90	113.55
2	A	501	HEM	CBA-CAA-C2A	-3.22	106.76	112.53
2	A	501	HEM	CBD-CAD-C3D	-3.13	104.44	113.55
2	D	504	HEM	C3C-CAC-CBC	-3.04	119.79	124.46
2	A	501	HEM	CAA-C2A-C1A	-2.97	123.78	127.01
2	D	504	HEM	CBA-CAA-C2A	-2.96	107.22	112.53
2	D	404	HEM	CBD-CAD-C3D	-2.81	105.38	113.55
2	C	403	HEM	C3B-C4B-NB	-2.76	106.35	111.63
2	C	503	HEM	C3C-CAC-CBC	-2.69	120.32	124.46
2	A	401	HEM	CAA-C2A-C1A	-2.65	124.13	127.01
2	B	502	HEM	CAA-C2A-C1A	-2.51	124.28	127.01
2	A	401	HEM	C3C-CAC-CBC	-2.49	120.63	124.46
2	A	501	HEM	C3B-C4B-NB	-2.48	106.88	111.63
2	B	502	HEM	CBA-CAA-C2A	-2.46	108.13	112.53
2	C	403	HEM	CMA-C3A-C4A	-2.40	124.39	128.36
2	B	502	HEM	CMA-C3A-C4A	-2.38	124.42	128.36
2	A	401	HEM	CBD-CAD-C3D	-2.34	106.75	113.55

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	HEM	CAA-CBA-CGA	-2.27	108.58	112.75
2	D	404	HEM	CMA-C3A-C4A	-2.21	124.70	128.36
2	D	504	HEM	C3B-C4B-NB	-2.19	107.45	111.63
2	A	401	HEM	C3B-C4B-NB	-2.14	107.54	111.63
2	B	502	HEM	C3B-C4B-NB	-2.14	107.54	111.63
2	C	503	HEM	C3B-C4B-NB	-2.11	107.60	111.63
2	D	404	HEM	C3C-CAC-CBC	-2.07	121.28	124.46
2	D	404	HEM	CAA-C2A-C1A	-2.03	124.81	127.01
2	B	402	HEM	C3B-C4B-NB	-2.03	107.75	111.63
2	D	404	HEM	C2C-C1C-CHC	2.10	126.87	123.68
2	D	404	HEM	C3B-C4B-CHC	2.11	126.14	123.16
2	B	502	HEM	C3B-C4B-CHC	2.14	126.18	123.16
2	B	402	HEM	C3B-C4B-CHC	2.23	126.30	123.16
2	B	402	HEM	CBA-CAA-C2A	2.24	116.54	112.53
2	B	402	HEM	C2C-C1C-CHC	2.34	127.23	123.68
2	A	401	HEM	C3B-C4B-CHC	2.42	126.57	123.16
2	A	401	HEM	C2C-C1C-CHC	2.48	127.45	123.68
2	C	403	HEM	CMD-C2D-C3D	2.62	125.96	114.35
2	B	502	HEM	CMD-C2D-C3D	2.66	126.12	114.35
2	C	503	HEM	CMD-C2D-C3D	2.69	126.26	114.35
2	C	503	HEM	C2D-C3D-C4D	2.76	106.18	101.50
2	C	403	HEM	C2D-C3D-C4D	2.79	106.23	101.50
2	B	402	HEM	C2D-C3D-C4D	2.81	106.26	101.50
2	D	504	HEM	CMD-C2D-C3D	2.86	127.00	114.35
2	D	504	HEM	C2D-C3D-C4D	2.87	106.37	101.50
2	D	404	HEM	C2D-C3D-C4D	2.91	106.43	101.50
2	A	501	HEM	CMD-C2D-C3D	2.99	127.55	114.35
2	D	404	HEM	CMD-C2D-C3D	3.00	127.60	114.35
2	A	401	HEM	CMD-C2D-C3D	3.02	127.71	114.35
2	B	402	HEM	CMD-C2D-C3D	3.21	128.55	114.35
2	A	401	HEM	C2D-C3D-C4D	3.23	106.97	101.50
2	A	501	HEM	C2D-C3D-C4D	3.27	107.03	101.50
2	B	502	HEM	C2D-C3D-C4D	3.28	107.06	101.50
2	C	403	HEM	CMC-C2C-C3C	3.56	125.41	116.53
2	A	501	HEM	C3B-C4B-CHC	3.59	128.22	123.16
2	C	403	HEM	C2C-C1C-CHC	3.72	129.34	123.68
2	A	501	HEM	CMC-C2C-C3C	3.76	125.92	116.53
2	C	503	HEM	CAD-C3D-C2D	3.91	124.45	113.22
2	B	402	HEM	CMC-C2C-C3C	3.96	126.42	116.53
2	A	401	HEM	CAD-C3D-C4D	4.03	126.69	112.47
2	B	402	HEM	CAD-C3D-C4D	4.13	127.03	112.47
2	B	502	HEM	CAD-C3D-C4D	4.18	127.22	112.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	HEM	CAD-C3D-C2D	4.19	125.28	113.22
2	A	401	HEM	CMB-C2B-C3B	4.22	127.07	116.53
2	D	404	HEM	CAD-C3D-C2D	4.23	125.37	113.22
2	A	501	HEM	CAD-C3D-C2D	4.23	125.38	113.22
2	A	501	HEM	CAD-C3D-C4D	4.28	127.58	112.47
2	B	502	HEM	CAD-C3D-C2D	4.32	125.64	113.22
2	C	403	HEM	CAD-C3D-C4D	4.36	127.85	112.47
2	C	403	HEM	CAD-C3D-C2D	4.41	125.89	113.22
2	D	404	HEM	CAD-C3D-C4D	4.44	128.14	112.47
2	D	504	HEM	CAD-C3D-C4D	4.49	128.31	112.47
2	D	404	HEM	CMB-C2B-C3B	4.49	127.75	116.53
2	A	401	HEM	CAD-C3D-C2D	4.56	126.33	113.22
2	D	404	HEM	CMC-C2C-C3C	4.61	128.04	116.53
2	A	501	HEM	CMB-C2B-C3B	4.64	128.12	116.53
2	B	402	HEM	CAD-C3D-C2D	4.68	126.67	113.22
2	C	503	HEM	CMB-C2B-C3B	4.68	128.22	116.53
2	B	502	HEM	CMC-C2C-C3C	4.75	128.38	116.53
2	D	504	HEM	CMC-C2C-C3C	4.76	128.41	116.53
2	C	503	HEM	CMC-C2C-C3C	4.76	128.42	116.53
2	B	502	HEM	CMB-C2B-C3B	4.77	128.44	116.53
2	C	503	HEM	CAD-C3D-C4D	4.77	129.31	112.47
2	D	504	HEM	CMB-C2B-C3B	4.78	128.46	116.53
2	C	403	HEM	CMB-C2B-C3B	4.87	128.69	116.53
2	B	402	HEM	CMB-C2B-C3B	4.88	128.70	116.53
2	A	401	HEM	CMC-C2C-C3C	4.88	128.71	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	HEM	11	0
2	A	501	HEM	11	0
2	B	402	HEM	10	0
2	B	502	HEM	9	0
2	C	403	HEM	4	0
2	C	503	HEM	9	0
2	D	404	HEM	9	0
2	D	504	HEM	11	0



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	308/320 (96%)	-0.48	0 100 100	11, 20, 33, 38	0
1	B	307/320 (95%)	-0.47	0 100 100	12, 20, 33, 41	1 (0%)
1	C	304/320 (95%)	-0.42	0 100 100	11, 20, 36, 42	1 (0%)
1	D	307/320 (95%)	-0.47	0 100 100	12, 20, 33, 41	0
All	All	1226/1280 (95%)	-0.46	0 100 100	11, 20, 34, 42	2 (0%)

There are no RSRZ outliers to report.

### 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	D	504	43/43	0.97	0.09	0.61	9,10,12,13	0
2	HEM	B	502	43/43	0.98	0.09	0.38	6,11,12,13	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	401	43/43	0.98	0.08	0.06	7,12,14,14	0
4	BU3	C	701	6/6	0.95	0.10	0.01	23,25,27,27	0
2	HEM	C	403	43/43	0.98	0.08	-0.12	7,10,12,14	0
2	HEM	C	503	43/43	0.98	0.08	-0.15	5,9,11,12	0
2	HEM	B	402	43/43	0.98	0.07	-0.26	9,12,15,16	0
2	HEM	A	501	43/43	0.98	0.07	-0.39	7,10,11,12	0
2	HEM	D	404	43/43	0.98	0.07	-0.42	8,12,13,14	0
3	CA	A	601	1/1	1.00	0.02	-4.23	13,13,13,13	0
3	CA	C	603	1/1	1.00	0.03	-4.78	11,11,11,11	0
3	CA	D	604	1/1	1.00	0.02	-6.47	13,13,13,13	0
3	CA	B	602	1/1	1.00	0.02	-9.41	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.