



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:22 PM GMT

PDB ID : 4RKN  
Title : Wolinella succinogenes octaheme sulfite reductase MccA, form II  
Authors : Hermann, B.; Kern, M.; La Pietra, L.; Simon, J.; Einsle, O.  
Deposited on : 2014-10-13  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (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

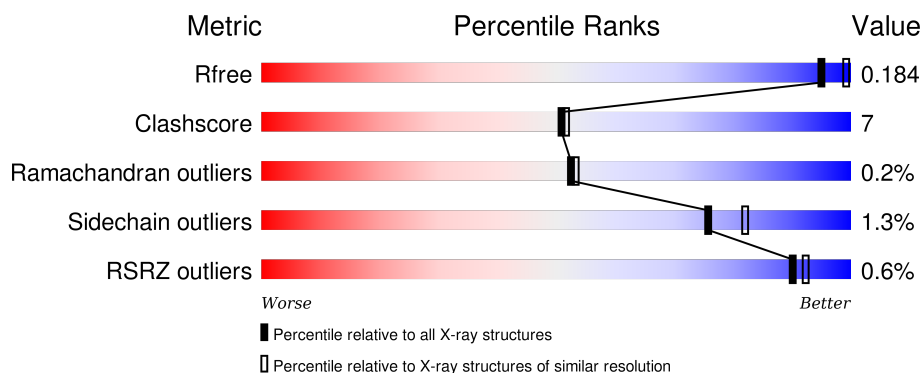
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	732	<div> <div></div> <div>84% 6% 10%</div> </div>
1	B	732	<div> <div></div> <div>% 84% 6% 10%</div> </div>
1	C	732	<div> <div></div> <div>% 84% 6% 10%</div> </div>
1	D	732	<div> <div></div> <div>83% 7% 10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTN	A	901	-	-	-	X
2	DTN	A	911	-	-	-	X
2	DTN	C	901	-	-	-	X
2	DTN	D	901	-	-	-	X
5	SO3	B	911	-	-	-	X
5	SO3	C	911	-	-	-	X
5	SO3	D	912	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23997 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 MccA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	3	0
			5250	3299	923	991	37			
1	B	660	Total	C	N	O	S	0	3	0
			5246	3295	923	991	37			
1	C	659	Total	C	N	O	S	0	3	0
			5240	3292	922	989	37			
1	D	660	Total	C	N	O	S	0	2	0
			5240	3291	922	990	37			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
A	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
A	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
A	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
A	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
A	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
A	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
A	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
A	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
A	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
A	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
A	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
A	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
A	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
A	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
A	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
A	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
A	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
B	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
B	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
B	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
B	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
B	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
B	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
B	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
B	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
B	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
B	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
B	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
B	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
B	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
B	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
B	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
B	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
B	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
B	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
C	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
C	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8

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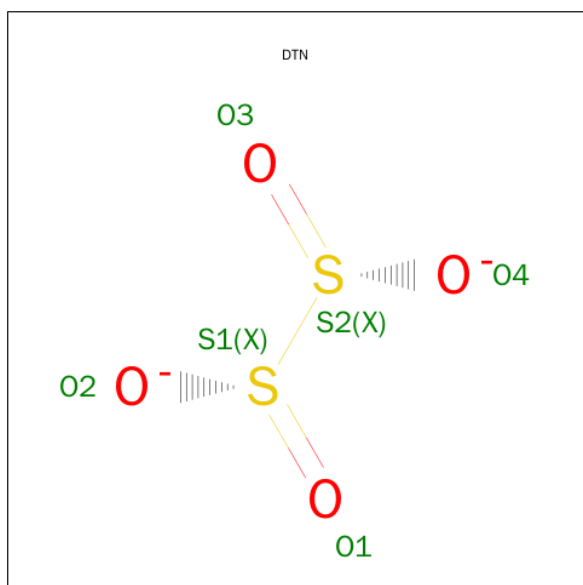
Chain	Residue	Modelled	Actual	Comment	Reference
C	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
C	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
C	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
C	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
C	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
C	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
C	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
C	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
C	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
C	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
C	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
C	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
C	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
C	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
C	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
D	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
D	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
D	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
D	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
D	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
D	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
D	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
D	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
D	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
D	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
D	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
D	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
D	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
D	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
D	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
D	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
D	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
D	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8

- Molecule 2 is DITHIONITE (three-letter code: DTN) (formula: O<sub>4</sub>S<sub>2</sub>).



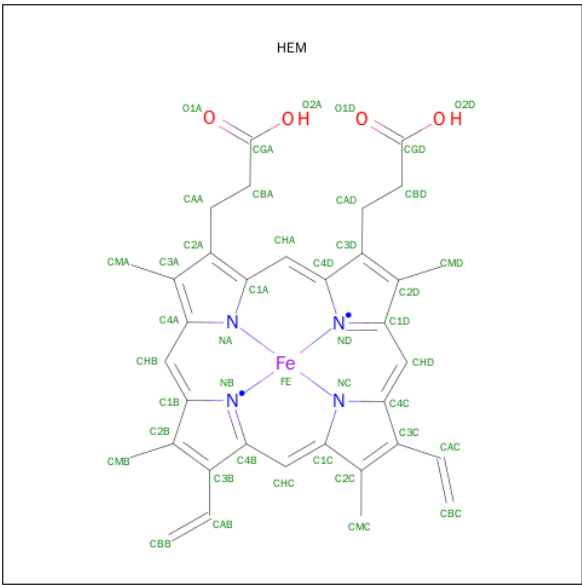
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			6	4	2		
2	A	1	Total	O	S	0	0
			6	4	2		
2	B	1	Total	O	S	0	0
			6	4	2		
2	C	1	Total	O	S	0	0
			6	4	2		

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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 86	C 68	Fe 2	N 8	O 8	0	1
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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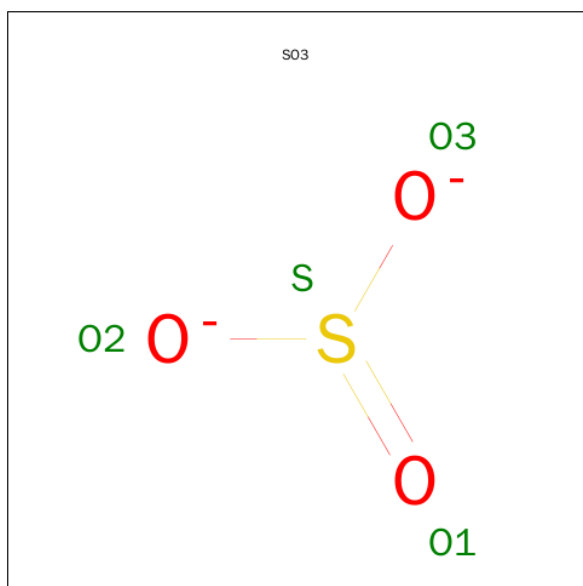
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cu	0	0
			1	1		
4	A	1	Total	Cu	0	0
			1	1		
4	D	1	Total	Cu	0	0
			1	1		
4	C	1	Total	Cu	0	0
			1	1		

- Molecule 5 is SULFITE ION (three-letter code: SO3) (formula: O<sub>3</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			4	3	1		
5	B	1	Total	O	S	0	0
			4	3	1		
5	C	1	Total	O	S	0	0
			4	3	1		
5	D	1	Total	O	S	0	0
			4	3	1		

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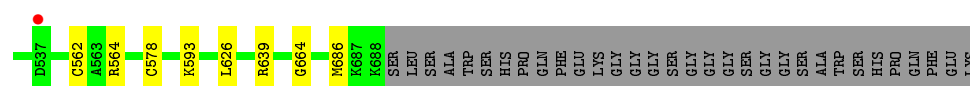
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			4	3	1		


- Molecule 6 is water.

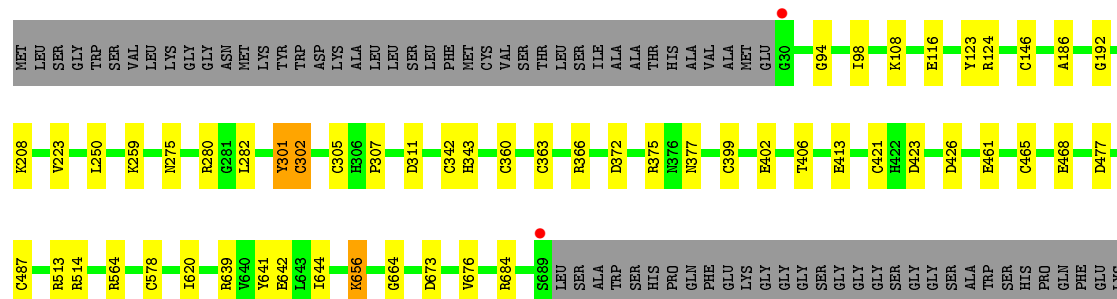
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	335	Total	O	0	0
			335	335		
6	B	355	Total	O	0	0
			355	355		
6	C	312	Total	O	0	0
			312	312		
6	D	417	Total	O	0	0
			417	417		





- Molecule 1: MccA

Chain D:  83% 7% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.47Å 186.47Å 232.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.26 – 2.10 47.22 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.26-2.10) 99.8 (47.22-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.135 , 0.175 0.149 , 0.184	Depositor DCC
$R_{free}$ test set	8789 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.2	EDS
Estimated twinning fraction	0.011 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.009 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.009 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.011 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.011 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.015 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.019 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 175765 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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: HEM, SO3, DTN, CU

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	0.88	0/5383	0.88	6/7251 (0.1%)
1	B	0.89	0/5379	0.92	14/7245 (0.2%)
1	C	0.88	0/5373	0.89	11/7237 (0.2%)
1	D	0.97	4/5370 (0.1%)	0.93	8/7233 (0.1%)
All	All	0.91	4/21505 (0.0%)	0.91	39/28966 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	413	GLU	CD-OE2	5.58	1.31	1.25
1	D	468	GLU	CD-OE2	-5.40	1.19	1.25
1	D	461	GLU	CD-OE2	5.11	1.31	1.25
1	D	641	TYR	CE1-CZ	5.06	1.45	1.38

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	B	514	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	B	505	ASP	CB-CG-OD1	8.74	126.17	118.30
1	A	526	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	D	280	ARG	NE-CZ-NH2	-8.47	116.06	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	5250	0	5072	73	0
1	B	5246	0	5063	72	0
1	C	5240	0	5059	71	0
1	D	5240	0	5054	72	0
2	A	12	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	387	0	270	56	0
3	B	387	0	270	61	0
3	C	387	0	270	64	0
3	D	387	0	270	57	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
5	D	8	0	0	3	0
6	A	335	0	0	4	0
6	B	355	0	0	3	0
6	C	312	0	0	2	0
6	D	417	0	0	4	0
All	All	23997	0	21328	301	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 7.

The worst 5 of 301 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:B:562:CYS:SG	3:B:909:HEM:CAB	2.01	1.48
1:D:578:CYS:SG	3:D:909:HEM:CAC	2.03	1.47
1:C:562:CYS:SG	3:C:909:HEM:CAB	2.02	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:CYS:SG	3:B:904[A]:HEM:CAB	2.03	1.47
1:D:305:CYS:SG	3:D:903:HEM:CAC	2.03	1.47

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	661/732 (90%)	631 (96%)	28 (4%)	2 (0%)	46	45
1	B	661/732 (90%)	635 (96%)	26 (4%)	0	100	100
1	C	660/732 (90%)	629 (95%)	30 (4%)	1 (0%)	52	53
1	D	660/732 (90%)	633 (96%)	25 (4%)	2 (0%)	46	45
All	All	2642/2928 (90%)	2528 (96%)	109 (4%)	5 (0%)	52	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	630	LYS
1	D	301	TYR
1	A	664	GLY
1	C	664	GLY
1	D	664	GLY

### 5.3.2 Protein sidechains [i](#)

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	563/613 (92%)	556 (99%)	7 (1%)	78	84
1	B	562/613 (92%)	552 (98%)	10 (2%)	66	72
1	C	561/613 (92%)	555 (99%)	6 (1%)	80	85
1	D	561/613 (92%)	555 (99%)	6 (1%)	80	85
All	All	2247/2452 (92%)	2218 (99%)	29 (1%)	76	82

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	441	SER
1	B	631	LYS
1	D	302	CYS
1	B	498	PHE
1	C	124	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	243	GLN
1	A	497	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

Of 50 ligands modelled in this entry, 4 are monoatomic - leaving 46 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	DTN	A	901	-	0,5,5	0.00	-	0,6,6	0.00	-
3	HEM	A	902	1	30,50,50	2.43	7 (23%)	24,82,82	2.54	10 (41%)
3	HEM	A	903	1,5	30,50,50	2.16	5 (16%)	24,82,82	2.62	12 (50%)
3	HEM	A	904[A]	1	30,50,50	2.10	5 (16%)	24,82,82	2.78	11 (45%)
3	HEM	A	904[B]	1	30,50,50	2.12	6 (20%)	24,82,82	2.92	13 (54%)
3	HEM	A	905	1	30,50,50	2.03	6 (20%)	24,82,82	2.30	8 (33%)
3	HEM	A	906	1	30,50,50	2.12	6 (20%)	24,82,82	2.29	8 (33%)
3	HEM	A	907	1	30,50,50	2.26	7 (23%)	24,82,82	2.74	12 (50%)
3	HEM	A	908	1	30,50,50	2.55	8 (26%)	24,82,82	2.38	8 (33%)
3	HEM	A	909	1	30,50,50	2.54	6 (20%)	24,82,82	2.53	12 (50%)
2	DTN	A	911	-	0,5,5	0.00	-	0,6,6	0.00	-
5	SO3	A	912	3,4	1,3,3	7.68	1 (100%)	0,3,3	0.00	-
2	DTN	B	901	-	0,5,5	0.00	-	0,6,6	0.00	-
3	HEM	B	902	1	30,50,50	2.30	7 (23%)	24,82,82	2.84	9 (37%)
3	HEM	B	903	1,5	30,50,50	1.92	6 (20%)	24,82,82	2.80	12 (50%)
3	HEM	B	904[A]	1	30,50,50	2.13	8 (26%)	24,82,82	2.99	12 (50%)
3	HEM	B	904[B]	1	30,50,50	2.17	8 (26%)	24,82,82	2.96	12 (50%)
3	HEM	B	905	1	30,50,50	2.07	9 (30%)	24,82,82	2.50	7 (29%)
3	HEM	B	906	1	30,50,50	2.32	6 (20%)	24,82,82	2.60	12 (50%)
3	HEM	B	907	1	30,50,50	2.48	6 (20%)	24,82,82	2.59	10 (41%)
3	HEM	B	908	1	30,50,50	1.93	6 (20%)	24,82,82	2.53	7 (29%)
3	HEM	B	909	1	30,50,50	2.58	7 (23%)	24,82,82	2.75	12 (50%)
5	SO3	B	911	3,4	1,3,3	5.11	1 (100%)	0,3,3	0.00	-
2	DTN	C	901	-	0,5,5	0.00	-	0,6,6	0.00	-
3	HEM	C	902	1	30,50,50	2.15	6 (20%)	24,82,82	2.63	11 (45%)
3	HEM	C	903	1,5	30,50,50	1.83	4 (13%)	24,82,82	2.45	7 (29%)
3	HEM	C	904[A]	1	30,50,50	2.20	7 (23%)	24,82,82	2.74	11 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEM	C	904[B]	1	30,50,50	2.17	7 (23%)	24,82,82	2.59	10 (41%)
3	HEM	C	905	1	30,50,50	2.13	6 (20%)	24,82,82	2.40	7 (29%)
3	HEM	C	906	1	30,50,50	2.43	9 (30%)	24,82,82	2.52	9 (37%)
3	HEM	C	907	1	30,50,50	2.58	8 (26%)	24,82,82	2.74	12 (50%)
3	HEM	C	908	1	30,50,50	2.33	8 (26%)	24,82,82	2.42	11 (45%)
3	HEM	C	909	1	30,50,50	2.36	7 (23%)	24,82,82	2.53	9 (37%)
5	SO3	C	911	3	1,3,3	5.84	1 (100%)	0,3,3	0.00	-
2	DTN	D	901	-	0,5,5	0.00	-	0,6,6	0.00	-
3	HEM	D	902	1	30,50,50	2.06	8 (26%)	24,82,82	2.80	13 (54%)
3	HEM	D	903	1,5	30,50,50	2.10	4 (13%)	24,82,82	2.47	5 (20%)
3	HEM	D	904[A]	1	30,50,50	2.27	7 (23%)	24,82,82	2.76	12 (50%)
3	HEM	D	904[B]	1	30,50,50	2.31	7 (23%)	24,82,82	2.81	13 (54%)
3	HEM	D	905	1	30,50,50	2.25	6 (20%)	24,82,82	2.25	6 (25%)
3	HEM	D	906	1	30,50,50	2.44	6 (20%)	24,82,82	2.73	13 (54%)
3	HEM	D	907	1	30,50,50	2.42	7 (23%)	24,82,82	2.88	13 (54%)
3	HEM	D	908	1	30,50,50	2.11	7 (23%)	24,82,82	2.61	10 (41%)
3	HEM	D	909	1	30,50,50	2.70	8 (26%)	24,82,82	2.97	14 (58%)
5	SO3	D	911	-	1,3,3	8.91	1 (100%)	0,3,3	0.00	-
5	SO3	D	912	3	1,3,3	6.47	1 (100%)	0,3,3	0.00	-

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	DTN	A	901	-	-	0/0/4/4	0/0/0/0
3	HEM	A	902	1	-	0/10/54/54	0/0/8/8
3	HEM	A	903	1,5	-	0/10/54/54	0/0/8/8
3	HEM	A	904[A]	1	-	0/10/54/54	0/0/8/8
3	HEM	A	904[B]	1	-	0/10/54/54	0/0/8/8
3	HEM	A	905	1	-	0/10/54/54	0/0/8/8
3	HEM	A	906	1	-	0/10/54/54	0/0/8/8
3	HEM	A	907	1	-	0/10/54/54	0/0/8/8
3	HEM	A	908	1	-	0/10/54/54	0/0/8/8
3	HEM	A	909	1	-	0/10/54/54	0/0/8/8
2	DTN	A	911	-	-	0/0/4/4	0/0/0/0
5	SO3	A	912	3,4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTN	B	901	-	-	0/0/4/4	0/0/0/0
3	HEM	B	902	1	-	0/10/54/54	0/0/8/8
3	HEM	B	903	1,5	-	0/10/54/54	0/0/8/8
3	HEM	B	904[A]	1	-	0/10/54/54	0/0/8/8
3	HEM	B	904[B]	1	-	0/10/54/54	0/0/8/8
3	HEM	B	905	1	-	0/10/54/54	0/0/8/8
3	HEM	B	906	1	-	0/10/54/54	0/0/8/8
3	HEM	B	907	1	-	0/10/54/54	0/0/8/8
3	HEM	B	908	1	-	0/10/54/54	0/0/8/8
3	HEM	B	909	1	-	0/10/54/54	0/0/8/8
5	SO3	B	911	3,4	-	0/0/0/0	0/0/0/0
2	DTN	C	901	-	-	0/0/4/4	0/0/0/0
3	HEM	C	902	1	-	0/10/54/54	0/0/8/8
3	HEM	C	903	1,5	-	0/10/54/54	0/0/8/8
3	HEM	C	904[A]	1	-	0/10/54/54	0/0/8/8
3	HEM	C	904[B]	1	-	0/10/54/54	0/0/8/8
3	HEM	C	905	1	-	0/10/54/54	0/0/8/8
3	HEM	C	906	1	-	0/10/54/54	0/0/8/8
3	HEM	C	907	1	-	0/10/54/54	0/0/8/8
3	HEM	C	908	1	-	0/10/54/54	0/0/8/8
3	HEM	C	909	1	-	0/10/54/54	0/0/8/8
5	SO3	C	911	3	-	0/0/0/0	0/0/0/0
2	DTN	D	901	-	-	0/0/4/4	0/0/0/0
3	HEM	D	902	1	-	0/10/54/54	0/0/8/8
3	HEM	D	903	1,5	-	0/10/54/54	0/0/8/8
3	HEM	D	904[A]	1	-	0/10/54/54	0/0/8/8
3	HEM	D	904[B]	1	-	0/10/54/54	0/0/8/8
3	HEM	D	905	1	-	0/10/54/54	0/0/8/8
3	HEM	D	906	1	-	0/10/54/54	0/0/8/8
3	HEM	D	907	1	-	0/10/54/54	0/0/8/8
3	HEM	D	908	1	-	0/10/54/54	0/0/8/8
3	HEM	D	909	1	-	0/10/54/54	0/0/8/8
5	SO3	D	911	-	-	0/0/0/0	0/0/0/0
5	SO3	D	912	3	-	0/0/0/0	0/0/0/0

The worst 5 of 246 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	907	HEM	C3B-C4B	-8.19	1.44	1.51
3	D	909	HEM	C3B-C4B	-8.02	1.44	1.51
3	A	908	HEM	C3B-C4B	-7.98	1.44	1.51
3	A	903	HEM	C2C-C1C	-7.74	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	909	HEM	C3B-C4B	-7.67	1.45	1.51

The worst 5 of 373 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	HEM	C3B-CAB-CBB	-7.24	113.34	124.46
3	D	909	HEM	CAA-CBA-CGA	-6.92	100.06	112.75
3	B	904[A]	HEM	C3B-CAB-CBB	-6.86	113.93	124.46
3	B	908	HEM	C3B-CAB-CBB	-6.68	114.21	124.46
3	B	904[B]	HEM	C3B-CAB-CBB	-6.57	114.39	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 244 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	HEM	5	0
3	A	903	HEM	11	0
3	A	904[A]	HEM	8	0
3	A	904[B]	HEM	7	0
3	A	905	HEM	5	0
3	A	906	HEM	7	0
3	A	907	HEM	5	0
3	A	908	HEM	4	0
3	A	909	HEM	4	0
5	A	912	SO3	1	0
3	B	902	HEM	5	0
3	B	903	HEM	13	0
3	B	904[A]	HEM	10	0
3	B	904[B]	HEM	9	0
3	B	906	HEM	4	0
3	B	907	HEM	4	0
3	B	908	HEM	4	0
3	B	909	HEM	12	0
5	B	911	SO3	1	0
3	C	902	HEM	5	0
3	C	903	HEM	15	0
3	C	904[A]	HEM	9	0
3	C	904[B]	HEM	4	0
3	C	905	HEM	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	906	HEM	6	0
3	C	907	HEM	6	0
3	C	908	HEM	6	0
3	C	909	HEM	8	0
5	C	911	SO3	1	0
3	D	902	HEM	5	0
3	D	903	HEM	16	0
3	D	904[A]	HEM	5	0
3	D	904[B]	HEM	5	0
3	D	905	HEM	9	0
3	D	906	HEM	5	0
3	D	907	HEM	4	0
3	D	908	HEM	4	0
3	D	909	HEM	4	0
5	D	912	SO3	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	660/732 (90%)	-0.43	3 (0%) 91 93	15, 26, 43, 82	0
1	B	660/732 (90%)	-0.45	7 (1%) 82 86	16, 24, 43, 67	0
1	C	659/732 (90%)	-0.39	4 (0%) 90 92	17, 27, 46, 71	0
1	D	660/732 (90%)	-0.45	2 (0%) 94 95	11, 21, 40, 76	0
All	All	2639/2928 (90%)	-0.43	16 (0%) 90 92	11, 25, 44, 82	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	630	LYS	4.1
1	C	379	LEU	3.9
1	D	689	SER	3.6
1	C	30	GLY	3.4
1	C	537	ASP	3.1

### 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	DTN	A	901	6/6	0.84	0.24	7.54	25,33,40,42	6
5	SO3	B	911	4/4	0.99	0.14	7.02	23,23,31,34	0
2	DTN	D	901	6/6	0.92	0.19	6.91	33,38,51,51	6
2	DTN	C	901	6/6	0.89	0.28	5.47	56,57,64,67	6
2	DTN	A	911	6/6	0.96	0.11	4.95	23,28,36,37	6
5	SO3	C	911	4/4	0.99	0.14	2.04	23,25,30,38	0
5	SO3	A	912	4/4	0.99	0.14	1.48	21,22,25,35	0
3	HEM	D	904[B]	43/43	0.96	0.15	0.99	9,12,14,15	43
3	HEM	D	904[A]	43/43	0.96	0.15	0.99	10,11,13,15	43
3	HEM	A	909	43/43	0.96	0.13	0.88	19,23,45,72	0
3	HEM	B	904[A]	43/43	0.97	0.14	0.82	15,16,18,20	43
3	HEM	B	904[B]	43/43	0.97	0.14	0.82	11,16,19,21	43
3	HEM	C	909	43/43	0.95	0.11	0.73	20,23,41,61	0
2	DTN	B	901	6/6	0.92	0.14	0.65	27,36,37,40	6
3	HEM	B	909	43/43	0.96	0.10	0.60	17,20,40,71	0
3	HEM	A	904[A]	43/43	0.97	0.13	0.56	14,17,18,20	43
3	HEM	A	904[B]	43/43	0.97	0.13	0.56	12,18,19,20	43
5	SO3	D	911	4/4	0.93	0.10	0.56	40,48,50,62	0
3	HEM	D	909	43/43	0.96	0.09	0.45	14,19,54,66	0
3	HEM	B	907	43/43	0.95	0.11	0.44	15,16,29,54	0
3	HEM	C	908	43/43	0.97	0.08	0.36	17,19,24,26	0
3	HEM	C	903	43/43	0.96	0.11	0.30	18,21,26,29	0
3	HEM	D	907	43/43	0.96	0.09	0.26	12,14,23,54	0
3	HEM	C	904[A]	43/43	0.96	0.14	0.23	14,17,19,21	43
3	HEM	C	904[B]	43/43	0.96	0.14	0.23	15,17,19,21	43
3	HEM	B	903	43/43	0.96	0.10	0.19	15,18,20,22	0
3	HEM	A	907	43/43	0.96	0.09	0.13	14,16,25,47	0
3	HEM	B	908	43/43	0.97	0.08	0.12	14,17,21,22	0
3	HEM	C	907	43/43	0.96	0.09	0.08	16,18,29,45	0
3	HEM	C	902	43/43	0.96	0.13	0.03	15,19,22,25	0
3	HEM	C	906	43/43	0.96	0.10	0.02	15,18,24,34	0
3	HEM	D	903	43/43	0.96	0.12	0.01	11,13,14,15	0
3	HEM	A	902	43/43	0.96	0.12	-0.02	17,19,24,28	0
3	HEM	A	903	43/43	0.96	0.10	-0.03	16,19,22,24	0
3	HEM	C	905	43/43	0.96	0.12	-0.03	16,18,20,21	0
3	HEM	D	905	43/43	0.97	0.12	-0.05	10,11,13,14	0
3	HEM	B	906	43/43	0.97	0.10	-0.10	13,16,25,34	0
3	HEM	D	902	43/43	0.97	0.12	-0.12	12,13,19,22	0
5	SO3	D	912	4/4	0.98	0.13	-0.20	15,17,21,24	0
3	HEM	A	908	43/43	0.97	0.08	-0.20	15,17,20,23	0
3	HEM	D	906	43/43	0.97	0.10	-0.24	9,12,17,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HEM	A	905	43/43	0.97	0.10	-0.32	13,17,19,21	0
3	HEM	B	905	43/43	0.97	0.10	-0.35	14,15,18,18	0
3	HEM	B	902	43/43	0.97	0.11	-0.39	16,18,22,25	0
3	HEM	A	906	43/43	0.97	0.09	-0.44	13,16,24,31	0
3	HEM	D	908	43/43	0.97	0.07	-0.75	12,14,21,22	0
4	CU	A	910	1/1	0.99	0.10	-1.22	15,15,15,15	1
4	CU	C	910	1/1	0.98	0.10	-1.61	17,17,17,17	1
4	CU	D	910	1/1	1.00	0.09	-2.52	9,9,9,9	1
4	CU	B	910	1/1	1.00	0.09	-2.81	11,11,11,11	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.