



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:24 PM GMT

PDB ID : 4RKM
Title : Wolinella succinogenes octaheme sulfite reductase MccA, form I
Authors : Hermann, B.; Kern, M.; La Pietra, L.; Simon, J.; Einsle, O.
Deposited on : 2014-10-13
Resolution : 2.20 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
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

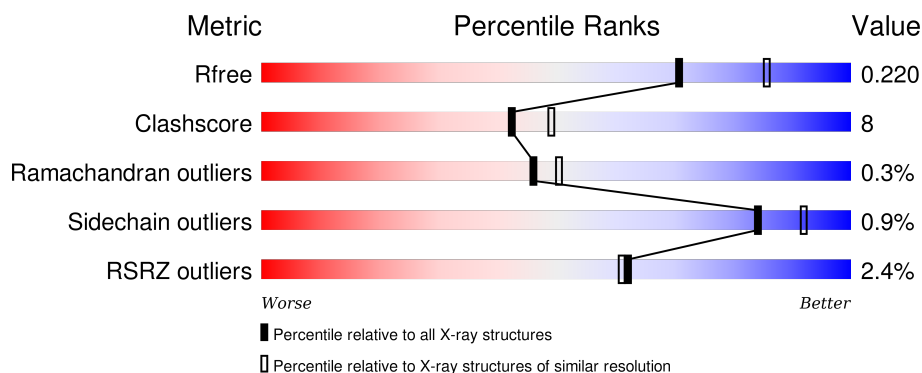
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 ≥ 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>2%</div> <div>85% 5% 10%</div> </div>
1	B	732	<div> <div>%</div> <div>85% 5% 10%</div> </div>
1	C	732	<div> <div>%</div> <div>84% 5% 10%</div> </div>
1	D	732	<div> <div>3%</div> <div>84% 5% 10%</div> </div>
1	E	732	<div> <div>%</div> <div>84% 6% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	732	
1	G	732	
1	H	732	
1	I	732	
1	J	732	
1	K	732	
1	L	732	

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
3	SX	B	802	-	-	-	X
3	SX	F	802	-	-	-	X
3	SX	H	802	-	-	-	X
4	BU3	A	804	-	-	-	X
4	BU3	B	804	-	-	-	X
4	BU3	B	805	-	-	-	X
4	BU3	C	804	-	-	-	X
4	BU3	E	804	-	-	-	X
4	BU3	G	804	-	-	-	X
4	BU3	H	804	-	-	-	X
4	BU3	H	805	-	-	-	X
4	BU3	I	804	-	-	-	X
4	BU3	J	804	-	-	-	X
4	BU3	K	804	-	-	-	X
5	ACT	A	805	-	-	-	X
5	ACT	B	806	-	-	-	X
5	ACT	C	805	-	-	-	X
5	ACT	D	805	-	-	-	X
5	ACT	E	805	-	-	-	X
5	ACT	F	806	-	-	-	X
5	ACT	G	805	-	-	-	X
5	ACT	H	806	-	-	-	X
5	ACT	J	805	-	-	-	X
5	ACT	K	805	-	-	-	X
5	ACT	L	805	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO2	G	814	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 70014 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	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	B	660	Total	C	N	O	S	0	0	0
			5232	3289	920	988	35			
1	C	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	D	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	E	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	F	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	H	660	Total	C	N	O	S	0	0	0
			5232	3289	920	988	35			
1	I	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	J	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	K	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	L	659	Total	C	N	O	S	0	0	0
			5224	3283	919	987	35			
1	G	658	Total	C	N	O	S	0	0	0
			5218	3280	918	985	35			

There are 360 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
E	691	SER	-	EXPRESSION TAG	UNP Q7MSJ8
E	692	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
E	693	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
E	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
E	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
E	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
E	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
E	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
E	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
E	700	LYS	-	EXPRESSION TAG	UNP Q7MSJ8
E	701	GLY	-	EXPRESSION TAG	UNP Q7MSJ8

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

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	702	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	703	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	704	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	705	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	706	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	707	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	708	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	709	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	710	GLY	-	EXPRESSION TAG	UNP Q7MSJ8
G	711	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	712	ALA	-	EXPRESSION TAG	UNP Q7MSJ8
G	713	TRP	-	EXPRESSION TAG	UNP Q7MSJ8
G	714	SER	-	EXPRESSION TAG	UNP Q7MSJ8
G	715	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
G	716	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
G	717	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
G	718	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
G	719	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
G	720	LYS	-	EXPRESSION TAG	UNP Q7MSJ8

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

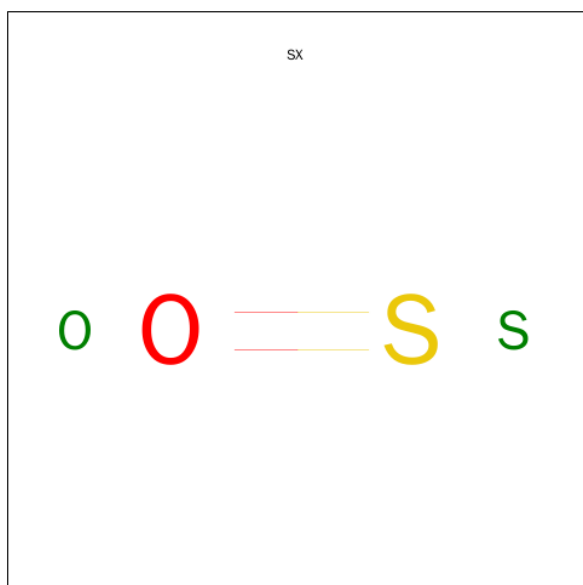
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cu 1 1	0	0
2	J	1	Total Cu 1 1	0	0
2	D	1	Total Cu 1 1	0	0
2	K	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0
2	H	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		

- Molecule 3 is SULFUR OXIDE (three-letter code: SX) (formula: OS).



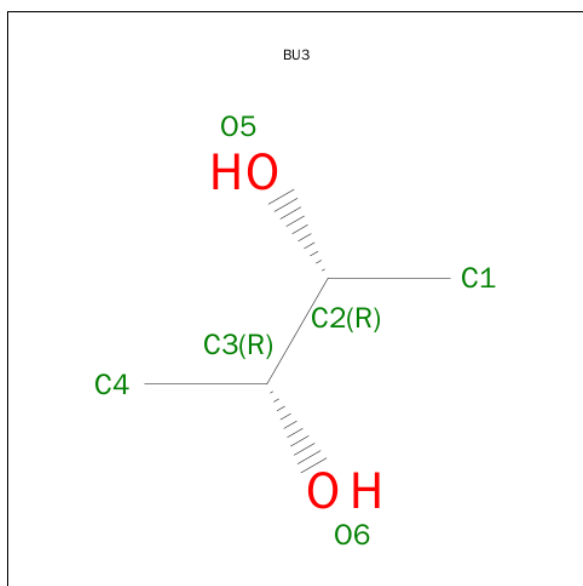
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			2	1	1		
3	B	1	Total	O	S	0	0
			2	1	1		
3	C	1	Total	O	S	0	0
			2	1	1		
3	E	1	Total	O	S	0	0
			2	1	1		
3	F	1	Total	O	S	0	0
			2	1	1		
3	H	1	Total	O	S	0	0
			2	1	1		
3	J	1	Total	O	S	0	0
			2	1	1		
3	K	1	Total	O	S	0	0
			2	1	1		
3	L	1	Total	O	S	0	0
			2	1	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			2	1	1		

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: C₄H₁₀O₂).



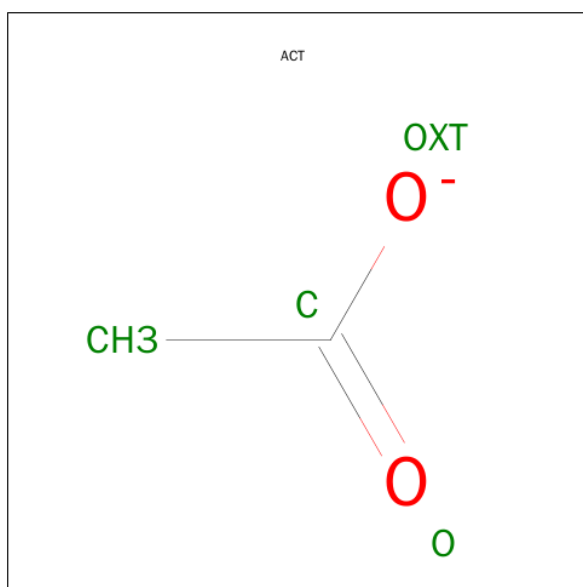
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			6	4	2		
4	D	1	Total	C	O	0	0
			6	4	2		
4	D	1	Total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

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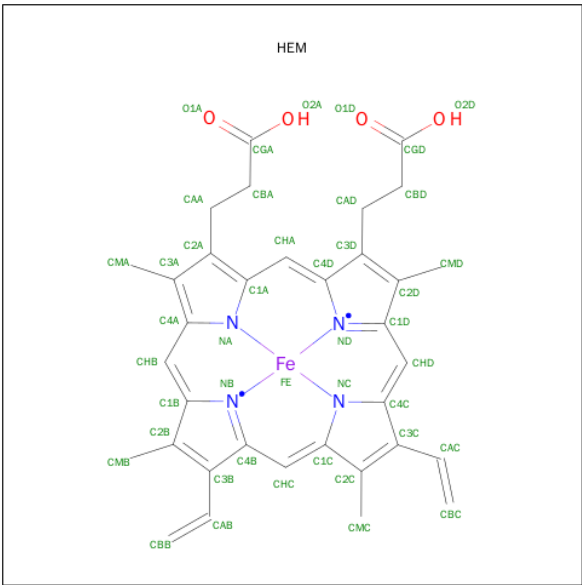
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	4	2		
4	F	1	Total	C	O	0	0
			6	4	2		
4	F	1	Total	C	O	0	0
			6	4	2		
4	F	1	Total	C	O	0	0
			6	4	2		
4	H	1	Total	C	O	0	0
			6	4	2		
4	H	1	Total	C	O	0	0
			6	4	2		
4	H	1	Total	C	O	0	0
			6	4	2		
4	I	1	Total	C	O	0	0
			6	4	2		
4	I	1	Total	C	O	0	0
			6	4	2		
4	J	1	Total	C	O	0	0
			6	4	2		
4	J	1	Total	C	O	0	0
			6	4	2		
4	K	1	Total	C	O	0	0
			6	4	2		
4	K	1	Total	C	O	0	0
			6	4	2		
4	L	1	Total	C	O	0	0
			6	4	2		
4	L	1	Total	C	O	0	0
			6	4	2		
4	G	1	Total	C	O	0	0
			6	4	2		
4	G	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	L	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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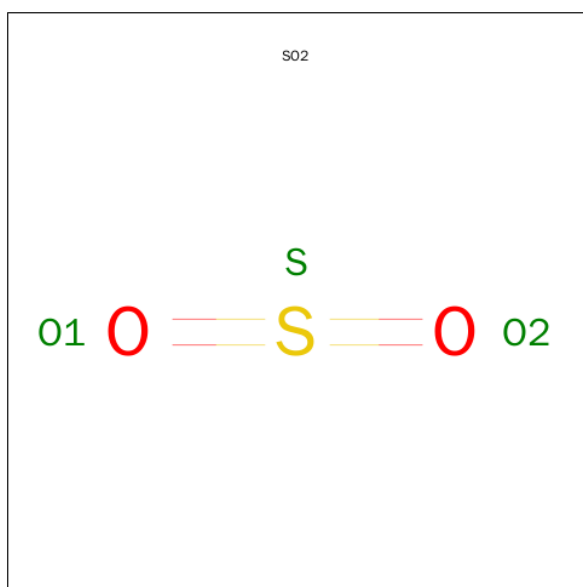
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is SULFUR DIOXIDE (three-letter code: SO2) (formula: O₂S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			3	2	1		
7	D	1	Total	O	S	0	0
			3	2	1		
7	I	1	Total	O	S	0	0
			3	2	1		
7	G	1	Total	O	S	0	0
			3	2	1		

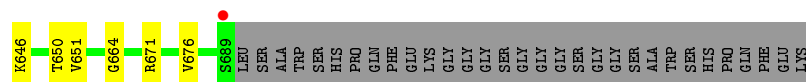
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	416	Total	O	0	0
			416	416		
8	B	298	Total	O	0	0
			298	298		
8	C	285	Total	O	0	0
			285	285		
8	D	307	Total	O	0	0
			307	307		
8	E	219	Total	O	0	0
			219	219		
8	F	245	Total	O	0	0
			245	245		
8	H	250	Total	O	0	0
			250	250		
8	I	218	Total	O	0	0
			218	218		

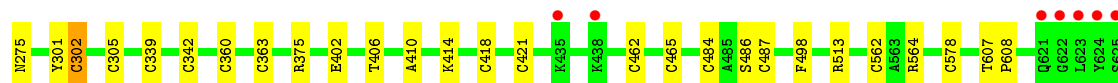
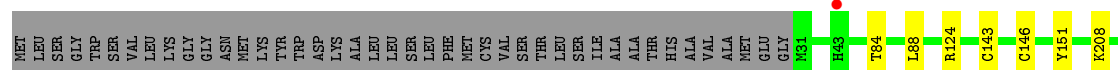
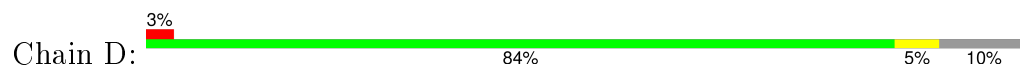
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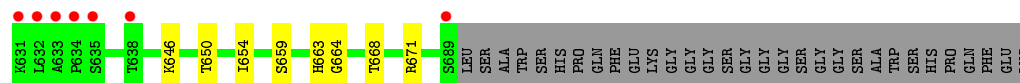
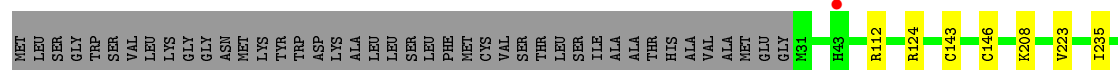
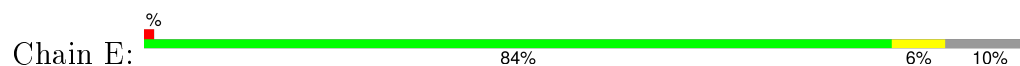
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	180	Total 180	O 180	0	0
8	K	158	Total 158	O 158	0	0
8	L	126	Total 126	O 126	0	0
8	G	232	Total 232	O 232	0	0



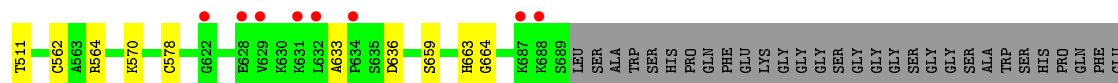
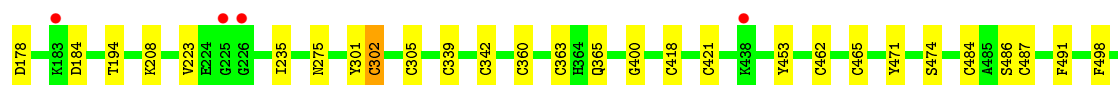
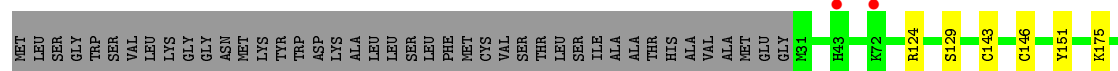
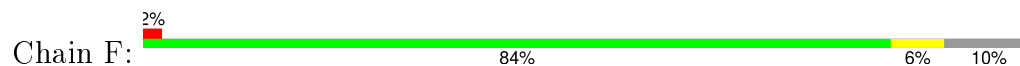
• Molecule 1: MccA



• Molecule 1: MccA

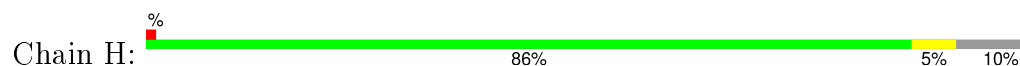


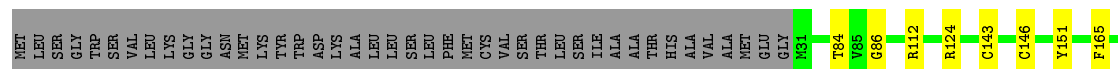
• Molecule 1: MccA

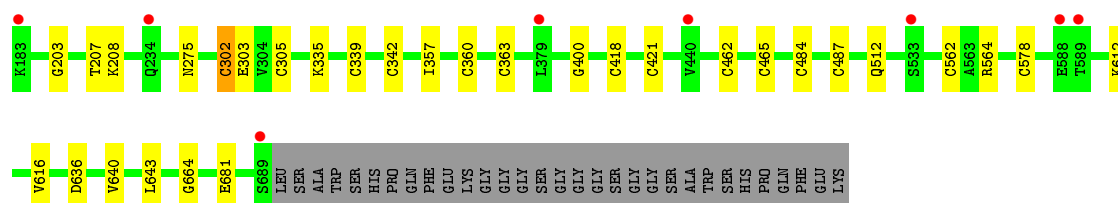


LYS

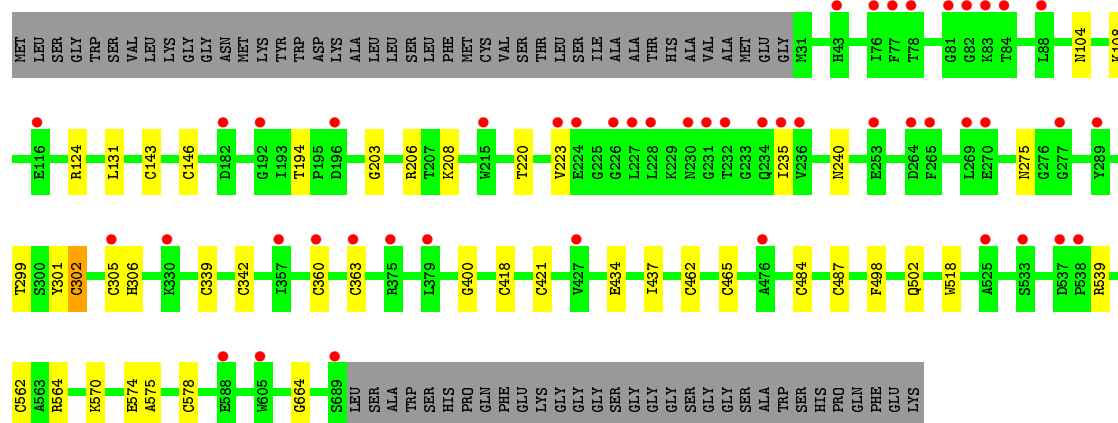
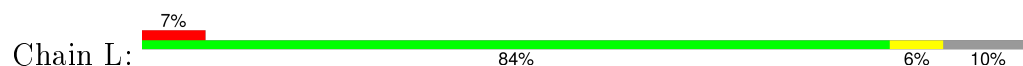
• Molecule 1: MccA



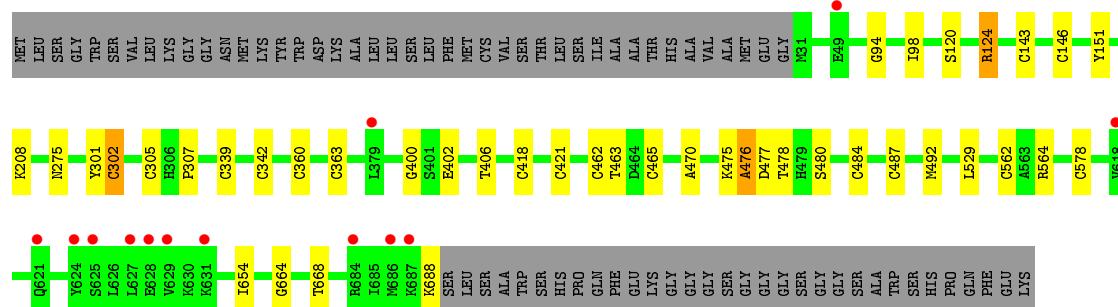
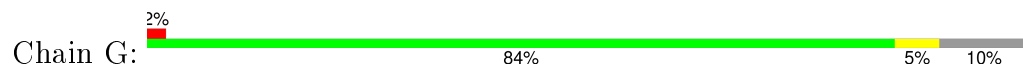




• Molecule 1: MccA



• Molecule 1: MccA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	211.12Å 103.04Å 233.07Å 90.00° 98.46° 90.00°	Depositor
Resolution (Å)	49.37 – 2.20 49.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.37-2.20) 99.8 (49.38-2.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.184 , 0.220 0.187 , 0.220	Depositor DCC
R_{free} test set	24857 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 500067 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	70014	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SX, CU1, BU3, SO2, ACT, 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	0.34	0/5354	0.57	0/7212
1	B	0.32	0/5362	0.54	0/7223
1	C	0.32	0/5354	0.54	0/7212
1	D	0.32	0/5354	0.55	0/7212
1	E	0.31	0/5354	0.52	0/7212
1	F	0.31	0/5354	0.53	0/7212
1	G	0.31	0/5348	0.54	0/7204
1	H	0.31	0/5362	0.52	0/7223
1	I	0.32	0/5354	0.53	0/7212
1	J	0.30	0/5354	0.52	0/7212
1	K	0.31	0/5354	0.52	0/7212
1	L	0.30	0/5354	0.52	0/7212
All	All	0.31	0/64258	0.53	0/86558

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5224	0	5051	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5232	0	5063	83	0
1	C	5224	0	5052	84	0
1	D	5224	0	5054	90	0
1	E	5224	0	5052	93	0
1	F	5224	0	5052	88	0
1	G	5218	0	5048	92	0
1	H	5232	0	5064	85	0
1	I	5224	0	5053	91	0
1	J	5224	0	5054	87	0
1	K	5224	0	5053	84	0
1	L	5224	0	5054	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	12	0	20	0	0
4	B	18	0	30	0	0
4	C	12	0	20	0	0
4	D	12	0	20	0	0
4	E	12	0	20	2	0
4	F	18	0	30	0	0
4	G	12	0	20	0	0
4	H	18	0	30	1	0
4	I	12	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	12	0	20	0	0
4	K	12	0	20	1	0
4	L	12	0	20	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	1	0
5	D	4	0	3	0	0
5	E	4	0	3	1	0
5	F	4	0	3	1	0
5	G	4	0	3	0	0
5	H	4	0	3	0	0
5	I	4	0	3	0	0
5	J	4	0	3	0	0
5	K	4	0	3	0	0
5	L	4	0	3	0	0
6	A	344	0	240	80	0
6	B	344	0	240	79	0
6	C	344	0	240	78	0
6	D	344	0	240	85	0
6	E	344	0	240	79	0
6	F	344	0	240	78	0
6	G	344	0	240	82	0
6	H	344	0	240	85	0
6	I	344	0	240	83	0
6	J	344	0	240	80	0
6	K	344	0	240	80	0
6	L	344	0	240	85	0
7	A	3	0	0	1	0
7	D	3	0	0	0	0
7	G	3	0	0	0	0
7	I	3	0	0	0	0
8	A	416	0	0	3	0
8	B	298	0	0	0	0
8	C	285	0	0	0	0
8	D	307	0	0	1	0
8	E	219	0	0	2	0
8	F	245	0	0	0	0
8	G	232	0	0	0	0
8	H	250	0	0	0	0
8	I	218	0	0	0	0
8	J	180	0	0	0	0
8	K	158	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	126	0	0	0	0
All	All	70014	0	63836	1090	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 8.

The worst 5 of 1090 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:CYS:SG	6:A:811:HEM:HAB	1.41	1.55
1:J:143:CYS:SG	6:J:806:HEM:HAB	1.47	1.51
1:A:462:CYS:SG	6:A:811:HEM:CAB	2.02	1.46
1:A:339:CYS:SG	6:A:808:HEM:CAB	2.04	1.46
1:F:462:CYS:SG	6:F:812:HEM:CAB	2.03	1.46

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	657/732 (90%)	632 (96%)	24 (4%)	1 (0%)	52	59
1	B	658/732 (90%)	628 (95%)	29 (4%)	1 (0%)	52	59
1	C	657/732 (90%)	632 (96%)	23 (4%)	2 (0%)	46	50
1	D	657/732 (90%)	624 (95%)	32 (5%)	1 (0%)	52	59
1	E	657/732 (90%)	625 (95%)	30 (5%)	2 (0%)	46	50
1	F	657/732 (90%)	626 (95%)	29 (4%)	2 (0%)	46	50
1	G	656/732 (90%)	625 (95%)	28 (4%)	3 (0%)	34	35
1	H	658/732 (90%)	631 (96%)	26 (4%)	1 (0%)	52	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	657/732 (90%)	626 (95%)	29 (4%)	2 (0%)	46	50
1	J	657/732 (90%)	623 (95%)	32 (5%)	2 (0%)	46	50
1	K	657/732 (90%)	625 (95%)	31 (5%)	1 (0%)	52	59
1	L	657/732 (90%)	628 (96%)	27 (4%)	2 (0%)	46	50
All	All	7885/8784 (90%)	7525 (95%)	340 (4%)	20 (0%)	46	50

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	476	ALA
1	K	664	GLY
1	L	664	GLY
1	C	301	TYR
1	F	301	TYR

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	559/613 (91%)	553 (99%)	6 (1%)	80	89
1	B	560/613 (91%)	555 (99%)	5 (1%)	84	92
1	C	559/613 (91%)	554 (99%)	5 (1%)	84	92
1	D	559/613 (91%)	553 (99%)	6 (1%)	80	89
1	E	559/613 (91%)	555 (99%)	4 (1%)	88	94
1	F	559/613 (91%)	552 (99%)	7 (1%)	76	87
1	G	558/613 (91%)	554 (99%)	4 (1%)	88	94
1	H	560/613 (91%)	555 (99%)	5 (1%)	84	92
1	I	559/613 (91%)	553 (99%)	6 (1%)	80	89
1	J	559/613 (91%)	555 (99%)	4 (1%)	88	94
1	K	559/613 (91%)	554 (99%)	5 (1%)	84	92
1	L	559/613 (91%)	553 (99%)	6 (1%)	80	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6709/7356 (91%)	6646 (99%)	63 (1%)	84 92

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	194	THR
1	H	302	CYS
1	L	564	ARG
1	F	275	ASN
1	F	498	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	683	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 161 ligands modelled in this entry, 12 are monoatomic - leaving 149 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
3	SX	A	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	A	803	-	4,5,5	0.43	0	6,6,6	0.32	0
4	BU3	A	804	-	4,5,5	0.43	0	6,6,6	0.31	0
5	ACT	A	805	-	1,3,3	1.43	0	0,3,3	0.00	-
6	HEM	A	806	1	30,50,50	2.72	11 (36%)	24,82,82	2.74	12 (50%)
6	HEM	A	807	1,3,7	30,50,50	2.59	10 (33%)	24,82,82	2.64	9 (37%)
6	HEM	A	808	1	30,50,50	2.78	10 (33%)	24,82,82	2.71	14 (58%)
6	HEM	A	809	1	30,50,50	2.67	10 (33%)	24,82,82	2.48	10 (41%)
6	HEM	A	810	1	30,50,50	2.86	10 (33%)	24,82,82	2.78	12 (50%)
6	HEM	A	811	1	30,50,50	2.67	11 (36%)	24,82,82	2.68	11 (45%)
6	HEM	A	812	1	30,50,50	2.88	10 (33%)	24,82,82	2.85	12 (50%)
6	HEM	A	813	1	30,50,50	2.85	11 (36%)	24,82,82	2.61	10 (41%)
7	SO2	A	814	6	2,2,2	1.61	0	1,1,1	1.47	0
3	SX	B	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	B	803	-	4,5,5	0.47	0	6,6,6	0.16	0
4	BU3	B	804	-	4,5,5	0.46	0	6,6,6	0.29	0
4	BU3	B	805	-	4,5,5	0.38	0	6,6,6	0.16	0
5	ACT	B	806	-	1,3,3	1.53	0	0,3,3	0.00	-
6	HEM	B	807	1	30,50,50	2.72	11 (36%)	24,82,82	2.63	10 (41%)
6	HEM	B	808	1,3	30,50,50	2.62	10 (33%)	24,82,82	2.57	10 (41%)
6	HEM	B	809	1	30,50,50	2.82	11 (36%)	24,82,82	2.83	15 (62%)
6	HEM	B	810	1	30,50,50	2.73	11 (36%)	24,82,82	2.50	10 (41%)
6	HEM	B	811	1	30,50,50	2.84	11 (36%)	24,82,82	2.73	12 (50%)
6	HEM	B	812	1	30,50,50	2.70	11 (36%)	24,82,82	2.59	12 (50%)
6	HEM	B	813	1	30,50,50	2.83	11 (36%)	24,82,82	2.68	11 (45%)
6	HEM	B	814	1	30,50,50	2.75	10 (33%)	24,82,82	2.51	11 (45%)
3	SX	C	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	C	803	-	4,5,5	0.41	0	6,6,6	0.29	0
4	BU3	C	804	-	4,5,5	0.38	0	6,6,6	0.28	0
5	ACT	C	805	-	1,3,3	1.31	0	0,3,3	0.00	-
6	HEM	C	806	1	30,50,50	2.81	10 (33%)	24,82,82	2.81	11 (45%)
6	HEM	C	807	1,3	30,50,50	2.64	10 (33%)	24,82,82	2.55	9 (37%)
6	HEM	C	808	1	30,50,50	2.84	12 (40%)	24,82,82	3.00	14 (58%)
6	HEM	C	809	1	30,50,50	2.67	9 (30%)	24,82,82	2.49	10 (41%)
6	HEM	C	810	1	30,50,50	2.86	10 (33%)	24,82,82	2.63	10 (41%)
6	HEM	C	811	1	30,50,50	2.88	11 (36%)	24,82,82	2.62	11 (45%)
6	HEM	C	812	1	30,50,50	2.78	11 (36%)	24,82,82	2.70	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEM	C	813	1	30,50,50	2.75	11 (36%)	24,82,82	2.55	13 (54%)
7	SO2	D	802	6	2,2,2	1.67	0	1,1,1	1.56	0
4	BU3	D	803	-	4,5,5	0.44	0	6,6,6	0.14	0
4	BU3	D	804	-	4,5,5	0.55	0	6,6,6	0.39	0
5	ACT	D	805	-	1,3,3	1.36	0	0,3,3	0.00	-
6	HEM	D	806	1	30,50,50	2.85	10 (33%)	24,82,82	2.70	13 (54%)
6	HEM	D	807	1,7	30,50,50	2.59	10 (33%)	24,82,82	2.61	9 (37%)
6	HEM	D	808	1	30,50,50	2.88	12 (40%)	24,82,82	3.01	12 (50%)
6	HEM	D	809	1	30,50,50	2.77	11 (36%)	24,82,82	2.48	9 (37%)
6	HEM	D	810	1	30,50,50	2.80	11 (36%)	24,82,82	2.68	10 (41%)
6	HEM	D	811	1	30,50,50	2.82	10 (33%)	24,82,82	2.67	12 (50%)
6	HEM	D	812	1	30,50,50	2.82	11 (36%)	24,82,82	2.71	11 (45%)
6	HEM	D	813	1	30,50,50	2.70	11 (36%)	24,82,82	2.53	11 (45%)
3	SX	E	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	E	803	-	4,5,5	0.37	0	6,6,6	0.12	0
4	BU3	E	804	-	4,5,5	0.35	0	6,6,6	0.17	0
5	ACT	E	805	-	1,3,3	1.22	0	0,3,3	0.00	-
6	HEM	E	806	1	30,50,50	2.80	10 (33%)	24,82,82	2.64	11 (45%)
6	HEM	E	807	1,3	30,50,50	2.58	10 (33%)	24,82,82	2.56	8 (33%)
6	HEM	E	808	1	30,50,50	2.79	11 (36%)	24,82,82	2.81	14 (58%)
6	HEM	E	809	1	30,50,50	2.75	11 (36%)	24,82,82	2.46	9 (37%)
6	HEM	E	810	1	30,50,50	2.77	11 (36%)	24,82,82	2.64	12 (50%)
6	HEM	E	811	1	30,50,50	2.76	11 (36%)	24,82,82	2.62	12 (50%)
6	HEM	E	812	1	30,50,50	2.80	11 (36%)	24,82,82	2.65	11 (45%)
6	HEM	E	813	1	30,50,50	2.76	11 (36%)	24,82,82	2.56	12 (50%)
3	SX	F	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	F	803	-	4,5,5	0.45	0	6,6,6	0.41	0
4	BU3	F	804	-	4,5,5	0.52	0	6,6,6	0.29	0
4	BU3	F	805	-	4,5,5	0.48	0	6,6,6	0.24	0
5	ACT	F	806	-	1,3,3	1.09	0	0,3,3	0.00	-
6	HEM	F	807	1	30,50,50	2.85	10 (33%)	24,82,82	2.63	11 (45%)
6	HEM	F	808	1,3	30,50,50	2.58	11 (36%)	24,82,82	2.62	9 (37%)
6	HEM	F	809	1	30,50,50	2.80	12 (40%)	24,82,82	2.84	13 (54%)
6	HEM	F	810	1	30,50,50	2.76	11 (36%)	24,82,82	2.47	9 (37%)
6	HEM	F	811	1	30,50,50	2.82	11 (36%)	24,82,82	2.77	14 (58%)
6	HEM	F	812	1	30,50,50	2.78	11 (36%)	24,82,82	2.70	13 (54%)
6	HEM	F	813	1	30,50,50	2.84	11 (36%)	24,82,82	2.76	11 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEM	F	814	1	30,50,50	2.78	11 (36%)	24,82,82	2.53	10 (41%)
3	SX	G	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	G	803	-	4,5,5	0.51	0	6,6,6	0.28	0
4	BU3	G	804	-	4,5,5	0.47	0	6,6,6	0.14	0
5	ACT	G	805	-	1,3,3	1.07	0	0,3,3	0.00	-
6	HEM	G	806	1	30,50,50	2.73	11 (36%)	24,82,82	2.56	10 (41%)
6	HEM	G	807	1,3,7	30,50,50	2.57	10 (33%)	24,82,82	2.65	10 (41%)
6	HEM	G	808	1	30,50,50	2.70	11 (36%)	24,82,82	2.73	13 (54%)
6	HEM	G	809	1	30,50,50	2.71	11 (36%)	24,82,82	2.47	10 (41%)
6	HEM	G	810	1	30,50,50	2.82	11 (36%)	24,82,82	2.60	12 (50%)
6	HEM	G	811	1	30,50,50	2.88	11 (36%)	24,82,82	2.73	13 (54%)
6	HEM	G	812	1	30,50,50	2.81	11 (36%)	24,82,82	2.68	11 (45%)
6	HEM	G	813	1	30,50,50	2.73	11 (36%)	24,82,82	2.57	14 (58%)
7	SO2	G	814	6	2,2,2	1.60	0	1,1,1	1.62	0
3	SX	H	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	H	803	-	4,5,5	0.36	0	6,6,6	0.20	0
4	BU3	H	804	-	4,5,5	0.45	0	6,6,6	0.26	0
4	BU3	H	805	-	4,5,5	0.32	0	6,6,6	0.41	0
5	ACT	H	806	-	1,3,3	1.18	0	0,3,3	0.00	-
6	HEM	H	807	1	30,50,50	2.83	11 (36%)	24,82,82	2.69	12 (50%)
6	HEM	H	808	1,3	30,50,50	2.62	10 (33%)	24,82,82	2.61	11 (45%)
6	HEM	H	809	1	30,50,50	2.83	12 (40%)	24,82,82	2.78	13 (54%)
6	HEM	H	810	1	30,50,50	2.73	11 (36%)	24,82,82	2.47	10 (41%)
6	HEM	H	811	1	30,50,50	2.72	11 (36%)	24,82,82	2.71	13 (54%)
6	HEM	H	812	1	30,50,50	2.74	11 (36%)	24,82,82	2.56	12 (50%)
6	HEM	H	813	1	30,50,50	2.78	11 (36%)	24,82,82	2.54	10 (41%)
6	HEM	H	814	1	30,50,50	2.72	11 (36%)	24,82,82	2.66	11 (45%)
7	SO2	I	802	6	2,2,2	1.69	0	1,1,1	1.54	0
4	BU3	I	803	-	4,5,5	0.46	0	6,6,6	0.14	0
4	BU3	I	804	-	4,5,5	0.60	0	6,6,6	0.31	0
5	ACT	I	805	-	1,3,3	1.20	0	0,3,3	0.00	-
6	HEM	I	806	1	30,50,50	2.76	11 (36%)	24,82,82	2.58	10 (41%)
6	HEM	I	807	1,7	30,50,50	2.66	11 (36%)	24,82,82	2.63	11 (45%)
6	HEM	I	808	1	30,50,50	2.72	11 (36%)	24,82,82	2.71	14 (58%)
6	HEM	I	809	1	30,50,50	2.66	11 (36%)	24,82,82	2.44	8 (33%)
6	HEM	I	810	1	30,50,50	2.76	10 (33%)	24,82,82	2.64	12 (50%)
6	HEM	I	811	1	30,50,50	2.75	11 (36%)	24,82,82	2.70	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEM	I	812	1	30,50,50	2.71	11 (36%)	24,82,82	2.67	11 (45%)
6	HEM	I	813	1	30,50,50	2.77	11 (36%)	24,82,82	2.55	11 (45%)
3	SX	J	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	J	803	-	4,5,5	0.38	0	6,6,6	0.27	0
4	BU3	J	804	-	4,5,5	0.54	0	6,6,6	0.15	0
5	ACT	J	805	-	1,3,3	1.20	0	0,3,3	0.00	-
6	HEM	J	806	1	30,50,50	2.66	12 (40%)	24,82,82	2.73	12 (50%)
6	HEM	J	807	1,3	30,50,50	2.60	10 (33%)	24,82,82	2.67	11 (45%)
6	HEM	J	808	1	30,50,50	2.84	11 (36%)	24,82,82	2.77	15 (62%)
6	HEM	J	809	1	30,50,50	2.77	10 (33%)	24,82,82	2.42	11 (45%)
6	HEM	J	810	1	30,50,50	2.80	11 (36%)	24,82,82	2.56	9 (37%)
6	HEM	J	811	1	30,50,50	2.78	11 (36%)	24,82,82	2.65	12 (50%)
6	HEM	J	812	1	30,50,50	2.81	12 (40%)	24,82,82	2.67	10 (41%)
6	HEM	J	813	1	30,50,50	2.71	11 (36%)	24,82,82	2.53	11 (45%)
3	SX	K	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	K	803	-	4,5,5	0.41	0	6,6,6	0.32	0
4	BU3	K	804	-	4,5,5	0.58	0	6,6,6	0.27	0
5	ACT	K	805	-	1,3,3	1.30	0	0,3,3	0.00	-
6	HEM	K	806	1	30,50,50	2.63	11 (36%)	24,82,82	2.66	10 (41%)
6	HEM	K	807	1,3	30,50,50	2.72	11 (36%)	24,82,82	2.64	9 (37%)
6	HEM	K	808	1	30,50,50	2.74	11 (36%)	24,82,82	2.66	13 (54%)
6	HEM	K	809	1	30,50,50	2.70	10 (33%)	24,82,82	2.52	12 (50%)
6	HEM	K	810	1	30,50,50	2.77	11 (36%)	24,82,82	2.63	13 (54%)
6	HEM	K	811	1	30,50,50	2.75	11 (36%)	24,82,82	2.59	11 (45%)
6	HEM	K	812	1	30,50,50	2.73	11 (36%)	24,82,82	2.57	10 (41%)
6	HEM	K	813	1	30,50,50	2.77	11 (36%)	24,82,82	2.55	10 (41%)
3	SX	L	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	L	803	-	4,5,5	0.53	0	6,6,6	0.21	0
4	BU3	L	804	-	4,5,5	0.49	0	6,6,6	0.32	0
5	ACT	L	805	-	1,3,3	1.24	0	0,3,3	0.00	-
6	HEM	L	806	1	30,50,50	2.81	10 (33%)	24,82,82	2.56	12 (50%)
6	HEM	L	807	1,3	30,50,50	2.63	10 (33%)	24,82,82	2.62	11 (45%)
6	HEM	L	808	1	30,50,50	2.72	11 (36%)	24,82,82	2.72	13 (54%)
6	HEM	L	809	1	30,50,50	2.69	11 (36%)	24,82,82	2.48	11 (45%)
6	HEM	L	810	1	30,50,50	2.76	11 (36%)	24,82,82	2.62	14 (58%)
6	HEM	L	811	1	30,50,50	2.80	11 (36%)	24,82,82	2.90	13 (54%)
6	HEM	L	812	1	30,50,50	2.70	11 (36%)	24,82,82	2.51	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEM	L	813	1	30,50,50	2.81	13 (43%)	24,82,82	2.39	13 (54%)

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
3	SX	A	802	6	-	0/0/0/0	0/0/0/0
4	BU3	A	803	-	-	0/4/4/4	0/0/0/0
4	BU3	A	804	-	-	0/4/4/4	0/0/0/0
5	ACT	A	805	-	-	0/0/0/0	0/0/0/0
6	HEM	A	806	1	-	0/10/54/54	0/0/8/8
6	HEM	A	807	1,3,7	-	0/10/54/54	0/0/8/8
6	HEM	A	808	1	-	0/10/54/54	0/0/8/8
6	HEM	A	809	1	-	0/10/54/54	0/0/8/8
6	HEM	A	810	1	-	0/10/54/54	0/0/8/8
6	HEM	A	811	1	-	0/10/54/54	0/0/8/8
6	HEM	A	812	1	-	0/10/54/54	0/0/8/8
6	HEM	A	813	1	-	0/10/54/54	0/0/8/8
7	SO2	A	814	6	-	0/0/0/0	0/0/0/0
3	SX	B	802	6	-	0/0/0/0	0/0/0/0
4	BU3	B	803	-	-	0/4/4/4	0/0/0/0
4	BU3	B	804	-	-	0/4/4/4	0/0/0/0
4	BU3	B	805	-	-	0/4/4/4	0/0/0/0
5	ACT	B	806	-	-	0/0/0/0	0/0/0/0
6	HEM	B	807	1	-	0/10/54/54	0/0/8/8
6	HEM	B	808	1,3	-	0/10/54/54	0/0/8/8
6	HEM	B	809	1	-	0/10/54/54	0/0/8/8
6	HEM	B	810	1	-	0/10/54/54	0/0/8/8
6	HEM	B	811	1	-	0/10/54/54	0/0/8/8
6	HEM	B	812	1	-	0/10/54/54	0/0/8/8
6	HEM	B	813	1	-	0/10/54/54	0/0/8/8
6	HEM	B	814	1	-	0/10/54/54	0/0/8/8
3	SX	C	802	6	-	0/0/0/0	0/0/0/0
4	BU3	C	803	-	-	0/4/4/4	0/0/0/0
4	BU3	C	804	-	-	0/4/4/4	0/0/0/0
5	ACT	C	805	-	-	0/0/0/0	0/0/0/0
6	HEM	C	806	1	-	0/10/54/54	0/0/8/8
6	HEM	C	807	1,3	-	0/10/54/54	0/0/8/8
6	HEM	C	808	1	-	0/10/54/54	0/0/8/8
6	HEM	C	809	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	C	810	1	-	0/10/54/54	0/0/8/8
6	HEM	C	811	1	-	0/10/54/54	0/0/8/8
6	HEM	C	812	1	-	0/10/54/54	0/0/8/8
6	HEM	C	813	1	-	0/10/54/54	0/0/8/8
7	SO2	D	802	6	-	0/0/0/0	0/0/0/0
4	BU3	D	803	-	-	0/4/4/4	0/0/0/0
4	BU3	D	804	-	-	0/4/4/4	0/0/0/0
5	ACT	D	805	-	-	0/0/0/0	0/0/0/0
6	HEM	D	806	1	-	0/10/54/54	0/0/8/8
6	HEM	D	807	1,7	-	0/10/54/54	0/0/8/8
6	HEM	D	808	1	-	0/10/54/54	0/0/8/8
6	HEM	D	809	1	-	0/10/54/54	0/0/8/8
6	HEM	D	810	1	-	0/10/54/54	0/0/8/8
6	HEM	D	811	1	-	0/10/54/54	0/0/8/8
6	HEM	D	812	1	-	0/10/54/54	0/0/8/8
6	HEM	D	813	1	-	0/10/54/54	0/0/8/8
3	SX	E	802	6	-	0/0/0/0	0/0/0/0
4	BU3	E	803	-	-	0/4/4/4	0/0/0/0
4	BU3	E	804	-	-	0/4/4/4	0/0/0/0
5	ACT	E	805	-	-	0/0/0/0	0/0/0/0
6	HEM	E	806	1	-	0/10/54/54	0/0/8/8
6	HEM	E	807	1,3	-	0/10/54/54	0/0/8/8
6	HEM	E	808	1	-	0/10/54/54	0/0/8/8
6	HEM	E	809	1	-	0/10/54/54	0/0/8/8
6	HEM	E	810	1	-	0/10/54/54	0/0/8/8
6	HEM	E	811	1	-	0/10/54/54	0/0/8/8
6	HEM	E	812	1	-	0/10/54/54	0/0/8/8
6	HEM	E	813	1	-	0/10/54/54	0/0/8/8
3	SX	F	802	6	-	0/0/0/0	0/0/0/0
4	BU3	F	803	-	-	0/4/4/4	0/0/0/0
4	BU3	F	804	-	-	0/4/4/4	0/0/0/0
4	BU3	F	805	-	-	0/4/4/4	0/0/0/0
5	ACT	F	806	-	-	0/0/0/0	0/0/0/0
6	HEM	F	807	1	-	0/10/54/54	0/0/8/8
6	HEM	F	808	1,3	-	0/10/54/54	0/0/8/8
6	HEM	F	809	1	-	0/10/54/54	0/0/8/8
6	HEM	F	810	1	-	0/10/54/54	0/0/8/8
6	HEM	F	811	1	-	0/10/54/54	0/0/8/8
6	HEM	F	812	1	-	0/10/54/54	0/0/8/8
6	HEM	F	813	1	-	0/10/54/54	0/0/8/8
6	HEM	F	814	1	-	0/10/54/54	0/0/8/8
3	SX	G	802	6	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BU3	G	803	-	-	0/4/4/4	0/0/0/0
4	BU3	G	804	-	-	0/4/4/4	0/0/0/0
5	ACT	G	805	-	-	0/0/0/0	0/0/0/0
6	HEM	G	806	1	-	0/10/54/54	0/0/8/8
6	HEM	G	807	1,3,7	-	0/10/54/54	0/0/8/8
6	HEM	G	808	1	-	0/10/54/54	0/0/8/8
6	HEM	G	809	1	-	0/10/54/54	0/0/8/8
6	HEM	G	810	1	-	0/10/54/54	0/0/8/8
6	HEM	G	811	1	-	0/10/54/54	0/0/8/8
6	HEM	G	812	1	-	0/10/54/54	0/0/8/8
6	HEM	G	813	1	-	0/10/54/54	0/0/8/8
7	SO2	G	814	6	-	0/0/0/0	0/0/0/0
3	SX	H	802	6	-	0/0/0/0	0/0/0/0
4	BU3	H	803	-	-	0/4/4/4	0/0/0/0
4	BU3	H	804	-	-	0/4/4/4	0/0/0/0
4	BU3	H	805	-	-	0/4/4/4	0/0/0/0
5	ACT	H	806	-	-	0/0/0/0	0/0/0/0
6	HEM	H	807	1	-	0/10/54/54	0/0/8/8
6	HEM	H	808	1,3	-	0/10/54/54	0/0/8/8
6	HEM	H	809	1	-	0/10/54/54	0/0/8/8
6	HEM	H	810	1	-	0/10/54/54	0/0/8/8
6	HEM	H	811	1	-	0/10/54/54	0/0/8/8
6	HEM	H	812	1	-	0/10/54/54	0/0/8/8
6	HEM	H	813	1	-	0/10/54/54	0/0/8/8
6	HEM	H	814	1	-	0/10/54/54	0/0/8/8
7	SO2	I	802	6	-	0/0/0/0	0/0/0/0
4	BU3	I	803	-	-	0/4/4/4	0/0/0/0
4	BU3	I	804	-	-	0/4/4/4	0/0/0/0
5	ACT	I	805	-	-	0/0/0/0	0/0/0/0
6	HEM	I	806	1	-	0/10/54/54	0/0/8/8
6	HEM	I	807	1,7	-	0/10/54/54	0/0/8/8
6	HEM	I	808	1	-	0/10/54/54	0/0/8/8
6	HEM	I	809	1	-	0/10/54/54	0/0/8/8
6	HEM	I	810	1	-	0/10/54/54	0/0/8/8
6	HEM	I	811	1	-	0/10/54/54	0/0/8/8
6	HEM	I	812	1	-	0/10/54/54	0/0/8/8
6	HEM	I	813	1	-	0/10/54/54	0/0/8/8
3	SX	J	802	6	-	0/0/0/0	0/0/0/0
4	BU3	J	803	-	-	0/4/4/4	0/0/0/0
4	BU3	J	804	-	-	0/4/4/4	0/0/0/0
5	ACT	J	805	-	-	0/0/0/0	0/0/0/0
6	HEM	J	806	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	J	807	1,3	-	0/10/54/54	0/0/8/8
6	HEM	J	808	1	-	0/10/54/54	0/0/8/8
6	HEM	J	809	1	-	0/10/54/54	0/0/8/8
6	HEM	J	810	1	-	0/10/54/54	0/0/8/8
6	HEM	J	811	1	-	0/10/54/54	0/0/8/8
6	HEM	J	812	1	-	0/10/54/54	0/0/8/8
6	HEM	J	813	1	-	0/10/54/54	0/0/8/8
3	SX	K	802	6	-	0/0/0/0	0/0/0/0
4	BU3	K	803	-	-	0/4/4/4	0/0/0/0
4	BU3	K	804	-	-	0/4/4/4	0/0/0/0
5	ACT	K	805	-	-	0/0/0/0	0/0/0/0
6	HEM	K	806	1	-	0/10/54/54	0/0/8/8
6	HEM	K	807	1,3	-	0/10/54/54	0/0/8/8
6	HEM	K	808	1	-	0/10/54/54	0/0/8/8
6	HEM	K	809	1	-	0/10/54/54	0/0/8/8
6	HEM	K	810	1	-	0/10/54/54	0/0/8/8
6	HEM	K	811	1	-	0/10/54/54	0/0/8/8
6	HEM	K	812	1	-	0/10/54/54	0/0/8/8
6	HEM	K	813	1	-	0/10/54/54	0/0/8/8
3	SX	L	802	6	-	0/0/0/0	0/0/0/0
4	BU3	L	803	-	-	0/4/4/4	0/0/0/0
4	BU3	L	804	-	-	0/4/4/4	0/0/0/0
5	ACT	L	805	-	-	0/0/0/0	0/0/0/0
6	HEM	L	806	1	-	0/10/54/54	0/0/8/8
6	HEM	L	807	1,3	-	0/10/54/54	0/0/8/8
6	HEM	L	808	1	-	0/10/54/54	0/0/8/8
6	HEM	L	809	1	-	0/10/54/54	0/0/8/8
6	HEM	L	810	1	-	0/10/54/54	0/0/8/8
6	HEM	L	811	1	-	0/10/54/54	0/0/8/8
6	HEM	L	812	1	-	0/10/54/54	0/0/8/8
6	HEM	L	813	1	-	0/10/54/54	0/0/8/8

The worst 5 of 1038 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	812	HEM	C3B-C4B	-7.55	1.45	1.51
6	A	810	HEM	C3B-C4B	-7.18	1.45	1.51
6	J	809	HEM	C2D-C3D	-7.14	1.33	1.54
6	D	806	HEM	C3B-C4B	-7.14	1.45	1.51
6	F	807	HEM	C3B-C4B	-7.12	1.45	1.51

The worst 5 of 1086 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	L	811	HEM	C3B-CAB-CBB	-7.44	113.04	124.46
6	D	808	HEM	C3B-CAB-CBB	-6.98	113.75	124.46
6	C	806	HEM	C3B-CAB-CBB	-6.65	114.26	124.46
6	A	806	HEM	C3B-CAB-CBB	-5.81	115.54	124.46
6	A	810	HEM	C3B-CAB-CBB	-5.79	115.58	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

103 monomers are involved in 982 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	806	HEM	9	0
6	A	807	HEM	12	0
6	A	808	HEM	9	0
6	A	809	HEM	13	0
6	A	810	HEM	10	0
6	A	811	HEM	7	0
6	A	812	HEM	11	0
6	A	813	HEM	10	0
7	A	814	SO2	1	0
6	B	807	HEM	11	0
6	B	808	HEM	13	0
6	B	809	HEM	9	0
6	B	810	HEM	10	0
6	B	811	HEM	11	0
6	B	812	HEM	8	0
6	B	813	HEM	9	0
6	B	814	HEM	9	0
5	C	805	ACT	1	0
6	C	806	HEM	9	0
6	C	807	HEM	14	0
6	C	808	HEM	10	0
6	C	809	HEM	11	0
6	C	810	HEM	9	0
6	C	811	HEM	8	0
6	C	812	HEM	8	0
6	C	813	HEM	9	0
6	D	806	HEM	10	0
6	D	807	HEM	13	0
6	D	808	HEM	11	0
6	D	809	HEM	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	810	HEM	11	0
6	D	811	HEM	10	0
6	D	812	HEM	9	0
6	D	813	HEM	9	0
4	E	804	BU3	2	0
5	E	805	ACT	1	0
6	E	806	HEM	11	0
6	E	807	HEM	11	0
6	E	808	HEM	9	0
6	E	809	HEM	12	0
6	E	810	HEM	9	0
6	E	811	HEM	7	0
6	E	812	HEM	10	0
6	E	813	HEM	10	0
5	F	806	ACT	1	0
6	F	807	HEM	12	0
6	F	808	HEM	12	0
6	F	809	HEM	8	0
6	F	810	HEM	11	0
6	F	811	HEM	10	0
6	F	812	HEM	7	0
6	F	813	HEM	9	0
6	F	814	HEM	9	0
6	G	806	HEM	12	0
6	G	807	HEM	12	0
6	G	808	HEM	8	0
6	G	809	HEM	11	0
6	G	810	HEM	9	0
6	G	811	HEM	8	0
6	G	812	HEM	13	0
6	G	813	HEM	9	0
4	H	803	BU3	1	0
6	H	807	HEM	10	0
6	H	808	HEM	14	0
6	H	809	HEM	9	0
6	H	810	HEM	10	0
6	H	811	HEM	13	0
6	H	812	HEM	7	0
6	H	813	HEM	11	0
6	H	814	HEM	12	0
6	I	806	HEM	10	0
6	I	807	HEM	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	808	HEM	10	0
6	I	809	HEM	11	0
6	I	810	HEM	11	0
6	I	811	HEM	10	0
6	I	812	HEM	11	0
6	I	813	HEM	8	0
6	J	806	HEM	11	0
6	J	807	HEM	12	0
6	J	808	HEM	8	0
6	J	809	HEM	12	0
6	J	810	HEM	8	0
6	J	811	HEM	8	0
6	J	812	HEM	8	0
6	J	813	HEM	13	0
4	K	803	BU3	1	0
6	K	806	HEM	10	0
6	K	807	HEM	14	0
6	K	808	HEM	11	0
6	K	809	HEM	12	0
6	K	810	HEM	9	0
6	K	811	HEM	10	0
6	K	812	HEM	8	0
6	K	813	HEM	7	0
6	L	806	HEM	9	0
6	L	807	HEM	17	0
6	L	808	HEM	10	0
6	L	809	HEM	14	0
6	L	810	HEM	8	0
6	L	811	HEM	9	0
6	L	812	HEM	9	0
6	L	813	HEM	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	659/732 (90%)	-0.20	14 (2%) 67 65	16, 24, 45, 95	0
1	B	660/732 (90%)	-0.25	6 (0%) 85 85	20, 33, 49, 82	0
1	C	659/732 (90%)	-0.19	5 (0%) 87 87	18, 32, 54, 86	0
1	D	659/732 (90%)	-0.19	21 (3%) 51 50	21, 32, 56, 102	0
1	E	659/732 (90%)	-0.10	10 (1%) 76 75	23, 38, 59, 104	0
1	F	659/732 (90%)	-0.02	14 (2%) 67 65	21, 38, 63, 107	0
1	G	658/732 (89%)	-0.20	13 (1%) 68 67	25, 37, 57, 93	0
1	H	660/732 (90%)	-0.16	7 (1%) 82 82	25, 37, 61, 95	0
1	I	659/732 (90%)	0.08	21 (3%) 51 50	26, 39, 58, 76	0
1	J	659/732 (90%)	0.08	21 (3%) 51 50	27, 46, 69, 96	0
1	K	659/732 (90%)	0.05	8 (1%) 81 80	25, 46, 68, 85	0
1	L	659/732 (90%)	0.45	48 (7%) 18 17	30, 51, 76, 89	0
All	All	7909/8784 (90%)	-0.05	188 (2%) 62 61	16, 37, 65, 107	0

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	629	VAL	7.7
1	F	629	VAL	7.4
1	A	629	VAL	6.7
1	G	379	LEU	5.4
1	H	629	VAL	5.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
5	ACT	A	805	4/4	0.81	0.28	7.67	47,50,50,51	0
5	ACT	D	805	4/4	0.81	0.27	7.28	59,62,62,63	0
5	ACT	H	806	4/4	0.81	0.28	6.84	59,63,64,64	0
4	BU3	B	805	6/6	0.89	0.26	6.63	55,59,59,60	0
5	ACT	K	805	4/4	0.76	0.20	6.20	58,58,58,59	0
5	ACT	F	806	4/4	0.92	0.19	6.01	54,56,56,56	0
4	BU3	A	804	6/6	0.87	0.20	5.83	40,41,42,43	0
5	ACT	B	806	4/4	0.82	0.29	5.74	46,47,48,49	0
4	BU3	E	804	6/6	0.86	0.30	4.89	77,79,79,79	0
5	ACT	J	805	4/4	0.85	0.26	4.86	62,62,62,63	0
4	BU3	G	804	6/6	0.94	0.18	4.70	58,59,61,61	0
5	ACT	C	805	4/4	0.87	0.25	4.36	58,59,61,61	0
4	BU3	H	805	6/6	0.84	0.25	4.32	49,50,51,53	0
4	BU3	K	804	6/6	0.77	0.31	3.78	74,77,78,79	0
5	ACT	L	805	4/4	0.86	0.34	3.74	61,63,63,64	0
5	ACT	E	805	4/4	0.83	0.23	3.65	58,60,61,61	0
3	SX	H	802	2/2	0.90	0.14	3.51	58,58,58,61	0
4	BU3	J	804	6/6	0.86	0.21	3.43	64,65,66,66	0
4	BU3	C	804	6/6	0.82	0.24	3.31	48,49,49,50	0
5	ACT	G	805	4/4	0.89	0.20	3.27	51,51,52,52	0
4	BU3	B	804	6/6	0.90	0.21	2.80	50,52,53,53	0
7	SO2	G	814	3/3	0.97	0.15	2.53	74,74,74,76	3
3	SX	B	802	2/2	0.88	0.18	2.42	51,51,51,52	0
4	BU3	H	804	6/6	0.90	0.18	2.23	61,62,62,64	0
4	BU3	I	804	6/6	0.87	0.28	2.17	60,61,62,62	0
3	SX	F	802	2/2	0.95	0.16	2.09	69,69,69,73	0
6	HEM	F	814	43/43	0.97	0.13	1.94	24,26,34,39	0
7	SO2	I	802	3/3	0.85	0.18	1.15	63,63,64,71	0
3	SX	C	802	2/2	0.90	0.16	1.15	55,55,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	HEM	B	813	43/43	0.97	0.12	1.15	24,26,29,30	0
6	HEM	C	807	43/43	0.98	0.17	1.08	21,23,23,24	0
6	HEM	L	812	43/43	0.96	0.14	1.05	37,39,41,42	0
3	SX	E	802	2/2	0.89	0.16	1.04	66,66,66,68	0
6	HEM	D	811	43/43	0.97	0.13	1.01	21,23,33,42	0
3	SX	G	802	2/2	0.98	0.13	1.00	31,31,31,32	2
6	HEM	D	812	43/43	0.98	0.12	0.92	20,22,24,27	0
6	HEM	D	813	43/43	0.97	0.12	0.90	25,26,34,36	0
5	ACT	I	805	4/4	0.94	0.24	0.86	50,50,52,52	0
6	HEM	E	813	43/43	0.96	0.14	0.79	30,32,44,55	0
6	HEM	H	814	43/43	0.97	0.12	0.73	25,26,36,40	0
6	HEM	B	809	43/43	0.98	0.17	0.72	20,22,23,27	0
4	BU3	D	804	6/6	0.94	0.13	0.71	45,46,47,47	0
6	HEM	E	812	43/43	0.97	0.11	0.67	26,28,31,32	0
6	HEM	G	809	43/43	0.97	0.14	0.67	24,27,28,28	0
4	BU3	F	804	6/6	0.93	0.15	0.66	62,63,64,65	0
6	HEM	F	808	43/43	0.97	0.13	0.65	25,28,32,35	0
6	HEM	E	811	43/43	0.97	0.11	0.65	27,29,36,43	0
6	HEM	H	811	43/43	0.97	0.13	0.64	25,27,30,33	0
6	HEM	C	813	43/43	0.96	0.14	0.62	30,32,45,50	0
6	HEM	K	810	43/43	0.97	0.12	0.61	27,29,33,37	0
6	HEM	B	807	43/43	0.97	0.14	0.61	21,22,23,24	0
6	HEM	E	808	43/43	0.97	0.18	0.59	23,24,25,27	0
6	HEM	F	812	43/43	0.96	0.12	0.58	21,23,32,42	0
6	HEM	B	814	43/43	0.96	0.15	0.56	29,31,43,46	0
6	HEM	C	809	43/43	0.98	0.16	0.56	18,20,21,21	0
6	HEM	E	807	43/43	0.97	0.17	0.53	28,29,31,33	0
6	HEM	L	807	43/43	0.97	0.20	0.52	37,39,42,44	0
6	HEM	F	811	43/43	0.98	0.14	0.50	21,22,26,31	0
6	HEM	A	812	43/43	0.97	0.13	0.49	18,19,22,25	0
6	HEM	K	808	43/43	0.97	0.14	0.48	27,27,29,31	0
6	HEM	K	806	43/43	0.97	0.18	0.48	26,28,31,32	0
6	HEM	E	810	43/43	0.97	0.14	0.48	24,25,29,34	0
6	HEM	K	807	43/43	0.97	0.14	0.46	38,41,45,49	0
6	HEM	A	807	43/43	0.97	0.14	0.46	16,16,17,17	0
6	HEM	E	806	43/43	0.98	0.16	0.45	23,24,26,26	0
6	HEM	A	813	43/43	0.97	0.13	0.43	21,23,31,34	0
6	HEM	J	811	43/43	0.96	0.12	0.43	29,31,41,51	0
6	HEM	C	812	43/43	0.97	0.11	0.41	23,25,28,31	0
6	HEM	B	811	43/43	0.97	0.15	0.37	21,22,28,34	0
6	HEM	C	811	43/43	0.97	0.12	0.37	24,26,36,46	0
6	HEM	A	809	43/43	0.98	0.16	0.36	14,15,17,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	HEM	L	809	43/43	0.97	0.21	0.36	32,34,38,40	0
6	HEM	J	813	43/43	0.97	0.14	0.31	37,40,53,62	0
6	HEM	C	806	43/43	0.98	0.15	0.31	16,17,18,19	0
6	HEM	B	812	43/43	0.97	0.14	0.30	23,24,33,43	0
6	HEM	L	813	43/43	0.94	0.17	0.29	46,48,58,65	0
6	HEM	F	809	43/43	0.97	0.19	0.28	28,29,30,31	0
6	HEM	J	810	43/43	0.97	0.13	0.28	26,28,33,37	0
6	HEM	I	808	43/43	0.97	0.21	0.27	27,28,30,30	0
6	HEM	A	806	43/43	0.97	0.14	0.27	19,20,21,21	0
6	HEM	E	809	43/43	0.97	0.17	0.27	24,25,26,26	0
6	HEM	K	812	43/43	0.96	0.11	0.24	31,34,36,37	0
6	HEM	H	810	43/43	0.97	0.12	0.23	28,30,31,32	0
6	HEM	K	811	43/43	0.97	0.12	0.23	27,30,39,47	0
6	HEM	L	810	43/43	0.96	0.17	0.22	31,32,39,43	0
6	HEM	J	809	43/43	0.98	0.13	0.22	29,31,33,35	0
6	HEM	B	808	43/43	0.98	0.14	0.21	24,25,26,28	0
6	HEM	A	808	43/43	0.98	0.16	0.21	17,18,20,23	0
6	HEM	F	807	43/43	0.97	0.21	0.21	25,29,32,33	0
6	HEM	I	809	43/43	0.96	0.21	0.20	26,27,30,32	0
6	HEM	D	809	43/43	0.98	0.12	0.19	21,22,23,25	0
6	HEM	I	813	43/43	0.95	0.14	0.18	33,35,46,49	0
6	HEM	A	811	43/43	0.97	0.14	0.18	19,20,28,33	0
6	HEM	F	810	43/43	0.98	0.15	0.17	25,27,27,27	0
6	HEM	H	807	43/43	0.97	0.18	0.16	32,33,35,36	0
6	HEM	J	806	43/43	0.97	0.14	0.15	28,30,32,34	0
6	HEM	I	812	43/43	0.97	0.11	0.15	27,28,31,33	0
6	HEM	G	811	43/43	0.97	0.12	0.15	28,31,43,49	0
4	BU3	L	804	6/6	0.89	0.18	0.13	69,70,70,72	0
6	HEM	H	809	43/43	0.97	0.16	0.13	29,31,34,39	0
6	HEM	C	808	43/43	0.98	0.16	0.12	18,19,21,23	0
6	HEM	G	807	43/43	0.98	0.11	0.09	25,26,28,29	0
6	HEM	G	810	43/43	0.97	0.12	0.09	24,24,29,31	0
6	HEM	K	813	43/43	0.95	0.13	0.08	39,41,52,55	0
6	HEM	J	808	43/43	0.97	0.13	0.08	27,28,29,30	0
6	HEM	I	811	43/43	0.96	0.13	0.07	25,26,35,43	0
6	HEM	L	806	43/43	0.97	0.14	0.02	24,30,33,34	0
6	HEM	G	808	43/43	0.97	0.13	0.01	25,26,28,30	0
6	HEM	L	808	43/43	0.97	0.16	0.01	31,33,35,38	0
6	HEM	H	812	43/43	0.96	0.12	-0.02	23,26,35,43	0
6	HEM	F	813	43/43	0.97	0.10	-0.03	21,23,24,26	0
6	HEM	G	812	43/43	0.97	0.10	-0.03	26,28,32,33	0
6	HEM	B	810	43/43	0.98	0.15	-0.03	20,23,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	HEM	C	810	43/43	0.97	0.14	-0.05	20,21,24,28	0
6	HEM	I	806	43/43	0.97	0.16	-0.06	27,30,32,32	0
7	SO2	A	814	3/3	0.96	0.12	-0.07	16,16,16,16	3
6	HEM	H	808	43/43	0.97	0.11	-0.07	24,29,31,33	0
6	HEM	I	810	43/43	0.96	0.15	-0.08	24,26,30,35	0
6	HEM	G	813	43/43	0.96	0.11	-0.09	28,31,38,45	0
6	HEM	A	810	43/43	0.97	0.14	-0.12	16,17,21,24	0
6	HEM	K	809	43/43	0.97	0.13	-0.14	28,31,34,35	0
6	HEM	H	813	43/43	0.97	0.11	-0.14	26,27,28,29	0
3	SX	K	802	2/2	0.94	0.13	-0.15	67,67,67,71	0
6	HEM	D	808	43/43	0.97	0.12	-0.17	25,27,31,35	0
6	HEM	I	807	43/43	0.97	0.15	-0.20	29,32,33,34	0
6	HEM	D	810	43/43	0.97	0.12	-0.20	21,22,25,28	0
6	HEM	D	807	43/43	0.97	0.11	-0.20	21,22,24,25	0
6	HEM	G	806	43/43	0.97	0.12	-0.22	27,28,29,29	0
6	HEM	J	812	43/43	0.97	0.10	-0.31	34,36,37,39	0
6	HEM	J	807	43/43	0.96	0.12	-0.37	34,36,38,39	0
6	HEM	L	811	43/43	0.96	0.12	-0.45	34,37,45,49	0
6	HEM	D	806	43/43	0.97	0.12	-0.48	28,30,32,33	0
3	SX	L	802	2/2	0.98	0.15	-0.76	65,65,65,68	0
7	SO2	D	802	3/3	0.97	0.09	-1.10	51,51,53,54	0
3	SX	J	802	2/2	0.96	0.10	-1.17	57,57,57,62	0
3	SX	A	802	2/2	0.94	0.10	-1.42	45,45,45,50	2
2	CU1	B	801	1/1	0.98	0.08	-	35,35,35,35	0
2	CU1	D	801	1/1	0.97	0.10	-	33,33,33,33	0
2	CU1	K	801	1/1	0.98	0.14	-	53,53,53,53	0
4	BU3	C	803	6/6	0.87	0.33	-	52,53,54,55	0
2	CU1	E	801	1/1	0.96	0.08	-	37,37,37,37	0
2	CU1	A	801	1/1	0.99	0.08	-	26,26,26,26	0
2	CU1	L	801	1/1	0.94	0.06	-	55,55,55,55	0
4	BU3	K	803	6/6	0.71	0.33	-	56,58,59,60	0
2	CU1	I	801	1/1	0.99	0.10	-	39,39,39,39	0
4	BU3	F	805	6/6	0.85	0.30	-	58,60,61,62	0
4	BU3	B	803	6/6	0.88	0.28	-	50,51,52,52	0
2	CU1	G	801	1/1	0.98	0.12	-	34,34,34,34	0
4	BU3	A	803	6/6	0.89	0.34	-	47,47,48,48	0
4	BU3	L	803	6/6	0.86	0.33	-	57,58,58,60	0
4	BU3	E	803	6/6	0.92	0.29	-	50,51,54,55	0
4	BU3	G	803	6/6	0.91	0.29	-	49,50,51,52	0
4	BU3	J	803	6/6	0.87	0.33	-	55,57,58,58	0
2	CU1	F	801	1/1	0.98	0.12	-	38,38,38,38	0
4	BU3	D	803	6/6	0.86	0.28	-	50,54,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BU3	F	803	6/6	0.86	0.26	-	49,50,50,50	0
4	BU3	H	803	6/6	0.87	0.30	-	62,63,64,65	0
2	CU1	C	801	1/1	0.97	0.07	-	31,31,31,31	0
2	CU1	H	801	1/1	0.97	0.17	-	45,45,45,45	0
2	CU1	J	801	1/1	0.94	0.08	-	51,51,51,51	0
4	BU3	I	803	6/6	0.90	0.44	-	48,50,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.