Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2017 – 02:57 PM EST

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	:	unknown
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

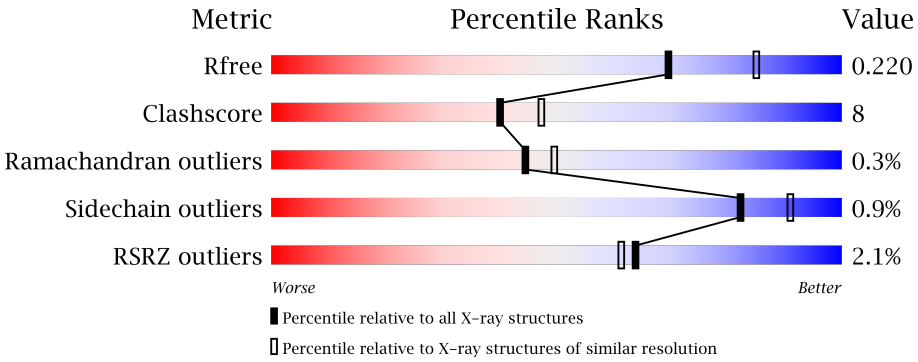
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

1 Overall quality at a glance (i)

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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (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 <=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	2% 85% 5% 10%
1	B	732	.% 85% 5% 10%
1	C	732	.% 84% 5% 10%
1	D	732	3% 84% 5% 10%
1	E	732	.% 84% 6% 10%

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Mol	Chain	Length	Quality of chain
1	F	732	2% 84% 6% 10%
1	G	732	2% 84% 5% 10%
1	H	732	.% 86% 5% 10%
1	I	732	2% 84% 6% 10%
1	J	732	2% 84% 6% 10%
1	K	732	.% 85% 5% 10%
1	L	732	5% 84% 6% 10%

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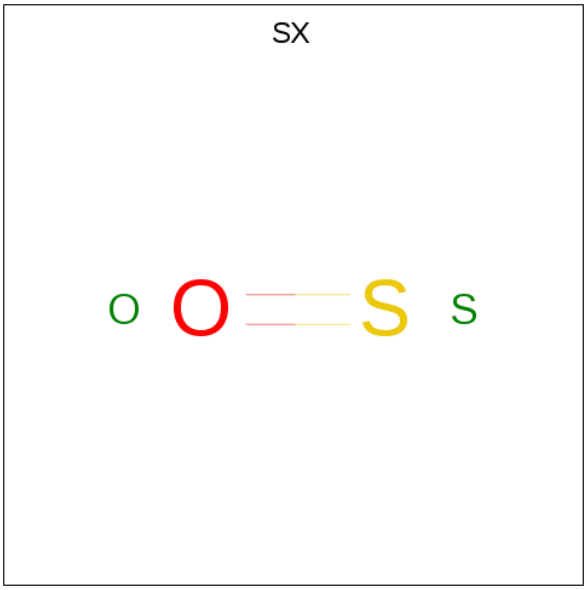
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0

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



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

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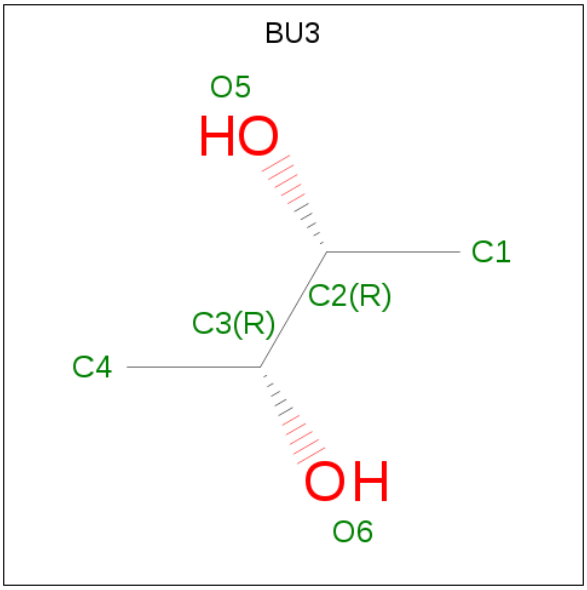
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total O S 2 1 1	0	0

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: $C_4H_{10}O_2$).



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

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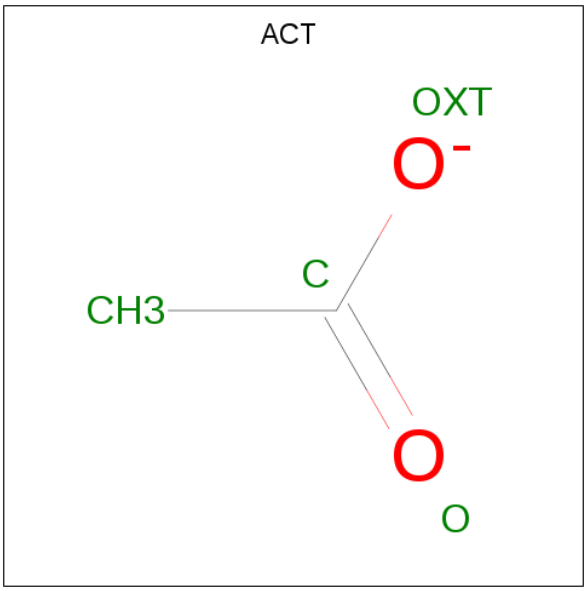
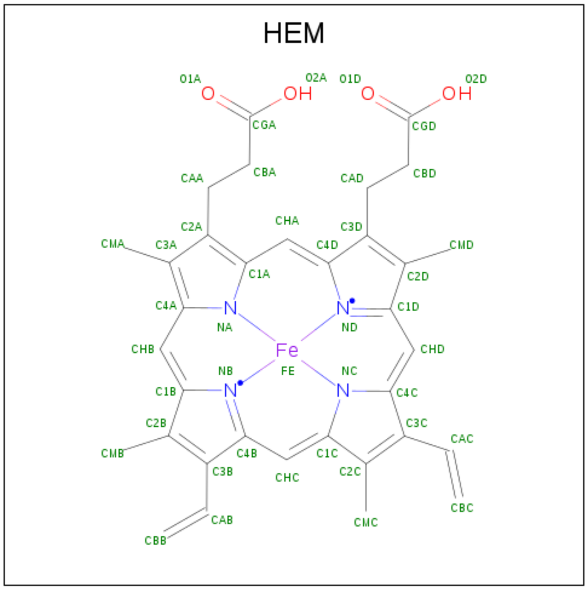
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 4 2	0	0
4	F	1	Total C O 6 4 2	0	0
4	F	1	Total C O 6 4 2	0	0
4	F	1	Total C O 6 4 2	0	0
4	H	1	Total C O 6 4 2	0	0
4	H	1	Total C O 6 4 2	0	0
4	H	1	Total C O 6 4 2	0	0
4	I	1	Total C O 6 4 2	0	0
4	I	1	Total C O 6 4 2	0	0
4	J	1	Total C O 6 4 2	0	0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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- 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	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 C Fe N O 43 34 1 4 4	0	0
6	B	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	C	1	Total C Fe N O 43 34 1 4 4	0	0
6	D	1	Total C Fe N O 43 34 1 4 4	0	0
6	D	1	Total C Fe N O 43 34 1 4 4	0	0
6	D	1	Total C Fe N O 43 34 1 4 4	0	0
6	D	1	Total C Fe N O 43 34 1 4 4	0	0
6	D	1	Total C Fe N O 43 34 1 4 4	0	0
6	D	1	Total C Fe N O 43 34 1 4 4	0	0
6	D	1	Total C Fe N O 43 34 1 4 4	0	0
6	D	1	Total C Fe N O 43 34 1 4 4	0	0
6	E	1	Total C Fe N O 43 34 1 4 4	0	0
6	E	1	Total C Fe N O 43 34 1 4 4	0	0
6	E	1	Total C Fe N O 43 34 1 4 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	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 C Fe N O 43 34 1 4 4	0	0
6	I	1	Total C Fe N O 43 34 1 4 4	0	0
6	I	1	Total C Fe N O 43 34 1 4 4	0	0
6	I	1	Total C Fe N O 43 34 1 4 4	0	0
6	I	1	Total C Fe N O 43 34 1 4 4	0	0
6	I	1	Total C Fe N O 43 34 1 4 4	0	0
6	I	1	Total C Fe N O 43 34 1 4 4	0	0
6	I	1	Total C Fe N O 43 34 1 4 4	0	0
6	J	1	Total C Fe N O 43 34 1 4 4	0	0
6	J	1	Total C Fe N O 43 34 1 4 4	0	0
6	J	1	Total C Fe N O 43 34 1 4 4	0	0
6	J	1	Total C Fe N O 43 34 1 4 4	0	0
6	J	1	Total C Fe N O 43 34 1 4 4	0	0
6	J	1	Total C Fe N O 43 34 1 4 4	0	0
6	J	1	Total C Fe N O 43 34 1 4 4	0	0
6	J	1	Total C Fe N O 43 34 1 4 4	0	0
6	K	1	Total C Fe N O 43 34 1 4 4	0	0
6	K	1	Total C Fe N O 43 34 1 4 4	0	0
6	K	1	Total C Fe N O 43 34 1 4 4	0	0
6	K	1	Total C Fe N O 43 34 1 4 4	0	0
6	K	1	Total C Fe N O 43 34 1 4 4	0	0

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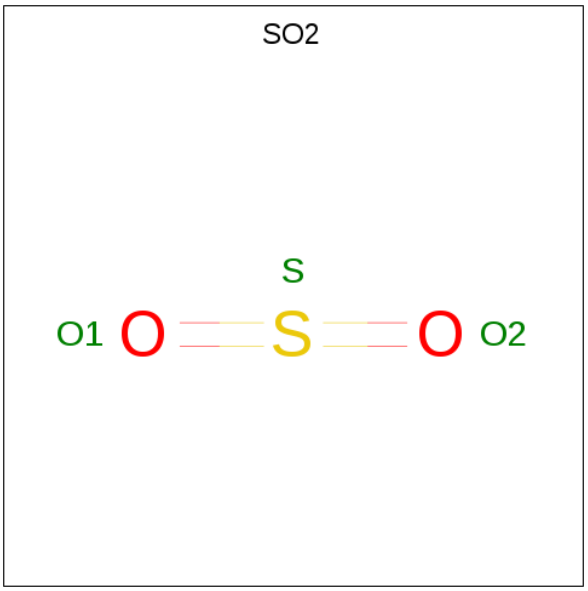
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	K	1	Total C Fe N O 43 34 1 4 4	0	0
6	K	1	Total C Fe N O 43 34 1 4 4	0	0
6	K	1	Total C Fe N O 43 34 1 4 4	0	0
6	L	1	Total C Fe N O 43 34 1 4 4	0	0
6	L	1	Total C Fe N O 43 34 1 4 4	0	0
6	L	1	Total C Fe N O 43 34 1 4 4	0	0
6	L	1	Total C Fe N O 43 34 1 4 4	0	0
6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

- Molecule 7 is SULFUR DIOXIDE (three-letter code: SO2) (formula: O_2S).



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

- Molecule 8 is water.

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

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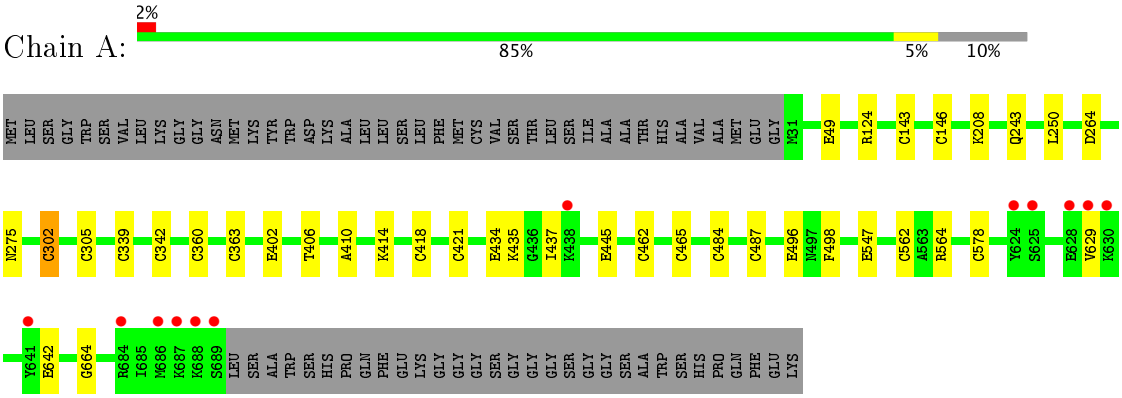
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	J	180	Total O 180 180	0	0
8	K	158	Total O 158 158	0	0
8	L	126	Total O 126 126	0	0
8	G	232	Total O 232 232	0	0

3 Residue-property plots (i)

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

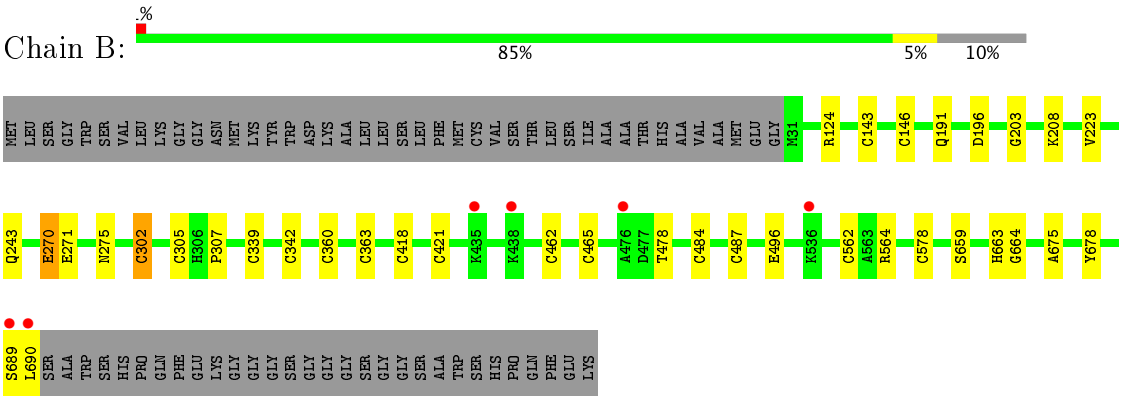
- Molecule 1: MccA

Chain A:



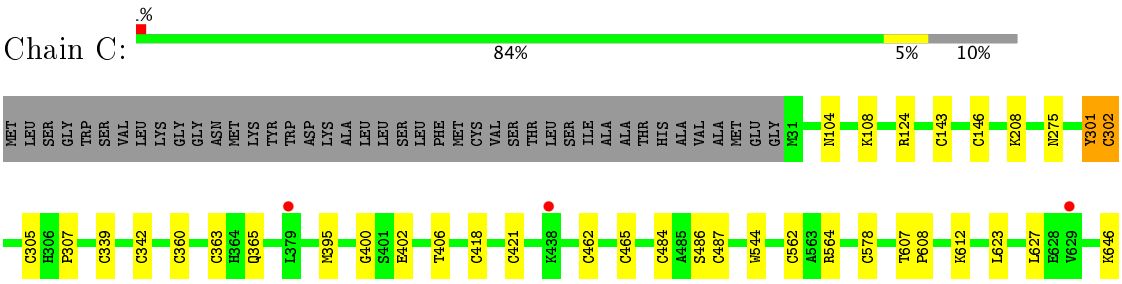
- Molecule 1: MccA

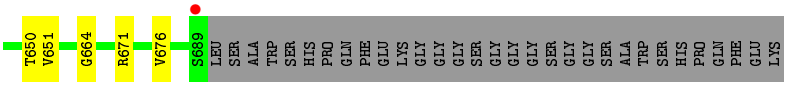
Chain B:



- Molecule 1: MccA

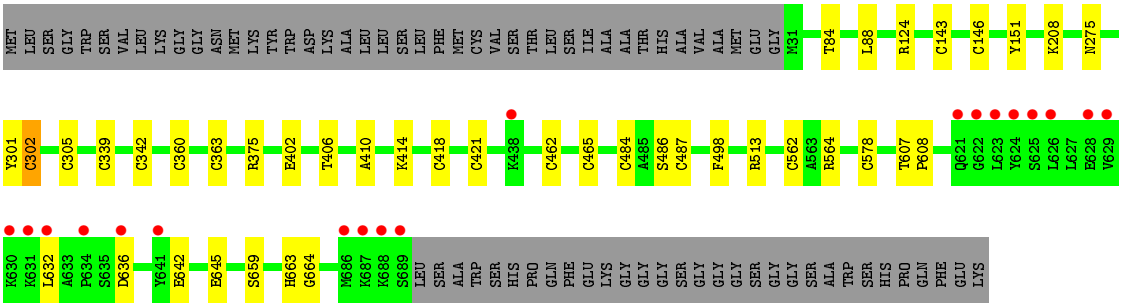
Chain C:





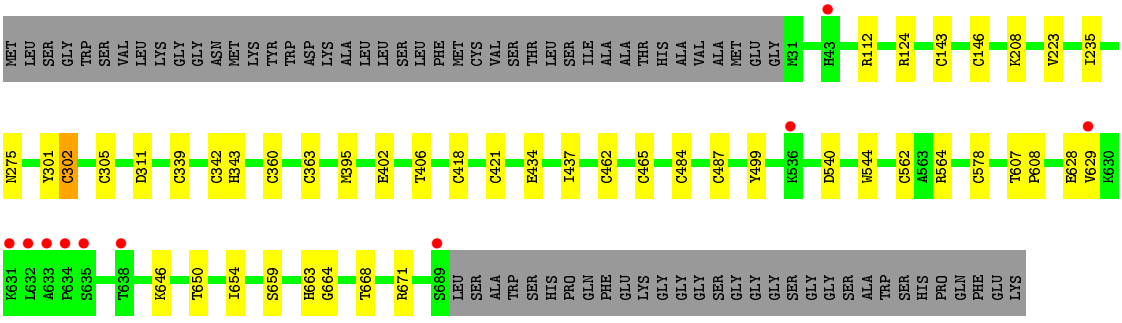
• Molecule 1: MccA

Chain D:



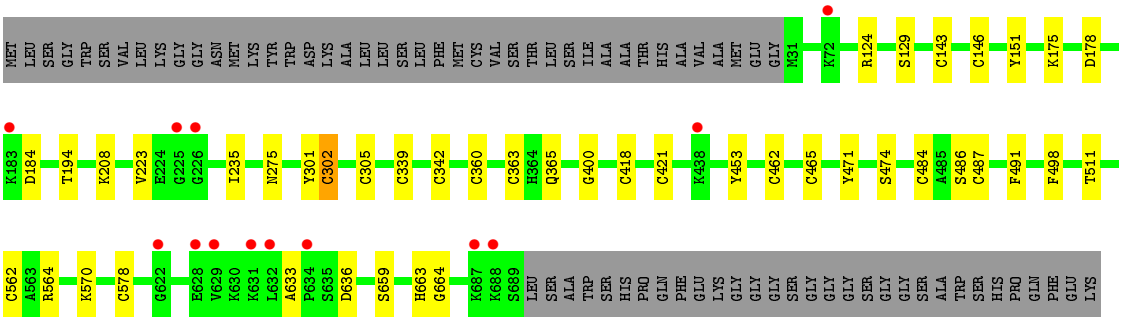
• Molecule 1: MccA

Chain E:



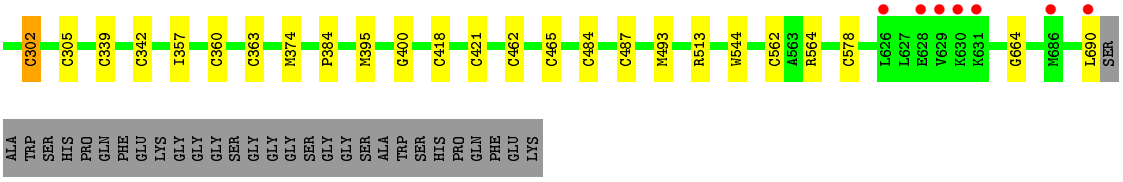
• Molecule 1: MccA

Chain F:



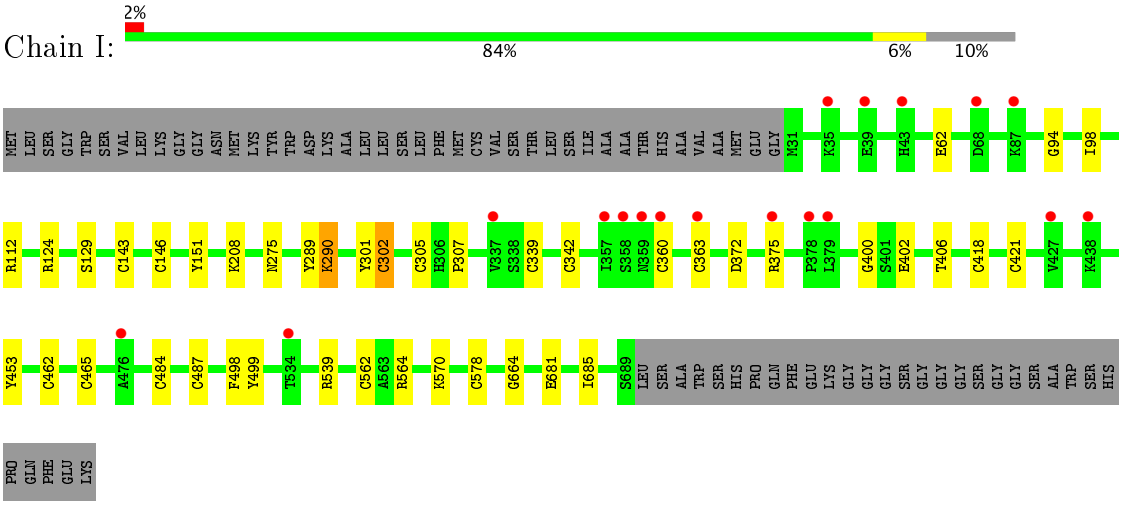
• Molecule 1: MccA

Chain H:



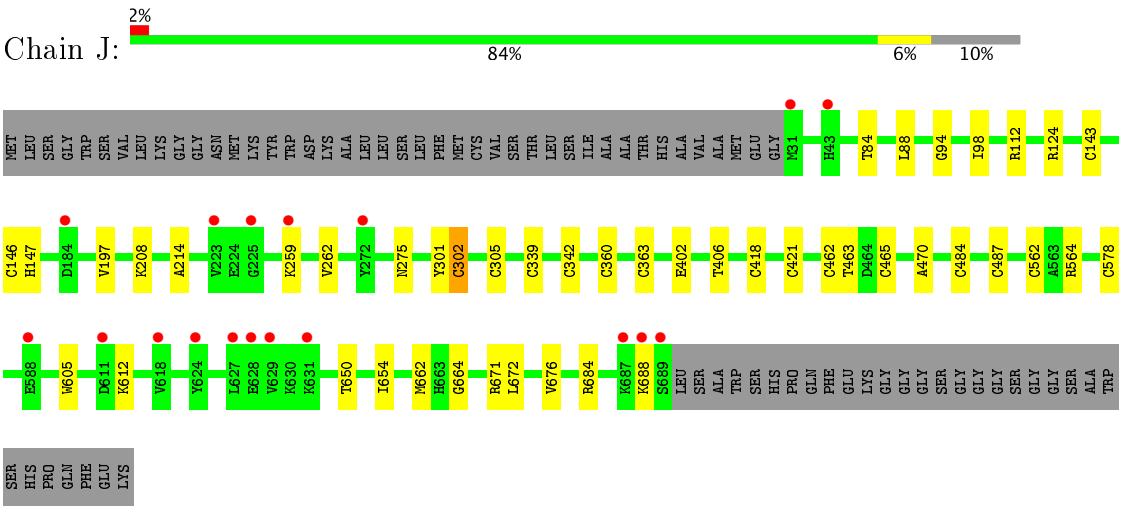
- Molecule 1: MccA

Chain I:



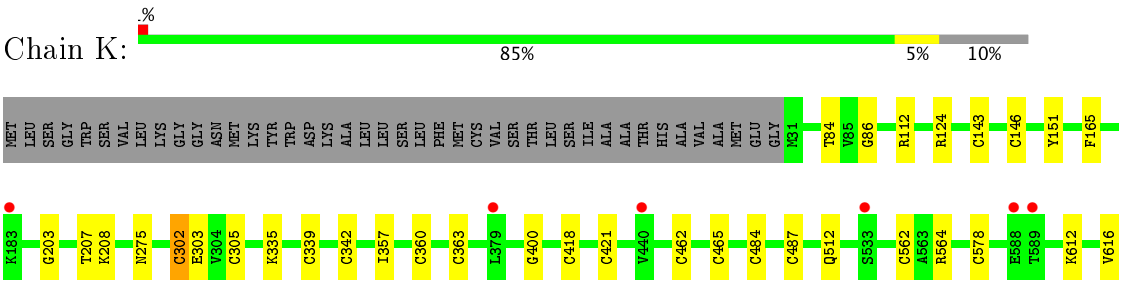
- Molecule 1: MccA

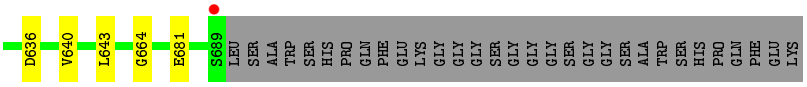
Chain J:



- Molecule 1: MccA

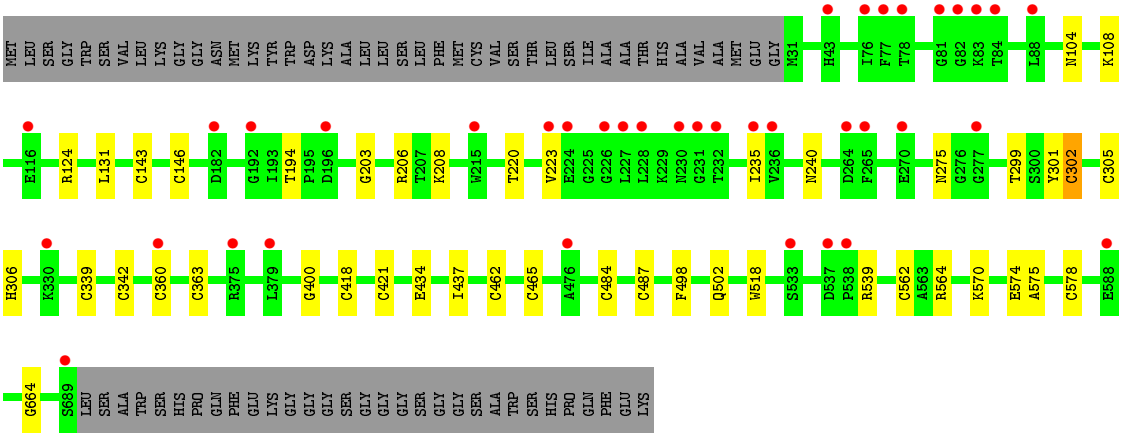
Chain K:





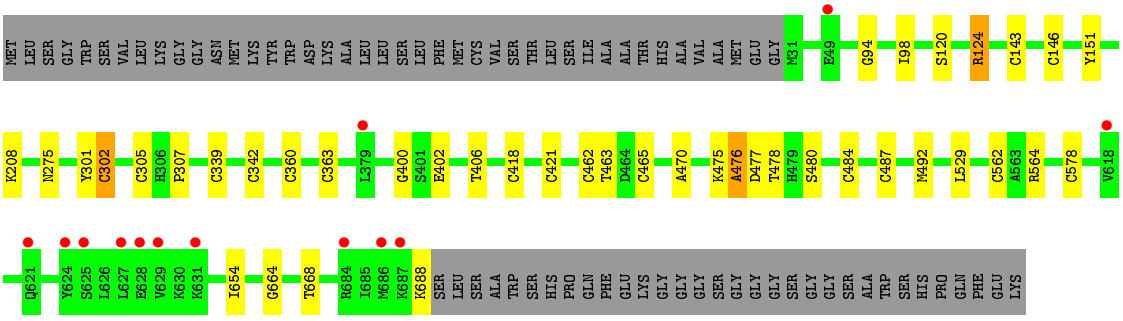
• Molecule 1: MccA

Chain L:



• Molecule 1: MccA

Chain G:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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.

All (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:339:CYS:SG	6:A:808:HEM:CAB	2.04	1.46
1:A:462:CYS:SG	6:A:811:HEM:CAB	2.02	1.46
1:F:462:CYS:SG	6:F:812:HEM:CAB	2.03	1.46
1:A:484:CYS:SG	6:A:812:HEM:CAB	2.05	1.45
1:F:484:CYS:SG	6:F:813:HEM:CAB	2.04	1.45
1:C:462:CYS:SG	6:C:811:HEM:CAB	2.03	1.45
1:B:339:CYS:SG	6:B:809:HEM:CAB	2.05	1.44
1:I:462:CYS:SG	6:I:811:HEM:CAB	2.06	1.44
1:K:418:CYS:SG	6:K:810:HEM:CAB	2.06	1.44
1:C:418:CYS:SG	6:C:810:HEM:CAB	2.03	1.44
1:H:484:CYS:SG	6:H:813:HEM:CAB	2.04	1.44
1:G:462:CYS:SG	6:G:811:HEM:CAB	2.06	1.43
1:E:339:CYS:SG	6:E:808:HEM:CAB	2.06	1.43
1:B:484:CYS:SG	6:B:813:HEM:CAB	2.05	1.43
1:E:462:CYS:SG	6:E:811:HEM:CAB	2.05	1.43
1:D:484:CYS:SG	6:D:812:HEM:CAB	2.07	1.43
1:F:562:CYS:SG	6:F:814:HEM:CAB	2.07	1.43
1:K:143:CYS:SG	6:K:806:HEM:HAB	1.57	1.43
1:A:143:CYS:SG	6:A:806:HEM:CAB	2.07	1.42
1:D:418:CYS:SG	6:D:810:HEM:CAB	2.07	1.42
1:I:339:CYS:SG	6:I:808:HEM:CAB	2.07	1.42
1:F:143:CYS:SG	6:F:807:HEM:CAB	2.07	1.42
1:C:562:CYS:SG	6:C:813:HEM:CAB	2.08	1.42
1:E:484:CYS:SG	6:E:812:HEM:CAB	2.08	1.41
1:C:339:CYS:SG	6:C:808:HEM:CAB	2.08	1.41
1:G:418:CYS:SG	6:G:810:HEM:CAB	2.06	1.41
1:K:462:CYS:SG	6:K:811:HEM:CAB	2.09	1.41
1:D:562:CYS:SG	6:D:813:HEM:CAB	2.08	1.41
1:A:418:CYS:SG	6:A:810:HEM:CAB	2.07	1.41
1:C:360:CYS:SG	6:C:809:HEM:CAB	2.09	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:CYS:SG	6:G:808:HEM:CAB	2.09	1.40
1:A:562:CYS:SG	6:A:813:HEM:CAB	2.08	1.40
1:C:484:CYS:SG	6:C:812:HEM:CAB	2.09	1.40
1:E:418:CYS:SG	6:E:810:HEM:CAB	2.09	1.40
1:D:462:CYS:SG	6:D:811:HEM:CAB	2.09	1.40
1:B:562:CYS:SG	6:B:814:HEM:CAB	2.08	1.40
1:I:484:CYS:SG	6:I:812:HEM:CAB	2.10	1.40
1:L:339:CYS:SG	6:L:808:HEM:CAB	2.10	1.40
1:B:418:CYS:SG	6:B:811:HEM:CAB	2.08	1.39
1:G:562:CYS:SG	6:G:813:HEM:CAB	2.11	1.39
1:G:484:CYS:SG	6:G:812:HEM:CAB	2.11	1.39
1:B:143:CYS:SG	6:B:807:HEM:CAB	2.10	1.39
1:D:339:CYS:SG	6:D:808:HEM:CAB	2.09	1.39
1:H:562:CYS:SG	6:H:814:HEM:CAB	2.10	1.39
1:J:462:CYS:SG	6:J:811:HEM:CAB	2.10	1.39
1:B:462:CYS:SG	6:B:812:HEM:CAB	2.11	1.39
1:F:339:CYS:SG	6:F:809:HEM:CAB	2.10	1.39
1:G:143:CYS:HG	6:G:806:HEM:CAB	1.36	1.39
1:I:418:CYS:SG	6:I:810:HEM:CAB	2.09	1.39
1:J:339:CYS:SG	6:J:808:HEM:CAB	2.11	1.39
1:A:305:CYS:SG	6:A:807:HEM:CAC	2.11	1.39
1:I:363:CYS:SG	6:I:809:HEM:CAC	2.11	1.39
1:J:562:CYS:SG	6:J:813:HEM:CAB	2.11	1.39
1:E:562:CYS:SG	6:E:813:HEM:CAB	2.09	1.38
1:L:562:CYS:SG	6:L:813:HEM:CAB	2.11	1.38
1:K:339:CYS:SG	6:K:808:HEM:CAB	2.10	1.38
1:K:484:CYS:SG	6:K:812:HEM:CAB	2.11	1.38
1:G:143:CYS:SG	6:G:806:HEM:CAB	2.10	1.38
1:H:462:CYS:SG	6:H:812:HEM:CAB	2.09	1.38
1:D:143:CYS:SG	6:D:806:HEM:CAB	2.11	1.38
1:F:418:CYS:SG	6:F:811:HEM:CAB	2.12	1.38
1:H:562:CYS:HG	6:H:814:HEM:CAB	1.33	1.38
1:J:484:CYS:SG	6:J:812:HEM:CAB	2.12	1.37
1:I:562:CYS:SG	6:I:813:HEM:CAB	2.12	1.37
1:H:418:CYS:SG	6:H:811:HEM:CAB	2.11	1.37
1:J:418:CYS:SG	6:J:810:HEM:CAB	2.10	1.37
1:K:143:CYS:SG	6:K:806:HEM:CAB	2.10	1.37
1:C:143:CYS:SG	6:C:806:HEM:CAB	2.13	1.36
1:C:363:CYS:SG	6:C:809:HEM:CAC	2.14	1.36
1:A:363:CYS:SG	6:A:809:HEM:CAC	2.13	1.36
1:H:339:CYS:SG	6:H:809:HEM:CAB	2.14	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:363:CYS:SG	6:H:810:HEM:CAC	2.14	1.35
1:J:143:CYS:SG	6:J:806:HEM:CAB	2.12	1.35
1:K:562:CYS:SG	6:K:813:HEM:CAB	2.12	1.35
1:D:363:CYS:SG	6:D:809:HEM:CAC	2.14	1.35
1:L:484:CYS:SG	6:L:812:HEM:CAB	2.14	1.35
1:E:360:CYS:SG	6:E:809:HEM:CAB	2.13	1.35
1:B:360:CYS:SG	6:B:810:HEM:CAB	2.15	1.35
1:D:360:CYS:SG	6:D:809:HEM:CAB	2.15	1.34
1:L:418:CYS:SG	6:L:810:HEM:CAB	2.15	1.34
1:F:363:CYS:SG	6:F:810:HEM:CAC	2.14	1.34
1:L:143:CYS:SG	6:L:806:HEM:CAB	2.15	1.34
1:A:578:CYS:SG	6:A:813:HEM:CAC	2.15	1.34
1:E:363:CYS:SG	6:E:809:HEM:CAC	2.16	1.34
1:G:363:CYS:SG	6:G:809:HEM:CAC	2.16	1.34
1:H:143:CYS:SG	6:H:807:HEM:CAB	2.15	1.33
1:C:305:CYS:SG	6:C:807:HEM:CAC	2.16	1.33
1:K:363:CYS:SG	6:K:809:HEM:CAC	2.16	1.33
1:L:360:CYS:SG	6:L:809:HEM:CAB	2.17	1.33
1:B:363:CYS:SG	6:B:810:HEM:CAC	2.16	1.33
1:E:418:CYS:HG	6:E:810:HEM:CAB	1.40	1.32
1:E:143:CYS:SG	6:E:806:HEM:CAB	2.17	1.32
1:L:363:CYS:SG	6:L:809:HEM:CAC	2.16	1.32
1:E:305:CYS:SG	6:E:807:HEM:CAC	2.17	1.32
1:J:360:CYS:SG	6:J:809:HEM:CAB	2.18	1.31
1:K:360:CYS:SG	6:K:809:HEM:CAB	2.18	1.31
1:H:487:CYS:SG	6:H:813:HEM:CAC	2.18	1.31
1:F:360:CYS:SG	6:F:810:HEM:CAB	2.18	1.31
1:H:360:CYS:SG	6:H:810:HEM:CAB	2.18	1.31
1:A:487:CYS:SG	6:A:812:HEM:CAC	2.18	1.31
1:I:143:CYS:SG	6:I:806:HEM:CAB	2.18	1.31
1:J:305:CYS:SG	6:J:807:HEM:CAC	2.19	1.31
1:L:462:CYS:SG	6:L:811:HEM:CAB	2.19	1.31
1:A:360:CYS:SG	6:A:809:HEM:CAB	2.18	1.31
1:G:360:CYS:SG	6:G:809:HEM:CAB	2.19	1.31
1:H:305:CYS:SG	6:H:808:HEM:CAC	2.19	1.30
1:I:305:CYS:SG	6:I:807:HEM:CAC	2.19	1.30
1:I:360:CYS:SG	6:I:809:HEM:CAB	2.19	1.30
1:G:146:CYS:SG	6:G:806:HEM:CAC	2.18	1.30
1:J:363:CYS:SG	6:J:809:HEM:CAC	2.19	1.30
1:D:305:CYS:SG	6:D:807:HEM:CAC	2.19	1.30
1:F:578:CYS:SG	6:F:814:HEM:CAC	2.19	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:CYS:SG	6:K:807:HEM:CAC	2.20	1.30
1:D:487:CYS:SG	6:D:812:HEM:CAC	2.20	1.30
1:C:342:CYS:SG	6:C:808:HEM:CAC	2.19	1.30
1:E:578:CYS:SG	6:E:813:HEM:CAC	2.19	1.29
1:F:342:CYS:SG	6:F:809:HEM:CAC	2.19	1.29
1:I:342:CYS:SG	6:I:808:HEM:CAC	2.20	1.29
1:C:146:CYS:SG	6:C:806:HEM:CAC	2.20	1.29
1:F:146:CYS:SG	6:F:807:HEM:CAC	2.20	1.29
1:B:305:CYS:SG	6:B:808:HEM:CAC	2.18	1.29
1:G:487:CYS:SG	6:G:812:HEM:CAC	2.21	1.29
1:E:487:CYS:SG	6:E:812:HEM:CAC	2.20	1.29
1:I:465:CYS:SG	6:I:811:HEM:CAC	2.21	1.29
1:K:487:CYS:SG	6:K:812:HEM:CAC	2.21	1.29
1:B:487:CYS:SG	6:B:813:HEM:CAC	2.21	1.29
1:H:465:CYS:SG	6:H:812:HEM:CAC	2.21	1.28
1:F:487:CYS:SG	6:F:813:HEM:CAC	2.22	1.28
1:A:146:CYS:SG	6:A:806:HEM:CAC	2.22	1.28
1:C:487:CYS:SG	6:C:812:HEM:CAC	2.20	1.28
1:H:578:CYS:HG	6:H:814:HEM:CAC	1.46	1.28
1:E:146:CYS:SG	6:E:806:HEM:CAC	2.22	1.28
1:G:465:CYS:SG	6:G:811:HEM:CAC	2.22	1.28
1:H:578:CYS:SG	6:H:814:HEM:CAC	2.20	1.28
1:J:578:CYS:SG	6:J:813:HEM:CAC	2.22	1.28
1:D:342:CYS:SG	6:D:808:HEM:CAC	2.22	1.28
1:D:363:CYS:HG	6:D:809:HEM:CAC	1.47	1.28
1:K:363:CYS:HG	6:K:809:HEM:CAC	1.42	1.28
1:B:465:CYS:SG	6:B:812:HEM:CAC	2.22	1.28
1:B:342:CYS:SG	6:B:809:HEM:CAC	2.22	1.27
1:E:363:CYS:HG	6:E:809:HEM:CAC	1.46	1.27
1:J:487:CYS:SG	6:J:812:HEM:CAC	2.22	1.27
1:K:578:CYS:SG	6:K:813:HEM:CAC	2.21	1.27
1:L:487:CYS:SG	6:L:812:HEM:CAC	2.22	1.27
1:K:465:CYS:SG	6:K:811:HEM:CAC	2.21	1.27
1:C:465:CYS:SG	6:C:811:HEM:CAC	2.23	1.27
1:K:146:CYS:SG	6:K:806:HEM:CAC	2.22	1.27
1:E:465:CYS:SG	6:E:811:HEM:CAC	2.23	1.27
1:I:487:CYS:SG	6:I:812:HEM:CAC	2.22	1.27
1:I:421:CYS:SG	6:I:810:HEM:CAC	2.23	1.27
1:A:421:CYS:SG	6:A:810:HEM:CAC	2.22	1.27
1:H:421:CYS:HG	6:H:811:HEM:CAC	1.45	1.27
1:J:146:CYS:SG	6:J:806:HEM:CAC	2.22	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:CYS:SG	6:D:813:HEM:CAC	2.21	1.27
1:D:146:CYS:SG	6:D:806:HEM:CAC	2.22	1.26
1:L:578:CYS:SG	6:L:813:HEM:HAC	1.73	1.26
1:L:146:CYS:SG	6:L:806:HEM:CAC	2.23	1.26
1:F:305:CYS:SG	6:F:808:HEM:CAC	2.23	1.26
1:L:342:CYS:SG	6:L:808:HEM:CAC	2.23	1.26
1:J:342:CYS:SG	6:J:808:HEM:CAC	2.22	1.26
1:L:305:CYS:SG	6:L:807:HEM:CAC	2.22	1.26
1:B:578:CYS:SG	6:B:814:HEM:CAC	2.24	1.26
1:L:578:CYS:SG	6:L:813:HEM:CAC	2.22	1.26
1:D:465:CYS:SG	6:D:811:HEM:CAC	2.24	1.26
1:K:342:CYS:SG	6:K:808:HEM:CAC	2.22	1.26
1:G:305:CYS:SG	6:G:807:HEM:CAC	2.23	1.25
1:B:146:CYS:SG	6:B:807:HEM:CAC	2.22	1.25
1:G:342:CYS:SG	6:G:808:HEM:CAC	2.23	1.25
1:I:146:CYS:SG	6:I:806:HEM:CAC	2.23	1.25
1:D:421:CYS:SG	6:D:810:HEM:CAC	2.24	1.25
1:I:578:CYS:SG	6:I:813:HEM:CAC	2.23	1.25
1:L:465:CYS:SG	6:L:811:HEM:CAC	2.24	1.25
1:F:465:CYS:SG	6:F:812:HEM:CAC	2.24	1.25
1:H:421:CYS:SG	6:H:811:HEM:CAC	2.25	1.25
1:H:342:CYS:SG	6:H:809:HEM:CAC	2.24	1.25
1:F:421:CYS:SG	6:F:811:HEM:CAC	2.25	1.24
1:J:465:CYS:SG	6:J:811:HEM:CAC	2.24	1.24
1:A:342:CYS:SG	6:A:808:HEM:CAC	2.24	1.24
1:L:421:CYS:SG	6:L:810:HEM:CAC	2.25	1.23
7:A:814:SO2:O1	8:A:1232:HOH:O	1.55	1.23
1:E:342:CYS:SG	6:E:808:HEM:CAC	2.26	1.23
1:H:146:CYS:SG	6:H:807:HEM:CAC	2.26	1.23
1:J:421:CYS:SG	6:J:810:HEM:CAC	2.27	1.23
1:A:465:CYS:SG	6:A:811:HEM:CAC	2.26	1.23
1:C:578:CYS:SG	6:C:813:HEM:CAC	2.25	1.23
1:A:487:CYS:HG	6:A:812:HEM:CAC	1.47	1.22
1:E:421:CYS:SG	6:E:810:HEM:CAC	2.27	1.22
1:G:578:CYS:SG	6:G:813:HEM:CAC	2.27	1.22
1:G:421:CYS:SG	6:G:810:HEM:CAC	2.27	1.22
1:C:421:CYS:SG	6:C:810:HEM:CAC	2.27	1.22
1:B:421:CYS:SG	6:B:811:HEM:CAC	2.27	1.22
1:K:302:CYS:SG	6:K:807:HEM:CAB	2.27	1.21
1:K:421:CYS:SG	6:K:810:HEM:CAC	2.29	1.21
1:H:487:CYS:HG	6:H:813:HEM:CAC	1.51	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:462:CYS:HG	6:L:811:HEM:CAB	1.50	1.19
1:H:302:CYS:SG	6:H:808:HEM:CAB	2.30	1.19
1:J:487:CYS:SG	6:J:812:HEM:CBC	2.31	1.19
1:K:462:CYS:HG	6:K:811:HEM:CAB	1.47	1.19
1:D:302:CYS:SG	6:D:807:HEM:CAB	2.31	1.18
1:L:302:CYS:SG	6:L:807:HEM:CAB	2.31	1.18
1:K:302:CYS:SG	6:K:807:HEM:C3B	2.37	1.18
1:D:339:CYS:SG	6:D:808:HEM:HAB	1.73	1.18
1:J:360:CYS:HG	6:J:809:HEM:CAB	1.55	1.18
1:G:360:CYS:HG	6:G:809:HEM:CAB	1.54	1.17
1:J:302:CYS:SG	6:J:807:HEM:CAB	2.33	1.17
1:E:562:CYS:HG	6:E:813:HEM:CAB	1.47	1.17
1:F:302:CYS:SG	6:F:808:HEM:CAB	2.34	1.16
1:C:339:CYS:HG	6:C:808:HEM:CAB	1.53	1.16
1:C:302:CYS:SG	6:C:807:HEM:CAB	2.33	1.16
1:F:418:CYS:HG	6:F:811:HEM:CAB	1.55	1.15
1:A:302:CYS:SG	6:A:807:HEM:CAB	2.34	1.15
1:B:302:CYS:SG	6:B:808:HEM:CAB	2.35	1.15
1:A:363:CYS:HG	6:A:809:HEM:CAC	1.55	1.14
1:A:562:CYS:HG	6:A:813:HEM:CAB	1.53	1.14
1:E:302:CYS:SG	6:E:807:HEM:CAB	2.36	1.13
1:I:302:CYS:SG	6:I:807:HEM:CAB	2.37	1.13
1:K:418:CYS:SG	6:K:810:HEM:CBB	2.36	1.12
1:J:562:CYS:HG	6:J:813:HEM:CAB	1.52	1.12
1:F:143:CYS:SG	6:F:807:HEM:CBB	2.36	1.12
1:H:578:CYS:SG	6:H:814:HEM:CBC	2.39	1.11
1:C:339:CYS:SG	6:C:808:HEM:HAB	1.83	1.11
1:I:418:CYS:HG	6:I:810:HEM:CAB	1.50	1.11
1:G:302:CYS:SG	6:G:807:HEM:CAB	2.39	1.11
1:I:465:CYS:HG	6:I:811:HEM:CAC	1.57	1.09
1:H:462:CYS:SG	6:H:812:HEM:CBB	2.41	1.08
1:J:363:CYS:HG	6:J:809:HEM:CAC	1.61	1.08
1:K:462:CYS:SG	6:K:811:HEM:CBB	2.41	1.08
1:K:578:CYS:SG	6:K:813:HEM:CBC	2.42	1.07
1:C:462:CYS:SG	6:C:811:HEM:CBB	2.43	1.07
1:H:484:CYS:SG	6:H:813:HEM:CBB	2.43	1.07
1:L:487:CYS:SG	6:L:812:HEM:CBC	2.43	1.06
1:L:462:CYS:SG	6:L:811:HEM:HAB	1.94	1.06
1:E:360:CYS:HG	6:E:809:HEM:CAB	1.57	1.06
1:F:484:CYS:SG	6:F:813:HEM:HAB	1.92	1.05
1:B:360:CYS:HG	6:B:810:HEM:CAB	1.60	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:CYS:SG	6:B:814:HEM:CBC	2.44	1.05
1:C:418:CYS:SG	6:C:810:HEM:CBB	2.44	1.05
1:I:339:CYS:HG	6:I:808:HEM:CAB	1.56	1.05
1:J:302:CYS:SG	6:J:807:HEM:C3B	2.50	1.05
1:L:570:LYS:NZ	1:L:574:GLU:OE2	1.87	1.05
1:F:462:CYS:SG	6:F:812:HEM:CBB	2.44	1.04
1:C:562:CYS:SG	6:C:813:HEM:CBB	2.45	1.04
1:J:462:CYS:SG	6:J:811:HEM:CBB	2.46	1.04
1:J:305:CYS:SG	6:J:807:HEM:CBC	2.45	1.04
1:L:146:CYS:SG	6:L:806:HEM:CBC	2.44	1.04
1:B:305:CYS:SG	6:B:808:HEM:CBC	2.46	1.04
1:D:360:CYS:HG	6:D:809:HEM:CAB	1.61	1.04
1:I:462:CYS:SG	6:I:811:HEM:CBB	2.44	1.04
1:L:562:CYS:SG	6:L:813:HEM:CBB	2.45	1.03
1:D:339:CYS:HG	6:D:808:HEM:CAB	1.59	1.03
1:H:302:CYS:SG	6:H:808:HEM:C3B	2.50	1.03
1:K:484:CYS:SG	6:K:812:HEM:CBB	2.46	1.03
1:K:562:CYS:SG	6:K:813:HEM:CBB	2.46	1.03
1:J:146:CYS:SG	6:J:806:HEM:CBC	2.47	1.02
1:I:562:CYS:SG	6:I:813:HEM:CBB	2.47	1.02
1:A:143:CYS:SG	6:A:806:HEM:HAB	1.93	1.02
1:D:302:CYS:SG	6:D:807:HEM:C3B	2.52	1.02
1:I:302:CYS:SG	6:I:807:HEM:C3B	2.53	1.02
1:L:302:CYS:SG	6:L:807:HEM:C3B	2.52	1.02
1:I:339:CYS:SG	6:I:808:HEM:HAB	2.00	1.02
1:L:305:CYS:SG	6:L:807:HEM:CBC	2.47	1.02
1:D:487:CYS:SG	6:D:812:HEM:CBC	2.48	1.01
1:F:360:CYS:HG	6:F:810:HEM:CAB	1.69	1.01
1:E:484:CYS:SG	6:E:812:HEM:CBB	2.47	1.01
1:E:418:CYS:SG	6:E:810:HEM:CBB	2.49	1.01
1:J:418:CYS:SG	6:J:810:HEM:CBB	2.48	1.01
1:I:363:CYS:HG	6:I:809:HEM:CAC	1.69	1.01
1:C:302:CYS:SG	6:C:807:HEM:C3B	2.53	1.01
1:B:462:CYS:SG	6:B:812:HEM:CBB	2.48	1.01
1:A:418:CYS:SG	6:A:810:HEM:HAB	1.95	1.00
1:I:418:CYS:SG	6:I:810:HEM:CBB	2.48	1.00
1:F:339:CYS:SG	6:F:809:HEM:HAB	1.96	1.00
1:D:562:CYS:SG	6:D:813:HEM:CBB	2.49	1.00
1:B:562:CYS:SG	6:B:814:HEM:CBB	2.50	1.00
1:C:363:CYS:HG	6:C:809:HEM:CAC	1.63	1.00
1:G:462:CYS:SG	6:G:811:HEM:CBB	2.50	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:487:CYS:SG	6:G:812:HEM:CBC	2.49	1.00
1:E:462:CYS:SG	6:E:811:HEM:CBB	2.48	1.00
1:L:418:CYS:SG	6:L:810:HEM:CBB	2.49	0.99
1:C:143:CYS:SG	6:C:806:HEM:HAB	1.99	0.99
1:E:305:CYS:SG	6:E:807:HEM:CBC	2.50	0.99
1:F:418:CYS:SG	6:F:811:HEM:HAB	2.01	0.99
1:B:302:CYS:SG	6:B:808:HEM:C3B	2.55	0.99
1:E:465:CYS:SG	6:E:811:HEM:CBC	2.50	0.99
1:C:305:CYS:SG	6:C:807:HEM:CBC	2.51	0.99
1:D:418:CYS:SG	6:D:810:HEM:HAB	2.01	0.99
1:H:578:CYS:HG	6:H:814:HEM:CBC	1.74	0.99
1:L:339:CYS:SG	6:L:808:HEM:CBB	2.51	0.99
1:H:487:CYS:SG	6:H:813:HEM:CBC	2.51	0.99
1:A:578:CYS:SG	6:A:813:HEM:CBC	2.51	0.99
1:A:484:CYS:SG	6:A:812:HEM:CBB	2.51	0.99
1:B:484:CYS:SG	6:B:813:HEM:CBB	2.49	0.99
1:E:302:CYS:SG	6:E:807:HEM:C3B	2.56	0.99
1:G:562:CYS:SG	6:G:813:HEM:CBB	2.51	0.99
1:A:339:CYS:SG	6:A:808:HEM:HAB	1.99	0.98
1:L:363:CYS:HG	6:L:809:HEM:CAC	1.65	0.98
1:B:339:CYS:SG	6:B:809:HEM:HAB	2.02	0.98
1:K:342:CYS:SG	6:K:808:HEM:CBC	2.51	0.98
1:A:418:CYS:HG	6:A:810:HEM:CAB	1.63	0.98
1:E:487:CYS:SG	6:E:812:HEM:CBC	2.51	0.97
1:G:146:CYS:SG	6:G:806:HEM:CBC	2.51	0.97
1:H:418:CYS:HG	6:H:811:HEM:CAB	1.66	0.97
1:H:360:CYS:HG	6:H:810:HEM:CAB	1.69	0.97
1:I:360:CYS:HG	6:I:809:HEM:CAB	1.69	0.97
1:B:418:CYS:SG	6:B:811:HEM:HAB	2.02	0.97
1:D:484:CYS:SG	6:D:812:HEM:CBB	2.53	0.97
1:E:339:CYS:SG	6:E:808:HEM:CBB	2.53	0.97
1:G:418:CYS:SG	6:G:810:HEM:HAB	2.03	0.97
1:H:339:CYS:SG	6:H:809:HEM:HAB	2.05	0.97
1:K:339:CYS:SG	6:K:808:HEM:HAB	2.05	0.97
1:F:562:CYS:SG	6:F:814:HEM:CBB	2.51	0.96
1:G:339:CYS:SG	6:G:808:HEM:CBB	2.53	0.96
1:B:487:CYS:SG	6:B:813:HEM:CBC	2.53	0.96
1:F:578:CYS:SG	6:F:814:HEM:CBC	2.53	0.96
1:A:484:CYS:SG	6:A:812:HEM:HAB	2.03	0.96
1:L:360:CYS:HG	6:L:809:HEM:CAB	1.70	0.96
1:D:462:CYS:SG	6:D:811:HEM:CBB	2.54	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:CYS:SG	6:F:808:HEM:C3B	2.59	0.95
1:G:143:CYS:SG	6:G:806:HEM:HAB	2.06	0.95
1:H:484:CYS:SG	6:H:813:HEM:HAB	2.06	0.95
1:L:421:CYS:SG	6:L:810:HEM:CBC	2.53	0.95
1:D:146:CYS:SG	6:D:806:HEM:CBC	2.54	0.95
1:I:484:CYS:SG	6:I:812:HEM:HAB	2.04	0.95
1:K:305:CYS:SG	6:K:807:HEM:CBC	2.53	0.95
1:G:418:CYS:SG	6:G:810:HEM:CBB	2.53	0.95
1:G:484:CYS:SG	6:G:812:HEM:CBB	2.54	0.95
1:H:487:CYS:HG	6:H:813:HEM:CBC	1.78	0.95
1:J:339:CYS:SG	6:J:808:HEM:HAB	2.07	0.95
1:L:484:CYS:SG	6:L:812:HEM:CBB	2.54	0.95
1:B:465:CYS:SG	6:B:812:HEM:CBC	2.54	0.95
1:E:578:CYS:SG	6:E:813:HEM:CBC	2.54	0.95
1:A:302:CYS:SG	6:A:807:HEM:C3B	2.59	0.95
1:A:305:CYS:SG	6:A:807:HEM:C3C	2.60	0.95
1:C:462:CYS:SG	6:C:811:HEM:HAB	2.06	0.95
1:J:484:CYS:SG	6:J:812:HEM:CBB	2.54	0.95
1:A:339:CYS:SG	6:A:808:HEM:CBB	2.55	0.95
1:C:465:CYS:SG	6:C:811:HEM:CBC	2.54	0.95
1:D:418:CYS:HG	6:D:810:HEM:CAB	1.59	0.95
1:B:484:CYS:SG	6:B:813:HEM:HAB	2.05	0.94
1:D:484:CYS:SG	6:D:812:HEM:HAB	2.03	0.94
1:G:339:CYS:SG	6:G:808:HEM:HAB	2.05	0.94
1:B:143:CYS:SG	6:B:807:HEM:HAB	2.05	0.94
1:F:487:CYS:SG	6:F:813:HEM:CBC	2.55	0.94
1:C:484:CYS:SG	6:C:812:HEM:HAB	2.05	0.94
1:D:578:CYS:SG	6:D:813:HEM:CBC	2.54	0.94
1:B:363:CYS:SG	6:B:810:HEM:CBC	2.55	0.94
1:D:143:CYS:SG	6:D:806:HEM:HAB	2.05	0.94
1:H:418:CYS:SG	6:H:811:HEM:CBB	2.55	0.94
1:J:562:CYS:SG	6:J:813:HEM:CBB	2.54	0.94
1:K:487:CYS:SG	6:K:812:HEM:CBC	2.56	0.94
1:B:418:CYS:HG	6:B:811:HEM:CAB	1.62	0.94
1:L:339:CYS:SG	6:L:808:HEM:HAB	2.06	0.93
1:C:418:CYS:SG	6:C:810:HEM:HAB	2.06	0.93
1:F:462:CYS:SG	6:F:812:HEM:HAB	2.05	0.93
1:A:360:CYS:HG	6:A:809:HEM:CAB	1.68	0.93
1:E:143:CYS:SG	6:E:806:HEM:HAB	2.09	0.93
1:G:462:CYS:SG	6:G:811:HEM:HAB	2.08	0.93
1:G:305:CYS:SG	6:G:807:HEM:CBC	2.56	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:CYS:SG	6:E:808:HEM:HAB	2.06	0.93
1:J:578:CYS:SG	6:J:813:HEM:CBC	2.56	0.92
1:D:305:CYS:SG	6:D:807:HEM:CBC	2.57	0.92
1:F:562:CYS:SG	6:F:814:HEM:HAB	2.07	0.92
1:H:421:CYS:HG	6:H:811:HEM:CBC	1.80	0.92
1:I:578:CYS:SG	6:I:813:HEM:CBC	2.57	0.92
1:H:143:CYS:SG	6:H:807:HEM:HAB	2.06	0.92
1:I:146:CYS:SG	6:I:806:HEM:CBC	2.57	0.92
1:H:146:CYS:SG	6:H:807:HEM:CBC	2.58	0.92
1:J:484:CYS:SG	6:J:812:HEM:HAB	2.09	0.92
1:H:360:CYS:SG	6:H:810:HEM:CBB	2.58	0.92
1:H:418:CYS:SG	6:H:811:HEM:HAB	2.10	0.92
1:B:421:CYS:SG	6:B:811:HEM:CBC	2.58	0.92
1:C:305:CYS:SG	6:C:807:HEM:C3C	2.63	0.92
1:A:305:CYS:SG	6:A:807:HEM:CBC	2.57	0.91
1:B:143:CYS:SG	6:B:807:HEM:CBB	2.58	0.91
1:C:578:CYS:SG	6:C:813:HEM:CBC	2.57	0.91
1:H:363:CYS:SG	6:H:810:HEM:CBC	2.58	0.91
1:I:339:CYS:SG	6:I:808:HEM:CBB	2.57	0.91
1:F:465:CYS:SG	6:F:812:HEM:CBC	2.57	0.91
1:G:143:CYS:SG	6:G:806:HEM:CBB	2.58	0.91
1:G:484:CYS:SG	6:G:812:HEM:HAB	2.09	0.91
1:I:484:CYS:SG	6:I:812:HEM:CBB	2.57	0.91
1:B:339:CYS:SG	6:B:809:HEM:CBB	2.57	0.91
1:H:465:CYS:SG	6:H:812:HEM:CBC	2.59	0.91
1:F:305:CYS:SG	6:F:808:HEM:CBC	2.59	0.91
1:H:305:CYS:SG	6:H:808:HEM:C3C	2.64	0.91
1:E:562:CYS:SG	6:E:813:HEM:CBB	2.58	0.91
1:I:487:CYS:SG	6:I:812:HEM:CBC	2.59	0.91
1:A:487:CYS:SG	6:A:812:HEM:CBC	2.58	0.90
1:D:465:CYS:SG	6:D:811:HEM:CBC	2.59	0.90
1:B:418:CYS:SG	6:B:811:HEM:CBB	2.60	0.90
1:D:418:CYS:SG	6:D:810:HEM:CBB	2.59	0.90
1:J:339:CYS:SG	6:J:808:HEM:CBB	2.58	0.90
1:C:342:CYS:SG	6:C:808:HEM:CBC	2.59	0.90
1:K:360:CYS:HG	6:K:809:HEM:CAB	1.74	0.90
1:D:562:CYS:SG	6:D:813:HEM:HAB	2.12	0.90
1:C:487:CYS:SG	6:C:812:HEM:CBC	2.59	0.90
1:E:462:CYS:SG	6:E:811:HEM:HAB	2.10	0.90
1:E:562:CYS:SG	6:E:813:HEM:HAB	2.11	0.90
1:I:143:CYS:SG	6:I:806:HEM:CBB	2.60	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:342:CYS:SG	6:L:808:HEM:CBC	2.58	0.90
1:G:478:THR:O	6:G:813:HEM:O2D	1.88	0.90
1:K:339:CYS:SG	6:K:808:HEM:CBB	2.58	0.89
1:H:562:CYS:SG	6:H:814:HEM:CBB	2.60	0.89
1:K:143:CYS:HG	6:K:806:HEM:HAB	1.12	0.89
1:K:465:CYS:SG	6:K:811:HEM:CBC	2.60	0.89
1:A:562:CYS:SG	6:A:813:HEM:CBB	2.60	0.89
1:I:418:CYS:SG	6:I:810:HEM:HAB	2.12	0.89
1:I:305:CYS:SG	6:I:807:HEM:CBC	2.60	0.89
1:A:465:CYS:SG	6:A:811:HEM:CBC	2.59	0.89
1:D:143:CYS:SG	6:D:806:HEM:CBB	2.59	0.89
1:H:421:CYS:SG	6:H:811:HEM:CBC	2.61	0.89
1:I:363:CYS:SG	6:I:809:HEM:C3C	2.65	0.89
1:J:462:CYS:SG	6:J:811:HEM:HAB	2.13	0.89
1:C:363:CYS:SG	6:C:809:HEM:HAC	2.12	0.89
1:E:146:CYS:SG	6:E:806:HEM:CBC	2.61	0.89
1:I:462:CYS:SG	6:I:811:HEM:HAB	2.11	0.89
1:J:418:CYS:SG	6:J:810:HEM:HAB	2.09	0.89
1:L:143:CYS:SG	6:L:806:HEM:CBB	2.61	0.89
1:E:421:CYS:SG	6:E:810:HEM:CBC	2.61	0.88
1:G:302:CYS:SG	6:G:807:HEM:C3B	2.66	0.88
1:D:360:CYS:SG	6:D:809:HEM:CBB	2.61	0.88
1:F:418:CYS:SG	6:F:811:HEM:CBB	2.62	0.88
1:E:484:CYS:SG	6:E:812:HEM:HAB	2.09	0.88
1:D:462:CYS:SG	6:D:811:HEM:HAB	2.11	0.88
1:H:562:CYS:HG	6:H:814:HEM:CBB	1.87	0.88
1:D:363:CYS:SG	6:D:809:HEM:CBC	2.60	0.88
1:E:418:CYS:SG	6:E:810:HEM:HAB	2.10	0.88
1:A:487:CYS:HG	6:A:812:HEM:CBC	1.88	0.88
1:I:363:CYS:SG	6:I:809:HEM:HAC	2.14	0.88
1:B:146:CYS:SG	6:B:807:HEM:CBC	2.62	0.87
1:G:143:CYS:HG	6:G:806:HEM:CBB	1.87	0.87
1:G:421:CYS:SG	6:G:810:HEM:CBC	2.61	0.87
1:H:462:CYS:SG	6:H:812:HEM:HAB	2.13	0.87
1:K:146:CYS:SG	6:K:806:HEM:CBC	2.61	0.87
1:F:146:CYS:SG	6:F:807:HEM:CBC	2.62	0.87
1:G:562:CYS:SG	6:G:813:HEM:HAB	2.14	0.87
1:D:305:CYS:SG	6:D:807:HEM:C3C	2.68	0.87
1:I:562:CYS:SG	6:I:813:HEM:HAB	2.15	0.87
1:L:143:CYS:SG	6:L:806:HEM:HAB	2.11	0.87
1:B:305:CYS:SG	6:B:808:HEM:C3C	2.68	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:339:CYS:HG	6:I:808:HEM:CBB	1.86	0.87
1:A:143:CYS:SG	6:A:806:HEM:CBB	2.62	0.87
1:A:562:CYS:SG	6:A:813:HEM:HAB	2.11	0.87
1:E:305:CYS:SG	6:E:807:HEM:C3C	2.68	0.86
1:H:363:CYS:SG	6:H:810:HEM:C3C	2.68	0.86
1:J:305:CYS:SG	6:J:807:HEM:C3C	2.67	0.86
1:A:363:CYS:SG	6:A:809:HEM:CBC	2.62	0.86
1:H:143:CYS:SG	6:H:807:HEM:CBB	2.62	0.86
1:J:421:CYS:SG	6:J:810:HEM:CBC	2.64	0.86
1:C:146:CYS:SG	6:C:806:HEM:CBC	2.63	0.86
1:F:484:CYS:SG	6:F:813:HEM:CBB	2.63	0.86
1:I:305:CYS:SG	6:I:807:HEM:C3C	2.68	0.86
1:A:342:CYS:SG	6:A:808:HEM:CBC	2.62	0.86
1:G:578:CYS:SG	6:G:813:HEM:CBC	2.64	0.86
1:J:342:CYS:SG	6:J:808:HEM:CBC	2.64	0.86
1:D:302:CYS:HG	6:D:807:HEM:CAB	1.83	0.86
1:G:342:CYS:SG	6:G:808:HEM:CBC	2.63	0.86
1:E:418:CYS:HG	6:E:810:HEM:CBB	1.85	0.86
1:G:465:CYS:SG	6:G:811:HEM:C3C	2.69	0.86
1:K:484:CYS:SG	6:K:812:HEM:HAB	2.15	0.86
1:F:363:CYS:SG	6:F:810:HEM:CBC	2.64	0.85
1:H:562:CYS:SG	6:H:814:HEM:HAB	2.11	0.85
1:K:305:CYS:SG	6:K:807:HEM:C3C	2.69	0.85
1:A:363:CYS:HG	6:A:809:HEM:CBC	1.88	0.85
1:F:305:CYS:SG	6:F:808:HEM:C3C	2.70	0.85
1:B:342:CYS:SG	6:B:809:HEM:CBC	2.64	0.85
1:C:360:CYS:SG	6:C:809:HEM:HAB	2.17	0.85
1:B:562:CYS:SG	6:B:814:HEM:HAB	2.16	0.85
1:D:342:CYS:SG	6:D:808:HEM:CBC	2.63	0.85
1:L:360:CYS:SG	6:L:809:HEM:CBB	2.64	0.85
1:A:418:CYS:SG	6:A:810:HEM:CBB	2.65	0.84
1:K:360:CYS:SG	6:K:809:HEM:CBB	2.64	0.84
1:C:360:CYS:SG	6:C:809:HEM:CBB	2.65	0.84
1:F:363:CYS:SG	6:F:810:HEM:HAC	2.16	0.84
1:C:562:CYS:SG	6:C:813:HEM:HAB	2.15	0.84
1:B:302:CYS:HG	6:B:808:HEM:CAB	1.84	0.84
1:E:360:CYS:SG	6:E:809:HEM:CBB	2.64	0.84
1:F:360:CYS:SG	6:F:810:HEM:CBB	2.64	0.84
1:H:305:CYS:SG	6:H:808:HEM:CBC	2.65	0.84
1:L:465:CYS:SG	6:L:811:HEM:CBC	2.65	0.84
1:D:363:CYS:SG	6:D:809:HEM:C3C	2.68	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:363:CYS:SG	6:L:809:HEM:C3C	2.68	0.84
1:L:484:CYS:SG	6:L:812:HEM:HAB	2.18	0.84
1:C:484:CYS:SG	6:C:812:HEM:CBB	2.64	0.84
1:I:465:CYS:SG	6:I:811:HEM:CBC	2.65	0.84
1:E:363:CYS:SG	6:E:809:HEM:CBC	2.66	0.83
1:A:146:CYS:SG	6:A:806:HEM:CBC	2.66	0.83
1:D:363:CYS:HG	6:D:809:HEM:CBC	1.90	0.83
1:C:363:CYS:SG	6:C:809:HEM:C3C	2.70	0.83
1:G:363:CYS:SG	6:G:809:HEM:C3C	2.70	0.83
1:A:421:CYS:SG	6:A:810:HEM:CBC	2.66	0.83
1:G:302:CYS:HG	6:G:807:HEM:CAB	1.88	0.83
1:J:465:CYS:SG	6:J:811:HEM:CBC	2.65	0.83
1:L:418:CYS:SG	6:L:810:HEM:HAB	2.16	0.83
1:E:363:CYS:SG	6:E:809:HEM:C3C	2.70	0.83
1:B:462:CYS:SG	6:B:812:HEM:HAB	2.14	0.83
1:F:421:CYS:SG	6:F:811:HEM:CBC	2.68	0.82
1:F:342:CYS:SG	6:F:809:HEM:CBC	2.67	0.82
1:A:360:CYS:SG	6:A:809:HEM:CBB	2.67	0.82
1:C:360:CYS:SG	6:C:809:HEM:C3B	2.66	0.82
1:H:342:CYS:SG	6:H:809:HEM:CBC	2.67	0.82
1:B:360:CYS:SG	6:B:810:HEM:CBB	2.66	0.82
1:F:143:CYS:SG	6:F:807:HEM:HAB	2.17	0.82
1:H:339:CYS:SG	6:H:809:HEM:CBB	2.67	0.82
1:D:421:CYS:SG	6:D:810:HEM:CBC	2.68	0.82
1:I:421:CYS:SG	6:I:810:HEM:C3C	2.72	0.82
1:B:478:THR:O	6:B:814:HEM:O2D	1.97	0.82
1:C:360:CYS:HG	6:C:809:HEM:CAB	1.76	0.82
1:H:302:CYS:HG	6:H:808:HEM:CAB	1.88	0.82
1:I:143:CYS:SG	6:I:806:HEM:HAB	2.18	0.82
1:J:363:CYS:SG	6:J:809:HEM:CBC	2.68	0.82
1:A:363:CYS:SG	6:A:809:HEM:HAC	2.19	0.81
1:I:421:CYS:SG	6:I:810:HEM:CBC	2.68	0.81
1:E:363:CYS:HG	6:E:809:HEM:CBC	1.94	0.81
1:J:143:CYS:HG	6:J:806:HEM:HAB	0.99	0.81
1:I:342:CYS:SG	6:I:808:HEM:CBC	2.68	0.81
1:F:146:CYS:SG	6:F:807:HEM:C3C	2.73	0.81
1:L:305:CYS:SG	6:L:807:HEM:C3C	2.72	0.81
1:C:421:CYS:SG	6:C:810:HEM:CBC	2.68	0.81
1:J:360:CYS:SG	6:J:809:HEM:CBB	2.69	0.81
1:K:363:CYS:SG	6:K:809:HEM:C3C	2.69	0.81
1:H:465:CYS:SG	6:H:812:HEM:C3C	2.73	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:360:CYS:SG	6:I:809:HEM:C3B	2.69	0.81
1:L:421:CYS:SG	6:L:810:HEM:C3C	2.74	0.81
1:E:342:CYS:SG	6:E:808:HEM:CBC	2.69	0.80
1:A:363:CYS:SG	6:A:809:HEM:C3C	2.74	0.80
1:K:418:CYS:SG	6:K:810:HEM:HAB	2.16	0.80
1:G:305:CYS:SG	6:G:807:HEM:C3C	2.74	0.80
1:I:465:CYS:HG	6:I:811:HEM:CBC	1.95	0.80
1:J:465:CYS:SG	6:J:811:HEM:C3C	2.75	0.80
1:K:465:CYS:SG	6:K:811:HEM:C3C	2.74	0.80
1:A:146:CYS:SG	6:A:806:HEM:C3C	2.75	0.80
1:B:360:CYS:SG	6:B:810:HEM:HAB	2.21	0.80
1:E:146:CYS:SG	6:E:806:HEM:C3C	2.74	0.80
1:L:562:CYS:SG	6:L:813:HEM:HAB	2.20	0.80
1:E:143:CYS:SG	6:E:806:HEM:CBB	2.69	0.80
1:G:360:CYS:SG	6:G:809:HEM:CBB	2.69	0.80
1:J:562:CYS:HG	6:J:813:HEM:CBB	1.95	0.80
1:E:562:CYS:HG	6:E:813:HEM:CBB	1.94	0.79
1:G:363:CYS:SG	6:G:809:HEM:HAC	2.22	0.79
1:J:363:CYS:SG	6:J:809:HEM:C3C	2.75	0.79
1:B:363:CYS:SG	6:B:810:HEM:C3C	2.75	0.79
1:F:339:CYS:SG	6:F:809:HEM:CBB	2.71	0.79
1:K:363:CYS:HG	6:K:809:HEM:CBC	1.94	0.79
1:K:363:CYS:SG	6:K:809:HEM:CBC	2.71	0.79
1:I:465:CYS:SG	6:I:811:HEM:C3C	2.74	0.79
1:A:360:CYS:SG	6:A:809:HEM:HAB	2.22	0.79
6:L:807:HEM:HMD1	6:L:807:HEM:CGD	2.12	0.79
6:J:807:HEM:HMD1	6:J:807:HEM:CGD	2.13	0.79
1:K:462:CYS:SG	6:K:811:HEM:HAB	2.20	0.79
1:B:146:CYS:SG	6:B:807:HEM:C3C	2.77	0.78
1:G:363:CYS:SG	6:G:809:HEM:CBC	2.72	0.78
1:D:146:CYS:SG	6:D:806:HEM:C3C	2.77	0.78
1:E:360:CYS:SG	6:E:809:HEM:HAB	2.20	0.78
1:K:363:CYS:SG	6:K:809:HEM:HAC	2.24	0.78
6:C:807:HEM:HMD1	6:C:807:HEM:CGD	2.14	0.78
1:I:418:CYS:HG	6:I:810:HEM:CBB	1.94	0.78
1:I:146:CYS:SG	6:I:806:HEM:C3C	2.77	0.78
1:E:465:CYS:SG	6:E:811:HEM:C3C	2.77	0.78
1:E:462:CYS:SG	6:E:811:HEM:C3B	2.77	0.78
1:B:339:CYS:SG	6:B:809:HEM:C3B	2.78	0.77
1:L:363:CYS:SG	6:L:809:HEM:HAC	2.24	0.77
1:A:562:CYS:SG	6:A:813:HEM:C3B	2.75	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:487:CYS:SG	6:E:812:HEM:C3C	2.76	0.77
1:L:360:CYS:SG	6:L:809:HEM:C3B	2.73	0.77
1:G:465:CYS:SG	6:G:811:HEM:CBC	2.72	0.77
1:K:487:CYS:SG	6:K:812:HEM:C3C	2.76	0.77
1:C:484:CYS:SG	6:C:812:HEM:C3B	2.78	0.77
1:F:418:CYS:HG	6:F:811:HEM:CBB	1.95	0.77
1:I:363:CYS:SG	6:I:809:HEM:CBC	2.73	0.77
1:F:342:CYS:SG	6:F:809:HEM:C3C	2.78	0.77
1:D:421:CYS:SG	6:D:810:HEM:C3C	2.79	0.76
1:C:146:CYS:SG	6:C:806:HEM:C3C	2.78	0.76
6:I:807:HEM:CGD	6:I:807:HEM:HMD1	2.14	0.76
6:K:807:HEM:HMD1	6:K:807:HEM:CGD	2.15	0.76
1:A:578:CYS:SG	6:A:813:HEM:C3C	2.78	0.76
1:G:146:CYS:SG	6:G:806:HEM:C3C	2.77	0.76
1:L:363:CYS:SG	6:L:809:HEM:CBC	2.73	0.76
1:A:465:CYS:SG	6:A:811:HEM:C3C	2.79	0.76
6:D:807:HEM:HMD1	6:D:807:HEM:CGD	2.14	0.76
1:J:562:CYS:SG	6:J:813:HEM:HAB	2.22	0.76
1:J:360:CYS:SG	6:J:809:HEM:C3B	2.71	0.76
1:L:146:CYS:SG	6:L:806:HEM:C3C	2.78	0.76
1:K:421:CYS:SG	6:K:810:HEM:CBC	2.73	0.76
1:E:339:CYS:SG	6:E:808:HEM:C3B	2.78	0.76
1:H:146:CYS:SG	6:H:807:HEM:C3C	2.78	0.76
1:H:421:CYS:SG	6:H:811:HEM:C3C	2.76	0.76
1:I:342:CYS:SG	6:I:808:HEM:C3C	2.79	0.76
1:J:421:CYS:SG	6:J:810:HEM:C3C	2.79	0.76
1:F:302:CYS:HG	6:F:808:HEM:CAB	1.99	0.76
1:F:363:CYS:SG	6:F:810:HEM:C3C	2.78	0.76
1:B:465:CYS:SG	6:B:812:HEM:C3C	2.79	0.75
1:B:562:CYS:SG	6:B:814:HEM:C3B	2.79	0.75
1:J:562:CYS:SG	6:J:813:HEM:C3B	2.74	0.75
1:E:421:CYS:SG	6:E:810:HEM:C3C	2.79	0.75
1:L:465:CYS:SG	6:L:811:HEM:C3C	2.79	0.75
1:F:421:CYS:SG	6:F:811:HEM:C3C	2.78	0.75
1:G:360:CYS:SG	6:G:809:HEM:HAB	2.25	0.75
1:E:302:CYS:HG	6:E:807:HEM:CAB	1.89	0.75
1:A:421:CYS:SG	6:A:810:HEM:C3C	2.79	0.75
1:C:143:CYS:SG	6:C:806:HEM:CBB	2.73	0.75
1:B:342:CYS:SG	6:B:809:HEM:C3C	2.79	0.75
1:B:360:CYS:SG	6:B:810:HEM:C3B	2.74	0.75
1:D:465:CYS:SG	6:D:811:HEM:C3C	2.80	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:342:CYS:SG	6:L:808:HEM:C3C	2.80	0.75
1:B:421:CYS:SG	6:B:811:HEM:C3C	2.79	0.74
1:F:342:CYS:SG	6:F:809:HEM:HAC	2.25	0.74
1:K:421:CYS:SG	6:K:810:HEM:C3C	2.80	0.74
1:A:562:CYS:HG	6:A:813:HEM:CBB	1.99	0.74
1:C:462:CYS:SG	6:C:811:HEM:C3B	2.80	0.74
1:D:360:CYS:SG	6:D:809:HEM:HAB	2.26	0.74
1:E:360:CYS:SG	6:E:809:HEM:C3B	2.73	0.74
1:F:462:CYS:SG	6:F:812:HEM:C3B	2.79	0.74
1:C:421:CYS:SG	6:C:810:HEM:C3C	2.81	0.74
1:H:360:CYS:SG	6:H:810:HEM:C3B	2.77	0.74
1:A:339:CYS:SG	6:A:808:HEM:C3B	2.81	0.74
1:J:302:CYS:HG	6:J:807:HEM:CAB	1.91	0.73
1:G:462:CYS:SG	6:G:811:HEM:C3B	2.81	0.73
1:F:465:CYS:SG	6:F:812:HEM:C3C	2.81	0.73
1:C:465:CYS:SG	6:C:811:HEM:C3C	2.81	0.73
6:A:807:HEM:HMD1	6:A:807:HEM:CGD	2.18	0.73
6:L:810:HEM:HMC1	6:L:810:HEM:HBC2	1.71	0.73
1:F:484:CYS:SG	6:F:813:HEM:C3B	2.82	0.73
1:F:360:CYS:SG	6:F:810:HEM:HAB	2.26	0.72
1:K:462:CYS:HG	6:K:811:HEM:CBB	1.90	0.72
1:I:360:CYS:SG	6:I:809:HEM:HAB	2.25	0.72
1:G:487:CYS:SG	6:G:812:HEM:C3C	2.82	0.72
1:I:360:CYS:SG	6:I:809:HEM:CBB	2.78	0.72
1:C:562:CYS:SG	6:C:813:HEM:C3B	2.82	0.72
1:H:487:CYS:SG	6:H:813:HEM:C3C	2.79	0.72
1:K:562:CYS:SG	6:K:813:HEM:C3B	2.82	0.72
1:D:462:CYS:SG	6:D:811:HEM:C3B	2.81	0.72
1:K:562:CYS:SG	6:K:813:HEM:HAB	2.24	0.72
1:C:418:CYS:SG	6:C:810:HEM:C3B	2.81	0.72
1:F:578:CYS:SG	6:F:814:HEM:C3C	2.83	0.72
1:H:342:CYS:SG	6:H:809:HEM:C3C	2.82	0.72
1:K:418:CYS:SG	6:K:810:HEM:C3B	2.82	0.72
1:F:562:CYS:SG	6:F:814:HEM:C3B	2.83	0.71
1:D:342:CYS:SG	6:D:808:HEM:HAC	2.30	0.71
1:I:462:CYS:SG	6:I:811:HEM:C3B	2.81	0.71
1:I:342:CYS:SG	6:I:808:HEM:HAC	2.27	0.71
1:D:339:CYS:SG	6:D:808:HEM:C3B	2.84	0.71
1:A:484:CYS:SG	6:A:812:HEM:C3B	2.83	0.71
1:C:363:CYS:SG	6:C:809:HEM:CBC	2.78	0.71
1:D:562:CYS:SG	6:D:813:HEM:C3B	2.82	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:146:CYS:SG	6:K:806:HEM:C3C	2.82	0.71
1:C:342:CYS:SG	6:C:808:HEM:HAC	2.28	0.71
1:K:360:CYS:SG	6:K:809:HEM:HAB	2.27	0.71
1:C:487:CYS:SG	6:C:812:HEM:HAC	2.30	0.70
1:C:487:CYS:SG	6:C:812:HEM:C3C	2.84	0.70
1:D:342:CYS:SG	6:D:808:HEM:C3C	2.83	0.70
1:D:487:CYS:SG	6:D:812:HEM:C3C	2.83	0.70
1:G:342:CYS:SG	6:G:808:HEM:HAC	2.30	0.70
1:G:418:CYS:SG	6:G:810:HEM:C3B	2.83	0.70
1:I:339:CYS:SG	6:I:808:HEM:C3B	2.84	0.70
1:J:578:CYS:SG	6:J:813:HEM:C3C	2.83	0.70
1:J:146:CYS:SG	6:J:806:HEM:C3C	2.83	0.70
1:L:462:CYS:SG	6:L:811:HEM:C3B	2.79	0.70
1:C:342:CYS:SG	6:C:808:HEM:C3C	2.83	0.70
1:C:578:CYS:SG	6:C:813:HEM:C3C	2.84	0.70
1:I:302:CYS:HG	6:I:807:HEM:CAB	1.91	0.70
1:B:487:CYS:SG	6:B:813:HEM:C3C	2.83	0.70
1:F:360:CYS:SG	6:F:810:HEM:C3B	2.78	0.70
1:A:487:CYS:SG	6:A:812:HEM:C3C	2.81	0.70
1:G:562:CYS:SG	6:G:813:HEM:C3B	2.85	0.70
1:G:421:CYS:SG	6:G:810:HEM:C3C	2.84	0.70
1:H:484:CYS:SG	6:H:813:HEM:C3B	2.84	0.70
1:J:363:CYS:HG	6:J:809:HEM:CBC	2.05	0.70
1:J:487:CYS:SG	6:J:812:HEM:C3C	2.84	0.70
1:E:578:CYS:SG	6:E:813:HEM:C3C	2.85	0.69
1:C:339:CYS:SG	6:C:808:HEM:C3B	2.83	0.69
1:A:578:CYS:SG	6:A:813:HEM:HAC	2.30	0.69
1:K:578:CYS:SG	6:K:813:HEM:C3C	2.84	0.69
1:L:562:CYS:SG	6:L:813:HEM:C3B	2.84	0.69
1:I:487:CYS:SG	6:I:812:HEM:C3C	2.85	0.69
1:K:360:CYS:SG	6:K:809:HEM:C3B	2.77	0.69
1:B:484:CYS:SG	6:B:813:HEM:C3B	2.84	0.69
1:E:578:CYS:SG	6:E:813:HEM:HAC	2.31	0.69
6:E:807:HEM:HMD1	6:E:807:HEM:CGD	2.23	0.69
1:A:208:LYS:HG3	6:A:807:HEM:HMA2	1.73	0.69
1:F:143:CYS:SG	6:F:807:HEM:C3B	2.85	0.69
1:F:143:CYS:HG	6:F:807:HEM:CAB	2.05	0.69
6:F:808:HEM:HMD1	6:F:808:HEM:CGD	2.23	0.69
1:I:578:CYS:SG	6:I:813:HEM:C3C	2.86	0.69
1:D:578:CYS:SG	6:D:813:HEM:C3C	2.85	0.68
1:A:487:CYS:SG	6:A:812:HEM:HAC	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:363:CYS:SG	6:J:809:HEM:HAC	2.28	0.68
1:L:487:CYS:SG	6:L:812:HEM:C3C	2.86	0.68
1:F:339:CYS:SG	6:F:809:HEM:C3B	2.85	0.68
6:G:807:HEM:HMD1	6:G:807:HEM:CGD	2.22	0.68
1:A:342:CYS:SG	6:A:808:HEM:HAC	2.32	0.68
1:K:342:CYS:SG	6:K:808:HEM:C3C	2.86	0.68
1:B:418:CYS:SG	6:B:811:HEM:C3B	2.85	0.68
1:J:339:CYS:SG	6:J:808:HEM:C3B	2.87	0.68
1:E:363:CYS:SG	6:E:809:HEM:HAC	2.26	0.68
6:H:808:HEM:HMD1	6:H:808:HEM:CGD	2.24	0.68
1:L:302:CYS:HG	6:L:807:HEM:CAB	2.06	0.68
1:E:342:CYS:SG	6:E:808:HEM:C3C	2.86	0.68
1:J:342:CYS:SG	6:J:808:HEM:C3C	2.85	0.68
1:A:302:CYS:HG	6:A:807:HEM:CAB	1.97	0.67
1:E:562:CYS:SG	6:E:813:HEM:C3B	2.78	0.67
1:F:487:CYS:SG	6:F:813:HEM:C3C	2.88	0.67
1:K:339:CYS:SG	6:K:808:HEM:C3B	2.88	0.67
1:H:360:CYS:SG	6:H:810:HEM:HAB	2.31	0.67
1:H:363:CYS:SG	6:H:810:HEM:HAC	2.31	0.67
6:B:808:HEM:HMD1	6:B:808:HEM:CGD	2.25	0.67
1:G:342:CYS:SG	6:G:808:HEM:C3C	2.88	0.67
1:D:363:CYS:SG	6:D:809:HEM:HAC	2.27	0.67
1:E:143:CYS:HG	6:E:806:HEM:HAB	1.58	0.67
1:E:143:CYS:HG	6:E:806:HEM:CAB	2.03	0.67
1:B:143:CYS:SG	6:B:807:HEM:C3B	2.88	0.67
1:E:342:CYS:SG	6:E:808:HEM:HAC	2.34	0.66
1:G:484:CYS:SG	6:G:812:HEM:C3B	2.88	0.66
1:J:342:CYS:SG	6:J:808:HEM:HAC	2.29	0.66
1:D:418:CYS:SG	6:D:810:HEM:C3B	2.84	0.66
1:G:578:CYS:SG	6:G:813:HEM:C3C	2.88	0.66
1:L:360:CYS:SG	6:L:809:HEM:HAB	2.28	0.66
1:J:360:CYS:SG	6:J:809:HEM:HAB	2.29	0.66
1:A:418:CYS:SG	6:A:810:HEM:C3B	2.85	0.66
1:H:339:CYS:SG	6:H:809:HEM:C3B	2.89	0.65
1:I:562:CYS:SG	6:I:813:HEM:C3B	2.90	0.65
1:I:484:CYS:SG	6:I:812:HEM:C3B	2.88	0.65
1:C:339:CYS:SG	6:C:808:HEM:CBB	2.84	0.65
1:J:462:CYS:SG	6:J:811:HEM:C3B	2.88	0.65
1:A:342:CYS:SG	6:A:808:HEM:C3C	2.89	0.65
1:K:146:CYS:SG	6:K:806:HEM:HAC	2.35	0.65
1:C:363:CYS:HG	6:C:809:HEM:CBC	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:SER:OG	1:G:124:ARG:HG3	1.97	0.65
1:B:363:CYS:SG	6:B:810:HEM:HAC	2.31	0.64
1:B:418:CYS:HG	6:B:811:HEM:CBB	2.05	0.64
1:I:487:CYS:SG	6:I:812:HEM:HAC	2.35	0.64
1:A:421:CYS:SG	6:A:810:HEM:HAC	2.33	0.64
1:D:484:CYS:SG	6:D:812:HEM:C3B	2.87	0.64
1:E:484:CYS:SG	6:E:812:HEM:C3B	2.88	0.64
1:L:484:CYS:SG	6:L:812:HEM:C3B	2.88	0.64
1:B:462:CYS:SG	6:B:812:HEM:C3B	2.89	0.64
1:C:143:CYS:SG	6:C:806:HEM:C3B	2.91	0.64
6:B:811:HEM:HMC1	6:B:811:HEM:HBC2	1.80	0.63
1:C:339:CYS:HG	6:C:808:HEM:CBB	2.10	0.63
1:H:342:CYS:SG	6:H:809:HEM:HAC	2.33	0.63
1:H:562:CYS:SG	6:H:814:HEM:C3B	2.80	0.63
1:C:146:CYS:SG	6:C:806:HEM:HAC	2.30	0.63
1:C:302:CYS:HG	6:C:807:HEM:CAB	2.08	0.63
1:G:339:CYS:SG	6:G:808:HEM:C3B	2.89	0.63
1:K:484:CYS:SG	6:K:812:HEM:C3B	2.90	0.63
1:I:465:CYS:SG	6:I:811:HEM:HAC	2.35	0.63
1:D:360:CYS:SG	6:D:809:HEM:C3B	2.74	0.63
1:D:143:CYS:SG	6:D:806:HEM:C3B	2.89	0.63
1:L:143:CYS:SG	6:L:806:HEM:C3B	2.91	0.63
1:A:305:CYS:SG	6:A:807:HEM:HAC	2.31	0.62
1:G:208:LYS:HG3	6:G:807:HEM:HMA3	1.82	0.62
1:F:487:CYS:SG	6:F:813:HEM:HAC	2.33	0.62
1:L:578:CYS:SG	6:L:813:HEM:C3C	2.93	0.62
1:E:143:CYS:SG	6:E:806:HEM:C3B	2.91	0.62
1:G:475:LYS:O	1:G:476:ALA:O	2.17	0.62
1:D:375:ARG:NH1	8:D:1036:HOH:O	2.31	0.62
1:J:484:CYS:SG	6:J:812:HEM:C3B	2.91	0.62
1:H:462:CYS:SG	6:H:812:HEM:C3B	2.91	0.61
1:B:689:SER:O	1:B:690:LEU:HB2	2.01	0.61
1:F:418:CYS:SG	6:F:811:HEM:C3B	2.92	0.61
1:H:418:CYS:SG	6:H:811:HEM:C3B	2.89	0.61
1:B:578:CYS:SG	6:B:814:HEM:C3C	2.92	0.61
1:B:487:CYS:SG	6:B:813:HEM:HAC	2.36	0.61
1:A:360:CYS:SG	6:A:809:HEM:C3B	2.80	0.61
1:D:421:CYS:SG	6:D:810:HEM:HAC	2.37	0.61
1:J:418:CYS:SG	6:J:810:HEM:C3B	2.92	0.61
1:B:342:CYS:SG	6:B:809:HEM:HAC	2.34	0.60
1:I:418:CYS:SG	6:I:810:HEM:C3B	2.86	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:502:GLN:O	1:L:539:ARG:NH2	2.35	0.60
1:G:360:CYS:SG	6:G:809:HEM:C3B	2.78	0.60
1:D:418:CYS:HG	6:D:810:HEM:CBB	2.07	0.60
1:A:143:CYS:SG	6:A:806:HEM:C3B	2.91	0.59
1:C:302:CYS:SG	6:C:807:HEM:CBB	2.89	0.59
1:H:418:CYS:HG	6:H:811:HEM:CBB	2.06	0.59
1:I:143:CYS:SG	6:I:806:HEM:C3B	2.93	0.59
1:L:339:CYS:SG	6:L:808:HEM:C3B	2.93	0.59
1:J:650:THR:HG23	1:J:671:ARG:HG2	1.84	0.59
1:E:418:CYS:SG	6:E:810:HEM:C3B	2.87	0.59
1:K:302:CYS:SG	6:K:807:HEM:C2B	2.95	0.58
1:L:418:CYS:SG	6:L:810:HEM:C3B	2.95	0.58
1:J:305:CYS:CB	6:J:807:HEM:C3C	2.86	0.58
1:K:302:CYS:SG	6:K:807:HEM:HAB	2.39	0.58
1:I:363:CYS:HG	6:I:809:HEM:CBC	2.14	0.58
1:I:208:LYS:HG3	6:I:807:HEM:HMA3	1.86	0.58
1:F:578:CYS:SG	6:F:814:HEM:HAC	2.34	0.58
1:G:465:CYS:SG	6:G:811:HEM:HAC	2.36	0.57
1:I:578:CYS:SG	6:I:813:HEM:HAC	2.37	0.57
1:B:146:CYS:SG	6:B:807:HEM:HAC	2.38	0.56
1:K:465:CYS:SG	6:K:811:HEM:HAC	2.40	0.56
1:F:146:CYS:SG	6:F:807:HEM:HAC	2.37	0.56
1:A:434:GLU:HB2	1:A:437:ILE:HD12	1.86	0.56
1:H:578:CYS:SG	6:H:814:HEM:C3C	2.86	0.56
6:L:812:HEM:HMC2	6:L:812:HEM:HBC2	1.88	0.56
1:H:143:CYS:SG	6:H:807:HEM:C3B	2.96	0.56
1:K:462:CYS:SG	6:K:811:HEM:C3B	2.80	0.56
1:A:302:CYS:SG	6:A:807:HEM:CBB	2.93	0.55
1:K:143:CYS:SG	6:K:806:HEM:CBB	2.90	0.55
1:L:575:ALA:HB3	6:L:813:HEM:HBC1	1.88	0.55
1:A:146:CYS:SG	6:A:806:HEM:HAC	2.36	0.55
1:D:302:CYS:SG	6:D:807:HEM:CBB	2.93	0.55
1:L:575:ALA:HB3	6:L:813:HEM:CBC	2.36	0.55
1:J:612:LYS:HE3	1:J:676:VAL:HG21	1.88	0.55
6:J:813:HEM:HBB2	6:J:813:HEM:HMB1	1.88	0.55
1:I:421:CYS:SG	6:I:810:HEM:HAC	2.38	0.54
1:K:305:CYS:CB	6:K:807:HEM:C3C	2.90	0.54
1:D:208:LYS:HG3	6:D:807:HEM:HMA2	1.88	0.54
1:A:402:GLU:O	1:A:406:THR:HG23	2.08	0.54
1:D:402:GLU:O	1:D:406:THR:HG23	2.07	0.54
1:G:578:CYS:SG	6:G:813:HEM:HAC	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:CYS:SG	6:E:807:HEM:CBB	2.95	0.54
1:G:476:ALA:O	1:G:480:SER:HB3	2.06	0.54
1:A:305:CYS:CB	6:A:807:HEM:C3C	2.90	0.53
1:B:146:CYS:CB	6:B:807:HEM:C3C	2.91	0.53
1:D:487:CYS:SG	6:D:812:HEM:HAC	2.39	0.53
1:D:578:CYS:SG	6:D:813:HEM:HAC	2.36	0.53
1:C:578:CYS:SG	6:C:813:HEM:HAC	2.42	0.53
1:A:462:CYS:SG	6:A:811:HEM:C3B	2.91	0.53
6:K:810:HEM:HMB1	6:K:810:HEM:HBB2	1.90	0.53
1:D:305:CYS:CB	6:D:807:HEM:C3C	2.92	0.53
1:H:400:GLY:HA3	6:H:808:HEM:HMD2	1.89	0.53
1:C:612:LYS:HE3	1:C:676:VAL:HG21	1.91	0.53
1:B:305:CYS:CB	6:B:808:HEM:C3C	2.92	0.53
1:H:487:CYS:SG	6:H:813:HEM:HAC	2.36	0.53
1:B:302:CYS:SG	6:B:808:HEM:CBB	2.95	0.52
1:E:208:LYS:HG3	6:E:807:HEM:HMA2	1.92	0.52
1:A:418:CYS:HG	6:A:810:HEM:CBB	2.13	0.52
1:E:484:CYS:CB	6:E:812:HEM:CAB	2.87	0.52
1:E:540:ASP:O	4:E:804:BU3:H3	2.10	0.52
1:F:146:CYS:CB	6:F:807:HEM:C3C	2.93	0.52
1:G:302:CYS:SG	6:G:807:HEM:CBB	2.98	0.52
1:F:302:CYS:SG	6:F:808:HEM:CBB	2.98	0.52
1:H:302:CYS:SG	6:H:808:HEM:CBB	2.96	0.52
1:F:208:LYS:HG3	6:F:808:HEM:HMA3	1.92	0.51
1:H:305:CYS:CB	6:H:808:HEM:C3C	2.93	0.51
1:L:208:LYS:HG3	6:L:807:HEM:HMA3	1.91	0.51
1:G:146:CYS:SG	6:G:806:HEM:HAC	2.38	0.51
1:B:208:LYS:HG3	6:B:808:HEM:HMA3	1.93	0.51
1:L:400:GLY:HA3	6:L:807:HEM:HMD2	1.92	0.51
1:L:305:CYS:CB	6:L:807:HEM:C3C	2.94	0.51
1:G:146:CYS:CB	6:G:806:HEM:C3C	2.93	0.51
1:L:146:CYS:CB	6:L:806:HEM:C3C	2.94	0.51
1:L:575:ALA:CB	6:L:813:HEM:CBC	2.89	0.51
1:J:578:CYS:SG	6:J:813:HEM:HAC	2.37	0.51
1:A:435:LYS:NZ	1:A:445:GLU:OE1	2.43	0.51
1:C:146:CYS:CB	6:C:806:HEM:C3C	2.94	0.51
1:D:146:CYS:CB	6:D:806:HEM:C3C	2.94	0.51
1:F:305:CYS:CB	6:F:808:HEM:C3C	2.94	0.51
1:G:484:CYS:CB	6:G:812:HEM:CAB	2.89	0.51
1:D:339:CYS:HG	6:D:808:HEM:CBB	2.22	0.51
1:C:395:MET:HG2	1:C:544:TRP:CE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:CYS:CB	6:I:807:HEM:C3C	2.93	0.50
1:A:49:GLU:HG2	8:A:1274:HOH:O	2.11	0.50
1:A:629:VAL:HG12	1:A:629:VAL:O	2.11	0.50
1:F:363:CYS:CB	6:F:810:HEM:C3C	2.95	0.50
1:L:465:CYS:SG	6:L:811:HEM:HAC	2.39	0.50
1:L:518:TRP:HE1	6:L:811:HEM:HBB2	1.76	0.50
1:E:146:CYS:CB	6:E:806:HEM:C3C	2.95	0.50
1:D:339:CYS:SG	6:D:808:HEM:CBB	2.95	0.49
1:I:484:CYS:HB3	6:I:812:HEM:C3B	2.48	0.49
1:D:632:LEU:HD13	1:D:636:ASP:CB	2.43	0.49
6:H:811:HEM:HBB2	6:H:811:HEM:HMB1	1.94	0.49
1:J:146:CYS:CB	6:J:806:HEM:C3C	2.96	0.49
1:L:104:ASN:O	1:L:108:LYS:HG2	2.12	0.49
1:L:342:CYS:SG	6:L:808:HEM:HAC	2.40	0.49
6:B:809:HEM:HBC1	6:B:810:HEM:CHC	2.42	0.49
1:C:421:CYS:SG	6:C:810:HEM:HAC	2.41	0.49
1:C:208:LYS:HG3	6:C:807:HEM:HMA3	1.95	0.49
1:L:363:CYS:HG	6:L:809:HEM:CBC	2.17	0.49
1:H:84:THR:OG1	1:H:86:GLY:O	2.25	0.49
1:B:465:CYS:SG	6:B:812:HEM:HAC	2.43	0.49
1:A:410:ALA:O	1:A:414:LYS:HG2	2.12	0.48
6:J:812:HEM:HMC2	6:J:812:HEM:HBC2	1.95	0.48
1:K:421:CYS:SG	6:K:810:HEM:HAC	2.43	0.48
1:J:360:CYS:HG	6:J:809:HEM:CBB	2.21	0.48
1:A:146:CYS:CB	6:A:806:HEM:C3C	2.96	0.48
1:K:342:CYS:SG	6:K:808:HEM:HAC	2.39	0.48
1:C:486:SER:HB2	6:C:813:HEM:HBC2	1.96	0.48
1:F:223:VAL:CG2	1:F:235:ILE:HD13	2.43	0.48
1:I:146:CYS:CB	6:I:806:HEM:C3C	2.96	0.48
1:G:487:CYS:SG	6:G:812:HEM:HAC	2.40	0.48
1:I:484:CYS:CB	6:I:812:HEM:CAB	2.89	0.48
6:L:806:HEM:HMC2	6:L:806:HEM:HBC2	1.96	0.48
1:I:146:CYS:SG	6:I:806:HEM:HAC	2.44	0.48
1:A:462:CYS:SG	6:A:811:HEM:CBB	2.94	0.47
1:D:360:CYS:HG	6:D:809:HEM:CBB	2.20	0.47
1:J:84:THR:HG21	1:J:88:LEU:HD21	1.95	0.47
1:E:146:CYS:SG	6:E:806:HEM:HAC	2.40	0.47
1:J:463:THR:HG22	1:J:470:ALA:HB2	1.96	0.47
1:G:484:CYS:HB3	6:G:812:HEM:C3B	2.49	0.47
1:I:681:GLU:O	1:I:685:ILE:HD12	2.14	0.47
1:J:421:CYS:SG	6:J:810:HEM:HAC	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:465:CYS:SG	6:J:811:HEM:HAC	2.41	0.47
1:K:165:PHE:CZ	1:K:335:LYS:HD3	2.49	0.47
1:C:465:CYS:SG	6:C:811:HEM:HAC	2.43	0.47
1:E:305:CYS:CB	6:E:807:HEM:C3C	2.97	0.47
1:K:487:CYS:SG	6:K:812:HEM:HAC	2.41	0.47
1:E:607:THR:HB	1:E:608:PRO:HD3	1.96	0.47
1:G:305:CYS:C	1:G:307:PRO:HD3	2.35	0.47
1:G:143:CYS:SG	6:G:806:HEM:C3B	2.87	0.47
1:I:400:GLY:HA3	6:I:807:HEM:HMD2	1.97	0.47
1:A:547:GLU:HG3	8:A:1296:HOH:O	2.15	0.47
1:G:305:CYS:CB	6:G:807:HEM:C3C	2.98	0.47
1:C:400:GLY:HA3	6:C:807:HEM:HMD2	1.98	0.47
1:C:623:LEU:O	1:C:627:LEU:HG	2.15	0.46
1:F:421:CYS:SG	6:F:811:HEM:HAC	2.40	0.46
1:K:208:LYS:HG3	6:K:807:HEM:HMA3	1.95	0.46
1:L:302:CYS:SG	6:L:807:HEM:CBB	2.99	0.46
6:I:810:HEM:HBB2	6:I:810:HEM:HMB1	1.96	0.46
1:C:305:CYS:CB	6:C:807:HEM:C3C	2.99	0.46
1:F:491:PHE:O	1:F:511:THR:HB	2.16	0.46
1:J:684:ARG:O	1:J:688:LYS:NZ	2.48	0.46
1:K:305:CYS:HB2	6:K:807:HEM:C3C	2.50	0.46
1:B:243:GLN:HB3	1:B:496:GLU:OE2	2.14	0.46
1:E:646:LYS:NZ	8:E:1118:HOH:O	2.49	0.46
1:H:146:CYS:CB	6:H:807:HEM:C3C	2.99	0.46
6:H:807:HEM:HBC2	6:H:807:HEM:HMC2	1.97	0.46
1:I:372:ASP:OD1	1:I:375:ARG:NH2	2.48	0.46
1:A:363:CYS:CB	6:A:809:HEM:C3C	2.99	0.46
6:L:808:HEM:HBC1	6:L:809:HEM:CHC	2.46	0.46
1:C:301:TYR:CD2	6:C:807:HEM:HAB	2.51	0.46
1:D:465:CYS:HG	6:D:811:HEM:CAC	2.26	0.46
1:I:289:TYR:CE2	1:I:290:LYS:HE2	2.51	0.46
1:J:146:CYS:SG	6:J:806:HEM:HAC	2.45	0.46
6:K:808:HEM:CMC	6:K:808:HEM:HBC2	2.46	0.46
6:L:807:HEM:HBC2	6:L:807:HEM:HMC2	1.97	0.46
1:D:484:CYS:CB	6:D:812:HEM:CAB	2.91	0.45
1:F:365:GLN:NE2	5:F:806:ACT:O	2.48	0.45
1:G:654:ILE:HD12	1:G:668:THR:HG23	1.98	0.45
1:I:305:CYS:SG	6:I:807:HEM:HAC	2.39	0.45
1:E:112:ARG:HB2	1:K:151:TYR:CE1	2.51	0.45
1:A:484:CYS:CB	6:A:812:HEM:CAB	2.93	0.45
1:B:675:ALA:HA	1:B:678:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:CYS:HG	6:K:807:HEM:CAB	2.10	0.45
1:C:650:THR:HG23	1:C:671:ARG:HG2	1.98	0.45
1:C:365:GLN:OE1	5:C:805:ACT:H1	2.17	0.45
1:F:486:SER:HB2	6:F:814:HEM:HBC2	1.98	0.45
1:F:143:CYS:CB	6:F:807:HEM:CAB	2.92	0.45
1:G:402:GLU:O	1:G:406:THR:HG23	2.16	0.45
1:A:305:CYS:HB2	6:A:807:HEM:C3C	2.51	0.45
1:G:487:CYS:HG	6:G:812:HEM:CAC	2.22	0.45
1:E:305:CYS:SG	6:E:807:HEM:HAC	2.43	0.45
1:E:659:SER:HB3	1:E:663:HIS:CE1	2.52	0.45
1:G:360:CYS:HG	6:G:809:HEM:CBB	2.16	0.45
1:I:499:TYR:O	1:I:539:ARG:NH2	2.50	0.45
1:G:208:LYS:HG3	6:G:807:HEM:CMA	2.48	0.44
6:I:806:HEM:HBC2	6:I:806:HEM:HMC2	1.99	0.44
1:K:146:CYS:CB	6:K:806:HEM:C3C	3.00	0.44
1:E:654:ILE:HD12	1:E:668:THR:HG23	1.99	0.44
1:K:357:ILE:HB	4:K:803:BU3:H11	1.99	0.44
1:F:363:CYS:HB2	6:F:810:HEM:C3C	2.51	0.44
1:G:94:GLY:O	1:G:98:ILE:HB	2.16	0.44
1:L:220:THR:HA	1:L:240:ASN:ND2	2.33	0.44
1:D:146:CYS:SG	6:D:806:HEM:HAC	2.44	0.44
1:D:465:CYS:SG	6:D:811:HEM:HAC	2.44	0.44
1:D:486:SER:HB2	6:D:813:HEM:HBC2	1.99	0.44
1:G:688:LYS:N	1:G:688:LYS:HD3	2.33	0.44
6:J:813:HEM:HBD1	6:J:813:HEM:HMD2	1.98	0.44
1:F:223:VAL:HG22	1:F:235:ILE:HD13	1.99	0.44
1:F:659:SER:HB3	1:F:663:HIS:CE1	2.53	0.44
1:A:243:GLN:HB3	1:A:496:GLU:OE2	2.18	0.44
1:E:402:GLU:O	1:E:406:THR:HG23	2.16	0.44
1:G:421:CYS:SG	6:G:810:HEM:HAC	2.45	0.44
1:B:305:CYS:C	1:B:307:PRO:HD3	2.37	0.44
1:J:208:LYS:HG3	6:J:807:HEM:HMA3	1.99	0.44
6:C:807:HEM:HBB2	6:C:807:HEM:HMB2	2.00	0.44
6:D:811:HEM:HMC2	6:D:811:HEM:HBC2	1.99	0.44
1:E:484:CYS:HB3	6:E:812:HEM:C3B	2.53	0.44
1:F:633:ALA:O	1:F:636:ASP:N	2.44	0.44
1:J:143:CYS:HG	6:J:806:HEM:CAB	1.88	0.44
1:B:578:CYS:SG	6:B:814:HEM:HAC	2.43	0.43
1:C:104:ASN:O	1:C:108:LYS:HG2	2.17	0.43
6:C:810:HEM:HMB1	6:C:810:HEM:HBB2	2.00	0.43
1:H:123:TYR:CE1	6:H:808:HEM:HBC2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:402:GLU:O	1:J:406:THR:HG23	2.19	0.43
1:J:305:CYS:HB2	6:J:807:HEM:C3C	2.53	0.43
1:K:400:GLY:HA3	6:K:807:HEM:HMD2	2.00	0.43
1:B:270:GLU:HG2	1:B:271:GLU:N	2.33	0.43
1:B:143:CYS:HG	6:B:807:HEM:CAB	2.21	0.43
1:F:453:TYR:CD2	1:F:570:LYS:HG2	2.54	0.43
1:H:203:GLY:HA3	6:H:808:HEM:HMA1	2.01	0.43
1:H:305:CYS:SG	6:H:808:HEM:HAC	2.39	0.43
1:D:410:ALA:O	1:D:414:LYS:HG2	2.19	0.43
1:E:343:HIS:CE1	6:E:808:HEM:ND	2.86	0.43
1:K:207:THR:HG23	1:K:512:GLN:HG3	2.00	0.43
1:J:302:CYS:SG	6:J:807:HEM:CBB	3.04	0.43
1:D:659:SER:HB3	1:D:663:HIS:CE1	2.54	0.43
1:D:305:CYS:HB2	6:D:807:HEM:C3C	2.53	0.43
1:F:484:CYS:CB	6:F:813:HEM:CAB	2.95	0.43
6:H:814:HEM:HMC2	6:H:814:HEM:HBC2	1.99	0.43
1:D:151:TYR:CE1	1:K:112:ARG:HB2	2.54	0.43
1:D:305:CYS:SG	6:D:807:HEM:HAC	2.43	0.43
1:G:400:GLY:HA3	6:G:807:HEM:HMD2	2.00	0.43
1:F:151:TYR:CE1	1:I:112:ARG:HB2	2.53	0.43
1:L:131:LEU:HD21	1:L:299:THR:HG21	2.01	0.43
1:L:434:GLU:HB2	1:L:437:ILE:HD12	2.01	0.43
6:D:808:HEM:HBC1	6:D:809:HEM:CHC	2.48	0.43
1:H:493:MET:HB2	1:H:513:ARG:HB2	2.01	0.43
1:I:151:TYR:CE1	1:J:112:ARG:HB2	2.53	0.43
1:I:402:GLU:O	1:I:406:THR:HG23	2.18	0.43
1:I:453:TYR:CD2	1:I:570:LYS:HD2	2.54	0.43
6:D:806:HEM:HBC2	6:D:806:HEM:HMC2	2.01	0.43
1:H:302:CYS:SG	6:H:808:HEM:HAB	2.48	0.43
6:A:808:HEM:HBC1	6:A:809:HEM:CHC	2.49	0.43
1:E:223:VAL:HG22	1:E:235:ILE:HD13	2.01	0.43
1:F:143:CYS:HG	6:F:807:HEM:CBB	2.19	0.43
1:K:143:CYS:SG	6:K:806:HEM:C3B	3.00	0.43
6:G:806:HEM:HMC2	6:G:806:HEM:HBC2	2.01	0.42
1:H:395:MET:HG2	1:H:544:TRP:CE2	2.54	0.42
1:K:84:THR:OG1	1:K:86:GLY:O	2.37	0.42
1:L:339:CYS:HA	6:L:808:HEM:CHC	2.49	0.42
6:L:807:HEM:HBB2	6:L:807:HEM:HMB2	2.00	0.42
1:B:487:CYS:HG	6:B:813:HEM:CAC	2.22	0.42
1:H:484:CYS:CB	6:H:813:HEM:CAB	2.95	0.42
1:K:612:LYS:O	1:K:616:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:223:VAL:HG22	1:L:235:ILE:HD13	2.01	0.42
6:K:808:HEM:HBC2	6:K:808:HEM:HMC2	2.01	0.42
1:L:305:CYS:HB2	6:L:807:HEM:C3C	2.55	0.42
1:E:499:TYR:CD1	4:E:804:BU3:H43	2.54	0.42
1:E:360:CYS:HG	6:E:809:HEM:CBB	2.19	0.42
1:G:363:CYS:CB	6:G:809:HEM:C3C	3.03	0.42
6:J:813:HEM:HBD1	6:J:813:HEM:CMD	2.50	0.42
1:B:191:GLN:HG2	1:B:223:VAL:O	2.19	0.42
6:B:808:HEM:HMB2	6:B:808:HEM:HBB2	2.00	0.42
6:C:807:HEM:HMD1	6:C:807:HEM:CBD	2.50	0.42
1:D:607:THR:HB	1:D:608:PRO:HD3	2.01	0.42
1:A:264:ASP:OD1	1:A:264:ASP:N	2.51	0.42
1:F:302:CYS:SG	6:F:808:HEM:HAB	2.50	0.42
6:H:807:HEM:HBC2	6:H:807:HEM:CMC	2.50	0.42
1:J:197:VAL:O	1:J:214:ALA:N	2.53	0.42
1:L:301:TYR:CD2	6:L:807:HEM:HAB	2.55	0.42
1:G:492:MET:CE	1:G:529:LEU:HD21	2.49	0.42
1:H:374:MET:CE	1:H:384:PRO:HA	2.50	0.42
6:L:812:HEM:HBC2	6:L:812:HEM:CMC	2.50	0.42
1:F:471:TYR:O	1:F:474:SER:OG	2.33	0.42
6:K:808:HEM:HBC1	6:K:809:HEM:CHC	2.49	0.42
1:G:402:GLU:HB2	6:G:810:HEM:HMB3	2.01	0.41
1:J:259:LYS:HA	1:J:262:VAL:O	2.20	0.41
1:J:654:ILE:CD1	1:J:672:LEU:HG	2.50	0.41
1:L:302:CYS:SG	6:L:807:HEM:HAB	2.47	0.41
1:C:607:THR:HB	1:C:608:PRO:HD3	2.02	0.41
1:E:395:MET:HG2	1:E:544:TRP:CE2	2.55	0.41
5:E:805:ACT:H1	8:E:1105:HOH:O	2.19	0.41
1:G:476:ALA:O	1:G:477:ASP:CB	2.68	0.41
1:G:484:CYS:CB	6:G:812:HEM:C3B	3.03	0.41
6:H:809:HEM:HBC1	6:H:810:HEM:CHC	2.50	0.41
1:I:302:CYS:SG	6:I:807:HEM:C2B	3.12	0.41
1:I:62:GLU:OE1	1:I:129:SER:OG	2.25	0.41
1:L:203:GLY:HA2	6:L:807:HEM:HBA2	2.02	0.41
1:C:305:CYS:C	1:C:307:PRO:HD3	2.40	0.41
1:E:628:GLU:O	1:E:629:VAL:HG22	2.19	0.41
1:A:642:GLU:OE2	1:C:646:LYS:HE3	2.21	0.41
1:D:642:GLU:HG3	1:E:646:LYS:HE3	2.03	0.41
1:F:400:GLY:HA3	6:F:808:HEM:HMD2	2.03	0.41
1:L:306:HIS:CE1	6:L:809:HEM:HMD2	2.56	0.41
1:B:418:CYS:CA	6:B:811:HEM:HAB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:GLU:O	1:C:406:THR:HG23	2.21	0.41
1:F:184:ASP:OD1	1:F:184:ASP:N	2.52	0.41
1:G:463:THR:HG22	1:G:470:ALA:HB2	2.03	0.41
1:H:112:ARG:HB2	1:G:151:TYR:CE1	2.56	0.41
1:K:636:ASP:O	1:K:640:VAL:HG23	2.21	0.41
1:D:301:TYR:CD2	6:D:807:HEM:HAB	2.56	0.41
1:I:305:CYS:C	1:I:307:PRO:HD3	2.40	0.41
1:I:484:CYS:CB	6:I:812:HEM:C3B	3.04	0.41
1:J:302:CYS:SG	6:J:807:HEM:C2B	3.10	0.41
1:K:643:LEU:HD11	1:K:681:GLU:HG2	2.02	0.41
1:B:143:CYS:HG	6:B:807:HEM:HAB	1.81	0.41
1:J:143:CYS:SG	6:J:806:HEM:C3B	3.03	0.41
1:E:311:ASP:C	1:E:311:ASP:OD1	2.59	0.41
1:G:475:LYS:O	1:G:476:ALA:C	2.60	0.41
1:J:94:GLY:O	1:J:98:ILE:HB	2.21	0.41
1:B:305:CYS:HB2	6:B:808:HEM:C3C	2.55	0.41
1:D:84:THR:HG21	1:D:88:LEU:HD21	2.03	0.41
1:E:434:GLU:HB2	1:E:437:ILE:HD12	2.03	0.41
1:F:175:LYS:HE3	1:F:178:ASP:OD2	2.21	0.41
1:B:196:ASP:N	1:B:196:ASP:OD1	2.54	0.40
1:B:659:SER:HB3	1:B:663:HIS:CE1	2.56	0.40
6:G:812:HEM:HMC2	6:G:812:HEM:HBC2	2.03	0.40
1:H:357:ILE:HB	4:H:803:BU3:H11	2.02	0.40
1:I:94:GLY:O	1:I:98:ILE:HB	2.20	0.40
1:B:203:GLY:HA3	6:B:808:HEM:HMA1	2.03	0.40
1:H:421:CYS:SG	6:H:811:HEM:HAC	2.45	0.40
1:J:147:HIS:CE1	6:J:806:HEM:ND	2.89	0.40
1:J:605:TRP:HE3	1:J:662:MET:SD	2.44	0.40
1:D:513:ARG:NH1	6:D:810:HEM:O1A	2.55	0.40
1:E:484:CYS:CB	6:E:812:HEM:C3B	3.05	0.40
1:E:650:THR:HG23	1:E:671:ARG:HB3	2.04	0.40
1:K:203:GLY:HA3	6:K:807:HEM:HMA1	2.03	0.40
6:L:809:HEM:HMB2	6:L:809:HEM:HBB2	2.04	0.40

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%)	51	58
1	B	658/732 (90%)	628 (95%)	29 (4%)	1 (0%)	51	58
1	C	657/732 (90%)	632 (96%)	23 (4%)	2 (0%)	44	49
1	D	657/732 (90%)	624 (95%)	32 (5%)	1 (0%)	51	58
1	E	657/732 (90%)	625 (95%)	30 (5%)	2 (0%)	44	49
1	F	657/732 (90%)	626 (95%)	29 (4%)	2 (0%)	44	49
1	G	656/732 (90%)	625 (95%)	28 (4%)	3 (0%)	32	34
1	H	658/732 (90%)	631 (96%)	26 (4%)	1 (0%)	51	58
1	I	657/732 (90%)	626 (95%)	29 (4%)	2 (0%)	44	49
1	J	657/732 (90%)	623 (95%)	32 (5%)	2 (0%)	44	49
1	K	657/732 (90%)	625 (95%)	31 (5%)	1 (0%)	51	58
1	L	657/732 (90%)	628 (96%)	27 (4%)	2 (0%)	44	49
All	All	7885/8784 (90%)	7525 (95%)	340 (4%)	20 (0%)	44	49

All (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
1	J	301	TYR
1	G	301	TYR
1	E	301	TYR
1	I	301	TYR
1	L	206	ARG
1	I	664	GLY
1	B	664	GLY

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Mol	Chain	Res	Type
1	D	664	GLY
1	A	664	GLY
1	F	664	GLY
1	H	664	GLY
1	G	664	GLY
1	C	664	GLY
1	E	664	GLY
1	J	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	559/613 (91%)	553 (99%)	6 (1%)	78	88
1	B	560/613 (91%)	555 (99%)	5 (1%)	82	91
1	C	559/613 (91%)	554 (99%)	5 (1%)	82	91
1	D	559/613 (91%)	553 (99%)	6 (1%)	78	88
1	E	559/613 (91%)	555 (99%)	4 (1%)	87	93
1	F	559/613 (91%)	552 (99%)	7 (1%)	73	85
1	G	558/613 (91%)	554 (99%)	4 (1%)	87	93
1	H	560/613 (91%)	555 (99%)	5 (1%)	82	91
1	I	559/613 (91%)	553 (99%)	6 (1%)	78	88
1	J	559/613 (91%)	555 (99%)	4 (1%)	87	93
1	K	559/613 (91%)	554 (99%)	5 (1%)	82	91
1	L	559/613 (91%)	553 (99%)	6 (1%)	78	88
All	All	6709/7356 (91%)	6646 (99%)	63 (1%)	82	91

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ARG
1	A	250	LEU

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Mol	Chain	Res	Type
1	A	275	ASN
1	A	302	CYS
1	A	498	PHE
1	A	564	ARG
1	B	124	ARG
1	B	270	GLU
1	B	275	ASN
1	B	302	CYS
1	B	564	ARG
1	C	124	ARG
1	C	275	ASN
1	C	302	CYS
1	C	564	ARG
1	C	651	VAL
1	D	124	ARG
1	D	275	ASN
1	D	302	CYS
1	D	498	PHE
1	D	564	ARG
1	D	645	GLU
1	E	124	ARG
1	E	275	ASN
1	E	302	CYS
1	E	564	ARG
1	F	124	ARG
1	F	129	SER
1	F	194	THR
1	F	275	ASN
1	F	302	CYS
1	F	498	PHE
1	F	564	ARG
1	H	124	ARG
1	H	275	ASN
1	H	302	CYS
1	H	564	ARG
1	H	690	LEU
1	I	124	ARG
1	I	275	ASN
1	I	290	LYS
1	I	302	CYS
1	I	498	PHE
1	I	564	ARG

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Mol	Chain	Res	Type
1	J	124	ARG
1	J	275	ASN
1	J	302	CYS
1	J	564	ARG
1	K	124	ARG
1	K	275	ASN
1	K	302	CYS
1	K	303	GLU
1	K	564	ARG
1	L	124	ARG
1	L	194	THR
1	L	275	ASN
1	L	302	CYS
1	L	498	PHE
1	L	564	ARG
1	G	124	ARG
1	G	275	ASN
1	G	302	CYS
1	G	564	ARG

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 (i)

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	0.33	0	6,6,6	0.32	0
4	BU3	A	804	-	4,5,5	0.33	0	6,6,6	0.39	0
5	ACT	A	805	-	1,3,3	1.60	0	0,3,3	0.00	-
6	HEM	A	806	1	28,50,50	1.34	4 (14%)	17,82,82	1.72	4 (23%)
6	HEM	A	807	1,3,7	28,50,50	1.42	4 (14%)	17,82,82	1.89	5 (29%)
6	HEM	A	808	1	28,50,50	1.46	4 (14%)	17,82,82	1.76	5 (29%)
6	HEM	A	809	1	28,50,50	1.34	4 (14%)	17,82,82	1.63	4 (23%)
6	HEM	A	810	1	28,50,50	1.52	4 (14%)	17,82,82	1.79	4 (23%)
6	HEM	A	811	1	28,50,50	1.54	5 (17%)	17,82,82	1.99	3 (17%)
6	HEM	A	812	1	28,50,50	1.54	4 (14%)	17,82,82	1.97	7 (41%)
6	HEM	A	813	1	28,50,50	1.47	4 (14%)	17,82,82	1.80	6 (35%)
7	SO2	A	814	6	2,2,2	1.65	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	0.36	0	6,6,6	0.19	0
4	BU3	B	804	-	4,5,5	0.36	0	6,6,6	0.32	0
4	BU3	B	805	-	4,5,5	0.30	0	6,6,6	0.26	0
5	ACT	B	806	-	1,3,3	1.71	0	0,3,3	0.00	-
6	HEM	B	807	1	28,50,50	1.36	4 (14%)	17,82,82	1.62	4 (23%)
6	HEM	B	808	1,3	28,50,50	1.32	4 (14%)	17,82,82	1.93	5 (29%)
6	HEM	B	809	1	28,50,50	1.44	4 (14%)	17,82,82	2.05	5 (29%)
6	HEM	B	810	1	28,50,50	1.44	4 (14%)	17,82,82	1.70	5 (29%)
6	HEM	B	811	1	28,50,50	1.45	4 (14%)	17,82,82	1.74	5 (29%)
6	HEM	B	812	1	28,50,50	1.41	4 (14%)	17,82,82	1.77	5 (29%)
6	HEM	B	813	1	28,50,50	1.39	4 (14%)	17,82,82	1.68	3 (17%)
6	HEM	B	814	1	28,50,50	1.38	4 (14%)	17,82,82	1.65	3 (17%)
3	SX	C	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	C	803	-	4,5,5	0.31	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BU3	C	804	-	4,5,5	0.31	0	6,6,6	0.28	0
5	ACT	C	805	-	1,3,3	1.47	0	0,3,3	0.00	-
6	HEM	C	806	1	28,50,50	1.38	4 (14%)	17,82,82	1.58	4 (23%)
6	HEM	C	807	1,3	28,50,50	1.39	4 (14%)	17,82,82	1.79	3 (17%)
6	HEM	C	808	1	28,50,50	1.41	4 (14%)	17,82,82	2.10	5 (29%)
6	HEM	C	809	1	28,50,50	1.41	4 (14%)	17,82,82	1.59	3 (17%)
6	HEM	C	810	1	28,50,50	1.49	4 (14%)	17,82,82	1.74	5 (29%)
6	HEM	C	811	1	28,50,50	1.39	4 (14%)	17,82,82	1.82	3 (17%)
6	HEM	C	812	1	28,50,50	1.42	4 (14%)	17,82,82	1.67	4 (23%)
6	HEM	C	813	1	28,50,50	1.42	4 (14%)	17,82,82	1.71	4 (23%)
7	SO2	D	802	6	2,2,2	1.71	0	1,1,1	1.56	0
4	BU3	D	803	-	4,5,5	0.35	0	6,6,6	0.15	0
4	BU3	D	804	-	4,5,5	0.43	0	6,6,6	0.37	0
5	ACT	D	805	-	1,3,3	1.52	0	0,3,3	0.00	-
6	HEM	D	806	1	28,50,50	1.34	4 (14%)	17,82,82	1.59	3 (17%)
6	HEM	D	807	1,7	28,50,50	1.36	4 (14%)	17,82,82	1.91	6 (35%)
6	HEM	D	808	1	28,50,50	1.50	4 (14%)	17,82,82	1.97	5 (29%)
6	HEM	D	809	1	28,50,50	1.40	4 (14%)	17,82,82	1.65	3 (17%)
6	HEM	D	810	1	28,50,50	1.41	4 (14%)	17,82,82	1.69	3 (17%)
6	HEM	D	811	1	28,50,50	1.48	4 (14%)	17,82,82	1.81	5 (29%)
6	HEM	D	812	1	28,50,50	1.47	4 (14%)	17,82,82	1.66	2 (11%)
6	HEM	D	813	1	28,50,50	1.40	4 (14%)	17,82,82	1.68	3 (17%)
3	SX	E	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	E	803	-	4,5,5	0.29	0	6,6,6	0.27	0
4	BU3	E	804	-	4,5,5	0.27	0	6,6,6	0.29	0
5	ACT	E	805	-	1,3,3	1.37	0	0,3,3	0.00	-
6	HEM	E	806	1	28,50,50	1.44	4 (14%)	17,82,82	1.59	3 (17%)
6	HEM	E	807	1,3	28,50,50	1.31	4 (14%)	17,82,82	1.85	4 (23%)
6	HEM	E	808	1	28,50,50	1.35	4 (14%)	17,82,82	1.96	5 (29%)
6	HEM	E	809	1	28,50,50	1.49	4 (14%)	17,82,82	1.69	4 (23%)
6	HEM	E	810	1	28,50,50	1.40	4 (14%)	17,82,82	1.77	3 (17%)
6	HEM	E	811	1	28,50,50	1.46	4 (14%)	17,82,82	2.06	5 (29%)
6	HEM	E	812	1	28,50,50	1.44	4 (14%)	17,82,82	1.62	4 (23%)
6	HEM	E	813	1	28,50,50	1.38	4 (14%)	17,82,82	1.70	3 (17%)
3	SX	F	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	F	803	-	4,5,5	0.36	0	6,6,6	0.41	0
4	BU3	F	804	-	4,5,5	0.41	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BU3	F	805	-	4,5,5	0.38	0	6,6,6	0.21	0
5	ACT	F	806	-	1,3,3	1.24	0	0,3,3	0.00	-
6	HEM	F	807	1	28,50,50	1.41	4 (14%)	17,82,82	1.65	3 (17%)
6	HEM	F	808	1,3	28,50,50	1.41	4 (14%)	17,82,82	2.03	6 (35%)
6	HEM	F	809	1	28,50,50	1.39	4 (14%)	17,82,82	1.94	5 (29%)
6	HEM	F	810	1	28,50,50	1.48	4 (14%)	17,82,82	1.64	3 (17%)
6	HEM	F	811	1	28,50,50	1.44	4 (14%)	17,82,82	1.84	4 (23%)
6	HEM	F	812	1	28,50,50	1.44	4 (14%)	17,82,82	2.02	4 (23%)
6	HEM	F	813	1	28,50,50	1.41	4 (14%)	17,82,82	1.74	2 (11%)
6	HEM	F	814	1	28,50,50	1.41	4 (14%)	17,82,82	1.65	2 (11%)
3	SX	G	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	G	803	-	4,5,5	0.40	0	6,6,6	0.28	0
4	BU3	G	804	-	4,5,5	0.37	0	6,6,6	0.27	0
5	ACT	G	805	-	1,3,3	1.21	0	0,3,3	0.00	-
6	HEM	G	806	1	28,50,50	1.36	4 (14%)	17,82,82	1.52	2 (11%)
6	HEM	G	807	1,3,7	28,50,50	1.35	4 (14%)	17,82,82	1.92	5 (29%)
6	HEM	G	808	1	28,50,50	1.37	4 (14%)	17,82,82	1.88	2 (11%)
6	HEM	G	809	1	28,50,50	1.37	3 (10%)	17,82,82	1.60	3 (17%)
6	HEM	G	810	1	28,50,50	1.48	4 (14%)	17,82,82	1.74	3 (17%)
6	HEM	G	811	1	28,50,50	1.44	4 (14%)	17,82,82	1.91	6 (35%)
6	HEM	G	812	1	28,50,50	1.46	4 (14%)	17,82,82	1.77	5 (29%)
6	HEM	G	813	1	28,50,50	1.38	4 (14%)	17,82,82	1.68	4 (23%)
7	SO2	G	814	6	2,2,2	1.64	0	1,1,1	1.61	0
3	SX	H	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	H	803	-	4,5,5	0.28	0	6,6,6	0.22	0
4	BU3	H	804	-	4,5,5	0.35	0	6,6,6	0.30	0
4	BU3	H	805	-	4,5,5	0.25	0	6,6,6	0.61	0
5	ACT	H	806	-	1,3,3	1.33	0	0,3,3	0.00	-
6	HEM	H	807	1	28,50,50	1.38	5 (17%)	17,82,82	1.69	4 (23%)
6	HEM	H	808	1,3	28,50,50	1.38	4 (14%)	17,82,82	1.89	5 (29%)
6	HEM	H	809	1	28,50,50	1.54	4 (14%)	17,82,82	1.81	5 (29%)
6	HEM	H	810	1	28,50,50	1.40	4 (14%)	17,82,82	1.63	4 (23%)
6	HEM	H	811	1	28,50,50	1.35	4 (14%)	17,82,82	1.88	6 (35%)
6	HEM	H	812	1	28,50,50	1.41	4 (14%)	17,82,82	1.85	5 (29%)
6	HEM	H	813	1	28,50,50	1.32	4 (14%)	17,82,82	1.63	2 (11%)
6	HEM	H	814	1	28,50,50	1.42	4 (14%)	17,82,82	1.72	3 (17%)
7	SO2	I	802	6	2,2,2	1.72	0	1,1,1	1.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BU3	I	803	-	4,5,5	0.36	0	6,6,6	0.18	0
4	BU3	I	804	-	4,5,5	0.47	0	6,6,6	0.32	0
5	ACT	I	805	-	1,3,3	1.35	0	0,3,3	0.00	-
6	HEM	I	806	1	28,50,50	1.35	4 (14%)	17,82,82	1.55	3 (17%)
6	HEM	I	807	1,7	28,50,50	1.36	4 (14%)	17,82,82	1.85	4 (23%)
6	HEM	I	808	1	28,50,50	1.39	4 (14%)	17,82,82	1.90	8 (47%)
6	HEM	I	809	1	28,50,50	1.35	4 (14%)	17,82,82	1.53	3 (17%)
6	HEM	I	810	1	28,50,50	1.37	4 (14%)	17,82,82	1.81	4 (23%)
6	HEM	I	811	1	28,50,50	1.36	4 (14%)	17,82,82	2.02	6 (35%)
6	HEM	I	812	1	28,50,50	1.33	4 (14%)	17,82,82	1.69	4 (23%)
6	HEM	I	813	1	28,50,50	1.47	4 (14%)	17,82,82	1.83	5 (29%)
3	SX	J	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	J	803	-	4,5,5	0.30	0	6,6,6	0.29	0
4	BU3	J	804	-	4,5,5	0.42	0	6,6,6	0.24	0
5	ACT	J	805	-	1,3,3	1.35	0	0,3,3	0.00	-
6	HEM	J	806	1	28,50,50	1.44	4 (14%)	17,82,82	1.81	2 (11%)
6	HEM	J	807	1,3	28,50,50	1.35	4 (14%)	17,82,82	1.93	4 (23%)
6	HEM	J	808	1	28,50,50	1.41	4 (14%)	17,82,82	1.88	5 (29%)
6	HEM	J	809	1	28,50,50	1.51	5 (17%)	17,82,82	1.72	4 (23%)
6	HEM	J	810	1	28,50,50	1.43	4 (14%)	17,82,82	1.69	3 (17%)
6	HEM	J	811	1	28,50,50	1.41	4 (14%)	17,82,82	1.86	3 (17%)
6	HEM	J	812	1	28,50,50	1.36	4 (14%)	17,82,82	1.73	5 (29%)
6	HEM	J	813	1	28,50,50	1.40	4 (14%)	17,82,82	1.69	3 (17%)
3	SX	K	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	K	803	-	4,5,5	0.33	0	6,6,6	0.37	0
4	BU3	K	804	-	4,5,5	0.45	0	6,6,6	0.28	0
5	ACT	K	805	-	1,3,3	1.45	0	0,3,3	0.00	-
6	HEM	K	806	1	28,50,50	1.47	4 (14%)	17,82,82	1.76	2 (11%)
6	HEM	K	807	1,3	28,50,50	1.38	4 (14%)	17,82,82	1.96	5 (29%)
6	HEM	K	808	1	28,50,50	1.35	4 (14%)	17,82,82	1.74	3 (17%)
6	HEM	K	809	1	28,50,50	1.42	4 (14%)	17,82,82	1.78	3 (17%)
6	HEM	K	810	1	28,50,50	1.39	4 (14%)	17,82,82	1.76	4 (23%)
6	HEM	K	811	1	28,50,50	1.40	4 (14%)	17,82,82	1.78	4 (23%)
6	HEM	K	812	1	28,50,50	1.34	4 (14%)	17,82,82	1.58	4 (23%)
6	HEM	K	813	1	28,50,50	1.40	4 (14%)	17,82,82	1.88	5 (29%)
3	SX	L	802	6	0,1,1	0.00	-	0,0,0	0.00	-
4	BU3	L	803	-	4,5,5	0.41	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BU3	L	804	-	4,5,5	0.38	0	6,6,6	0.35	0
5	ACT	L	805	-	1,3,3	1.39	0	0,3,3	0.00	-
6	HEM	L	806	1	28,50,50	1.46	4 (14%)	17,82,82	1.59	4 (23%)
6	HEM	L	807	1,3	28,50,50	1.42	4 (14%)	17,82,82	1.78	4 (23%)
6	HEM	L	808	1	28,50,50	1.42	4 (14%)	17,82,82	1.79	4 (23%)
6	HEM	L	809	1	28,50,50	1.45	3 (10%)	17,82,82	1.58	2 (11%)
6	HEM	L	810	1	28,50,50	1.41	4 (14%)	17,82,82	1.75	4 (23%)
6	HEM	L	811	1	28,50,50	1.32	4 (14%)	17,82,82	1.84	4 (23%)
6	HEM	L	812	1	28,50,50	1.34	4 (14%)	17,82,82	1.50	2 (11%)
6	HEM	L	813	1	28,50,50	1.40	5 (17%)	17,82,82	1.73	5 (29%)

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	-	0/6/54/54	0/0/8/8
6	HEM	A	807	1,3,7	-	0/6/54/54	0/0/8/8
6	HEM	A	808	1	-	0/6/54/54	0/0/8/8
6	HEM	A	809	1	-	0/6/54/54	0/0/8/8
6	HEM	A	810	1	-	0/6/54/54	0/0/8/8
6	HEM	A	811	1	-	0/6/54/54	0/0/8/8
6	HEM	A	812	1	-	0/6/54/54	0/0/8/8
6	HEM	A	813	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	B	808	1,3	-	0/6/54/54	0/0/8/8
6	HEM	B	809	1	-	0/6/54/54	0/0/8/8
6	HEM	B	810	1	-	0/6/54/54	0/0/8/8
6	HEM	B	811	1	-	0/6/54/54	0/0/8/8
6	HEM	B	812	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	B	813	1	-	0/6/54/54	0/0/8/8
6	HEM	B	814	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	C	807	1,3	-	0/6/54/54	0/0/8/8
6	HEM	C	808	1	-	0/6/54/54	0/0/8/8
6	HEM	C	809	1	-	0/6/54/54	0/0/8/8
6	HEM	C	810	1	-	0/6/54/54	0/0/8/8
6	HEM	C	811	1	-	0/6/54/54	0/0/8/8
6	HEM	C	812	1	-	0/6/54/54	0/0/8/8
6	HEM	C	813	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	D	807	1,7	-	0/6/54/54	0/0/8/8
6	HEM	D	808	1	-	0/6/54/54	0/0/8/8
6	HEM	D	809	1	-	0/6/54/54	0/0/8/8
6	HEM	D	810	1	-	0/6/54/54	0/0/8/8
6	HEM	D	811	1	-	0/6/54/54	0/0/8/8
6	HEM	D	812	1	-	0/6/54/54	0/0/8/8
6	HEM	D	813	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	E	807	1,3	-	0/6/54/54	0/0/8/8
6	HEM	E	808	1	-	0/6/54/54	0/0/8/8
6	HEM	E	809	1	-	0/6/54/54	0/0/8/8
6	HEM	E	810	1	-	0/6/54/54	0/0/8/8
6	HEM	E	811	1	-	0/6/54/54	0/0/8/8
6	HEM	E	812	1	-	0/6/54/54	0/0/8/8
6	HEM	E	813	1	-	0/6/54/54	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACT	F	806	-	-	0/0/0/0	0/0/0/0
6	HEM	F	807	1	-	0/6/54/54	0/0/8/8
6	HEM	F	808	1,3	-	0/6/54/54	0/0/8/8
6	HEM	F	809	1	-	0/6/54/54	0/0/8/8
6	HEM	F	810	1	-	0/6/54/54	0/0/8/8
6	HEM	F	811	1	-	0/6/54/54	0/0/8/8
6	HEM	F	812	1	-	0/6/54/54	0/0/8/8
6	HEM	F	813	1	-	0/6/54/54	0/0/8/8
6	HEM	F	814	1	-	0/6/54/54	0/0/8/8
3	SX	G	802	6	-	0/0/0/0	0/0/0/0
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	-	0/6/54/54	0/0/8/8
6	HEM	G	807	1,3,7	-	0/6/54/54	0/0/8/8
6	HEM	G	808	1	-	0/6/54/54	0/0/8/8
6	HEM	G	809	1	-	0/6/54/54	0/0/8/8
6	HEM	G	810	1	-	0/6/54/54	0/0/8/8
6	HEM	G	811	1	-	0/6/54/54	0/0/8/8
6	HEM	G	812	1	-	0/6/54/54	0/0/8/8
6	HEM	G	813	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	H	808	1,3	-	0/6/54/54	0/0/8/8
6	HEM	H	809	1	-	0/6/54/54	0/0/8/8
6	HEM	H	810	1	-	0/6/54/54	0/0/8/8
6	HEM	H	811	1	-	0/6/54/54	0/0/8/8
6	HEM	H	812	1	-	0/6/54/54	0/0/8/8
6	HEM	H	813	1	-	0/6/54/54	0/0/8/8
6	HEM	H	814	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	I	807	1,7	-	0/6/54/54	0/0/8/8
6	HEM	I	808	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	I	809	1	-	0/6/54/54	0/0/8/8
6	HEM	I	810	1	-	0/6/54/54	0/0/8/8
6	HEM	I	811	1	-	0/6/54/54	0/0/8/8
6	HEM	I	812	1	-	0/6/54/54	0/0/8/8
6	HEM	I	813	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	J	807	1,3	-	0/6/54/54	0/0/8/8
6	HEM	J	808	1	-	0/6/54/54	0/0/8/8
6	HEM	J	809	1	-	0/6/54/54	0/0/8/8
6	HEM	J	810	1	-	0/6/54/54	0/0/8/8
6	HEM	J	811	1	-	0/6/54/54	0/0/8/8
6	HEM	J	812	1	-	0/6/54/54	0/0/8/8
6	HEM	J	813	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	K	807	1,3	-	0/6/54/54	0/0/8/8
6	HEM	K	808	1	-	0/6/54/54	0/0/8/8
6	HEM	K	809	1	-	0/6/54/54	0/0/8/8
6	HEM	K	810	1	-	0/6/54/54	0/0/8/8
6	HEM	K	811	1	-	0/6/54/54	0/0/8/8
6	HEM	K	812	1	-	0/6/54/54	0/0/8/8
6	HEM	K	813	1	-	0/6/54/54	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	-	0/6/54/54	0/0/8/8
6	HEM	L	807	1,3	-	0/6/54/54	0/0/8/8
6	HEM	L	808	1	-	0/6/54/54	0/0/8/8
6	HEM	L	809	1	-	0/6/54/54	0/0/8/8
6	HEM	L	810	1	-	0/6/54/54	0/0/8/8
6	HEM	L	811	1	-	0/6/54/54	0/0/8/8
6	HEM	L	812	1	-	0/6/54/54	0/0/8/8
6	HEM	L	813	1	-	0/6/54/54	0/0/8/8

All (386) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	810	HEM	C1B-NB	-5.89	1.29	1.36
6	H	809	HEM	C1B-NB	-5.54	1.30	1.36
6	A	812	HEM	C1B-NB	-5.50	1.30	1.36
6	D	811	HEM	C1B-NB	-5.45	1.30	1.36
6	G	812	HEM	C1B-NB	-5.44	1.30	1.36
6	A	808	HEM	C1B-NB	-5.36	1.30	1.36
6	C	810	HEM	C1B-NB	-5.29	1.30	1.36
6	G	810	HEM	C1B-NB	-5.28	1.30	1.36
6	E	809	HEM	C1B-NB	-5.26	1.30	1.36
6	B	811	HEM	C1B-NB	-5.23	1.30	1.36
6	J	809	HEM	C1B-NB	-5.17	1.30	1.36
6	L	810	HEM	C1B-NB	-5.16	1.30	1.36
6	F	808	HEM	C1B-NB	-5.16	1.30	1.36
6	A	813	HEM	C1B-NB	-5.15	1.30	1.36
6	E	806	HEM	C1B-NB	-5.12	1.30	1.36
6	E	812	HEM	C1B-NB	-5.09	1.30	1.36
6	F	810	HEM	C1B-NB	-5.08	1.30	1.36
6	I	813	HEM	C1B-NB	-5.08	1.30	1.36
6	A	811	HEM	C1B-NB	-5.07	1.30	1.36
6	D	810	HEM	C1B-NB	-5.04	1.30	1.36
6	B	810	HEM	C1B-NB	-5.03	1.30	1.36
6	B	812	HEM	C1B-NB	-5.02	1.30	1.36
6	A	807	HEM	C1B-NB	-5.01	1.30	1.36
6	C	809	HEM	C1B-NB	-5.01	1.30	1.36
6	L	808	HEM	C1B-NB	-5.01	1.30	1.36
6	E	811	HEM	C1B-NB	-5.00	1.30	1.36
6	C	813	HEM	C1B-NB	-5.00	1.30	1.36
6	L	809	HEM	C1B-NB	-5.00	1.30	1.36
6	L	806	HEM	C1B-NB	-4.98	1.30	1.36
6	G	811	HEM	C1B-NB	-4.93	1.30	1.36
6	F	811	HEM	C1B-NB	-4.92	1.31	1.36
6	D	812	HEM	C1B-NB	-4.92	1.31	1.36
6	K	810	HEM	C1B-NB	-4.91	1.31	1.36
6	E	810	HEM	C1B-NB	-4.91	1.31	1.36
6	D	808	HEM	C1B-NB	-4.91	1.31	1.36
6	F	807	HEM	C1B-NB	-4.90	1.31	1.36
6	H	808	HEM	C1B-NB	-4.89	1.31	1.36
6	I	810	HEM	C1B-NB	-4.89	1.31	1.36
6	I	808	HEM	C1B-NB	-4.87	1.31	1.36
6	C	807	HEM	C1B-NB	-4.85	1.31	1.36
6	L	807	HEM	C1B-NB	-4.85	1.31	1.36
6	B	809	HEM	C1B-NB	-4.85	1.31	1.36
6	B	813	HEM	C1B-NB	-4.84	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	812	HEM	C1B-NB	-4.84	1.31	1.36
6	F	813	HEM	C1B-NB	-4.84	1.31	1.36
6	J	810	HEM	C1B-NB	-4.81	1.31	1.36
6	K	809	HEM	C1B-NB	-4.81	1.31	1.36
6	H	814	HEM	C1B-NB	-4.80	1.31	1.36
6	F	812	HEM	C1B-NB	-4.79	1.31	1.36
6	D	807	HEM	C1B-NB	-4.78	1.31	1.36
6	D	813	HEM	C1B-NB	-4.76	1.31	1.36
6	J	811	HEM	C1B-NB	-4.75	1.31	1.36
6	F	814	HEM	C1B-NB	-4.73	1.31	1.36
6	I	809	HEM	C1B-NB	-4.73	1.31	1.36
6	K	807	HEM	C1B-NB	-4.73	1.31	1.36
6	H	810	HEM	C1B-NB	-4.72	1.31	1.36
6	J	807	HEM	C1B-NB	-4.70	1.31	1.36
6	B	814	HEM	C1B-NB	-4.69	1.31	1.36
6	D	809	HEM	C1B-NB	-4.69	1.31	1.36
6	K	813	HEM	C1B-NB	-4.67	1.31	1.36
6	H	812	HEM	C1B-NB	-4.67	1.31	1.36
6	G	809	HEM	C1B-NB	-4.67	1.31	1.36
6	G	813	HEM	C1B-NB	-4.66	1.31	1.36
6	G	808	HEM	C1B-NB	-4.66	1.31	1.36
6	K	811	HEM	C1B-NB	-4.66	1.31	1.36
6	K	812	HEM	C1B-NB	-4.66	1.31	1.36
6	I	811	HEM	C1B-NB	-4.65	1.31	1.36
6	K	806	HEM	C1B-NB	-4.64	1.31	1.36
6	I	806	HEM	C1B-NB	-4.59	1.31	1.36
6	I	807	HEM	C1B-NB	-4.57	1.31	1.36
6	K	808	HEM	C1B-NB	-4.57	1.31	1.36
6	H	811	HEM	C1B-NB	-4.56	1.31	1.36
6	J	813	HEM	C1B-NB	-4.54	1.31	1.36
6	L	812	HEM	C1B-NB	-4.53	1.31	1.36
6	E	807	HEM	C1B-NB	-4.52	1.31	1.36
6	L	813	HEM	C1B-NB	-4.52	1.31	1.36
6	J	808	HEM	C1B-NB	-4.51	1.31	1.36
6	B	807	HEM	C1B-NB	-4.47	1.31	1.36
6	F	809	HEM	C1B-NB	-4.46	1.31	1.36
6	C	806	HEM	C1B-NB	-4.43	1.31	1.36
6	B	808	HEM	C1B-NB	-4.43	1.31	1.36
6	E	813	HEM	C1B-NB	-4.42	1.31	1.36
6	C	811	HEM	C1B-NB	-4.40	1.31	1.36
6	I	812	HEM	C1B-NB	-4.39	1.31	1.36
6	G	807	HEM	C1B-NB	-4.38	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	806	HEM	C1B-NB	-4.35	1.31	1.36
6	L	811	HEM	C1B-NB	-4.34	1.31	1.36
6	J	812	HEM	C1B-NB	-4.32	1.31	1.36
6	G	806	HEM	C1B-NB	-4.31	1.31	1.36
6	D	806	HEM	C1B-NB	-4.30	1.31	1.36
6	H	807	HEM	C1B-NB	-4.24	1.31	1.36
6	C	808	HEM	C1B-NB	-4.18	1.31	1.36
6	A	809	HEM	C1B-NB	-4.18	1.31	1.36
6	H	813	HEM	C1B-NB	-4.12	1.31	1.36
6	J	806	HEM	C1B-NB	-4.10	1.31	1.36
6	E	808	HEM	C1B-NB	-4.04	1.32	1.36
6	K	806	HEM	C3B-C2B	-3.24	1.36	1.40
6	F	812	HEM	C4B-NB	-3.03	1.29	1.36
6	J	806	HEM	C3B-C2B	-3.00	1.36	1.40
6	D	812	HEM	C4B-NB	-2.98	1.29	1.36
6	E	812	HEM	C4B-NB	-2.88	1.29	1.36
6	A	811	HEM	C3B-C2B	-2.88	1.36	1.40
6	H	814	HEM	C4B-NB	-2.76	1.30	1.36
6	D	808	HEM	C4B-NB	-2.74	1.30	1.36
6	H	812	HEM	C4B-NB	-2.72	1.30	1.36
6	E	811	HEM	C4B-NB	-2.71	1.30	1.36
6	F	807	HEM	C4B-NB	-2.69	1.30	1.36
6	C	813	HEM	C4B-NB	-2.67	1.30	1.36
6	A	812	HEM	C4B-NB	-2.67	1.30	1.36
6	H	809	HEM	C4B-NB	-2.66	1.30	1.36
6	C	811	HEM	C4B-NB	-2.66	1.30	1.36
6	J	808	HEM	C4B-NB	-2.65	1.30	1.36
6	B	807	HEM	C4B-NB	-2.65	1.30	1.36
6	I	811	HEM	C4B-NB	-2.65	1.30	1.36
6	A	808	HEM	C4B-NB	-2.65	1.30	1.36
6	C	810	HEM	C4B-NB	-2.64	1.30	1.36
6	C	812	HEM	C4B-NB	-2.64	1.30	1.36
6	F	813	HEM	C4B-NB	-2.64	1.30	1.36
6	A	806	HEM	C4B-NB	-2.63	1.30	1.36
6	C	806	HEM	C4B-NB	-2.63	1.30	1.36
6	A	813	HEM	C4B-NB	-2.62	1.30	1.36
6	C	808	HEM	C4B-NB	-2.61	1.30	1.36
6	B	813	HEM	C4B-NB	-2.61	1.30	1.36
6	B	811	HEM	C4B-NB	-2.60	1.30	1.36
6	D	811	HEM	C4B-NB	-2.60	1.30	1.36
6	K	811	HEM	C4B-NB	-2.60	1.30	1.36
6	J	811	HEM	C4B-NB	-2.58	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	813	HEM	C4B-NB	-2.58	1.30	1.36
6	A	809	HEM	C4B-NB	-2.58	1.30	1.36
6	A	810	HEM	C4B-NB	-2.57	1.30	1.36
6	G	808	HEM	C4B-NB	-2.57	1.30	1.36
6	G	811	HEM	C4B-NB	-2.55	1.30	1.36
6	I	812	HEM	C4B-NB	-2.54	1.30	1.36
6	A	807	HEM	C4B-NB	-2.54	1.30	1.36
6	I	808	HEM	C4B-NB	-2.53	1.30	1.36
6	F	809	HEM	C4B-NB	-2.52	1.30	1.36
6	G	812	HEM	C4B-NB	-2.51	1.30	1.36
6	E	808	HEM	C4B-NB	-2.50	1.30	1.36
6	B	814	HEM	C4B-NB	-2.49	1.30	1.36
6	D	810	HEM	C4B-NB	-2.48	1.30	1.36
6	G	810	HEM	C4B-NB	-2.47	1.30	1.36
6	D	806	HEM	C4B-NB	-2.46	1.30	1.36
6	J	813	HEM	C4B-NB	-2.46	1.30	1.36
6	E	806	HEM	C4B-NB	-2.46	1.30	1.36
6	F	811	HEM	C4B-NB	-2.46	1.30	1.36
6	L	806	HEM	C4B-NB	-2.45	1.30	1.36
6	K	810	HEM	C4B-NB	-2.45	1.30	1.36
6	J	810	HEM	C4B-NB	-2.44	1.30	1.36
6	E	813	HEM	C4B-NB	-2.44	1.30	1.36
6	L	808	HEM	C4B-NB	-2.44	1.30	1.36
6	E	810	HEM	C4B-NB	-2.43	1.30	1.36
6	H	807	HEM	C4B-NB	-2.42	1.30	1.36
6	F	814	HEM	C4B-NB	-2.41	1.30	1.36
6	C	807	HEM	C4B-NB	-2.40	1.30	1.36
6	D	813	HEM	C4B-NB	-2.40	1.30	1.36
6	K	807	HEM	C4B-NB	-2.40	1.30	1.36
6	E	807	HEM	C4B-NB	-2.40	1.30	1.36
6	G	807	HEM	C4B-NB	-2.38	1.31	1.36
6	J	812	HEM	C4B-NB	-2.37	1.31	1.36
6	D	807	HEM	C4B-NB	-2.37	1.31	1.36
6	B	809	HEM	C4B-NB	-2.36	1.31	1.36
6	G	806	HEM	C4B-NB	-2.35	1.31	1.36
6	L	813	HEM	C4B-NB	-2.31	1.31	1.36
6	K	808	HEM	C4B-NB	-2.31	1.31	1.36
6	K	809	HEM	C4B-NB	-2.31	1.31	1.36
6	I	807	HEM	C4B-NB	-2.30	1.31	1.36
6	L	812	HEM	C4B-NB	-2.30	1.31	1.36
6	E	809	HEM	C4B-NB	-2.29	1.31	1.36
6	D	809	HEM	C4B-NB	-2.29	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	813	HEM	C4B-NB	-2.28	1.31	1.36
6	L	811	HEM	C4B-NB	-2.28	1.31	1.36
6	H	811	HEM	C4B-NB	-2.26	1.31	1.36
6	L	807	HEM	C4B-NB	-2.25	1.31	1.36
6	B	812	HEM	C4B-NB	-2.25	1.31	1.36
6	I	809	HEM	C4B-NB	-2.24	1.31	1.36
6	I	813	HEM	C4B-NB	-2.24	1.31	1.36
6	B	808	HEM	C4B-NB	-2.24	1.31	1.36
6	I	810	HEM	C4B-NB	-2.22	1.31	1.36
6	I	806	HEM	C4B-NB	-2.22	1.31	1.36
6	C	809	HEM	C4B-NB	-2.21	1.31	1.36
6	F	810	HEM	C4B-NB	-2.20	1.31	1.36
6	L	810	HEM	C4B-NB	-2.19	1.31	1.36
6	J	807	HEM	C4B-NB	-2.19	1.31	1.36
6	H	808	HEM	C4B-NB	-2.18	1.31	1.36
6	B	810	HEM	C4B-NB	-2.12	1.31	1.36
6	F	808	HEM	C4B-NB	-2.11	1.31	1.36
6	H	810	HEM	C4B-NB	-2.10	1.31	1.36
6	K	813	HEM	C4B-NB	-2.10	1.31	1.36
6	J	809	HEM	C4B-NB	-2.10	1.31	1.36
6	A	811	HEM	C4B-NB	-2.09	1.31	1.36
6	K	812	HEM	C4B-NB	-2.06	1.31	1.36
6	J	809	HEM	C4D-ND	-2.05	1.34	1.36
6	H	807	HEM	C4D-ND	-2.03	1.34	1.36
6	L	813	HEM	C3C-C2C	-2.01	1.37	1.40
6	L	813	HEM	CBC-CAC	2.40	1.45	1.28
6	D	806	HEM	CBB-CAB	2.51	1.46	1.28
6	F	812	HEM	CBB-CAB	2.57	1.46	1.28
6	B	809	HEM	CBC-CAC	2.57	1.47	1.28
6	D	808	HEM	CBC-CAC	2.59	1.47	1.28
6	A	810	HEM	CBC-CAC	2.59	1.47	1.28
6	J	808	HEM	CBC-CAC	2.60	1.47	1.28
6	K	807	HEM	CBB-CAB	2.60	1.47	1.28
6	I	808	HEM	CBC-CAC	2.61	1.47	1.28
6	K	806	HEM	CBB-CAB	2.61	1.47	1.28
6	A	811	HEM	CBB-CAB	2.61	1.47	1.28
6	C	810	HEM	CBC-CAC	2.61	1.47	1.28
6	B	811	HEM	CBC-CAC	2.61	1.47	1.28
6	A	808	HEM	CBC-CAC	2.61	1.47	1.28
6	F	807	HEM	CBB-CAB	2.62	1.47	1.28
6	F	809	HEM	CBC-CAC	2.62	1.47	1.28
6	K	810	HEM	CBC-CAC	2.62	1.47	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	808	HEM	CBB-CAB	2.63	1.47	1.28
6	E	810	HEM	CBC-CAC	2.63	1.47	1.28
6	J	806	HEM	CBB-CAB	2.63	1.47	1.28
6	C	807	HEM	CBB-CAB	2.64	1.47	1.28
6	I	807	HEM	CBB-CAB	2.64	1.47	1.28
6	D	812	HEM	CBB-CAB	2.64	1.47	1.28
6	B	813	HEM	CBC-CAC	2.65	1.47	1.28
6	I	809	HEM	CBB-CAB	2.65	1.47	1.28
6	A	807	HEM	CBB-CAB	2.65	1.47	1.28
6	H	808	HEM	CBC-CAC	2.65	1.47	1.28
6	B	807	HEM	CBB-CAB	2.65	1.47	1.28
6	H	811	HEM	CBC-CAC	2.65	1.47	1.28
6	E	808	HEM	CBC-CAC	2.65	1.47	1.28
6	E	808	HEM	CBB-CAB	2.66	1.47	1.28
6	D	807	HEM	CBB-CAB	2.66	1.47	1.28
6	H	810	HEM	CBB-CAB	2.66	1.47	1.28
6	L	810	HEM	CBC-CAC	2.66	1.47	1.28
6	K	812	HEM	CBC-CAC	2.66	1.47	1.28
6	L	808	HEM	CBB-CAB	2.66	1.47	1.28
6	G	810	HEM	CBC-CAC	2.66	1.47	1.28
6	K	807	HEM	CBC-CAC	2.66	1.47	1.28
6	F	811	HEM	CBB-CAB	2.67	1.47	1.28
6	A	808	HEM	CBB-CAB	2.67	1.47	1.28
6	D	807	HEM	CBC-CAC	2.67	1.47	1.28
6	I	811	HEM	CBB-CAB	2.67	1.47	1.28
6	F	812	HEM	CBC-CAC	2.67	1.47	1.28
6	E	807	HEM	CBB-CAB	2.68	1.47	1.28
6	I	810	HEM	CBC-CAC	2.68	1.47	1.28
6	J	808	HEM	CBB-CAB	2.68	1.47	1.28
6	D	808	HEM	CBB-CAB	2.68	1.47	1.28
6	E	812	HEM	CBB-CAB	2.68	1.47	1.28
6	A	809	HEM	CBB-CAB	2.68	1.47	1.28
6	K	809	HEM	CBB-CAB	2.68	1.47	1.28
6	C	808	HEM	CBC-CAC	2.68	1.47	1.28
6	G	808	HEM	CBC-CAC	2.68	1.47	1.28
6	A	806	HEM	CBB-CAB	2.68	1.47	1.28
6	F	813	HEM	CBC-CAC	2.68	1.47	1.28
6	H	808	HEM	CBB-CAB	2.68	1.47	1.28
6	C	812	HEM	CBB-CAB	2.68	1.47	1.28
6	I	808	HEM	CBB-CAB	2.69	1.47	1.28
6	B	808	HEM	CBC-CAC	2.69	1.47	1.28
6	F	810	HEM	CBB-CAB	2.69	1.47	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	809	HEM	CBC-CAC	2.69	1.47	1.28
6	C	806	HEM	CBC-CAC	2.69	1.47	1.28
6	B	807	HEM	CBC-CAC	2.69	1.47	1.28
6	F	811	HEM	CBC-CAC	2.70	1.47	1.28
6	K	808	HEM	CBB-CAB	2.70	1.47	1.28
6	H	813	HEM	CBB-CAB	2.70	1.47	1.28
6	I	810	HEM	CBB-CAB	2.70	1.47	1.28
6	D	809	HEM	CBB-CAB	2.70	1.47	1.28
6	C	812	HEM	CBC-CAC	2.70	1.47	1.28
6	B	811	HEM	CBB-CAB	2.70	1.47	1.28
6	I	812	HEM	CBC-CAC	2.70	1.47	1.28
6	L	811	HEM	CBB-CAB	2.70	1.47	1.28
6	L	808	HEM	CBC-CAC	2.70	1.47	1.28
6	G	807	HEM	CBC-CAC	2.70	1.47	1.28
6	I	812	HEM	CBB-CAB	2.70	1.47	1.28
6	B	809	HEM	CBB-CAB	2.71	1.47	1.28
6	C	811	HEM	CBB-CAB	2.71	1.47	1.28
6	D	810	HEM	CBC-CAC	2.71	1.47	1.28
6	H	812	HEM	CBB-CAB	2.71	1.48	1.28
6	C	809	HEM	CBC-CAC	2.71	1.48	1.28
6	D	810	HEM	CBB-CAB	2.72	1.48	1.28
6	A	811	HEM	CBC-CAC	2.72	1.48	1.28
6	H	813	HEM	CBC-CAC	2.72	1.48	1.28
6	D	809	HEM	CBC-CAC	2.72	1.48	1.28
6	A	806	HEM	CBC-CAC	2.72	1.48	1.28
6	H	811	HEM	CBB-CAB	2.72	1.48	1.28
6	L	807	HEM	CBB-CAB	2.72	1.48	1.28
6	J	810	HEM	CBC-CAC	2.72	1.48	1.28
6	E	813	HEM	CBB-CAB	2.72	1.48	1.28
6	F	814	HEM	CBC-CAC	2.72	1.48	1.28
6	L	807	HEM	CBC-CAC	2.72	1.48	1.28
6	H	809	HEM	CBB-CAB	2.72	1.48	1.28
6	F	808	HEM	CBC-CAC	2.73	1.48	1.28
6	A	813	HEM	CBB-CAB	2.73	1.48	1.28
6	E	809	HEM	CBB-CAB	2.73	1.48	1.28
6	I	807	HEM	CBC-CAC	2.73	1.48	1.28
6	C	813	HEM	CBC-CAC	2.73	1.48	1.28
6	L	806	HEM	CBB-CAB	2.73	1.48	1.28
6	I	809	HEM	CBC-CAC	2.73	1.48	1.28
6	K	811	HEM	CBC-CAC	2.73	1.48	1.28
6	B	814	HEM	CBC-CAC	2.73	1.48	1.28
6	A	812	HEM	CBC-CAC	2.73	1.48	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	810	HEM	CBB-CAB	2.73	1.48	1.28
6	D	812	HEM	CBC-CAC	2.73	1.48	1.28
6	D	811	HEM	CBB-CAB	2.74	1.48	1.28
6	K	808	HEM	CBC-CAC	2.74	1.48	1.28
6	D	813	HEM	CBB-CAB	2.74	1.48	1.28
6	F	810	HEM	CBC-CAC	2.74	1.48	1.28
6	H	814	HEM	CBC-CAC	2.74	1.48	1.28
6	L	812	HEM	CBC-CAC	2.74	1.48	1.28
6	B	810	HEM	CBB-CAB	2.74	1.48	1.28
6	G	813	HEM	CBC-CAC	2.74	1.48	1.28
6	J	807	HEM	CBB-CAB	2.74	1.48	1.28
6	K	812	HEM	CBB-CAB	2.75	1.48	1.28
6	G	812	HEM	CBC-CAC	2.75	1.48	1.28
6	I	813	HEM	CBC-CAC	2.75	1.48	1.28
6	D	813	HEM	CBC-CAC	2.75	1.48	1.28
6	G	809	HEM	CBC-CAC	2.75	1.48	1.28
6	A	813	HEM	CBC-CAC	2.75	1.48	1.28
6	K	809	HEM	CBC-CAC	2.75	1.48	1.28
6	E	806	HEM	CBC-CAC	2.75	1.48	1.28
6	J	811	HEM	CBC-CAC	2.75	1.48	1.28
6	G	807	HEM	CBB-CAB	2.75	1.48	1.28
6	G	812	HEM	CBB-CAB	2.76	1.48	1.28
6	A	807	HEM	CBC-CAC	2.76	1.48	1.28
6	E	807	HEM	CBC-CAC	2.76	1.48	1.28
6	I	806	HEM	CBB-CAB	2.76	1.48	1.28
6	D	806	HEM	CBC-CAC	2.76	1.48	1.28
6	E	809	HEM	CBC-CAC	2.76	1.48	1.28
6	E	810	HEM	CBB-CAB	2.76	1.48	1.28
6	J	807	HEM	CBC-CAC	2.76	1.48	1.28
6	J	809	HEM	CBC-CAC	2.76	1.48	1.28
6	J	812	HEM	CBC-CAC	2.76	1.48	1.28
6	K	813	HEM	CBC-CAC	2.76	1.48	1.28
6	C	808	HEM	CBB-CAB	2.77	1.48	1.28
6	J	811	HEM	CBB-CAB	2.77	1.48	1.28
6	B	810	HEM	CBC-CAC	2.77	1.48	1.28
6	C	807	HEM	CBC-CAC	2.77	1.48	1.28
6	G	813	HEM	CBB-CAB	2.77	1.48	1.28
6	G	808	HEM	CBB-CAB	2.77	1.48	1.28
6	F	808	HEM	CBB-CAB	2.77	1.48	1.28
6	E	806	HEM	CBB-CAB	2.77	1.48	1.28
6	I	813	HEM	CBB-CAB	2.77	1.48	1.28
6	G	806	HEM	CBB-CAB	2.77	1.48	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	813	HEM	CBB-CAB	2.77	1.48	1.28
6	K	811	HEM	CBB-CAB	2.78	1.48	1.28
6	K	813	HEM	CBB-CAB	2.78	1.48	1.28
6	A	812	HEM	CBB-CAB	2.78	1.48	1.28
6	J	812	HEM	CBB-CAB	2.78	1.48	1.28
6	B	814	HEM	CBB-CAB	2.78	1.48	1.28
6	L	810	HEM	CBB-CAB	2.78	1.48	1.28
6	J	806	HEM	CBC-CAC	2.79	1.48	1.28
6	H	807	HEM	CBB-CAB	2.79	1.48	1.28
6	J	809	HEM	CBB-CAB	2.79	1.48	1.28
6	B	812	HEM	CBB-CAB	2.79	1.48	1.28
6	H	814	HEM	CBB-CAB	2.79	1.48	1.28
6	E	811	HEM	CBC-CAC	2.79	1.48	1.28
6	E	811	HEM	CBB-CAB	2.79	1.48	1.28
6	J	813	HEM	CBB-CAB	2.79	1.48	1.28
6	B	812	HEM	CBC-CAC	2.79	1.48	1.28
6	J	813	HEM	CBC-CAC	2.79	1.48	1.28
6	C	806	HEM	CBB-CAB	2.79	1.48	1.28
6	D	811	HEM	CBC-CAC	2.79	1.48	1.28
6	L	809	HEM	CBB-CAB	2.79	1.48	1.28
6	K	810	HEM	CBB-CAB	2.79	1.48	1.28
6	H	812	HEM	CBC-CAC	2.79	1.48	1.28
6	L	811	HEM	CBC-CAC	2.79	1.48	1.28
6	E	812	HEM	CBC-CAC	2.80	1.48	1.28
6	G	811	HEM	CBB-CAB	2.80	1.48	1.28
6	F	814	HEM	CBB-CAB	2.80	1.48	1.28
6	F	807	HEM	CBC-CAC	2.80	1.48	1.28
6	E	813	HEM	CBC-CAC	2.80	1.48	1.28
6	I	806	HEM	CBC-CAC	2.80	1.48	1.28
6	C	810	HEM	CBB-CAB	2.81	1.48	1.28
6	I	811	HEM	CBC-CAC	2.81	1.48	1.28
6	A	809	HEM	CBC-CAC	2.81	1.48	1.28
6	B	813	HEM	CBB-CAB	2.81	1.48	1.28
6	H	807	HEM	CBC-CAC	2.81	1.48	1.28
6	C	811	HEM	CBC-CAC	2.81	1.48	1.28
6	L	809	HEM	CBC-CAC	2.81	1.48	1.28
6	F	809	HEM	CBB-CAB	2.81	1.48	1.28
6	G	809	HEM	CBB-CAB	2.82	1.48	1.28
6	K	806	HEM	CBC-CAC	2.82	1.48	1.28
6	F	813	HEM	CBB-CAB	2.82	1.48	1.28
6	C	809	HEM	CBB-CAB	2.83	1.48	1.28
6	C	813	HEM	CBB-CAB	2.83	1.48	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	806	HEM	CBC-CAC	2.83	1.48	1.28
6	G	811	HEM	CBC-CAC	2.83	1.48	1.28
6	G	806	HEM	CBC-CAC	2.84	1.48	1.28
6	J	810	HEM	CBB-CAB	2.84	1.48	1.28
6	L	812	HEM	CBB-CAB	2.85	1.48	1.28
6	H	810	HEM	CBC-CAC	2.86	1.49	1.28
6	G	810	HEM	CBB-CAB	2.88	1.49	1.28

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	806	HEM	C3B-C4B-NB	-5.88	101.61	109.21
6	A	811	HEM	C3B-C4B-NB	-5.75	101.77	109.21
6	J	806	HEM	C3B-C4B-NB	-5.74	101.79	109.21
6	F	813	HEM	C3B-C4B-NB	-5.05	102.68	109.21
6	I	811	HEM	C3B-C4B-NB	-4.95	102.81	109.21
6	B	809	HEM	C3B-C4B-NB	-4.91	102.86	109.21
6	F	812	HEM	C3B-C4B-NB	-4.90	102.88	109.21
6	E	811	HEM	C3B-C4B-NB	-4.88	102.90	109.21
6	C	811	HEM	C3B-C4B-NB	-4.88	102.90	109.21
6	D	808	HEM	C3B-C4B-NB	-4.85	102.94	109.21
6	A	812	HEM	C3B-C4B-NB	-4.75	103.06	109.21
6	J	811	HEM	C3B-C4B-NB	-4.74	103.08	109.21
6	A	806	HEM	C3B-C4B-NB	-4.64	103.21	109.21
6	C	808	HEM	C3B-C4B-NB	-4.61	103.26	109.21
6	J	812	HEM	C3B-C4B-NB	-4.60	103.26	109.21
6	G	811	HEM	C3B-C4B-NB	-4.59	103.28	109.21
6	D	810	HEM	C3B-C4B-NB	-4.58	103.28	109.21
6	C	812	HEM	C3B-C4B-NB	-4.58	103.29	109.21
6	D	811	HEM	C3B-C4B-NB	-4.57	103.31	109.21
6	G	806	HEM	C3B-C4B-NB	-4.56	103.31	109.21
6	H	807	HEM	C3B-C4B-NB	-4.54	103.34	109.21
6	D	807	HEM	C3B-C4B-NB	-4.54	103.34	109.21
6	F	807	HEM	C3B-C4B-NB	-4.54	103.34	109.21
6	A	810	HEM	C3B-C4B-NB	-4.53	103.35	109.21
6	D	812	HEM	C3B-C4B-NB	-4.52	103.37	109.21
6	F	809	HEM	C3B-C4B-NB	-4.50	103.39	109.21
6	L	807	HEM	C3B-C4B-NB	-4.50	103.39	109.21
6	E	808	HEM	C3B-C4B-NB	-4.50	103.39	109.21
6	H	811	HEM	C3B-C4B-NB	-4.49	103.41	109.21
6	I	807	HEM	C3B-C4B-NB	-4.48	103.41	109.21
6	I	812	HEM	C3B-C4B-NB	-4.48	103.42	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	813	HEM	C3B-C4B-NB	-4.48	103.42	109.21
6	F	811	HEM	C3B-C4B-NB	-4.47	103.43	109.21
6	G	807	HEM	C3B-C4B-NB	-4.47	103.43	109.21
6	K	807	HEM	C3B-C4B-NB	-4.46	103.44	109.21
6	C	806	HEM	C3B-C4B-NB	-4.43	103.48	109.21
6	H	808	HEM	C3B-C4B-NB	-4.43	103.48	109.21
6	F	814	HEM	C3B-C4B-NB	-4.42	103.50	109.21
6	E	810	HEM	C3B-C4B-NB	-4.42	103.50	109.21
6	G	810	HEM	C3B-C4B-NB	-4.41	103.50	109.21
6	J	807	HEM	C3B-C4B-NB	-4.40	103.52	109.21
6	B	813	HEM	C3B-C4B-NB	-4.40	103.52	109.21
6	E	807	HEM	C3B-C4B-NB	-4.40	103.52	109.21
6	C	810	HEM	C3B-C4B-NB	-4.39	103.53	109.21
6	B	807	HEM	C3B-C4B-NB	-4.39	103.53	109.21
6	K	811	HEM	C3B-C4B-NB	-4.37	103.56	109.21
6	B	812	HEM	C3B-C4B-NB	-4.35	103.59	109.21
6	B	808	HEM	C3B-C4B-NB	-4.32	103.63	109.21
6	A	807	HEM	C3B-C4B-NB	-4.32	103.63	109.21
6	E	812	HEM	C3B-C4B-NB	-4.29	103.66	109.21
6	D	813	HEM	C3B-C4B-NB	-4.29	103.67	109.21
6	J	810	HEM	C3B-C4B-NB	-4.29	103.67	109.21
6	A	808	HEM	C3B-C4B-NB	-4.27	103.68	109.21
6	I	813	HEM	C3B-C4B-NB	-4.27	103.69	109.21
6	K	812	HEM	C3B-C4B-NB	-4.26	103.70	109.21
6	G	812	HEM	C3B-C4B-NB	-4.26	103.71	109.21
6	E	806	HEM	C3B-C4B-NB	-4.26	103.71	109.21
6	C	813	HEM	C3B-C4B-NB	-4.25	103.71	109.21
6	L	808	HEM	C3B-C4B-NB	-4.23	103.74	109.21
6	K	810	HEM	C3B-C4B-NB	-4.22	103.75	109.21
6	E	813	HEM	C3B-C4B-NB	-4.22	103.75	109.21
6	E	811	HEM	CAD-CBD-CGD	-4.21	105.47	112.66
6	D	806	HEM	C3B-C4B-NB	-4.20	103.78	109.21
6	F	808	HEM	C3B-C4B-NB	-4.19	103.80	109.21
6	I	810	HEM	C3B-C4B-NB	-4.18	103.80	109.21
6	H	812	HEM	C3B-C4B-NB	-4.18	103.80	109.21
6	C	808	HEM	CBA-CAA-C2A	-4.18	104.50	112.48
6	K	808	HEM	C3B-C4B-NB	-4.16	103.83	109.21
6	H	809	HEM	CBA-CAA-C2A	-4.16	104.53	112.48
6	B	811	HEM	C3B-C4B-NB	-4.16	103.84	109.21
6	I	808	HEM	C3B-C4B-NB	-4.14	103.86	109.21
6	K	813	HEM	C3B-C4B-NB	-4.13	103.87	109.21
6	G	808	HEM	C3B-C4B-NB	-4.11	103.89	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	808	HEM	CBA-CAA-C2A	-4.11	104.63	112.48
6	C	807	HEM	C3B-C4B-NB	-4.10	103.90	109.21
6	L	810	HEM	C3B-C4B-NB	-4.08	103.94	109.21
6	L	812	HEM	C3B-C4B-NB	-3.99	104.05	109.21
6	H	810	HEM	C3B-C4B-NB	-3.97	104.08	109.21
6	I	806	HEM	C3B-C4B-NB	-3.96	104.09	109.21
6	J	808	HEM	CBA-CAA-C2A	-3.96	104.91	112.48
6	E	808	HEM	CBA-CAA-C2A	-3.96	104.91	112.48
6	H	814	HEM	C3B-C4B-NB	-3.96	104.10	109.21
6	L	808	HEM	CBA-CAA-C2A	-3.94	104.95	112.48
6	B	810	HEM	C3B-C4B-NB	-3.94	104.11	109.21
6	A	813	HEM	C3B-C4B-NB	-3.94	104.12	109.21
6	H	809	HEM	C3B-C4B-NB	-3.91	104.15	109.21
6	L	806	HEM	C3B-C4B-NB	-3.89	104.18	109.21
6	C	809	HEM	C3B-C4B-NB	-3.88	104.19	109.21
6	L	809	HEM	C3B-C4B-NB	-3.86	104.22	109.21
6	D	809	HEM	C3B-C4B-NB	-3.86	104.22	109.21
6	J	808	HEM	C3B-C4B-NB	-3.86	104.22	109.21
6	G	813	HEM	C3B-C4B-NB	-3.83	104.26	109.21
6	D	808	HEM	CBA-CAA-C2A	-3.81	105.21	112.48
6	K	809	HEM	CBD-CAD-C3D	-3.80	105.22	112.47
6	F	812	HEM	CAD-CBD-CGD	-3.79	106.19	112.66
6	J	813	HEM	C3B-C4B-NB	-3.78	104.32	109.21
6	B	814	HEM	C3B-C4B-NB	-3.77	104.33	109.21
6	A	811	HEM	CAD-CBD-CGD	-3.76	106.24	112.66
6	B	809	HEM	CBA-CAA-C2A	-3.75	105.31	112.48
6	I	811	HEM	CAD-CBD-CGD	-3.75	106.26	112.66
6	L	811	HEM	C3B-C4B-NB	-3.73	104.38	109.21
6	L	811	HEM	CAD-CBD-CGD	-3.72	106.30	112.66
6	K	808	HEM	CBA-CAA-C2A	-3.70	105.41	112.48
6	F	809	HEM	CBA-CAA-C2A	-3.66	105.48	112.48
6	E	809	HEM	C3B-C4B-NB	-3.65	104.48	109.21
6	J	809	HEM	CBD-CAD-C3D	-3.65	105.51	112.47
6	A	808	HEM	CBA-CAA-C2A	-3.62	105.56	112.48
6	G	809	HEM	C3B-C4B-NB	-3.60	104.55	109.21
6	F	808	HEM	CMA-C3A-C4A	-3.56	122.99	128.46
6	I	809	HEM	C3B-C4B-NB	-3.54	104.63	109.21
6	A	809	HEM	C3B-C4B-NB	-3.53	104.64	109.21
6	F	810	HEM	C3B-C4B-NB	-3.52	104.66	109.21
6	J	809	HEM	C3B-C4B-NB	-3.50	104.69	109.21
6	B	808	HEM	CMA-C3A-C4A	-3.46	123.15	128.46
6	J	811	HEM	CAD-CBD-CGD	-3.41	106.83	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	812	HEM	CAD-CBD-CGD	-3.39	106.88	112.66
6	K	807	HEM	CMA-C3A-C4A	-3.37	123.28	128.46
6	J	807	HEM	CMA-C3A-C4A	-3.37	123.29	128.46
6	K	809	HEM	C3B-C4B-NB	-3.34	104.89	109.21
6	I	813	HEM	CAD-CBD-CGD	-3.30	107.03	112.66
6	L	813	HEM	C3B-C4B-NB	-3.26	105.00	109.21
6	C	811	HEM	CAD-CBD-CGD	-3.25	107.10	112.66
6	G	812	HEM	CMA-C3A-C4A	-3.22	123.52	128.46
6	A	812	HEM	CAD-CBD-CGD	-3.18	107.23	112.66
6	H	808	HEM	CMA-C3A-C4A	-3.18	123.58	128.46
6	G	807	HEM	CMA-C3A-C4A	-3.15	123.63	128.46
6	H	814	HEM	CAA-CBA-CGA	-3.14	107.30	112.66
6	I	810	HEM	CAA-CBA-CGA	-3.12	107.33	112.66
6	G	813	HEM	CAA-CBA-CGA	-3.09	107.38	112.66
6	K	810	HEM	CAA-CBA-CGA	-3.09	107.38	112.66
6	L	813	HEM	CAA-CBA-CGA	-3.08	107.40	112.66
6	F	811	HEM	CAA-CBA-CGA	-3.07	107.42	112.66
6	A	807	HEM	CMA-C3A-C4A	-3.02	123.82	128.46
6	C	807	HEM	CMA-C3A-C4A	-2.97	123.90	128.46
6	E	807	HEM	CMA-C3A-C4A	-2.91	124.00	128.46
6	D	807	HEM	CMA-C3A-C4A	-2.90	124.01	128.46
6	C	813	HEM	CBD-CAD-C3D	-2.87	106.98	112.47
6	D	811	HEM	CAD-CBD-CGD	-2.86	107.78	112.66
6	C	809	HEM	CMA-C3A-C4A	-2.82	124.13	128.46
6	I	807	HEM	CMA-C3A-C4A	-2.82	124.14	128.46
6	G	811	HEM	CAD-CBD-CGD	-2.81	107.86	112.66
6	E	809	HEM	CBD-CAD-C3D	-2.75	107.22	112.47
6	B	808	HEM	CMD-C2D-C1D	-2.73	124.27	128.46
6	B	810	HEM	CBD-CAD-C3D	-2.73	107.27	112.47
6	F	809	HEM	CMA-C3A-C4A	-2.71	124.29	128.46
6	C	808	HEM	CMA-C3A-C4A	-2.71	124.30	128.46
6	L	809	HEM	CBD-CAD-C3D	-2.71	107.30	112.47
6	I	808	HEM	CBA-CAA-C2A	-2.69	107.33	112.48
6	H	811	HEM	CBD-CAD-C3D	-2.68	107.35	112.47
6	A	809	HEM	CMA-C3A-C4A	-2.67	124.36	128.46
6	K	813	HEM	CBD-CAD-C3D	-2.67	107.38	112.47
6	G	809	HEM	CMA-C3A-C4A	-2.66	124.37	128.46
6	G	810	HEM	CAA-CBA-CGA	-2.64	108.15	112.66
6	K	813	HEM	CAD-CBD-CGD	-2.63	108.17	112.66
6	L	807	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
6	B	812	HEM	CAD-CBD-CGD	-2.59	108.24	112.66
6	K	809	HEM	CMA-C3A-C4A	-2.59	124.49	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	810	HEM	CBD-CAD-C3D	-2.56	107.59	112.47
6	B	812	HEM	CBA-CAA-C2A	-2.56	107.60	112.48
6	E	813	HEM	CAD-CBD-CGD	-2.55	108.31	112.66
6	A	810	HEM	CAA-CBA-CGA	-2.53	108.33	112.66
6	B	811	HEM	CAA-CBA-CGA	-2.52	108.35	112.66
6	G	811	HEM	CMA-C3A-C4A	-2.51	124.61	128.46
6	L	813	HEM	C3C-C4C-NC	-2.50	106.22	110.94
6	J	812	HEM	CMA-C3A-C4A	-2.49	124.63	128.46
6	K	811	HEM	CMA-C3A-C4A	-2.49	124.64	128.46
6	H	810	HEM	CMA-C3A-C4A	-2.48	124.66	128.46
6	H	807	HEM	CMA-C3A-C4A	-2.46	124.68	128.46
6	J	808	HEM	CMA-C3A-C4A	-2.46	124.69	128.46
6	I	808	HEM	CMA-C3A-C4A	-2.46	124.69	128.46
6	E	811	HEM	CMA-C3A-C4A	-2.45	124.69	128.46
6	A	813	HEM	CAD-CBD-CGD	-2.43	108.50	112.66
6	B	809	HEM	CMA-C3A-C4A	-2.43	124.72	128.46
6	D	809	HEM	CMA-C3A-C4A	-2.37	124.82	128.46
6	B	814	HEM	CMA-C3A-C4A	-2.36	124.83	128.46
6	I	811	HEM	CMA-C3A-C4A	-2.35	124.86	128.46
6	A	810	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
6	J	806	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
6	A	813	HEM	CBD-CAD-C3D	-2.32	108.04	112.47
6	D	809	HEM	CBD-CAD-C3D	-2.32	108.04	112.47
6	A	811	HEM	CBA-CAA-C2A	-2.31	108.06	112.48
6	L	811	HEM	CMA-C3A-C4A	-2.30	124.92	128.46
6	H	810	HEM	CBD-CAD-C3D	-2.30	108.08	112.47
6	A	808	HEM	CMA-C3A-C4A	-2.30	124.93	128.46
6	J	813	HEM	CMA-C3A-C4A	-2.29	124.95	128.46
6	A	806	HEM	CMA-C3A-C4A	-2.28	124.95	128.46
6	L	806	HEM	CBA-CAA-C2A	-2.28	108.13	112.48
6	H	811	HEM	CAA-CBA-CGA	-2.26	108.79	112.66
6	A	812	HEM	CMA-C3A-C4A	-2.26	124.99	128.46
6	F	809	HEM	C3C-C4C-NC	-2.25	106.70	110.94
6	I	813	HEM	CAA-CBA-CGA	-2.25	108.82	112.66
6	I	807	HEM	CMD-C2D-C1D	-2.24	125.02	128.46
6	L	807	HEM	CBA-CAA-C2A	-2.24	108.20	112.48
6	A	812	HEM	C1D-C2D-C3D	-2.23	105.44	107.00
6	L	813	HEM	CMA-C3A-C4A	-2.23	125.04	128.46
6	G	813	HEM	CMA-C3A-C4A	-2.22	125.05	128.46
6	L	812	HEM	CMA-C3A-C4A	-2.22	125.06	128.46
6	L	813	HEM	CAD-CBD-CGD	-2.21	108.88	112.66
6	I	812	HEM	CMA-C3A-C4A	-2.21	125.07	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	811	HEM	CAD-CBD-CGD	-2.21	108.89	112.66
6	H	812	HEM	CMA-C3A-C4A	-2.21	125.07	128.46
6	K	807	HEM	CMD-C2D-C1D	-2.19	125.10	128.46
6	D	808	HEM	CMA-C3A-C4A	-2.18	125.11	128.46
6	F	810	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
6	C	812	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
6	L	808	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
6	B	810	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
6	L	807	HEM	CMD-C2D-C1D	-2.16	125.15	128.46
6	K	808	HEM	CMA-C3A-C4A	-2.15	125.15	128.46
6	L	810	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
6	G	811	HEM	CBD-CAD-C3D	-2.14	108.38	112.47
6	I	809	HEM	CBD-CAD-C3D	-2.14	108.38	112.47
6	K	806	HEM	CMA-C3A-C4A	-2.13	125.20	128.46
6	B	812	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
6	E	808	HEM	CAD-CBD-CGD	-2.11	109.05	112.66
6	K	813	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
6	D	807	HEM	CMD-C2D-C1D	-2.10	125.23	128.46
6	F	808	HEM	CMD-C2D-C1D	-2.10	125.23	128.46
6	A	813	HEM	C1D-C2D-C3D	-2.10	105.53	107.00
6	B	811	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
6	G	813	HEM	C1D-C2D-C3D	-2.08	105.55	107.00
6	I	808	HEM	C3C-C4C-NC	-2.08	107.02	110.94
6	L	806	HEM	CMA-C3A-C4A	-2.08	125.27	128.46
6	F	810	HEM	CBD-CAD-C3D	-2.08	108.51	112.47
6	I	806	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
6	I	811	HEM	CBA-CAA-C2A	-2.07	108.53	112.48
6	D	806	HEM	CBA-CAA-C2A	-2.07	108.53	112.48
6	A	812	HEM	CAA-CBA-CGA	-2.07	109.13	112.66
6	D	811	HEM	CMA-C3A-C4A	-2.06	125.30	128.46
6	J	812	HEM	CAA-CBA-CGA	-2.05	109.15	112.66
6	H	811	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
6	H	809	HEM	C3C-C4C-NC	-2.05	107.08	110.94
6	K	812	HEM	CMA-C3A-C4A	-2.04	125.32	128.46
6	B	813	HEM	CMA-C3A-C4A	-2.04	125.33	128.46
6	E	812	HEM	CMA-C3A-C4A	-2.04	125.33	128.46
6	H	808	HEM	CMD-C2D-C1D	-2.03	125.34	128.46
6	A	809	HEM	CBD-CAD-C3D	-2.03	108.60	112.47
6	J	807	HEM	CMD-C2D-C1D	-2.03	125.35	128.46
6	G	812	HEM	CAA-CBA-CGA	-2.02	109.20	112.66
6	E	813	HEM	CAA-CBA-CGA	-2.02	109.20	112.66
6	C	810	HEM	CAA-CBA-CGA	-2.02	109.21	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	810	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
6	B	807	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
6	A	808	HEM	C3C-C4C-NC	-2.01	107.14	110.94
6	I	813	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
6	A	807	HEM	CMD-C2D-C1D	-2.01	125.38	128.46
6	J	809	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
6	D	811	HEM	CBA-CAA-C2A	-2.00	108.65	112.48
6	E	808	HEM	CMA-C3A-C4A	-2.00	125.38	128.46
6	C	806	HEM	CMA-C3A-C4A	-2.00	125.39	128.46
6	D	808	HEM	C3C-C4C-NC	-2.00	107.17	110.94
6	A	813	HEM	CMB-C2B-C3B	2.00	128.61	124.89
6	I	810	HEM	CMB-C2B-C3B	2.01	128.61	124.89
6	A	808	HEM	CMB-C2B-C3B	2.01	128.62	124.89
6	J	808	HEM	CMC-C2C-C3C	2.01	128.62	124.89
6	C	806	HEM	C4A-C3A-C2A	2.01	108.40	107.00
6	K	811	HEM	C4A-C3A-C2A	2.02	108.40	107.00
6	B	809	HEM	CMB-C2B-C3B	2.02	128.65	124.89
6	H	809	HEM	CMB-C2B-C3B	2.02	128.65	124.89
6	E	806	HEM	CMB-C2B-C3B	2.04	128.67	124.89
6	A	812	HEM	CMC-C2C-C3C	2.04	128.68	124.89
6	H	807	HEM	CMB-C2B-C3B	2.04	128.68	124.89
6	F	811	HEM	CMC-C2C-C3C	2.05	128.69	124.89
6	C	810	HEM	CMB-C2B-C3B	2.05	128.70	124.89
6	E	811	HEM	CMB-C2B-C3B	2.05	128.70	124.89
6	B	811	HEM	CMB-C2B-C3B	2.06	128.71	124.89
6	B	810	HEM	CMB-C2B-C3B	2.06	128.71	124.89
6	G	811	HEM	CMB-C2B-C3B	2.06	128.71	124.89
6	G	806	HEM	CMB-C2B-C3B	2.07	128.73	124.89
6	D	810	HEM	CMB-C2B-C3B	2.08	128.74	124.89
6	C	812	HEM	C4A-C3A-C2A	2.08	108.44	107.00
6	I	812	HEM	C4A-C3A-C2A	2.08	108.45	107.00
6	E	812	HEM	C4A-C3A-C2A	2.09	108.45	107.00
6	G	812	HEM	CMB-C2B-C3B	2.09	128.77	124.89
6	H	812	HEM	CMB-C2B-C3B	2.09	128.78	124.89
6	I	808	HEM	C4C-C3C-C2C	2.10	108.36	106.90
6	H	811	HEM	CMB-C2B-C3B	2.11	128.80	124.89
6	F	814	HEM	C4A-C3A-C2A	2.11	108.46	107.00
6	J	807	HEM	C4A-C3A-C2A	2.11	108.47	107.00
6	E	808	HEM	C4A-C3A-C2A	2.11	108.47	107.00
6	C	810	HEM	CMC-C2C-C3C	2.12	128.83	124.89
6	K	810	HEM	CMB-C2B-C3B	2.13	128.84	124.89
6	D	808	HEM	C4A-C3A-C2A	2.13	108.48	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	811	HEM	C4A-C3A-C2A	2.13	108.48	107.00
6	B	807	HEM	C4A-C3A-C2A	2.13	108.48	107.00
6	C	813	HEM	CMB-C2B-C3B	2.13	128.85	124.89
6	D	813	HEM	CMB-C2B-C3B	2.14	128.86	124.89
6	F	807	HEM	C4A-C3A-C2A	2.14	108.48	107.00
6	C	808	HEM	C4A-C3A-C2A	2.14	108.49	107.00
6	H	808	HEM	C4A-C3A-C2A	2.14	108.49	107.00
6	J	812	HEM	C4A-C3A-C2A	2.15	108.49	107.00
6	I	808	HEM	CMC-C2C-C3C	2.15	128.89	124.89
6	D	806	HEM	CMB-C2B-C3B	2.16	128.90	124.89
6	H	809	HEM	CMC-C2C-C3C	2.16	128.90	124.89
6	F	808	HEM	CMB-C2B-C3B	2.17	128.91	124.89
6	K	812	HEM	C4A-C3A-C2A	2.17	108.50	107.00
6	D	813	HEM	C4A-C3A-C2A	2.17	108.51	107.00
6	G	807	HEM	CBD-CAD-C3D	2.18	116.62	112.47
6	C	813	HEM	C4A-C3A-C2A	2.19	108.52	107.00
6	F	809	HEM	CMB-C2B-C3B	2.19	128.95	124.89
6	K	807	HEM	C4A-C3A-C2A	2.19	108.52	107.00
6	K	812	HEM	CMB-C2B-C3B	2.20	128.97	124.89
6	D	807	HEM	C4A-C3A-C2A	2.20	108.53	107.00
6	B	807	HEM	CMB-C2B-C3B	2.21	128.98	124.89
6	I	809	HEM	CMB-C2B-C3B	2.21	128.99	124.89
6	C	811	HEM	CMB-C2B-C3B	2.21	129.00	124.89
6	H	813	HEM	C4A-C3A-C2A	2.22	108.54	107.00
6	A	806	HEM	CMB-C2B-C3B	2.23	129.04	124.89
6	J	812	HEM	CMB-C2B-C3B	2.23	129.04	124.89
6	A	809	HEM	C4A-C3A-C2A	2.25	108.56	107.00
6	I	813	HEM	C4A-C3A-C2A	2.25	108.56	107.00
6	E	809	HEM	CMB-C2B-C3B	2.26	129.09	124.89
6	F	813	HEM	CMB-C2B-C3B	2.26	129.09	124.89
6	D	807	HEM	CMB-C2B-C3B	2.26	129.09	124.89
6	B	808	HEM	C4A-C3A-C2A	2.27	108.58	107.00
6	A	807	HEM	CMB-C2B-C3B	2.27	129.11	124.89
6	C	806	HEM	CMB-C2B-C3B	2.28	129.12	124.89
6	H	814	HEM	CMB-C2B-C3B	2.29	129.14	124.89
6	B	812	HEM	C4A-C3A-C2A	2.29	108.59	107.00
6	D	807	HEM	CBD-CAD-C3D	2.30	116.85	112.47
6	I	810	HEM	C4A-C3A-C2A	2.30	108.59	107.00
6	I	808	HEM	C4A-C3A-C2A	2.30	108.59	107.00
6	G	809	HEM	C4A-C3A-C2A	2.31	108.60	107.00
6	L	808	HEM	CMB-C2B-C3B	2.31	129.18	124.89
6	D	811	HEM	CMB-C2B-C3B	2.32	129.19	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	808	HEM	C4A-C3A-C2A	2.32	108.61	107.00
6	F	812	HEM	C4A-C3A-C2A	2.35	108.63	107.00
6	I	811	HEM	C4A-C3A-C2A	2.37	108.64	107.00
6	A	813	HEM	C4A-C3A-C2A	2.37	108.65	107.00
6	G	807	HEM	C4A-C3A-C2A	2.37	108.65	107.00
6	G	807	HEM	CMB-C2B-C3B	2.37	129.30	124.89
6	J	811	HEM	C4A-C3A-C2A	2.38	108.65	107.00
6	C	807	HEM	CBD-CAD-C3D	2.38	117.01	112.47
6	I	811	HEM	CMB-C2B-C3B	2.40	129.34	124.89
6	B	810	HEM	C4A-C3A-C2A	2.41	108.67	107.00
6	E	807	HEM	C4A-C3A-C2A	2.41	108.67	107.00
6	L	806	HEM	C4A-C3A-C2A	2.42	108.68	107.00
6	H	812	HEM	C4A-C3A-C2A	2.43	108.69	107.00
6	H	810	HEM	C4A-C3A-C2A	2.43	108.69	107.00
6	G	811	HEM	C4A-C3A-C2A	2.43	108.69	107.00
6	G	812	HEM	C4A-C3A-C2A	2.44	108.69	107.00
6	L	810	HEM	C4A-C3A-C2A	2.45	108.70	107.00
6	E	812	HEM	CMB-C2B-C3B	2.45	129.44	124.89
6	F	807	HEM	CMB-C2B-C3B	2.45	129.44	124.89
6	I	807	HEM	C4A-C3A-C2A	2.46	108.70	107.00
6	I	808	HEM	CMB-C2B-C3B	2.46	129.45	124.89
6	I	812	HEM	CMB-C2B-C3B	2.46	129.46	124.89
6	C	812	HEM	CMB-C2B-C3B	2.46	129.46	124.89
6	H	808	HEM	CBD-CAD-C3D	2.47	117.18	112.47
6	H	807	HEM	C4A-C3A-C2A	2.47	108.72	107.00
6	F	811	HEM	CMB-C2B-C3B	2.48	129.49	124.89
6	B	808	HEM	CMD-C2D-C3D	2.49	129.63	124.94
6	A	806	HEM	C4A-C3A-C2A	2.50	108.74	107.00
6	D	810	HEM	C4A-C3A-C2A	2.51	108.74	107.00
6	G	810	HEM	C4A-C3A-C2A	2.51	108.74	107.00
6	B	813	HEM	CMB-C2B-C3B	2.51	129.55	124.89
6	C	808	HEM	CMB-C2B-C3B	2.51	129.56	124.89
6	B	811	HEM	C4A-C3A-C2A	2.51	108.75	107.00
6	K	807	HEM	CBD-CAD-C3D	2.52	117.27	112.47
6	C	809	HEM	C4A-C3A-C2A	2.52	108.75	107.00
6	E	810	HEM	CMB-C2B-C3B	2.52	129.57	124.89
6	D	812	HEM	CMB-C2B-C3B	2.53	129.58	124.89
6	F	812	HEM	CMB-C2B-C3B	2.55	129.63	124.89
6	E	807	HEM	CBD-CAD-C3D	2.57	117.37	112.47
6	E	809	HEM	C4A-C3A-C2A	2.57	108.78	107.00
6	A	810	HEM	CMB-C2B-C3B	2.59	129.69	124.89
6	A	807	HEM	CBD-CAD-C3D	2.60	117.43	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	810	HEM	C4A-C3A-C2A	2.60	108.81	107.00
6	B	809	HEM	C4A-C3A-C2A	2.61	108.81	107.00
6	F	808	HEM	CBD-CAD-C3D	2.62	117.46	112.47
6	A	812	HEM	CMB-C2B-C3B	2.65	129.81	124.89
6	E	806	HEM	C4A-C3A-C2A	2.69	108.86	107.00
6	H	811	HEM	C4A-C3A-C2A	2.74	108.90	107.00
6	J	813	HEM	C4A-C3A-C2A	2.75	108.91	107.00
6	E	810	HEM	C4A-C3A-C2A	2.76	108.92	107.00
6	E	811	HEM	C4A-C3A-C2A	2.77	108.92	107.00
6	J	809	HEM	C4A-C3A-C2A	2.81	108.95	107.00
6	K	813	HEM	C4A-C3A-C2A	2.82	108.96	107.00
6	B	814	HEM	C4A-C3A-C2A	2.84	108.97	107.00
6	I	806	HEM	C4A-C3A-C2A	2.85	108.98	107.00
6	C	810	HEM	C4A-C3A-C2A	2.96	109.06	107.00
6	J	810	HEM	C4A-C3A-C2A	3.01	109.09	107.00
6	F	808	HEM	C4A-C3A-C2A	3.26	109.26	107.00

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	813	HEM	10	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.24	12 (1%)	69	66	16, 24, 45, 95	0
1	B	660/732 (90%)	-0.29	6 (0%)	84	83	20, 33, 49, 82	0
1	C	659/732 (90%)	-0.24	4 (0%)	89	88	18, 32, 54, 86	0
1	D	659/732 (90%)	-0.23	19 (2%)	52	50	21, 32, 56, 102	0
1	E	659/732 (90%)	-0.15	10 (1%)	74	72	23, 38, 59, 104	0
1	F	659/732 (90%)	-0.07	13 (1%)	65	63	21, 38, 63, 107	0
1	G	658/732 (89%)	-0.25	13 (1%)	65	63	25, 37, 57, 93	0
1	H	660/732 (90%)	-0.20	7 (1%)	80	79	25, 37, 61, 95	0
1	I	659/732 (90%)	0.02	18 (2%)	55	52	26, 39, 58, 76	0
1	J	659/732 (90%)	0.02	18 (2%)	55	52	27, 46, 69, 96	0
1	K	659/732 (90%)	-0.01	7 (1%)	80	79	25, 46, 68, 85	0
1	L	659/732 (90%)	0.39	38 (5%)	24	23	30, 51, 76, 89	0
All	All	7909/8784 (90%)	-0.10	165 (2%)	64	61	16, 37, 65, 107	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	629	VAL	7.4
1	F	629	VAL	7.1
1	A	629	VAL	6.5
1	G	379	LEU	5.2
1	H	629	VAL	5.2
1	F	628	GLU	4.8
1	H	628	GLU	4.8
1	L	81	GLY	4.7
1	G	629	VAL	4.6
1	H	631	LYS	4.4
1	D	628	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	624	TYR	4.2
1	L	231	GLY	4.2
1	A	688	LYS	4.1
1	G	625	SER	4.1
1	L	223	VAL	4.0
1	G	627	LEU	4.0
1	L	379	LEU	3.9
1	F	687	LYS	3.9
1	D	629	VAL	3.8
1	E	634	PRO	3.8
1	L	78	THR	3.8
1	L	537	ASP	3.8
1	A	624	TYR	3.8
1	D	634	PRO	3.8
1	J	689	SER	3.7
1	D	641	TYR	3.6
1	L	689	SER	3.6
1	B	435	LYS	3.6
1	E	629	VAL	3.5
1	D	621	GLN	3.5
1	F	631	LYS	3.4
1	L	82	GLY	3.4
1	H	690	LEU	3.4
1	J	688	LYS	3.4
1	L	277	GLY	3.3
1	A	625	SER	3.3
1	A	630	LYS	3.3
1	L	538	PRO	3.3
1	L	235	ILE	3.3
1	D	623	LEU	3.2
1	G	628	GLU	3.2
1	I	357	ILE	3.2
1	G	687	LYS	3.2
1	E	689	SER	3.2
1	J	627	LEU	3.1
1	K	689	SER	3.1
1	G	624	TYR	3.0
1	E	638	THR	3.0
1	K	589	THR	3.0
1	A	641	TYR	3.0
1	L	227	LEU	3.0
1	D	689	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	630	LYS	3.0
1	I	35	LYS	3.0
1	I	379	LEU	3.0
1	E	633	ALA	3.0
1	E	635	SER	3.0
1	B	690	LEU	2.9
1	H	626	LEU	2.9
1	L	230	ASN	2.9
1	D	625	SER	2.9
1	F	688	LYS	2.9
1	D	632	LEU	2.9
1	L	228	LEU	2.9
1	I	39	GLU	2.8
1	C	438	LYS	2.8
1	A	438	LYS	2.8
1	B	476	ALA	2.8
1	L	196	ASP	2.8
1	L	84	THR	2.8
1	L	236	VAL	2.8
1	L	264	ASP	2.7
1	L	226	GLY	2.7
1	I	360	CYS	2.7
1	D	687	LYS	2.7
1	J	628	GLU	2.7
1	I	378	PRO	2.7
1	L	476	ALA	2.7
1	D	688	LYS	2.7
1	L	215	TRP	2.6
1	G	618	VAL	2.6
1	D	438	LYS	2.6
1	L	83	LYS	2.6
1	D	626	LEU	2.6
1	K	183	LYS	2.6
1	F	632	LEU	2.6
1	D	622	GLY	2.6
1	L	43	HIS	2.5
1	B	536	LYS	2.5
1	A	628	GLU	2.5
1	F	225	GLY	2.5
1	F	622	GLY	2.5
1	I	363	CYS	2.5
1	L	76	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	634	PRO	2.5
1	G	621	GLN	2.5
1	C	629	VAL	2.5
1	L	330	LYS	2.5
1	D	631	LYS	2.5
1	K	379	LEU	2.5
1	L	224	GLU	2.4
1	A	687	LYS	2.4
1	J	184	ASP	2.4
1	L	360	CYS	2.4
1	I	375	ARG	2.4
1	F	226	GLY	2.4
1	L	232	THR	2.4
1	G	631	LYS	2.4
1	A	686	MET	2.4
1	J	31	MET	2.4
1	D	630	LYS	2.4
1	F	438	LYS	2.4
1	L	116	GLU	2.4
1	J	43	HIS	2.3
1	I	438	LYS	2.3
1	L	375	ARG	2.3
1	C	379	LEU	2.3
1	F	183	LYS	2.3
1	J	588	GLU	2.3
1	I	87	LYS	2.3
1	B	438	LYS	2.3
1	I	337	VAL	2.3
1	L	77	PHE	2.3
1	L	265	PHE	2.3
1	I	534	THR	2.2
1	E	43	HIS	2.2
1	A	689	SER	2.2
1	B	689	SER	2.2
1	I	427	VAL	2.2
1	I	43	HIS	2.2
1	D	686	MET	2.2
1	K	533	SER	2.2
1	I	476	ALA	2.2
1	C	689	SER	2.2
1	J	223	VAL	2.2
1	J	618	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	636	ASP	2.2
1	G	49	GLU	2.2
1	E	631	LYS	2.2
1	L	88	LEU	2.2
1	I	358	SER	2.2
1	J	631	LYS	2.1
1	J	687	LYS	2.1
1	K	440	VAL	2.1
1	L	533	SER	2.1
1	E	632	LEU	2.1
1	L	270	GLU	2.1
1	E	536	LYS	2.1
1	J	225	GLY	2.1
1	J	272	TYR	2.1
1	L	192	GLY	2.1
1	J	611	ASP	2.1
1	L	182	ASP	2.1
1	I	359	ASN	2.1
1	J	259	LYS	2.1
1	J	624	TYR	2.1
1	G	686	MET	2.0
1	K	588	GLU	2.0
1	L	588	GLU	2.0
1	G	684	ARG	2.0
1	F	72	LYS	2.0
1	H	686	MET	2.0
1	A	684	ARG	2.0
1	I	68	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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.