



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:22 PM GMT

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

This is a 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

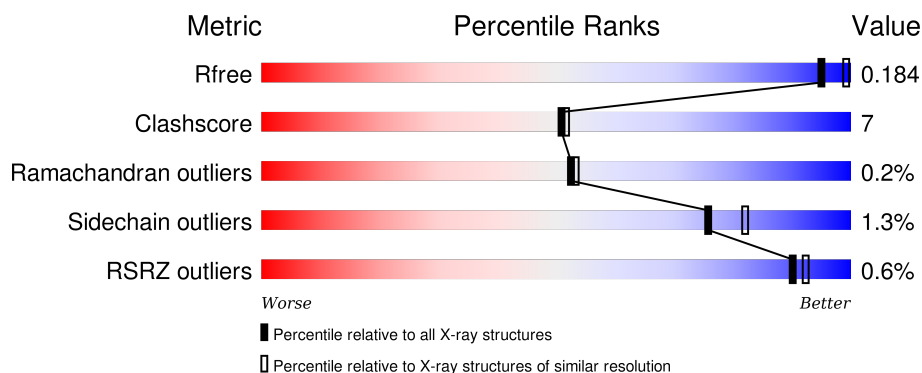
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	732	
1	B	732	
1	C	732	
1	D	732	

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

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

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23997 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MccA.

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

There are 120 discrepancies between the modelled and reference sequences:

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

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

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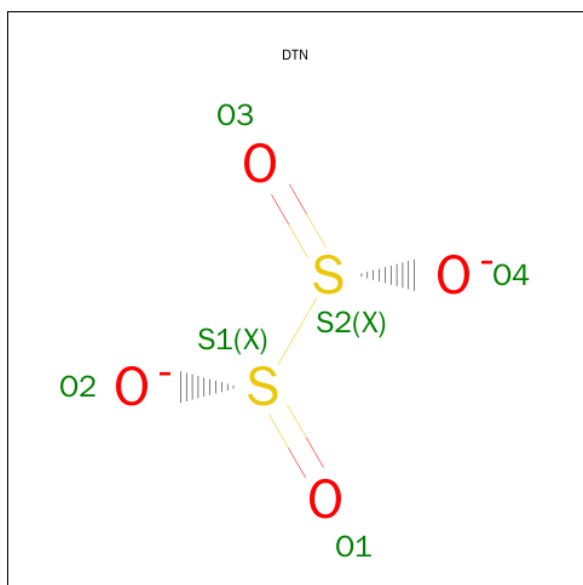
Chain	Residue	Modelled	Actual	Comment	Reference
C	694	SER	-	EXPRESSION TAG	UNP Q7MSJ8
C	695	HIS	-	EXPRESSION TAG	UNP Q7MSJ8
C	696	PRO	-	EXPRESSION TAG	UNP Q7MSJ8
C	697	GLN	-	EXPRESSION TAG	UNP Q7MSJ8
C	698	PHE	-	EXPRESSION TAG	UNP Q7MSJ8
C	699	GLU	-	EXPRESSION TAG	UNP Q7MSJ8
C	700	LYS	-	EXPRESSION TAG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

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

- Molecule 2 is DITHIONITE (three-letter code: DTN) (formula: O_4S_2).



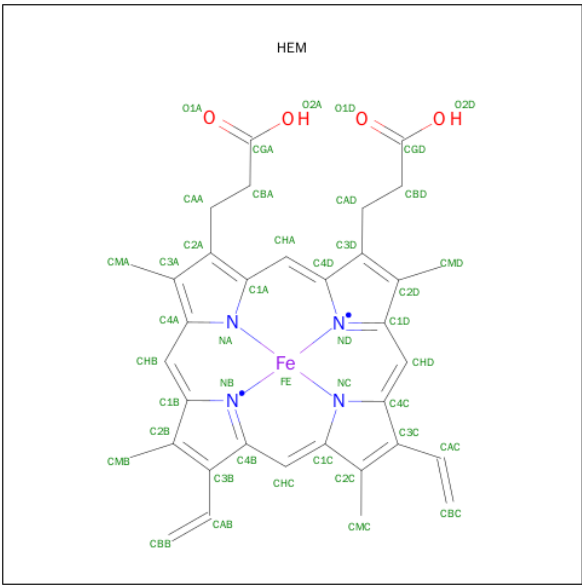
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			6	4	2		
2	A	1	Total	O	S	0	0
			6	4	2		
2	B	1	Total	O	S	0	0
			6	4	2		
2	C	1	Total	O	S	0	0
			6	4	2		

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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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

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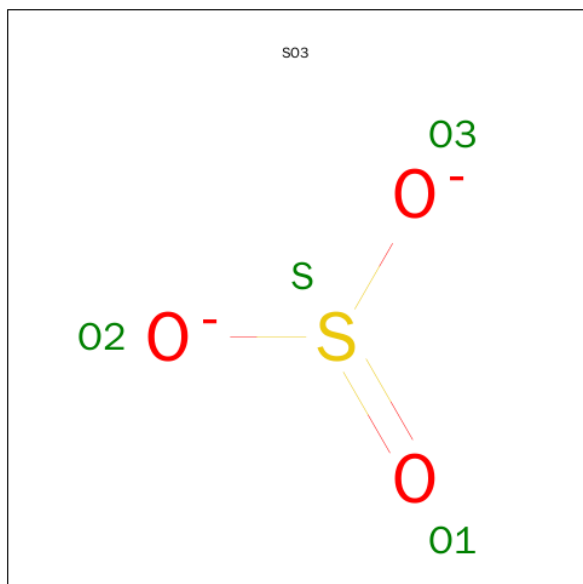
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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

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

- Molecule 5 is SULFITE ION (three-letter code: SO3) (formula: O₃S).



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

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

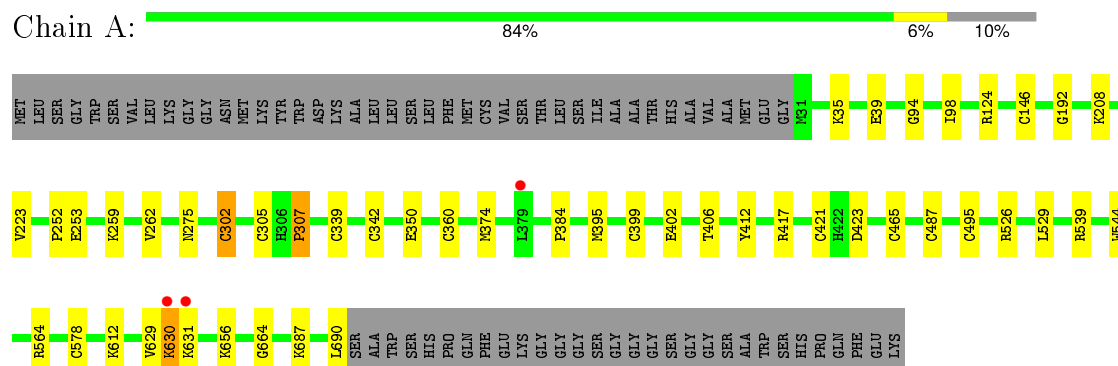
- Molecule 6 is water.

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

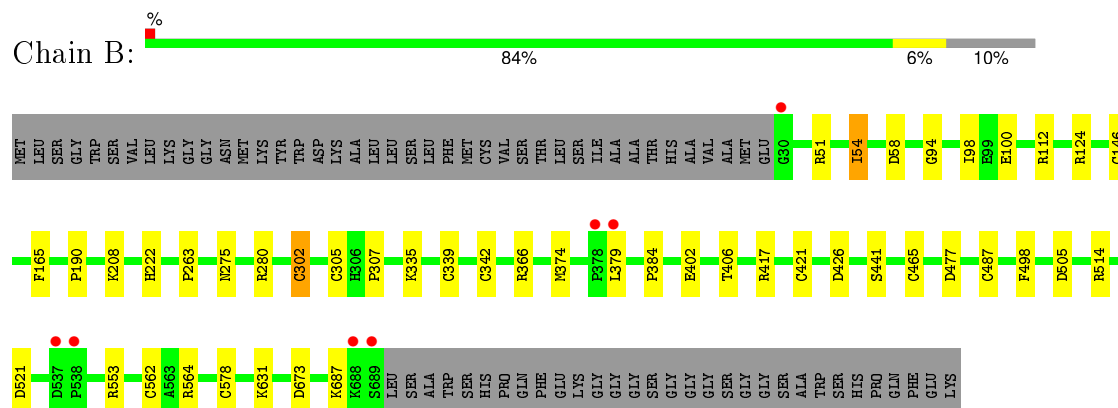
3 Residue-property plots [i](#)

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

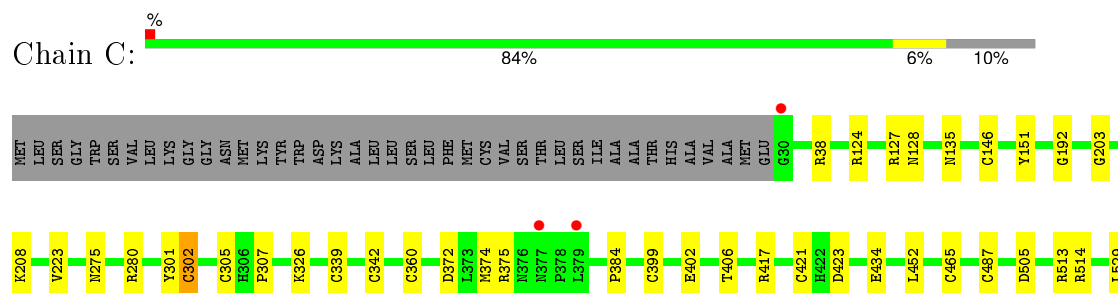
• Molecule 1: MccA

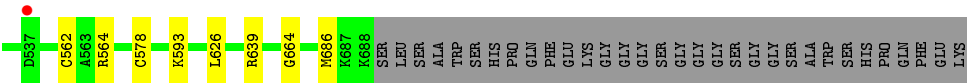


• Molecule 1: MccA

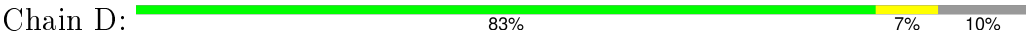


• Molecule 1: MccA





● Molecule 1: MccA



4 Data and refinement statistics

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO3, DTN, CU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.88	0/5383	0.88	6/7251 (0.1%)
1	B	0.89	0/5379	0.92	14/7245 (0.2%)
1	C	0.88	0/5373	0.89	11/7237 (0.2%)
1	D	0.97	4/5370 (0.1%)	0.93	8/7233 (0.1%)
All	All	0.91	4/21505 (0.0%)	0.91	39/28966 (0.1%)

All (4) bond length outliers are listed below:

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

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	B	514	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	B	505	ASP	CB-CG-OD1	8.74	126.17	118.30
1	A	526	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	D	280	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	C	514	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	D	280	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	417	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	417	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	539	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	C	280	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	539	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	B	521	ASP	CB-CG-OD2	6.68	124.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	366	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	D	423	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	366	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	B	514	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	423	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	505	ASP	CB-CG-OD1	6.43	124.08	118.30
1	C	417	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	553	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	526	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	D	311	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	514	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	423	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	477	ASP	CB-CG-OD1	5.74	123.47	118.30
1	D	477	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	127	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	426	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	553	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	38	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	426	ASP	CB-CG-OD1	5.34	123.10	118.30
1	C	639	ARG	CG-CD-NE	-5.31	100.66	111.80
1	B	58	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	B	505	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	280	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	280	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	C	38	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	673	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5250	0	5072	73	0
1	B	5246	0	5063	72	0
1	C	5240	0	5059	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	5240	0	5054	72	0
2	A	12	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	387	0	270	56	0
3	B	387	0	270	61	0
3	C	387	0	270	64	0
3	D	387	0	270	57	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
5	D	8	0	0	3	0
6	A	335	0	0	4	0
6	B	355	0	0	3	0
6	C	312	0	0	2	0
6	D	417	0	0	4	0
All	All	23997	0	21328	301	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (301) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:CYS:SG	3:B:909:HEM:CAB	2.01	1.48
1:D:578:CYS:SG	3:D:909:HEM:CAC	2.03	1.47
1:C:562:CYS:SG	3:C:909:HEM:CAB	2.02	1.47
1:B:339:CYS:SG	3:B:904[A]:HEM:CAB	2.03	1.47
1:D:305:CYS:SG	3:D:903:HEM:CAC	2.03	1.47
1:D:360:CYS:SG	3:D:905:HEM:CAB	2.02	1.46
1:C:339:CYS:SG	3:C:904[A]:HEM:CAB	2.03	1.46
1:A:339:CYS:SG	3:A:904[A]:HEM:CAB	2.04	1.45
1:B:339:CYS:SG	3:B:904[B]:HEM:CAB	2.05	1.44
1:D:487:CYS:SG	3:D:908:HEM:CAC	2.06	1.44
1:B:578:CYS:SG	3:B:909:HEM:CAC	2.07	1.43
1:A:360:CYS:SG	3:A:905:HEM:CAB	2.07	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:CYS:SG	3:D:905:HEM:CAC	2.08	1.42
1:A:421:CYS:SG	3:A:906:HEM:CAC	2.07	1.41
1:C:487:CYS:SG	3:C:908:HEM:CAC	2.08	1.41
1:A:421:CYS:HG	3:A:906:HEM:CAC	1.33	1.40
1:A:339:CYS:SG	3:A:904[B]:HEM:CAB	2.07	1.39
1:D:146:CYS:SG	3:D:902:HEM:CAC	2.11	1.39
1:D:421:CYS:SG	3:D:906:HEM:CAC	2.10	1.39
1:A:487:CYS:SG	3:A:908:HEM:CAC	2.09	1.38
1:B:305:CYS:SG	3:B:903:HEM:CAC	2.12	1.38
1:C:360:CYS:SG	3:C:905:HEM:CAB	2.11	1.37
1:C:305:CYS:SG	3:C:903:HEM:CAC	2.13	1.37
1:C:421:CYS:SG	3:C:906:HEM:CAC	2.13	1.36
1:A:578:CYS:SG	3:A:909:HEM:CAC	2.12	1.36
1:C:146:CYS:SG	3:C:902:HEM:CAC	2.13	1.36
1:D:342:CYS:SG	3:D:904[B]:HEM:CAC	2.13	1.36
1:B:487:CYS:SG	3:B:908:HEM:CAC	2.13	1.36
1:D:465:CYS:SG	3:D:907:HEM:CAC	2.14	1.35
1:A:305:CYS:SG	3:A:903:HEM:CAC	2.14	1.35
1:C:578:CYS:SG	3:C:909:HEM:CAC	2.15	1.35
1:B:578:CYS:HG	3:B:909:HEM:CAC	1.33	1.34
1:D:342:CYS:SG	3:D:904[A]:HEM:CAC	2.15	1.34
1:B:421:CYS:SG	3:B:906:HEM:CAC	2.16	1.32
1:C:342:CYS:SG	3:C:904[A]:HEM:CAC	2.20	1.30
1:B:146:CYS:SG	3:B:902:HEM:CAC	2.18	1.30
1:A:342:CYS:SG	3:A:904[B]:HEM:CAC	2.19	1.29
1:A:146:CYS:SG	3:A:902:HEM:CAC	2.19	1.29
1:B:342:CYS:SG	3:B:904[B]:HEM:CAC	2.21	1.29
1:B:342:CYS:SG	3:B:904[A]:HEM:CAC	2.21	1.27
1:C:342:CYS:SG	3:C:904[B]:HEM:CAC	2.22	1.27
1:A:465:CYS:SG	3:A:907:HEM:CAC	2.21	1.27
1:A:342:CYS:SG	3:A:904[A]:HEM:CAC	2.23	1.26
1:B:465:CYS:SG	3:B:907:HEM:CAC	2.25	1.24
1:D:302:CYS:SG	3:D:903:HEM:CAB	2.28	1.22
1:C:465:CYS:SG	3:C:907:HEM:CAC	2.28	1.20
1:A:360:CYS:HG	3:A:905:HEM:CAB	1.52	1.17
1:C:421:CYS:HG	3:C:906:HEM:CAC	1.49	1.16
1:B:339:CYS:SG	3:B:904[B]:HEM:HAB	1.85	1.14
1:B:302:CYS:SG	3:B:903:HEM:CAB	2.33	1.14
1:D:360:CYS:SG	3:D:905:HEM:HAB	1.87	1.14
1:B:562:CYS:SG	3:B:909:HEM:HAB	1.88	1.14
1:A:302:CYS:SG	3:A:903:HEM:CAB	2.36	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:CYS:SG	3:C:909:HEM:HAB	1.82	1.08
1:D:487:CYS:SG	3:D:908:HEM:HAC	1.91	1.08
1:C:302:CYS:SG	3:C:903:HEM:CAB	2.42	1.07
1:A:421:CYS:SG	3:A:906:HEM:HAC	1.92	1.06
1:A:339:CYS:SG	3:A:904[A]:HEM:HAB	1.90	1.06
1:B:339:CYS:SG	3:B:904[A]:HEM:HAB	1.85	1.05
1:D:363:CYS:SG	3:D:905:HEM:HAC	1.94	1.04
1:C:360:CYS:HG	3:C:905:HEM:CAB	1.62	1.03
1:D:342:CYS:SG	3:D:904[B]:HEM:CBC	2.46	1.03
1:B:578:CYS:SG	3:B:909:HEM:HAC	1.96	1.01
1:D:578:CYS:SG	3:D:909:HEM:HAC	1.98	1.01
1:B:305:CYS:SG	3:B:903:HEM:CBC	2.48	1.01
1:B:146:CYS:SG	3:B:902:HEM:CBC	2.48	1.00
1:A:487:CYS:SG	3:A:908:HEM:HAC	1.99	0.99
1:D:259:LYS:HE3	6:D:1403:HOH:O	1.63	0.99
1:D:305:CYS:SG	3:D:903:HEM:HAC	2.04	0.97
1:D:305:CYS:SG	3:D:903:HEM:C3C	2.59	0.96
1:C:339:CYS:SG	3:C:904[A]:HEM:HAB	1.85	0.96
1:B:562:CYS:SG	3:B:909:HEM:CBB	2.53	0.96
1:A:339:CYS:SG	3:A:904[B]:HEM:HAB	1.91	0.95
1:A:360:CYS:SG	3:A:905:HEM:HAB	2.02	0.95
1:C:487:CYS:SG	3:C:908:HEM:HAC	2.06	0.95
1:D:342:CYS:SG	3:D:904[A]:HEM:CBC	2.47	0.95
1:D:421:CYS:SG	3:D:906:HEM:CBC	2.54	0.95
1:B:302:CYS:HG	3:B:903:HEM:CAB	1.80	0.95
1:A:578:CYS:SG	3:A:909:HEM:HAC	2.04	0.95
1:D:302:CYS:HG	3:D:903:HEM:CAB	1.76	0.93
1:A:339:CYS:SG	3:A:904[A]:HEM:CBB	2.57	0.92
1:A:305:CYS:SG	3:A:903:HEM:CBC	2.58	0.92
1:C:305:CYS:SG	3:C:903:HEM:C3C	2.62	0.92
1:D:578:CYS:SG	3:D:909:HEM:CBC	2.58	0.91
1:B:487:CYS:SG	3:B:908:HEM:HAC	2.09	0.91
1:C:578:CYS:SG	3:C:909:HEM:CBC	2.58	0.91
1:A:339:CYS:SG	3:A:904[B]:HEM:CBB	2.57	0.91
1:C:146:CYS:SG	3:C:902:HEM:HAC	2.11	0.91
1:C:421:CYS:SG	3:C:906:HEM:CBC	2.59	0.90
1:C:360:CYS:SG	3:C:905:HEM:CBB	2.61	0.89
1:A:342:CYS:SG	3:A:904[B]:HEM:CBC	2.60	0.89
1:C:305:CYS:SG	3:C:903:HEM:CBC	2.59	0.89
1:C:487:CYS:SG	3:C:908:HEM:CBC	2.60	0.89
1:C:360:CYS:SG	3:C:905:HEM:HAB	2.12	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:CYS:SG	3:D:902:HEM:HAC	2.11	0.89
1:A:146:CYS:SG	3:A:902:HEM:CBC	2.62	0.88
1:D:302:CYS:SG	3:D:903:HEM:C3B	2.65	0.88
1:B:305:CYS:SG	3:B:903:HEM:C3C	2.67	0.88
1:B:487:CYS:SG	3:B:908:HEM:CBC	2.61	0.88
1:C:562:CYS:SG	3:C:909:HEM:CBB	2.62	0.87
1:B:339:CYS:SG	3:B:904[A]:HEM:CBB	2.61	0.87
1:D:146:CYS:SG	3:D:902:HEM:CBC	2.62	0.87
1:C:578:CYS:SG	3:C:909:HEM:HAC	2.14	0.87
1:B:421:CYS:SG	3:B:906:HEM:HAC	2.15	0.87
1:D:578:CYS:SG	3:D:909:HEM:C3C	2.67	0.87
1:D:305:CYS:SG	3:D:903:HEM:CBC	2.62	0.86
1:C:302:CYS:HG	3:C:903:HEM:CAB	1.88	0.85
1:B:578:CYS:HG	3:B:909:HEM:CBC	1.88	0.85
1:C:421:CYS:SG	3:C:906:HEM:HAC	2.16	0.85
1:D:465:CYS:SG	3:D:907:HEM:HAC	2.16	0.85
1:C:342:CYS:SG	3:C:904[A]:HEM:CBC	2.65	0.85
1:D:465:CYS:SG	3:D:907:HEM:C3C	2.70	0.85
1:D:421:CYS:SG	3:D:906:HEM:HAC	2.15	0.84
1:B:578:CYS:SG	3:B:909:HEM:CBC	2.65	0.84
1:A:487:CYS:SG	3:A:908:HEM:CBC	2.66	0.84
1:B:342:CYS:SG	3:B:904[B]:HEM:CBC	2.65	0.83
1:C:146:CYS:SG	3:C:902:HEM:CBC	2.66	0.83
1:A:305:CYS:SG	3:A:903:HEM:C3C	2.71	0.83
1:B:342:CYS:SG	3:B:904[B]:HEM:HAC	2.18	0.83
1:C:465:CYS:HG	3:C:907:HEM:CAC	1.88	0.83
1:D:360:CYS:SG	3:D:905:HEM:C3B	2.71	0.83
1:D:360:CYS:SG	3:D:905:HEM:CBB	2.67	0.82
1:D:465:CYS:SG	3:D:907:HEM:CBC	2.66	0.82
1:A:302:CYS:SG	3:A:903:HEM:C3B	2.71	0.82
1:B:421:CYS:SG	3:B:906:HEM:CBC	2.67	0.82
1:D:342:CYS:SG	3:D:904[B]:HEM:HAC	2.20	0.82
1:D:146:CYS:SG	3:D:902:HEM:C3C	2.72	0.82
1:A:421:CYS:HG	3:A:906:HEM:CBC	1.92	0.81
1:D:363:CYS:SG	3:D:905:HEM:C3C	2.72	0.81
1:C:302:CYS:SG	3:C:903:HEM:C3B	2.72	0.81
1:C:146:CYS:SG	3:C:902:HEM:C3C	2.72	0.81
1:A:465:CYS:SG	3:A:907:HEM:CBC	2.68	0.81
1:D:421:CYS:SG	3:D:906:HEM:C3C	2.73	0.81
1:A:578:CYS:SG	3:A:909:HEM:CBC	2.68	0.81
1:C:421:CYS:SG	3:C:906:HEM:C3C	2.73	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:CYS:HG	3:A:903:HEM:CAB	1.90	0.80
1:A:421:CYS:SG	3:A:906:HEM:C3C	2.70	0.79
1:A:146:CYS:SG	3:A:902:HEM:C3C	2.74	0.79
1:A:360:CYS:SG	3:A:905:HEM:CBB	2.69	0.79
1:C:487:CYS:SG	3:C:908:HEM:C3C	2.76	0.79
1:A:305:CYS:SG	3:A:903:HEM:HAC	2.21	0.79
1:D:487:CYS:SG	3:D:908:HEM:C3C	2.76	0.78
1:D:487:CYS:SG	3:D:908:HEM:CBC	2.72	0.78
1:B:342:CYS:SG	3:B:904[A]:HEM:HAC	2.18	0.78
1:C:342:CYS:SG	3:C:904[A]:HEM:HAC	2.23	0.78
1:A:465:CYS:SG	3:A:907:HEM:C3C	2.76	0.78
4:D:910:CU:CU	5:D:912:SO3:O3	1.32	0.78
1:D:363:CYS:SG	3:D:905:HEM:CBC	2.71	0.78
1:C:305:CYS:SG	3:C:903:HEM:HAC	2.24	0.77
1:B:421:CYS:SG	3:B:906:HEM:C3C	2.77	0.77
1:C:360:CYS:SG	3:C:905:HEM:C3B	2.71	0.77
1:B:302:CYS:SG	3:B:903:HEM:C3B	2.75	0.77
1:A:578:CYS:SG	3:A:909:HEM:C3C	2.77	0.76
1:B:578:CYS:SG	3:B:909:HEM:C3C	2.75	0.76
1:B:465:CYS:SG	3:B:907:HEM:CBC	2.73	0.76
1:C:465:CYS:SG	3:C:907:HEM:C3C	2.78	0.76
1:A:487:CYS:SG	3:A:908:HEM:C3C	2.79	0.75
1:B:146:CYS:SG	3:B:902:HEM:C3C	2.79	0.75
1:C:421:CYS:HG	3:C:906:HEM:CBC	1.93	0.75
1:C:342:CYS:SG	3:C:904[A]:HEM:C3C	2.80	0.75
1:C:339:CYS:SG	3:C:904[A]:HEM:CBB	2.54	0.75
1:A:421:CYS:SG	3:A:906:HEM:CBC	2.75	0.75
1:B:465:CYS:SG	3:B:907:HEM:C3C	2.79	0.75
1:B:487:CYS:SG	3:B:908:HEM:C3C	2.80	0.74
1:A:342:CYS:SG	3:A:904[A]:HEM:CBC	2.63	0.74
1:B:562:CYS:SG	3:B:909:HEM:C3B	2.81	0.74
1:A:342:CYS:SG	3:A:904[B]:HEM:HAC	2.23	0.74
1:A:146:CYS:SG	3:A:902:HEM:HAC	2.28	0.74
1:C:342:CYS:SG	3:C:904[B]:HEM:CBC	2.66	0.73
1:B:342:CYS:SG	3:B:904[A]:HEM:CBC	2.67	0.73
1:A:360:CYS:SG	3:A:905:HEM:C3B	2.66	0.73
1:C:465:CYS:SG	3:C:907:HEM:CBC	2.76	0.73
1:B:339:CYS:SG	3:B:904[A]:HEM:C3B	2.82	0.72
1:C:302:CYS:SG	3:C:903:HEM:CBB	2.78	0.72
1:C:578:CYS:SG	3:C:909:HEM:C3C	2.82	0.72
1:D:342:CYS:SG	3:D:904[B]:HEM:C3C	2.84	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:CYS:SG	3:A:904[B]:HEM:C3C	2.83	0.71
1:A:339:CYS:SG	3:A:904[A]:HEM:C3B	2.83	0.70
1:B:339:CYS:SG	3:B:904[B]:HEM:CBB	2.62	0.70
1:B:305:CYS:SG	3:B:903:HEM:HAC	2.27	0.70
1:B:342:CYS:SG	3:B:904[A]:HEM:C3C	2.85	0.69
1:B:146:CYS:SG	3:B:902:HEM:HAC	2.31	0.69
1:C:562:CYS:SG	3:C:909:HEM:C3B	2.84	0.68
1:B:302:CYS:SG	3:B:903:HEM:CBB	2.82	0.68
1:A:465:CYS:SG	3:A:907:HEM:HAC	2.30	0.68
1:D:302:CYS:SG	3:D:903:HEM:CBB	2.80	0.68
3:C:904[A]:HEM:HHA	3:C:904[A]:HEM:HBA2	1.74	0.68
1:B:465:CYS:SG	3:B:907:HEM:HAC	2.28	0.68
3:A:907:HEM:O2D	6:A:1332:HOH:O	2.13	0.66
1:A:302:CYS:SG	3:A:903:HEM:CBB	2.84	0.65
1:D:684:ARG:HH11	1:D:684:ARG:HG2	1.61	0.65
5:D:912:SO3:O1	6:D:1404:HOH:O	2.14	0.64
1:D:208:LYS:HG3	3:D:903:HEM:HMA2	1.81	0.61
1:D:399[A]:CYS:SG	5:D:912:SO3:O3	2.58	0.61
3:B:903:HEM:CGD	3:B:903:HEM:HMD1	2.31	0.60
3:A:903:HEM:CGD	3:A:903:HEM:HMD1	2.30	0.60
1:C:465:CYS:SG	3:C:907:HEM:HAC	2.35	0.59
3:D:903:HEM:CGD	3:D:903:HEM:HMD1	2.33	0.58
1:D:402:GLU:O	1:D:406:THR:HG23	2.04	0.58
1:C:342:CYS:SG	3:C:904[B]:HEM:C3C	2.80	0.57
1:A:252:PRO:HG2	1:A:253:GLU:OE1	2.04	0.57
1:B:342:CYS:HG	3:B:904[B]:HEM:CAC	2.16	0.57
1:B:342:CYS:HG	3:B:904[A]:HEM:CAC	2.16	0.57
1:A:687:LYS:O	1:A:690:LEU:HG	2.05	0.57
1:B:342:CYS:HG	3:B:904[A]:HEM:HAC	1.70	0.56
1:A:612:LYS:HG3	6:A:1234:HOH:O	2.05	0.56
1:A:342:CYS:SG	3:A:904[A]:HEM:C3C	2.84	0.56
1:B:342:CYS:HG	3:B:904[B]:HEM:HAC	1.70	0.56
1:D:684:ARG:HG2	1:D:684:ARG:NH1	2.21	0.55
1:D:377:ASN:HB2	6:D:1326:HOH:O	2.06	0.55
1:C:301:TYR:CD2	3:C:903:HEM:HAB	2.42	0.55
1:B:402:GLU:O	1:B:406:THR:HG23	2.07	0.55
3:C:903:HEM:CGD	3:C:903:HEM:HMD1	2.37	0.54
1:C:192:GLY:HA3	1:C:223:VAL:HB	1.89	0.54
1:C:402:GLU:O	1:C:406:THR:HG23	2.07	0.54
1:B:54:ILE:CG2	6:B:1199:HOH:O	2.55	0.54
1:C:305:CYS:CB	3:C:903:HEM:C3C	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HG3	3:A:903:HEM:HMA2	1.90	0.53
1:A:35:LYS:O	1:A:39:GLU:HG2	2.08	0.53
1:D:302:CYS:SG	3:D:903:HEM:HAB	2.41	0.53
1:B:305:CYS:CB	3:B:903:HEM:C3C	2.91	0.53
1:C:487:CYS:HG	3:C:908:HEM:HAC	1.74	0.52
1:C:465:CYS:HG	3:C:907:HEM:CBC	2.20	0.52
5:B:911:SO3:O3	6:B:1351:HOH:O	2.19	0.52
1:A:402:GLU:O	1:A:406:THR:HG23	2.10	0.52
1:D:305:CYS:CB	3:D:903:HEM:C3C	2.93	0.51
1:C:374:MET:CE	1:C:384:PRO:HA	2.40	0.51
1:C:626:LEU:HD13	1:C:686:MET:HG2	1.92	0.51
1:B:302:CYS:SG	3:B:903:HEM:HAB	2.42	0.51
1:A:690:LEU:HD12	1:A:690:LEU:C	2.32	0.51
1:C:146:CYS:CB	3:C:902:HEM:C3C	2.94	0.50
3:C:903:HEM:HMB2	3:C:903:HEM:HBB2	1.94	0.49
3:D:904[A]:HEM:CMC	3:D:904[A]:HEM:HBC2	2.43	0.49
1:B:342:CYS:SG	3:B:904[B]:HEM:C3C	2.87	0.48
1:D:146:CYS:CB	3:D:902:HEM:C3C	2.95	0.48
1:B:165:PHE:CZ	1:B:335:LYS:HD3	2.48	0.48
1:A:146:CYS:CB	3:A:902:HEM:C3C	2.96	0.48
1:A:612:LYS:CG	6:A:1234:HOH:O	2.61	0.48
1:D:123:TYR:CE1	3:D:903:HEM:HBC2	2.49	0.48
1:B:374:MET:CE	1:B:384:PRO:HA	2.44	0.48
3:D:904[B]:HEM:CMC	3:D:904[B]:HEM:HBC2	2.44	0.47
1:B:94:GLY:O	1:B:98:ILE:HB	2.14	0.47
1:B:562:CYS:CB	3:B:909:HEM:CAB	2.90	0.47
1:B:305:CYS:HB2	3:B:903:HEM:C3C	2.50	0.47
1:D:94:GLY:O	1:D:98:ILE:HB	2.14	0.47
1:A:94:GLY:O	1:A:98:ILE:HB	2.14	0.47
1:D:342:CYS:SG	3:D:904[A]:HEM:C3C	2.84	0.47
1:D:620:ILE:HG23	1:D:644:ILE:HG23	1.96	0.46
1:A:342:CYS:SG	3:A:904[A]:HEM:HAC	2.28	0.46
1:B:146:CYS:CB	3:B:902:HEM:C3C	2.98	0.46
1:C:372:ASP:OD1	1:C:375:ARG:NH2	2.45	0.46
1:B:305:CYS:C	1:B:307:PRO:HD3	2.36	0.46
1:B:208:LYS:HG3	3:B:903:HEM:HMA2	1.98	0.45
1:A:253:GLU:CD	1:A:253:GLU:H	2.20	0.45
1:D:639:ARG:NH1	1:D:642:GLU:OE1	2.45	0.45
1:A:421:CYS:CB	3:A:906:HEM:C3C	3.00	0.45
1:C:434:GLU:HG2	1:C:452:LEU:HG	1.98	0.45
1:C:208:LYS:HG3	3:C:903:HEM:HMA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLY:HA3	1:A:223:VAL:HB	1.98	0.45
1:A:305:CYS:C	1:A:307:PRO:HD3	2.38	0.44
1:A:350:GLU:HG3	1:C:128:ASN:CG	2.37	0.44
1:D:305:CYS:HB2	3:D:903:HEM:C3C	2.52	0.44
1:D:343:HIS:CE1	3:D:904[A]:HEM:ND	2.86	0.44
1:C:487:CYS:HG	3:C:908:HEM:CAC	2.18	0.44
1:B:112:ARG:HB2	1:C:151:TYR:CE1	2.53	0.44
1:A:374:MET:CE	1:A:384:PRO:HA	2.49	0.43
1:D:656:LYS:HA	1:D:656:LYS:HD2	1.86	0.43
1:C:203:GLY:HA3	3:C:903:HEM:HMA1	2.01	0.43
1:A:259:LYS:HA	1:A:262:VAL:O	2.19	0.42
3:C:904[A]:HEM:HBC1	3:C:905:HEM:CHC	2.50	0.42
1:D:399[B]:CYS:SG	1:D:513:ARG:HG3	2.59	0.42
1:A:629:VAL:C	1:A:630:LYS:O	2.57	0.42
1:D:259:LYS:CE	6:D:1403:HOH:O	2.43	0.42
1:D:186:ALA:HB1	1:D:282:LEU:HG	2.01	0.42
5:C:911:SO3:O3	6:C:1308:HOH:O	2.22	0.42
1:D:305:CYS:C	1:D:307:PRO:HD3	2.40	0.42
3:C:904[B]:HEM:HBC1	3:C:905:HEM:CHC	2.50	0.42
1:C:593:LYS:NZ	6:C:1287:HOH:O	2.26	0.42
1:D:301:TYR:CE2	3:D:903:HEM:HHC	2.55	0.42
1:D:363:CYS:CB	3:D:905:HEM:C3C	3.03	0.42
1:A:305:CYS:CB	3:A:903:HEM:C3C	3.02	0.42
1:B:687:LYS:HE3	1:B:687:LYS:HB2	1.88	0.42
1:B:190:PRO:HB2	1:B:222:HIS:HB3	2.02	0.42
5:A:912:SO3:O1	6:A:1327:HOH:O	2.21	0.41
1:D:108:LYS:NZ	1:D:116:GLU:OE1	2.46	0.41
1:C:305:CYS:C	1:C:307:PRO:HD3	2.40	0.41
1:B:263:PRO:HD2	6:B:1318:HOH:O	2.21	0.41
1:B:51:ARG:NH2	1:C:135:ASN:OD1	2.53	0.41
1:B:562:CYS:HB3	3:B:909:HEM:C3B	2.55	0.41
1:D:208:LYS:HE3	3:D:903:HEM:C3A	2.55	0.41
1:B:54:ILE:CG2	1:B:54:ILE:O	2.69	0.41
1:D:673:ASP:HA	1:D:676:VAL:HG22	2.03	0.41
1:A:395:MET:HG2	1:A:544:TRP:CE2	2.55	0.41
1:A:399[B]:CYS:SG	1:A:495[B]:CYS:N	2.93	0.41
1:D:372:ASP:OD1	1:D:375:ARG:NH1	2.54	0.41
1:D:192:GLY:HA3	1:D:223:VAL:HB	2.02	0.41
1:A:406:THR:O	1:A:412:TYR:HB2	2.20	0.40
1:C:305:CYS:HB2	3:C:903:HEM:C3C	2.56	0.40
1:A:630:LYS:O	1:A:631:LYS:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:CYS:CB	3:D:906:HEM:C3C	3.04	0.40
1:C:399[B]:CYS:SG	1:C:513:ARG:HG3	2.61	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	661/732 (90%)	631 (96%)	28 (4%)	2 (0%)	46	45
1	B	661/732 (90%)	635 (96%)	26 (4%)	0	100	100
1	C	660/732 (90%)	629 (95%)	30 (4%)	1 (0%)	52	53
1	D	660/732 (90%)	633 (96%)	25 (4%)	2 (0%)	46	45
All	All	2642/2928 (90%)	2528 (96%)	109 (4%)	5 (0%)	52	53

All (5) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

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

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

Mol	Chain	Res	Type
1	A	124	ARG
1	A	275	ASN
1	A	302	CYS
1	A	307	PRO
1	A	529	LEU
1	A	564	ARG
1	A	656	LYS
1	B	54	ILE
1	B	100	GLU
1	B	124	ARG
1	B	275	ASN
1	B	302	CYS
1	B	379	LEU
1	B	441	SER
1	B	498	PHE
1	B	564	ARG
1	B	631	LYS
1	C	124	ARG
1	C	275	ASN
1	C	302	CYS
1	C	326	LYS
1	C	529	LEU
1	C	564	ARG
1	D	124	ARG
1	D	250	LEU
1	D	275	ASN
1	D	302	CYS
1	D	564	ARG
1	D	656	LYS

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

sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 4 are monoatomic - leaving 46 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DTN	A	901	-	0,5,5	0.00	-	0,6,6	0.00	-
3	HEM	A	902	1	30,50,50	2.43	7 (23%)	24,82,82	2.54	10 (41%)
3	HEM	A	903	1,5	30,50,50	2.16	5 (16%)	24,82,82	2.62	12 (50%)
3	HEM	A	904[A]	1	30,50,50	2.10	5 (16%)	24,82,82	2.78	11 (45%)
3	HEM	A	904[B]	1	30,50,50	2.12	6 (20%)	24,82,82	2.92	13 (54%)
3	HEM	A	905	1	30,50,50	2.03	6 (20%)	24,82,82	2.30	8 (33%)
3	HEM	A	906	1	30,50,50	2.12	6 (20%)	24,82,82	2.29	8 (33%)
3	HEM	A	907	1	30,50,50	2.26	7 (23%)	24,82,82	2.74	12 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	908	1	30,50,50	2.55	8 (26%)	24,82,82	2.38	8 (33%)
3	HEM	A	909	1	30,50,50	2.54	6 (20%)	24,82,82	2.53	12 (50%)
2	DTN	A	911	-	0,5,5	0.00	-	0,6,6	0.00	-
5	SO3	A	912	3,4	1,3,3	7.68	1 (100%)	0,3,3	0.00	-
2	DTN	B	901	-	0,5,5	0.00	-	0,6,6	0.00	-
3	HEM	B	902	1	30,50,50	2.30	7 (23%)	24,82,82	2.84	9 (37%)
3	HEM	B	903	1,5	30,50,50	1.92	6 (20%)	24,82,82	2.80	12 (50%)
3	HEM	B	904[A]	1	30,50,50	2.13	8 (26%)	24,82,82	2.99	12 (50%)
3	HEM	B	904[B]	1	30,50,50	2.17	8 (26%)	24,82,82	2.96	12 (50%)
3	HEM	B	905	1	30,50,50	2.07	9 (30%)	24,82,82	2.50	7 (29%)
3	HEM	B	906	1	30,50,50	2.32	6 (20%)	24,82,82	2.60	12 (50%)
3	HEM	B	907	1	30,50,50	2.48	6 (20%)	24,82,82	2.59	10 (41%)
3	HEM	B	908	1	30,50,50	1.93	6 (20%)	24,82,82	2.53	7 (29%)
3	HEM	B	909	1	30,50,50	2.58	7 (23%)	24,82,82	2.75	12 (50%)
5	SO3	B	911	3,4	1,3,3	5.11	1 (100%)	0,3,3	0.00	-
2	DTN	C	901	-	0,5,5	0.00	-	0,6,6	0.00	-
3	HEM	C	902	1	30,50,50	2.15	6 (20%)	24,82,82	2.63	11 (45%)
3	HEM	C	903	1,5	30,50,50	1.83	4 (13%)	24,82,82	2.45	7 (29%)
3	HEM	C	904[A]	1	30,50,50	2.20	7 (23%)	24,82,82	2.74	11 (45%)
3	HEM	C	904[B]	1	30,50,50	2.17	7 (23%)	24,82,82	2.59	10 (41%)
3	HEM	C	905	1	30,50,50	2.13	6 (20%)	24,82,82	2.40	7 (29%)
3	HEM	C	906	1	30,50,50	2.43	9 (30%)	24,82,82	2.52	9 (37%)
3	HEM	C	907	1	30,50,50	2.58	8 (26%)	24,82,82	2.74	12 (50%)
3	HEM	C	908	1	30,50,50	2.33	8 (26%)	24,82,82	2.42	11 (45%)
3	HEM	C	909	1	30,50,50	2.36	7 (23%)	24,82,82	2.53	9 (37%)
5	SO3	C	911	3	1,3,3	5.84	1 (100%)	0,3,3	0.00	-
2	DTN	D	901	-	0,5,5	0.00	-	0,6,6	0.00	-
3	HEM	D	902	1	30,50,50	2.06	8 (26%)	24,82,82	2.80	13 (54%)
3	HEM	D	903	1,5	30,50,50	2.10	4 (13%)	24,82,82	2.47	5 (20%)
3	HEM	D	904[A]	1	30,50,50	2.27	7 (23%)	24,82,82	2.76	12 (50%)
3	HEM	D	904[B]	1	30,50,50	2.31	7 (23%)	24,82,82	2.81	13 (54%)
3	HEM	D	905	1	30,50,50	2.25	6 (20%)	24,82,82	2.25	6 (25%)
3	HEM	D	906	1	30,50,50	2.44	6 (20%)	24,82,82	2.73	13 (54%)
3	HEM	D	907	1	30,50,50	2.42	7 (23%)	24,82,82	2.88	13 (54%)
3	HEM	D	908	1	30,50,50	2.11	7 (23%)	24,82,82	2.61	10 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	D	909	1	30,50,50	2.70	8 (26%)	24,82,82	2.97	14 (58%)
5	SO3	D	911	-	1,3,3	8.91	1 (100%)	0,3,3	0.00	-
5	SO3	D	912	3	1,3,3	6.47	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

All (246) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	907	HEM	C3B-C4B	-8.19	1.44	1.51
3	D	909	HEM	C3B-C4B	-8.02	1.44	1.51
3	A	908	HEM	C3B-C4B	-7.98	1.44	1.51
3	A	903	HEM	C2C-C1C	-7.74	1.37	1.52
3	B	909	HEM	C3B-C4B	-7.67	1.45	1.51
3	D	905	HEM	C2D-C3D	-7.40	1.32	1.54
3	B	906	HEM	C2D-C3D	-7.28	1.32	1.54
3	A	909	HEM	C3B-C4B	-7.27	1.45	1.51
3	B	907	HEM	C2D-C3D	-7.26	1.32	1.54
3	D	906	HEM	C2D-C3D	-7.24	1.32	1.54
3	A	902	HEM	C3B-C4B	-7.15	1.45	1.51
3	B	902	HEM	C2D-C3D	-7.14	1.33	1.54
3	B	907	HEM	C3B-C4B	-7.11	1.45	1.51
3	D	903	HEM	C2D-C3D	-7.11	1.33	1.54
3	A	909	HEM	C2D-C3D	-7.05	1.33	1.54
3	B	905	HEM	C2D-C3D	-6.98	1.33	1.54
3	A	907	HEM	C2D-C3D	-6.82	1.34	1.54
3	C	906	HEM	C2D-C3D	-6.79	1.34	1.54
3	A	908	HEM	C2D-C3D	-6.79	1.34	1.54
3	B	903	HEM	C2D-C3D	-6.75	1.34	1.54
3	A	904[B]	HEM	C2D-C3D	-6.69	1.34	1.54
3	A	905	HEM	C2D-C3D	-6.68	1.34	1.54
3	A	904[A]	HEM	C2D-C3D	-6.67	1.34	1.54
3	A	906	HEM	C2D-C3D	-6.64	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	909	HEM	C2D-C3D	-6.62	1.34	1.54
3	C	905	HEM	C2D-C3D	-6.61	1.34	1.54
3	D	909	HEM	C2D-C3D	-6.59	1.34	1.54
3	D	904[B]	HEM	C2D-C3D	-6.57	1.34	1.54
3	A	903	HEM	C2D-C3D	-6.55	1.34	1.54
3	C	909	HEM	C2D-C3D	-6.54	1.34	1.54
3	D	905	HEM	C2C-C1C	-6.53	1.40	1.52
3	D	904[A]	HEM	C2D-C3D	-6.45	1.35	1.54
3	A	902	HEM	C2D-C3D	-6.42	1.35	1.54
3	C	904[A]	HEM	C2D-C3D	-6.41	1.35	1.54
3	C	907	HEM	C2D-C3D	-6.37	1.35	1.54
3	C	904[B]	HEM	C2D-C3D	-6.36	1.35	1.54
3	A	909	HEM	C2C-C1C	-6.27	1.40	1.52
3	C	902	HEM	C2D-C3D	-6.27	1.35	1.54
3	B	908	HEM	C2D-C3D	-6.26	1.35	1.54
3	D	907	HEM	C2D-C3D	-6.24	1.35	1.54
3	D	908	HEM	C2C-C1C	-6.19	1.40	1.52
3	B	904[A]	HEM	C2D-C3D	-6.12	1.36	1.54
3	B	904[B]	HEM	C2D-C3D	-6.10	1.36	1.54
3	A	907	HEM	C3B-C4B	-6.10	1.46	1.51
3	A	904[A]	HEM	C2C-C1C	-6.09	1.41	1.52
3	C	909	HEM	C2C-C1C	-6.08	1.41	1.52
3	C	908	HEM	C3B-C4B	-6.06	1.46	1.51
3	C	903	HEM	C2D-C3D	-6.05	1.36	1.54
3	B	904[A]	HEM	C2C-C1C	-6.01	1.41	1.52
3	B	904[B]	HEM	C2C-C1C	-6.01	1.41	1.52
3	A	904[B]	HEM	C2C-C1C	-6.00	1.41	1.52
3	C	904[B]	HEM	C2C-C1C	-5.99	1.41	1.52
3	C	905	HEM	C2C-C1C	-5.99	1.41	1.52
3	B	902	HEM	C3B-C4B	-5.98	1.46	1.51
3	B	907	HEM	C2C-C1C	-5.98	1.41	1.52
3	D	906	HEM	C3B-C4B	-5.97	1.46	1.51
3	C	904[A]	HEM	C2C-C1C	-5.95	1.41	1.52
3	C	902	HEM	C2C-C1C	-5.91	1.41	1.52
3	D	902	HEM	C2D-C3D	-5.90	1.36	1.54
3	A	902	HEM	C2C-C1C	-5.84	1.41	1.52
3	D	908	HEM	C2D-C3D	-5.83	1.37	1.54
3	C	906	HEM	C3B-C4B	-5.82	1.46	1.51
3	D	907	HEM	C2C-C1C	-5.77	1.41	1.52
3	C	908	HEM	C2D-C3D	-5.59	1.37	1.54
3	D	906	HEM	C2C-C1C	-5.55	1.42	1.52
3	B	906	HEM	C3B-C4B	-5.54	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	HEM	C2C-C1C	-5.53	1.42	1.52
3	C	903	HEM	C2C-C1C	-5.47	1.42	1.52
3	B	906	HEM	C2C-C1C	-5.46	1.42	1.52
3	A	906	HEM	C2C-C1C	-5.44	1.42	1.52
3	D	904[A]	HEM	C2C-C1C	-5.40	1.42	1.52
3	D	909	HEM	C2C-C1C	-5.40	1.42	1.52
3	D	902	HEM	C2C-C1C	-5.37	1.42	1.52
3	D	904[B]	HEM	C2C-C1C	-5.30	1.42	1.52
3	C	906	HEM	C2C-C1C	-5.24	1.42	1.52
3	A	908	HEM	C2C-C1C	-5.15	1.42	1.52
3	D	904[B]	HEM	C3B-C4B	-5.07	1.47	1.51
3	B	908	HEM	C2C-C1C	-5.05	1.43	1.52
3	C	904[A]	HEM	C3B-C4B	-5.03	1.47	1.51
3	C	908	HEM	C2C-C1C	-5.02	1.43	1.52
3	B	909	HEM	C3D-C4D	-4.98	1.45	1.51
3	D	907	HEM	C3B-C4B	-4.97	1.47	1.51
3	D	906	HEM	C3D-C4D	-4.95	1.45	1.51
3	C	904[B]	HEM	C3B-C4B	-4.92	1.47	1.51
3	B	903	HEM	C2C-C1C	-4.91	1.43	1.52
3	C	907	HEM	C2C-C1C	-4.90	1.43	1.52
3	C	909	HEM	C3B-C4B	-4.85	1.47	1.51
3	D	907	HEM	C3D-C4D	-4.83	1.45	1.51
3	D	903	HEM	C2C-C1C	-4.77	1.43	1.52
3	D	904[A]	HEM	C3B-C4B	-4.76	1.47	1.51
3	A	907	HEM	C2C-C1C	-4.73	1.43	1.52
3	D	904[B]	HEM	C3D-C4D	-4.73	1.45	1.51
3	B	909	HEM	C2C-C1C	-4.71	1.43	1.52
3	C	907	HEM	C3D-C4D	-4.66	1.45	1.51
3	A	905	HEM	C2C-C1C	-4.62	1.43	1.52
3	B	904[B]	HEM	C3B-C4B	-4.54	1.47	1.51
3	C	909	HEM	C3D-C4D	-4.24	1.46	1.51
3	D	909	HEM	C2B-C1B	-4.20	1.38	1.51
3	C	902	HEM	C3D-C4D	-4.19	1.46	1.51
3	C	906	HEM	C3D-C4D	-4.11	1.46	1.51
3	D	904[A]	HEM	C3D-C4D	-4.07	1.46	1.51
3	B	904[A]	HEM	C3B-C4B	-4.00	1.48	1.51
3	D	908	HEM	C3B-C4B	-3.94	1.48	1.51
3	A	904[B]	HEM	C3B-C4B	-3.86	1.48	1.51
3	B	905	HEM	C2C-C1C	-3.85	1.45	1.52
3	D	905	HEM	C3B-C4B	-3.84	1.48	1.51
3	D	909	HEM	C3D-C4D	-3.68	1.46	1.51
3	C	908	HEM	C3D-C4D	-3.63	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	909	HEM	C3D-C4D	-3.61	1.46	1.51
3	A	909	HEM	C2B-C1B	-3.60	1.40	1.51
3	A	902	HEM	C2B-C1B	-3.52	1.40	1.51
3	B	909	HEM	C2B-C1B	-3.45	1.40	1.51
3	A	904[A]	HEM	C3B-C4B	-3.41	1.48	1.51
3	D	902	HEM	C3B-CAB	-3.38	1.45	1.51
3	A	908	HEM	C3D-C4D	-3.35	1.47	1.51
3	B	906	HEM	C2B-C1B	-3.16	1.41	1.51
3	B	904[B]	HEM	C3D-C4D	-3.15	1.47	1.51
3	B	908	HEM	C3B-C4B	-3.14	1.49	1.51
3	D	902	HEM	C3D-C4D	-3.05	1.47	1.51
3	B	904[A]	HEM	C3D-C4D	-2.94	1.47	1.51
3	D	907	HEM	C3B-CAB	-2.88	1.45	1.51
3	A	908	HEM	C2B-C1B	-2.87	1.42	1.51
3	A	906	HEM	C3B-C4B	-2.86	1.49	1.51
3	B	907	HEM	C3D-C4D	-2.84	1.47	1.51
3	C	908	HEM	C3B-CAB	-2.83	1.46	1.51
3	B	906	HEM	C3D-C4D	-2.83	1.47	1.51
3	D	906	HEM	C2B-C1B	-2.83	1.42	1.51
3	C	904[A]	HEM	C3D-C4D	-2.83	1.48	1.51
3	D	908	HEM	C3D-C4D	-2.80	1.48	1.51
3	A	905	HEM	C2B-C1B	-2.79	1.42	1.51
3	B	907	HEM	C2B-C1B	-2.78	1.42	1.51
3	C	908	HEM	C2B-C1B	-2.76	1.42	1.51
3	C	909	HEM	C2B-C1B	-2.75	1.42	1.51
3	C	903	HEM	C2B-C1B	-2.73	1.42	1.51
3	C	907	HEM	C3B-CAB	-2.67	1.46	1.51
3	B	904[A]	HEM	C2B-C1B	-2.66	1.43	1.51
3	C	904[B]	HEM	C3B-CAB	-2.62	1.46	1.51
3	C	904[B]	HEM	C3D-C4D	-2.62	1.48	1.51
3	C	904[A]	HEM	C3B-CAB	-2.61	1.46	1.51
3	B	903	HEM	C2B-C1B	-2.61	1.43	1.51
3	D	904[A]	HEM	C3B-CAB	-2.59	1.46	1.51
3	C	902	HEM	C3B-CAB	-2.59	1.46	1.51
3	C	905	HEM	C3D-C4D	-2.57	1.48	1.51
3	C	906	HEM	C3B-CAB	-2.54	1.46	1.51
3	D	904[B]	HEM	C3B-CAB	-2.54	1.46	1.51
3	A	907	HEM	C3B-CAB	-2.54	1.46	1.51
3	C	904[B]	HEM	C2B-C1B	-2.53	1.43	1.51
3	B	902	HEM	C2B-C1B	-2.52	1.43	1.51
3	C	908	HEM	C2D-C1D	-2.51	1.43	1.51
3	A	906	HEM	C2B-C1B	-2.48	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	HEM	C2B-C1B	-2.47	1.43	1.51
3	D	909	HEM	C3C-CAC	-2.47	1.46	1.51
3	D	908	HEM	C3B-CAB	-2.46	1.46	1.51
3	D	904[A]	HEM	C2B-C1B	-2.45	1.43	1.51
3	C	909	HEM	C3C-CAC	-2.43	1.46	1.51
3	C	904[A]	HEM	C2B-C1B	-2.43	1.43	1.51
3	B	905	HEM	C3C-CAC	-2.41	1.46	1.51
3	A	907	HEM	C2B-C1B	-2.41	1.44	1.51
3	D	903	HEM	C2B-C1B	-2.40	1.44	1.51
3	A	903	HEM	C2B-C1B	-2.39	1.44	1.51
3	C	907	HEM	C2B-C1B	-2.39	1.44	1.51
3	A	904[A]	HEM	C2B-C1B	-2.38	1.44	1.51
3	B	905	HEM	C3B-C4B	-2.37	1.49	1.51
3	B	904[B]	HEM	C2B-C1B	-2.35	1.44	1.51
3	B	905	HEM	C3D-C4D	-2.34	1.48	1.51
3	B	903	HEM	C3C-CAC	-2.27	1.47	1.51
3	A	904[B]	HEM	C3D-C4D	-2.26	1.48	1.51
3	B	904[A]	HEM	C3B-CAB	-2.26	1.47	1.51
3	D	907	HEM	C2B-C1B	-2.24	1.44	1.51
3	C	902	HEM	C2B-C1B	-2.24	1.44	1.51
3	A	905	HEM	C3B-C4B	-2.23	1.49	1.51
3	C	906	HEM	C2B-C1B	-2.22	1.44	1.51
3	B	905	HEM	C2B-C1B	-2.21	1.44	1.51
3	B	908	HEM	C2D-C1D	-2.18	1.44	1.51
3	D	904[B]	HEM	C2B-C1B	-2.16	1.44	1.51
3	B	908	HEM	C2B-C1B	-2.14	1.44	1.51
3	B	902	HEM	C3D-C4D	-2.14	1.48	1.51
3	A	908	HEM	CMB-C2B	-2.13	1.48	1.53
3	A	904[B]	HEM	C2B-C1B	-2.13	1.44	1.51
3	A	903	HEM	CAD-C3D	-2.12	1.49	1.54
3	D	908	HEM	C2B-C1B	-2.11	1.45	1.51
3	B	904[B]	HEM	C3B-CAB	-2.10	1.47	1.51
3	C	905	HEM	C3B-CAB	-2.09	1.47	1.51
3	D	902	HEM	C3C-CAC	-2.03	1.47	1.51
3	D	902	HEM	C3B-C4B	-2.03	1.50	1.51
3	B	902	HEM	C3C-CAC	-2.03	1.47	1.51
3	A	902	HEM	C3C-CAC	-2.02	1.47	1.51
3	B	909	HEM	C3B-CAB	-2.00	1.47	1.51
3	B	903	HEM	C4C-NC	2.01	1.38	1.36
3	B	905	HEM	FE-NB	2.02	2.08	1.97
3	A	908	HEM	CHC-C1C	2.04	1.41	1.36
3	C	906	HEM	CHD-C4C	2.06	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	905	HEM	FE-NC	2.06	2.03	1.95
3	B	904[A]	HEM	FE-NB	2.09	2.08	1.97
3	B	904[B]	HEM	FE-NB	2.15	2.08	1.97
3	A	907	HEM	CHD-C4C	2.17	1.41	1.36
3	B	904[A]	HEM	FE-NC	2.17	2.04	1.95
3	A	903	HEM	FE-NC	2.17	2.04	1.95
3	C	907	HEM	C1C-NC	2.18	1.38	1.36
3	D	909	HEM	CBB-CAB	2.19	1.42	1.29
3	C	906	HEM	CAA-C2A	2.25	1.55	1.52
3	A	906	HEM	CHC-C1C	2.27	1.41	1.36
3	D	905	HEM	C1C-NC	2.34	1.38	1.36
3	A	902	HEM	FE-NB	2.34	2.09	1.97
3	C	904[B]	HEM	FE-NC	2.36	2.05	1.95
3	C	904[A]	HEM	FE-NC	2.37	2.05	1.95
3	D	905	HEM	C4C-NC	2.38	1.38	1.36
3	A	907	HEM	FE-NC	2.46	2.05	1.95
3	D	906	HEM	FE-NC	2.48	2.05	1.95
3	B	904[B]	HEM	FE-NC	2.51	2.05	1.95
3	A	904[A]	HEM	FE-NC	2.56	2.05	1.95
3	B	908	HEM	FE-NC	2.58	2.06	1.95
3	C	908	HEM	FE-NC	2.59	2.06	1.95
3	A	902	HEM	FE-NC	2.64	2.06	1.95
3	C	902	HEM	FE-NC	2.68	2.06	1.95
3	D	904[A]	HEM	FE-NC	2.72	2.06	1.95
3	C	909	HEM	FE-NC	2.75	2.06	1.95
3	A	904[B]	HEM	FE-NC	2.76	2.06	1.95
3	C	903	HEM	FE-NC	2.77	2.06	1.95
3	B	907	HEM	FE-NC	2.79	2.06	1.95
3	B	905	HEM	C1C-NC	2.80	1.39	1.36
3	C	905	HEM	FE-NB	2.83	2.12	1.97
3	B	902	HEM	FE-NC	2.85	2.07	1.95
3	A	905	HEM	C4C-NC	2.86	1.39	1.36
3	D	904[B]	HEM	FE-NC	2.86	2.07	1.95
3	A	908	HEM	FE-NC	2.90	2.07	1.95
3	B	903	HEM	FE-NC	2.92	2.07	1.95
3	D	902	HEM	FE-NC	2.93	2.07	1.95
3	B	906	HEM	FE-NC	2.94	2.07	1.95
3	A	909	HEM	FE-NC	3.05	2.07	1.95
3	C	907	HEM	FE-NC	3.06	2.07	1.95
3	A	905	HEM	FE-NB	3.07	2.13	1.97
3	C	905	HEM	FE-NC	3.21	2.08	1.95
3	B	909	HEM	FE-NC	3.25	2.08	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	908	HEM	FE-NC	3.29	2.08	1.95
3	A	906	HEM	FE-NC	3.39	2.09	1.95
3	D	909	HEM	FE-NC	3.50	2.09	1.95
3	D	907	HEM	FE-NC	3.52	2.09	1.95
3	B	905	HEM	FE-NC	3.62	2.10	1.95
3	C	906	HEM	FE-NC	3.66	2.10	1.95
3	D	903	HEM	FE-NC	3.75	2.10	1.95
5	B	911	SO3	O1-S	5.11	1.66	1.44
5	C	911	SO3	O1-S	5.84	1.69	1.44
5	D	912	SO3	O1-S	6.47	1.72	1.44
5	A	912	SO3	O1-S	7.68	1.77	1.44
5	D	911	SO3	O1-S	8.91	1.83	1.44

All (373) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	HEM	C3B-CAB-CBB	-7.24	113.34	124.46
3	D	909	HEM	CAA-CBA-CGA	-6.92	100.06	112.75
3	B	904[A]	HEM	C3B-CAB-CBB	-6.86	113.93	124.46
3	B	908	HEM	C3B-CAB-CBB	-6.68	114.21	124.46
3	B	904[B]	HEM	C3B-CAB-CBB	-6.57	114.39	124.46
3	D	908	HEM	C3B-CAB-CBB	-5.93	115.36	124.46
3	C	906	HEM	C3B-CAB-CBB	-5.83	115.51	124.46
3	D	906	HEM	C3B-CAB-CBB	-5.72	115.68	124.46
3	A	904[A]	HEM	C3B-CAB-CBB	-5.21	116.47	124.46
3	C	907	HEM	C3B-CAB-CBB	-4.82	117.06	124.46
3	C	908	HEM	C3B-CAB-CBB	-4.79	117.11	124.46
3	A	904[B]	HEM	C3B-CAB-CBB	-4.70	117.25	124.46
3	B	907	HEM	C3B-CAB-CBB	-4.68	117.28	124.46
3	A	907	HEM	C3B-CAB-CBB	-4.67	117.30	124.46
3	A	908	HEM	C3B-CAB-CBB	-4.59	117.42	124.46
3	B	909	HEM	CAA-CBA-CGA	-4.54	104.42	112.75
3	B	904[A]	HEM	CAA-C2A-C1A	-4.48	122.14	127.01
3	A	902	HEM	C3B-CAB-CBB	-4.47	117.59	124.46
3	D	907	HEM	CMA-C3A-C4A	-4.47	120.97	128.36
3	B	906	HEM	C3B-CAB-CBB	-4.42	117.68	124.46
3	B	903	HEM	CMA-C3A-C4A	-4.26	121.32	128.36
3	D	904[A]	HEM	C3B-CAB-CBB	-4.25	117.94	124.46
3	B	909	HEM	C3B-CAB-CBB	-4.11	118.16	124.46
3	C	902	HEM	C3B-CAB-CBB	-4.10	118.17	124.46
3	C	909	HEM	C3B-CAB-CBB	-4.02	118.29	124.46
3	B	909	HEM	CMA-C3A-C4A	-4.01	121.72	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	907	HEM	C1D-CHD-C4C	-3.98	119.17	125.82
3	D	904[B]	HEM	C3B-CAB-CBB	-3.97	118.36	124.46
3	B	904[B]	HEM	CMA-C3A-C4A	-3.97	121.79	128.36
3	D	909	HEM	C3B-CAB-CBB	-3.92	118.45	124.46
3	D	907	HEM	C1D-CHD-C4C	-3.88	119.34	125.82
3	C	904[B]	HEM	C3B-CAB-CBB	-3.87	118.53	124.46
3	D	907	HEM	CBA-CAA-C2A	-3.82	105.68	112.53
3	D	904[B]	HEM	CMA-C3A-C4A	-3.81	122.06	128.36
3	D	904[A]	HEM	C3C-CAC-CBC	-3.76	118.69	124.46
3	D	904[B]	HEM	C3C-CAC-CBC	-3.75	118.70	124.46
3	C	904[A]	HEM	CMA-C3A-C4A	-3.74	122.18	128.36
3	C	904[A]	HEM	C3B-CAB-CBB	-3.73	118.73	124.46
3	A	903	HEM	CMA-C3A-C4A	-3.69	122.26	128.36
3	C	902	HEM	CMA-C3A-C4A	-3.68	122.28	128.36
3	A	904[B]	HEM	CMA-C3A-C4A	-3.67	122.30	128.36
3	D	906	HEM	CMA-C3A-C4A	-3.56	122.47	128.36
3	C	909	HEM	C1D-CHD-C4C	-3.44	120.07	125.82
3	D	902	HEM	CMA-C3A-C4A	-3.36	122.80	128.36
3	A	906	HEM	C3B-CAB-CBB	-3.36	119.30	124.46
3	B	905	HEM	CAA-C2A-C1A	-3.28	123.45	127.01
3	D	902	HEM	C3B-CAB-CBB	-3.27	119.44	124.46
3	A	909	HEM	C3B-CAB-CBB	-3.26	119.45	124.46
3	D	904[A]	HEM	C1D-CHD-C4C	-3.24	120.40	125.82
3	C	904[A]	HEM	C1D-CHD-C4C	-3.24	120.40	125.82
3	D	907	HEM	C3B-CAB-CBB	-3.24	119.49	124.46
3	A	904[A]	HEM	C3C-CAC-CBC	-3.20	119.55	124.46
3	B	904[A]	HEM	CBA-CAA-C2A	-3.19	106.81	112.53
3	D	904[B]	HEM	C1D-CHD-C4C	-3.17	120.52	125.82
3	C	904[B]	HEM	C1D-CHD-C4C	-3.16	120.53	125.82
3	A	909	HEM	C3C-CAC-CBC	-3.15	119.62	124.46
3	C	907	HEM	CMA-C3A-C4A	-3.13	123.19	128.36
3	A	904[B]	HEM	C3C-CAC-CBC	-3.11	119.69	124.46
3	C	905	HEM	CMA-C3A-C4A	-2.96	123.47	128.36
3	A	902	HEM	C3B-C4B-NB	-2.90	106.08	111.63
3	D	909	HEM	C1D-CHD-C4C	-2.89	120.99	125.82
3	D	909	HEM	CAA-C2A-C1A	-2.87	123.89	127.01
3	D	904[A]	HEM	CBA-CAA-C2A	-2.87	107.39	112.53
3	A	907	HEM	CBA-CAA-C2A	-2.85	107.42	112.53
3	B	902	HEM	C1D-CHD-C4C	-2.80	121.14	125.82
3	C	902	HEM	C1D-CHD-C4C	-2.79	121.16	125.82
3	B	902	HEM	CMA-C3A-C4A	-2.72	123.86	128.36
3	A	903	HEM	C4B-CHC-C1C	-2.71	121.30	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904[A]	HEM	C1D-CHD-C4C	-2.65	121.39	125.82
3	B	907	HEM	C3B-C4B-NB	-2.65	106.57	111.63
3	D	909	HEM	CMA-C3A-C4A	-2.64	123.99	128.36
3	B	906	HEM	C3B-C4B-NB	-2.63	106.60	111.63
3	C	906	HEM	CAA-CBA-CGA	-2.62	107.94	112.75
3	D	909	HEM	C3B-C4B-NB	-2.62	106.62	111.63
3	A	904[B]	HEM	C1D-CHD-C4C	-2.61	121.46	125.82
3	A	909	HEM	C1D-CHD-C4C	-2.58	121.50	125.82
3	C	907	HEM	C1D-CHD-C4C	-2.50	121.65	125.82
3	A	904[A]	HEM	CBA-CAA-C2A	-2.49	108.06	112.53
3	B	903	HEM	C3B-C4B-NB	-2.49	106.88	111.63
3	A	909	HEM	CMA-C3A-C4A	-2.48	124.25	128.36
3	C	904[B]	HEM	CMA-C3A-C4A	-2.48	124.26	128.36
3	D	904[A]	HEM	CAA-C2A-C1A	-2.47	124.32	127.01
3	B	906	HEM	CAA-CBA-CGA	-2.47	108.22	112.75
3	B	906	HEM	CMA-C3A-C4A	-2.46	124.29	128.36
3	C	909	HEM	CAA-CBA-CGA	-2.46	108.24	112.75
3	C	904[A]	HEM	C3C-CAC-CBC	-2.43	120.72	124.46
3	A	902	HEM	C1D-CHD-C4C	-2.43	121.76	125.82
3	B	904[A]	HEM	CMA-C3A-C4A	-2.38	124.43	128.36
3	A	909	HEM	C3B-C4B-NB	-2.37	107.09	111.63
3	B	904[A]	HEM	C3B-C4B-NB	-2.37	107.10	111.63
3	C	904[B]	HEM	C3C-CAC-CBC	-2.36	120.83	124.46
3	A	903	HEM	CAA-C2A-C1A	-2.32	124.49	127.01
3	D	904[B]	HEM	CAA-C2A-C1A	-2.31	124.50	127.01
3	A	907	HEM	CMA-C3A-C4A	-2.31	124.54	128.36
3	B	907	HEM	C1D-CHD-C4C	-2.28	122.01	125.82
3	A	904[B]	HEM	C3B-C4B-NB	-2.28	107.28	111.63
3	A	908	HEM	C4B-CHC-C1C	-2.27	122.03	125.82
3	A	904[A]	HEM	C3B-C4B-NB	-2.27	107.29	111.63
3	A	905	HEM	C3B-CAB-CBB	-2.27	120.98	124.46
3	D	908	HEM	C3C-CAC-CBC	-2.27	120.98	124.46
3	C	908	HEM	C1D-CHD-C4C	-2.26	122.04	125.82
3	D	908	HEM	C3B-C4B-NB	-2.24	107.34	111.63
3	D	906	HEM	C1D-CHD-C4C	-2.24	122.08	125.82
3	D	906	HEM	C3B-C4B-NB	-2.22	107.39	111.63
3	B	904[B]	HEM	C3B-C4B-NB	-2.21	107.40	111.63
3	D	902	HEM	C1D-CHD-C4C	-2.20	122.15	125.82
3	A	907	HEM	C3B-C4B-NB	-2.17	107.47	111.63
3	C	907	HEM	CBA-CAA-C2A	-2.17	108.64	112.53
3	C	904[B]	HEM	C3B-C4B-NB	-2.17	107.49	111.63
3	C	904[A]	HEM	C3B-C4B-NB	-2.17	107.49	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	908	HEM	C3B-C4B-NB	-2.13	107.55	111.63
3	D	904[A]	HEM	C3B-C4B-NB	-2.12	107.58	111.63
3	C	903	HEM	C3B-C4B-NB	-2.11	107.59	111.63
3	D	902	HEM	CAA-C2A-C1A	-2.10	124.73	127.01
3	D	904[A]	HEM	CMA-C3A-C4A	-2.08	124.92	128.36
3	A	906	HEM	CMA-C3A-C4A	-2.08	124.92	128.36
3	D	906	HEM	CAA-CBA-CGA	-2.07	108.95	112.75
3	D	904[B]	HEM	C3B-C4B-NB	-2.07	107.67	111.63
3	A	907	HEM	C3C-CAC-CBC	-2.04	121.32	124.46
3	D	902	HEM	C3B-C4B-NB	-2.02	107.76	111.63
3	B	904[B]	HEM	CAA-C2A-C1A	-2.02	124.81	127.01
3	B	906	HEM	C1D-CHD-C4C	-2.02	122.45	125.82
3	B	906	HEM	CBD-CAD-C3D	-2.00	107.73	113.55
3	D	907	HEM	CAA-C2A-C1A	-2.00	124.84	127.01
3	A	904[B]	HEM	C2D-C3D-C4D	2.00	104.90	101.50
3	C	902	HEM	CAA-CBA-CGA	2.02	116.45	112.75
3	D	906	HEM	CMA-C3A-C2A	2.03	129.48	125.24
3	C	907	HEM	CHD-C1D-ND	2.03	129.41	124.52
3	B	904[A]	HEM	CHC-C4B-NB	2.05	129.45	124.52
3	B	904[B]	HEM	C2D-C3D-C4D	2.07	105.00	101.50
3	B	908	HEM	CHC-C4B-NB	2.07	129.52	124.52
3	B	909	HEM	C2C-C1C-CHC	2.08	126.85	123.68
3	B	902	HEM	CHC-C4B-NB	2.08	129.54	124.52
3	A	903	HEM	C3C-CAC-CBC	2.09	127.67	124.46
3	A	908	HEM	CHC-C4B-NB	2.09	129.56	124.52
3	D	904[B]	HEM	CMA-C3A-C2A	2.10	129.62	125.24
3	D	906	HEM	CHC-C4B-NB	2.10	129.57	124.52
3	D	908	HEM	CHC-C4B-NB	2.12	129.62	124.52
3	C	906	HEM	C2D-C3D-C4D	2.14	105.12	101.50
3	B	904[A]	HEM	CAA-CBA-CGA	2.14	116.68	112.75
3	C	908	HEM	CHD-C1D-ND	2.15	129.71	124.52
3	C	907	HEM	C2D-C3D-C4D	2.17	105.18	101.50
3	B	908	HEM	CMD-C2D-C3D	2.19	124.03	114.35
3	A	909	HEM	C2D-C3D-C4D	2.19	105.22	101.50
3	D	907	HEM	C2D-C3D-C4D	2.22	105.26	101.50
3	B	903	HEM	C2C-C1C-CHC	2.24	127.09	123.68
3	B	904[B]	HEM	CHC-C4B-NB	2.24	129.93	124.52
3	A	903	HEM	C2D-C3D-C4D	2.25	105.31	101.50
3	D	902	HEM	C2D-C3D-C4D	2.26	105.34	101.50
3	A	904[A]	HEM	CHC-C4B-NB	2.28	130.01	124.52
3	D	909	HEM	CHC-C4B-NB	2.28	130.02	124.52
3	D	909	HEM	C2C-C1C-CHC	2.30	127.18	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	HEM	CHC-C4B-NB	2.30	130.06	124.52
3	B	907	HEM	CHC-C4B-NB	2.30	130.07	124.52
3	B	906	HEM	CHC-C4B-NB	2.31	130.07	124.52
3	A	908	HEM	CMD-C2D-C3D	2.32	124.60	114.35
3	C	902	HEM	CBA-CAA-C2A	2.36	116.76	112.53
3	D	902	HEM	CHC-C4B-NB	2.36	130.22	124.52
3	C	907	HEM	CAA-CBA-CGA	2.37	117.08	112.75
3	A	902	HEM	CHC-C4B-NB	2.37	130.24	124.52
3	A	905	HEM	CAA-CBA-CGA	2.40	117.14	112.75
3	A	903	HEM	CMA-C3A-C2A	2.40	130.26	125.24
3	D	909	HEM	CMD-C2D-C3D	2.40	124.98	114.35
3	A	906	HEM	CMD-C2D-C3D	2.41	125.00	114.35
3	C	906	HEM	C3C-CAC-CBC	2.41	128.15	124.46
3	A	903	HEM	C3B-CAB-CBB	2.41	128.16	124.46
3	A	909	HEM	CMD-C2D-C3D	2.42	125.05	114.35
3	B	909	HEM	CMA-C3A-C2A	2.44	130.34	125.24
3	C	908	HEM	C2C-C1C-CHC	2.49	127.47	123.68
3	B	909	HEM	CHC-C4B-NB	2.52	130.60	124.52
3	B	906	HEM	CMD-C2D-C3D	2.53	125.56	114.35
3	D	907	HEM	CMA-C3A-C2A	2.54	130.55	125.24
3	A	909	HEM	CHC-C4B-NB	2.55	130.65	124.52
3	A	904[B]	HEM	CHC-C4B-NB	2.55	130.66	124.52
3	B	902	HEM	CMD-C2D-C3D	2.60	125.84	114.35
3	D	907	HEM	CHC-C4B-NB	2.60	130.78	124.52
3	A	905	HEM	CMD-C2D-C3D	2.63	125.99	114.35
3	D	908	HEM	CMD-C2D-C3D	2.64	126.02	114.35
3	B	907	HEM	CAA-CBA-CGA	2.66	117.61	112.75
3	C	907	HEM	CMD-C2D-C3D	2.67	126.14	114.35
3	B	903	HEM	CMA-C3A-C2A	2.69	130.85	125.24
3	C	904[A]	HEM	CMD-C2D-C3D	2.69	126.24	114.35
3	B	905	HEM	CMD-C2D-C3D	2.69	126.26	114.35
3	C	903	HEM	CAD-C3D-C4D	2.71	122.02	112.47
3	C	904[B]	HEM	CMD-C2D-C3D	2.71	126.35	114.35
3	C	906	HEM	CMD-C2D-C3D	2.71	126.36	114.35
3	B	903	HEM	CBA-CAA-C2A	2.73	117.41	112.53
3	C	909	HEM	CMD-C2D-C3D	2.74	126.47	114.35
3	C	908	HEM	CMD-C2D-C3D	2.76	126.55	114.35
3	B	903	HEM	CAD-C3D-C4D	2.84	122.49	112.47
3	A	907	HEM	CMD-C2D-C3D	2.86	127.01	114.35
3	A	906	HEM	C2D-C3D-C4D	2.88	106.39	101.50
3	C	908	HEM	C2D-C3D-C4D	2.89	106.40	101.50
3	D	904[B]	HEM	CMD-C2D-C3D	2.91	127.22	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	HEM	C3C-CAC-CBC	2.94	128.97	124.46
3	C	902	HEM	CMD-C2D-C3D	2.96	127.43	114.35
3	D	904[A]	HEM	CMD-C2D-C3D	2.99	127.56	114.35
3	D	908	HEM	C2C-C1C-CHC	3.03	128.29	123.68
3	D	906	HEM	CMD-C2D-C3D	3.05	127.83	114.35
3	B	907	HEM	CMD-C2D-C3D	3.09	128.01	114.35
3	C	904[A]	HEM	CAA-CBA-CGA	3.11	118.45	112.75
3	D	902	HEM	CMD-C2D-C3D	3.13	128.18	114.35
3	D	905	HEM	CMD-C2D-C3D	3.13	128.20	114.35
3	B	909	HEM	CMD-C2D-C3D	3.13	128.21	114.35
3	A	907	HEM	C2D-C3D-C4D	3.14	106.81	101.50
3	B	904[B]	HEM	CMD-C2D-C3D	3.15	128.26	114.35
3	B	904[A]	HEM	CMD-C2D-C3D	3.15	128.27	114.35
3	C	905	HEM	C2D-C3D-C4D	3.16	106.85	101.50
3	A	902	HEM	CMD-C2D-C3D	3.18	128.43	114.35
3	D	903	HEM	CAD-C3D-C4D	3.23	123.86	112.47
3	B	909	HEM	C2D-C3D-C4D	3.26	107.02	101.50
3	D	905	HEM	C2D-C3D-C4D	3.26	107.03	101.50
3	C	908	HEM	CMB-C2B-C3B	3.28	124.73	116.53
3	C	903	HEM	C2D-C3D-C4D	3.31	107.10	101.50
3	A	903	HEM	CAD-C3D-C4D	3.32	124.18	112.47
3	D	906	HEM	C2D-C3D-C4D	3.32	107.13	101.50
3	A	905	HEM	C2D-C3D-C4D	3.36	107.20	101.50
3	B	908	HEM	CMB-C2B-C3B	3.39	125.01	116.53
3	A	904[A]	HEM	CMD-C2D-C3D	3.40	129.40	114.35
3	C	905	HEM	CMD-C2D-C3D	3.42	129.46	114.35
3	A	904[B]	HEM	CMD-C2D-C3D	3.42	129.50	114.35
3	C	905	HEM	CAD-C3D-C4D	3.43	124.58	112.47
3	D	903	HEM	CMD-C2D-C3D	3.46	129.64	114.35
3	B	905	HEM	C2D-C3D-C4D	3.46	107.36	101.50
3	B	909	HEM	CAD-C3D-C4D	3.49	124.77	112.47
3	B	909	HEM	CMB-C2B-C3B	3.50	125.27	116.53
3	A	903	HEM	CMD-C2D-C3D	3.51	129.86	114.35
3	B	903	HEM	C3B-CAB-CBB	3.52	129.86	124.46
3	A	902	HEM	CAA-CBA-CGA	3.63	119.39	112.75
3	D	909	HEM	CMC-C2C-C3C	3.70	125.78	116.53
3	D	908	HEM	CMC-C2C-C3C	3.71	125.78	116.53
3	D	909	HEM	CAD-C3D-C2D	3.71	123.87	113.22
3	D	907	HEM	CMD-C2D-C3D	3.72	130.81	114.35
3	A	905	HEM	CAD-C3D-C2D	3.73	123.95	113.22
3	A	908	HEM	CMC-C2C-C3C	3.76	125.91	116.53
3	C	909	HEM	CAD-C3D-C2D	3.76	124.04	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	909	HEM	CMC-C2C-C3C	3.78	125.95	116.53
3	D	904[B]	HEM	CAA-CBA-CGA	3.79	119.69	112.75
3	C	904[B]	HEM	CAD-C3D-C2D	3.81	124.18	113.22
3	D	907	HEM	CMB-C2B-C3B	3.81	126.05	116.53
3	D	905	HEM	CMC-C2C-C3C	3.87	126.20	116.53
3	D	905	HEM	CAD-C3D-C4D	3.88	126.14	112.47
3	B	906	HEM	CMB-C2B-C3B	3.88	126.21	116.53
3	B	905	HEM	CAD-C3D-C4D	3.89	126.20	112.47
3	C	903	HEM	CMD-C2D-C3D	3.90	131.59	114.35
3	C	904[A]	HEM	CAD-C3D-C2D	3.90	124.43	113.22
3	C	909	HEM	C2D-C3D-C4D	3.91	108.13	101.50
3	C	905	HEM	CMC-C2C-C3C	3.92	126.32	116.53
3	D	906	HEM	CMB-C2B-C3B	3.92	126.32	116.53
3	C	906	HEM	CMC-C2C-C3C	3.95	126.39	116.53
3	A	902	HEM	CMB-C2B-C3B	3.96	126.41	116.53
3	B	907	HEM	CMB-C2B-C3B	3.96	126.41	116.53
3	D	907	HEM	CAD-C3D-C4D	3.97	126.48	112.47
3	A	906	HEM	CAD-C3D-C2D	3.97	124.64	113.22
3	C	908	HEM	CMC-C2C-C3C	3.98	126.46	116.53
3	B	903	HEM	CMB-C2B-C3B	3.99	126.48	116.53
3	B	907	HEM	CAD-C3D-C4D	4.01	126.61	112.47
3	B	903	HEM	CMD-C2D-C3D	4.01	132.10	114.35
3	A	905	HEM	CMC-C2C-C3C	4.02	126.57	116.53
3	A	909	HEM	CMC-C2C-C3C	4.02	126.57	116.53
3	C	906	HEM	CMB-C2B-C3B	4.13	126.84	116.53
3	B	904[A]	HEM	CMC-C2C-C3C	4.14	126.86	116.53
3	D	904[B]	HEM	CMB-C2B-C3B	4.15	126.90	116.53
3	B	908	HEM	CAD-C3D-C2D	4.17	125.19	113.22
3	D	909	HEM	CAD-C3D-C4D	4.18	127.21	112.47
3	D	902	HEM	CAD-C3D-C4D	4.19	127.24	112.47
3	A	907	HEM	CAD-C3D-C4D	4.19	127.24	112.47
3	B	904[B]	HEM	CMC-C2C-C3C	4.19	126.99	116.53
3	A	909	HEM	CAD-C3D-C2D	4.19	125.27	113.22
3	B	903	HEM	CMC-C2C-C3C	4.21	127.03	116.53
3	C	907	HEM	CAD-C3D-C2D	4.21	125.32	113.22
3	A	906	HEM	CMB-C2B-C3B	4.22	127.07	116.53
3	D	906	HEM	CAD-C3D-C4D	4.23	127.40	112.47
3	D	908	HEM	CAD-C3D-C4D	4.26	127.48	112.47
3	D	906	HEM	CAD-C3D-C2D	4.26	125.47	113.22
3	D	904[B]	HEM	CMC-C2C-C3C	4.27	127.19	116.53
3	C	908	HEM	CAD-C3D-C4D	4.29	127.61	112.47
3	A	906	HEM	CMC-C2C-C3C	4.31	127.29	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	904[A]	HEM	CAD-C3D-C2D	4.32	125.62	113.22
3	C	903	HEM	CMB-C2B-C3B	4.32	127.32	116.53
3	D	904[A]	HEM	CMC-C2C-C3C	4.32	127.32	116.53
3	A	908	HEM	CMB-C2B-C3B	4.32	127.32	116.53
3	C	906	HEM	CAD-C3D-C4D	4.33	127.73	112.47
3	A	908	HEM	CAD-C3D-C2D	4.33	125.67	113.22
3	A	909	HEM	CMB-C2B-C3B	4.34	127.36	116.53
3	D	909	HEM	C2D-C3D-C4D	4.35	108.87	101.50
3	C	902	HEM	CMC-C2C-C3C	4.35	127.38	116.53
3	C	909	HEM	CAD-C3D-C4D	4.36	127.83	112.47
3	D	902	HEM	CMB-C2B-C3B	4.37	127.44	116.53
3	A	907	HEM	CAD-C3D-C2D	4.42	125.92	113.22
3	B	904[B]	HEM	CAD-C3D-C2D	4.42	125.92	113.22
3	D	909	HEM	CMB-C2B-C3B	4.43	127.59	116.53
3	C	908	HEM	CAD-C3D-C2D	4.44	125.99	113.22
3	A	902	HEM	CMC-C2C-C3C	4.46	127.67	116.53
3	B	904[A]	HEM	CAD-C3D-C2D	4.49	126.12	113.22
3	B	902	HEM	CAD-C3D-C2D	4.51	126.17	113.22
3	B	906	HEM	CAD-C3D-C2D	4.51	126.18	113.22
3	C	907	HEM	CMB-C2B-C3B	4.52	127.81	116.53
3	A	904[B]	HEM	CAD-C3D-C2D	4.52	126.21	113.22
3	A	902	HEM	CAD-C3D-C2D	4.53	126.23	113.22
3	A	903	HEM	CMC-C2C-C3C	4.54	127.87	116.53
3	C	902	HEM	CMB-C2B-C3B	4.56	127.92	116.53
3	D	908	HEM	CMB-C2B-C3B	4.59	127.99	116.53
3	A	903	HEM	CMB-C2B-C3B	4.59	127.99	116.53
3	D	904[B]	HEM	CAD-C3D-C4D	4.60	128.68	112.47
3	B	905	HEM	CAD-C3D-C2D	4.60	126.44	113.22
3	C	902	HEM	CAD-C3D-C2D	4.62	126.49	113.22
3	A	905	HEM	CAD-C3D-C4D	4.63	128.78	112.47
3	A	904[B]	HEM	CAD-C3D-C4D	4.64	128.83	112.47
3	A	904[B]	HEM	CMB-C2B-C3B	4.65	128.13	116.53
3	B	909	HEM	CMC-C2C-C3C	4.66	128.15	116.53
3	C	902	HEM	CAD-C3D-C4D	4.66	128.90	112.47
3	A	902	HEM	CAD-C3D-C4D	4.66	128.91	112.47
3	A	906	HEM	CAD-C3D-C4D	4.68	128.97	112.47
3	B	904[B]	HEM	CAD-C3D-C4D	4.69	129.00	112.47
3	D	904[A]	HEM	CAD-C3D-C2D	4.69	126.69	113.22
3	D	904[A]	HEM	CMB-C2B-C3B	4.70	128.27	116.53
3	B	906	HEM	CAD-C3D-C4D	4.72	129.11	112.47
3	D	905	HEM	CAD-C3D-C2D	4.73	126.82	113.22
3	B	904[B]	HEM	CMB-C2B-C3B	4.75	128.39	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	908	HEM	CMC-C2C-C3C	4.77	128.43	116.53
3	B	904[A]	HEM	CAD-C3D-C4D	4.77	129.30	112.47
3	C	904[A]	HEM	CMB-C2B-C3B	4.77	128.45	116.53
3	B	902	HEM	CMB-C2B-C3B	4.78	128.46	116.53
3	C	903	HEM	CMC-C2C-C3C	4.78	128.47	116.53
3	D	904[A]	HEM	CAD-C3D-C4D	4.79	129.38	112.47
3	D	904[B]	HEM	CAD-C3D-C2D	4.80	127.02	113.22
3	C	907	HEM	CAD-C3D-C4D	4.82	129.47	112.47
3	C	909	HEM	CMB-C2B-C3B	4.82	128.57	116.53
3	A	909	HEM	CAD-C3D-C4D	4.83	129.50	112.47
3	A	907	HEM	CMB-C2B-C3B	4.83	128.59	116.53
3	B	905	HEM	CMB-C2B-C3B	4.84	128.60	116.53
3	C	906	HEM	CAD-C3D-C2D	4.84	127.12	113.22
3	A	908	HEM	CAD-C3D-C4D	4.84	129.53	112.47
3	A	904[A]	HEM	CAD-C3D-C4D	4.89	129.70	112.47
3	A	904[B]	HEM	CMC-C2C-C3C	4.93	128.82	116.53
3	D	902	HEM	CAA-CBA-CGA	4.93	121.78	112.75
3	D	902	HEM	CAD-C3D-C2D	4.93	127.39	113.22
3	C	904[B]	HEM	CMB-C2B-C3B	4.96	128.91	116.53
3	A	904[A]	HEM	CMC-C2C-C3C	5.00	129.02	116.53
3	A	904[B]	HEM	CAA-CBA-CGA	5.02	121.94	112.75
3	B	908	HEM	CAD-C3D-C4D	5.03	130.23	112.47
3	C	904[A]	HEM	CMC-C2C-C3C	5.05	129.12	116.53
3	C	904[B]	HEM	CMC-C2C-C3C	5.07	129.19	116.53
3	D	903	HEM	CMB-C2B-C3B	5.09	129.23	116.53
3	B	902	HEM	CMC-C2C-C3C	5.09	129.25	116.53
3	B	902	HEM	CAD-C3D-C4D	5.10	130.47	112.47
3	B	904[B]	HEM	CAA-CBA-CGA	5.12	122.13	112.75
3	B	907	HEM	CMC-C2C-C3C	5.13	129.34	116.53
3	B	909	HEM	CAD-C3D-C2D	5.16	128.06	113.22
3	D	908	HEM	CAD-C3D-C2D	5.18	128.10	113.22
3	D	907	HEM	CAD-C3D-C2D	5.20	128.16	113.22
3	A	904[A]	HEM	CMB-C2B-C3B	5.21	129.53	116.53
3	D	905	HEM	CMB-C2B-C3B	5.27	129.68	116.53
3	C	904[A]	HEM	CAD-C3D-C4D	5.32	131.24	112.47
3	C	905	HEM	CMB-C2B-C3B	5.33	129.82	116.53
3	C	905	HEM	CAD-C3D-C2D	5.33	128.53	113.22
3	A	907	HEM	CMC-C2C-C3C	5.33	129.83	116.53
3	B	907	HEM	CAD-C3D-C2D	5.37	128.65	113.22
3	D	906	HEM	CMC-C2C-C3C	5.39	129.99	116.53
3	A	905	HEM	CMB-C2B-C3B	5.44	130.11	116.53
3	C	904[B]	HEM	CAD-C3D-C4D	5.44	131.67	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	904[A]	HEM	CMB-C2B-C3B	5.45	130.13	116.53
3	D	903	HEM	CMC-C2C-C3C	5.45	130.13	116.53
3	D	907	HEM	CMC-C2C-C3C	5.46	130.17	116.53
3	B	906	HEM	CMC-C2C-C3C	5.61	130.54	116.53
3	B	905	HEM	CMC-C2C-C3C	5.67	130.68	116.53
3	D	902	HEM	CMC-C2C-C3C	5.78	130.96	116.53
3	C	907	HEM	CMC-C2C-C3C	5.86	131.16	116.53
3	A	903	HEM	CAD-C3D-C2D	5.99	130.44	113.22
3	C	903	HEM	CAD-C3D-C2D	6.14	130.87	113.22
3	D	903	HEM	CAD-C3D-C2D	6.54	132.01	113.22
3	B	903	HEM	CAD-C3D-C2D	6.93	133.15	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 244 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	905	HEM	7	0
3	C	906	HEM	6	0
3	C	907	HEM	6	0
3	C	908	HEM	6	0
3	C	909	HEM	8	0
5	C	911	SO3	1	0
3	D	902	HEM	5	0
3	D	903	HEM	16	0
3	D	904[A]	HEM	5	0
3	D	904[B]	HEM	5	0
3	D	905	HEM	9	0
3	D	906	HEM	5	0
3	D	907	HEM	4	0
3	D	908	HEM	4	0
3	D	909	HEM	4	0
5	D	912	SO3	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	660/732 (90%)	-0.43	3 (0%) 91 93	15, 26, 43, 82	0
1	B	660/732 (90%)	-0.45	7 (1%) 82 86	16, 24, 43, 67	0
1	C	659/732 (90%)	-0.39	4 (0%) 90 92	17, 27, 46, 71	0
1	D	660/732 (90%)	-0.45	2 (0%) 94 95	11, 21, 40, 76	0
All	All	2639/2928 (90%)	-0.43	16 (0%) 90 92	11, 25, 44, 82	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	630	LYS	4.1
1	C	379	LEU	3.9
1	D	689	SER	3.6
1	C	30	GLY	3.4
1	C	537	ASP	3.1
1	A	631	LYS	3.1
1	D	30	GLY	3.0
1	B	379	LEU	2.9
1	B	689	SER	2.7
1	B	538	PRO	2.5
1	B	30	GLY	2.4
1	B	688	LYS	2.3
1	A	379	LEU	2.3
1	B	378	PRO	2.2
1	B	537	ASP	2.1
1	C	377	ASN	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	DTN	A	901	6/6	0.84	0.24	7.54	25,33,40,42	6
5	SO3	B	911	4/4	0.99	0.14	7.02	23,23,31,34	0
2	DTN	D	901	6/6	0.92	0.19	6.91	33,38,51,51	6
2	DTN	C	901	6/6	0.89	0.28	5.47	56,57,64,67	6
2	DTN	A	911	6/6	0.96	0.11	4.95	23,28,36,37	6
5	SO3	C	911	4/4	0.99	0.14	2.04	23,25,30,38	0
5	SO3	A	912	4/4	0.99	0.14	1.48	21,22,25,35	0
3	HEM	D	904[B]	43/43	0.96	0.15	0.99	9,12,14,15	43
3	HEM	D	904[A]	43/43	0.96	0.15	0.99	10,11,13,15	43
3	HEM	A	909	43/43	0.96	0.13	0.88	19,23,45,72	0
3	HEM	B	904[A]	43/43	0.97	0.14	0.82	15,16,18,20	43
3	HEM	B	904[B]	43/43	0.97	0.14	0.82	11,16,19,21	43
3	HEM	C	909	43/43	0.95	0.11	0.73	20,23,41,61	0
2	DTN	B	901	6/6	0.92	0.14	0.65	27,36,37,40	6
3	HEM	B	909	43/43	0.96	0.10	0.60	17,20,40,71	0
3	HEM	A	904[A]	43/43	0.97	0.13	0.56	14,17,18,20	43
3	HEM	A	904[B]	43/43	0.97	0.13	0.56	12,18,19,20	43
5	SO3	D	911	4/4	0.93	0.10	0.56	40,48,50,62	0
3	HEM	D	909	43/43	0.96	0.09	0.45	14,19,54,66	0
3	HEM	B	907	43/43	0.95	0.11	0.44	15,16,29,54	0
3	HEM	C	908	43/43	0.97	0.08	0.36	17,19,24,26	0
3	HEM	C	903	43/43	0.96	0.11	0.30	18,21,26,29	0
3	HEM	D	907	43/43	0.96	0.09	0.26	12,14,23,54	0
3	HEM	C	904[A]	43/43	0.96	0.14	0.23	14,17,19,21	43
3	HEM	C	904[B]	43/43	0.96	0.14	0.23	15,17,19,21	43
3	HEM	B	903	43/43	0.96	0.10	0.19	15,18,20,22	0
3	HEM	A	907	43/43	0.96	0.09	0.13	14,16,25,47	0
3	HEM	B	908	43/43	0.97	0.08	0.12	14,17,21,22	0
3	HEM	C	907	43/43	0.96	0.09	0.08	16,18,29,45	0
3	HEM	C	902	43/43	0.96	0.13	0.03	15,19,22,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEM	C	906	43/43	0.96	0.10	0.02	15,18,24,34	0
3	HEM	D	903	43/43	0.96	0.12	0.01	11,13,14,15	0
3	HEM	A	902	43/43	0.96	0.12	-0.02	17,19,24,28	0
3	HEM	A	903	43/43	0.96	0.10	-0.03	16,19,22,24	0
3	HEM	C	905	43/43	0.96	0.12	-0.03	16,18,20,21	0
3	HEM	D	905	43/43	0.97	0.12	-0.05	10,11,13,14	0
3	HEM	B	906	43/43	0.97	0.10	-0.10	13,16,25,34	0
3	HEM	D	902	43/43	0.97	0.12	-0.12	12,13,19,22	0
5	SO3	D	912	4/4	0.98	0.13	-0.20	15,17,21,24	0
3	HEM	A	908	43/43	0.97	0.08	-0.20	15,17,20,23	0
3	HEM	D	906	43/43	0.97	0.10	-0.24	9,12,17,30	0
3	HEM	A	905	43/43	0.97	0.10	-0.32	13,17,19,21	0
3	HEM	B	905	43/43	0.97	0.10	-0.35	14,15,18,18	0
3	HEM	B	902	43/43	0.97	0.11	-0.39	16,18,22,25	0
3	HEM	A	906	43/43	0.97	0.09	-0.44	13,16,24,31	0
3	HEM	D	908	43/43	0.97	0.07	-0.75	12,14,21,22	0
4	CU	A	910	1/1	0.99	0.10	-1.22	15,15,15,15	1
4	CU	C	910	1/1	0.98	0.10	-1.61	17,17,17,17	1
4	CU	D	910	1/1	1.00	0.09	-2.52	9,9,9,9	1
4	CU	B	910	1/1	1.00	0.09	-2.81	11,11,11,11	1

6.5 Other polymers ⓘ

There are no such residues in this entry.