WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

PDB ID	:	1IW0
Title	:	Crystal structure of a heme oxygenase (HmuO) from Corynebacterium diphtheriae complexed with heme in the ferric state
Authors	:	Hirotsu, S.; Unno, M.; Chu, G.C.; Lee, D.S.; Park, S.Y.; Shiro, Y.; Ikeda-Saito, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2002-04-04
Resolution	:	1.40 Å(reported)

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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	Percentile Ranks	Value
Rfree		0.193
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		4.0%

Worse　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
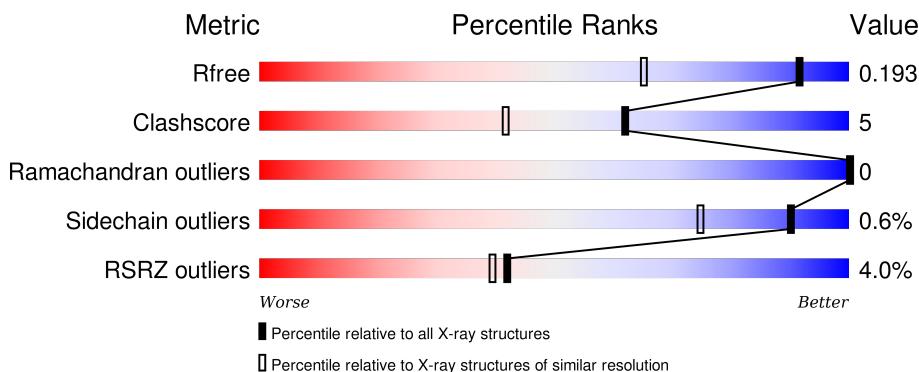
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1199 (1.40-1.40)
Clashscore	102246	1295 (1.40-1.40)
Ramachandran outliers	100387	1259 (1.40-1.40)
Sidechain outliers	100360	1258 (1.40-1.40)
RSRZ outliers	91569	1198 (1.40-1.40)

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	215	5% / 90% / 7% •
1	B	215	2% / 84% / 12% • •
1	C	215	5% / 88% / 8% •
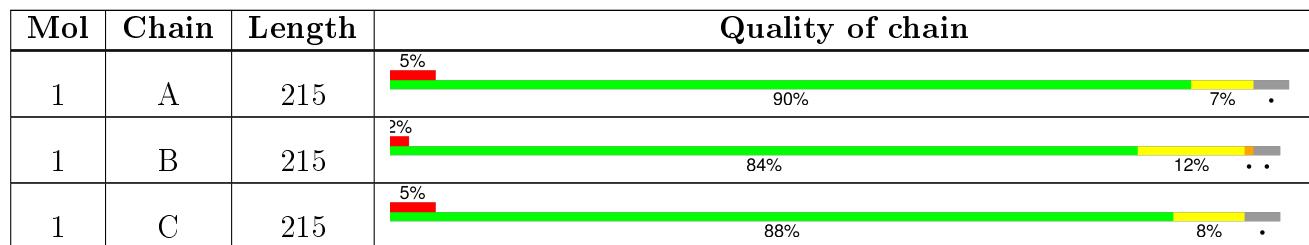
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SUC	B	904	-	-	-	X
3	SO4	B	907	-	-	-	X
3	SO4	C	910	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5838 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 Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1652	1042	293	314	3			
1	B	209	Total	C	N	O	S	0	5	0
			1678	1058	297	320	3			
1	C	207	Total	C	N	O	S	0	5	0
			1666	1051	293	319	3			

- Molecule 2 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).
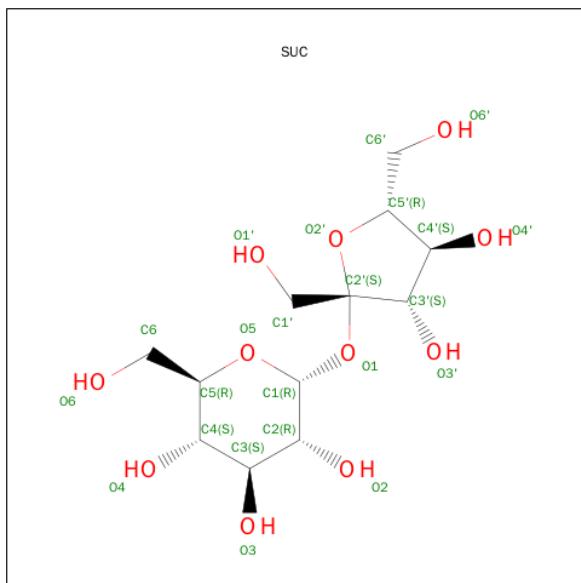
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
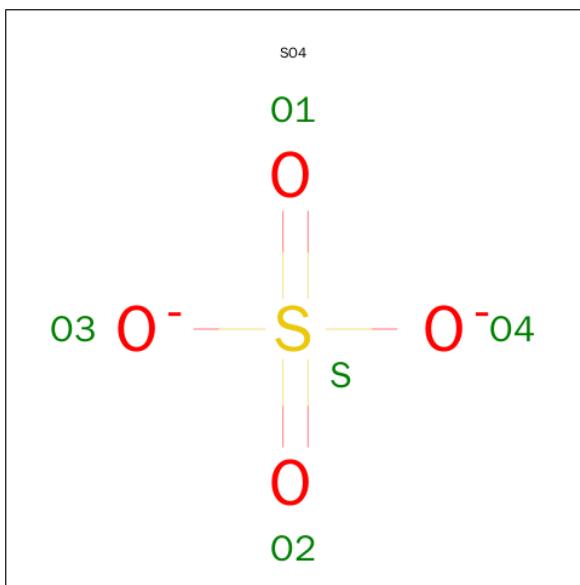
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

HEM
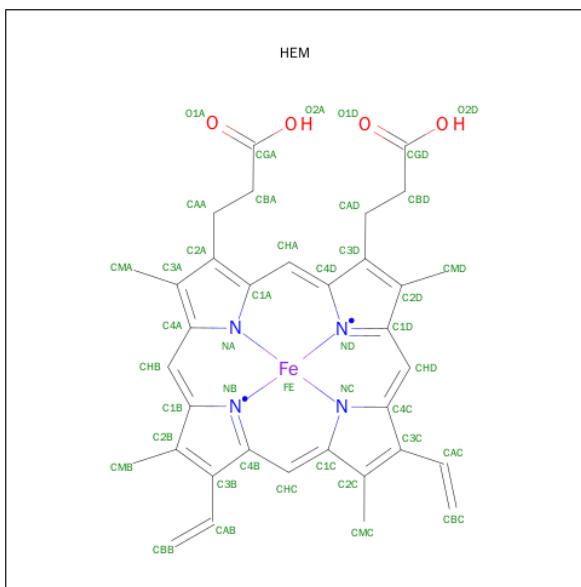
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	1
			46	35	1	4	6		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	2
			205	205		
5	B	239	Total	O	0	0
			239	239		
5	C	213	Total	O	0	0
			213	213		

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: Heme oxygenase
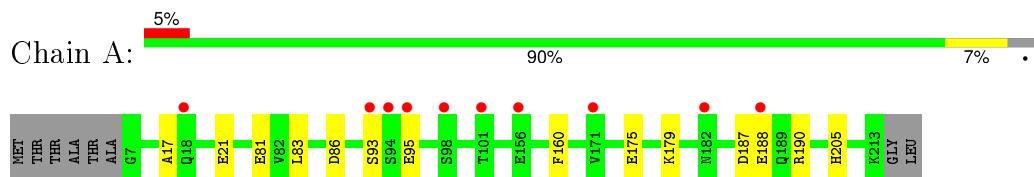
- Molecule 1: Heme oxygenase
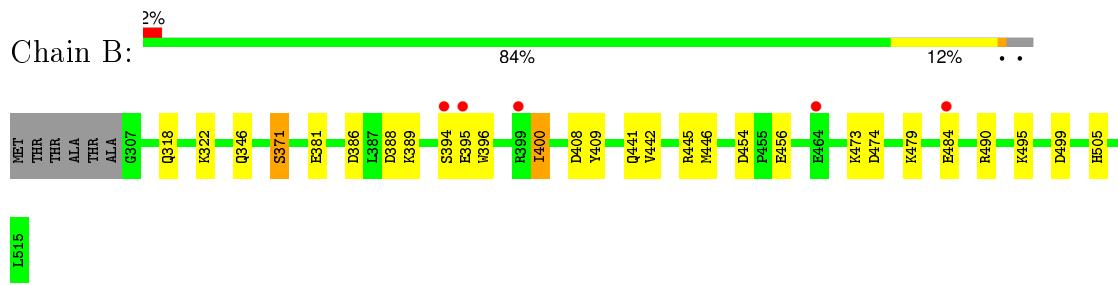
- Molecule 1: Heme oxygenase
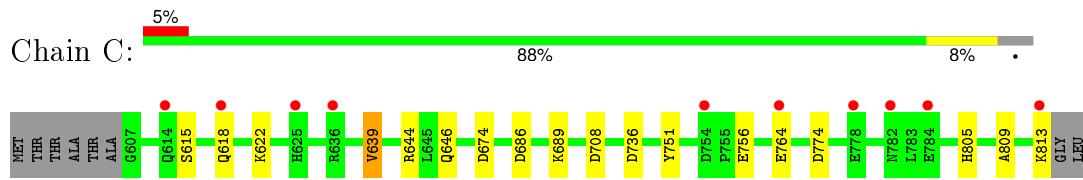
4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.56Å　　62.84Å　　107.66Å 90.00°　　100.86°　　90.00°	Depositor
Resolution (Å)	12.00　–　1.40 19.95　–　1.30	Depositor EDS
% Data completeness (in resolution range)	90.1 (12.00-1.40) 85.0 (19.95-1.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.15 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.165　,　0.192 0.167　,　0.193	Depositor DCC
R_{free} test set	12388 reflections (11.08%)	DCC
Wilson B-factor (Å²)	13.5	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.52 , 61.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	0 of 146824 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5838	wwPDB-VP
Average B, all atoms (Å²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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, SUC, SO4

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	0.53	0/1684	0.78	2/2274 (0.1%)
1	B	0.60	0/1728	0.82	4/2333 (0.2%)
1	C	0.60	0/1723	0.84	6/2327 (0.3%)
All	All	0.58	0/5135	0.81	12/6934 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	639[A]	VAL	CG1-CB-CG2	-8.18	97.82	110.90
1	C	639[B]	VAL	CG1-CB-CG2	-8.18	97.82	110.90
1	B	386	ASP	CB-CG-OD2	6.73	124.36	118.30
1	A	187	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	388	ASP	CB-CG-OD2	6.05	123.75	118.30
1	C	686	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	86	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	408	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	674	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	708	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	474	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	736	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1652	0	1611	9	0
1	B	1678	0	1632	24	1
1	C	1666	0	1620	20	0
2	B	23	0	22	0	0
3	B	15	0	0	2	0
3	C	15	0	0	0	0
4	A	46	0	4	2	0
4	B	43	0	30	0	0
4	C	43	0	30	0	0
5	A	205	0	0	7	1
5	B	239	0	0	7	0
5	C	213	0	0	9	0
All	All	5838	0	4949	55	1

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 5.

All (55) 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)
4:A:901[B]:HEM:O1D	5:A:1419:HOH:O	1.53	1.23
1:B:441:GLN:HB2	5:B:1575:HOH:O	1.45	1.14
1:C:689:LYS:HD3	1:C:756:GLU:HG3	1.42	0.99
1:A:205:HIS:ND1	5:A:1406:HOH:O	2.02	0.92
1:B:395:GLU:HA	5:B:1475:HOH:O	1.70	0.91
1:A:179:LYS:HE3	5:A:1400:HOH:O	1.71	0.89
1:C:644:ARG:NH1	5:C:1373:HOH:O	2.05	0.88
1:C:774:ASP:HB3	5:C:1384:HOH:O	1.81	0.79
1:B:454:ASP:HB3	1:B:456:GLU:OE1	1.86	0.75
1:C:774:ASP:CB	5:C:1384:HOH:O	2.39	0.71
1:B:396:TRP:O	1:B:400[A]:ILE:HD12	1.92	0.70
1:C:639[A]:VAL:HG23	1:C:751:TYR:HB3	1.74	0.70
1:B:394:SER:O	1:B:395:GLU:HB3	1.96	0.65
1:A:190:ARG:NH1	5:A:1262:HOH:O	2.28	0.65
1:C:689:LYS:HD2	1:C:756:GLU:O	1.97	0.65
1:C:644:ARG:NH1	5:C:1246:HOH:O	2.34	0.60
1:C:618:GLN:H	1:C:618:GLN:NE2	1.99	0.60
1:B:442:VAL:HG12	1:B:446:MET:HE2	1.84	0.60
1:A:175:GLU:HB3	5:A:1400:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LYS:HG2	5:B:1551:HOH:O	2.04	0.57
4:A:901[A]:HEM:O1D	5:A:1377:HOH:O	2.08	0.57
1:B:442:VAL:HG12	1:B:446:MET:CE	2.35	0.56
1:C:764:GLU:OE2	5:C:1260:HOH:O	2.18	0.56
1:B:381:GLU:HG2	5:B:1481:HOH:O	2.05	0.55
1:B:490:ARG:NH1	5:B:1632:HOH:O	2.34	0.55
1:C:809:ALA:O	1:C:813:LYS:HE2	2.07	0.55
1:C:774:ASP:CG	5:C:1384:HOH:O	2.45	0.54
1:C:764:GLU:HG2	5:C:1050:HOH:O	2.10	0.52
1:A:188:GLU:OE2	5:A:1256:HOH:O	2.18	0.51
1:B:394:SER:O	1:B:395:GLU:CB	2.52	0.51
1:B:394:SER:C	1:B:396:TRP:H	2.13	0.51
1:B:445:ARG:NE	5:B:1171:HOH:O	2.33	0.51
1:C:646:GLN:HA	1:C:646:GLN:NE2	2.27	0.49
1:C:615[A]:SER:OG	5:C:1079:HOH:O	2.12	0.49
1:B:495:LYS:CE	1:B:499:ASP:OD2	2.62	0.48
1:C:689:LYS:HD3	1:C:756:GLU:CG	2.30	0.47
1:B:394:SER:C	1:B:396:TRP:N	2.68	0.47
1:B:505:HIS:HE1	3:B:907:SO4:O1	1.98	0.47
1:A:93:SER:OG	1:A:95:GLU:HG2	2.16	0.46
1:C:646:GLN:HA	1:C:646:GLN:HE21	1.81	0.46
1:B:318:GLN:NE2	5:B:1569:HOH:O	2.49	0.46
1:C:813:LYS:HG3	5:C:1313:HOH:O	2.16	0.45
1:B:346:GLN:NE2	1:B:346:GLN:HA	2.32	0.45
1:B:389:LYS:NZ	1:B:456:GLU:HB3	2.32	0.44
1:B:389:LYS:HD2	1:B:456:GLU:O	2.18	0.44
1:C:618:GLN:H	1:C:618:GLN:CD	2.21	0.44
1:C:622:LYS:HD3	1:C:805:HIS:CE1	2.53	0.43
1:A:81:GLU:CD	1:A:81:GLU:H	2.23	0.43
1:C:689:LYS:CD	1:C:756:GLU:O	2.67	0.42
1:B:495:LYS:NZ	1:B:499:ASP:OD2	2.53	0.42
1:A:83:LEU:HG	1:A:160:PHE:HD1	1.86	0.41
1:B:371[A]:SER:OG	1:B:479:LYS:HE2	2.21	0.40
1:A:17:ALA:O	1:A:21:GLU:HG3	2.21	0.40
1:B:318:GLN:O	1:B:322:LYS:HG2	2.21	0.40
1:B:473:LYS:HE3	3:B:906:SO4:O3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:GLU:OE2	5:A:1250:HOH:O[1_455]	2.13	0.07

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	205/215 (95%)	200 (98%)	5 (2%)	0	100	100
1	B	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
1	C	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
All	All	627/645 (97%)	612 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	170/175 (97%)	170 (100%)	0	100	100
1	B	175/175 (100%)	170 (97%)	5 (3%)	50	13
1	C	175/175 (100%)	175 (100%)	0	100	100
All	All	520/525 (99%)	515 (99%)	5 (1%)	90	59

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	371[A]	SER
1	B	371[B]	SER
1	B	400[A]	ILE
1	B	400[B]	ILE
1	B	409	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	182	ASN
1	B	346	GLN
1	B	378	ASN
1	B	441	GLN
1	B	462	HIS
1	B	505	HIS
1	B	506	GLN
1	C	618	GLN
1	C	646	GLN
1	C	678	ASN
1	C	748	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

11 ligands are modelled in this entry.

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	#$|Z| > 2$
4	HEM	A	901[A]	-	30,50,50	2.06	7 (23%)	24,82,82	4.02	15 (62%)
4	HEM	A	901[B]	-	30,50,50	2.06	7 (23%)	24,82,82	3.94	15 (62%)
4	HEM	B	902	1,5	30,50,50	2.90	8 (26%)	24,82,82	3.84	15 (62%)
2	SUC	B	904	-	24,24,24	0.38	0	36,36,36	0.58	0
3	SO4	B	906	-	4,4,4	0.11	0	6,6,6	0.17	0
3	SO4	B	907	-	4,4,4	0.17	0	6,6,6	0.27	0
3	SO4	B	908	-	4,4,4	0.14	0	6,6,6	0.36	0
4	HEM	C	903	1,5	30,50,50	2.70	8 (26%)	24,82,82	3.42	12 (50%)
3	SO4	C	905	-	4,4,4	0.40	0	6,6,6	0.43	0
3	SO4	C	909	-	4,4,4	0.23	0	6,6,6	0.27	0
3	SO4	C	910	-	4,4,4	0.41	0	6,6,6	0.20	0

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
4	HEM	A	901[A]	-	-	0/10/54/54	0/0/8/8
4	HEM	A	901[B]	-	-	0/10/54/54	0/0/8/8
4	HEM	B	902	1,5	-	0/10/54/54	0/0/8/8
2	SUC	B	904	-	-	0/12/51/51	0/2/2/2
3	SO4	B	906	-	-	0/0/0/0	0/0/0/0
3	SO4	B	907	-	-	0/0/0/0	0/0/0/0
3	SO4	B	908	-	-	0/0/0/0	0/0/0/0
4	HEM	C	903	1,5	-	0/10/54/54	0/0/8/8
3	SO4	C	905	-	-	0/0/0/0	0/0/0/0
3	SO4	C	909	-	-	0/0/0/0	0/0/0/0
3	SO4	C	910	-	-	0/0/0/0	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	HEM	C3B-C4B	-11.06	1.42	1.51
4	C	903	HEM	C3B-C4B	-10.09	1.42	1.51
4	A	901[B]	HEM	C1C-NC	-6.81	1.27	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901[A]	HEM	C1C-NC	-6.81	1.27	1.36
4	B	902	HEM	C2D-C3D	-5.08	1.39	1.54
4	A	901[B]	HEM	C3B-C4B	-5.02	1.47	1.51
4	A	901[A]	HEM	C3B-C4B	-5.02	1.47	1.51
4	C	903	HEM	C2C-C1C	-4.35	1.44	1.52
4	B	902	HEM	C2C-C1C	-4.33	1.44	1.52
4	B	902	HEM	C2D-C1D	-4.27	1.37	1.51
4	C	903	HEM	C2D-C3D	-4.25	1.41	1.54
4	B	902	HEM	C3D-C4D	-3.99	1.46	1.51
4	C	903	HEM	C2B-C1B	-3.61	1.40	1.51
4	C	903	HEM	C3D-C4D	-3.54	1.47	1.51
4	B	902	HEM	C2B-C1B	-3.28	1.41	1.51
4	A	901[B]	HEM	C2C-C1C	-3.24	1.46	1.52
4	A	901[A]	HEM	C2C-C1C	-3.24	1.46	1.52
4	C	903	HEM	C2D-C1D	-3.01	1.42	1.51
4	A	901[B]	HEM	CMC-C2C	-2.68	1.46	1.53
4	A	901[A]	HEM	CMC-C2C	-2.68	1.46	1.53
4	A	901[B]	HEM	C2D-C1D	-2.24	1.44	1.51
4	A	901[A]	HEM	C2D-C1D	-2.24	1.44	1.51
4	A	901[B]	HEM	C2B-C1B	-2.03	1.45	1.51
4	A	901[A]	HEM	C2B-C1B	-2.03	1.45	1.51
4	C	903	HEM	FE-NC	2.09	2.04	1.95
4	B	902	HEM	C3C-CAC	2.41	1.55	1.51
4	A	901[B]	HEM	C4C-NC	2.57	1.39	1.36
4	A	901[A]	HEM	C4C-NC	2.57	1.39	1.36
4	B	902	HEM	FE-NC	3.43	2.09	1.95
4	C	903	HEM	C4C-NC	4.65	1.41	1.36

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	HEM	C3C-CAC-CBC	-9.57	109.78	124.46
4	C	903	HEM	C3C-CAC-CBC	-9.02	110.61	124.46
4	A	901[B]	HEM	C3C-CAC-CBC	-8.30	111.73	124.46
4	A	901[A]	HEM	C3C-CAC-CBC	-8.30	111.73	124.46
4	A	901[B]	HEM	CMA-C3A-C4A	-7.16	116.51	128.36
4	A	901[A]	HEM	CMA-C3A-C4A	-7.16	116.51	128.36
4	B	902	HEM	CMA-C3A-C4A	-6.09	118.28	128.36
4	C	903	HEM	CMA-C3A-C4A	-5.85	118.68	128.36
4	B	902	HEM	C3B-C4B-CHC	-4.51	116.82	123.16
4	C	903	HEM	CBD-CAD-C3D	-3.93	102.11	113.55
4	B	902	HEM	CAA-CBA-CGA	-3.88	105.63	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	HEM	C4B-CHC-C1C	-3.28	120.34	125.82
4	A	901[B]	HEM	CBD-CAD-C3D	-2.93	105.02	113.55
4	A	901[A]	HEM	CBD-CAD-C3D	-2.93	105.02	113.55
4	C	903	HEM	CAA-CBA-CGA	-2.79	107.63	112.75
4	A	901[B]	HEM	CAA-CBA-CGA	-2.74	107.72	112.75
4	A	901[A]	HEM	CAA-CBA-CGA	-2.74	107.72	112.75
4	A	901[B]	HEM	C3B-CAB-CBB	-2.68	120.35	124.46
4	A	901[A]	HEM	C3B-CAB-CBB	-2.68	120.35	124.46
4	A	901[B]	HEM	C3B-C4B-CHC	-2.50	119.64	123.16
4	A	901[A]	HEM	C3B-C4B-CHC	-2.50	119.64	123.16
4	B	902	HEM	C2C-C1C-NC	-2.44	106.10	110.21
4	A	901[B]	HEM	C4B-CHC-C1C	-2.41	121.79	125.82
4	A	901[A]	HEM	C4B-CHC-C1C	-2.41	121.79	125.82
4	B	902	HEM	CHC-C4B-NB	2.33	130.12	124.52
4	A	901[B]	HEM	CAD-C3D-C2D	2.33	119.93	113.22
4	A	901[A]	HEM	CAD-C3D-C2D	2.33	119.93	113.22
4	B	902	HEM	C3B-CAB-CBB	2.39	128.13	124.46
4	C	903	HEM	C1D-CHD-C4C	2.44	129.90	125.82
4	A	901[B]	HEM	CMD-C2D-C3D	2.54	125.61	114.35
4	A	901[A]	HEM	CMD-C2D-C3D	2.54	125.61	114.35
4	C	903	HEM	CMC-C2C-C3C	2.59	123.00	116.53
4	C	903	HEM	CAA-C2A-C1A	2.71	129.95	127.01
4	A	901[B]	HEM	CAD-CBD-CGD	2.73	124.14	113.02
4	A	901[B]	HEM	CHC-C4B-NB	3.00	131.75	124.52
4	A	901[A]	HEM	CHC-C4B-NB	3.00	131.75	124.52
4	B	902	HEM	CMD-C2D-C3D	3.07	127.93	114.35
4	B	902	HEM	CAA-C2A-C1A	3.12	130.40	127.01
4	C	903	HEM	CMA-C3A-C2A	3.23	131.98	125.24
4	C	903	HEM	C3B-CAB-CBB	3.31	129.53	124.46
4	C	903	HEM	CAD-C3D-C4D	4.68	128.96	112.47
4	B	902	HEM	C1D-CHD-C4C	4.69	133.67	125.82
4	C	903	HEM	CMB-C2B-C3B	4.76	128.41	116.53
4	A	901[A]	HEM	CAD-CBD-CGD	4.76	132.43	113.02
4	B	902	HEM	CMC-C2C-C3C	4.82	128.57	116.53
4	B	902	HEM	CAD-C3D-C2D	5.02	127.65	113.22
4	B	902	HEM	CAD-C3D-C4D	5.03	130.23	112.47
4	C	903	HEM	CAD-C3D-C2D	6.00	130.48	113.22
4	B	902	HEM	CMB-C2B-C3B	6.19	131.98	116.53
4	A	901[B]	HEM	CMC-C2C-C3C	6.30	132.25	116.53
4	A	901[A]	HEM	CMC-C2C-C3C	6.30	132.25	116.53
4	A	901[B]	HEM	CMB-C2B-C3B	6.31	132.27	116.53
4	A	901[A]	HEM	CMB-C2B-C3B	6.31	132.27	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901[B]	HEM	CAA-C2A-C1A	6.62	134.19	127.01
4	A	901[A]	HEM	CAA-C2A-C1A	6.62	134.19	127.01
4	A	901[B]	HEM	CAD-C3D-C4D	7.27	138.12	112.47
4	A	901[A]	HEM	CAD-C3D-C4D	7.27	138.12	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901[A]	HEM	1	0
4	A	901[B]	HEM	1	0
3	B	906	SO4	1	0
3	B	907	SO4	1	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	207/215 (96%)	0.11	10 (4%)	34	31	11, 18, 30, 39	0
1	B	209/215 (97%)	0.00	5 (2%)	62	59	8, 16, 26, 31	0
1	C	207/215 (96%)	0.09	10 (4%)	34	31	9, 16, 27, 35	0
All	All	623/645 (96%)	0.07	25 (4%)	42	39	8, 17, 28, 39	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	GLU	3.8
1	A	98	SER	3.8
1	B	394	SER	3.6
1	B	484	GLU	3.2
1	A	18	GLN	3.0
1	C	614	GLN	3.0
1	C	618	GLN	3.0
1	C	813	LYS	2.9
1	C	636	ARG	2.9
1	A	94	SER	2.9
1	C	784	GLU	2.8
1	C	754	ASP	2.7
1	B	399	ARG	2.6
1	C	625	HIS	2.6
1	C	764	GLU	2.5
1	A	93	SER	2.4
1	A	101	THR	2.4
1	B	395	GLU	2.3
1	C	782	ASN	2.3
1	C	778	GLU	2.3
1	A	182	ASN	2.2
1	A	188	GLU	2.1
1	A	171	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	464	GLU	2.1
1	A	156	GLU	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, 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
3	SO4	C	910	5/5	0.91	0.17	3.35	13,13,14,15	5
3	SO4	B	907	5/5	0.92	0.25	2.88	34,34,35,37	0
2	SUC	B	904	23/23	0.84	0.19	2.74	21,25,28,30	0
4	HEM	A	901[B]	43/43	0.97	0.09	0.07	11,17,28,31	3
4	HEM	A	901[A]	43/43	0.97	0.09	0.07	11,17,27,31	3
3	SO4	C	905	5/5	0.97	0.08	-0.21	18,18,19,21	5
4	HEM	B	902	43/43	0.98	0.08	-0.57	9,13,21,28	0
4	HEM	C	903	43/43	0.98	0.07	-0.77	10,12,19,25	0
3	SO4	C	909	5/5	0.91	0.22	-	14,16,16,17	5
3	SO4	B	906	5/5	0.97	0.24	-	32,32,33,33	0
3	SO4	B	908	5/5	0.93	0.24	-	36,36,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.