



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:23 AM GMT

PDB ID : 3I8R  
Title : Crystal structure of the heme oxygenase from *Corynebacterium diphtheriae* (HmuO) in complex with heme binding dithiothreitol (DTT)  
Authors : Matsui, T.; Unno, M.; Ikeda-Saito, M.  
Deposited on : 2009-07-10  
Resolution : 1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

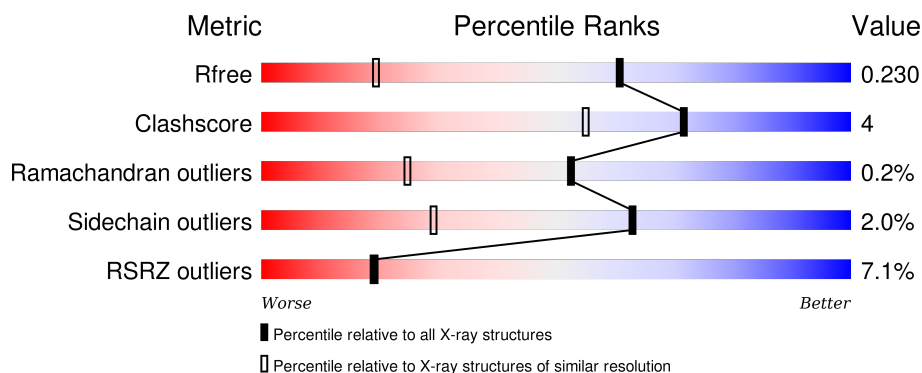
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	215	<div> <div>9%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	B	215	<div> <div>%</div> <div>80%</div> <div>14%</div> <div>.</div> <div>.</div> </div>
1	C	215	<div> <div>10%</div> <div>80%</div> <div>16%</div> <div>.</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	1008	-	-	-	X
3	SO4	C	1010	-	-	-	X

## 2 Entry composition [i](#)

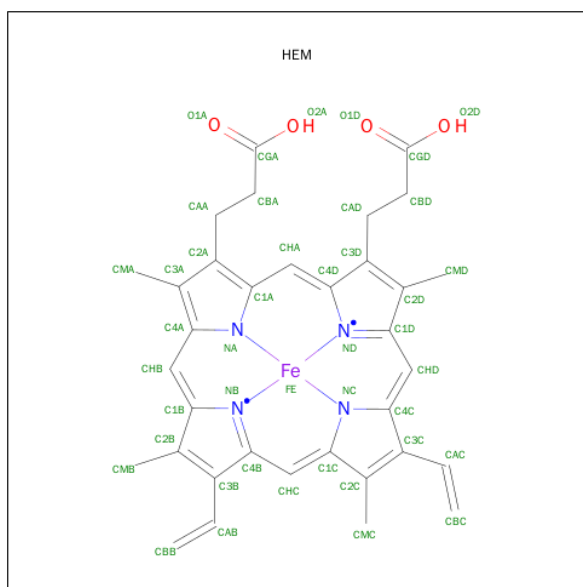
There are 5 unique types of molecules in this entry. The entry contains 5643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			1656	1043	296	314	3			
1	B	209	Total	C	N	O	S	0	0	0
			1665	1050	295	317	3			
1	C	207	Total	C	N	O	S	0	0	0
			1640	1034	290	313	3			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



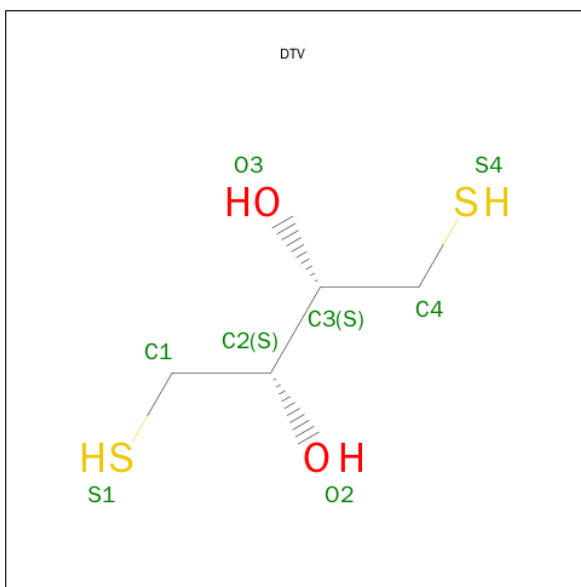
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		
4	B	1	Total	C	O	S	0	0
			8	4	2	2		
4	C	1	Total	C	O	S	0	0
			8	4	2	2		

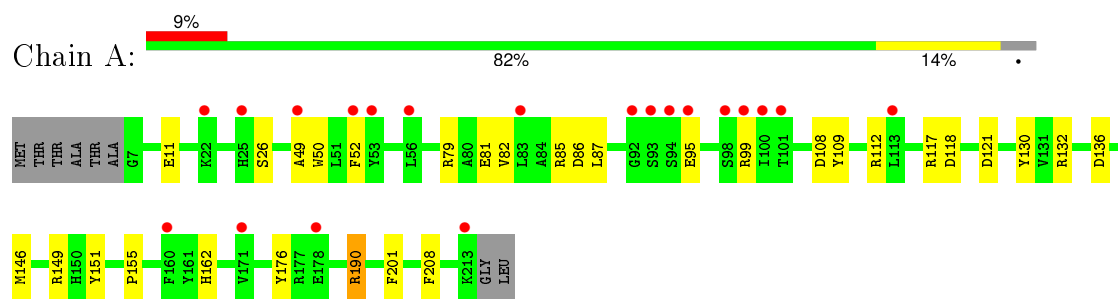
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	195	Total	O	0	0
			195	195		
5	C	126	Total	O	0	0
			126	126		

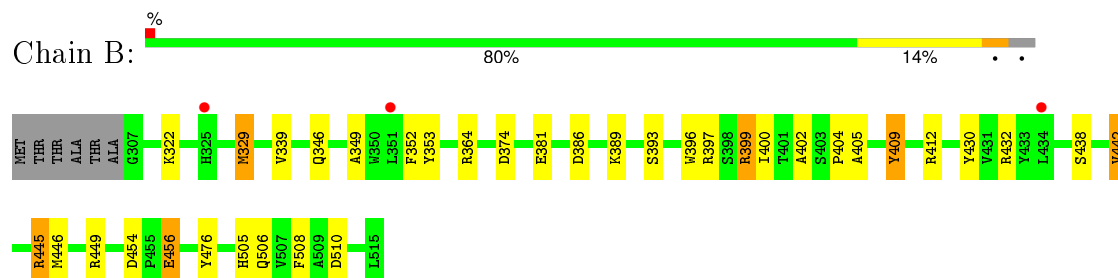
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

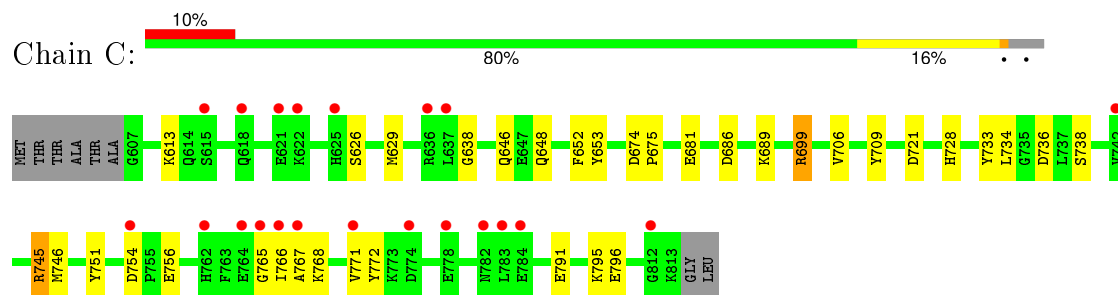
#### • Molecule 1: Heme oxygenase



#### • Molecule 1: Heme oxygenase



#### • Molecule 1: Heme oxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.12Å 62.56Å 108.00Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 30.80 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.50) 98.0 (30.80-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.194 , 0.224 0.202 , 0.230	Depositor DCC
$R_{free}$ test set	11109 reflections (11.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 111053 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5643	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4, DTV

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	1.44	7/1695 (0.4%)	1.44	23/2288 (1.0%)
1	B	1.50	14/1697 (0.8%)	1.44	17/2290 (0.7%)
1	C	1.38	6/1672 (0.4%)	1.26	11/2261 (0.5%)
All	All	1.44	27/5064 (0.5%)	1.38	51/6839 (0.7%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	681	GLU	CD-OE2	7.39	1.33	1.25
1	B	432	ARG	CZ-NH2	7.15	1.42	1.33
1	C	681	GLU	CG-CD	7.05	1.62	1.51
1	B	456	GLU	CG-CD	7.05	1.62	1.51
1	A	95	GLU	CB-CG	6.92	1.65	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	TYR	CB-CG-CD2	-10.54	114.67	121.00
1	A	109	TYR	CB-CG-CD1	9.70	126.82	121.00
1	A	109	TYR	CB-CG-CD2	-9.18	115.49	121.00
1	B	352	PHE	CB-CG-CD2	-9.10	114.43	120.80
1	B	409	TYR	CB-CG-CD1	8.62	126.17	121.00

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	1656	0	1612	8	0
1	B	1665	0	1625	16	0
1	C	1640	0	1583	17	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
4	A	8	0	6	0	0
4	B	8	0	9	0	0
4	C	8	0	9	1	0
5	A	163	0	0	1	0
5	B	195	0	0	2	0
5	C	126	0	0	0	0
All	All	5643	0	4934	43	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 4.

The worst 5 of 43 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:454:ASP:HB3	1:B:456:GLU:OE2	1.77	0.84
1:C:745:ARG:HG3	1:C:746:MET:CE	2.12	0.80
1:C:768:LYS:CB	1:C:771:VAL:HG12	2.17	0.75
1:C:745:ARG:HG3	1:C:746:MET:HE2	1.74	0.70
1:C:728:HIS:HE1	1:C:796:GLU:OE2	1.76	0.69

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	206/215 (96%)	201 (98%)	5 (2%)	0	100	100
1	B	207/215 (96%)	203 (98%)	4 (2%)	0	100	100
1	C	205/215 (95%)	200 (98%)	4 (2%)	1 (0%)	34	10
All	All	618/645 (96%)	604 (98%)	13 (2%)	1 (0%)	52	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	766	ILE

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/175 (98%)	169 (99%)	2 (1%)	78	54
1	B	171/175 (98%)	166 (97%)	5 (3%)	50	16
1	C	167/175 (95%)	164 (98%)	3 (2%)	66	35
All	All	509/525 (97%)	499 (98%)	10 (2%)	63	29

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	399	ARG
1	B	404	PRO

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Mol	Chain	Res	Type
1	C	675	PRO
1	B	393	SER
1	B	409	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	378	ASN
1	C	728	HIS
1	C	646	GLN
1	A	182	ASN
1	C	678	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 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	$\# Z  > 2$
3	SO4	A	1001	-	4,4,4	0.40	0	6,6,6	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	1005	-	4,4,4	0.17	0	6,6,6	0.29	0
4	DTV	A	2001	2	7,7,7	1.81	1 (14%)	4,8,8	7.56	2 (50%)
2	HEM	A	901	1,4	30,50,50	1.92	5 (16%)	24,82,82	3.08	13 (54%)
3	SO4	B	1002	-	4,4,4	0.44	0	6,6,6	0.62	0
3	SO4	B	1003	-	4,4,4	0.46	0	6,6,6	0.76	0
3	SO4	B	1004	-	4,4,4	0.32	0	6,6,6	1.14	1 (16%)
3	SO4	B	1008	-	4,4,4	1.50	1 (25%)	6,6,6	1.24	1 (16%)
4	DTV	B	2002	2	7,7,7	1.18	1 (14%)	4,8,8	1.78	1 (25%)
2	HEM	B	902	1,4	30,50,50	2.45	12 (40%)	24,82,82	3.38	18 (75%)
3	SO4	C	1009	-	4,4,4	0.27	0	6,6,6	0.69	0
3	SO4	C	1010	-	4,4,4	0.70	0	6,6,6	0.58	0
3	SO4	C	1011	-	4,4,4	0.17	0	6,6,6	0.12	0
4	DTV	C	2003	2	7,7,7	1.37	1 (14%)	4,8,8	2.49	1 (25%)
2	HEM	C	903	1,4	30,50,50	3.11	11 (36%)	24,82,82	2.66	15 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
4	DTV	A	2001	2	-	0/8/8/8	0/0/0/0
2	HEM	A	901	1,4	-	0/10/54/54	0/0/8/8
3	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1004	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1008	-	-	0/0/0/0	0/0/0/0
4	DTV	B	2002	2	-	0/8/8/8	0/0/0/0
2	HEM	B	902	1,4	-	0/10/54/54	0/0/8/8
3	SO4	C	1009	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1010	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1011	-	-	0/0/0/0	0/0/0/0
4	DTV	C	2003	2	-	0/8/8/8	0/0/0/0
2	HEM	C	903	1,4	-	0/10/54/54	0/0/8/8

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	903	HEM	C3B-C4B	-7.99	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	HEM	C3B-C4B	-7.08	1.45	1.51
2	A	901	HEM	C3D-C4D	-4.71	1.45	1.51
2	C	903	HEM	C2B-C1B	-4.71	1.36	1.51
2	B	902	HEM	C3D-C4D	-4.17	1.46	1.51

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	DTV	C3-C4-S4	-11.33	95.13	113.91
4	A	2001	DTV	C2-C1-S1	-9.71	97.80	113.91
2	B	902	HEM	CMA-C3A-C4A	-7.85	115.38	128.36
2	A	901	HEM	C3C-CAC-CBC	-6.75	114.11	124.46
2	C	903	HEM	C3C-CAC-CBC	-4.77	117.14	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	HEM	2	0
4	C	2003	DTV	1	0
2	C	903	HEM	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	207/215 (96%)	0.54	20 (9%) 10 9	13, 22, 36, 42	0
1	B	209/215 (97%)	0.08	3 (1%) 78 81	12, 21, 33, 42	0
1	C	207/215 (96%)	0.74	21 (10%) 9 8	16, 26, 42, 54	0
All	All	623/645 (96%)	0.45	44 (7%) 19 19	12, 23, 37, 54	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	767	ALA	9.2
1	C	765	GLY	5.8
1	C	771	VAL	5.3
1	C	636	ARG	3.9
1	C	764	GLU	3.9

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	1008	5/5	0.91	0.20	6.44	35,35,44,46	0
3	SO4	C	1010	5/5	0.79	0.28	5.61	55,58,61,62	0
3	SO4	A	1001	5/5	0.96	0.17	1.06	43,43,46,51	0
3	SO4	C	1009	5/5	0.89	0.20	1.01	56,58,60,60	0
4	DTV	A	2001	8/8	0.96	0.14	0.66	20,30,32,32	0
3	SO4	B	1004	5/5	0.94	0.14	0.62	41,44,47,51	0
2	HEM	C	903	43/43	0.96	0.11	0.15	18,26,39,50	0
2	HEM	B	902	43/43	0.97	0.10	0.03	14,19,30,51	0
2	HEM	A	901	43/43	0.97	0.10	-0.25	16,22,33,39	0
4	DTV	B	2002	8/8	0.98	0.08	-0.29	18,21,24,28	0
4	DTV	C	2003	8/8	0.96	0.10	-0.30	27,30,39,45	0
3	SO4	B	1002	5/5	0.96	0.28	-	45,49,51,52	0
3	SO4	C	1011	5/5	0.94	0.28	-	95,96,97,97	0
3	SO4	A	1005	5/5	0.62	0.29	-	108,109,109,109	0
3	SO4	B	1003	5/5	0.98	0.08	-	35,37,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.