



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:22 PM GMT

PDB ID : 1WNW  
Title : D136N mutant of Heme Oxygenase from *Corynebacterium diphtheriae* (HmuO)  
Authors : Unno, M.; Matsui, T.; Ikeda-Saito, M.  
Deposited on : 2004-08-10  
Resolution : 1.70 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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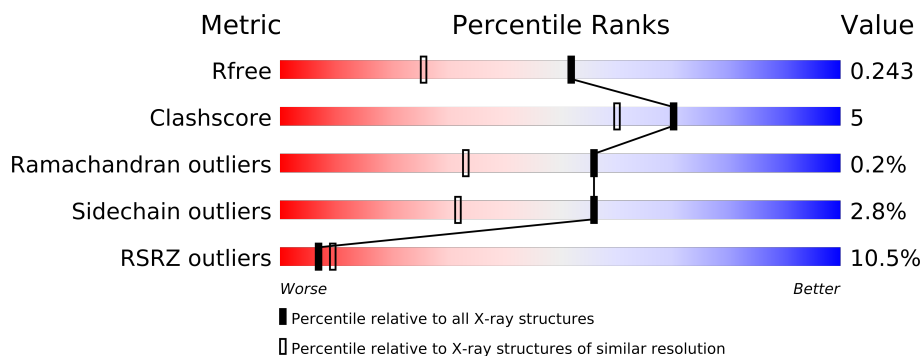
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	215	
1	B	215	
1	C	215	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NA	B	4001	-	X
3	NA	B	4002	-	X
4	SO4	A	2007	-	X
4	SO4	A	2009	-	X
4	SO4	A	2011	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	B	2003	-	X
4	SO4	B	2004	-	X
4	SO4	B	2008	-	X
4	SO4	C	2001	-	X
4	SO4	C	2012	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5538 atoms, of which 0 are hydrogen and 0 are deuterium.

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	208	Total	C	N	O	S	0	1	0
			1653	1042	298	310	3			
1	B	210	Total	C	N	O	S	0	1	0
			1668	1050	300	315	3			
1	C	206	Total	C	N	O	S	0	0	0
			1635	1031	291	310	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	LYS	GLU	SEE REMARK 999	UNP P71119
A	60	VAL	ALA	SEE REMARK 999	UNP P71119
A	92	GLY	ASP	SEE REMARK 999	UNP P71119
A	93	SER	GLY	SEE REMARK 999	UNP P71119
A	136	ASN	ASP	ENGINEERED	UNP P71119
A	192	HIS	ASN	SEE REMARK 999	UNP P71119
B	34	LYS	GLU	SEE REMARK 999	UNP P71119
B	60	VAL	ALA	SEE REMARK 999	UNP P71119
B	92	GLY	ASP	SEE REMARK 999	UNP P71119
B	93	SER	GLY	SEE REMARK 999	UNP P71119
B	136	ASN	ASP	ENGINEERED	UNP P71119
B	192	HIS	ASN	SEE REMARK 999	UNP P71119
C	34	LYS	GLU	SEE REMARK 999	UNP P71119
C	60	VAL	ALA	SEE REMARK 999	UNP P71119
C	92	GLY	ASP	SEE REMARK 999	UNP P71119
C	93	SER	GLY	SEE REMARK 999	UNP P71119
C	136	ASN	ASP	ENGINEERED	UNP P71119
C	192	HIS	ASN	SEE REMARK 999	UNP P71119

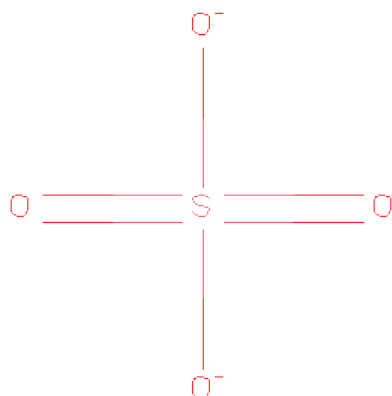
- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total I 4 4	0	0
2	A	4	Total I 4 4	0	0
2	C	1	Total I 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Na 2 2	0	0

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



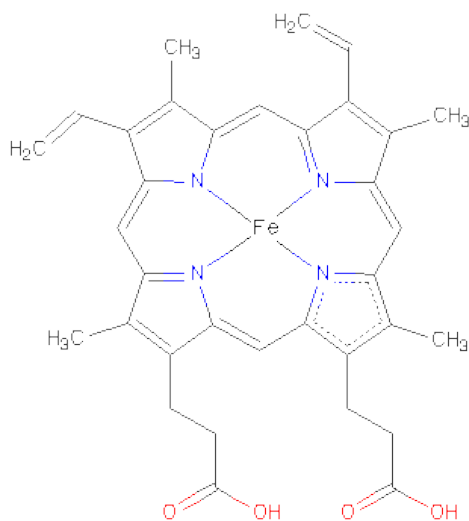
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 6 is water.

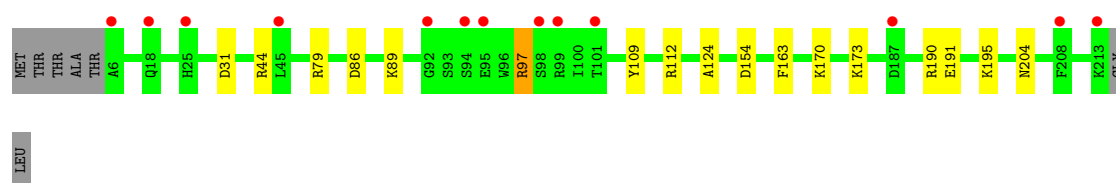
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total 128	O 128	0	0
6	B	157	Total 157	O 157	0	0
6	C	97	Total 97	O 97	0	0

### 3 Residue-property plots

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.

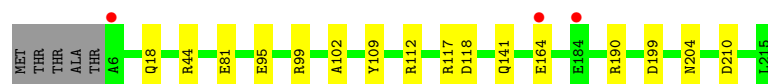
- Molecule 1: Heme oxygenase

Chain A: 



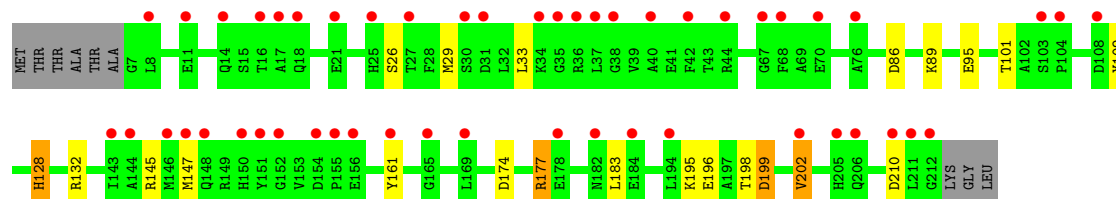
- Molecule 1: Heme oxygenase

Chain B: 



- Molecule 1: Heme oxygenase

Chain C: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.06Å 63.10Å 107.16Å 90.00° 101.03° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 23.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-1.70) 97.1 (23.84-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.196 , 0.233 0.209 , 0.243	Depositor DCC
$R_{free}$ test set	7616 reflections (11.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 75503 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.09	1/1692 (0.1%)	1.11	12/2285 (0.5%)
1	B	1.05	2/1707 (0.1%)	1.04	7/2303 (0.3%)
1	C	1.09	4/1667 (0.2%)	1.06	6/2254 (0.3%)
All	All	1.07	7/5066 (0.1%)	1.07	25/6842 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	TYR	CD1-CE1	-6.46	1.29	1.39
1	C	128	HIS	C-O	-6.46	1.11	1.23
1	B	109	TYR	CD1-CE1	5.92	1.48	1.39
1	C	145	ARG	C-O	5.89	1.34	1.23
1	A	124	ALA	CA-CB	-5.80	1.40	1.52
1	B	102	ALA	CA-CB	-5.58	1.40	1.52
1	C	161	TYR	CE1-CZ	5.26	1.45	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ASP	CB-CG-OD2	9.53	126.88	118.30
1	C	177	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	109	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	A	86	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	79	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	44	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	109	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	C	210	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	31	ASP	CB-CG-OD1	6.28	123.96	118.30
1	A	109	TYR	CB-CG-CD1	6.16	124.70	121.00
1	C	86	ASP	CB-CG-OD2	6.09	123.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	154	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	118	ASP	CB-CG-OD1	5.92	123.62	118.30
1	C	199	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	210	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	190	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	97	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	97	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	199	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	112[A]	ARG	CG-CD-NE	5.28	122.88	111.80
1	A	112[B]	ARG	CG-CD-NE	5.28	122.88	111.80
1	B	117	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	177	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	109	TYR	CB-CG-CD1	5.04	124.02	121.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1653	0	16	5	0
1	B	1668	0	30	6	0
1	C	1635	0	0	6	0
2	A	4	0	0	5	0
2	B	4	0	0	1	0
2	C	1	0	0	0	0
3	B	2	0	0	0	0
4	A	15	0	0	1	0
4	B	25	0	0	0	0
4	C	20	0	0	0	0
5	A	43	0	0	2	0
5	B	43	0	0	1	0
5	C	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	128	0	0	7	0
6	B	157	0	0	6	0
6	C	97	0	0	4	0
All	All	5538	0	46	24	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1006:IOD:I	6:A:2132:HOH:O	2.23	1.23
2:B:1002:IOD:I	6:B:4097:HOH:O	2.50	0.98
2:A:1008:IOD:I	6:A:2127:HOH:O	2.57	0.92
1:A:204:ASN:ND2	5:A:901:HEM:CBB	2.38	0.87
2:A:1006:IOD:I	2:A:1007:IOD:I	3.47	0.72
2:A:1006:IOD:I	6:A:2083:HOH:O	2.81	0.69
2:A:1007:IOD:I	6:A:2032:HOH:O	2.84	0.65
1:A:173:LYS:NZ	4:A:2011:SO4:O4	2.29	0.65
1:B:190:ARG:NH1	6:B:4092:HOH:O	2.33	0.61
5:A:901:HEM:CBD	6:A:2126:HOH:O	2.49	0.60
5:B:902:HEM:CBC	5:B:902:HEM:CHD	2.80	0.60
1:C:89:LYS:NZ	6:C:2099:HOH:O	2.35	0.57
1:B:99:ARG:NH2	6:B:4140:HOH:O	2.37	0.56
1:C:177:ARG:NH1	6:C:2078:HOH:O	2.38	0.56
1:B:141:GLN:NE2	6:B:4119:HOH:O	2.40	0.55
1:A:89:LYS:NZ	6:A:2130:HOH:O	2.44	0.50
1:C:95:GLU:CD	6:C:2069:HOH:O	2.52	0.48
1:B:44:ARG:NH2	6:B:4124:HOH:O	2.46	0.47
1:C:128:HIS:CE1	1:C:196:GLU:OE2	2.68	0.46
1:A:195:LYS:NZ	1:B:164:GLU:O	2.52	0.43
1:C:199:ASP:O	1:C:202:VAL:CG1	2.67	0.42
1:C:183:LEU:O	6:C:2057:HOH:O	2.21	0.42
1:A:97:ARG:NH2	6:A:2115:HOH:O	2.52	0.42
1:B:81:GLU:OE1	6:B:4057:HOH:O	2.22	0.41

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	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	38	17
1	B	209/215 (97%)	205 (98%)	4 (2%)	0	100	100
1	C	204/215 (95%)	201 (98%)	3 (2%)	0	100	100
All	All	620/645 (96%)	607 (98%)	12 (2%)	1 (0%)	56	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PHE

### 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	169/175 (97%)	167 (99%)	2 (1%)	82	69
1	B	170/175 (97%)	167 (98%)	3 (2%)	71	53
1	C	167/175 (95%)	158 (95%)	9 (5%)	31	11
All	All	506/525 (96%)	492 (97%)	14 (3%)	56	32

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	191	GLU
1	B	18	GLN
1	B	95	GLU
1	B	204	ASN

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Mol	Chain	Res	Type
1	C	26	SER
1	C	29	MET
1	C	33	LEU
1	C	101	THR
1	C	132	ARG
1	C	147	MET
1	C	195	LYS
1	C	198	THR
1	C	202	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 26 ligands modelled in this entry, 11 are monoatomic - leaving 15 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	$\# Z  > 2$
4	SO4	A	2007	-	4,4,4	0.19	0	6,6,6	0.28	0
4	SO4	A	2009	-	4,4,4	0.29	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	2011	-	4,4,4	0.32	0	6,6,6	0.37	0
5	HEM	A	901	1,6	49,50,50	2.64	16 (32%)	46,82,82	2.79	13 (28%)
4	SO4	B	2003	-	4,4,4	0.33	0	6,6,6	0.91	1 (16%)
4	SO4	B	2004	-	4,4,4	0.41	0	6,6,6	0.42	0
4	SO4	B	2005	-	4,4,4	0.14	0	6,6,6	0.49	0
4	SO4	B	2006	-	4,4,4	0.19	0	6,6,6	0.45	0
4	SO4	B	2008	-	4,4,4	0.15	0	6,6,6	0.17	0
5	HEM	B	902	1,6	49,50,50	2.96	13 (26%)	46,82,82	2.38	14 (30%)
4	SO4	C	2001	-	4,4,4	0.22	0	6,6,6	0.80	0
4	SO4	C	2002	-	4,4,4	0.41	0	6,6,6	0.89	0
4	SO4	C	2010	-	4,4,4	0.69	0	6,6,6	0.50	0
4	SO4	C	2012	-	4,4,4	0.09	0	6,6,6	0.09	0
5	HEM	C	903	1,6	49,50,50	2.34	14 (28%)	46,82,82	1.91	10 (21%)

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	SO4	A	2007	-	-	0/0/0/0	0/0/0/0
4	SO4	A	2009	-	-	0/0/0/0	0/0/0/0
4	SO4	A	2011	-	-	0/0/0/0	0/0/0/0
5	HEM	A	901	1,6	-	0/14/114/114	0/0/8/8
4	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2004	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2005	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2006	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2008	-	-	0/0/0/0	0/0/0/0
5	HEM	B	902	1,6	-	0/14/114/114	0/0/8/8
4	SO4	C	2001	-	-	0/0/0/0	0/0/0/0
4	SO4	C	2002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	2010	-	-	0/0/0/0	0/0/0/0
4	SO4	C	2012	-	-	0/0/0/0	0/0/0/0
5	HEM	C	903	1,6	-	0/14/114/114	0/0/8/8

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	HEM	C2D-C1D	-14.46	1.40	1.44
5	A	901	HEM	C2D-C1D	-10.61	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	903	HEM	C3D-C4D	6.57	1.46	1.44
5	B	902	HEM	C3C-C2C	-6.53	1.32	1.43
5	B	902	HEM	C3B-C2B	-6.52	1.32	1.43
5	A	901	HEM	C3B-C2B	-6.13	1.33	1.43
5	C	903	HEM	C3B-C2B	-5.97	1.33	1.43
5	C	903	HEM	C3C-C2C	-5.86	1.33	1.43
5	A	901	HEM	C3C-C2C	-5.59	1.34	1.43
5	C	903	HEM	C3C-CAC	4.91	1.55	1.40
5	C	903	HEM	C3D-C2D	4.89	1.52	1.43
5	C	903	HEM	C3B-CAB	4.27	1.53	1.40
5	A	901	HEM	C2B-C1B	4.25	1.45	1.44
5	B	902	HEM	C3B-CAB	4.06	1.53	1.40
5	A	901	HEM	C3C-CAC	3.95	1.52	1.40
5	C	903	HEM	C2D-C1D	3.89	1.45	1.44
5	A	901	HEM	C3D-C2D	3.71	1.50	1.43
5	A	901	HEM	C3D-C4D	-3.66	1.43	1.44
5	B	902	HEM	C3C-CAC	3.49	1.51	1.40
5	C	903	HEM	CMB-C2B	3.43	1.58	1.47
5	B	902	HEM	C3D-C2D	3.42	1.49	1.43
5	A	901	HEM	C3B-CAB	3.39	1.51	1.40
5	B	902	HEM	C2B-C1B	3.37	1.45	1.44
5	A	901	HEM	CHA-C4D	-3.36	1.31	1.35
5	B	902	HEM	C3D-C4D	3.25	1.45	1.44
5	B	902	HEM	C4A-C3A	3.21	1.44	1.40
5	A	901	HEM	CBD-CGD	2.93	1.58	1.50
5	A	901	HEM	C1B-NB	-2.89	1.33	1.39
5	B	902	HEM	FE-ND	2.76	2.07	1.97
5	A	901	HEM	C4A-C3A	2.70	1.43	1.40
5	C	903	HEM	C4A-C3A	2.60	1.43	1.40
5	A	901	HEM	FE-NB	2.42	2.06	1.97
5	B	902	HEM	CAA-C2A	2.40	1.56	1.52
5	A	901	HEM	C3B-C4B	-2.32	1.41	1.44
5	C	903	HEM	O1A-CGA	2.27	1.30	1.22
5	C	903	HEM	CMC-C2C	2.20	1.54	1.47
5	B	902	HEM	CMC-C2C	2.20	1.54	1.47
5	B	902	HEM	CHD-C4C	2.18	1.40	1.36
5	C	903	HEM	CMD-C2D	2.12	1.54	1.47
5	A	901	HEM	FE-NA	2.07	2.01	1.92
5	A	901	HEM	C1D-ND	2.05	1.42	1.37
5	C	903	HEM	C3B-C4B	2.01	1.46	1.44
5	C	903	HEM	FE-NC	2.01	2.05	1.97

All (38) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	HEM	C3B-C4B-NB	-12.71	104.90	114.00
5	B	902	HEM	C3B-C4B-NB	-7.73	108.47	114.00
5	C	903	HEM	C3B-C4B-NB	-6.78	109.15	114.00
5	A	901	HEM	C1B-NB-C4B	6.13	111.43	105.16
5	B	902	HEM	CHD-C1D-ND	5.57	129.21	124.58
5	B	902	HEM	C4D-ND-C1D	5.52	110.81	105.16
5	A	901	HEM	C1A-CHA-C4D	-5.33	120.46	127.47
5	B	902	HEM	CBD-CAD-C3D	-5.30	102.81	114.37
5	C	903	HEM	C4D-ND-C1D	4.84	110.11	105.16
5	C	903	HEM	CHD-C1D-ND	3.80	127.74	124.58
5	B	902	HEM	CMA-C3A-C4A	-3.73	122.88	128.62
5	A	901	HEM	C4C-NC-C1C	3.62	109.30	105.53
5	B	902	HEM	C2D-C1D-ND	-3.51	108.78	112.93
5	C	903	HEM	C2D-C1D-ND	-3.35	108.98	112.93
5	A	901	HEM	CHD-C4C-NC	3.31	127.60	124.73
5	C	903	HEM	CHC-C4B-NB	-3.20	121.92	124.58
5	C	903	HEM	CMA-C3A-C4A	-3.18	123.72	128.62
5	A	901	HEM	CMA-C3A-C4A	-3.04	123.94	128.62
5	A	901	HEM	CMB-C2B-C3B	3.01	133.24	126.16
5	B	902	HEM	CHC-C1C-NC	2.85	127.20	124.73
5	B	902	HEM	CAA-CBA-CGA	-2.84	104.34	113.47
5	C	903	HEM	CAA-CBA-CGA	-2.77	104.56	113.47
5	B	902	HEM	C4A-CHB-C1B	-2.70	123.91	127.47
5	A	901	HEM	CHC-C1C-NC	2.68	127.06	124.73
5	B	902	HEM	C1B-NB-C4B	2.66	107.89	105.16
5	A	901	HEM	C2D-C1D-ND	-2.65	109.81	112.93
5	A	901	HEM	CAA-CBA-CGA	-2.59	105.15	113.47
5	A	901	HEM	CHA-C4D-ND	2.54	127.80	124.31
5	B	902	HEM	C4A-C3A-C2A	2.48	108.72	107.00
5	B	902	HEM	CAD-C3D-C4D	2.45	128.94	124.53
5	C	903	HEM	C4A-C3A-C2A	2.43	108.68	107.00
5	A	901	HEM	C4A-C3A-C2A	2.34	108.62	107.00
5	C	903	HEM	CHA-C4D-ND	2.16	127.28	124.31
4	B	2003	SO4	O2-S-O1	2.16	116.66	109.53
5	B	902	HEM	CHA-C4D-ND	2.09	127.18	124.31
5	C	903	HEM	CHD-C4C-NC	-2.05	122.95	124.73
5	A	901	HEM	CHD-C1D-ND	2.04	126.28	124.58
5	B	902	HEM	O1A-CGA-CBA	-2.01	116.12	123.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	208/215 (96%)	0.28	13 (6%) 19 24	17, 27, 45, 51	0
1	B	210/215 (97%)	0.22	3 (1%) 72 78	16, 26, 38, 43	0
1	C	206/215 (95%)	1.30	50 (24%) 1 2	19, 40, 61, 78	0
All	All	624/645 (96%)	0.60	66 (10%) 7 9	16, 29, 53, 78	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	36	ARG	6.4
1	C	212	GLY	5.9
1	B	6	ALA	5.8
1	A	6	ALA	5.4
1	C	152	GLY	5.2
1	C	206	GLN	5.0
1	C	27	THR	4.7
1	C	35	GLY	4.5
1	C	210	ASP	4.2
1	B	184	GLU	3.9
1	C	150	HIS	3.9
1	A	101	THR	3.9
1	C	21	GLU	3.8
1	C	184	GLU	3.8
1	C	18	GLN	3.7
1	A	213	LYS	3.6
1	C	151	TYR	3.6
1	C	143	ILE	3.5
1	A	187	ASP	3.4
1	C	165	GLY	3.3
1	C	202	VAL	3.3
1	C	147	MET	3.2
1	C	34	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	25	HIS	3.2
1	A	92	GLY	3.2
1	A	98	SER	3.0
1	C	37	LEU	2.9
1	C	17	ALA	2.9
1	C	156	GLU	2.9
1	A	99	ARG	2.8
1	C	154	ASP	2.8
1	B	164	GLU	2.8
1	C	211	LEU	2.7
1	C	104	PRO	2.7
1	C	76	ALA	2.6
1	C	16	THR	2.6
1	C	8	LEU	2.5
1	C	14	GLN	2.5
1	C	169	LEU	2.5
1	C	67	GLY	2.5
1	C	182	ASN	2.5
1	C	148	GLN	2.5
1	A	25	HIS	2.4
1	C	42	PHE	2.4
1	C	178	GLU	2.4
1	C	103	SER	2.4
1	C	38	GLY	2.4
1	C	146	MET	2.4
1	C	194	LEU	2.3
1	A	95	GLU	2.3
1	A	18	GLN	2.3
1	C	31	ASP	2.2
1	C	155	PRO	2.2
1	C	161	TYR	2.2
1	C	70	GLU	2.2
1	C	44	ARG	2.2
1	A	94	SER	2.2
1	C	11	GLU	2.1
1	C	205	HIS	2.1
1	C	68	PHE	2.1
1	A	208	PHE	2.1
1	C	108	ASP	2.1
1	C	40	ALA	2.1
1	C	30	SER	2.1
1	C	144	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	45	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	B	4002	1/1	0.30	12.34	57,57,57,57	0
4	SO4	A	2009	5/5	0.28	10.08	62,64,68,69	0
4	SO4	A	2011	5/5	0.14	6.69	51,55,56,58	0
4	SO4	B	2003	5/5	0.29	5.76	63,64,66,67	0
4	SO4	C	2012	5/5	0.34	4.40	76,76,77,77	0
3	NA	B	4001	1/1	0.23	3.84	50,50,50,50	0
4	SO4	B	2004	5/5	0.27	3.79	40,43,45,47	0
4	SO4	C	2001	5/5	0.25	2.60	53,55,57,57	0
4	SO4	B	2008	5/5	0.29	2.01	95,95,96,96	0
4	SO4	A	2007	5/5	0.24	2.00	79,79,80,81	0
4	SO4	B	2005	5/5	0.23	1.70	62,67,68,69	0
2	IOD	B	1003	1/1	0.14	1.38	64,64,64,64	0
2	IOD	A	1009	1/1	0.15	1.35	49,49,49,49	0
4	SO4	C	2002	5/5	0.20	1.31	62,62,64,64	0
4	SO4	B	2006	5/5	0.23	1.23	80,80,81,82	0
4	SO4	C	2010	5/5	0.30	1.17	40,49,54,54	0
5	HEM	A	901	43/43	0.12	0.51	18,28,46,56	0
5	HEM	B	902	43/43	0.11	0.11	18,26,41,54	0
2	IOD	B	1002	1/1	0.12	-0.07	45,45,45,45	0
5	HEM	C	903	43/43	0.14	-0.15	31,38,52,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IOD	A	1007	1/1	0.12	-0.53	54,54,54,54	0
2	IOD	A	1006	1/1	0.11	-0.86	77,77,77,77	0
2	IOD	C	1001	1/1	0.07	-1.43	41,41,41,41	0
2	IOD	B	1005	1/1	0.06	-1.91	44,44,44,44	0
2	IOD	B	1004	1/1	0.04	-4.94	74,74,74,74	0
2	IOD	A	1008	1/1	0.04	-9.76	56,56,56,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.