Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:47 PM GMT

PDB ID	:	1V8X
Title	:	Crystal Structure of the Dioxygen-bound Heme Oxygenase from Corynebacterium diphtheriae
Authors	:	Unno, M.; Matsui, T.; Chu, G.C.; Couture, M.; Yoshida, T.; Rousseau, D.L.; Olson, J.S.; Ikeda-Saito, M.
Deposited on	:	2004-01-15
Resolution	:	1.85 Å(reported)

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

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

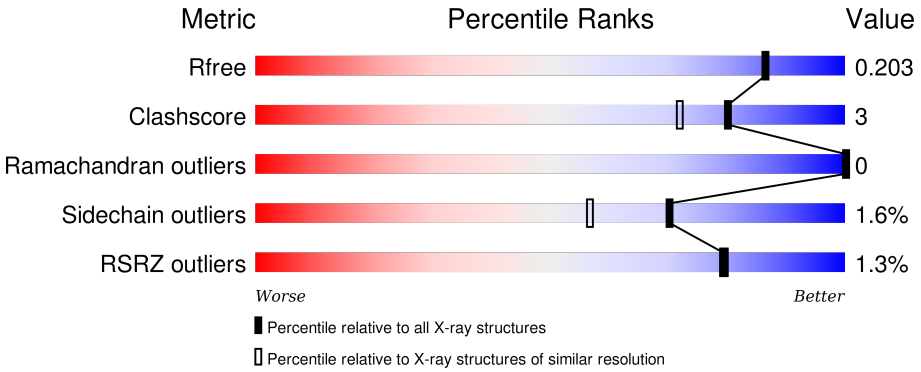
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	2% 88% 9%
1	B	215	88% 8%
1	C	215	2% 89% 7%

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	A	2003	-	-	-	X
3	SO4	A	2007	-	-	-	X
3	SO4	B	2006	-	-	-	X
3	SO4	B	2008	-	-	-	X
3	SO4	C	2002	-	-	-	X
3	SO4	C	2004	-	-	-	X
3	SO4	C	2005	-	-	-	X
3	SO4	C	2012	-	-	-	X
5	OXY	B	5002	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5679 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.

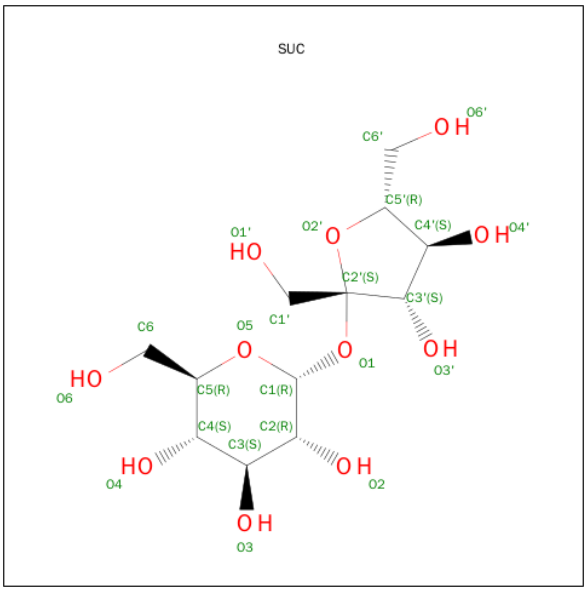
- Molecule 1 is a protein called Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	1	0
			1674	1054	299	318	3			
1	B	209	Total	C	N	O	S	0	3	0
			1676	1054	298	321	3			
1	C	208	Total	C	N	O	S	0	1	0
			1662	1048	294	317	3			

There are 15 discrepancies between the modelled and reference sequences:

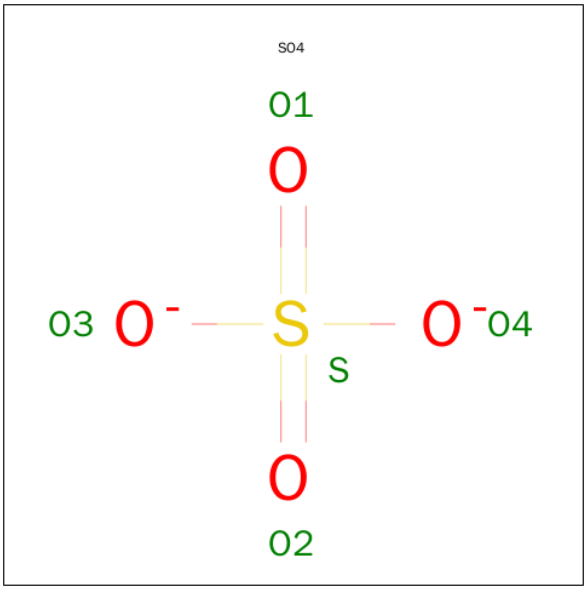
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	LYS	GLU	SEE REMARK 999	UNP P71119
A	60	VAL	ALA	SEE REMARK 999	UNP P71119
A	92	GLY	ASP	SEE REMARK 999	UNP P71119
A	93	SER	GLY	SEE REMARK 999	UNP P71119
A	192	HIS	ASN	SEE REMARK 999	UNP P71119
B	334	LYS	GLU	SEE REMARK 999	UNP P71119
B	360	VAL	ALA	SEE REMARK 999	UNP P71119
B	392	GLY	ASP	SEE REMARK 999	UNP P71119
B	393	SER	GLY	SEE REMARK 999	UNP P71119
B	492	HIS	ASN	SEE REMARK 999	UNP P71119
C	634	LYS	GLU	SEE REMARK 999	UNP P71119
C	660	VAL	ALA	SEE REMARK 999	UNP P71119
C	692	GLY	ASP	SEE REMARK 999	UNP P71119
C	693	SER	GLY	SEE REMARK 999	UNP P71119
C	792	HIS	ASN	SEE REMARK 999	UNP P71119

- Molecule 2 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



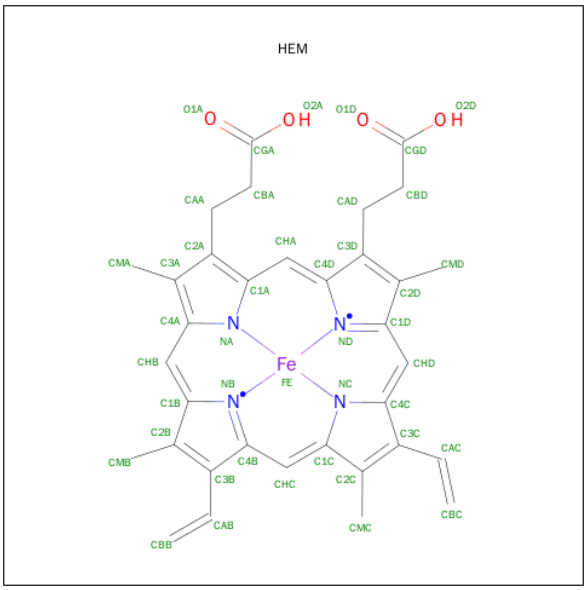
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

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



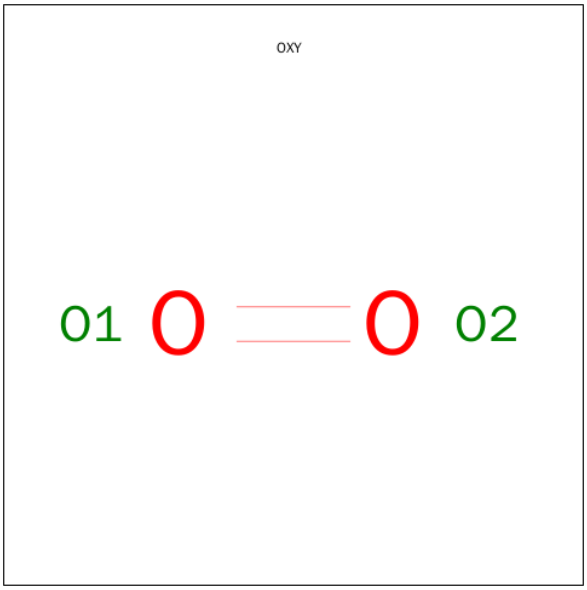
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Fe N O 43 34 1 4 4	0	0
4	B	1	Total C Fe N O 43 34 1 4 4	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		
5	C	1	Total	O	0	0
			2	2		

- Molecule 6 is water.

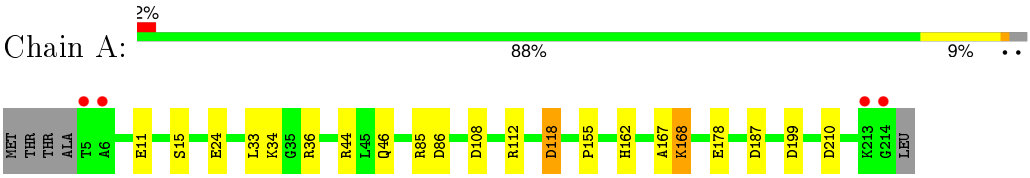
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	152	Total	O	0	0
			152	152		
6	B	164	Total	O	0	0
			164	164		
6	C	133	Total	O	0	0
			133	133		

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.

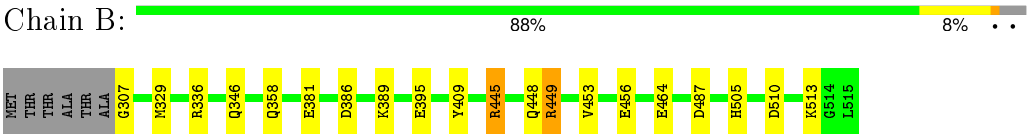
- Molecule 1: Heme oxygenase

Chain A:



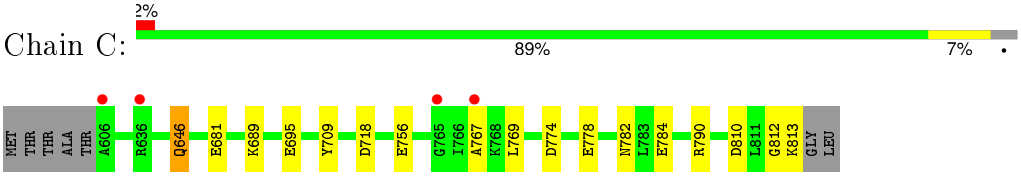
- Molecule 1: Heme oxygenase

Chain B:



- Molecule 1: Heme oxygenase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.00Å 62.97Å 107.49Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 40.56 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.85) 100.0 (40.56-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.153 , 0.193 0.166 , 0.203	Depositor DCC
R_{free} test set	6150 reflections (11.30%)	DCC
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 60599 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5679	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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, SUC, OXY, 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	0.94	0/1711	0.96	7/2310 (0.3%)
1	B	0.97	1/1725 (0.1%)	1.01	9/2328 (0.4%)
1	C	0.94	1/1698 (0.1%)	0.96	5/2293 (0.2%)
All	All	0.95	2/5134 (0.0%)	0.98	21/6931 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	681	GLU	CD-OE1	7.22	1.33	1.25
1	B	381	GLU	CD-OE1	5.93	1.32	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	445[A]	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	445[B]	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	C	718	ASP	CB-CG-OD2	7.61	125.15	118.30
1	C	790	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	445[A]	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	B	445[B]	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	B	487	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	386	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	86	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	449	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	108	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	810	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	329	MET	CG-SD-CE	-5.84	90.85	100.20
1	A	210	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	85	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	336	ARG	NE-CZ-NH2	-5.67	117.46	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	187	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	709	TYR	CB-CG-CD1	5.39	124.24	121.00
1	A	118	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	44	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	774	ASP	CB-CG-OD2	5.07	122.86	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	1674	0	1635	10	1
1	B	1676	0	1628	11	1
1	C	1662	0	1618	11	0
2	A	23	0	22	0	0
3	A	15	0	0	1	0
3	B	20	0	0	0	0
3	C	25	0	0	0	0
4	A	43	0	30	4	0
4	B	43	0	30	0	0
4	C	43	0	30	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	A	152	0	0	2	0
6	B	164	0	0	5	0
6	C	133	0	0	4	0
All	All	5679	0	4993	35	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 3.

All (35) 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)
3:A:2003:SO4:O3	6:A:5149:HOH:O	1.97	0.81
4:A:901:HEM:HHD	4:A:901:HEM:HBC2	1.67	0.77
1:A:168:LYS:HD2	1:A:168:LYS:H	1.61	0.63
1:B:307:GLY:N	6:B:5163:HOH:O	2.31	0.63
1:A:118:ASP:OD2	1:B:445[A]:ARG:NH2	2.32	0.61
1:B:358:GLN:NE2	6:B:5141:HOH:O	2.35	0.58
1:C:767:ALA:HA	6:C:272:HOH:O	2.02	0.58
1:C:695:GLU:HG3	6:C:438:HOH:O	2.04	0.57
1:C:646:GLN:HA	1:C:646:GLN:HE21	1.70	0.57
1:C:646:GLN:NE2	1:C:646:GLN:HA	2.20	0.55
1:B:448:GLN:HG2	1:B:453:VAL:O	2.07	0.55
1:B:389:LYS:CE	6:B:5080:HOH:O	2.56	0.54
1:B:510:ASP:HA	1:B:513:LYS:HE2	1.90	0.54
1:C:812:GLY:O	1:C:813:LYS:HB2	2.10	0.52
1:B:389:LYS:HE2	6:B:5080:HOH:O	2.11	0.50
1:A:34:LYS:HG3	1:A:36:ARG:HG3	1.92	0.50
1:C:689:LYS:HD2	1:C:756:GLU:O	2.14	0.48
1:B:389:LYS:HE3	6:B:5080:HOH:O	2.14	0.47
1:A:155:PRO:O	1:A:162:HIS:HE1	1.99	0.46
1:A:11:GLU:O	1:A:15:SER:HB2	2.16	0.45
1:A:168:LYS:H	1:A:168:LYS:CD	2.21	0.44
1:B:346:GLN:HA	1:B:346:GLN:NE2	2.33	0.44
1:A:178:GLU:HG3	6:A:5142:HOH:O	2.17	0.44
1:B:505:HIS:HD2	1:B:505:HIS:O	2.01	0.43
1:C:689:LYS:HE3	6:C:362:HOH:O	2.18	0.43
1:A:46:GLN:HA	1:A:46:GLN:NE2	2.32	0.43
1:A:33:LEU:HD11	4:A:901:HEM:HMC1	2.01	0.42
1:C:778[B]:GLU:HG3	1:C:782:ASN:ND2	2.34	0.42
1:C:689:LYS:CE	6:C:362:HOH:O	2.67	0.42
4:A:901:HEM:CHD	4:A:901:HEM:HBC2	2.37	0.42
1:B:389:LYS:HD2	1:B:456:GLU:O	2.20	0.42
1:C:812:GLY:O	1:C:813:LYS:CB	2.68	0.42
1:A:112[B]:ARG:NH1	1:A:199:ASP:OD2	2.50	0.42
1:C:646:GLN:CA	1:C:646:GLN:HE21	2.33	0.41
4:A:901:HEM:HBB2	4:A:901:HEM:CMB	2.51	0.41

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:A:167:ALA:O	1:B:449:ARG:NH2[2_645]	2.18	0.02

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	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
1	B	210/215 (98%)	206 (98%)	4 (2%)	0	100	100
1	C	207/215 (96%)	203 (98%)	4 (2%)	0	100	100
All	All	626/645 (97%)	612 (98%)	14 (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	172/175 (98%)	170 (99%)	2 (1%)	78	69
1	B	174/175 (99%)	171 (98%)	3 (2%)	68	54
1	C	171/175 (98%)	168 (98%)	3 (2%)	66	52
All	All	517/525 (98%)	509 (98%)	8 (2%)	70	60

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	168	LYS
1	B	395	GLU
1	B	409	TYR
1	B	464	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	646	GLN
1	C	769	LEU
1	C	784	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	B	346	GLN
1	B	358	GLN
1	B	506	GLN
1	C	625	HIS
1	C	646	GLN
1	C	762	HIS
1	C	782	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)

19 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	2003	-	4,4,4	0.51	0	6,6,6	0.64	0
3	SO4	A	2007	-	4,4,4	0.26	0	6,6,6	0.38	0
3	SO4	A	2011	-	4,4,4	0.29	0	6,6,6	0.69	0
2	SUC	A	3001	-	24,24,24	0.82	0	36,36,36	1.04	4 (11%)
5	OXY	A	5001	4	1,1,1	0.19	0	0,0,0	0.00	-
4	HEM	A	901	1,5	30,50,50	2.31	7 (23%)	24,82,82	2.39	9 (37%)
3	SO4	B	2001	-	4,4,4	0.32	0	6,6,6	0.35	0
3	SO4	B	2006	-	4,4,4	1.39	1 (25%)	6,6,6	0.78	0
3	SO4	B	2008	-	4,4,4	0.42	0	6,6,6	0.34	0
3	SO4	B	2009	-	4,4,4	0.13	0	6,6,6	0.26	0
5	OXY	B	5002	4	1,1,1	0.30	0	0,0,0	0.00	-
4	HEM	B	902	1,5	30,50,50	2.45	6 (20%)	24,82,82	2.78	16 (66%)
3	SO4	C	2002	-	4,4,4	0.37	0	6,6,6	0.38	0
3	SO4	C	2004	-	4,4,4	0.14	0	6,6,6	0.19	0
3	SO4	C	2005	-	4,4,4	0.60	0	6,6,6	0.73	0
3	SO4	C	2010	-	4,4,4	0.09	0	6,6,6	0.35	0
3	SO4	C	2012	-	4,4,4	0.05	0	6,6,6	0.26	0
5	OXY	C	5003	4	1,1,1	0.41	0	0,0,0	0.00	-
4	HEM	C	903	1,5	30,50,50	2.59	7 (23%)	24,82,82	2.72	13 (54%)

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	2003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2007	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2011	-	-	0/0/0/0	0/0/0/0
2	SUC	A	3001	-	-	0/12/51/51	0/2/2/2
5	OXY	A	5001	4	-	0/0/0/0	0/0/0/0
4	HEM	A	901	1,5	-	0/10/54/54	0/0/8/8
3	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2006	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2008	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2009	-	-	0/0/0/0	0/0/0/0
5	OXY	B	5002	4	-	0/0/0/0	0/0/0/0
4	HEM	B	902	1,5	-	0/10/54/54	0/0/8/8
3	SO4	C	2002	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2004	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2005	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	C	2010	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2012	-	-	0/0/0/0	0/0/0/0
5	OXY	C	5003	4	-	0/0/0/0	0/0/0/0
4	HEM	C	903	1,5	-	0/10/54/54	0/0/8/8

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	HEM	C3B-C4B	-10.03	1.42	1.51
4	C	903	HEM	C3B-C4B	-9.61	1.43	1.51
4	A	901	HEM	C3B-C4B	-8.03	1.44	1.51
4	C	903	HEM	C3D-C4D	-6.27	1.43	1.51
4	A	901	HEM	C3D-C4D	-6.06	1.43	1.51
4	A	901	HEM	C2C-C1C	-4.61	1.43	1.52
4	B	902	HEM	C3D-C4D	-4.30	1.46	1.51
4	B	902	HEM	C2C-C1C	-3.50	1.45	1.52
4	C	903	HEM	C2C-C1C	-3.22	1.46	1.52
4	B	902	HEM	C2B-C1B	-2.81	1.42	1.51
4	C	903	HEM	C2B-C1B	-2.45	1.43	1.51
4	A	901	HEM	C2B-C1B	-2.36	1.44	1.51
4	A	901	HEM	C2D-C1D	-2.30	1.44	1.51
4	B	902	HEM	C2D-C1D	-2.20	1.44	1.51
4	C	903	HEM	C4C-NC	2.13	1.38	1.36
3	B	2006	SO4	O3-S	2.40	1.56	1.47
4	A	901	HEM	FE-NC	2.52	2.05	1.95
4	A	901	HEM	C1C-NC	2.73	1.39	1.36
4	C	903	HEM	C1C-NC	2.98	1.39	1.36
4	C	903	HEM	FE-NC	4.06	2.11	1.95
4	B	902	HEM	FE-NC	4.31	2.12	1.95

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	903	HEM	C3C-CAC-CBC	-5.67	115.76	124.46
4	B	902	HEM	C3C-CAC-CBC	-5.14	116.57	124.46
4	B	902	HEM	CMA-C3A-C4A	-3.89	121.92	128.36
4	A	901	HEM	CMA-C3A-C4A	-3.67	122.29	128.36
4	B	902	HEM	C3B-CAB-CBB	-3.63	118.89	124.46
4	B	902	HEM	CAA-CBA-CGA	-3.55	106.24	112.75
4	A	901	HEM	C3C-CAC-CBC	-3.39	119.26	124.46
4	C	903	HEM	CBD-CAD-C3D	-3.37	103.74	113.55
4	C	903	HEM	CAA-C2A-C1A	-3.27	123.46	127.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	903	HEM	C3B-CAB-CBB	-2.89	120.02	124.46
2	A	3001	SUC	O1'-C1'-C2'	-2.81	102.92	111.91
4	A	901	HEM	C3B-CAB-CBB	-2.79	120.18	124.46
4	C	903	HEM	CAA-CBA-CGA	-2.57	108.03	112.75
4	B	902	HEM	C3B-C4B-NB	-2.51	106.83	111.63
4	B	902	HEM	CBD-CAD-C3D	-2.50	106.27	113.55
4	B	902	HEM	CAA-C2A-C1A	-2.45	124.35	127.01
2	A	3001	SUC	C4-C3-C2	-2.35	106.40	110.79
2	A	3001	SUC	O4-C4-C3	-2.23	105.31	110.34
4	C	903	HEM	C3B-C4B-NB	-2.14	107.53	111.63
4	A	901	HEM	CAA-CBA-CGA	-2.08	108.93	112.75
4	C	903	HEM	C2D-C3D-C4D	2.01	104.91	101.50
4	B	902	HEM	CMA-C3A-C2A	2.01	129.45	125.24
4	B	902	HEM	CHC-C4B-NB	2.02	129.38	124.52
4	A	901	HEM	CMD-C2D-C3D	2.07	123.49	114.35
4	B	902	HEM	CHD-C1D-ND	2.30	130.07	124.52
4	A	901	HEM	CMC-C2C-C3C	2.33	122.36	116.53
4	C	903	HEM	CHD-C1D-ND	2.45	130.42	124.52
4	B	902	HEM	C2D-C3D-C4D	2.62	105.94	101.50
4	B	902	HEM	CMD-C2D-C3D	2.67	126.17	114.35
4	C	903	HEM	CMD-C2D-C3D	2.82	126.84	114.35
4	B	902	HEM	CMC-C2C-C3C	2.93	123.85	116.53
2	A	3001	SUC	O3-C3-C2	3.00	117.10	110.34
4	C	903	HEM	CMB-C2B-C3B	3.33	124.84	116.53
4	C	903	HEM	CAD-C3D-C4D	3.87	126.11	112.47
4	B	902	HEM	CAD-C3D-C2D	4.15	125.14	113.22
4	C	903	HEM	CMC-C2C-C3C	4.44	127.61	116.53
4	B	902	HEM	CMB-C2B-C3B	4.51	127.78	116.53
4	B	902	HEM	CAD-C3D-C4D	4.66	128.91	112.47
4	A	901	HEM	CAD-C3D-C4D	4.68	128.97	112.47
4	A	901	HEM	CAD-C3D-C2D	4.91	127.33	113.22
4	C	903	HEM	CAD-C3D-C2D	5.48	128.96	113.22
4	A	901	HEM	CMB-C2B-C3B	5.52	130.31	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2003	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	HEM	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	210/215 (97%)	-0.15	4 (1%) 70 69	11, 20, 35, 48	0
1	B	209/215 (97%)	-0.35	0 100 100	10, 19, 35, 40	1 (0%)
1	C	208/215 (96%)	-0.31	4 (1%) 70 69	12, 22, 40, 49	0
All	All	627/645 (97%)	-0.27	8 (1%) 79 79	10, 20, 36, 49	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	GLY	4.6
1	C	606	ALA	4.4
1	C	767	ALA	3.5
1	A	213	LYS	3.2
1	C	765	GLY	2.9
1	A	5	THR	2.7
1	C	636	ARG	2.5
1	A	6	ALA	2.3

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	OXY	B	5002	2/2	0.99	0.20	17.47	26,26,26,32	0
3	SO4	C	2005	5/5	0.89	0.36	8.30	45,51,52,53	0
3	SO4	B	2006	5/5	0.87	0.25	8.11	28,34,44,45	0
3	SO4	C	2012	5/5	0.71	0.25	4.77	80,81,82,83	0
3	SO4	A	2007	5/5	0.92	0.25	4.00	52,53,57,58	0
3	SO4	B	2008	5/5	0.93	0.25	3.33	56,58,60,61	0
3	SO4	C	2002	5/5	0.90	0.22	2.83	45,45,50,50	0
3	SO4	A	2003	5/5	0.86	0.15	2.19	55,56,59,60	0
3	SO4	C	2004	5/5	0.82	0.32	2.05	74,75,76,76	0
5	OXY	C	5003	2/2	0.98	0.12	1.89	33,33,33,33	0
2	SUC	A	3001	23/23	0.88	0.14	0.46	21,27,30,35	0
3	SO4	A	2011	5/5	0.83	0.17	0.38	68,71,72,73	0
4	HEM	B	902	43/43	0.97	0.09	-0.00	15,22,43,57	0
5	OXY	A	5001	2/2	0.99	0.11	-0.05	31,31,31,31	0
4	HEM	A	901	43/43	0.99	0.10	-0.10	10,16,23,31	0
4	HEM	C	903	43/43	0.98	0.08	-0.37	17,22,36,48	0
3	SO4	C	2010	5/5	0.78	0.25	-	92,93,94,94	0
3	SO4	B	2001	5/5	0.97	0.11	-	39,39,42,43	0
3	SO4	B	2009	5/5	0.94	0.30	-	52,52,53,56	0

6.5 Other polymers (i)

There are no such residues in this entry.