



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:23 PM GMT

PDB ID : 3ON5  
Title : Crystal structure of a xanthine dehydrogenase (BH1974) from *Bacillus halodurans* at 2.80 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2010-08-27  
Resolution : 2.80 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>

---

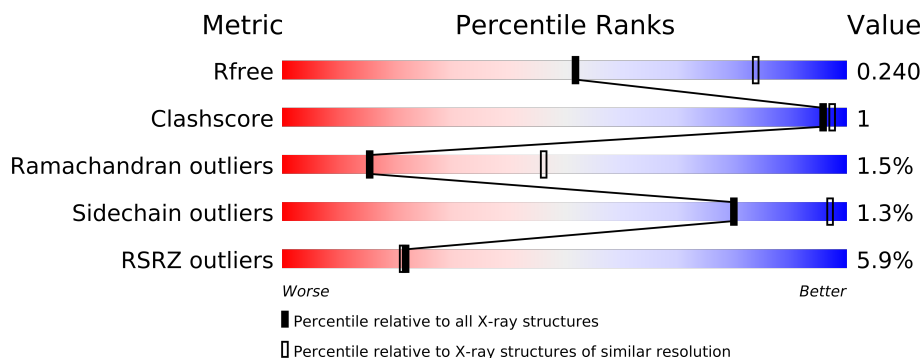
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	362	
1	B	362	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5218 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 BH1974 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	Se	0	5	0
			2651	1714	443	485	4	5			
1	B	323	Total	C	N	O	S	Se	0	1	0
			2514	1637	414	454	3	6			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MSE	-	EXPRESSION TAG	UNP Q9KBF4
A	-17	GLY	-	EXPRESSION TAG	UNP Q9KBF4
A	-16	SER	-	EXPRESSION TAG	UNP Q9KBF4
A	-15	ASP	-	EXPRESSION TAG	UNP Q9KBF4
A	-14	LYS	-	EXPRESSION TAG	UNP Q9KBF4
A	-13	ILE	-	EXPRESSION TAG	UNP Q9KBF4
A	-12	HIS	-	EXPRESSION TAG	UNP Q9KBF4
A	-11	HIS	-	EXPRESSION TAG	UNP Q9KBF4
A	-10	HIS	-	EXPRESSION TAG	UNP Q9KBF4
A	-9	HIS	-	EXPRESSION TAG	UNP Q9KBF4
A	-8	HIS	-	EXPRESSION TAG	UNP Q9KBF4
A	-7	HIS	-	EXPRESSION TAG	UNP Q9KBF4
A	-6	GLU	-	EXPRESSION TAG	UNP Q9KBF4
A	-5	ASN	-	EXPRESSION TAG	UNP Q9KBF4
A	-4	LEU	-	EXPRESSION TAG	UNP Q9KBF4
A	-3	TYR	-	EXPRESSION TAG	UNP Q9KBF4
A	-2	PHE	-	EXPRESSION TAG	UNP Q9KBF4
A	-1	GLN	-	EXPRESSION TAG	UNP Q9KBF4
A	0	GLY	-	EXPRESSION TAG	UNP Q9KBF4
B	-18	MSE	-	EXPRESSION TAG	UNP Q9KBF4
B	-17	GLY	-	EXPRESSION TAG	UNP Q9KBF4
B	-16	SER	-	EXPRESSION TAG	UNP Q9KBF4
B	-15	ASP	-	EXPRESSION TAG	UNP Q9KBF4
B	-14	LYS	-	EXPRESSION TAG	UNP Q9KBF4
B	-13	ILE	-	EXPRESSION TAG	UNP Q9KBF4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	EXPRESSION TAG	UNP Q9KBF4
B	-11	HIS	-	EXPRESSION TAG	UNP Q9KBF4
B	-10	HIS	-	EXPRESSION TAG	UNP Q9KBF4
B	-9	HIS	-	EXPRESSION TAG	UNP Q9KBF4
B	-8	HIS	-	EXPRESSION TAG	UNP Q9KBF4
B	-7	HIS	-	EXPRESSION TAG	UNP Q9KBF4
B	-6	GLU	-	EXPRESSION TAG	UNP Q9KBF4
B	-5	ASN	-	EXPRESSION TAG	UNP Q9KBF4
B	-4	LEU	-	EXPRESSION TAG	UNP Q9KBF4
B	-3	TYR	-	EXPRESSION TAG	UNP Q9KBF4
B	-2	PHE	-	EXPRESSION TAG	UNP Q9KBF4
B	-1	GLN	-	EXPRESSION TAG	UNP Q9KBF4
B	0	GLY	-	EXPRESSION TAG	UNP Q9KBF4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	29	Total O 29 29	0	0
3	B	22	Total O 22 22	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.24Å 94.24Å 245.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.24 – 2.80 74.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (94.24-2.80) 99.8 (74.76-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.195 , 0.222 0.212 , 0.240	Depositor DCC
$R_{free}$ test set	1418 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.1	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 28133 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: CL

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	0.50	0/2725	0.70	0/3701
1	B	0.49	0/2575	0.67	0/3500
All	All	0.50	0/5300	0.69	0/7201

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	GLN	Mainchain,Peptide

### 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	2651	0	0	4	0
1	B	2514	0	0	3	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
3	A	29	0	0	0	0
3	B	22	0	0	0	0
All	All	5218	0	0	6	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 1.

All (6) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:257:ASP:OD2	1:B:280:ARG:NH2	2.27	0.68
1:A:19:MSE:CE	1:A:36:MSE:SE	3.02	0.57
1:A:257:ASP:OD2	1:A:280:ARG:NH2	2.37	0.57
1:A:287:ASN:CA	2:A:345:CL:CL	2.94	0.52
1:B:152:TRP:NE1	1:B:154:SER:O	2.45	0.50
1:A:90:SER:O	1:B:280:ARG:NH1	2.50	0.44

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	339/362 (94%)	313 (92%)	17 (5%)	9 (3%)	8	25
1	B	318/362 (88%)	295 (93%)	21 (7%)	2 (1%)	33	72
All	All	657/724 (91%)	608 (92%)	38 (6%)	11 (2%)	15	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	14[A]	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	14[B]	ASP
1	A	155	GLY
1	A	166	GLU
1	A	84	LEU
1	A	154	SER
1	A	168	GLU
1	A	12	GLY
1	B	0	GLY
1	B	82	ASP

### 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	279/316 (88%)	275 (99%)	4 (1%)	78	96
1	B	254/316 (80%)	251 (99%)	3 (1%)	82	97
All	All	533/632 (84%)	526 (99%)	7 (1%)	80	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	92	CYS
1	A	230	ASP
1	A	287	ASN
1	B	54	LEU
1	B	78	LEU
1	B	230	ASP

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	336/362 (92%)	0.29	10 (2%) 48 49	39, 63, 105, 135	0
1	B	323/362 (89%)	0.48	29 (8%) 10 8	36, 79, 135, 155	0
All	All	659/724 (91%)	0.38	39 (5%) 22 21	36, 69, 123, 155	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	ASN	8.1
1	A	81	GLU	7.0
1	B	334	TYR	6.2
1	A	166	GLU	5.6
1	B	327	GLN	5.3
1	B	330	SER	5.0
1	B	332	PHE	4.1
1	B	161	ILE	4.1
1	B	336	PHE	4.1
1	A	49	LEU	4.1
1	B	338	PRO	4.0
1	B	329	SER	4.0
1	B	165	ASP	4.0
1	A	168	GLU	3.9
1	B	142	ILE	3.8
1	B	337	GLN	3.7
1	A	165	ASP	3.5
1	A	170	PRO	3.4
1	A	327	GLN	3.3
1	B	335	LEU	3.3
1	B	147	VAL	3.2
1	B	144	ASP	3.0
1	B	333	SER	3.0
1	B	42	ASP	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	15	GLN	2.9
1	B	331	PRO	2.8
1	A	164	ILE	2.7
1	B	115	TYR	2.7
1	B	156	HIS	2.5
1	B	146	SER	2.5
1	B	143	LEU	2.4
1	B	28	SER	2.4
1	B	160	TRP	2.3
1	B	164	ILE	2.3
1	B	120	ALA	2.2
1	B	167	ASN	2.2
1	B	166	GLU	2.2
1	A	147	VAL	2.1
1	B	103	VAL	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
2	CL	B	344	1/1	0.15	-0.95	63,63,63,63	0
2	CL	A	345	1/1	0.13	-2.02	121,121,121,121	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.