



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:43 am GMT

PDB ID : 2RDY  
Title : Crystal structure of a putative glycoside hydrolase family protein from *Bacillus halodurans*  
Authors : Sugadev, R.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-09-25  
Resolution : 2.03 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

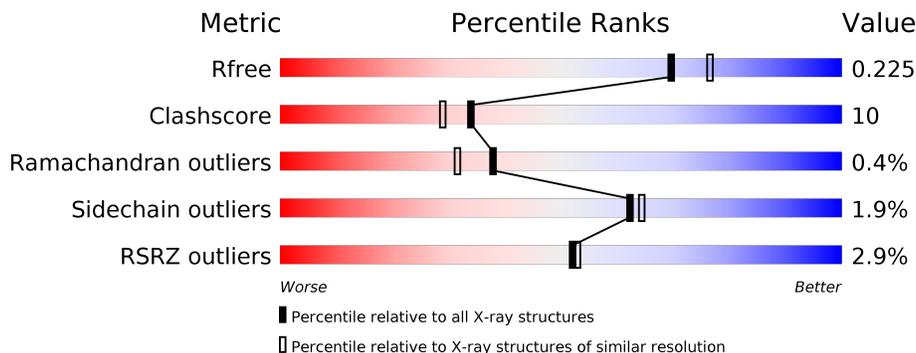
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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))
$R_{free}$	100719	8396 (2.04-2.00)
Clashscore	112137	9678 (2.04-2.00)
Ramachandran outliers	110173	9566 (2.04-2.00)
Sidechain outliers	110143	9565 (2.04-2.00)
RSRZ outliers	101464	8490 (2.04-2.00)

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	803	 2% 79% 18% ..
1	B	803	 3% 80% 17% ..

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13037 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 BH0842 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	787	6239	3955	1076	1181	9	18	0	0	0
1	B	787	6239	3955	1076	1181	9	18	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q9KEL0
A	2	SER	-	EXPRESSION TAG	UNP Q9KEL0
A	3	LEU	-	EXPRESSION TAG	UNP Q9KEL0
A	796	GLU	-	EXPRESSION TAG	UNP Q9KEL0
A	797	GLY	-	EXPRESSION TAG	UNP Q9KEL0
A	798	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	799	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	800	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	801	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	802	HIS	-	EXPRESSION TAG	UNP Q9KEL0
A	803	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	1	MSE	-	EXPRESSION TAG	UNP Q9KEL0
B	2	SER	-	EXPRESSION TAG	UNP Q9KEL0
B	3	LEU	-	EXPRESSION TAG	UNP Q9KEL0
B	796	GLU	-	EXPRESSION TAG	UNP Q9KEL0
B	797	GLY	-	EXPRESSION TAG	UNP Q9KEL0
B	798	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	799	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	800	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	801	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	802	HIS	-	EXPRESSION TAG	UNP Q9KEL0
B	803	HIS	-	EXPRESSION TAG	UNP Q9KEL0

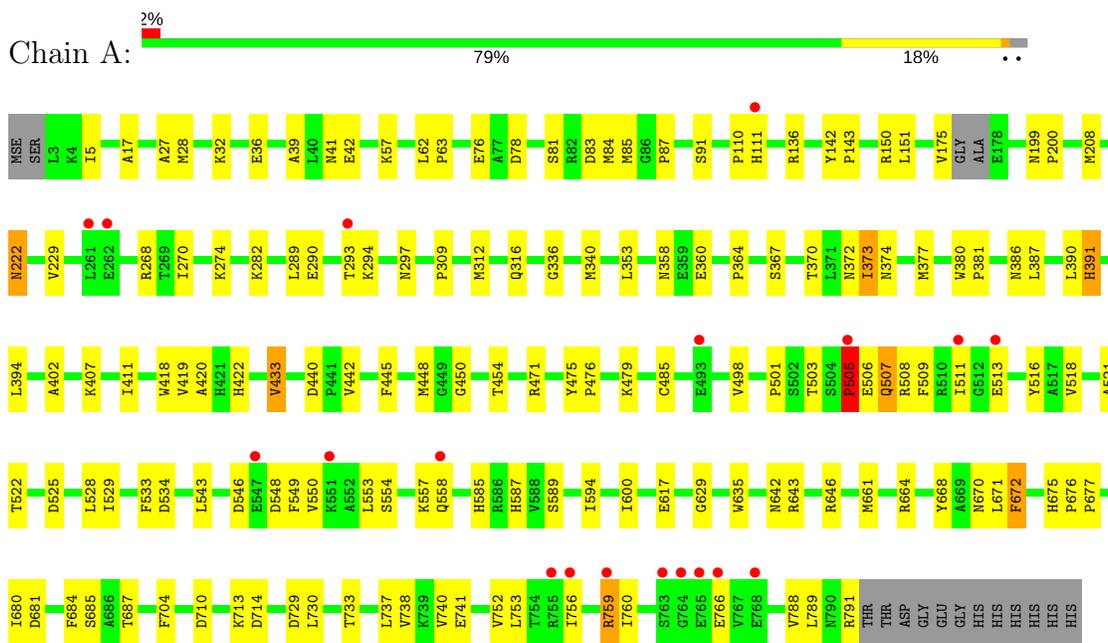
- Molecule 2 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	A	275	Total 275	O 275	0	0
2	B	284	Total 284	O 284	0	0

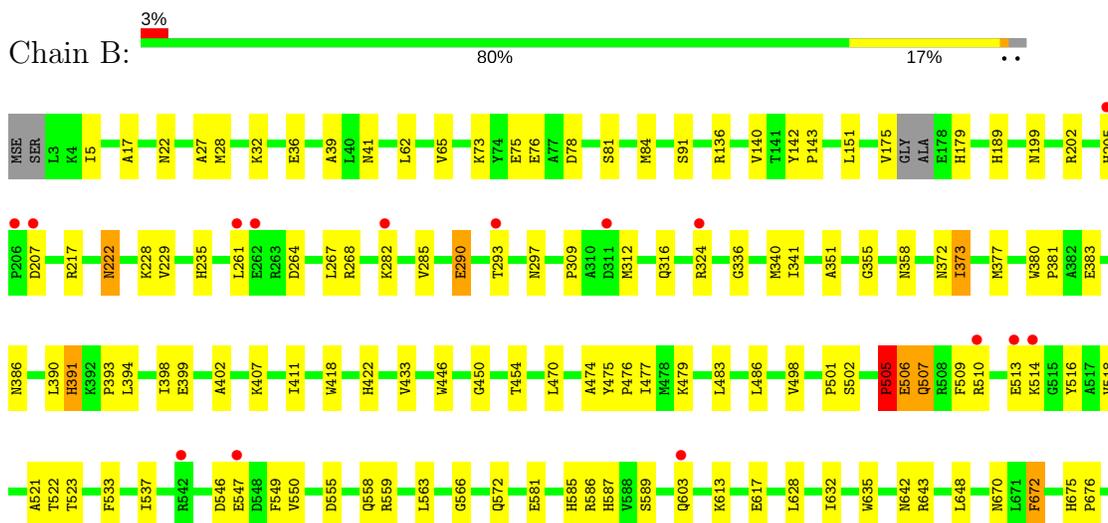
### 3 Residue-property plots i

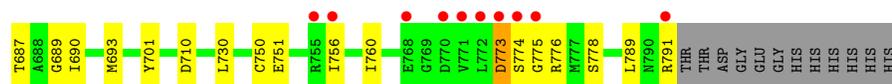
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: BH0842 protein



- Molecule 1: BH0842 protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.61Å 149.07Å 164.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 2.03 47.57 – 2.03	Depositor EDS
% Data completeness (in resolution range)	93.6 (47.57-2.03) 93.8 (47.57-2.03)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.55 (at 2.03Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.198 , 0.225 0.197 , 0.225	Depositor DCC
$R_{free}$ test set	6536 reflections (6.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.9	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.94 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.4057e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.33	0/6378	0.60	2/8621 (0.0%)
1	B	0.34	0/6378	0.60	1/8621 (0.0%)
All	All	0.33	0/12756	0.60	3/17242 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	ILE	N-CA-C	-5.28	96.75	111.00
1	A	42	GLU	N-CA-C	-5.14	97.13	111.00
1	A	5	ILE	N-CA-C	-5.10	97.23	111.00

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	6239	0	6036	123	0
1	B	6239	0	6036	112	0
2	A	275	0	0	5	0
2	B	284	0	0	2	0
All	All	13037	0	12072	235	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 10.

The worst 5 of 235 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:A:448:MSE:HE2	1:A:525:ASP:HA	1.22	1.17
1:B:690:ILE:HA	1:B:693:MSE:HE3	1.43	0.97
1:B:407:LYS:HE3	1:B:411:ILE:HD11	1.49	0.93
1:B:84:MSE:HE1	1:B:501:PRO:HG2	1.48	0.93
1:A:448:MSE:HE3	1:A:528:LEU:HB2	1.53	0.91

There are no symmetry-related clashes.

## 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	783/803 (98%)	749 (96%)	31 (4%)	3 (0%)	38	31
1	B	783/803 (98%)	750 (96%)	29 (4%)	4 (0%)	32	25
All	All	1566/1606 (98%)	1499 (96%)	60 (4%)	7 (0%)	38	31

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	ILE
1	B	373	ILE
1	A	505	PRO
1	B	505	PRO
1	B	773	ASP

### 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	661/654 (101%)	647 (98%)	14 (2%)	59	60
1	B	661/654 (101%)	650 (98%)	11 (2%)	66	68
All	All	1322/1308 (101%)	1297 (98%)	25 (2%)	62	64

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	730	LEU
1	A	766	GLU
1	B	558	GLN
1	A	759	ARG
1	B	91	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	ASN
1	B	179	HIS
1	B	662	GLN
1	B	133	GLN
1	B	189	HIS

### 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](#)

There are no ligands in this entry.

## 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	769/803 (95%)	0.08	19 (2%) 58 58	7, 14, 28, 42	0
1	B	769/803 (95%)	0.15	25 (3%) 47 48	6, 14, 30, 49	0
All	All	1538/1606 (95%)	0.12	44 (2%) 52 53	6, 14, 28, 49	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	775	GLY	6.4
1	B	773	ASP	5.0
1	B	261	LEU	4.9
1	B	774	SER	4.8
1	B	756	ILE	4.4

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.