



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TVL  
Title : Structure of YTNJ from Bacillus subtilis  
Authors : Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2004-06-29  
Resolution : 2.10 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](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

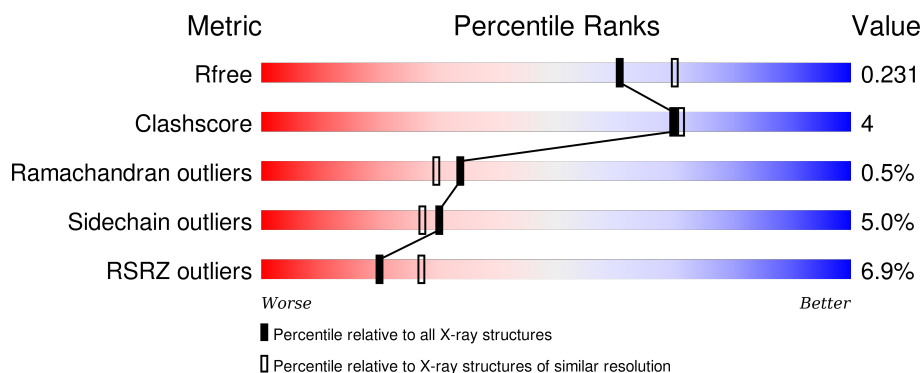
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	454	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3299 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 protein YTNJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3068	1945	538	581	4			

There are 13 discrepancies between the modelled and reference sequences:

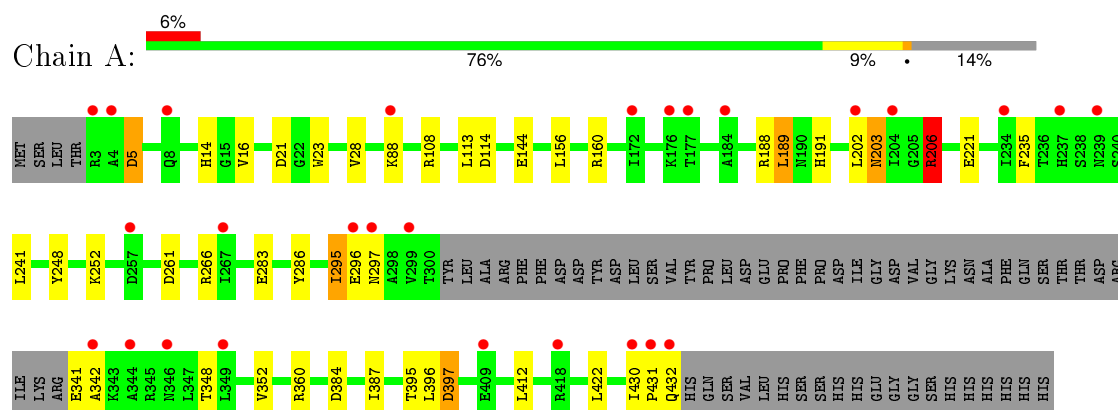
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	CLONING ARTIFACT	UNP O34974
A	0	SER	-	CLONING ARTIFACT	UNP O34974
A	1	LEU	-	CLONING ARTIFACT	UNP O34974
A	443	GLU	-	EXPRESSION TAG	UNP O34974
A	444	GLY	-	EXPRESSION TAG	UNP O34974
A	445	GLY	-	EXPRESSION TAG	UNP O34974
A	446	SER	-	EXPRESSION TAG	UNP O34974
A	447	HIS	-	EXPRESSION TAG	UNP O34974
A	448	HIS	-	EXPRESSION TAG	UNP O34974
A	449	HIS	-	EXPRESSION TAG	UNP O34974
A	450	HIS	-	EXPRESSION TAG	UNP O34974
A	451	HIS	-	EXPRESSION TAG	UNP O34974
A	452	HIS	-	EXPRESSION TAG	UNP O34974

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	231	Total	O	0	0
			231	231		



- Molecule 1: protein YTNJ



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.94Å 85.94Å 196.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.10) 99.1 (19.86-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.79 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.207 , 0.228 0.211 , 0.231	Depositor DCC
$R_{free}$ test set	2179 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 43147 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3299	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

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	0.48	0/3140	0.77	11/4247 (0.3%)

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	A	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	261	ASP	CB-CG-OD2	7.90	125.41	118.30
1	A	188	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	206	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	384	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	397	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	188	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	266	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	114	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	21	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	5	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	206	ARG	NE-CZ-NH1	5.52	123.06	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ASN	Peptide

## 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	3068	0	2987	27	0
2	A	231	0	0	7	0
All	All	3299	0	2987	27	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.

All (27) 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:395:THR:HG21	2:A:464:HOH:O	1.88	0.72
1:A:206:ARG:CD	1:A:432:GLN:HE21	2.06	0.69
1:A:203:ASN:H	1:A:203:ASN:HD22	1.42	0.65
1:A:206:ARG:HD3	1:A:432:GLN:NE2	2.12	0.64
1:A:206:ARG:HD3	1:A:432:GLN:HE21	1.63	0.63
1:A:108:ARG:NE	1:A:203:ASN:HD21	1.99	0.59
1:A:108:ARG:HG3	1:A:202:LEU:HD11	1.84	0.59
1:A:283:GLU:OE2	1:A:360:ARG:NH1	2.36	0.59
1:A:108:ARG:CD	1:A:203:ASN:HD21	2.16	0.58
1:A:360:ARG:NE	2:A:679:HOH:O	2.38	0.57
1:A:206:ARG:HD2	1:A:432:GLN:HE21	1.72	0.53
1:A:286:TYR:CD1	1:A:360:ARG:NH1	2.78	0.52
1:A:295:ILE:HD13	2:A:683:HOH:O	2.09	0.52
1:A:203:ASN:H	1:A:203:ASN:ND2	2.09	0.50
1:A:203:ASN:HD22	1:A:203:ASN:N	2.04	0.50
1:A:341:GLU:HA	2:A:682:HOH:O	2.10	0.50
1:A:430:ILE:HG22	1:A:432:GLN:HG3	1.93	0.49
1:A:206:ARG:CD	1:A:432:GLN:NE2	2.71	0.49
1:A:248:TYR:CZ	1:A:252:LYS:HE3	2.50	0.46
1:A:23:TRP:HA	1:A:28:VAL:HG11	1.97	0.46
1:A:342:ALA:HA	2:A:647:HOH:O	2.17	0.45
1:A:235:PHE:CD2	1:A:387:ILE:HG13	2.52	0.44
1:A:14:HIS:HE1	2:A:513:HOH:O	2.02	0.43
1:A:348:THR:O	1:A:352:VAL:HG23	2.18	0.43
1:A:108:ARG:HD2	1:A:203:ASN:HD21	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:NH1	2:A:586:HOH:O	2.47	0.41
1:A:189:LEU:HD22	1:A:191:HIS:HB2	2.02	0.40

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	386/454 (85%)	380 (98%)	4 (1%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	GLU
1	A	431	PRO

### 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	322/380 (85%)	306 (95%)	16 (5%)	30	27

All (16) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	5	ASP
1	A	16	VAL
1	A	88	LYS
1	A	113	LEU
1	A	144	GLU
1	A	156	LEU
1	A	189	LEU
1	A	203	ASN
1	A	206	ARG
1	A	221	GLU
1	A	241	LEU
1	A	295	ILE
1	A	396	LEU
1	A	397	ASP
1	A	412	LEU
1	A	422	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	141	ASN
1	A	173	HIS
1	A	203	ASN
1	A	432	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

There are no ligands in this entry.

## 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	390/454 (85%)	0.22	27 (6%)	20 27	29, 42, 62, 79	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	VAL	7.2
1	A	297	ASN	5.0
1	A	346	ASN	4.3
1	A	4	ALA	4.3
1	A	342	ALA	4.2
1	A	176	LYS	4.0
1	A	430	ILE	3.9
1	A	349	LEU	3.4
1	A	234	ILE	3.1
1	A	344	ALA	3.0
1	A	409	GLU	3.0
1	A	239	ASN	3.0
1	A	432	GLN	2.9
1	A	202	LEU	2.8
1	A	3	ARG	2.7
1	A	204	ILE	2.7
1	A	237	HIS	2.6
1	A	296	GLU	2.6
1	A	431	PRO	2.6
1	A	267	ILE	2.5
1	A	257	ASP	2.3
1	A	177	THR	2.3
1	A	88	LYS	2.2
1	A	418	ARG	2.2
1	A	8	GLN	2.2
1	A	172	ILE	2.0
1	A	184	ALA	2.0

## 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.