



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:23 PM GMT

PDB ID : 4JBF  
Title : Crystal structure of peptidoglycan glycosyltransferase from *Atopobium parvulum* DSM 20469.  
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Deposited on : 2013-02-19  
Resolution : 1.92 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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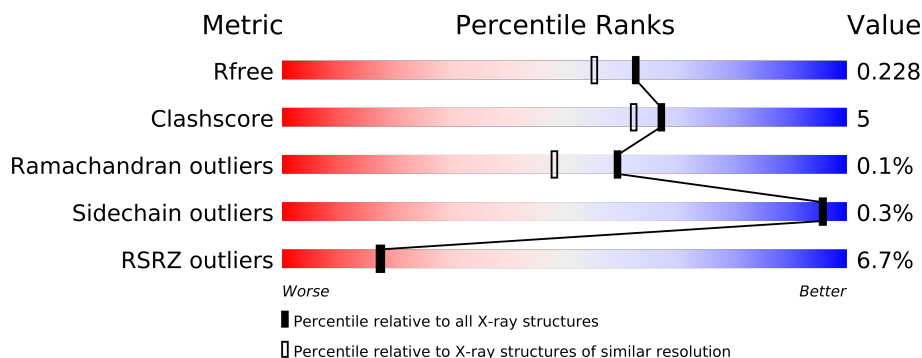
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.92 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	4387 (1.94-1.90)
Clashscore	79885	5258 (1.94-1.90)
Ramachandran outliers	78287	5193 (1.94-1.90)
Sidechain outliers	78261	5194 (1.94-1.90)
RSRZ outliers	66119	4389 (1.94-1.90)

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	482	
1	B	482	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	PG4	B	1001	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6378 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 Peptidoglycan glycosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	Se	0	1	0
			2948	1833	499	601	2	13			
1	B	410	Total	C	N	O	S	Se	0	2	0
			2953	1832	501	605	2	13			

There are 64 discrepancies between the modelled and reference sequences:

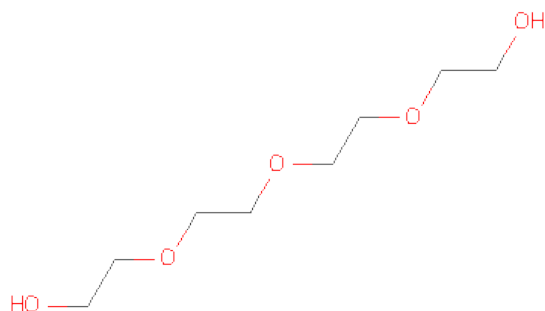
Chain	Residue	Modelled	Actual	Comment	Reference
A	473	MSE	-	EXPRESSION TAG	UNP C8W8H7
A	474	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	475	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	476	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	477	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	478	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	479	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	480	SER	-	EXPRESSION TAG	UNP C8W8H7
A	481	SER	-	EXPRESSION TAG	UNP C8W8H7
A	482	GLY	-	EXPRESSION TAG	UNP C8W8H7
A	483	VAL	-	EXPRESSION TAG	UNP C8W8H7
A	484	ASP	-	EXPRESSION TAG	UNP C8W8H7
A	485	LEU	-	EXPRESSION TAG	UNP C8W8H7
A	486	TRP	-	EXPRESSION TAG	UNP C8W8H7
A	487	SER	-	EXPRESSION TAG	UNP C8W8H7
A	488	HIS	-	EXPRESSION TAG	UNP C8W8H7
A	489	PRO	-	EXPRESSION TAG	UNP C8W8H7
A	490	GLN	-	EXPRESSION TAG	UNP C8W8H7
A	491	PHE	-	EXPRESSION TAG	UNP C8W8H7
A	492	GLU	-	EXPRESSION TAG	UNP C8W8H7
A	493	LYS	-	EXPRESSION TAG	UNP C8W8H7
A	494	GLY	-	EXPRESSION TAG	UNP C8W8H7
A	495	THR	-	EXPRESSION TAG	UNP C8W8H7
A	496	GLU	-	EXPRESSION TAG	UNP C8W8H7
A	497	ASN	-	EXPRESSION TAG	UNP C8W8H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	EXPRESSION TAG	UNP C8W8H7
A	499	TYR	-	EXPRESSION TAG	UNP C8W8H7
A	500	PHE	-	EXPRESSION TAG	UNP C8W8H7
A	501	GLN	-	EXPRESSION TAG	UNP C8W8H7
A	502	SER	-	EXPRESSION TAG	UNP C8W8H7
A	503	ASN	-	EXPRESSION TAG	UNP C8W8H7
A	504	ALA	-	EXPRESSION TAG	UNP C8W8H7
B	473	MSE	-	EXPRESSION TAG	UNP C8W8H7
B	474	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	475	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	476	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	477	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	478	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	479	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	480	SER	-	EXPRESSION TAG	UNP C8W8H7
B	481	SER	-	EXPRESSION TAG	UNP C8W8H7
B	482	GLY	-	EXPRESSION TAG	UNP C8W8H7
B	483	VAL	-	EXPRESSION TAG	UNP C8W8H7
B	484	ASP	-	EXPRESSION TAG	UNP C8W8H7
B	485	LEU	-	EXPRESSION TAG	UNP C8W8H7
B	486	TRP	-	EXPRESSION TAG	UNP C8W8H7
B	487	SER	-	EXPRESSION TAG	UNP C8W8H7
B	488	HIS	-	EXPRESSION TAG	UNP C8W8H7
B	489	PRO	-	EXPRESSION TAG	UNP C8W8H7
B	490	GLN	-	EXPRESSION TAG	UNP C8W8H7
B	491	PHE	-	EXPRESSION TAG	UNP C8W8H7
B	492	GLU	-	EXPRESSION TAG	UNP C8W8H7
B	493	LYS	-	EXPRESSION TAG	UNP C8W8H7
B	494	GLY	-	EXPRESSION TAG	UNP C8W8H7
B	495	THR	-	EXPRESSION TAG	UNP C8W8H7
B	496	GLU	-	EXPRESSION TAG	UNP C8W8H7
B	497	ASN	-	EXPRESSION TAG	UNP C8W8H7
B	498	LEU	-	EXPRESSION TAG	UNP C8W8H7
B	499	TYR	-	EXPRESSION TAG	UNP C8W8H7
B	500	PHE	-	EXPRESSION TAG	UNP C8W8H7
B	501	GLN	-	EXPRESSION TAG	UNP C8W8H7
B	502	SER	-	EXPRESSION TAG	UNP C8W8H7
B	503	ASN	-	EXPRESSION TAG	UNP C8W8H7
B	504	ALA	-	EXPRESSION TAG	UNP C8W8H7

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	218	Total	O	0	4
			222	222		
3	B	247	Total	O	0	1
			248	248		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.93Å 70.17Å 114.82Å 90.00° 97.35° 90.00°	Depositor
Resolution (Å)	29.48 – 1.92 29.48 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.48-1.92) 98.4 (29.48-1.92)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.195 , 0.237 0.193 , 0.228	Depositor DCC
$R_{free}$ test set	4008 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 79987 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: PG4

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	0.74	0/2982	0.88	1/4044 (0.0%)
1	B	0.81	1/2985 (0.0%)	0.91	3/4047 (0.1%)
All	All	0.78	1/5967 (0.0%)	0.89	4/8091 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	812	MSE	N-CA	5.59	1.57	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	759[B]	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	759[C]	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	920	VAL	CB-CA-C	-5.59	100.77	111.40
1	A	865	ARG	NE-CZ-NH1	5.59	123.09	120.30

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	2948	0	2863	22	0
1	B	2953	0	2874	36	0
2	B	7	0	9	0	0
3	A	222	0	0	4	0
3	B	248	0	0	3	0
All	All	6378	0	5746	58	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.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:759[C]:ARG:HG2	1:B:759[C]:ARG:HH21	1.27	0.98
1:B:878:MSE:CE	1:B:881:ARG:HH11	1.90	0.84
1:B:759[C]:ARG:HH21	1:B:759[C]:ARG:CG	1.90	0.84
1:B:878:MSE:HE2	1:B:881:ARG:HH11	1.45	0.80
1:A:545:GLN:HA	3:A:1146:HOH:O	1.83	0.77

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	395/482 (82%)	385 (98%)	10 (2%)	0	100	100
1	B	400/482 (83%)	384 (96%)	15 (4%)	1 (0%)	50	37
All	All	795/964 (82%)	769 (97%)	25 (3%)	1 (0%)	59	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	925	ASN

### 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	311/356 (87%)	310 (100%)	1 (0%)	96	96
1	B	311/356 (87%)	310 (100%)	1 (0%)	96	96
All	All	622/712 (87%)	620 (100%)	2 (0%)	96	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	900	ASN
1	B	900	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	527	GLN
1	B	925	ASN
1	B	722	ASN
1	A	722	ASN
1	B	570	GLN

### 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 ⓘ

1 ligand is 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	$\# Z  > 2$
2	PG4	B	1001	-	6,6,12	0.88	0	5,5,11	1.24	1 (20%)

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
2	PG4	B	1001	-	-	0/4/4/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	PG4	O3-C4-C3	-2.35	106.66	114.71

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	410/482 (85%)	0.15	27 (6%) 18 17	21, 37, 80, 125	0
1	B	410/482 (85%)	0.09	28 (6%) 17 17	21, 34, 76, 97	0
All	All	820/964 (85%)	0.12	55 (6%) 17 17	21, 35, 79, 125	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	603	ILE	5.6
1	B	525	TYR	5.5
1	B	526	VAL	4.7
1	A	926	GLY	4.4
1	A	898	ASN	4.4

### 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( $\text{\AA}^2$ )	Q<0.9
2	PG4	B	1001	7/13	0.14	2.43	42,44,49,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.