



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3BCV / pdb\_00003bcv  
Title : Crystal structure of a putative glycosyltransferase from *Bacteroides fragilis*  
Authors : Palani, K.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX  
Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-11-13  
Resolution : 2.35 Å (reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

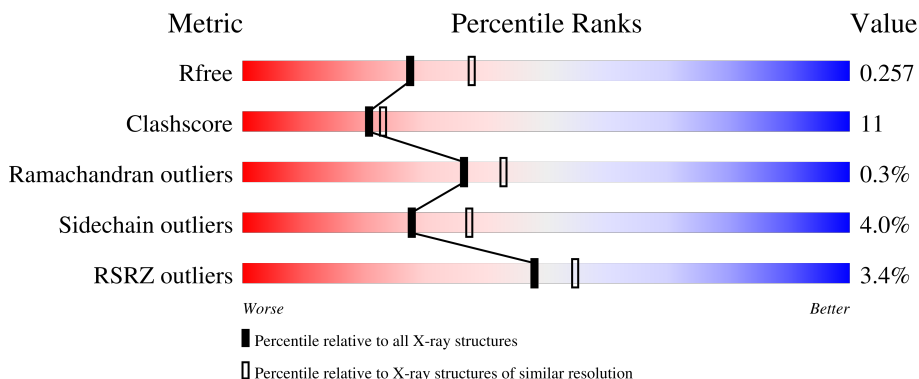
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	240	
1	B	240	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 3214 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 Putative glycosyltransferase protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	196	1555	993	252	299	7	4	0	0	0
1	B	196	1555	993	252	299	7	4	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 Q5LBM4
A	2	SER	-	expression tag	UNP Q5LBM4
A	3	LEU	-	expression tag	UNP Q5LBM4
A	233	GLU	-	expression tag	UNP Q5LBM4
A	234	GLY	-	expression tag	UNP Q5LBM4
A	235	HIS	-	expression tag	UNP Q5LBM4
A	236	HIS	-	expression tag	UNP Q5LBM4
A	237	HIS	-	expression tag	UNP Q5LBM4
A	238	HIS	-	expression tag	UNP Q5LBM4
A	239	HIS	-	expression tag	UNP Q5LBM4
A	240	HIS	-	expression tag	UNP Q5LBM4
B	1	MSE	-	expression tag	UNP Q5LBM4
B	2	SER	-	expression tag	UNP Q5LBM4
B	3	LEU	-	expression tag	UNP Q5LBM4
B	233	GLU	-	expression tag	UNP Q5LBM4
B	234	GLY	-	expression tag	UNP Q5LBM4
B	235	HIS	-	expression tag	UNP Q5LBM4
B	236	HIS	-	expression tag	UNP Q5LBM4
B	237	HIS	-	expression tag	UNP Q5LBM4
B	238	HIS	-	expression tag	UNP Q5LBM4
B	239	HIS	-	expression tag	UNP Q5LBM4
B	240	HIS	-	expression tag	UNP Q5LBM4

- Molecule 2 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	A	42	Total 42	O 42	0	0
2	B	62	Total 62	O 62	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.43Å 152.43Å 152.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.83 – 2.35 27.83 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.4 (27.83-2.35) 94.4 (27.83-2.35)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.34Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.257 0.230 , 0.257	Depositor DCC
$R_{free}$ test set	1119 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.031 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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, 0.333 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	0.47	0/1577	0.98	12/2134 (0.6%)
1	B	0.51	0/1577	1.07	11/2134 (0.5%)
All	All	0.49	0/3154	1.03	23/4268 (0.5%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	SER	N-CA-C	10.53	122.52	111.14
1	B	212	ASN	N-CA-C	-9.22	94.38	109.40
1	A	68	LYS	N-CA-C	-7.86	97.26	109.76
1	B	13	ILE	N-CA-C	7.70	118.89	108.11
1	B	97	VAL	N-CA-C	7.40	119.28	109.21
1	B	115	ASP	N-CA-C	-7.28	104.42	113.38
1	A	13	ILE	N-CA-C	6.79	117.62	108.11
1	B	144	LYS	N-CA-C	6.70	119.42	111.71
1	A	115	ASP	N-CA-C	-6.51	105.50	113.50
1	A	159	SER	N-CA-C	6.29	117.80	111.07
1	A	191	VAL	N-CA-C	-6.06	99.66	108.87
1	A	97	VAL	N-CA-C	6.00	118.60	109.12
1	A	101	MSE	N-CA-C	5.74	118.03	111.02
1	B	191	VAL	N-CA-C	-5.71	100.09	109.12
1	B	159	SER	N-CA-C	5.53	116.98	111.07
1	A	20	LEU	N-CA-C	5.43	117.62	111.11
1	A	195	ILE	N-CA-C	-5.41	106.91	111.56
1	A	180	ARG	N-CA-C	5.41	117.87	111.33
1	B	180	ARG	N-CA-C	5.38	117.56	111.11
1	B	99	SER	N-CA-C	5.26	117.75	111.71
1	A	118	PHE	N-CA-C	5.25	118.38	109.76
1	A	144	LYS	N-CA-C	5.08	118.74	112.54
1	B	68	LYS	N-CA-C	-5.03	101.52	109.96

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	1555	0	1562	33	0
1	B	1555	0	1562	37	0
2	A	42	0	0	0	0
2	B	62	0	0	2	0
All	All	3214	0	3124	69	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 11.

All (69) 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:101:MSE:HG2	1:A:105:MSE:HE2	1.27	1.12
1:B:101:MSE:HG2	1:B:105:MSE:HE2	1.25	1.09
1:B:77:ASN:HD21	1:B:190:PHE:H	1.19	0.89
1:A:77:ASN:HD21	1:A:190:PHE:H	1.23	0.87
1:B:101:MSE:CG	1:B:105:MSE:HE2	2.12	0.79
1:B:141:LYS:HD3	1:B:143:TYR:OH	1.82	0.79
1:A:152:LEU:HD12	1:A:167:ARG:HH21	1.49	0.76
1:A:152:LEU:HG	1:A:167:ARG:HE	1.56	0.68
1:A:192:SER:HB3	1:A:195:ILE:HD13	1.78	0.66
1:B:5:PRO:HG2	1:B:85:GLY:HA2	1.78	0.66
1:A:155:ASP:HB2	1:A:167:ARG:HG3	1.78	0.66
1:B:143:TYR:O	1:B:213:ILE:HA	2.01	0.61
1:A:167:ARG:HH11	1:A:167:ARG:HG2	1.67	0.59
1:B:92:ASP:HB2	1:B:95:ASP:OD2	2.03	0.59
1:A:101:MSE:HE3	1:A:105:MSE:HE1	1.85	0.59
1:B:56:ALA:HB2	1:B:64:VAL:HG23	1.84	0.58
1:B:72:LEU:HD22	1:B:72:LEU:H	1.70	0.57
1:B:102:TYR:CD2	1:B:105:MSE:HE3	2.39	0.57
1:A:167:ARG:HG2	1:A:167:ARG:NH1	2.19	0.56
1:A:115:ASP:HB3	1:A:182:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASP:HB3	2:B:247:HOH:O	2.07	0.54
1:A:31:THR:OG1	1:A:103:MSE:HG3	2.07	0.54
1:B:53:ASP:OD1	1:B:66:HIS:HE1	1.91	0.54
1:B:74:MSE:HE1	2:B:254:HOH:O	2.07	0.53
1:B:41:ASP:OD2	1:B:66:HIS:HD2	1.91	0.53
1:B:115:ASP:HB3	1:B:182:LEU:HD22	1.91	0.53
1:B:101:MSE:HE3	1:B:105:MSE:HE1	1.90	0.52
1:B:145:ASN:ND2	1:B:147:ASN:HB3	2.25	0.52
1:A:191:VAL:O	1:A:199:GLU:HG3	2.10	0.52
1:B:5:PRO:HG2	1:B:85:GLY:CA	2.40	0.51
1:B:156:LEU:O	1:B:164:ARG:HD3	2.11	0.51
1:A:38:ILE:HD13	1:A:82:VAL:HG23	1.93	0.50
1:B:65:ILE:HD11	1:B:82:VAL:HG11	1.93	0.50
1:A:65:ILE:HD11	1:A:82:VAL:HG11	1.94	0.49
1:A:16:VAL:HG21	1:A:93:SER:CB	2.42	0.49
1:B:16:VAL:HG11	1:B:93:SER:OG	2.13	0.48
1:B:152:LEU:O	1:B:167:ARG:NH1	2.46	0.47
1:B:145:ASN:HD22	1:B:145:ASN:C	2.23	0.47
1:A:32:LEU:HB2	1:A:103:MSE:HG2	1.95	0.47
1:B:191:VAL:O	1:B:199:GLU:HG3	2.15	0.46
1:A:4:ILE:HD12	1:A:4:ILE:N	2.30	0.46
1:B:67:LYS:HG2	1:B:68:LYS:O	2.15	0.46
1:B:145:ASN:ND2	1:B:148:GLU:H	2.13	0.46
1:B:193:GLU:H	1:B:193:GLU:CD	2.24	0.46
1:A:143:TYR:O	1:A:213:ILE:HA	2.17	0.46
1:B:119:THR:HG22	1:B:173:ALA:HB2	1.97	0.45
1:B:119:THR:HG22	1:B:173:ALA:CB	2.46	0.45
1:B:48:CYS:N	1:B:49:PRO:CD	2.80	0.44
1:A:152:LEU:CG	1:A:167:ARG:HE	2.29	0.44
1:A:140:PHE:C	1:A:141:LYS:HD2	2.43	0.44
1:B:37:ILE:HB	1:B:62:ILE:HG12	1.99	0.44
1:B:72:LEU:HD22	1:B:72:LEU:N	2.30	0.44
1:A:17:GLU:OE2	1:A:47:ASN:HB2	2.17	0.43
1:A:104:THR:O	1:A:108:VAL:HG23	2.19	0.43
1:A:145:ASN:OD1	1:A:148:GLU:HG3	2.18	0.43
1:B:188:LEU:HD22	1:B:206:ASP:HB3	2.01	0.42
1:B:76:CYS:HB3	1:B:90:PHE:CE2	2.55	0.42
1:A:97:VAL:HG11	1:A:101:MSE:HE1	2.02	0.41
1:A:3:LEU:HB3	1:A:4:ILE:HD12	2.02	0.41
1:A:17:GLU:OE1	1:A:46:ASP:HB2	2.20	0.41
1:A:102:TYR:CD2	1:A:105:MSE:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ALA:HA	1:A:177:LEU:O	2.20	0.41
1:A:167:ARG:HD3	1:A:167:ARG:HA	1.88	0.41
1:A:188:LEU:HD13	1:A:206:ASP:HB3	2.03	0.41
1:A:30:GLN:NE2	1:A:99:SER:HA	2.36	0.40
1:B:196:LEU:HD21	1:B:202:ILE:HG13	2.02	0.40
1:A:16:VAL:HG21	1:A:93:SER:HB3	2.03	0.40
1:A:165:GLU:HG3	1:B:191:VAL:HG21	2.04	0.40
1:B:115:ASP:OD2	1:B:212:ASN:O	2.39	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	192/240 (80%)	185 (96%)	7 (4%)	0	100	100
1	B	192/240 (80%)	186 (97%)	5 (3%)	1 (0%)	24	27
All	All	384/480 (80%)	371 (97%)	12 (3%)	1 (0%)	36	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	ILE

### 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	177/210 (84%)	170 (96%)	7 (4%)	28	37
1	B	177/210 (84%)	170 (96%)	7 (4%)	28	37
All	All	354/420 (84%)	340 (96%)	14 (4%)	28	37

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	17	GLU
1	A	72	LEU
1	A	103	MSE
1	A	167	ARG
1	A	193	GLU
1	A	199	GLU
1	B	27	LEU
1	B	100	ASP
1	B	113	THR
1	B	145	ASN
1	B	193	GLU
1	B	199	GLU
1	B	217	LEU

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	77	ASN
1	A	170	GLN
1	B	58	GLN
1	B	66	HIS
1	B	77	ASN
1	B	145	ASN
1	B	181	ASN

### 5.3.3 RNA

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 oligosaccharides 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	192/240 (80%)	0.30	8 (4%) 40 46	26, 40, 54, 64	0
1	B	192/240 (80%)	0.21	5 (2%) 57 63	25, 37, 50, 59	0
All	All	384/480 (80%)	0.26	13 (3%) 48 55	25, 38, 52, 64	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	5.2
1	A	96	TYR	4.1
1	B	119	THR	3.9
1	A	162	TYR	3.8
1	B	72	LEU	3.5
1	A	3	LEU	3.2
1	A	218	PRO	3.1
1	B	218	PRO	2.9
1	A	94	ASP	2.9
1	A	93	SER	2.7
1	A	166	GLU	2.7
1	B	140	PHE	2.6
1	A	215	CYS	2.2

### 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 oligosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.