

Supplementary Data Set 1: Summary of Glycosyltransferase structures in PDB (January 2019)

Glycosyltransferase structures in PDB as of January 1, 2019 have been previously cataloged in the CAZy database (1) and were used to populate the table below. Structure entries in the table are organized by CAZy family. Annotation information was provided for each protein structure, including gene symbol, protein name, and UniProt accession number (all collected from the respective UniProt entry (2)), species source and Kingdom for the coding region, and the species source of the expression system (derived from the respective PDB record (3)). The PDB ID codes for the respective protein structures are listed in many instances there are multiple PDB files deposited for a given protein with the year of first deposit for the protein coding region, and the year(s) of subsequent deposits of protein structures. The protein fold class designation was derived from the respective CAZy family record and visual inspection of the protein structure. The glycosyltransferase mechanism (inverting or retaining catalytic mechanisms) were derived from the respective CAZy family record or the primary citation of the structure. The dependence for a metal cation in the catalytic mechanism (Metal dep) was determined by the requirement of a metal for binding the donor analog in the respective protein structure for at least one member of the respective CAZy family. Donor and acceptor ligand structures were listed for analog complexes that bound to the respective substrates and do not include molecules bound to inhibitory or allosteric sites. Publications of the respective structures are listed by digital object identifiers (doi) based on citation information in the PDB record. If a publication doi is not available, then a PubMed ID is listed. In some instances no publication is listed if the Literature field of the PDB record indicates that the structure is to be published.

CAZy family	Gene symbol	Protein name	Uniprot	Species	Kingdom	Expression	PDB ID	Year first deposited	Year subsequent deposits	Fold class	Mechanism	Metal dep	Donor ligand analog	Acceptor ligand analog	Pub doi or PubMed ID
1	ase2	End2 glucosyltransferase	A0M999	Actinomyces viscosus	Bacteria	E. coli	5DQ2	2015		GT-B	inverting	N.D.			
	glfA	ETP-epi-sialosyltransferase	P9558	Amphibacillus oryzae	Bacteria	E. coli	1P93, 1P94, 1B61, 1B67	2003	2009	GT-B	inverting	no	UDP-Glc-UDP	Glc, sialosamine	10.1073/pdb.13337720.10.10161.chembl.2009.04.031
	glfB	Vancomycin-sulfonyl glycosyltransferase	P9559	Amphibacillus oryzae	Bacteria	E. coli	1B68	2001		GT-B	inverting	no			10.1016/S0969-2196(01)00616-5
	glfC	Vancomycin-sulfonyl glycosyltransferase	P9560	Amphibacillus oryzae	Bacteria	E. coli	1B69	2001		GT-B	inverting	no			
	glfD	Vancomycin-sulfonyl glycosyltransferase	P9561	Amphibacillus oryzae	Bacteria	E. coli	1B70	2001		GT-B	inverting	no			
	glfE	Vancomycin-sulfonyl glycosyltransferase	P9562	Amphibacillus oryzae	Bacteria	E. coli	1B71	2001		GT-B	inverting	no			
	glfF	Vancomycin-sulfonyl glycosyltransferase	P9563	Amphibacillus oryzae	Bacteria	E. coli	1B72	2001		GT-B	inverting	no			
	glfG	Vancomycin-sulfonyl glycosyltransferase	P9564	Amphibacillus oryzae	Bacteria	E. coli	1B73	2001		GT-B	inverting	no			
	glfH	Vancomycin-sulfonyl glycosyltransferase	P9565	Amphibacillus oryzae	Bacteria	E. coli	1B74	2001		GT-B	inverting	no			
	glfI	Vancomycin-sulfonyl glycosyltransferase	P9566	Amphibacillus oryzae	Bacteria	E. coli	1B75	2001		GT-B	inverting	no			
	glfJ	Vancomycin-sulfonyl glycosyltransferase	P9567	Amphibacillus oryzae	Bacteria	E. coli	1B76	2001		GT-B	inverting	no			
	glfK	Vancomycin-sulfonyl glycosyltransferase	P9568	Amphibacillus oryzae	Bacteria	E. coli	1B77	2001		GT-B	inverting	no			
	glfL	Vancomycin-sulfonyl glycosyltransferase	P9569	Amphibacillus oryzae	Bacteria	E. coli	1B78	2001		GT-B	inverting	no			
	glfM	Vancomycin-sulfonyl glycosyltransferase	P9570	Amphibacillus oryzae	Bacteria	E. coli	1B79	2001		GT-B	inverting	no			
	glfN	Vancomycin-sulfonyl glycosyltransferase	P9571	Amphibacillus oryzae	Bacteria	E. coli	1B80	2001		GT-B	inverting	no			
	glfO	Vancomycin-sulfonyl glycosyltransferase	P9572	Amphibacillus oryzae	Bacteria	E. coli	1B81	2001		GT-B	inverting	no			
	glfP	Vancomycin-sulfonyl glycosyltransferase	P9573	Amphibacillus oryzae	Bacteria	E. coli	1B82	2001		GT-B	inverting	no			
	glfQ	Vancomycin-sulfonyl glycosyltransferase	P9574	Amphibacillus oryzae	Bacteria	E. coli	1B83	2001		GT-B	inverting	no			
	glfR	Vancomycin-sulfonyl glycosyltransferase	P9575	Amphibacillus oryzae	Bacteria	E. coli	1B84	2001		GT-B	inverting	no			
	glfS	Vancomycin-sulfonyl glycosyltransferase	P9576	Amphibacillus oryzae	Bacteria	E. coli	1B85	2001		GT-B	inverting	no			
	glfT	Vancomycin-sulfonyl glycosyltransferase	P9577	Amphibacillus oryzae	Bacteria	E. coli	1B86	2001		GT-B	inverting	no			
	glfU	Vancomycin-sulfonyl glycosyltransferase	P9578	Amphibacillus oryzae	Bacteria	E. coli	1B87	2001		GT-B	inverting	no			
	glfV	Vancomycin-sulfonyl glycosyltransferase	P9579	Amphibacillus oryzae	Bacteria	E. coli	1B88	2001		GT-B	inverting	no			
	glfW	Vancomycin-sulfonyl glycosyltransferase	P9580	Amphibacillus oryzae	Bacteria	E. coli	1B89	2001		GT-B	inverting	no			
	glfX	Vancomycin-sulfonyl glycosyltransferase	P9581	Amphibacillus oryzae	Bacteria	E. coli	1B90	2001		GT-B	inverting	no			
glfY	Vancomycin-sulfonyl glycosyltransferase	P9582	Amphibacillus oryzae	Bacteria	E. coli	1B91	2001		GT-B	inverting	no				
glfZ	Vancomycin-sulfonyl glycosyltransferase	P9583	Amphibacillus oryzae	Bacteria	E. coli	1B92	2001		GT-B	inverting	no				
glfAA	Vancomycin-sulfonyl glycosyltransferase	P9584	Amphibacillus oryzae	Bacteria	E. coli	1B93	2001		GT-B	inverting	no				
glfAB	Vancomycin-sulfonyl glycosyltransferase	P9585	Amphibacillus oryzae	Bacteria	E. coli	1B94	2001		GT-B	inverting	no				
glfAC	Vancomycin-sulfonyl glycosyltransferase	P9586	Amphibacillus oryzae	Bacteria	E. coli	1B95	2001		GT-B	inverting	no				
glfAD	Vancomycin-sulfonyl glycosyltransferase	P9587	Amphibacillus oryzae	Bacteria	E. coli	1B96	2001		GT-B	inverting	no				
glfAE	Vancomycin-sulfonyl glycosyltransferase	P9588	Amphibacillus oryzae	Bacteria	E. coli	1B97	2001		GT-B	inverting	no				
glfAF	Vancomycin-sulfonyl glycosyltransferase	P9589	Amphibacillus oryzae	Bacteria	E. coli	1B98	2001		GT-B	inverting	no				
glfAG	Vancomycin-sulfonyl glycosyltransferase	P9590	Amphibacillus oryzae	Bacteria	E. coli	1B99	2001		GT-B	inverting	no				
glfAH	Vancomycin-sulfonyl glycosyltransferase	P9591	Amphibacillus oryzae	Bacteria	E. coli	1B00	2001		GT-B	inverting	no				
glfAI	Vancomycin-sulfonyl glycosyltransferase	P9592	Amphibacillus oryzae	Bacteria	E. coli	1B01	2001		GT-B	inverting	no				
glfAJ	Vancomycin-sulfonyl glycosyltransferase	P9593	Amphibacillus oryzae	Bacteria	E. coli	1B02	2001		GT-B	inverting	no				
glfAK	Vancomycin-sulfonyl glycosyltransferase	P9594	Amphibacillus oryzae	Bacteria	E. coli	1B03	2001		GT-B	inverting	no				
glfAL	Vancomycin-sulfonyl glycosyltransferase	P9595	Amphibacillus oryzae	Bacteria	E. coli	1B04	2001		GT-B	inverting	no				
glfAM	Vancomycin-sulfonyl glycosyltransferase	P9596	Amphibacillus oryzae	Bacteria	E. coli	1B05	2001		GT-B	inverting	no				
glfAN	Vancomycin-sulfonyl glycosyltransferase	P9597	Amphibacillus oryzae	Bacteria	E. coli	1B06	2001		GT-B	inverting	no				
glfAO	Vancomycin-sulfonyl glycosyltransferase	P9598	Amphibacillus oryzae	Bacteria	E. coli	1B07	2001		GT-B	inverting	no				
glfAP	Vancomycin-sulfonyl glycosyltransferase	P9599	Amphibacillus oryzae	Bacteria	E. coli	1B08	2001		GT-B	inverting	no				
glfAQ	Vancomycin-sulfonyl glycosyltransferase	P9600	Amphibacillus oryzae	Bacteria	E. coli	1B09	2001		GT-B	inverting	no				
glfAR	Vancomycin-sulfonyl glycosyltransferase	P9601	Amphibacillus oryzae	Bacteria	E. coli	1B10	2001		GT-B	inverting	no				
glfAS	Vancomycin-sulfonyl glycosyltransferase	P9602	Amphibacillus oryzae	Bacteria	E. coli	1B11	2001		GT-B	inverting	no				
glfAT	Vancomycin-sulfonyl glycosyltransferase	P9603	Amphibacillus oryzae	Bacteria	E. coli	1B12	2001		GT-B	inverting	no				
glfAU	Vancomycin-sulfonyl glycosyltransferase	P9604	Amphibacillus oryzae	Bacteria	E. coli	1B13	2001		GT-B	inverting	no				
glfAV	Vancomycin-sulfonyl glycosyltransferase	P9605	Amphibacillus oryzae	Bacteria	E. coli	1B14	2001		GT-B	inverting	no				
glfAW	Vancomycin-sulfonyl glycosyltransferase	P9606	Amphibacillus oryzae	Bacteria	E. coli	1B15	2001		GT-B	inverting	no				
glfAX	Vancomycin-sulfonyl glycosyltransferase	P9607	Amphibacillus oryzae	Bacteria	E. coli	1B16	2001		GT-B	inverting	no				
glfAY	Vancomycin-sulfonyl glycosyltransferase	P9608	Amphibacillus oryzae	Bacteria	E. coli	1B17	2001		GT-B	inverting	no				
glfAZ	Vancomycin-sulfonyl glycosyltransferase	P9609	Amphibacillus oryzae	Bacteria	E. coli	1B18	2001		GT-B	inverting	no				
glfBA	Vancomycin-sulfonyl glycosyltransferase	P9610	Amphibacillus oryzae	Bacteria	E. coli	1B19	2001		GT-B	inverting	no				
glfBB	Vancomycin-sulfonyl glycosyltransferase	P9611	Amphibacillus oryzae	Bacteria	E. coli	1B20	2001		GT-B	inverting	no				
glfBC	Vancomycin-sulfonyl glycosyltransferase	P9612	Amphibacillus oryzae	Bacteria	E. coli	1B21	2001		GT-B	inverting	no				
glfBD	Vancomycin-sulfonyl glycosyltransferase	P9613	Amphibacillus oryzae	Bacteria	E. coli	1B22	2001		GT-B	inverting	no				
glfBE	Vancomycin-sulfonyl glycosyltransferase	P9614	Amphibacillus oryzae	Bacteria	E. coli	1B23	2001		GT-B	inverting	no				
glfBF	Vancomycin-sulfonyl glycosyltransferase	P9615	Amphibacillus oryzae	Bacteria	E. coli	1B24	2001		GT-B	inverting	no				
glfBG	Vancomycin-sulfonyl glycosyltransferase	P9616	Amphibacillus oryzae	Bacteria	E. coli	1B25	2001		GT-B	inverting	no				
glfBH	Vancomycin-sulfonyl glycosyltransferase	P9617	Amphibacillus oryzae	Bacteria	E. coli	1B26	2001		GT-B	inverting	no				
glfBI	Vancomycin-sulfonyl glycosyltransferase	P9618	Amphibacillus oryzae	Bacteria	E. coli	1B27	2001		GT-B	inverting	no				
glfBJ	Vancomycin-sulfonyl glycosyltransferase	P9619	Amphibacillus oryzae	Bacteria	E. coli	1B28	2001		GT-B	inverting	no				
glfBK	Vancomycin-sulfonyl glycosyltransferase	P9620	Amphibacillus oryzae	Bacteria	E. coli	1B29	2001		GT-B	inverting	no				
glfBL	Vancomycin-sulfonyl glycosyltransferase	P9621	Amphibacillus oryzae	Bacteria	E. coli	1B30	2001		GT-B	inverting	no				
glfBM	Vancomycin-sulfonyl glycosyltransferase	P9622	Amphibacillus oryzae	Bacteria	E. coli	1B31	2001		GT-B	inverting	no				
glfBN	Vancomycin-sulfonyl glycosyltransferase	P9623	Amphibacillus oryzae	Bacteria	E. coli	1B32	2001		GT-B	inverting	no				
glfBO	Vancomycin-sulfonyl glycosyltransferase	P9624	Amphibacillus oryzae	Bacteria	E. coli	1B33	2001		GT-B	inverting	no				
glfBP	Vancomycin-sulfonyl glycosyltransferase	P9625	Amphibacillus oryzae	Bacteria	E. coli	1B34	2001		GT-B	inverting	no				
glfBQ	Vancomycin-sulfonyl glycosyltransferase	P9626	Amphibacillus oryzae	Bacteria	E. coli	1B35	2001		GT-B	inverting	no				
glfBR	Vancomycin-sulfonyl glycosyltransferase	P9627	Amphibacillus oryzae	Bacteria	E. coli	1B36	2001		GT-B	inverting	no				
glfBS	Vancomycin-sulfonyl glycosyltransferase	P9628	Amphibacillus oryzae	Bacteria	E. coli	1B37	2001		GT-B	inverting	no				
glfBT	Vancomycin-sulfonyl glycosyltransferase	P9629	Amphibacillus oryzae	Bacteria	E. coli	1B38	2001		GT-B	inverting	no				
glfBU	Vancomycin-sulfonyl glycosyltransferase	P9630	Amphibacillus oryzae	Bacteria	E. coli	1B39	2001		GT-B	inverting	no				
glfBV	Vancomycin-sulfonyl glycosyltransferase	P9631	Amphibacillus oryzae	Bacteria	E. coli	1B40	2001		GT-B	inverting	no				
glfBW	Vancomycin-sulfonyl glycosyltransferase	P9632	Amphibacillus oryzae	Bacteria	E. coli	1B41	2001		GT-B	inverting	no				
glfBX	Vancomycin-sulfonyl glycosyltransferase	P9633	Amphibacillus oryzae	Bacteria	E. coli	1B42	2001		GT-B	inverting	no				
glfBY	Vancomycin-sulfonyl glycosyltransferase	P9634	Amphibacillus oryzae	Bacteria	E. coli	1B43	2001		GT-B	inverting	no				
glfBZ	Vancomycin-sulfonyl glycosyltransferase	P9635	Amphibacillus oryzae	Bacteria	E. coli	1B44	2001		GT-B	inverting	no				
glfCA	Vancomycin-sulfonyl glycosyltransferase	P9636	Amphibacillus oryzae	Bacteria	E. coli	1B45	2001		GT-B	inverting	no				
glfCB	Vancomycin-sulfonyl glycosyltransferase	P9637	Amphibacillus oryzae	Bacteria	E. coli	1B46	2001		GT-B	inverting	no				
glfCC	Vancomycin-sulfonyl glycosyltransferase	P9638	Amphibacillus oryzae	Bacteria	E. coli	1B47	2001		GT-B	inverting	no				
glfCD	Vancomycin-sulfonyl glycosyltransferase	P9639	Amphibacillus oryzae	Bacteria	E. coli	1B48	2001		GT-B	inverting	no				
glfCE	Vancomycin-sulfonyl glycosyltransferase	P9640	Amphibacillus oryzae	Bacteria	E. coli	1B49	2001		GT-B	inverting	no				
glfCF	Vancomycin-sulfonyl glycosyltransferase	P9641	Amphibacillus oryzae	Bacteria	E. coli	1B50	2001		GT-B						



