

Supplemental data

STRUCTURAL INSIGHTS INTO THE CATALYTIC MECHANISM OF BACTERIAL GUANOSINE-DIPHOSPHO-D-MANNOSE PYROPHOSPHORYLASE AND ITS REGULATION BY DIVALENT IONS

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Supplementary Table I : Residues involved in polar contacts with bound substrates/product

		TmGMP-Man1P	TmGMP-GTP	TmGMP-GDPMan
<i>Mannose moiety</i>	C ₂ -OH	Asn189 SC Asp239 SC		Asp239 SC
	C ₃ -OH	Glu170 SC Asn189 SC Asp239 SC		Gly150 MC Glu170 SC Asn189 SC
	C ₄ -OH	Gly150 MC Asn189 MC		Gly150 MC Asn189 MC
	C ₆ -OH	-		His110 SC
<i>Guanosine moiety</i>	N ₁ H		Glu80 SC	-
	C ₂ -NH ₂		Val56 MC Glu80 SC	Val56 MC Glu80 SC
	N ₃		Gly9 MC	-
	C ₆ =O		Asn85 MC	Asn85 MC
	C ₂ '-OH		Gly10 MC	Gly9 MC
	C ₃ '-OH		Leu7 MC Ala108 MC	Leu7 MC Ala108 MC
<i>Phosphate moieties</i>	P _α		Arg14 SC Lys25 SC	-
	P _β / P _{Man}	Lys171 SC	Gly12 MC	Lys171 SC
	P _γ		Glu13 MC Arg14 MC Arg14 SC Arg326 SC	
MC : Main chain SC : Side chain				

Supplementary Figure 1: Alignment of GMP sequences from different bacterial sources.

Sequence alignment of TmGMP with orthologs from *T. thermophilus* (TtGMP) *C. perfringens* (CpGMP), and *L. interrogans* (LiGMP) belonging to the monofunctional GMP class and *H. pylori* (HPGMP-PMI), *P. aeruginosa* (PaGMP-PMI), *E. coli* (EcPMI-GMP) and *P. furiosus* (PfGMP-PMI) belonging to the bifunctional GMP-PMI class. Asterisks and filled circles indicate residues that interact with the nucleotide and sugar moieties, respectively. Triangles denote residues buried at the dimeric interface.

