Mevalonate 5-diphosphate mediates ATP binding to the mevalonate diphosphate decarboxylase from the bacterial pathogen *Enterococcus faecalis*

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Supplementary Table S1. Structural information of the published structures of MDD from *S. epidermidis* (27)*.

PDB accession code	4DPT	4DPU	4DPW	4DU7
Protein	$\text{MDD}_{\text{SE*}}$	MDD_{SE}	MDD_{SE}	MDD_{SE}
Wild type/mutation	Wild type	S192A	D283A	Wild type
Ligands**	FMVAPP	FMVAPP	MVAPP	MVAPP
	ATPγS	ATPγS	ATPγS	--
Resolution (Å)	2.2	1.9	2.6	2.2
Undefined region	184-193	--	--	183-186
Metal ion	No	No	No	No
Distance between 3’-O of MVAPP (or FMVAPP) and γ-P of ATPγS (Å)**	5.5	5.9	6.1	--
*MDD stands for the mevalonate diphosphate decarboxylase and $_{\text{SE}}$ stands for *Staphylococcus epidermidis*. **FMVAPP: 6-fluoromevlonate diphosphate, ATPγS: adenosine 5’-(γ-thio)triphosphate				

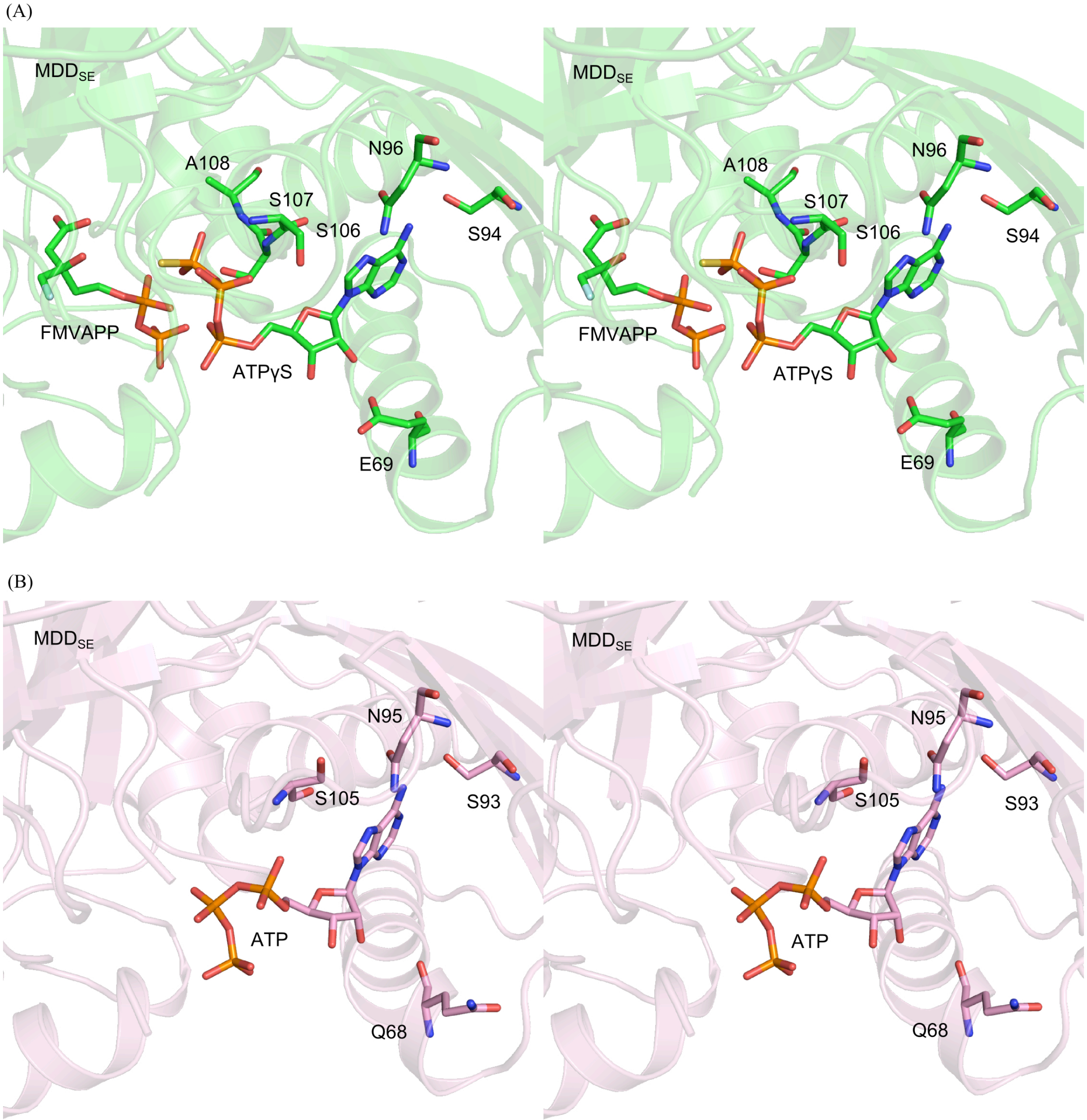
Supplementary Table S2. Patterns of dead-end inhibition of a bi-substrate reaction*

Mechanism	Competitive inhibitor mimicking a substrate	Inhibition pattern**	
		Varied [A]	Varied [B]
Sequential ordered with A binding first	A	Competitive	Noncompetitive
Sequential ordered with A binding first	B	Uncompetitive	Competitive
Sequential ordered with B binding first	A	Competitive	Uncompetitive
Sequential ordered with B binding first	B	Noncompetitive	Competitive
Sequential random	A	Competitive	Noncompetitive
Sequential random	B	Noncompetitive	Competitive
Ping-Pong	A	Competitive	Uncompetitive
Ping-Pong	B	Uncompetitive	Competitive

*The table is modified from Table 11.2 in the text book “Enzymes: A Practical Introduction to Structure, Mechanism and Data Analysis” edit by Robert A. Copeland(33).

**The reactions would be conducted at a non-saturating concentration (about the K_m value) of the fixed substrate.

Supplementary Figure S1 Active-site structural comparison of MDD_{SE}-FMVAPP-ATPγS and MDD_{EF}-ATP. (A) Stereo view of the ligands in the active site of MDD_{SE} and interacting residues around the ATP binding pocket of MDD_{SE}. (B) Stereo view of ATP in the active site of MDD_{EF} and interacting residues around the ATP binding pocket of MDD_{EF}.



Supplementary Figure S1*A* and S1*B*