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Supporting information for article:

Identification, structure determination and analysis of *Mycobacterium smegmatis* acyl-carrier protein synthase (AcpS) crystallized serendipitously

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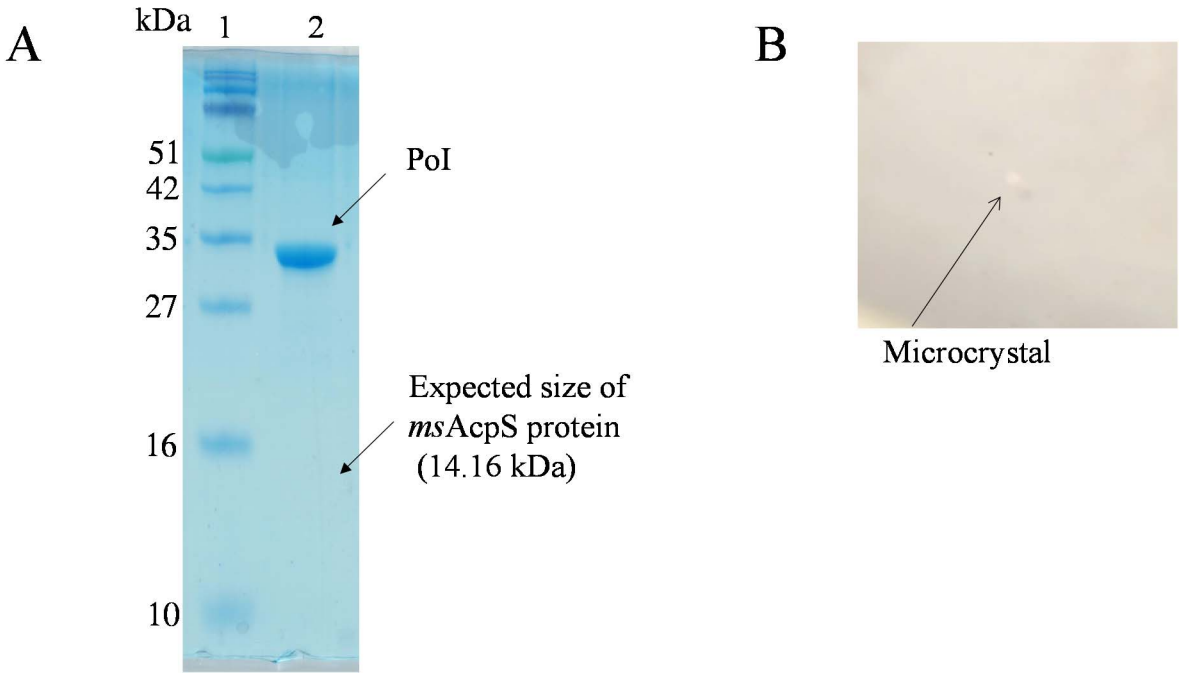

Figure S1 Purification and crystallization of protein of interest. **(A)** 15% SDS-PAGE analysis of purified PoI showing no traces of host protein *(ms*AcpS). **(B)** Crystals of *ms*AcpS protein which were initially expected to be of PoI.

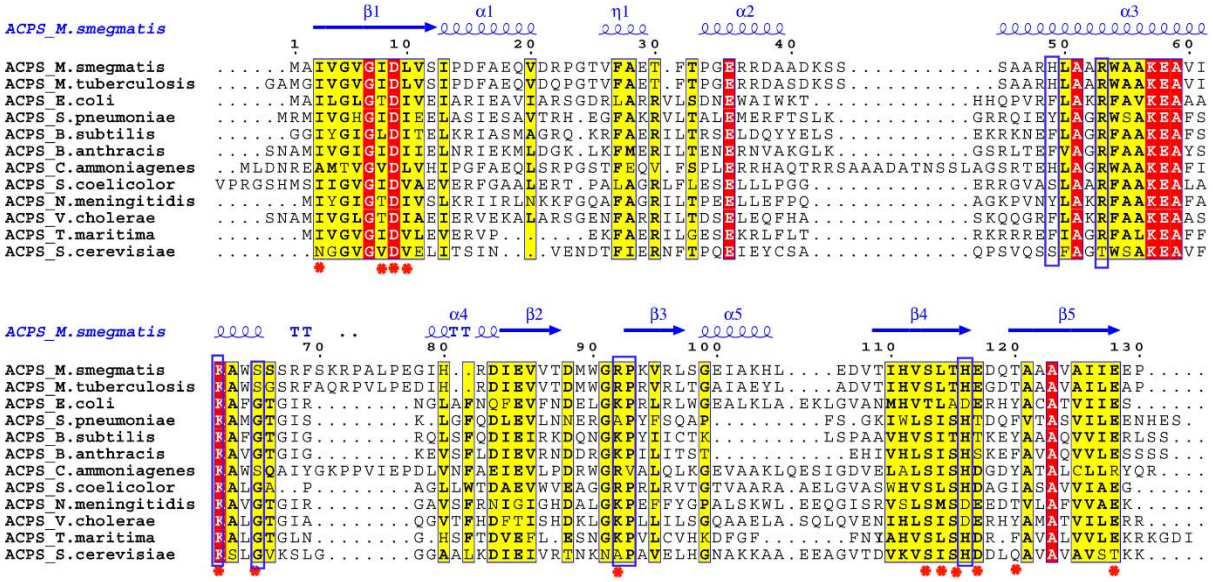

Figure S2 Multiple sequence alignment of AcpS protein sequences from various bacteria showing the active site and residues involved in the trimer formation. The active site residues are boxed in blue and residues involved in trimer formation in *ms*AcpS and corresponding columns are marked with red star.

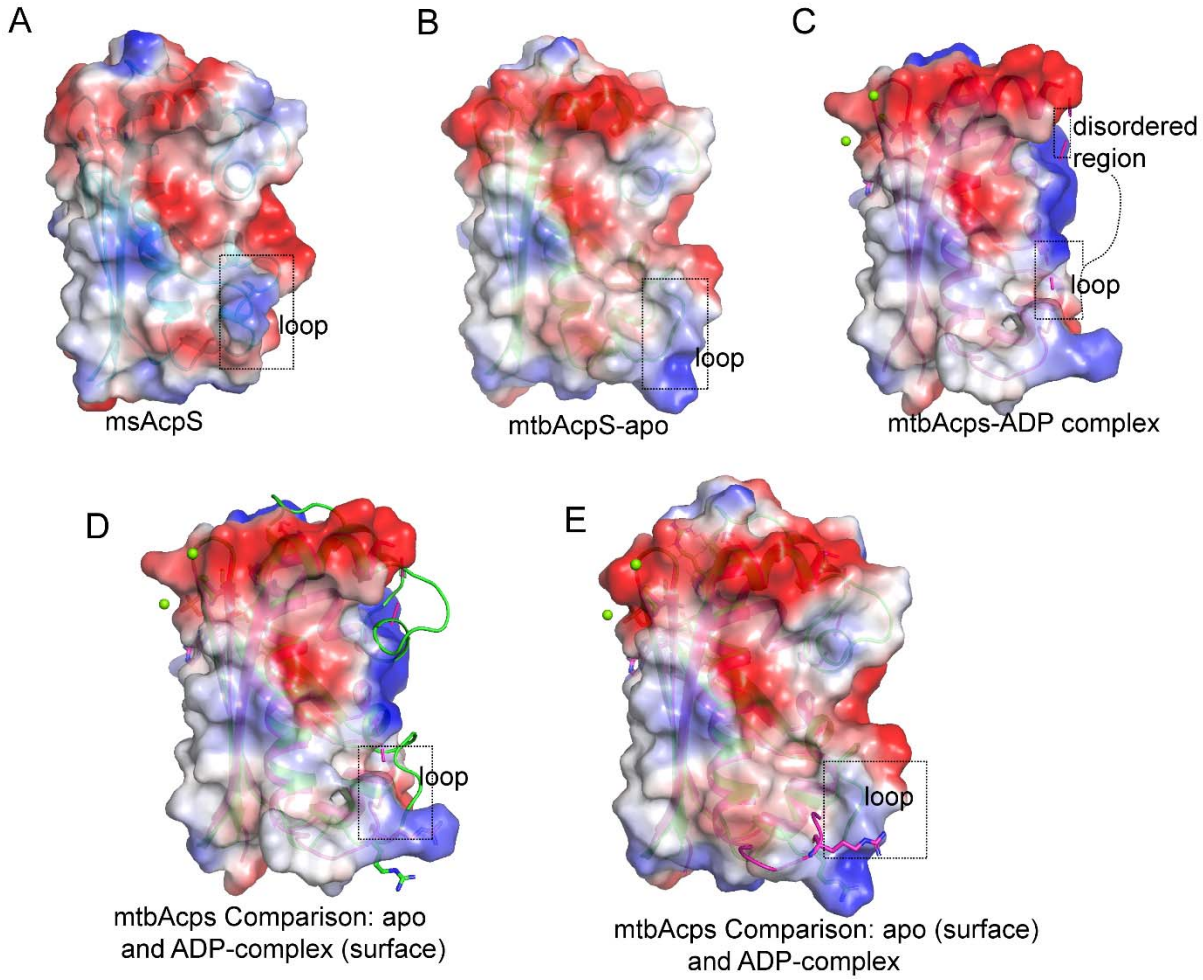

Figure S3 The electrostatic potential mapped onto the accessible surface area of AcpS protein structures from *M. smegmatis and M. tuberculosis* (both apo and in complex with 3',5' ADP). (A). Surface representation of *ms*AcpS with cartoon shown in cyan. (B). Surface representation of *mtb*AcpS-apo. Cartoon presentation is in green. (C) Surface representation of *mtb*AcpS (cartoon-magenta) in complex with 3',5' ADP. (D) Superposition *mtb*AcpS (apo) and *mtb*AcpS-ADP complex. The surface representation is of *mtb*AcpS-ADP complex. (E) Superposition *mtb*AcpS (apo) and *mtb*AcpS-ADP complex. The surface representation is of *mtb*AcpS-apo. Regions of negative potential are colored red, those of positive potential are colored blue, neutral regions are shown in white. The protein is represented as cartoon. The surface representations illustrate the similarities and differences of the structural and electrostatic environments of structural elements mainly in the loop connecting the α3-α4 helices in AcpS proteins.