Crystal structure of diaminopimelate epimerase *Mycobacterium tuberculosis* DapF

Veeraraghavan Usha[1], Lynn G. Dover[1,3], David I. Roper[2], Klaus Fütterer[1,*], Gurdyal S. Besra[1,*]

[1]School of Biosciences, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK.
[2] Department of Biological Sciences, University of Warwick, Gibbet Hill Rd, Coventry, CV4 7AL, UK
[3] Present address: Biomedical Sciences, School of Applied Sciences, Northumbria University, Ellison Place, Newcastle upon Tyne, NE1 8ST, UK

*Contact: (KF) Email K.Futterer@bham.ac.uk; Phone +44 – 121 – 414 5895; Fax +44 – 121 – 414 5925
(GSB) Email G.Besra@bham.ac.uk; Phone +44 – 121 – 415 8125; Fax +44 – 121 – 414 5925

Captions for Supplementary Figures

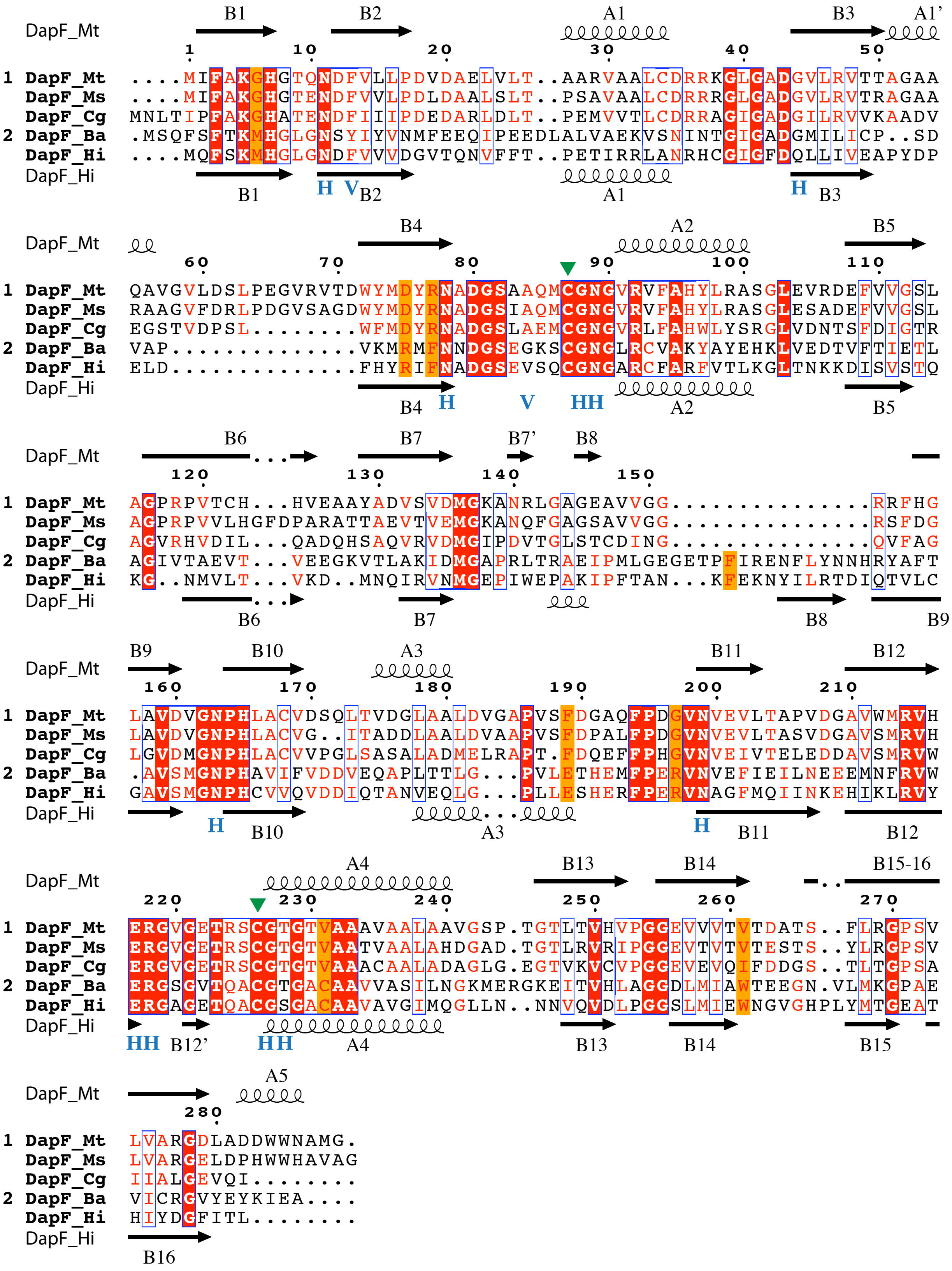
Supplementary Figure S1. Sequence alignment and secondary structure assignment of DapF.

Amino acid sequences of DapF orthologues aligned using ClustalW. Species abbreviations: Mt = *M. tuberculosis*, Ms = *Mycobacterium smegmatis*, Cg = *Corynebacterium glutamicum*, Ba = *Bacillus anthracis*, Hi = *Haemophilus influenzae*. Secondary structure assignments of the bottom sequence reflects that of PDB entry 1bwz. Green triangles mark the catalytic Cys residues. Blue letters H, V denote residues in H-bond or van der Waals contact, respectively, with L,L-AziDAP in PDB entry 2gke (Pillai et al., 2006). Alignment formatted using ESPript (http://espript.ibcp.fr/).

Supplementary Figure S2. Distribution of atomic displacement factors

Ribbon diagram of *Mt*DapF coloured according to atomic displacement factors. Colour ramp is from dark blue (min. B = 31 Å^2) to dark red (max. B = 110 Å^2).

Supplementary Figure S1



Supplementary Figure S2