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Supporting information for article:

Mutational and structural study of RipA, a key enzyme for *Mycobacterium tuberculosis* cell division: evidence for the L to D inversion of configuration of the catalytic cysteine

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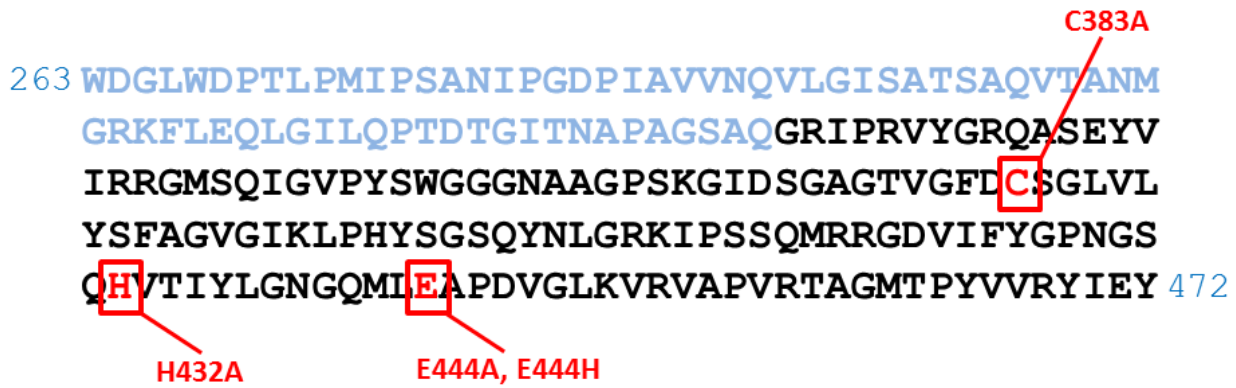
(A)



(B)

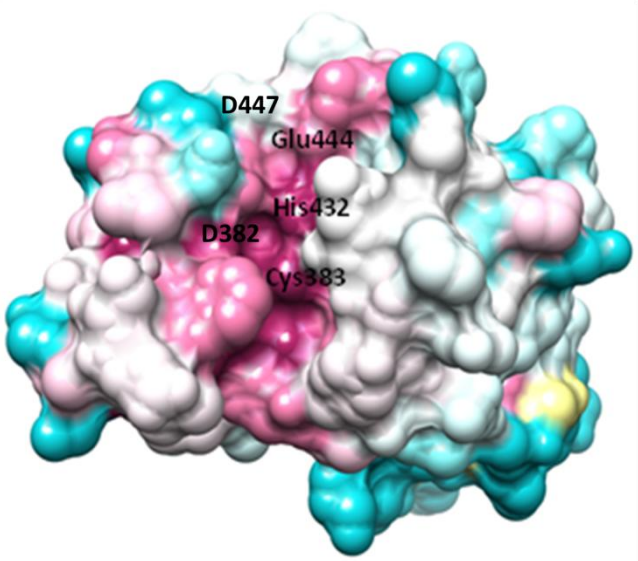


Figure S1 (A) Aminoacid sequence of $RipA_{263\text{-}472}$ variants studied in this work. The black region corresponds to $RipA_{332\text{-}472}$ whereas mutations are shown in red. (B) Map of conserved residues on $RipA_{332\text{-}472}$ surface, as calculated by ConSurf sequence alignment (Goldenberg *et al.*, 2009). Residue colouring, reflecting the degree of residue conservation over the entire NlpC/P60 domain family, ranges from magenta (highly conserved) to cyan (variable).

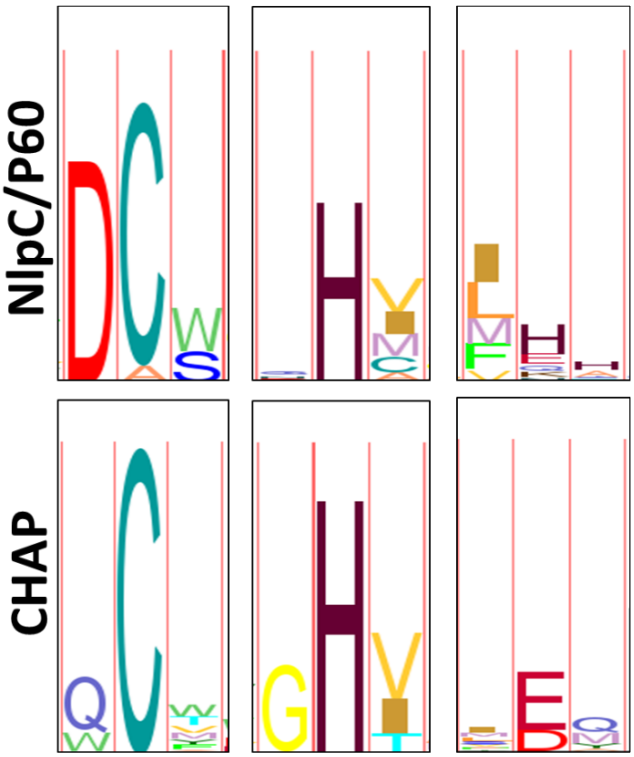


Figure S2 HMM logo showing conservation of the catalytic triad in NlpC/P60 (top) and CHAP (bottom) domains.

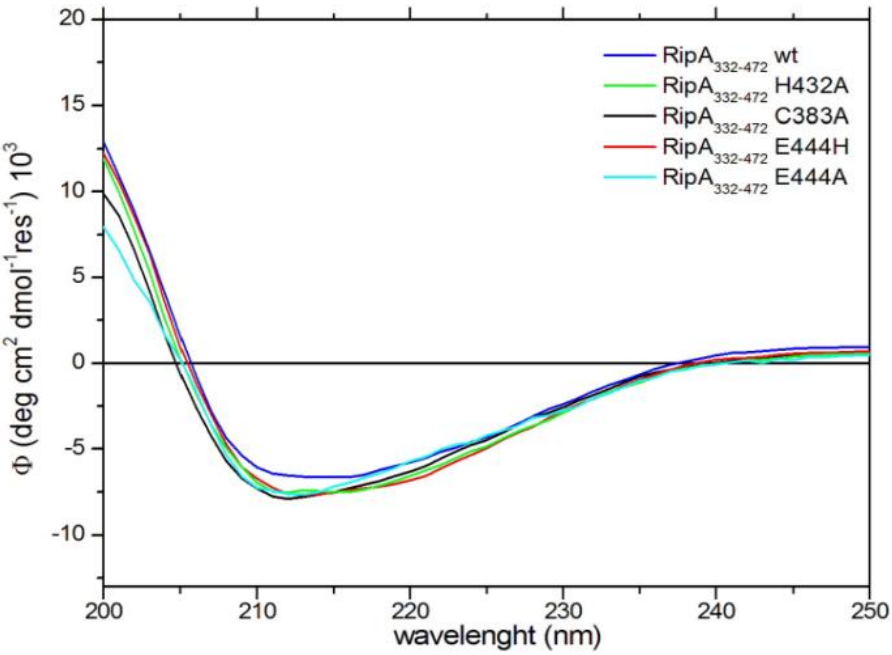


Figure S3 CD spectra showing that mutations do not affect $RipA_{332-472}$ overall structural integrity. Colour code is explained in the inset.

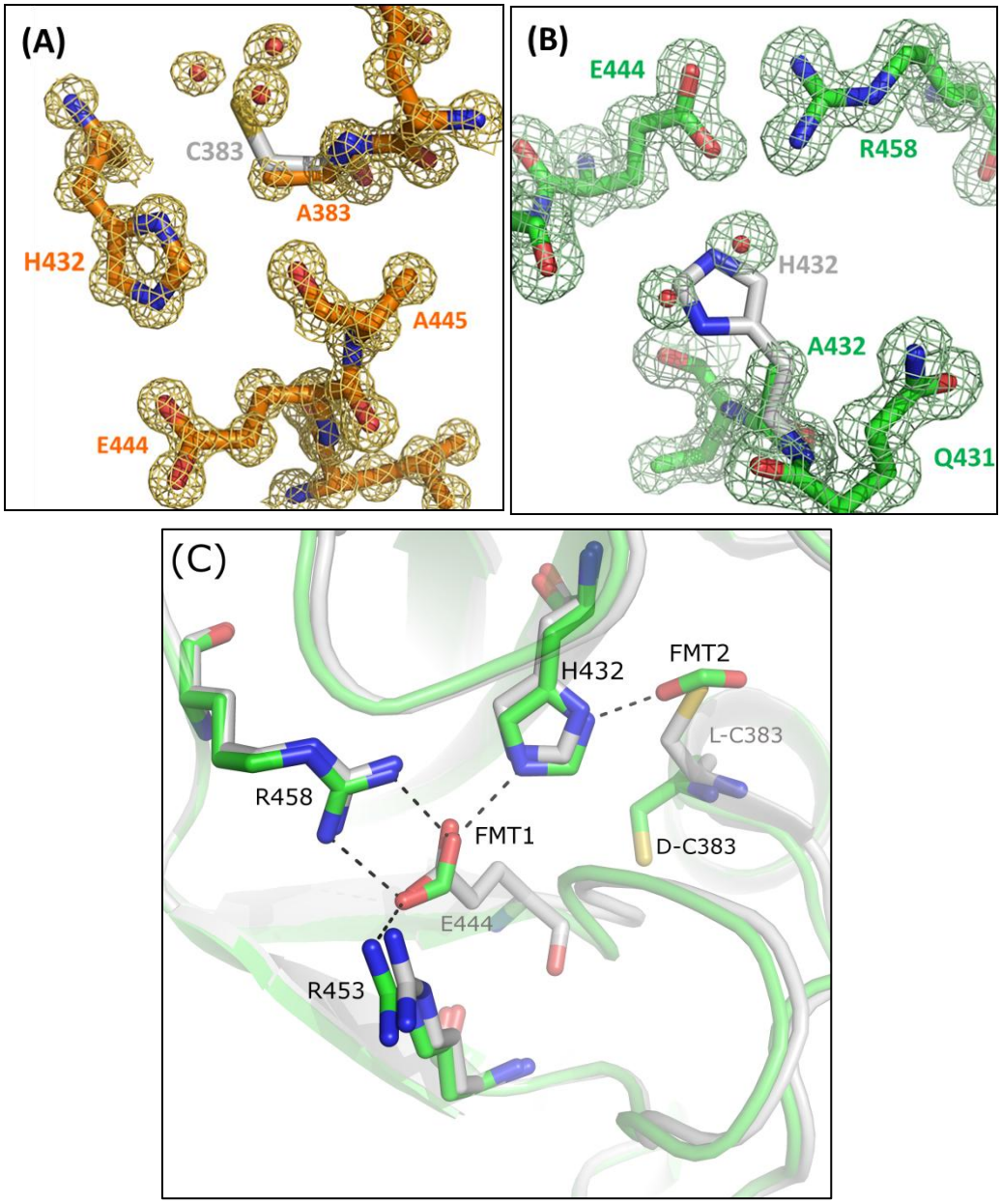


Figure S4 (A) Omit (2Fo-Fc) electron density map of the catalytic site in the C383A mutant (orange) and (B) in the H432A mutant (green). (C) Residues of the wild type protein are shown in grey for comparison.

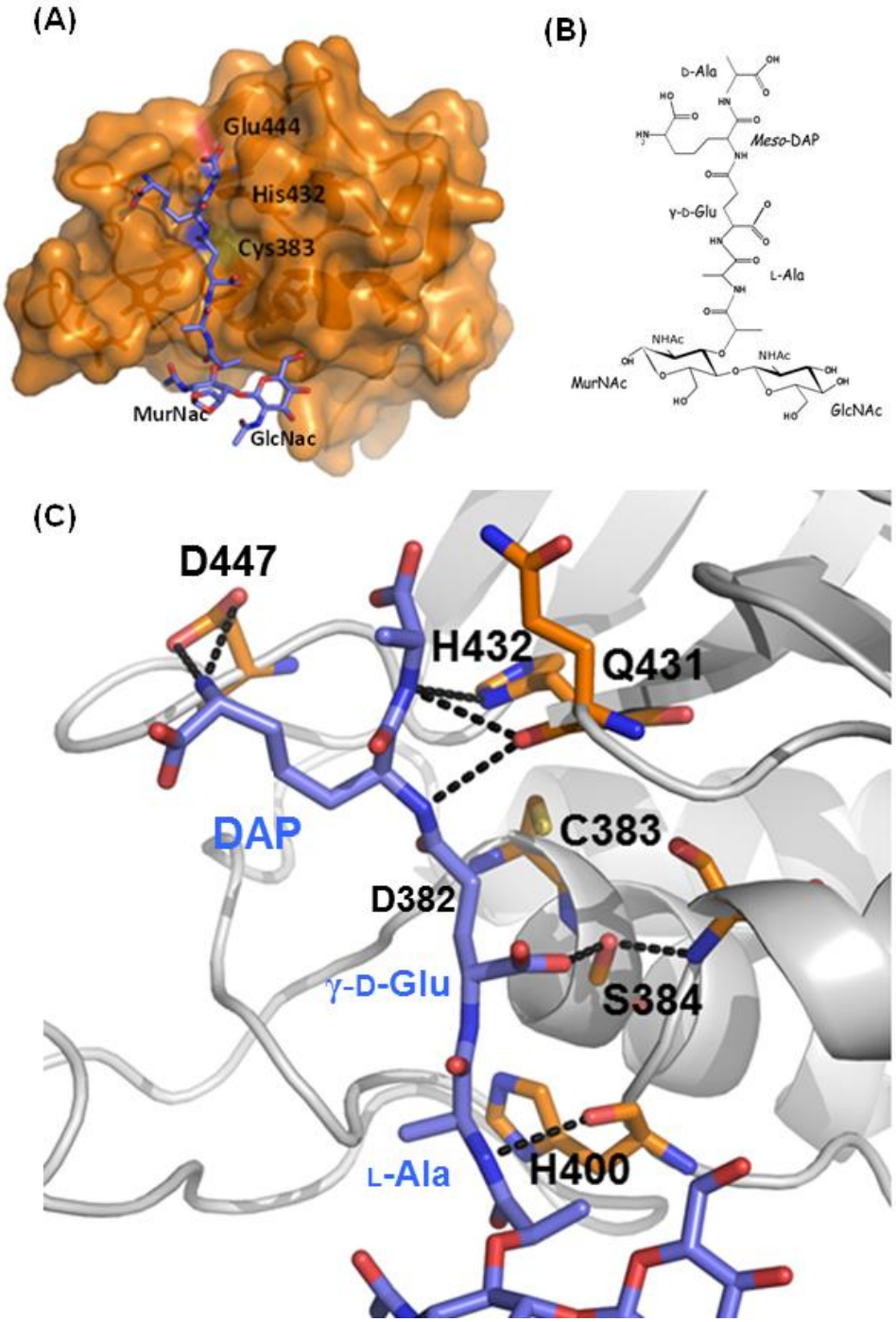


Figure S5 **(A)** Modeling of the muropeptide GlcNAc-MurNAc-L-Ala-γ-D-Glu-mesoDAP-D-Ala in RipA catalytic site cleft; (B) Chemical structure of studied muropeptide; (C) Details of muropeptide binding with RipA catalytic site cleft.

Supplementary reference

Goldenberg, O., Erez, E., Nimrod, G. & Ben-Tal, N. (2009). *Nucleic Acids Res* **37**, D323-D327.