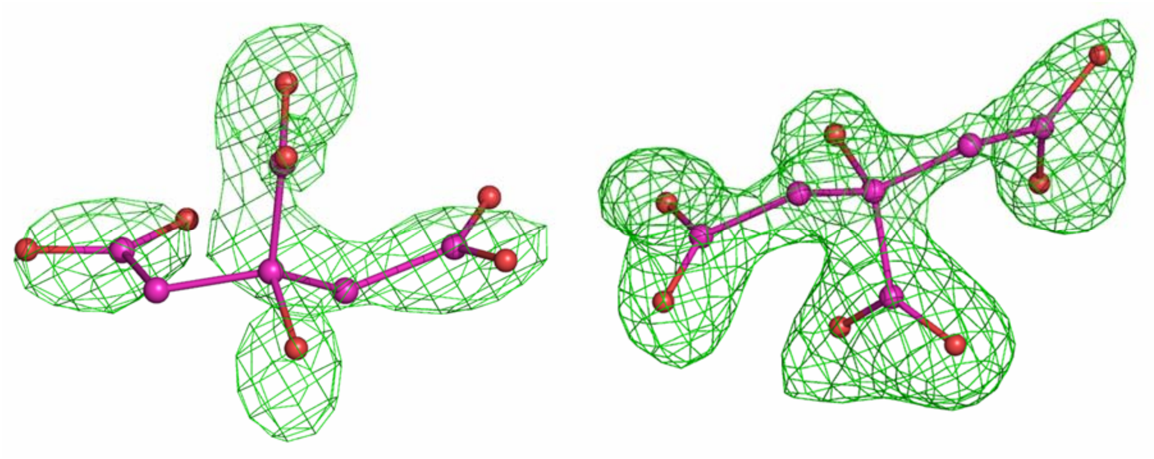
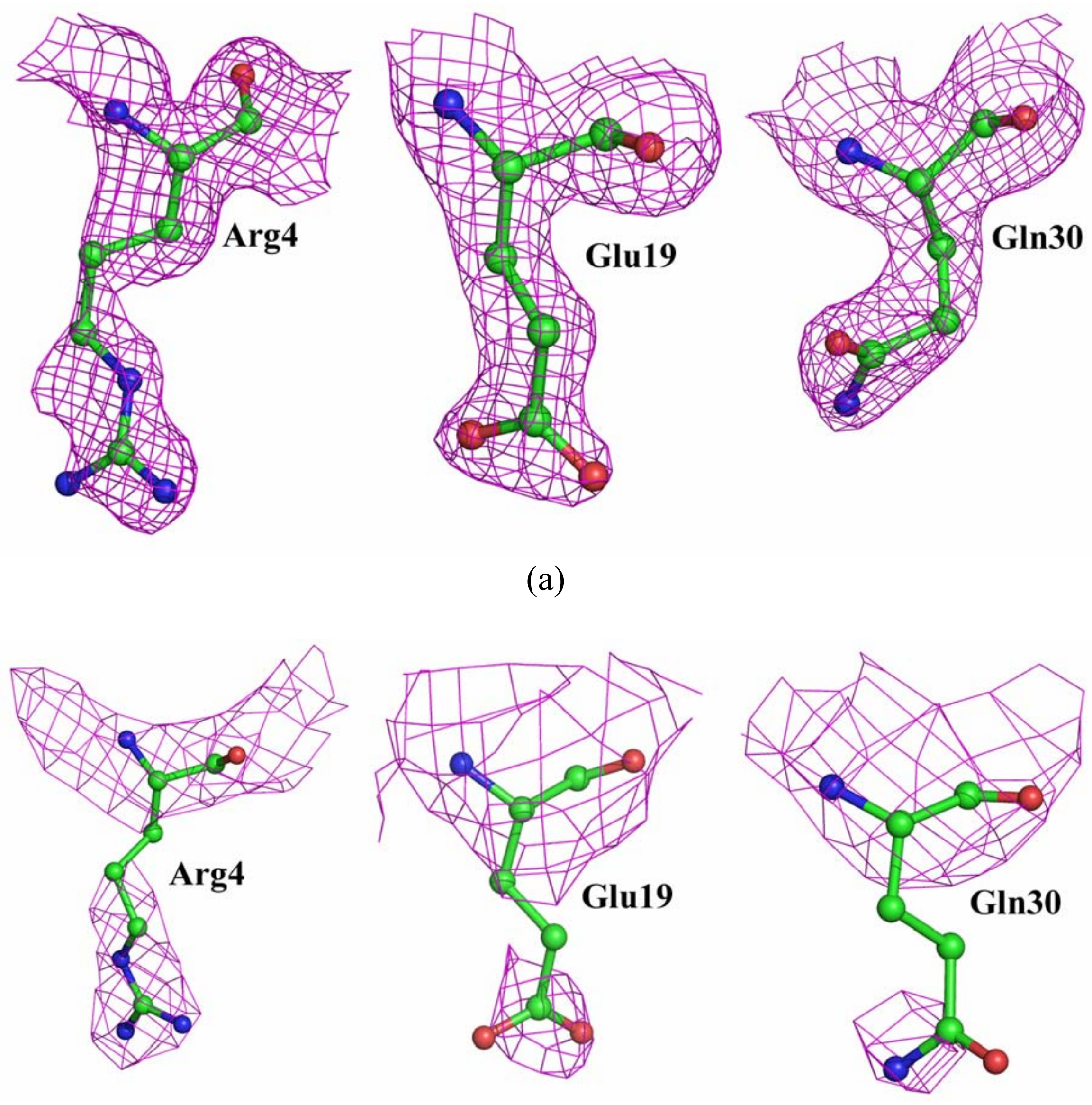


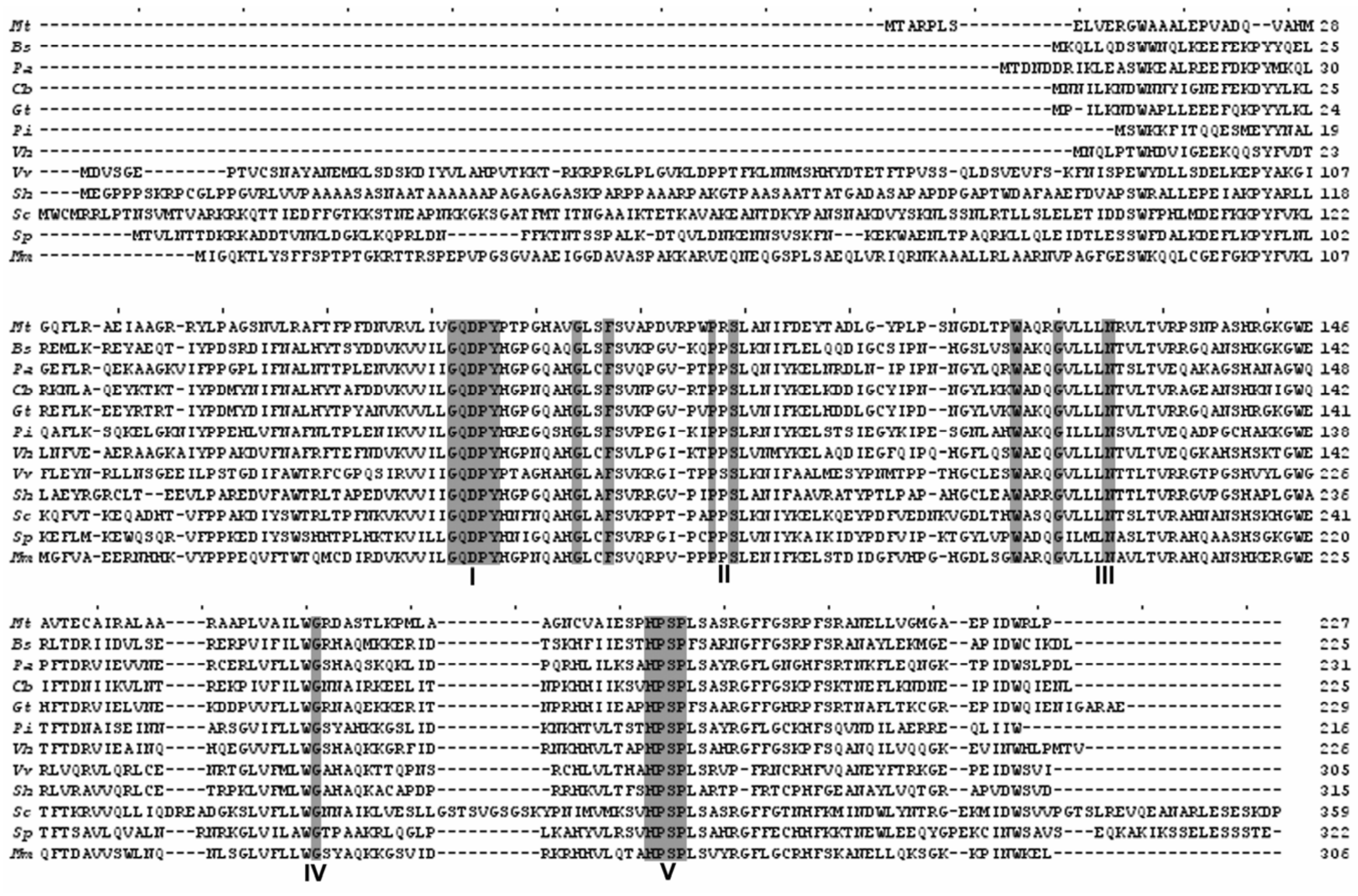
Supplementary Figure S1. Unexplained electron density in the Fo-Fc map which could be interpreted as that for two citrate ions. The contours are at 3σ level.



(a)

(b)

Supplementary Figure S2. Electron density in 2Fo-Fc maps for representative residues in the structures (a) MtUng and (b) the MtUng-Ugi complex. The contours are at 1 σ level



Supplementary Figure S3. Alignment of typical sequences among the 293 that are homologous to MtUng. Totally conserved residues are highlighted. Mt: *Mycobacterium tuberculosis*; accession No. P67071 (High G+C Gram-positeve bacterium), Bs: *Bacillus* *subtilis*; P39615 (Low G+C Gram-positive bacterium), Pa: *Pseudomonas aeruginosa*; A6VAM7 (Gram-negative bacterium), Cd: *Clostridium botulinum*; B2V017 (Anaerobai bacterium), Gt: *Geobacillus thermodenitrificans* A4ITQ2 (Thermophilic bacterium), Pi: *Psychromonas ingrahamii*; A1SUE5 (Psychrophilic bacterium), Vh: *Vibrio harveyi*; A7MS85 (Halophilic bacterium), Vv: Varicella-zoster virus; P09307 (Huamn herpesvvirus), Sh: Suid herpesvirus 1; P52506 (Porcine herpesvirus 1), Sc: *Saccharomyces cerevisiae*; P12887 (Yeast mitochondrial), Sp: *Schizosaccharomyces pombe*; O74834 (yeast), Ms: *Mus musculus*; P97931 (Mouse).