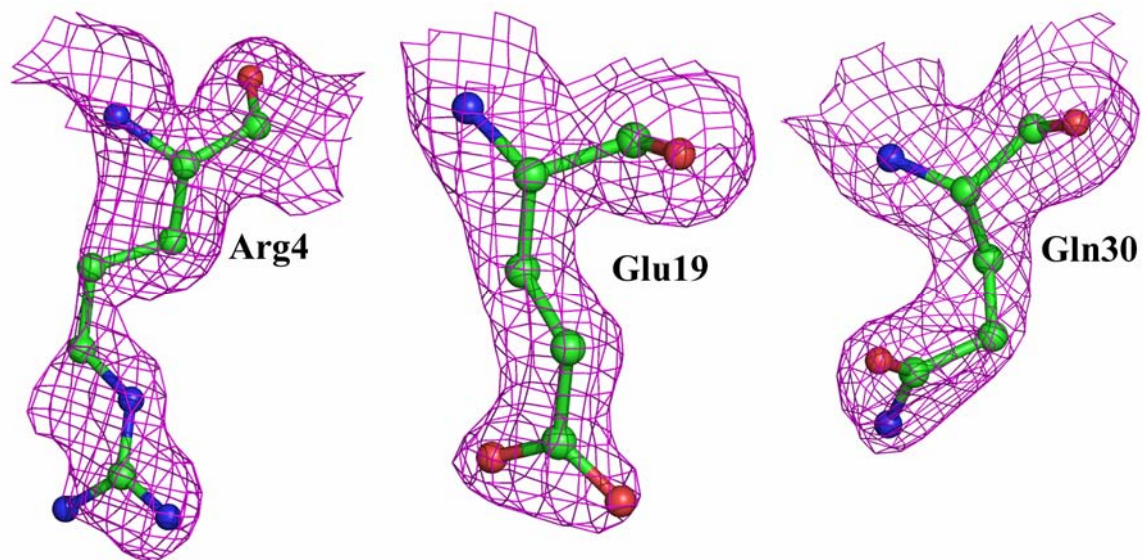
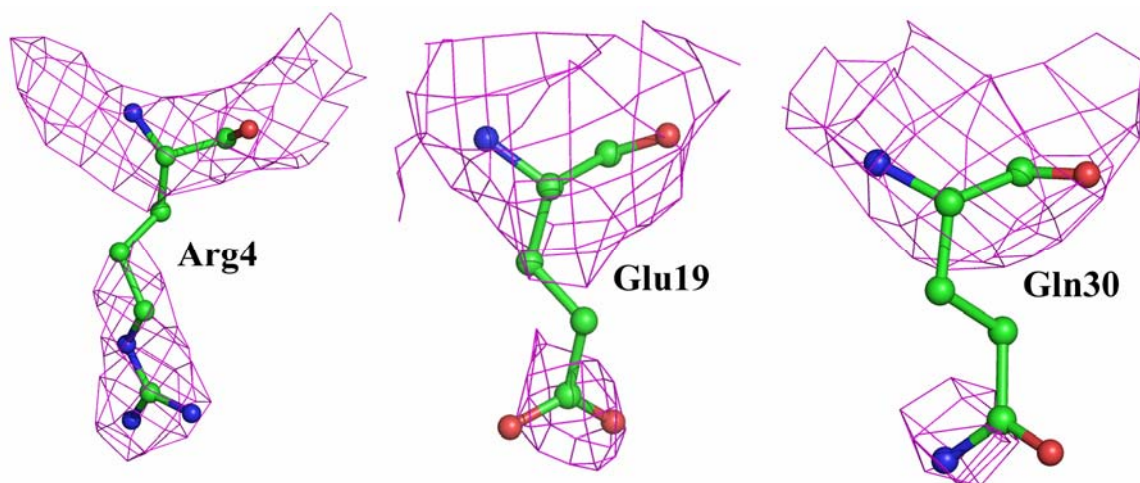


**Supplementary Figure S1.** Unexplained electron density in the Fo-Fc map which could be interpreted as that for two citrate ions. The contours are at  $3\sigma$  level.



(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  $\sigma$  level

Mt -----MTARPLS-----ELVERGWAAALEPVADQ--VAHM 28  
 Bs -----MKQLLQDSWNNQLKEEFKPYQEL 25  
 Pa -----MTDNDRIKLEASWKEALREEFDKPYMKQL 30  
 Cb -----MMHILKMDWNNYIGNEFEKPYLKL 25  
 Gt -----MP-ILKMDWAPLLEEFQKPYLKL 24  
 Pi -----MSWKKFITQESMEYYNAL 19  
 Vh -----MNQLPTWHDVIGEEKQQSYFVD 23  
 Vy -----MDVSGE-----PTVCSNAYANEMKLSDSKD IYVLAMPVTKKT-RKRPRGLPLGVKLDPPFTKLNNMSHNYDTETFTPVSS-QLDSVEVFS-KFNISPEWYDLSDELKEPYAKGI 107  
 Sh -----MEGPPPSKRPCGLPPGVRLVUPAAAASASNAATAAAAAAPAGAGAGASKPARPPAAARPAGKTPAASAAATATGADASAPAPDPGAPTWDAAFAAEFDVAPSWRALLEPEIAKPYARLL 118  
 Sc MWCMRRLPTNSVMTVARKKQTTIEDFFGTHKSTNEAPHKKGKSGATFMTITNGAAIKTETKAVAKEANTDKYPANSHAKDVYSKQLSSNLRTLLSLELETIDDSWFFPHLMDEFKGPYFVKL 122  
 Sp -----MTVLNTTDKPKADDTVHKLDGKLGKQPRLDN-----FFKTNTSSPALK-DTQVLDNKENHNSVSKFN--KEKWAENLTPAQKLLQLEIDTLESSWFDALKDEFLKPYFLNL 102  
 Ma -----MIGQKTLYSFFSPTPTGKRTTRSPPEVPGSGVAAEIGGDAVASPAKKARVEQNEQGSPLSAEQLVRIQRNKAALLRLAARNUPAGFGESWKKQLCGEFGKPYFVKL 107

Mt GQFLR-AEIAAGR-RYLPAGSHVLRAFTFPFDIVRVLIVGQDPYPTPGHAGVLSFSVAPDVWPERSLANIFDEYTAGDLG-YPLP-SHGDLTPWAQRGVULLLHVLTVRPSPHPASHRGKGWE 146  
 Bs REMLK-REYAEQT-IYDSDRIFNALHYTSYDDVKVWILGQDPYHGPQGQAGLSFSVVKPGV-KQPPSLKNIIFLELQDDIGCSIPN--HGSLVSWAKQGVULLLNTVLTVRRGQANSHRGKGWE 142  
 Pa GEFLR-QEKAAGKVIFPPGPIFNALNTTPLENVKVVILGQDPYHGPQGQAGLCSFVQPGV-PTPPLSLNIYKELNRLN-IPIPN-HGYLQSWAEQGVULLLNTSLTVEQAKAGSHANAGWQ 148  
 Cb RQHLA-QEYKTKT-IYDMDYIFNALHYTAFDDVKVWILGQDPYHGPQGQAGLCSFVQPGV-RTPPSLNIIYKELKDDIGCYIPN--HGYLKQWADQGVULLLNTVLTVRAGEANSHRGIGWQ 142  
 Gt REFLK-EEYRTRT-IYDMDYIFNALHYTPYANVKVWLLGQDPYHGPQGQAGLCSFVVKPGV-PVPPSLVNIYKELHDDLGCYIPD--HGYLKQWAKQGVULLLNTVLTVRRGQANSHRGKGWE 141  
 Pi QATLK-SQKELGKNIYPPHVLNFNALTPLENIKVVILGQDPYHGPQGQAGLCSFVPEGI-KIPPSLNIYKELSTSIEGYKIPESGNLAKWAKQGILLNLSVLTVEQADPGCHAKKGWE 138  
 Vh LNFVE-AERAAGKAIYPPAKDVFNAPRTEFNDVKVWILGQDPYHGPQGQAGLCSFVLPGI-KTPPSLVNMYKELAQDIEGFQIPQ-HGFLQSWAEQGVULLLNTVLTVEQKAKSHSKTGWE 142  
 Vy FLEYN-RLNLSGEEILPSTGDIFAWTRFCGPGSIRVVIIGQDPYPTAGHAGLAFSVKRGITPPPSLKNIFAALMESYPMTTP-TNGCLESWARQGVULLLNTLTVRRGTPGSHVYLGW 226  
 Sh LAEYRGRCIT--EEVLPAREDVFAWTRLTAPEDVKVWILGQDPYHGPQGQAGLAFSVKRGV-PIPPSLANIFAAVRATYPTLPAP-ANGCLEAWARRGVULLLNTLTVRRGTPGSHAPLGWA 236  
 Sc KQFVT-KEQADHT-VFPPAKDIYSWTRLTTPFNKVKVWILGQDPYHGPQGQAGLAFSVKPGT-PAPPSLKNIIYKELKQEPDFVEDNKGVDLTHWASQGVULLLNTSLTVRAHNIANSKSHGW 241  
 Sp KEFLM-KEWQSQR-VFPPKEDIYSWSHRTPLHKTIVILLGQDPYHGPQGQAGLAFSVKPGI-PCPPSLVNIYKAIKIDYDIPVIP-KTGYPVWADQGILMLNASLTVRAHQASHSGKGWE 220  
 Ma MGIVA-EERNHKK-VYPPPEQVFTWTQCDIRDVKVWILGQDPYHGPQGQAGLAFSVKPGV-PPPPSLNIIYKELSTDIDGFVHPG-HGDLSCWARQGVULLLNTVRAHQANSHKRGWE 225

I II III

Mt AVTECAIRALAA---RAAPLVAAILWGRDASTLKPMLA-----AGNCVAIESPHPSPLSASRGFFGSRPFSRANELLVGMGA--EPIDWRLP----- 227  
 Bs RLTDRIIDVLS---RERPVIIFLWGRHAQMKKERID-----TSKRFIIESTHPSPLSARNGFFGSRPFSRANAYLEKMG--APIDWCIKDL----- 225  
 Pa PFTDRVIEVVTE---RCERLVFLLWGRSHAQSKQKLID-----PQRHLILKSANPSPLSAYRGFLGNHFSRTHKFLQNGK--TPIDWSLPDL----- 231  
 Cb IFTDNIIVKLT---REKPIVIFLWGNNAIRKEELIT-----NPKQHIIKSVHPSPLSASRGFFGSKPFSKTHFLKNDNE--IPIDWQIENL----- 223  
 Gt HFTDRVIELVNE---KDDPVVFLWGRNAQEKKERIT-----NPRRHIIEAPHPSPSFAARGFFGHRPFSRTNAFLTCKGR--EPIDWQIENIGARAE----- 229  
 Pi TFTDHAISEINN---ARSGVIFLLWGRSYAHKKGSLID-----KHKGTULTSTHPSPLSAYRGFLGCKHFSQVNDILAERRE--QLIIW----- 216  
 Vh TFTDRVIEAINQ---HQEGVVFLWGRSHAQKGRFID-----RHKQHVLTAPHPSPSFAHRGFFGSKPFSQANQLVQQGGK--EVINWHLPMTV----- 226  
 Vy RLVRQLVQLCE---NRTGLVFMWGRANAQKTTQPHS-----RCHLVLTNHPSPLSRVP-FRNCRHVQANEYFTRKGE--PEIDWSVI----- 305  
 Sh RLVRVAVQLCE---TRPKLVFMWGRANAQKACAPD-----RRHKVLTFSHPSPSLARTP-FRNCPHGEANAYLVQGTGR--APVDWSVD----- 315  
 Sc TTFKRVVQLLIQDREADGKSLVFLWGNNAIKLVESLLGSTSVGSGSKYPHIMVMSKVPSPSASRGFFGTNHFIMINDWLYNTRG-EKMDWSVVPGTSLREVQEAHARLESESKDP 359  
 Sp TFTSAVLQVALN---RNRKGLVILAWGTPAAKRLQGLP-----LKARYVLRSVHPSPLSARNGFFECHNFKKTHEWLEEQYGPKECINWSAVS--EQKAKIKSSELESSTE- 322  
 Ma QFTDAVWSVLNQ---NLSGLVFLWGRSYAQKKGSVID-----RKRHVLTQTHPSPLSVYRGFLGCKHFSKANELLQKSGK--KPINWKL----- 306

IV V

**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-positive 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 herpesvivirus), Sh: Suid herpesvirus 1; P52506 (Porcine herpesvirus 1), Sc: *Saccharomyces cerevisiae*; P12887 (Yeast mitochondrial), Sp: *Schizosaccharomyces pombe*; O74834 (yeast), Ms: *Mus musculus*; P97931 (Mouse).