



Supplemental Figure SF1. Conformational changes for Asn104 and Tyr105 in the ES*-acylation structure. Glu166His with the “flipped-out” conformation forms H-bond with Asn104. Tyr105 becomes more flexible as indicated by the electron density. Fo-Fc omit map (purple) is drawn in mesh format and contoured at 2.0 σ .