



FIGURE S1. Related to Fig. 3. 2Fo-Fc electron density maps of drugs bound to allβ3 headpiece in the order of their appearance in the main text. Metal conditions (Mg or Mn) for compound soaking are described in Table S1. Electron density (cyan mesh) is contoured around atoms at 1.5 σ . Colors are as in Fig. 2: Mg²⁺ and Mn²⁺ ions as gold and purple spheres, respectively, and waters as smaller red spheres. Black dashes represent metal coordination and key hydrogen bonds.