



Figure S4. Substrate binding in MdfA

(a-c) Stick models of the substrate binding sites in Cm, deoxycholate (Dxc), and LDAO complex structures, respectively. Omit maps are contoured at 3.0σ around the substrate molecules (magenta). Oxygen and nitrogen atoms are in red and blue, respectively. Molecular surface representation is from the MdfA structure. (d) Superimposition of the three ligands. Stick model of Cm is shown in magenta, and others in grey.