



Figure S3. Diagram illustrating the comparison of the Toll-like receptor 4/myeloid differentiation factor-2/lipopolysaccharide (TLR4/MD-2/LPS) complex structures with HDCK and X-ray crystallography data. The three-dimensional (3D) structures of TLR4 and MD-2 are presented in a cartoon style, whereas LPS (core oligosaccharide and lipid A) is depicted in stick representation. TLR4 and MD-2 are shown in light blue and dark pink, respectively. (a) 3D structures of the TLR4/MD-2/LPS complexes determined by X-ray crystallography. The core oligosaccharide and lipid A of LPS are shown in orange and dark green, respectively. (b) 3D structure of the TLR4/MD-2/LPS complexes of HDCK data. The core oligosaccharide and lipid A of LPS are shown in yellow and light green, respectively. (c) Superimposition 3D model of the TLR4/MD-2/LPS complexes of HDCK and X-ray crystallography data.