



Figure S2. Atomic distances (upper subplots), and effective Mulliken atomic charges (lower subplots) of atoms directly involved in the reaction pathway, presented for BBI docked to β -lactamases which

belong to the A, C, and D classes, respectively. The simulation results in the plots are based on the “first simulation” described in **Table 2**. The reaction steps, marked with vertical dashed lines, correspond to denotations in **Table 2** and in **Figure 7**.