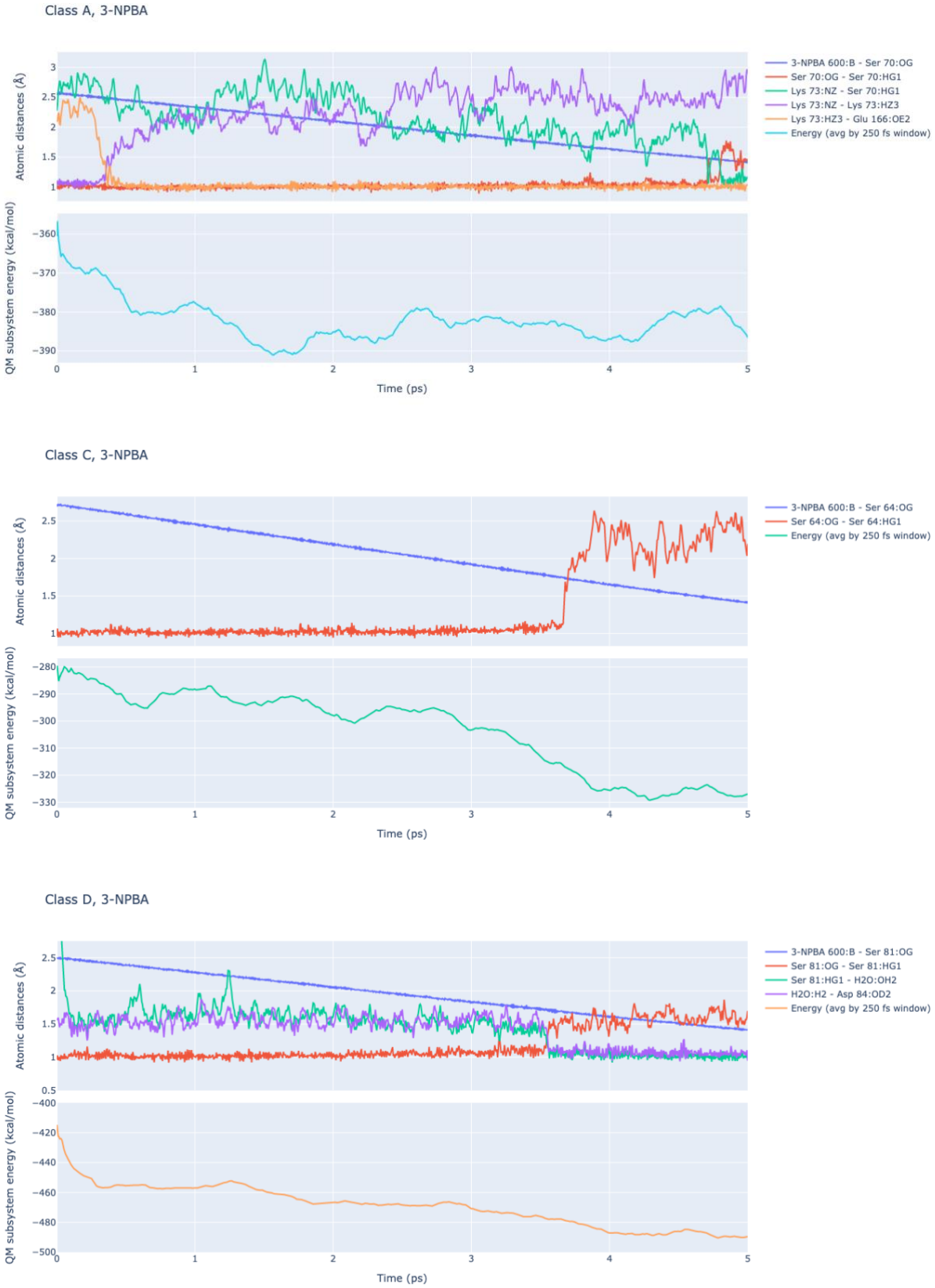

Figure S3. Steered molecular dynamics (SMD) simulations results for the complexes of 3-NPBA and β-lactamases which belong to the A, C, and D classes, respectively. The distance between the boron atom of 3-NPBA and the oxygen atom of Ser OG was gradually reduced. Atomic distances (upper

subplots) and the QM subsystem energy of the residues and the inhibitor directly involved in the reaction (lower subplots).