

Supporting Information for

Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Study
of the Deacylation Reaction in a Penicillin Binding Protein (PBP)
Versus in a Class C β -Lactamase

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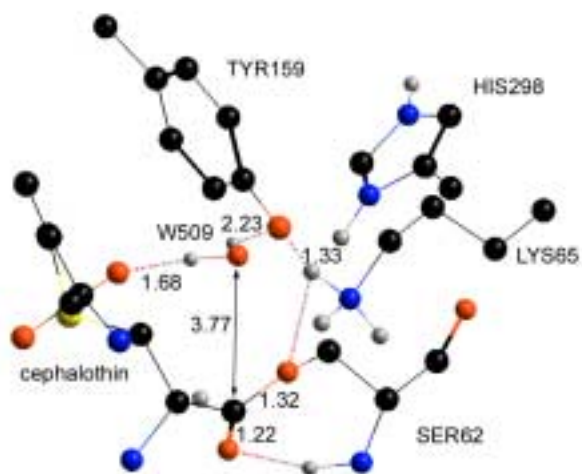
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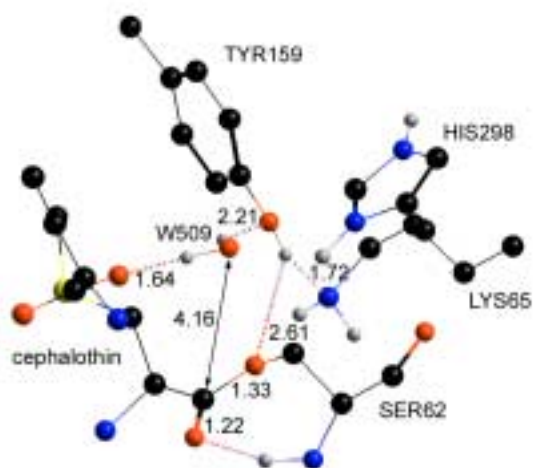
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Figure S1. Active site geometries for the QM/MM-optimized R61 acyl-enzyme intermediate protonation/hydrogen bond configurations. Dashed lines indicate hydrogen bonds. Single numbers indicate distances (Å). Color coding: C-black, N-blue, O-red, H-gray, S-yellow.

(1)



(2a)



(3)

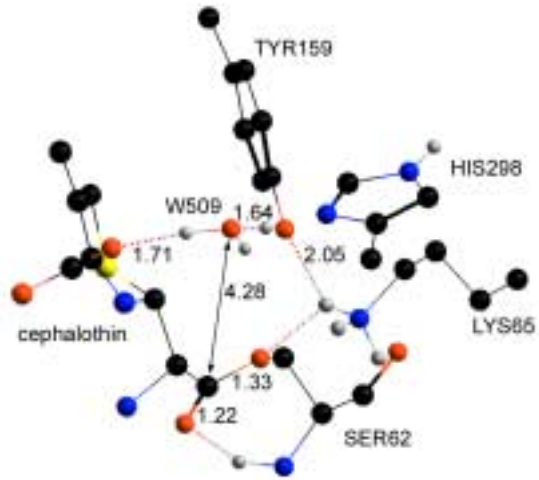
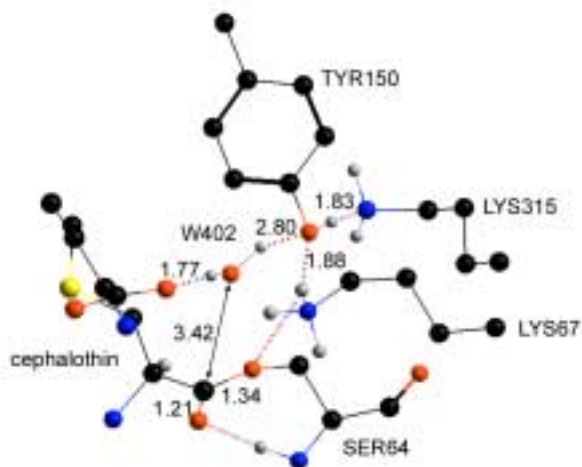
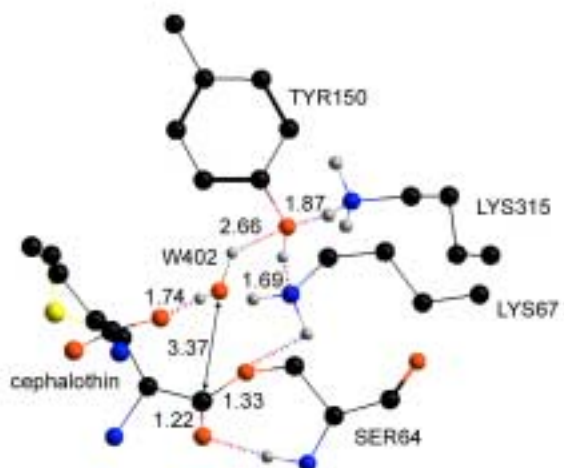


Figure S2. Active site geometries for the QM/MM-optimized P99 acyl-enzyme intermediate protonation/hydrogen bond configurations. Dashed lines indicate hydrogen bonds. Single numbers indicate distances (Å). Color coding: C-black, N-blue, O-red, H-gray, S-yellow.

(1)



(2)



(3)

