Mechanochemical Function of Myosin II: Investigation into the Recovery Stroke and ATP Hydrolysis

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Supplemental Information:

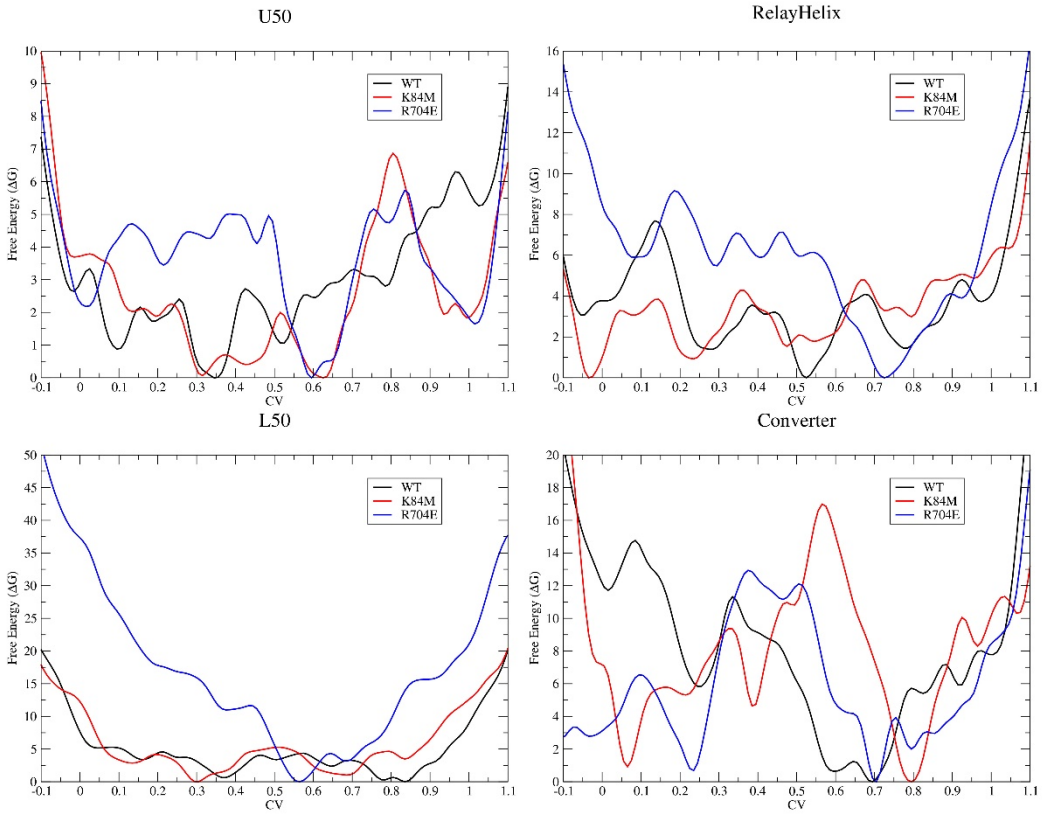

Figure S1. Coverged FES profiles for the U50 (top left), relayhelix (top right), L50 (bottom left, and converter (bottom right) domains for the recovery stroke.

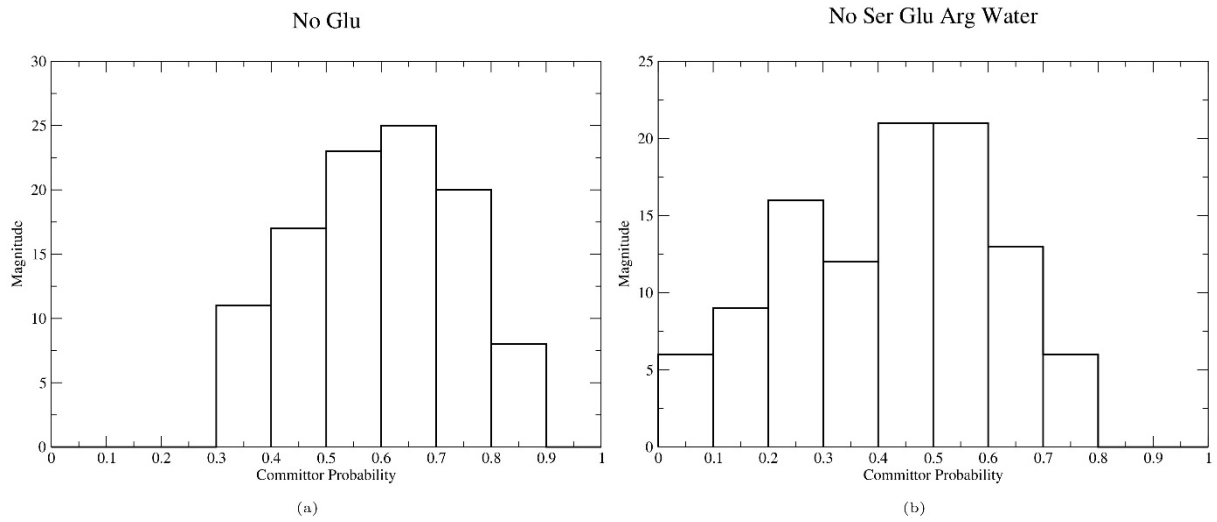

Figure S2. Committor distribution for a constrained QM region when a) Glu459 is unconstrained and b) Ser181, Glu459, Arg238, and a water are unconstrained.

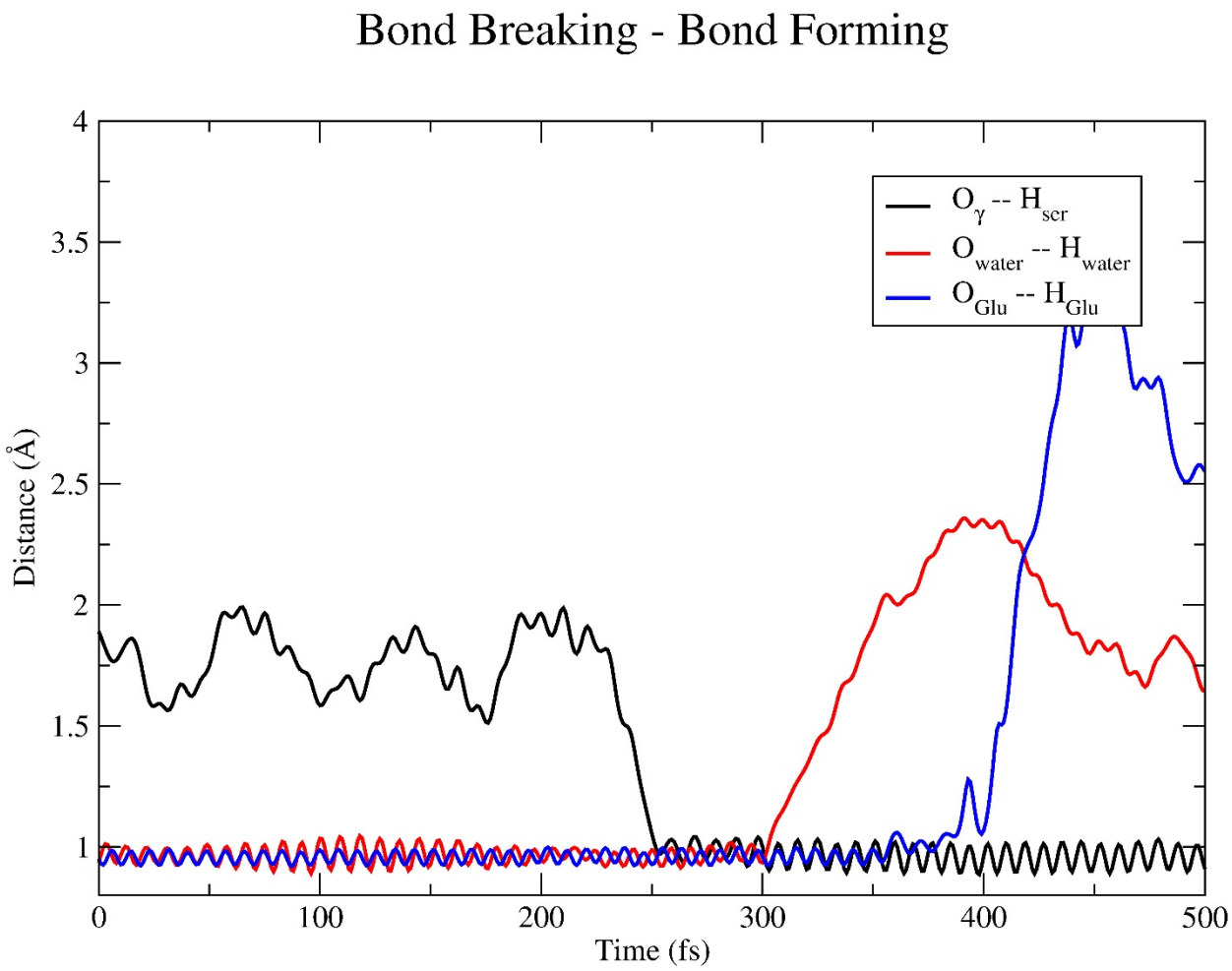

Figure S3. Mechanism for the formation of H_2PO_4 from the Ser181 ensemble. The proton from Ser181 (H_{ser}) transfers to an oxygen (O_γ) of HPO_4 and afterwards Ser181 abstracts the hydrogen from a nearby water (H_{water}) and Glu459 is then deprotonated (H_{Glu}) by the newly formed hydroxide.