

Supporting Information

For the manuscript: “**Exploring the dynamics of holo-Shikimate Kinase through molecular mechanics**” by Pedro Ojeda-May. High Performance Computing Center North (HPC2N), Umeå University, S-90187 Umeå, Sweden. (pedro.ojeda-may@umu.se)

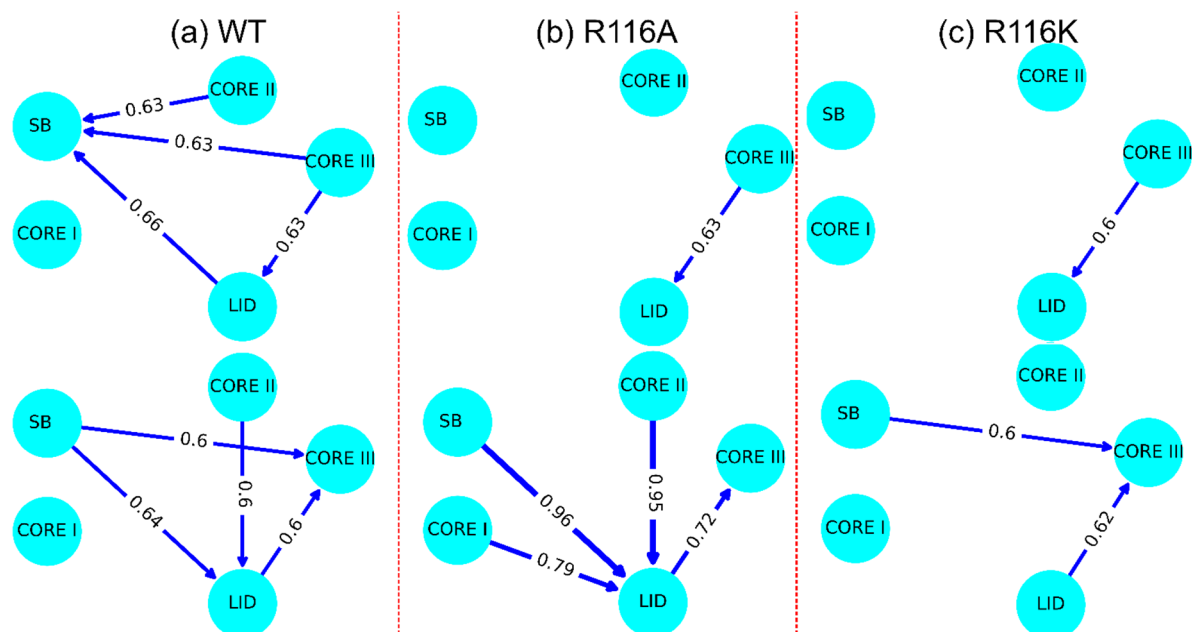


Figure S1. Directed graphs obtained from a 0.6 probability threshold with the Neural Relational Inference (NRI) method for the WT, R116A, and R116K variants in (a)-(c), respectively.