

Table S2. Docking figures for the best scoring structures, comparing the DHp domain in different conformational states

DHp functional state	Haddock's global score	Buried surface area (\AA^2)	Haddock energy (kJ/mol)	Distance ATP γ P - His188 N_ϵ (\AA)
kinase	-99.2	1540	-620	3.08
phosphotransferase	-73.3	1271	-263	3.02
phosphatase	-135	1890	-761	8.7