Figure 5-figure supplement 1

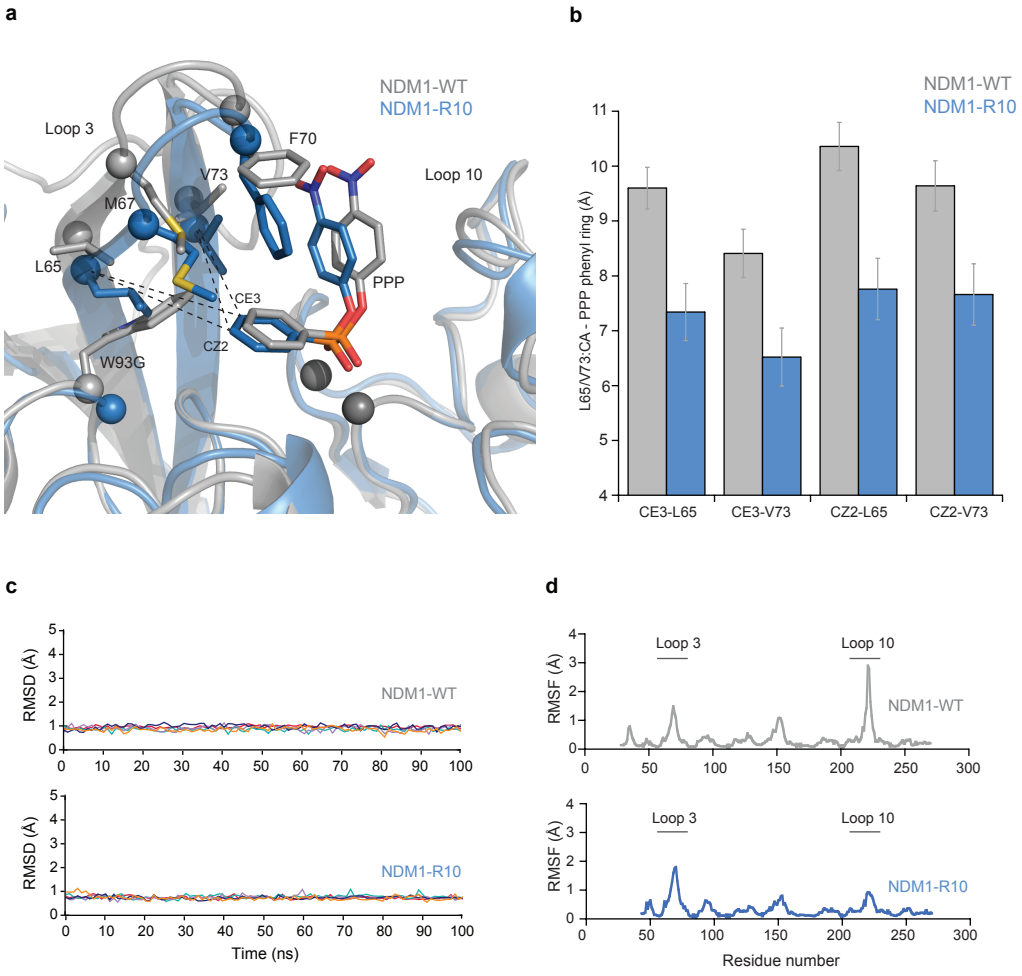

Figure 5-figure supplement 1. The molecular dynamics (MD) simulations of NDM1-WT and NDM1-R10. (**A**) Overlay of representative structures from the MD simulations of NDM1-WT (grey), NDM1-W93G (blue) in complex with the PPP substrate (**B**) The average distance between the substrate and active site residues Leu65 and Val73 during the MD simulation of NDM1-WT and R10. (**C**) Root-mean square deviations (RMSD, Å) of all C-α atoms from the MD simulations of the NDM1-WT and NDM1-R10 in complex with PPP. The relevant enzyme variants are indicated on each panel. The data is presented individually for five independent 100 ns trajectories in each system, and for clarity the data was plotted using cspline smoothing function implemented in Gnuplot. (**D**) Root-mean square fluctuations (RMSF, Å) of C-α atoms calculated from the last 50 ns of all five 100 ns simulations of NDM1-WT and NDM1-R10 in complex with the PPP substrate.