Figure 5-figure supplement 2

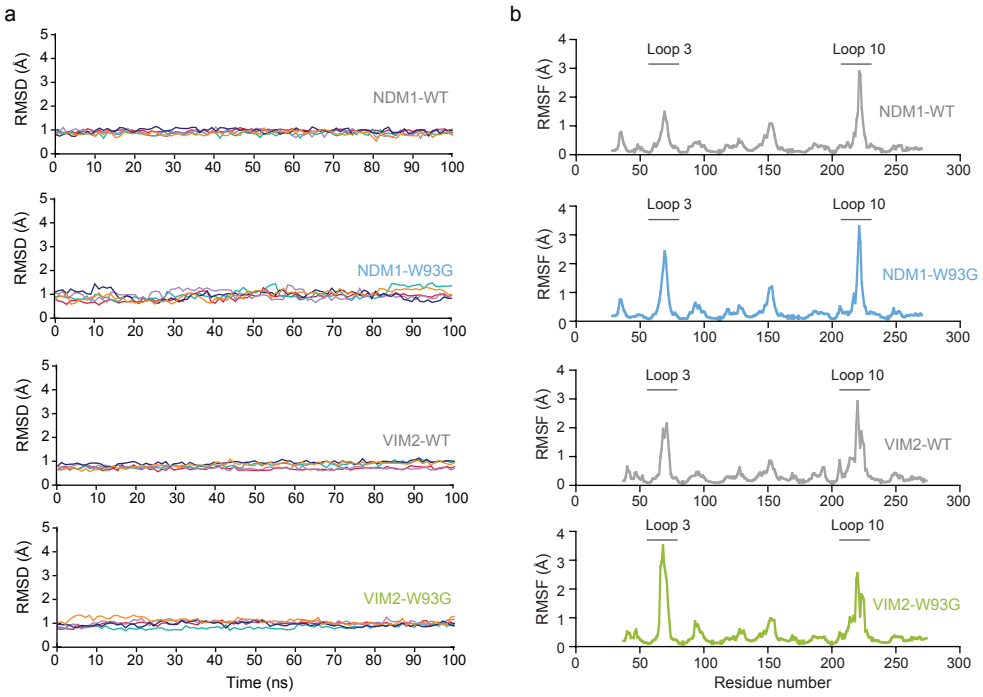

Figure 5-figure supplement 2. The molecular dynamics (MD) simulations of NDM1-WT, NDM1-W93G, VIM2-WT, and VIM2-W93G. (**A**) Root-mean square deviations (RMSD, Å) of all C-α atoms from the MD simulations of NDM1-WT, NDM1-W93, VIM2-WT and VIM2-W93G in complex with PPP. The relevant enzyme variants are 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. (**B**) Root-mean square fluctuations (RMSF, Å) of C-α atoms during the MD simulations. The data was calculated from the last 50 ns of all five 100 ns simulations of each of the four enzyme-PPP complexes (specific variant indicated in each panel).