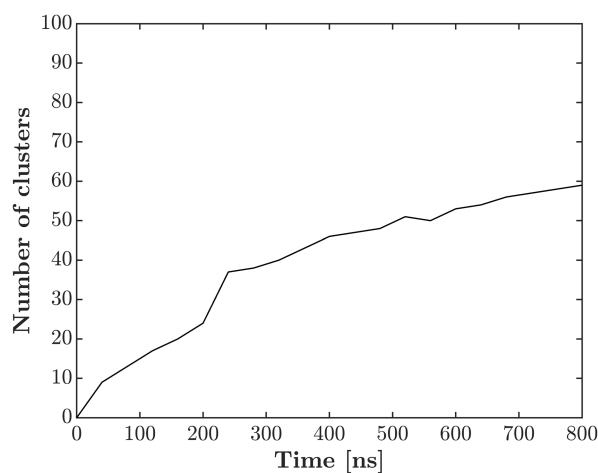


1 Supplementary material to

2 Pembrolizumab induces an unexpected

3 conformational change in the CC'-loop of PD-1



4 **Figure S1.** Number of clusters increasing with total simulation time. Daura clustering was
5 performed over increasing portions (every 50 ns) of total simulation time (0-800 ns) of the four
6 systems, PD-1_{Apo}, PD-1_{PD-L1} (red), PD-1_{Niv} (blue) and PD-1_{Pem}. First the number of clusters increases
7 significantly and shows some levelling off later on, indicating that simulations have fairly
8 converged.
9