

## **Supporting Information**

Molecular Dynamic Simulation of the Self-Assembly of DAP12-NKG2C Activating Immunoreceptor Complex

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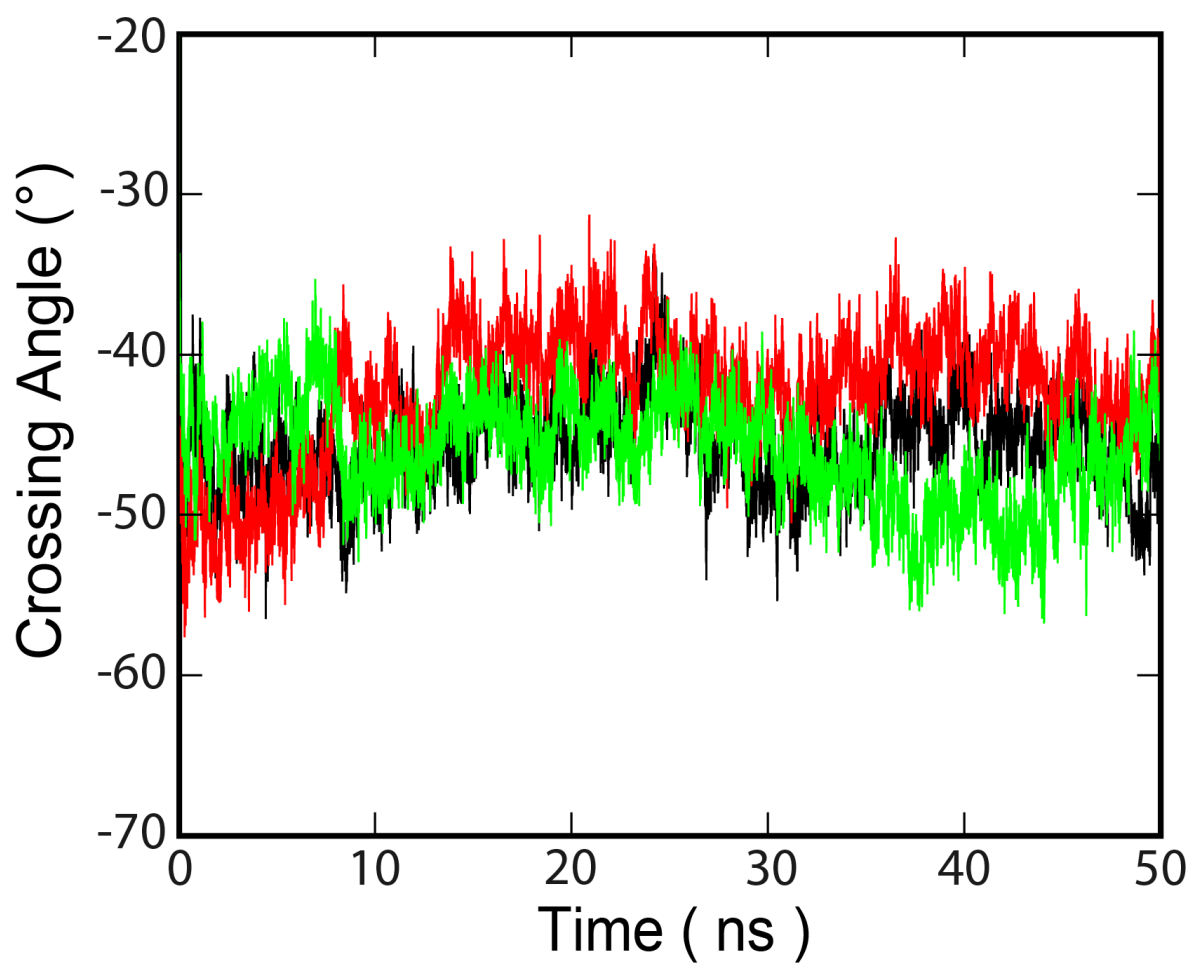


Figure S1: Crossing angle analysis based on AT-MD simulation of DAP12-NKG2C-DAP12 trimer. The figure shows the evolution of crossing angles of the DAP12 dimer. The analysis is carried out on all the three simulations (black, red, and green).

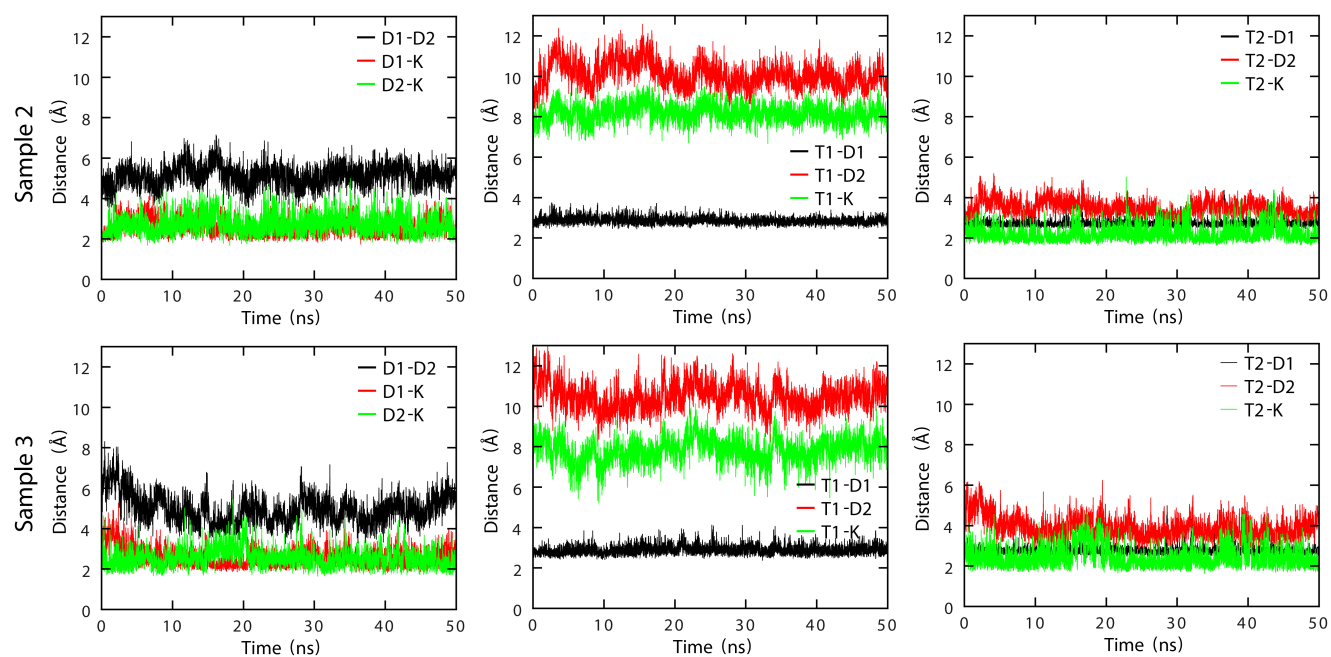


Figure S2: Distance between the key residues versus time in AT-MD simulation of DAP12-NKG2C-DAP12 trimer. Sample 2 and Sample 3 were shown; and Sample 1 was shown in Figure 3.

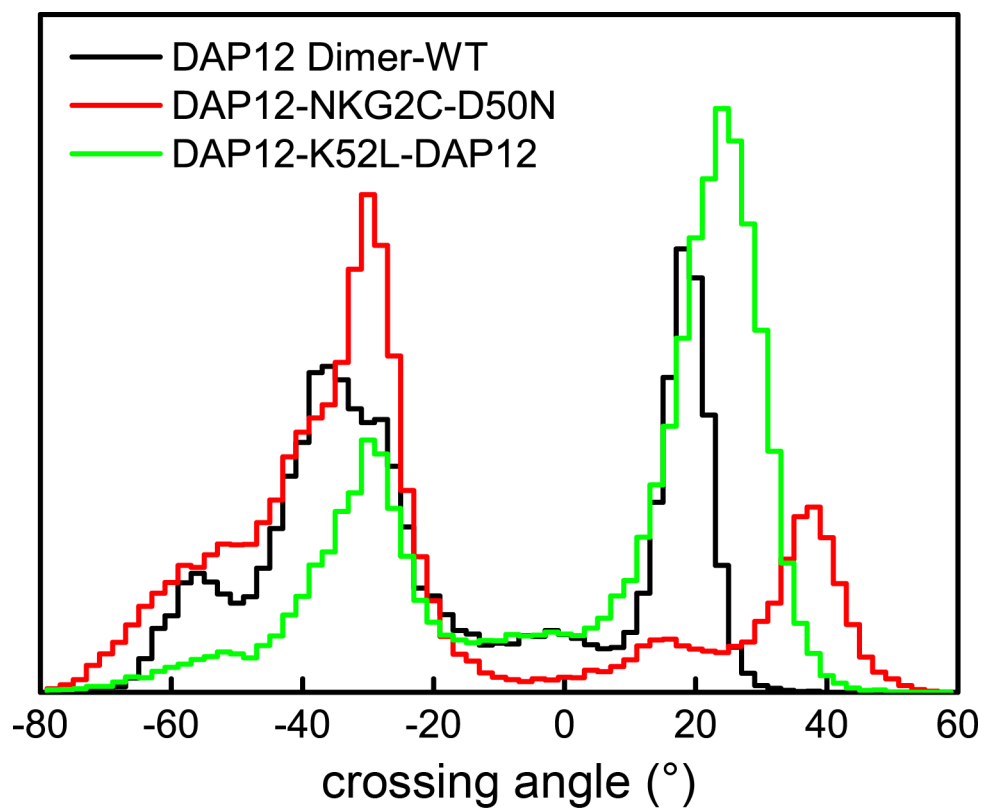


Figure S3: Convergence analysis of CG-MD simulations based on crossing angle analysis. The figure shows the distribution of the DAP12 dimer in wild type (black), DAP12-NKG2C-DAP12 (red), and DAP12-K52L-DAP12 (green) crossing angles. The analysis is carried out on all the three simulations.

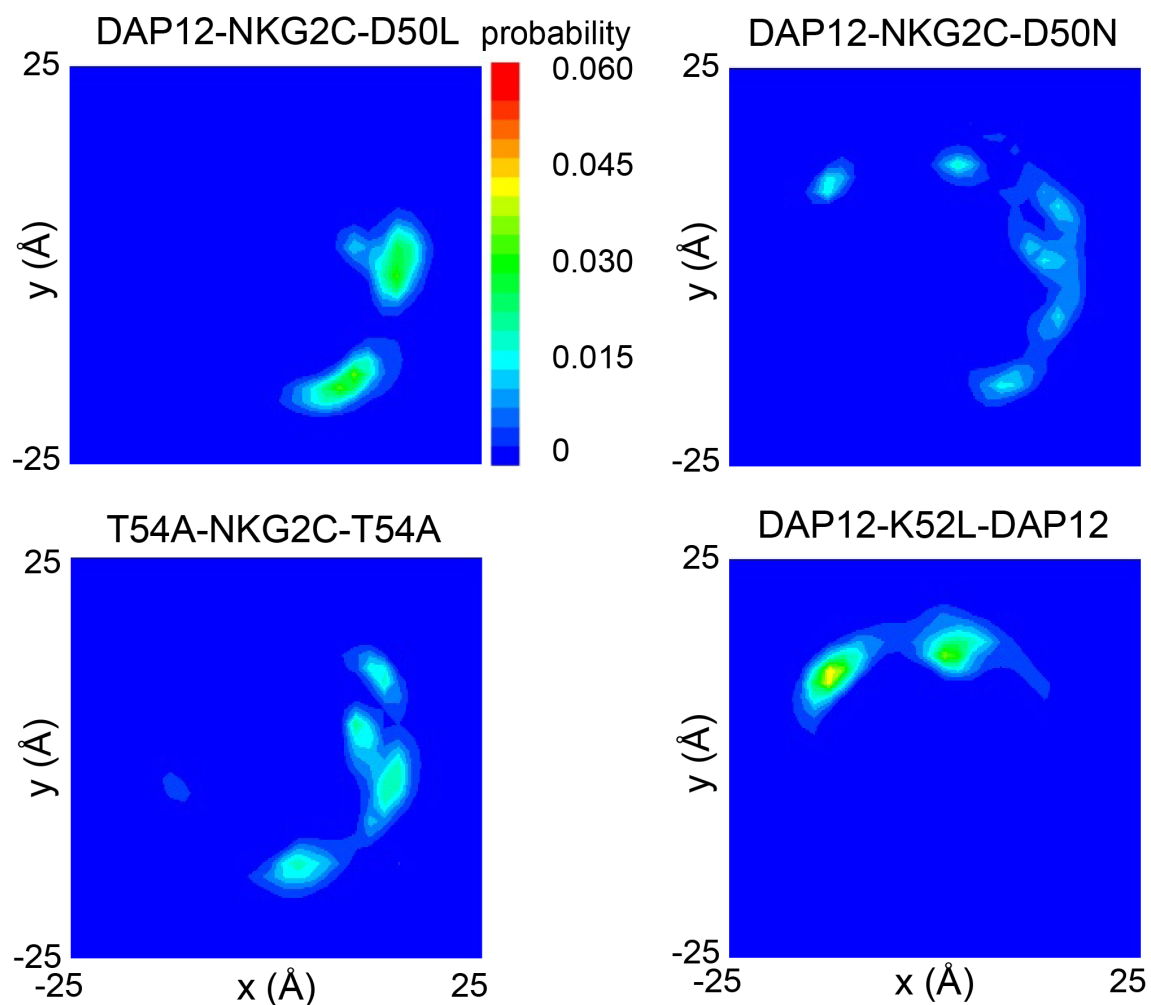


Figure S4: Convergence analysis based on the spatial distribution of the DAP12 dimer in mutants of DAP12-NKG2C-DAP12 trimer with respect to NKG2C. Blue and red indicate low and high probabilities of finding two DAP12 helices at that position.