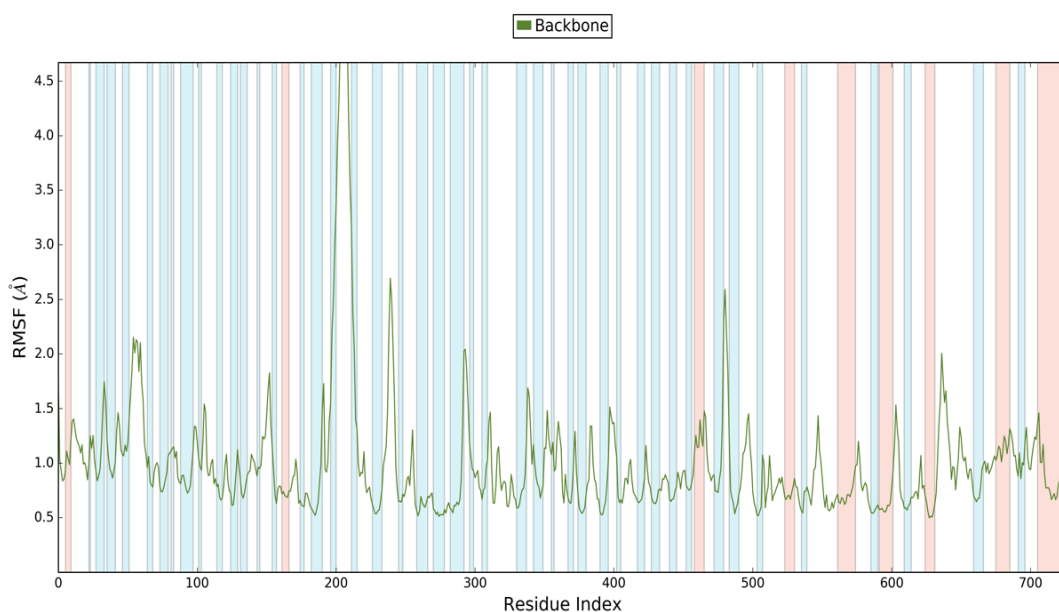


1 **Supplementary materials**

2 Figure S1. Root mean square fluctuation (RMSF) of the backbone of DPP4  
3 during 100-ns MD simulation.

4 Figure S2. A representation of the interactions and contacts over time. The  
5 top panel shows the total number of specific contacts DPP4 makes with  
6 EGCG over the simulation. The bottom panel shows which residues  
7 interact with EGCG in each trajectory frame.

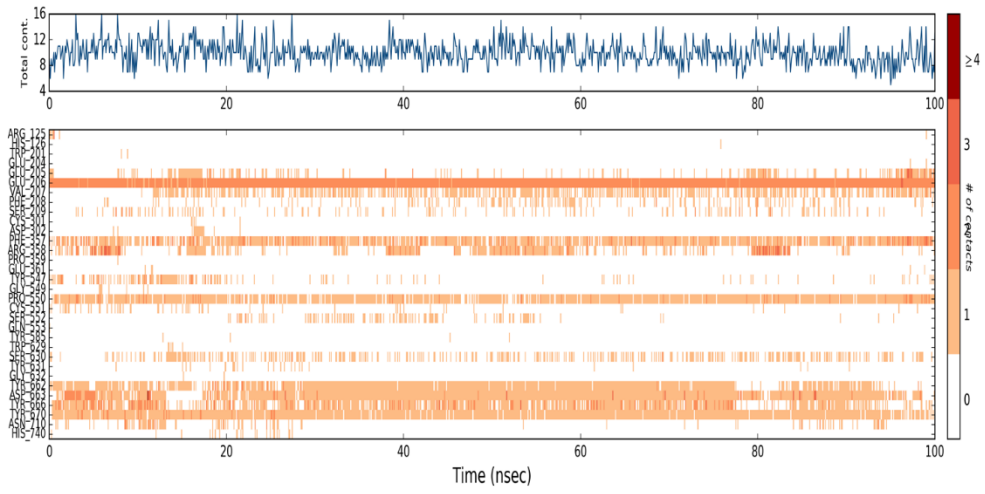
8 Figure S3. Normalized stacked bar chart representation of interactions and  
9 contacts over the course of the MD simulation trajectory.



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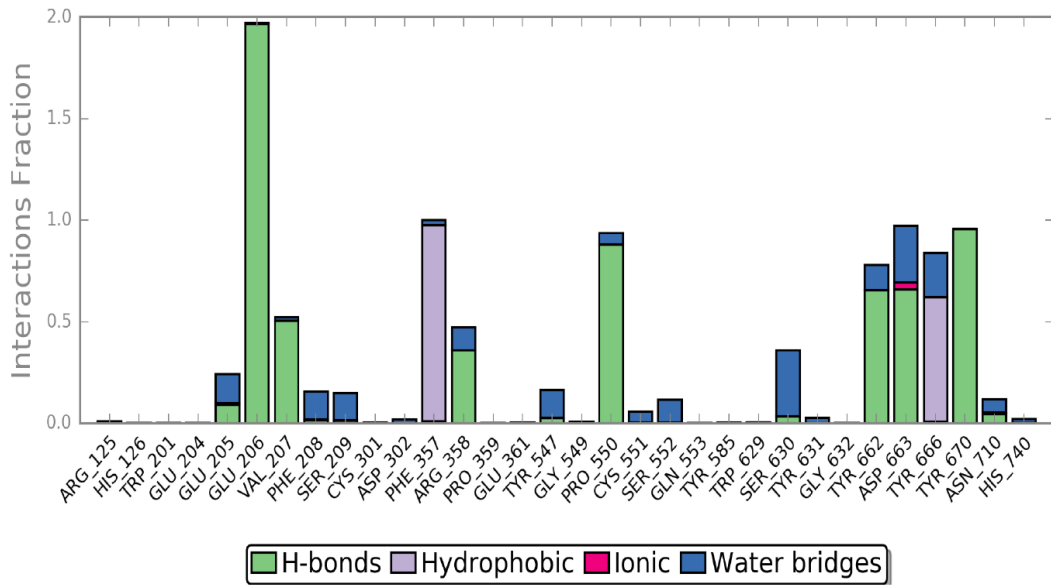
Figure S1



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Figure S2



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Figure S3