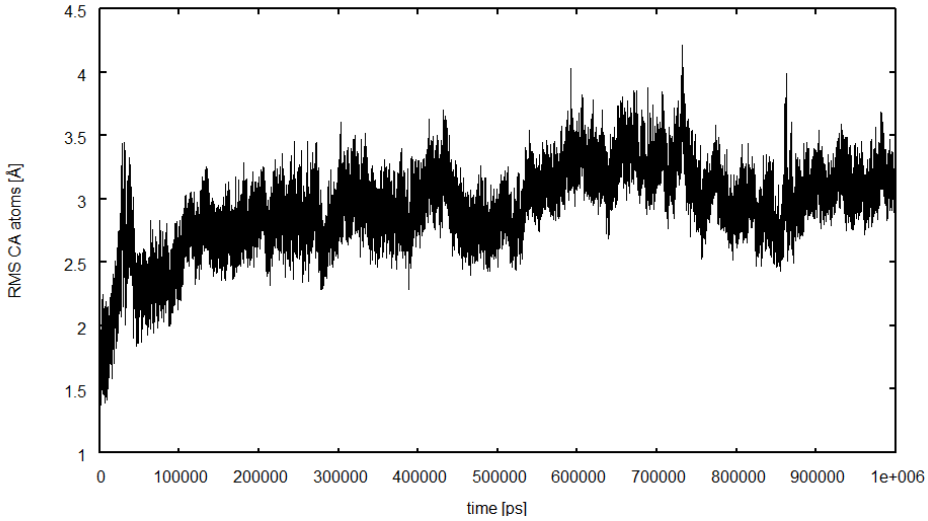
S6 Text

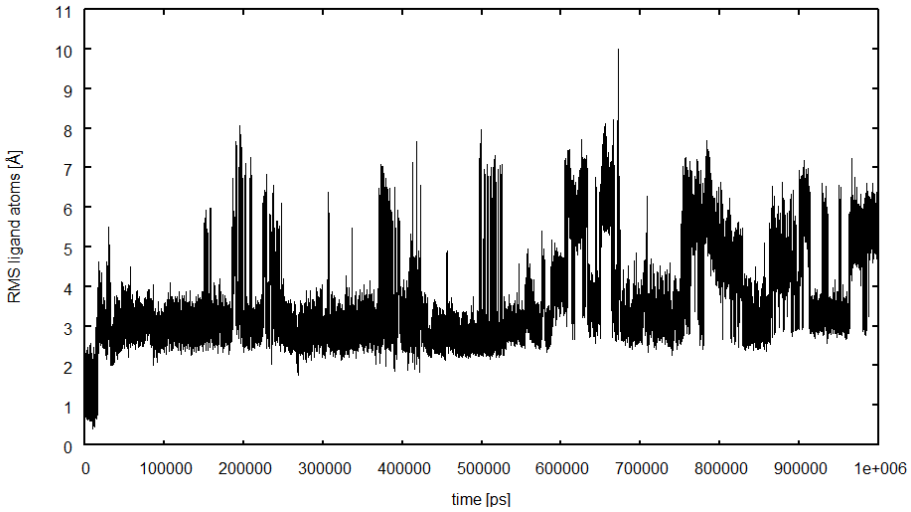
RMSD data ligand 1 complex

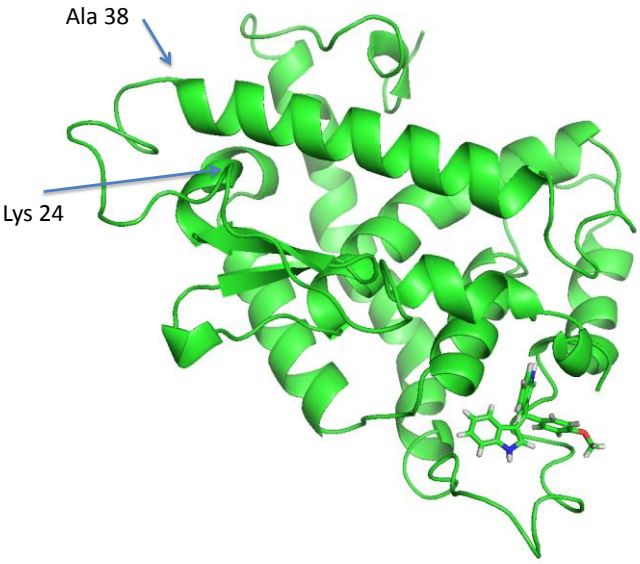
The poses obtained by docking the putative ligands into the binding site occurred during the MD simulation of the un-complexed protein served as starting point for MD simulations of the respective complexes. Ligand **1** stays within the binding site even after 1µs simulation time illustrating an extraordinary stability for the protein-ligand complex.

RMS Cα atoms 1µs simulation with bound ligand **1**

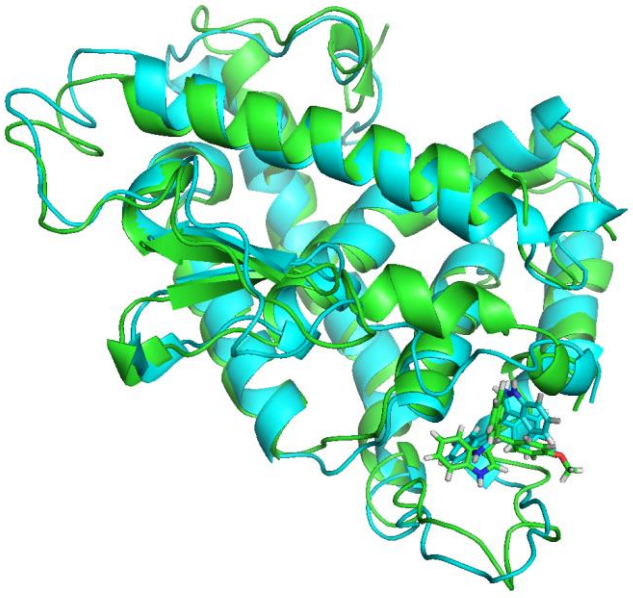


RMS ligand atoms 1µs simulation with bound ligand **1**

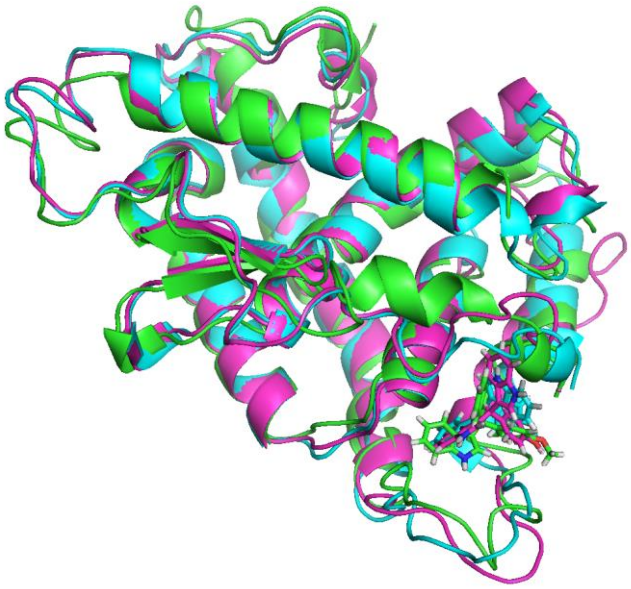




0 ns (start)



100 ns



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