Additional file 10: Stereo figure of Compound 24 in the crystal structure compared to the docking pose obtained with 2PC4. A) Comparison between the docked pose (cyan sticks) and the observed orientation of compound 24 (orange sticks) in Chain A of the PfAldolase tetramer. The coordinates of 2PC4 are represented as ribbons and the corresponding TRAP-tail is shown in magenta sticks. The TRAP-tail of the ternary co-crystal structure 4TR9 is shown in orange sticks. B) Approximate rotation of 90 degrees towards the viewer compared to figure A.

A


B


