

## **S1 File1. Statistical analysis of the ranking of poses and chains obtained by biased docking.**

At the poses level:

For 1B7F, 18 of the 20 poses with RMSD < 2 Å were ranked in the top 22 out of 53, and the 31 poses with RMSD > 5 Å were all ranked in the last 37 (p-values  $2 \cdot 10^{-6}$  and  $5 \cdot 10^{-9}$ ).

For 1CVJ, 14 of the 15 poses with RMSD < 2 Å were ranked in the top 15 out of 24, and the 5 poses with RMSD > 4 Å were ranked in the last 7 (p-values  $1 \cdot 10^{-4}$  and 0.008).

At the chains level:

For 1B7F, 34 of the 35 chains with RMSD < 2 Å were ranked in the top 100 out of 166, and 63 of the 121 chains with RMSD > 5 Å were ranked in the last 69 chains (p-value  $4 \cdot 10^{-8}$  and  $3 \cdot 10^{-6}$ ).

For 1CVJ, the 31 chains with RMSD < 1 Å were all ranked in the top 47 out of 69, and 20 of the 25 chains with RMSD > 2 Å were ranked in the last 20 chains (p-values  $4 \cdot 10^{-8}$  and  $5 \cdot 10^{-13}$ ).