Text S6. Error Analysis on Case 1RLB

In addition to case 1ML0 in the subsection of "Error Analysis", we identified another case, 1RLB, for which 2 out of the top 5 ranked DockRank conformations have unusually large L-RMSDs (> 79 Å) while the interface predictions from PS-HomPPI are in Safe Zone.
Examination of the structure of 1RLB downloaded from the PDB (the Protein Data Bank) [50] reveals that the 1RLB bound complex has two identical ligands (chain E and chain F), which bind on both sides of the receptor; however, the authors of BM3 (Docking Benchmark 3.0) chose to include only chain E in the docking case included in Docking Benchmark 3.0 and excluded chain F. As shown in Figure S7, all top 5 DockRank conformations are on *both* sides of the receptor overlaping with the bound ligands positions, while two of the top 5 ClusPro conformations are out of place relative to either of two bound ligands.
We recalculated the L-RMSD for all the docked conformations for case 1RLB by considering both the two identical bound ligands to correspond to native ligand positions. The smaller of the two L-RMSD values between a docked ligand and two possible positions of the bound ligand is used as the overall L-RMSD for the conformation. Based on the preceding calculation, we found that two conformations have $L\text{-}RMSD \leq 10$ Å (with DockRank's rank of 3 and 5 compared with ClusPro's rank of 3 and 13), and three conformations have $L\text{-}RMSD \leq 15$ Å(with DockRank's rank of 3, 4, 5, compared with ClusPro's rank of 3, 11, 13). Thus, we conclude that DockRank performs better than ClusPro on case 1RLB.