**3DRobot: Automated Generation of Diverse and Well-packed Protein Structure Decoys**

Haiyou Deng, Ya Jia, Yang Zhang

**SUPPLEMENTAL INFORMATION**

**Figure S1.** Illustrative examples from the widely used decoy sets showing strong correlation between RMSD and secondary structure density or radius of gyration. (A) 1ubi from Rosetta_set; (b) 1V14A from QUARK decoy set; (c) 1lga from Modeller_set; (d) 1thx_ from the I-TASSER_set.
**Figure S2.** An illustrative example showing how decoys are selected from outputs of simulation based different structural template.
Figure S3. Average RMSD of random protein structure pairs for a given length ($L$) with a given distance ($r$) to the reference protein structures.
Figure S4. The Pearson correlation depends on the range of RMSD of the decoys.