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

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SUPPLEMENTAL INFORMATION

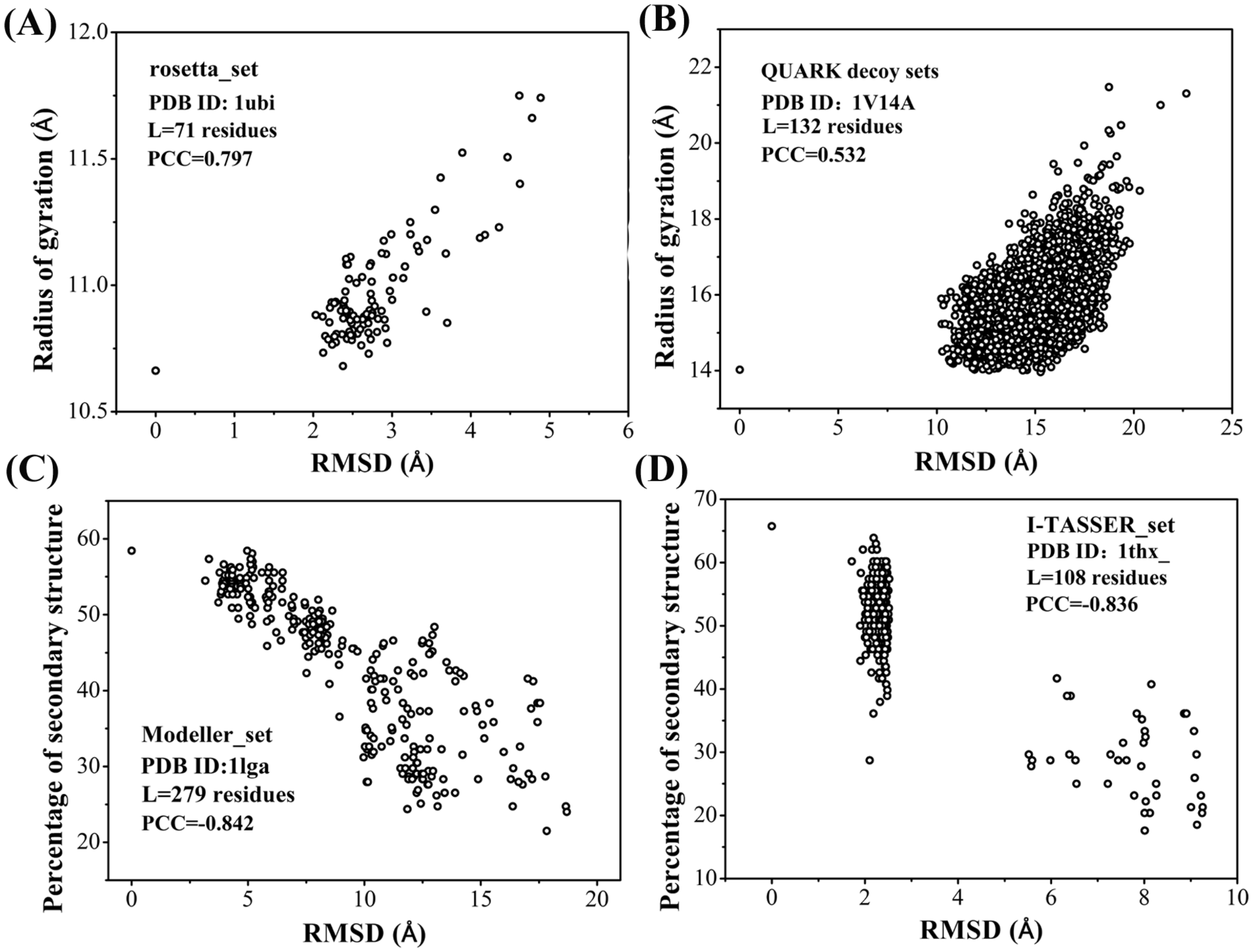

Figure S1. Illustrative examples from the widely used decoy sets showing strong correlation between RMSD and secondary structure density or radius of gyration. (A) 1ubi from Rosetta_set; (b) 1V14A from QUARK decoy set; (c) 1lga from Modeller_set; (d) 1thx_ from the I-TASSER_set.

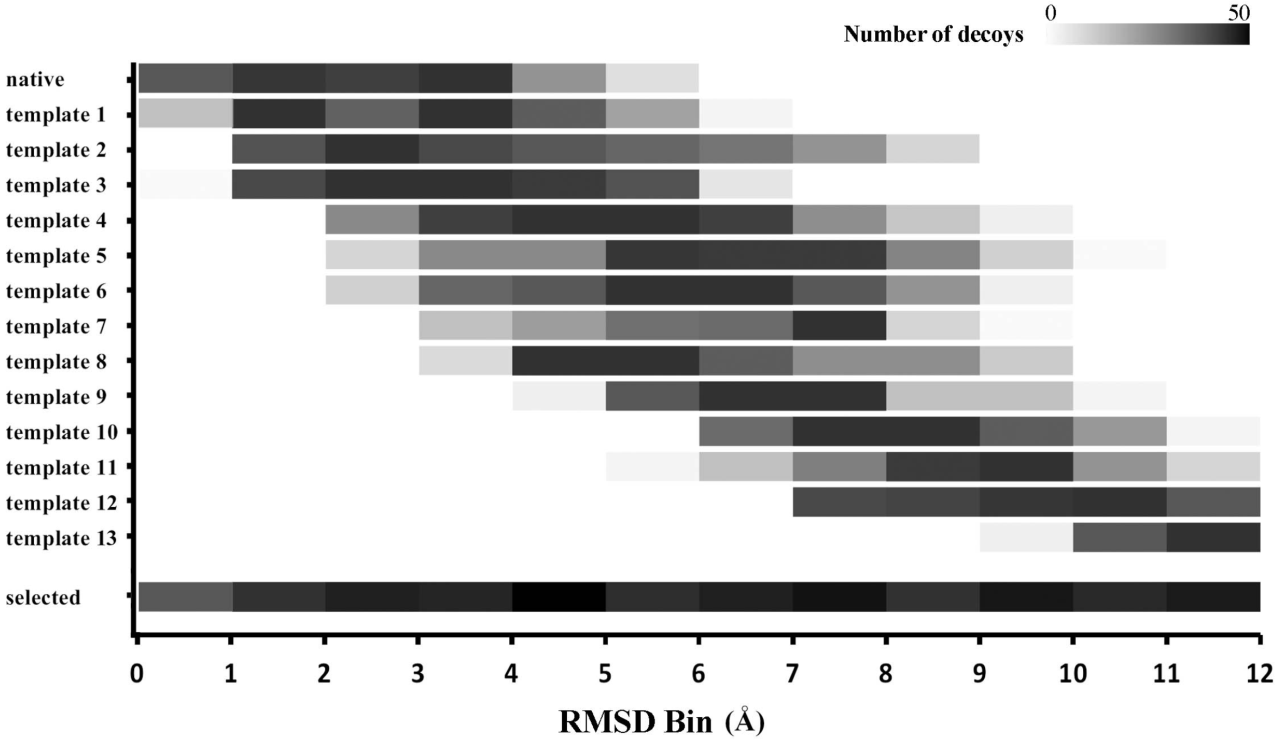

Figure S2. An illustrative example showing how decoys are selected from outputs of simulation based different structural template.

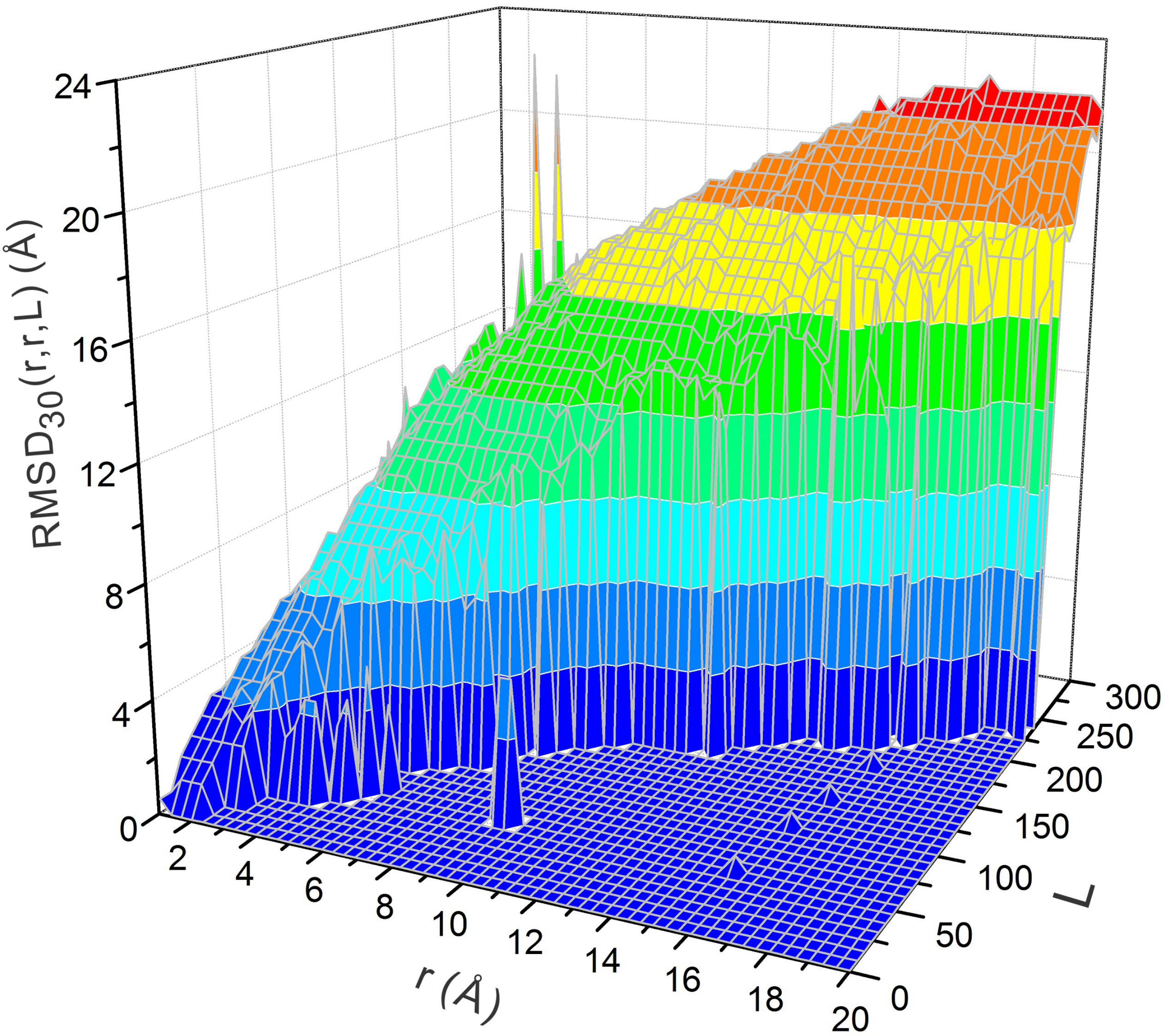

Figure S3. Average RMSD of random protein structure pairs for a given length (*L*) with a given distance (*r*) to the reference protein structures.

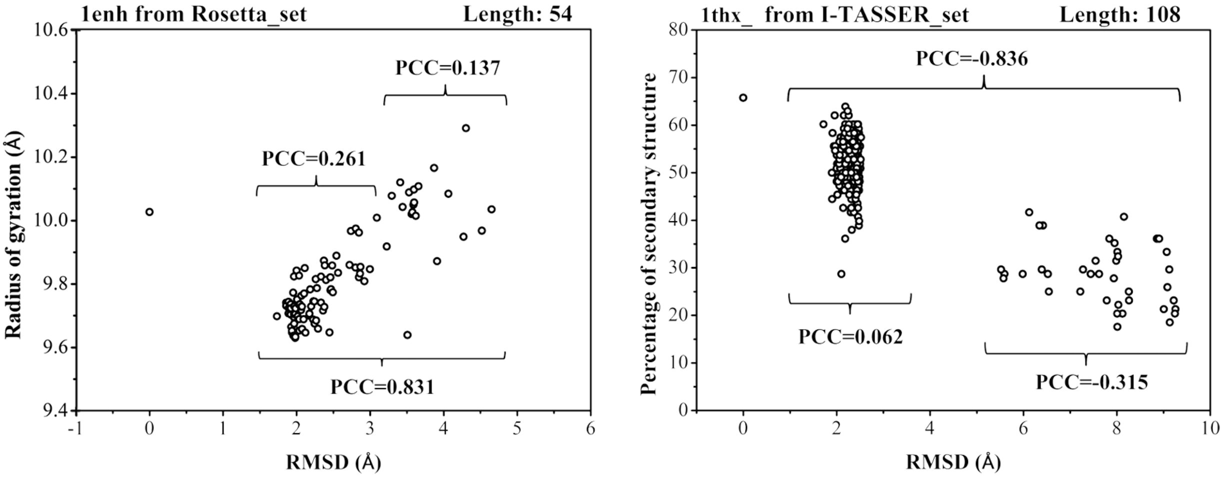

Figure S4. The Pearson correlation depends on the range of RMSD of the decoys.