Sampling and refinement protocols for template-based macrocycle docking: 2018 D3R Grand Challenge 4: Supplementary Material

Sergei Kotelnikov[1,2,3,*] and Andrey Alekseenko[1,2,*], Cong Liu[1,4], Mikhail Ignatov[1,2,5], Dzmitry Padhorny[1,2], Emiliano Brini[1], Mark Lukin[6], Evangelos Coutsias[1,2], Ken A. Dill[1,4,7], Dima Kozakov[1,2,5]

1 Laufer Center for Physical and Quantitative Biology, Stony Brook University, Stony Brook, NY, USA
2 Department of Applied Mathematics and Statistics, Stony Brook University, Stony Brook, NY, USA
3 Innopolis University, Innopolis, Russia
4 Department of Chemistry, Stony Brook University, Stony Brook, NY, USA
5 Institute for Advanced Computational Sciences, Stony Brook University, Stony Brook, NY, USA
6 Department of Pharmacological Sciences, Stony Brook University, Stony Brook, NY, USA
7 Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY, USA
* These authors contributed equally to this work

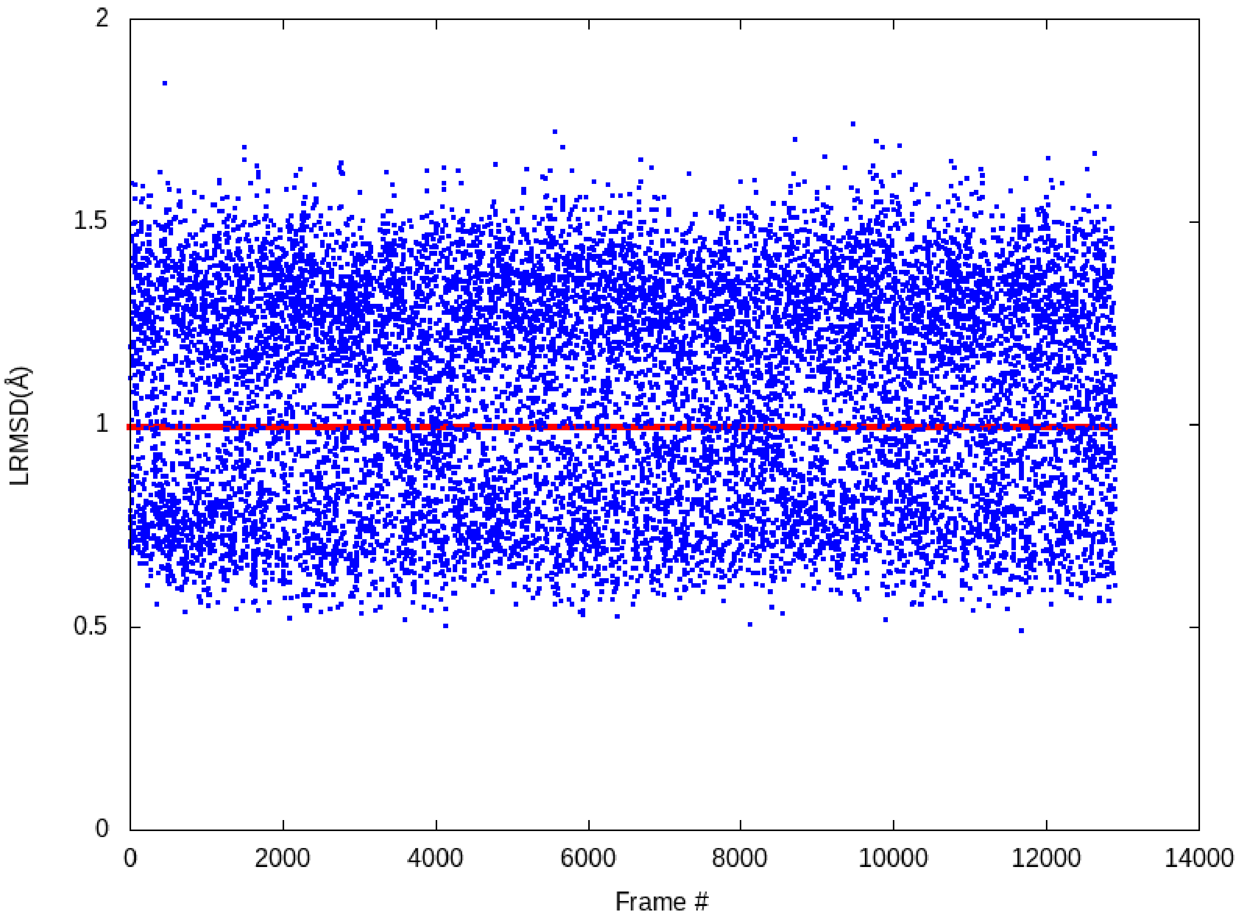

Fig. S1. LRMSD of MELD trajectory for BACE_18. The LRMSD of all poses sampled during MELD simulation and the final best MELD refined pose are depicted as blue dots and a red line, respectively. MELD samples poses closer to native, but the current clustering protocol fails to extract them

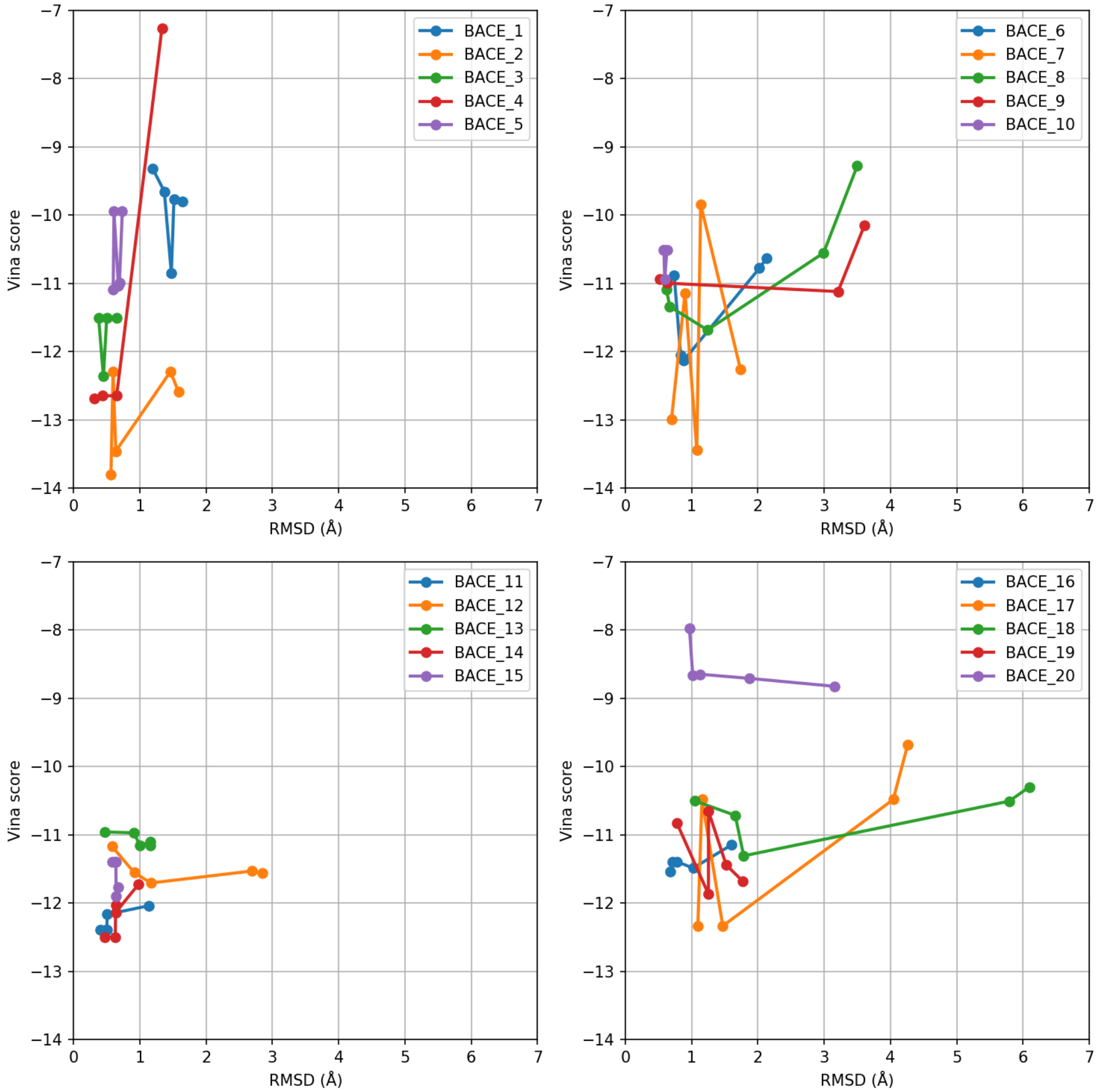

Fig. S2. Vina scores and RMSD for the submitted Stage 1a poses. Each line connects points for the same target ligand. Vina score tends to be higher for high-RMSD structures, but is not suitable as the single measure of structure quality, as there are many cases with either low score for high-RMSD structure or high score for a low-RMSD structure