Scores distribution [pKd] MLT-LE **GraphDTA** 2.0 CDN 3.0 GMDLDR 2.5 LigDream 1.5 REINVENT 2.0 **REINVENT 3.0** Transmol 1.0 1.5 TransVAE 1.0 0.5 0.5 0.0 0.0 2.0 3.0 2.5 1.5 2.0 P **Density** 1.0 1.0 0.5 0.5 0.0 0.0 2.0 3.0 2.5 1.5 2.0 1.0 1.5 1.0 0.5 0.5 0.0 0.0 10 9 5 5 10 3 4 6 9 7 8 6 8 Score