**RUN965** binding 1.5  $\Delta\Delta G$  / kcal mol<sup>-1</sup> binding (all GENS) 1.0 0.5 0.0 -9.0solvent complex  $\Delta G$  / kcal mol<sup>-1</sup> -9.5 -10.0-10.5-11.0

**GEN**