**RUN606** binding 0.5  $\Delta\Delta G$  / kcal mol $^{-1}$ binding (all GENS) 0.4 0.3 0.2 0.1 0.0 -146.8solvent complex  $\Delta G$  / kcal mol<sup>-1</sup> -147.0-147.2-147.4

**GEN**