

**Fig. 1. Distribution of  $\Delta G^{\text{off}}$  over all structures vs. interface quality parameter  $I_{\text{rms}}$ .** Each dot represents one structure in the Score set of Targets. The x axis shows the RMSD of backbone atoms of interface residues between docking decoys and the crystal structure; the y axis represents the  $\Delta G^{\text{off}}$  which describes the binding strength.

