Electronic Supplementary Information

Figure S1 Ligand bound structures of HIV1TAR deposited in the PDB (green dots) superimposed to the MaxOcc landscape (color coded) as function of α_h, β_h and γ_h angles (2D projections). White areas correspond to not sampled regions.
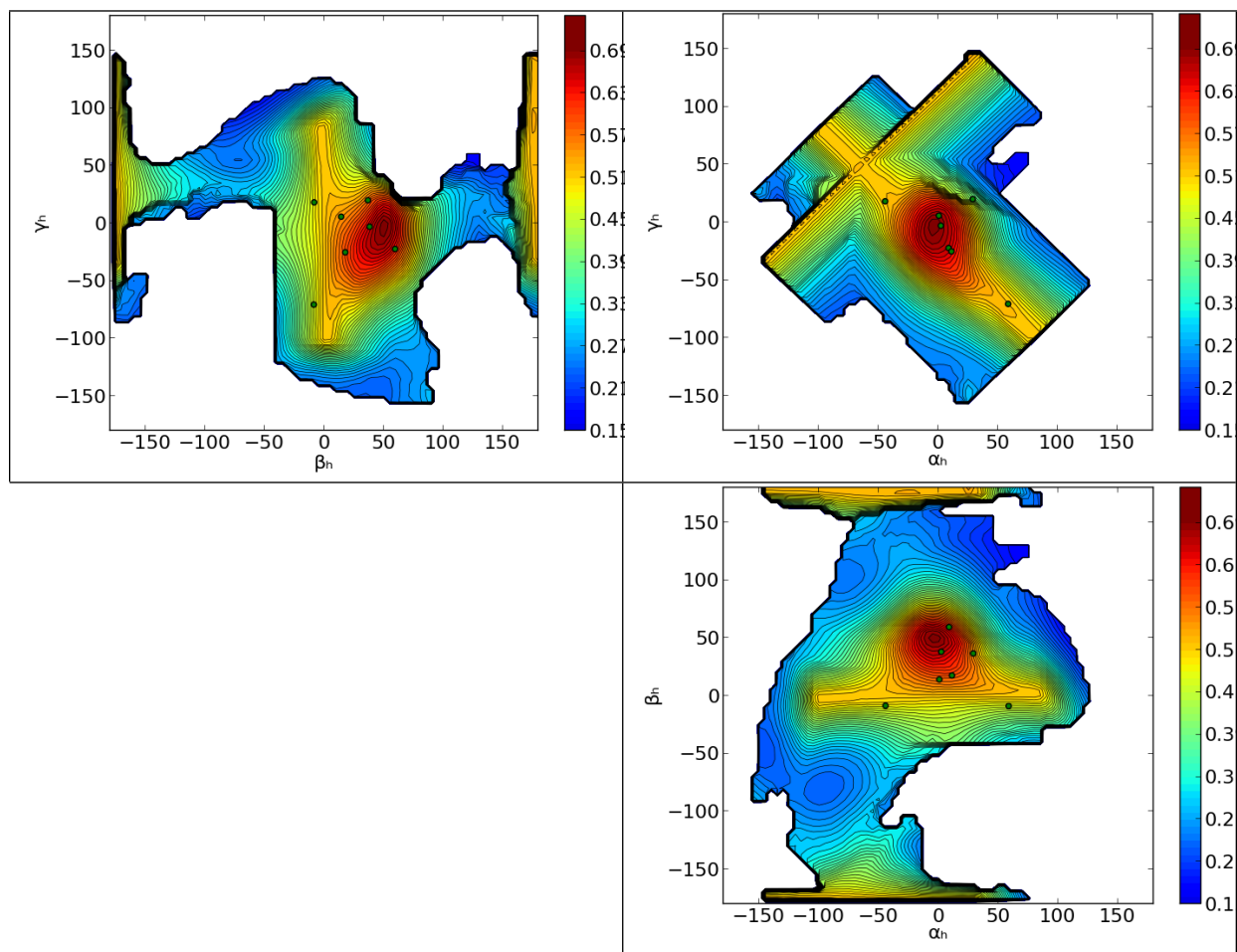
Figure S2. In order to identify two-centered compact regions which can explain the experimental data, two subregions are selected in the conformational space. The subregion composing the peak of the MaxOcc profile ($-10 < \alpha_h < 5°$, $45 < \beta_h < 55°$, $-15 < \gamma_h < 5°$) is complemented by another subregion of size of 5°·5° in the (β_h, $\alpha_h + \gamma_h$) 2D projection of the conformational space. This second subregion was changed in the different calculations in a systematic way in order to cover the whole (β_h, $\alpha_h + \gamma_h$) space. The figure shows the MaxOR of the two-centered regions as a function of the (β_h, $\alpha_h + \gamma_h$) position of the second subregion. The red rectangle indicates the position of the first subregion, at the peak of the MaxOcc profile, used together with the second subregion.
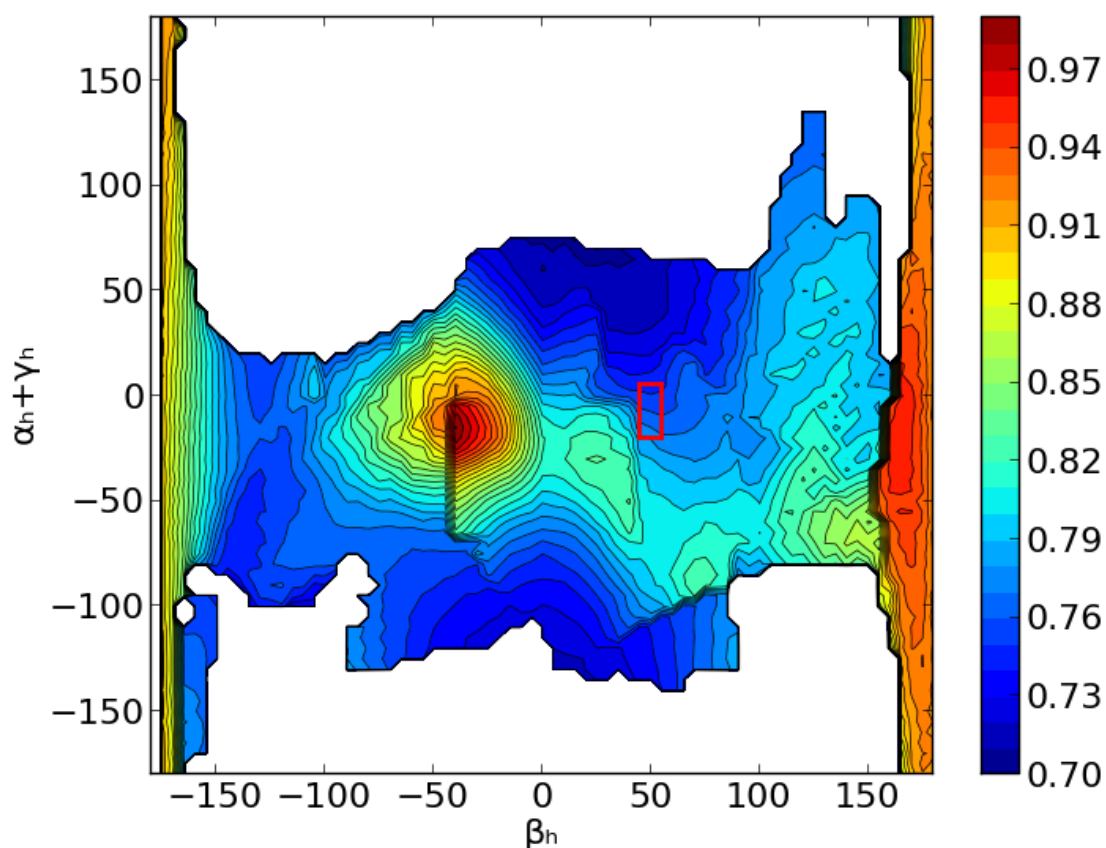
Figure S3. MaxOR of the two-centered ensembles as a function of the α_h coordinate of the region complementing that at the peak of the MaxOcc profile (see text) when the other coordinates are fixed to β_h =-40 and γ_h =-α_h -15°.