

Supplementary Material for the manuscript ‘Numerical errors and chaotic behavior in docking simulations by Miklos Feher and Christopher I. Williams

Figure S1: A representative subset of each pose cluster after docking 40000 structures to 2br1. The average pairwise RMSD within the cluster and the number of members in each cluster (**N**) are also given. The top-scoring pose from all runs (a member of pose cluster 1), colored black and rendered in ball-and-stick mode, is drawn for comparison. The spread within each cluster is summarized as the intra-cluster average pairwise RMSD.

Figure S2: Histograms of the scores within each pose cluster after docking 40000 structures to 2br1. The individual histograms are scaled according to the percentage of solutions within each cluster rather than overall percentage; otherwise the cluster 1 histogram would dominate the plot. The score histogram for pose cluster 1 shows that the scores group into 3 distinct Gaussian peaks. Pose cluster 4 has a distinctly bimodal score and pose distribution, representing two pose groups within the cluster, one shifted from the other by ~ 1 Å. Other pose clusters produce multi-modal score distributions with less distinct maxima.

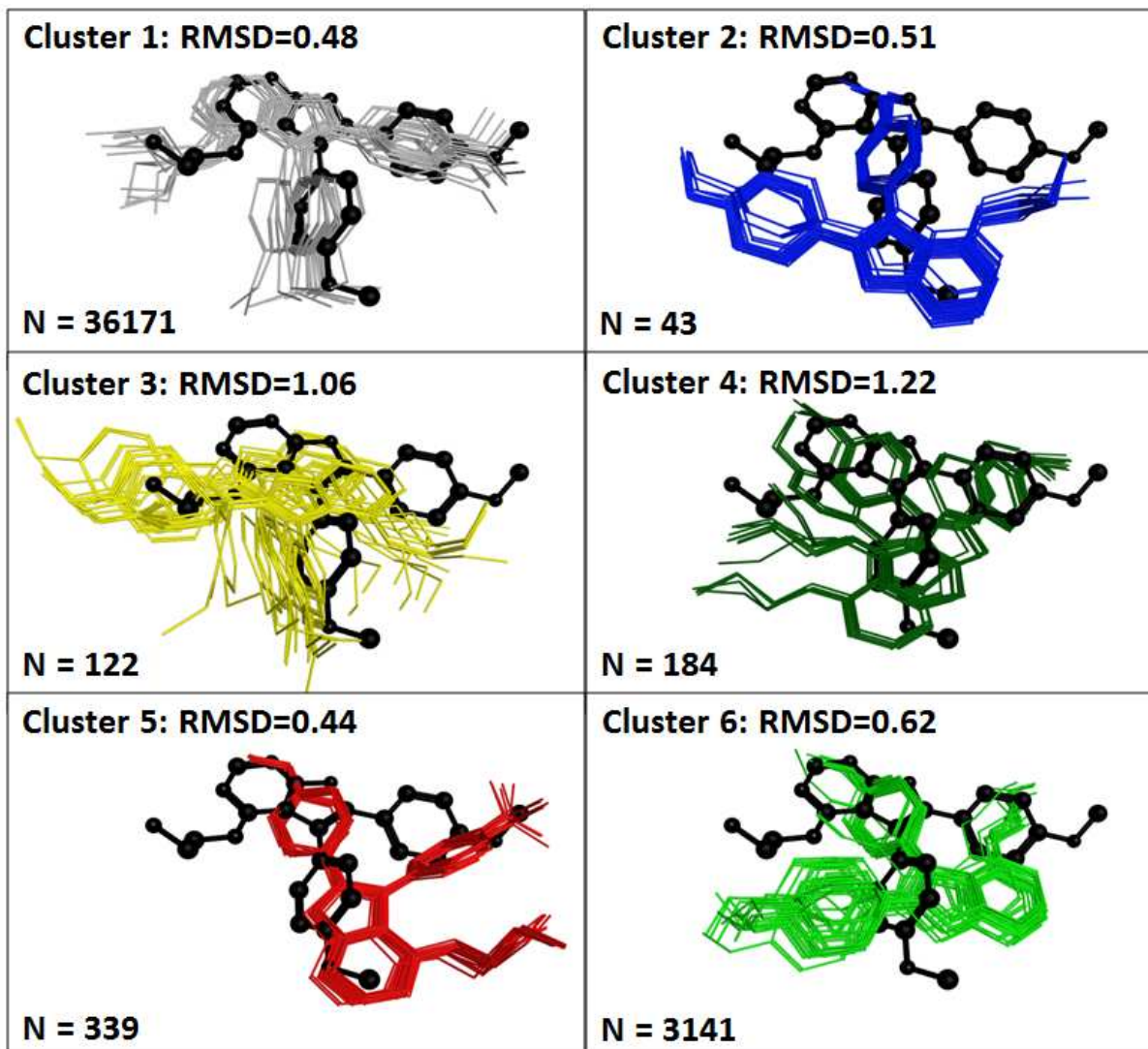


Figure S1

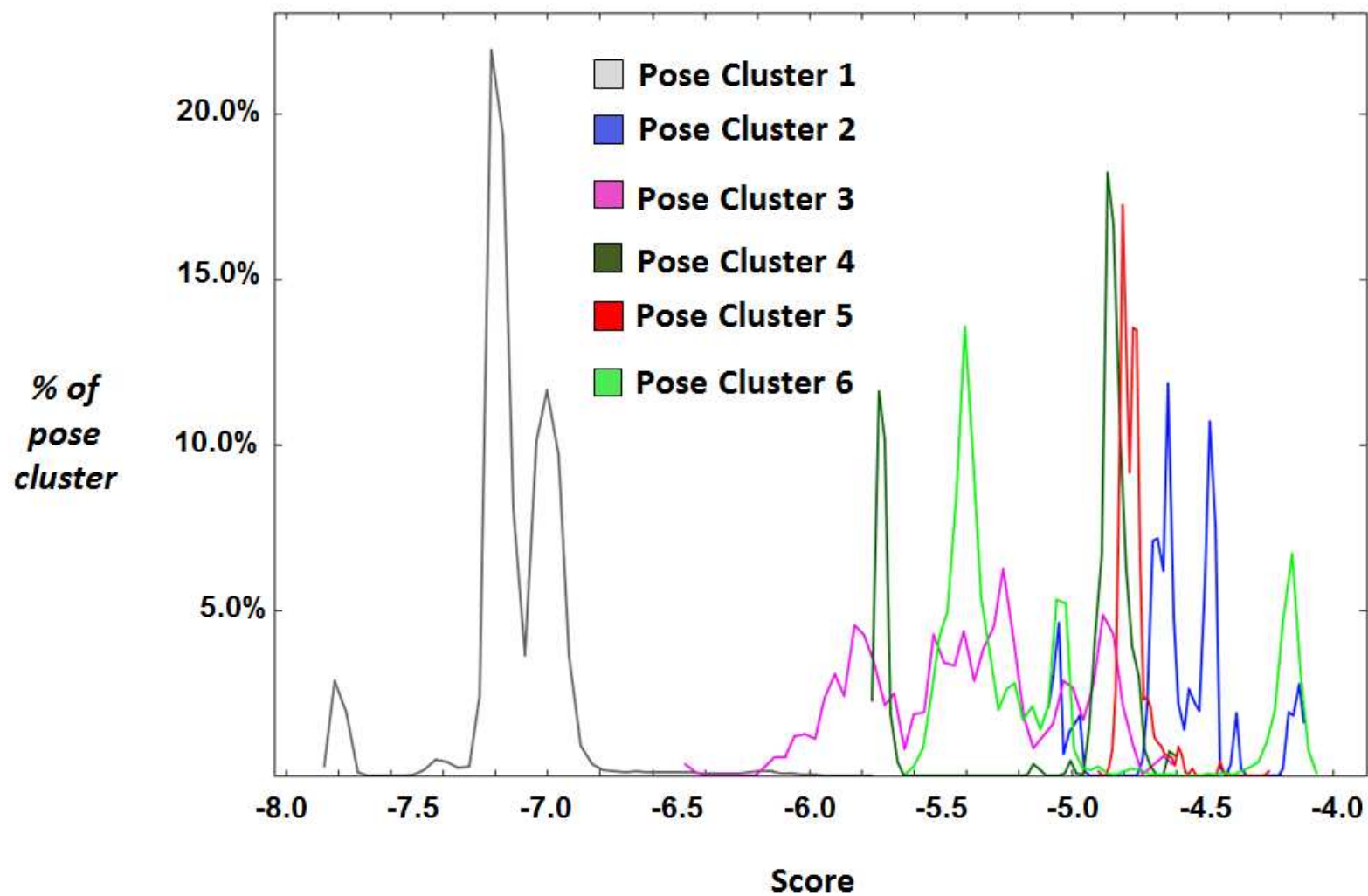


Figure S2