**Supplementary data 1. Optimization of gap penalties and anchor weight.** (A) The percentage of alignments with best $N_{\text{dist}}$ score (dark blue) is plotted for different combination of gap initiation and extension penalties. The scores close to the maximum $N_{\text{dist}}$ score (maximum $N_{\text{dist}} - 3$) are considered as good scores (light blue). (B) The distribution of percentage of good scores with different anchor weights.
Supplementary data 2. Alignment of Armadillo/Beta-catenin like repeats. Alignment of 3 structures (PDB ID+chain: 1BK5b (green), 1IALa (blue) and 3BCT (red)) using (A) mulPBA, (B) HOMSTRAD and (C) MULTIPROT. The quality scores in terms of $N_{\text{rms}}$, $N_{\text{dist}}$ and $N_{3.5}$ are also given. Figures are rendered in PyMol (Delano Scientific Inc.)
Supplementary data 3. Overfitting by flexible alignment tools. From the multiple alignment of 5 structures with cupin fold (PDB ID+chain: 1DZR (green), 1O5U (blue), 1QXR (red), 1V70 (yellow) and 1VJ2 (orange)) using Posa, two structures (1O5U (blue), 1QXR (red)) are shown. The structural segments of 1O5U moved for flexible fitting is indicated using thick backbone.