

Supplementary Material

Figure S1: Root mean-square deviation of the C α carbon atom positions in all the systems as a function of time, computed per chains.

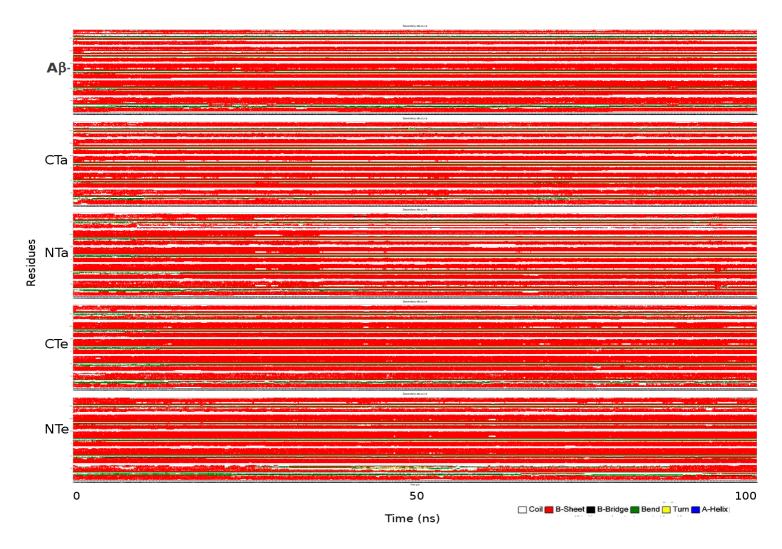


Figure S2: Secondary structures as function of time for each systems, indicated by the labels, as calculated by DSSP.

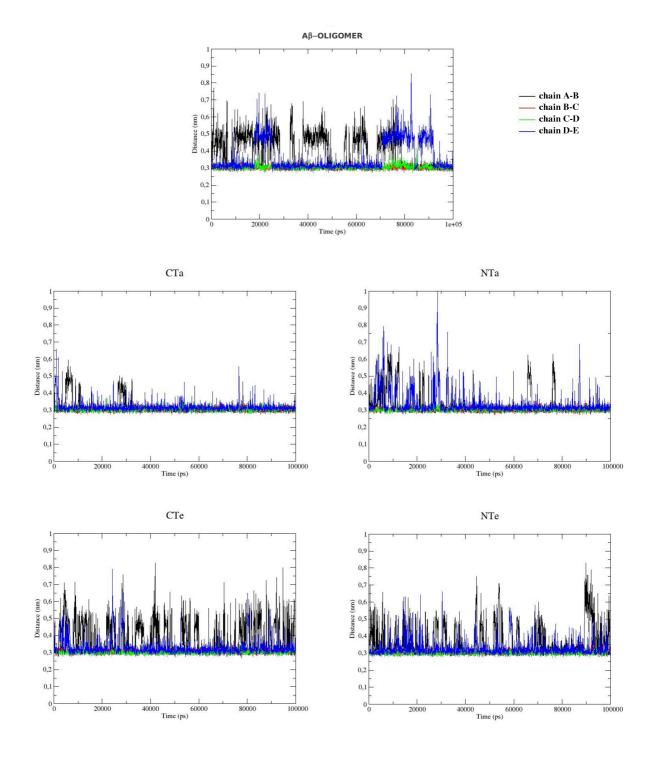


Figure S3: D23-K28 distances as a function of time for the all the systems.