

Supplementary Material for: A Unique Binding Mode of the Eukaryotic Translation Initiation Factor 4E for Guiding the Design of Novel Peptide Inhibitors

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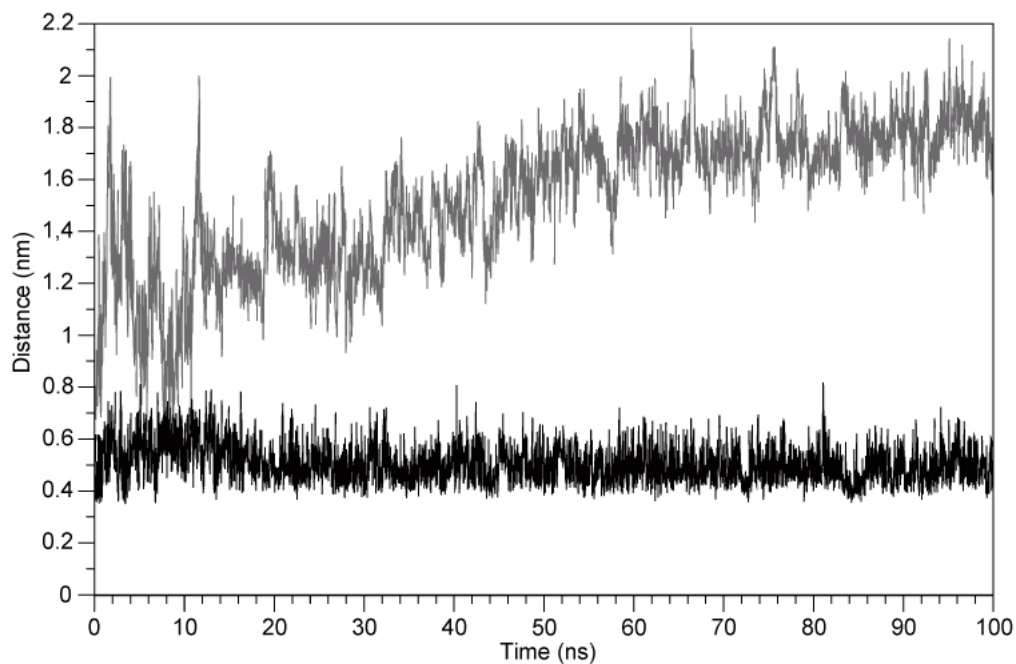


Figure 1: Atomic distance between the CD1 atoms of L1 and L5 residues of CYFIP1p (black line) and of the center of mass of the guanidinium group of R186 of eIF4E and the lateral chain N atom of residues of CYFIP1p (gray line).

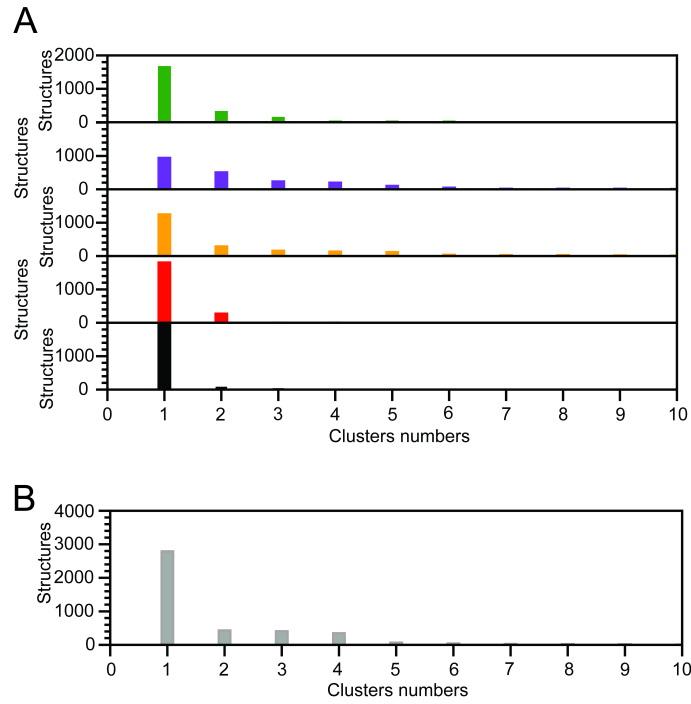
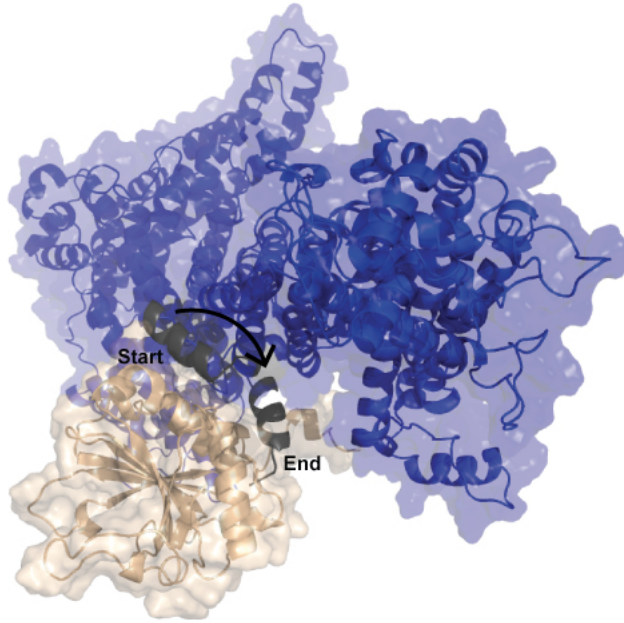


Figure 2: Number of structures in each cluster of the 4E-BPs' and 4Gs' peptides (A) and CYFIP1p (B). Color code as in Fig. 3 and Table 1.

A



B

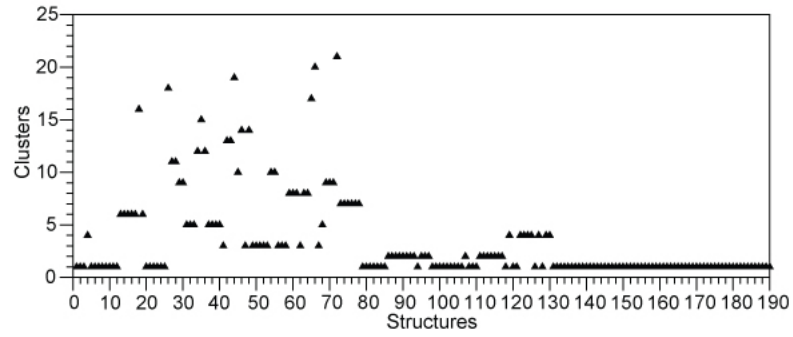


Figure 3: (A) Comparison between the initial and final structures of CYFIP1p (dark gray), eIF4E is shown in salmon color, CYFIP1 in blue. (B) Cluster populations for the ensemble of structures at $\lambda = 1$ and 300 K of CYFIP1p complexes with eIF4E produced by the BEDAM simulation.

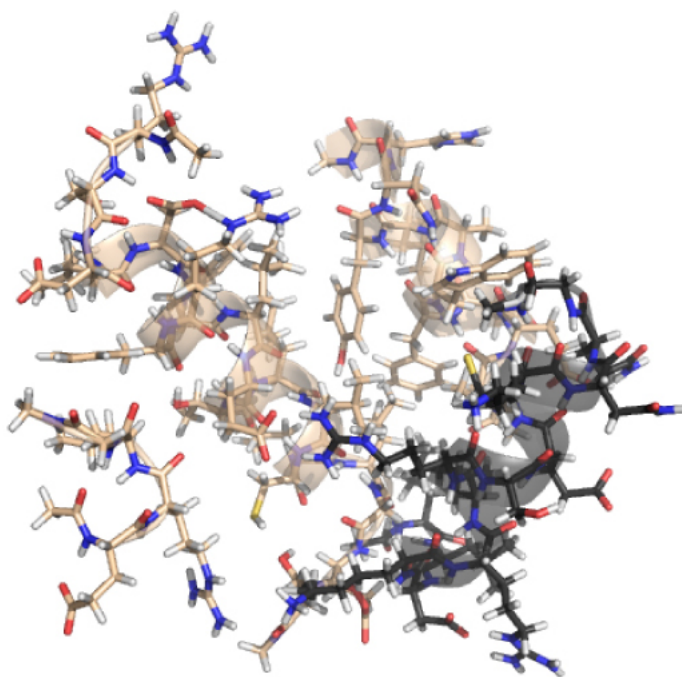


Figure 4: Model of the eIF4E receptor used for the BEDAM simulations (salmon color). The CYFIP1 peptide is also included for reference (dark gray).



Figure 5: The relatively small rearrangement of the BEDAM-predicted structure of CYFIP1 (blue) after 50 ns of explicit solvent refinement (cyan). eIF4E is shown in red. The structure file of the final structure is attached (CYFIP1p-eIF4E.pdb)