Supporting Materials

Insights into the effect of Curcumin and (-)-epigallocatechin-3-gallate on the aggregation of Aβ(1-40) monomers by means of molecular dynamics

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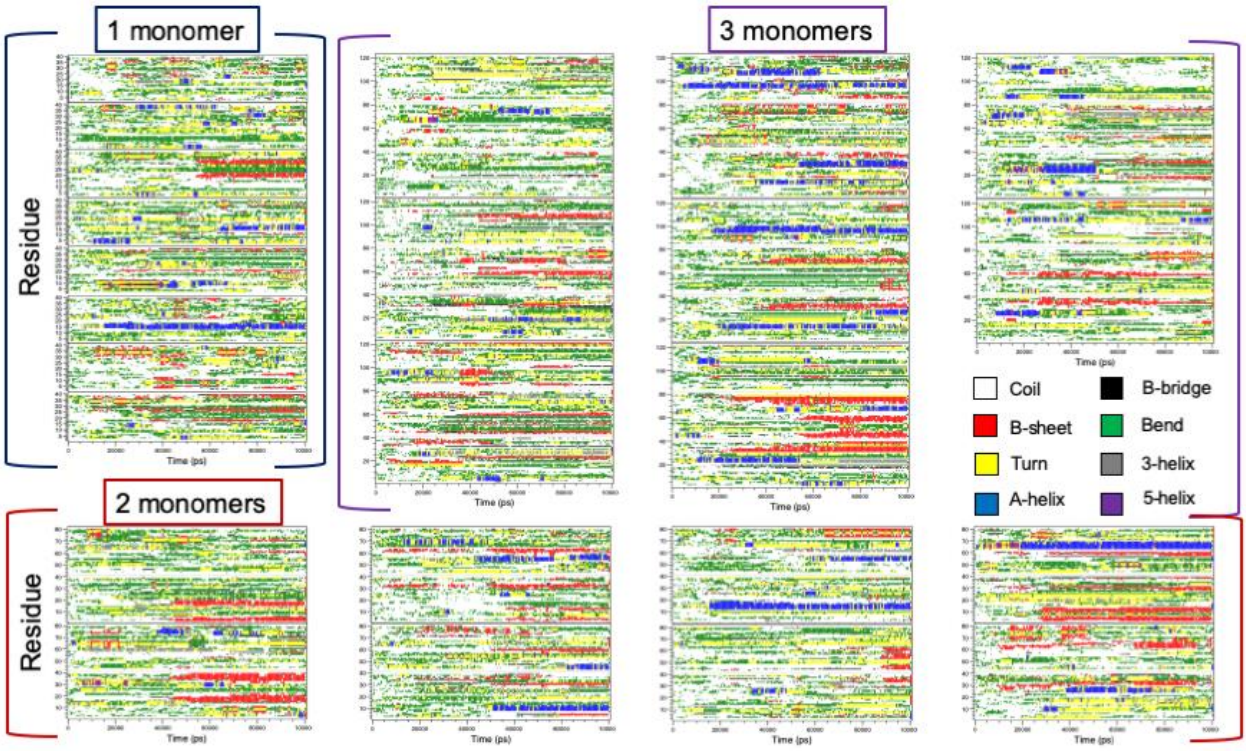

Figure S 1: Time evolution of the secondary structure for each residue of the Aβ-amyloid monomeric, dimeric, and trimeric models obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend on the right.

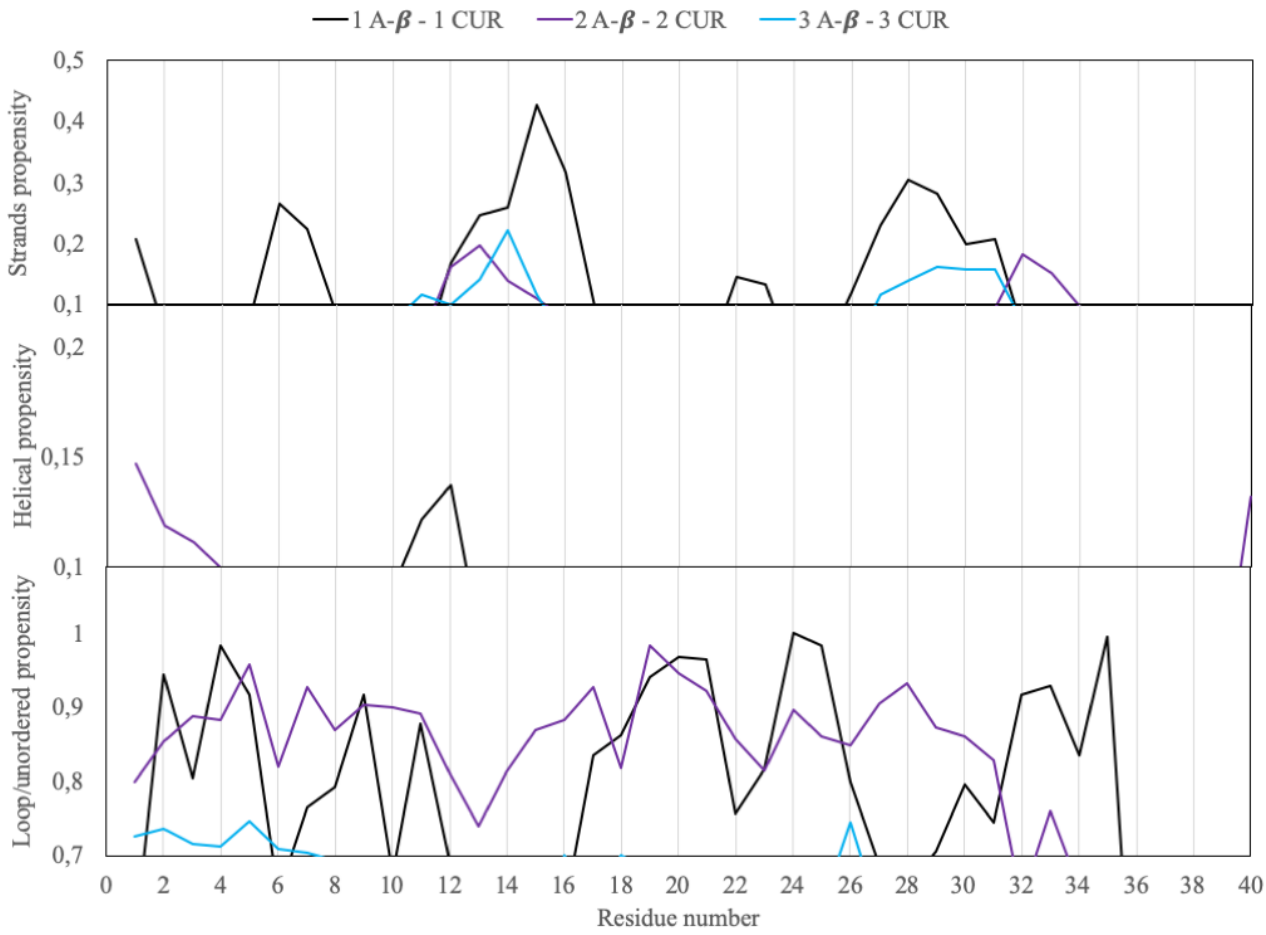

Figure S 2: secondary structure propensity for Aβ monomers interacting with CUR.

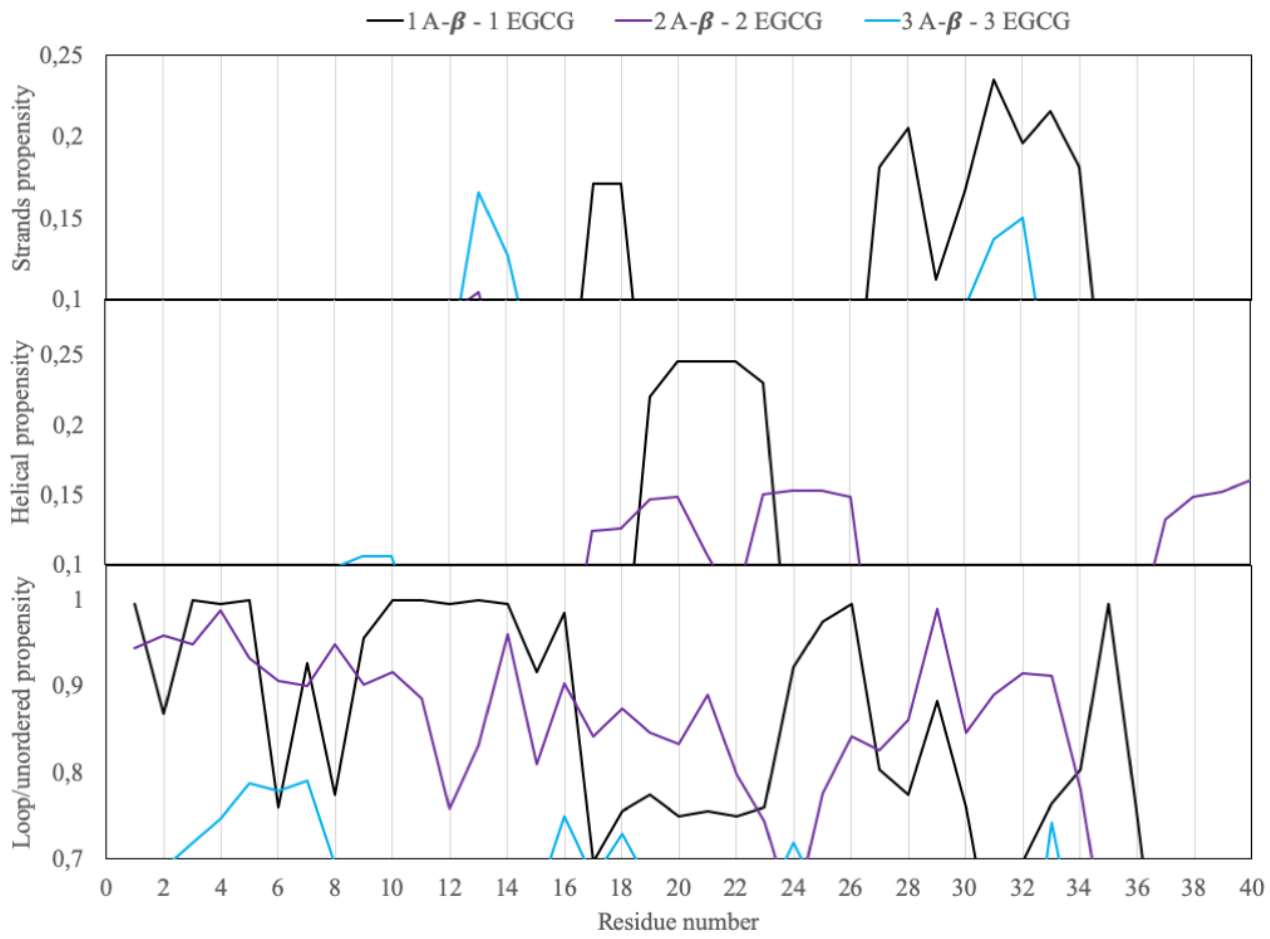

Figure S 3: secondary structure propensity for Aβ monomers interacting with EGCG.

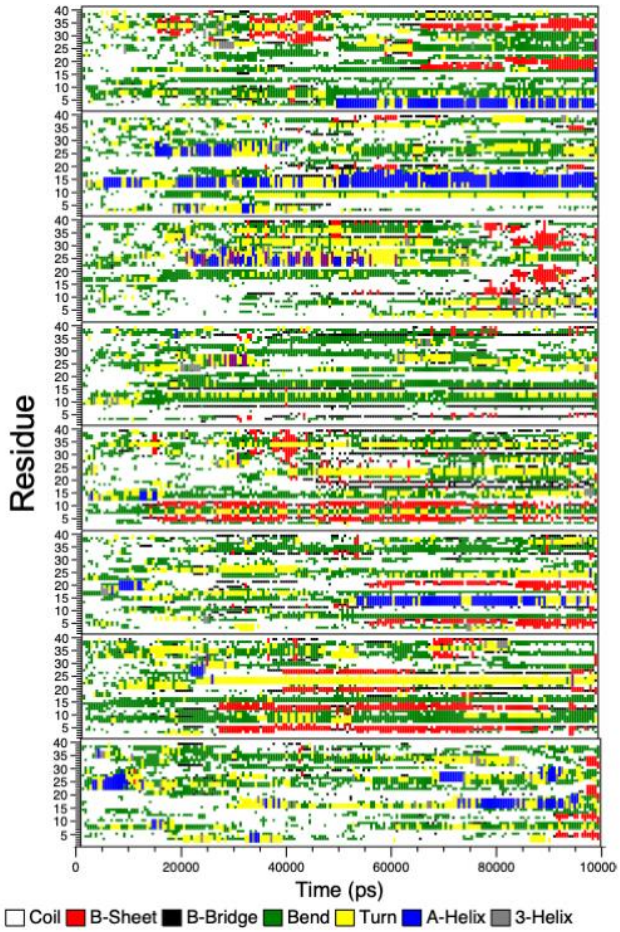

Figure S 4: Secondary structure assignment of the single monomer for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + CUR.

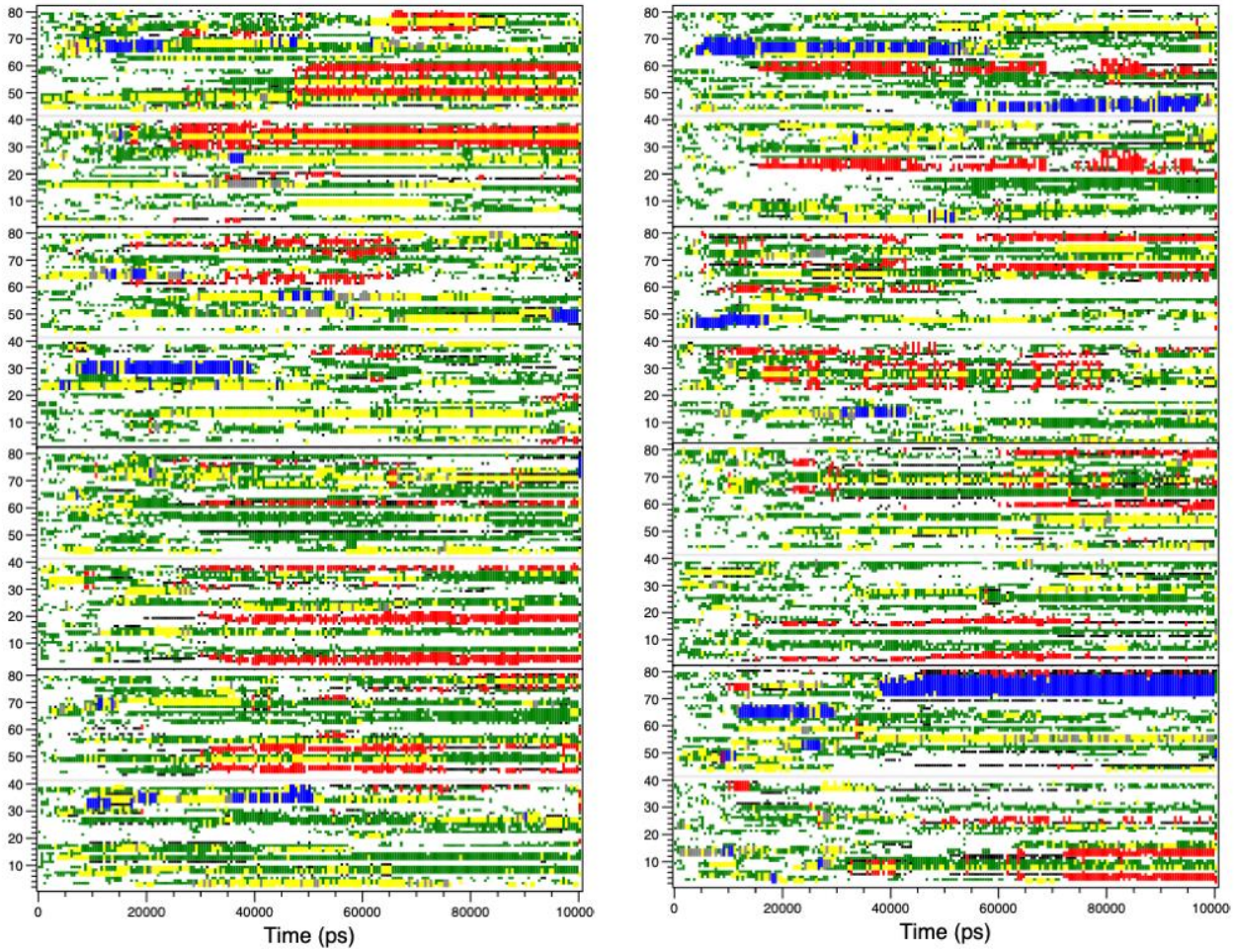

Figure S 5: Secondary structure assignment of two monomers for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + CUR

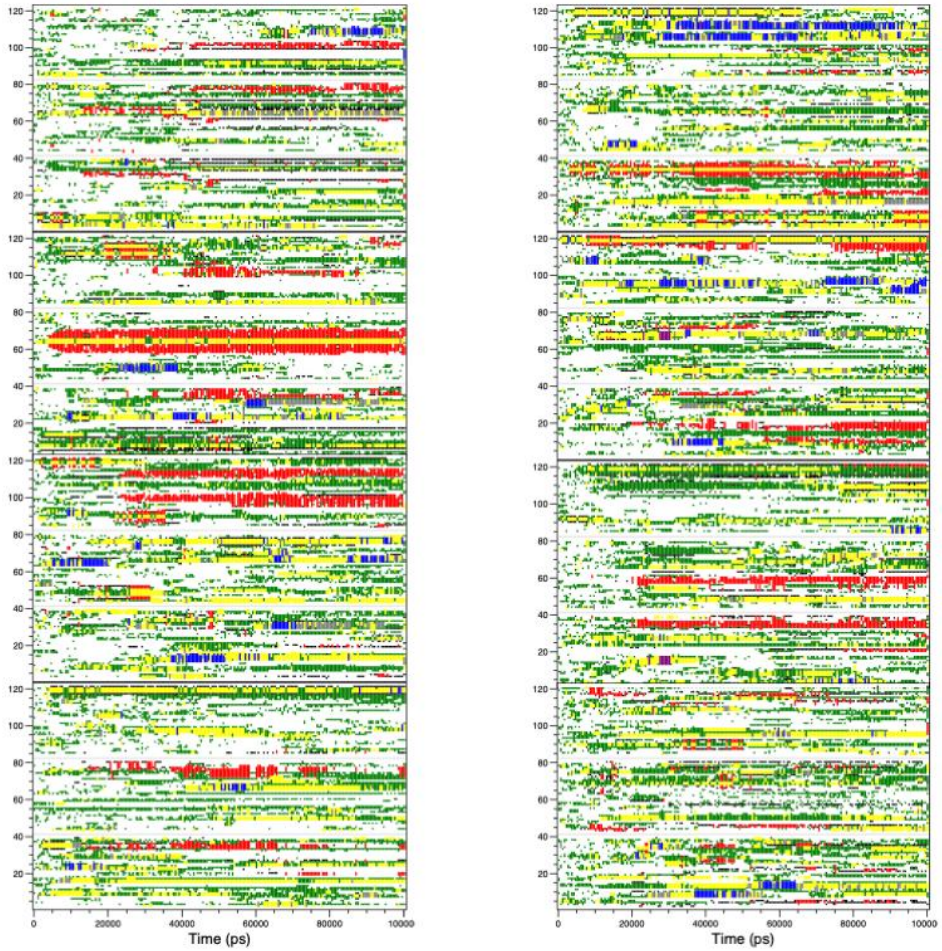

Figure S 6: Secondary structure assignment of three monomers for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + CUR

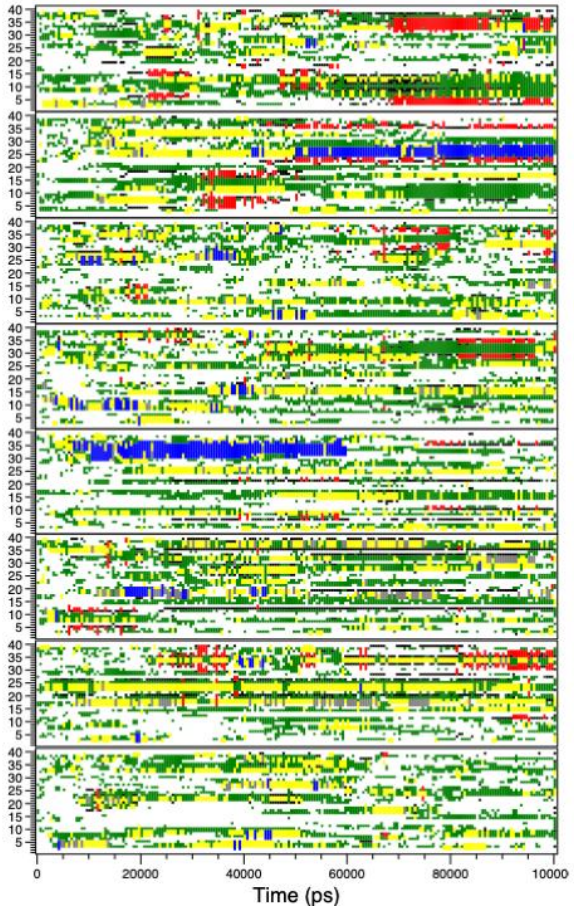

Figure S 7: Secondary structure assignment of the single monomer for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + EGCG

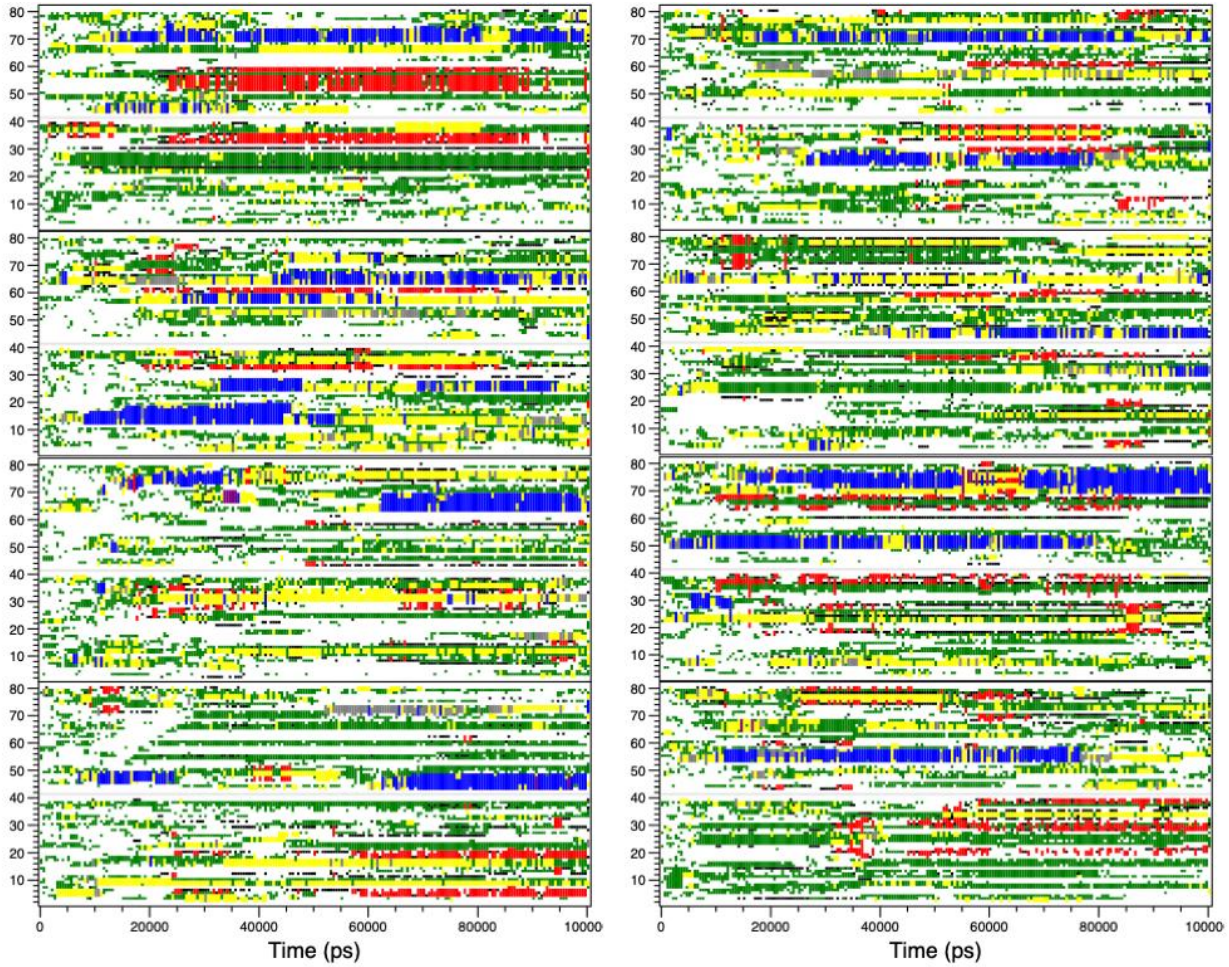

Figure S 8: Secondary structure assignment of two monomers for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + EGCG

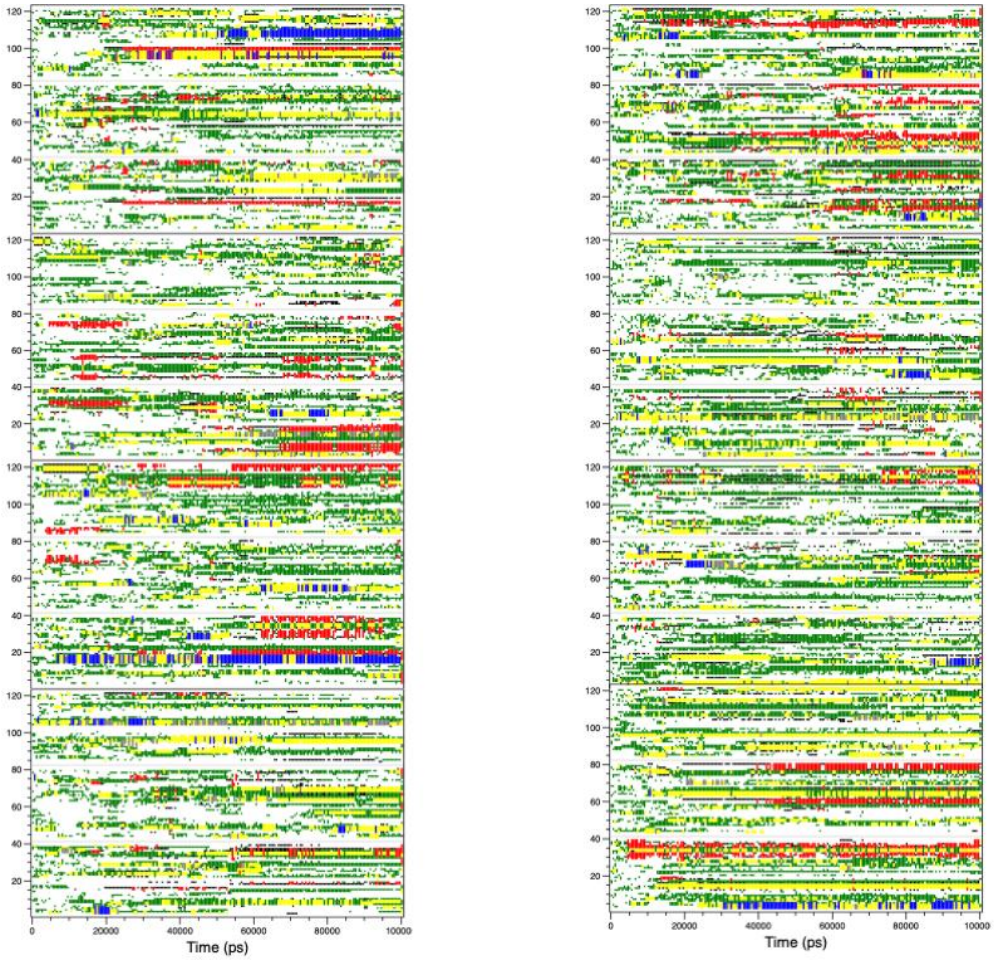

Figure S 9: Secondary structure assignment of three monomers for each residue obtained using the DSSP software for the eight REST simulations. Each color represents a different secondary structure as explained in the legend at the bottom. Monomers + EGCG