SUPPLEMENTARY DATA

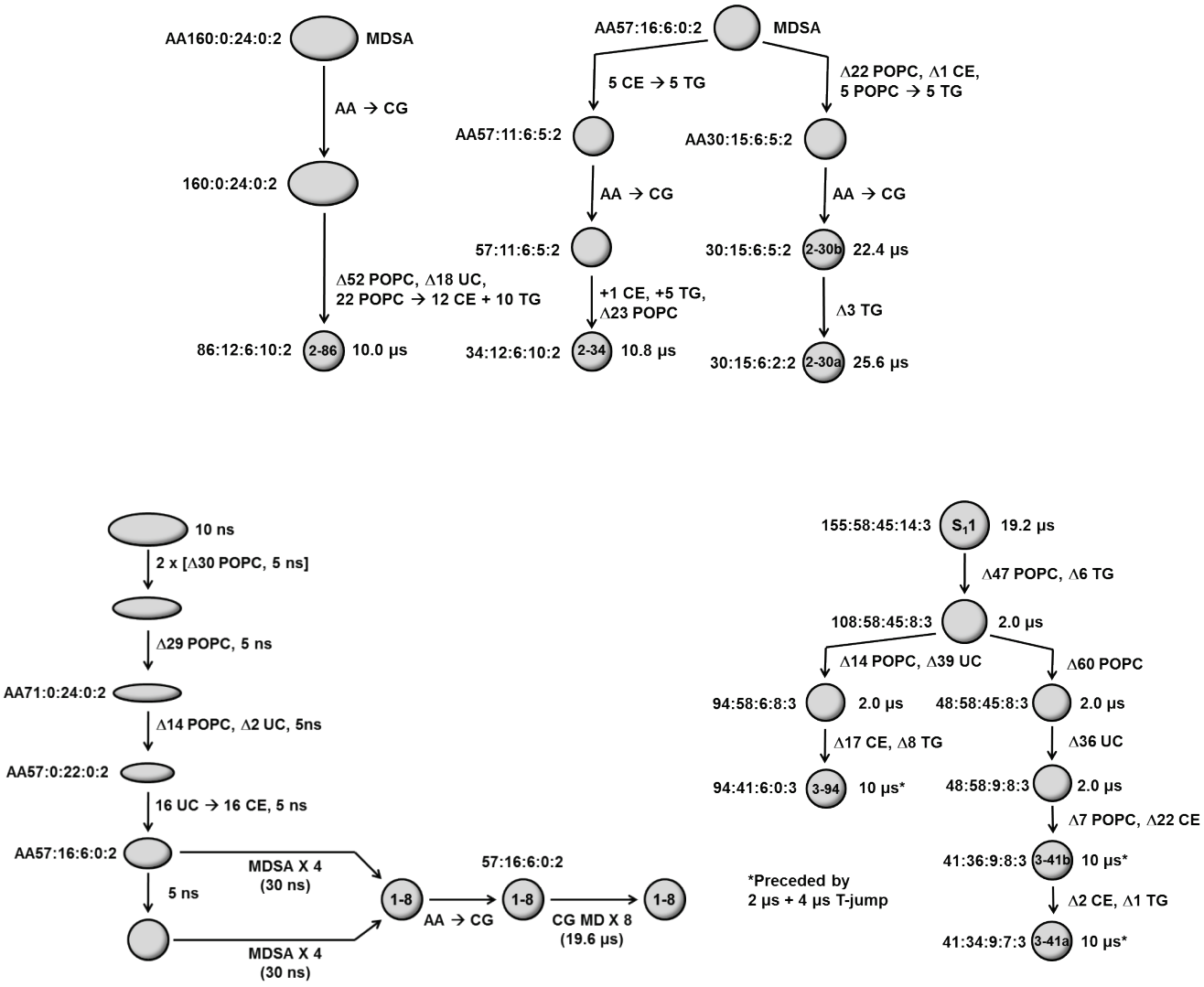

Figure S1A. Flow diagrams for the construction and MD simulation of AA and CG sHDL particles. Upper panels show the construction and simulation of some of the particles with two apoA-I: S2-86, S2-34, S2-30a, and S2-30b. Lower left panel shows the construction and simulation of the rest of the particles with two apoA-I: AA and CG S2-57. Lower right panel shows the construction and simulation of some of the particles with three apoA-I: S3-94, S3-41a, and S3-41b.

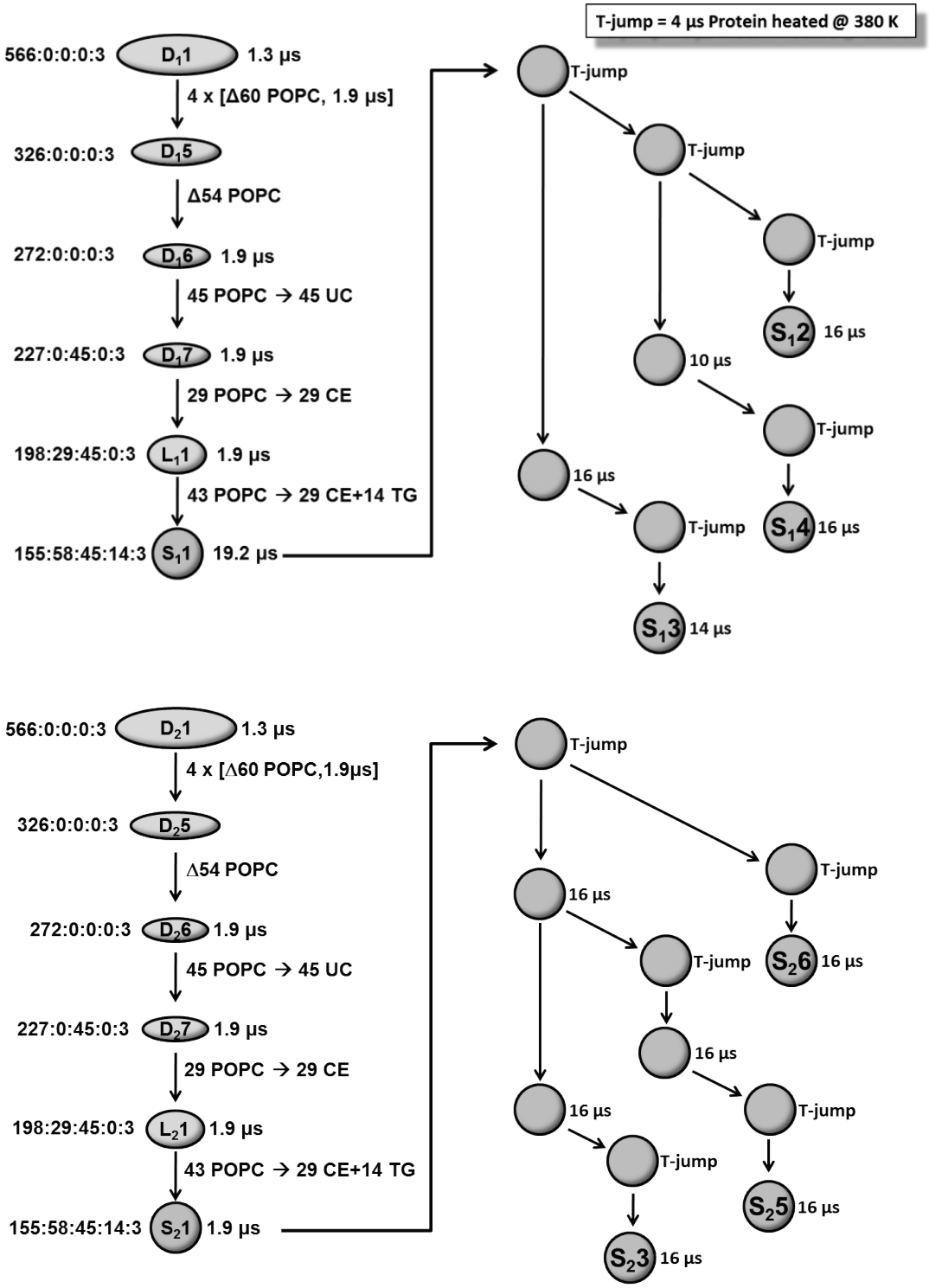

Figure S1B. Flow diagrams for the construction and MD simulation of CG sHDL particles. Upper and lower panels show construction and simulation of the remaining particles with three apoA-I: S3-155.

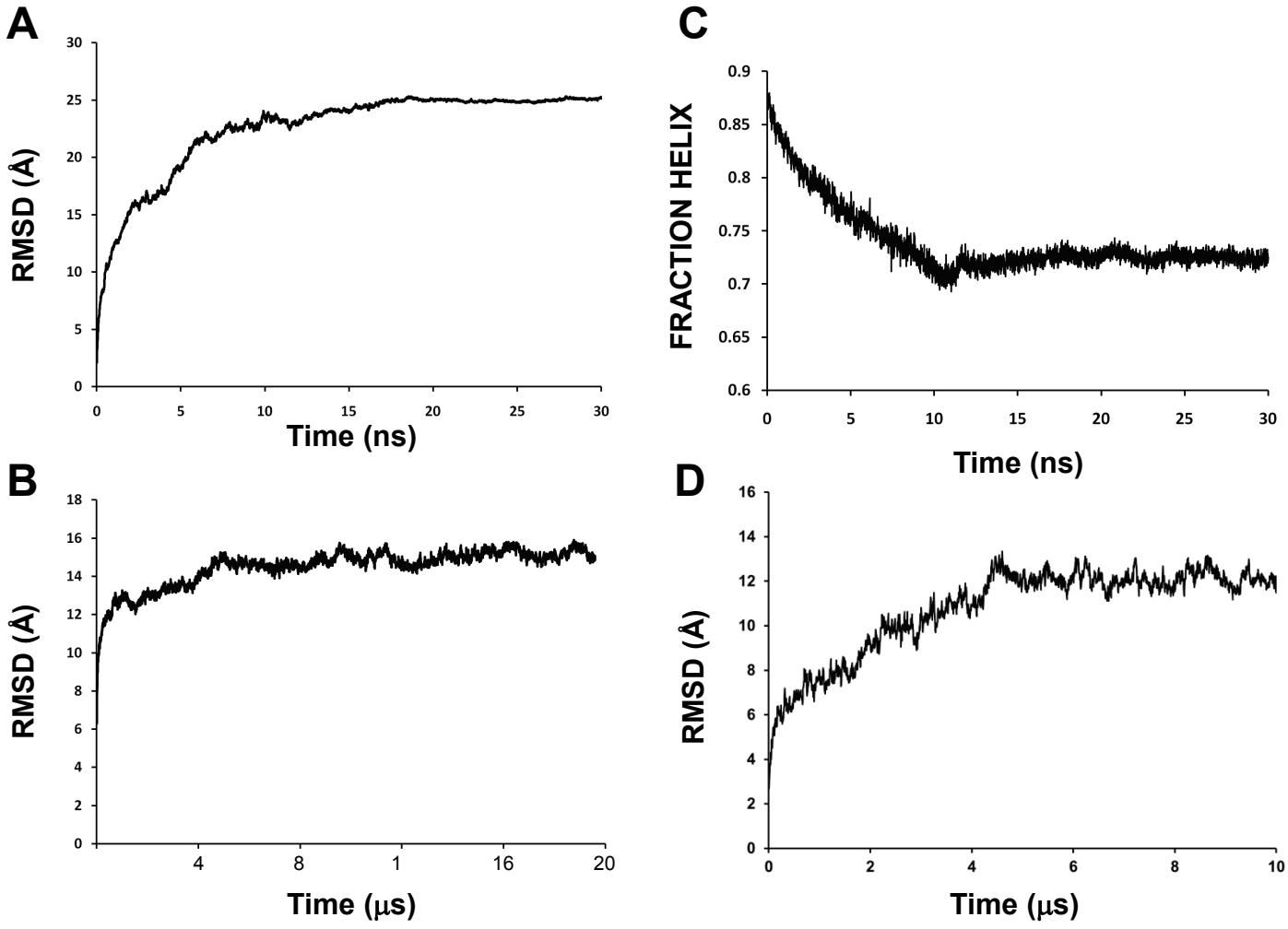

Figure S2. Equilibration dynamics of S2-57 and S3-41 particles. A. Average RMSD changes with time during the eight 30 ns MDSA simulations of S2-57. **B.** Average RMSD changes with time during the eight 19.6 μs CGMD simulations of S2-57. **C**. Average changes in total helicity with time during the eight MDSA simulations of S2-57. **D.** RMSD changes with time during the 10.0 μs CGMD simulation of S3-41.

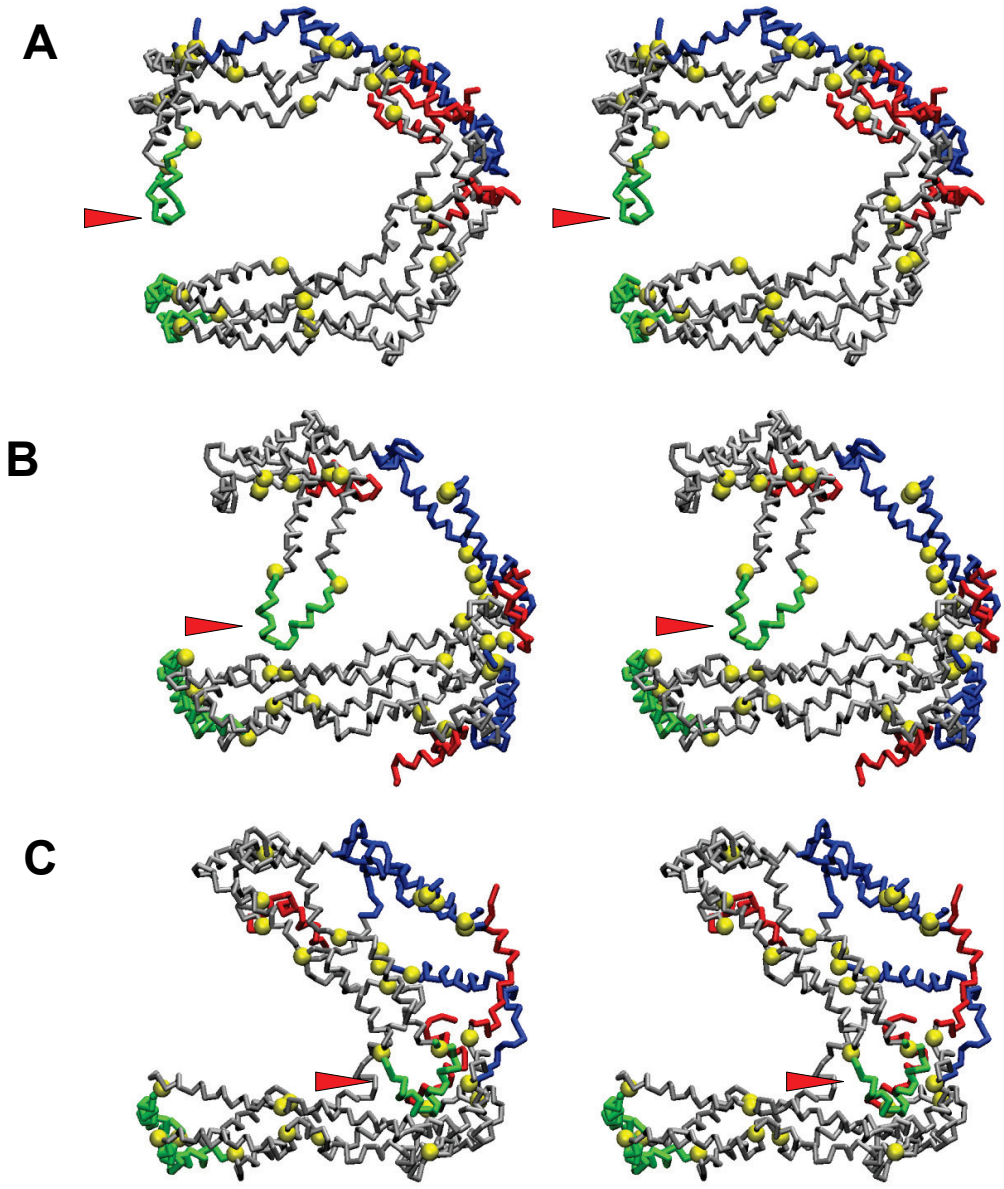

Figure S3. Three CGMD simulation frames illustrating the dynamics of motion of the hairpin portion of S3-155. The hairpin portion of the model swings in a right handed spiral (red arrowheads) from the helix 5 pair to the N-terminal domains with time of simulation. Protein backbone color code: Aligned residues 78-188, green; residues 1-43, blue; helix 10, red; prolines, yellow spacefilling; remainder, silver.