Supporting Information for Phase Behavior of AB/CD Diblock Copolymer Blends via Coarse-Grained Simulation

1. Simulation Termination

Simulations were stopped and analyzed when the domain size and structure factor were unchanging. A representative example is shown in Figure S1. This simulation stopped changing after $\sim 1 \times 10^7$ timesteps.

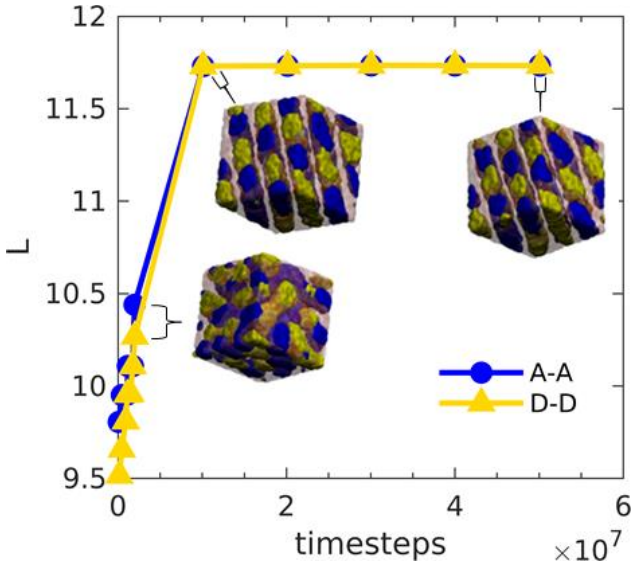

Figure S1. Domain size vs timestep for $A_6B_8C_8D_6$. Domain size (and structure factor) are unchanging after $\sim 1 \times 10^7$ timesteps. Example snapshots are shown inset. A domains are represented in blue, D in yellow, and the BC domains as red/silver and transparent. All bead representations are done using VMD's[1] quicksurf method.

2. S(q) and mixing determination

The plots show here were calculated using Equation 5 in the main text. S(q*) is the maximum value of S(q). All 3 S(q*) plots (see main text Figure 3 for S(q*) for $N_A = 1$) show a significant drop as N_B increase, though the decrease is significantly smaller for larger N_A. This is partly due to the decrease in φ_A as N_B increases caused by the simultaneous increase in N_C, but also due to the change in morphology. The pair distribution function $g(r)$ is calculated using VMD.

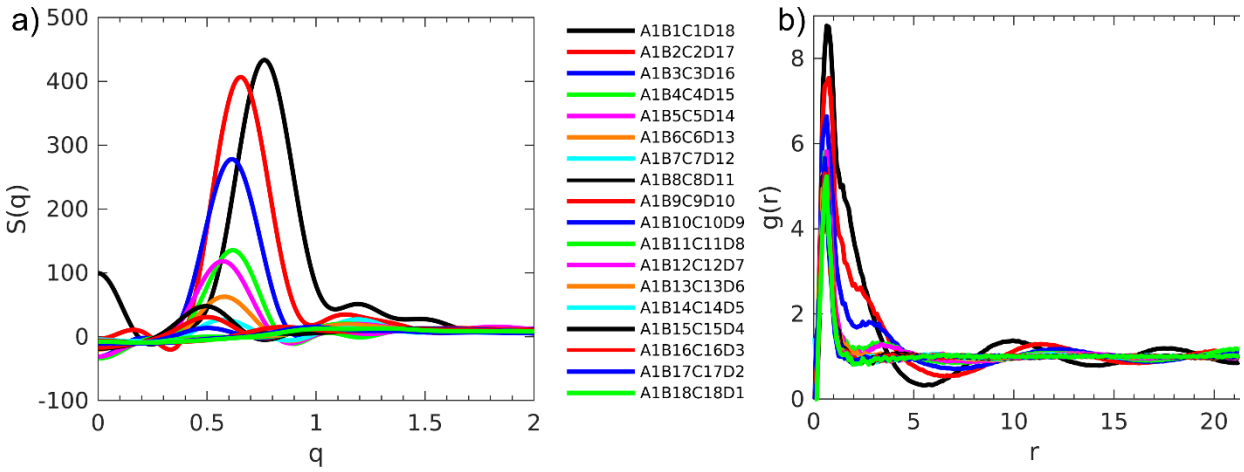

Figure S2. a) S(q) for N_A=1, and b) corresponding pair distribution function g(r).

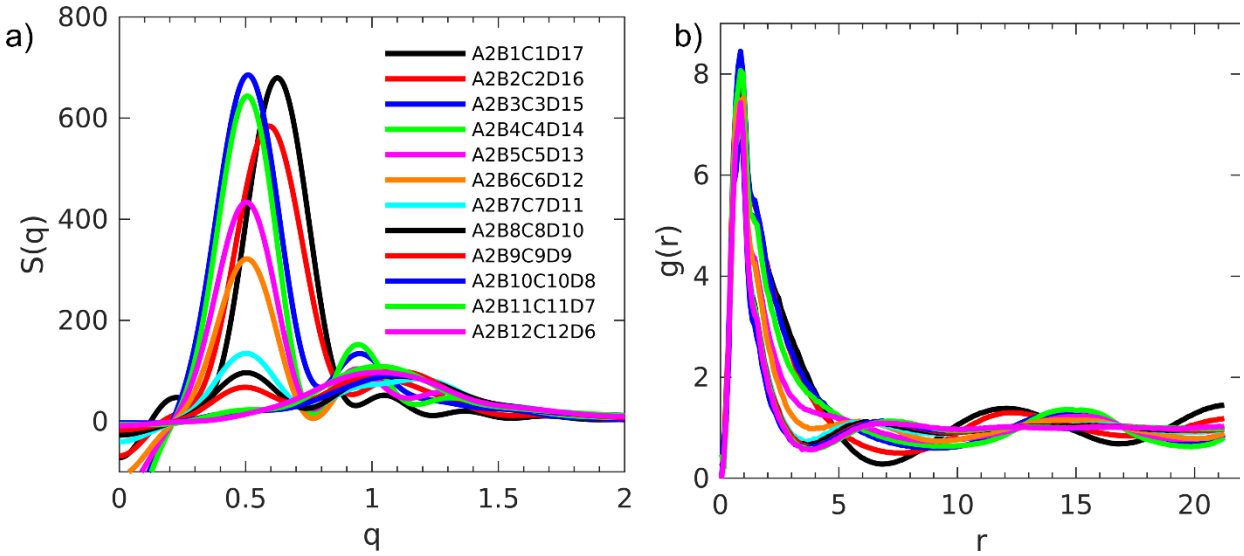

Figure S3. a) S(q) for N_A=2 and corresponding pair distribution function g(r).

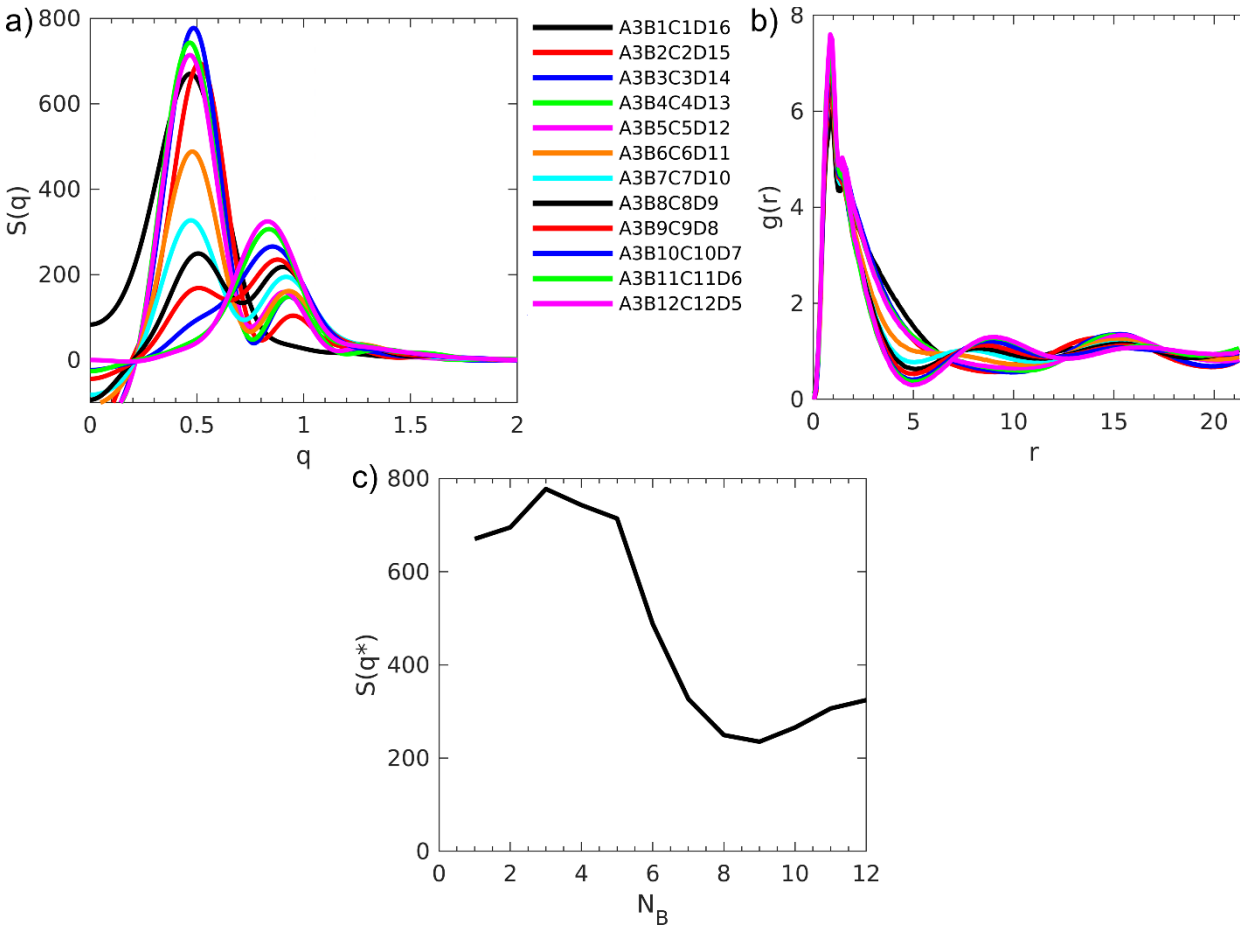

Figure S4. a) S(q) for N_A=3, b) the corresponding g(r)S(q*) for N_A=3.

3. Number of Nearest Neighbors

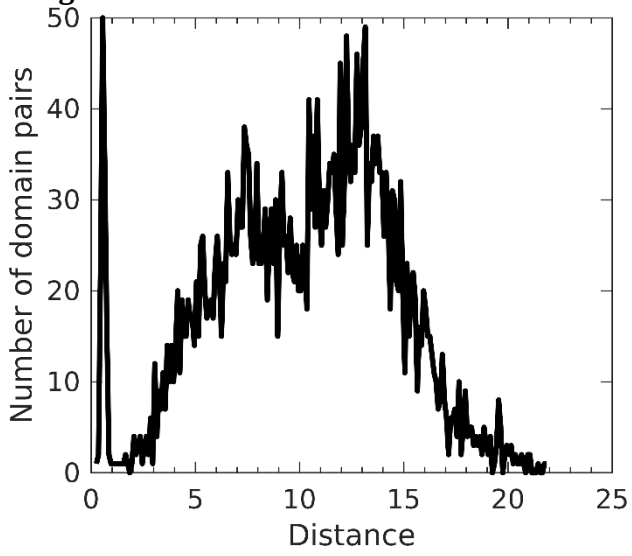

Figure S5. Representative distance between domains histogram used to calculate the number of nearest neighbors.

4. Shape Determination Sensitivity

As described in the text, the sensitivity of the cutoff values was measured by incrementally changing the cutoffs keeping each other cutoff constant. The number of changed data points (n_{diff}) were then recorded. Figure S6 plots n_{diff} versus the cutoff criteria shown in Table 1. In general, there is a fairly wide region where the determination remains unchanged. However, the sphere cutoff is more sensitive and the transition from sphere to cylinder, specifically for the minor A or D phase, is slow. The phases change from spheres to short cylinders before they finally form cylinders. Such types of structures are sometimes found in triblock BCPs,[2] diblocks under external forces,[3] defective BCP films,[4] and diblocks in solution.[5]

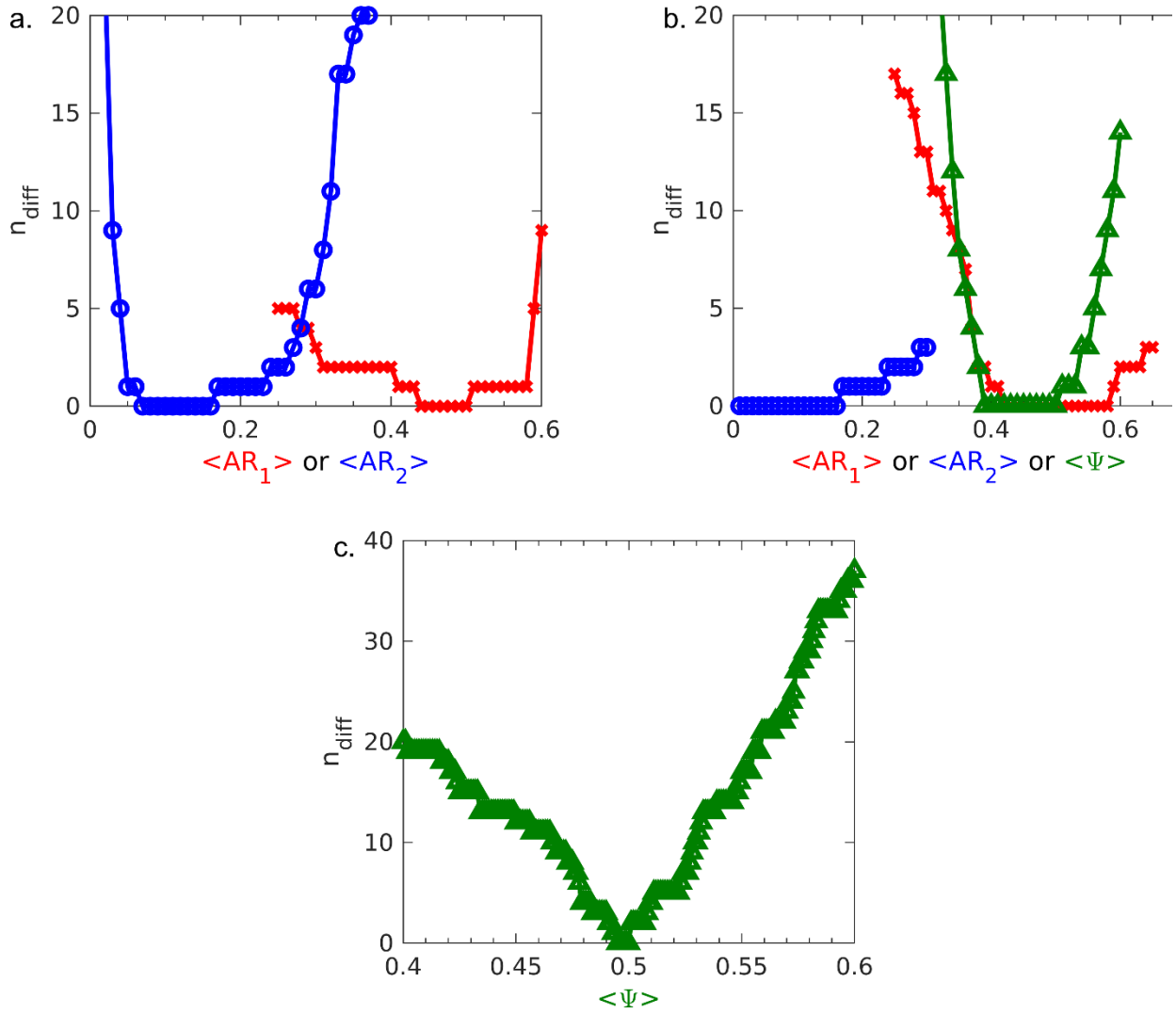

Figure S6. Changed evaluations (n_{diff}) versus cutoff values for a) lamellae, b) branched/gyroid, and c) spheres.

References

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