SUPPORTING INFORMATION: Aggregation of Alzheimer's Amyloid β-Peptide in Biological Membranes: A Molecular Dynamics Study

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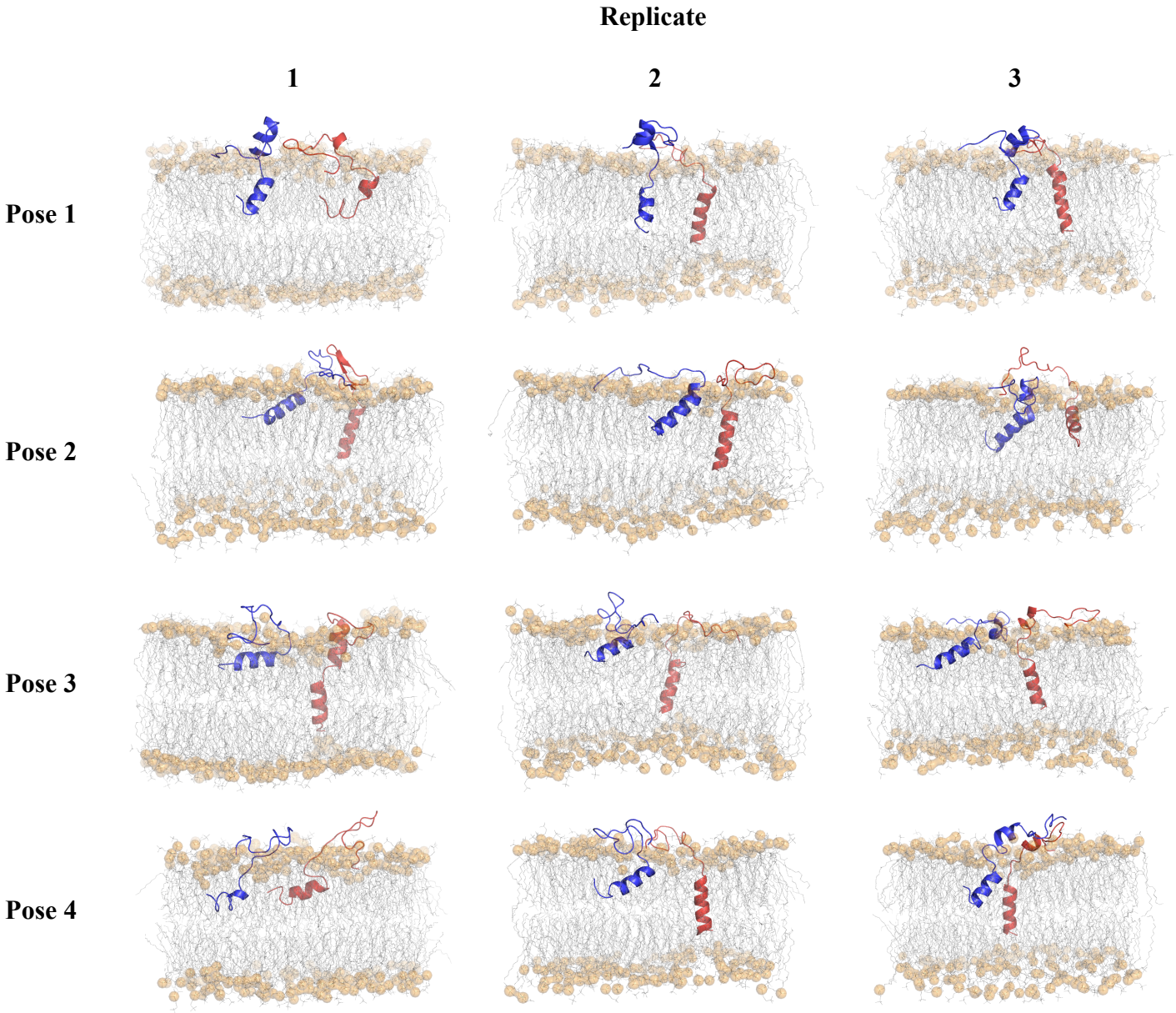

Figure S1. Side-on views of all POPC-CH systems from snapshots at 200 ns. Peptide 1 (blue) and peptide 2 (red) are shown as cartoons. Lipids are shown as gray lines, with phosphorus atoms highlighted as translucent gold spheres to give perspective of membrane dimensions.

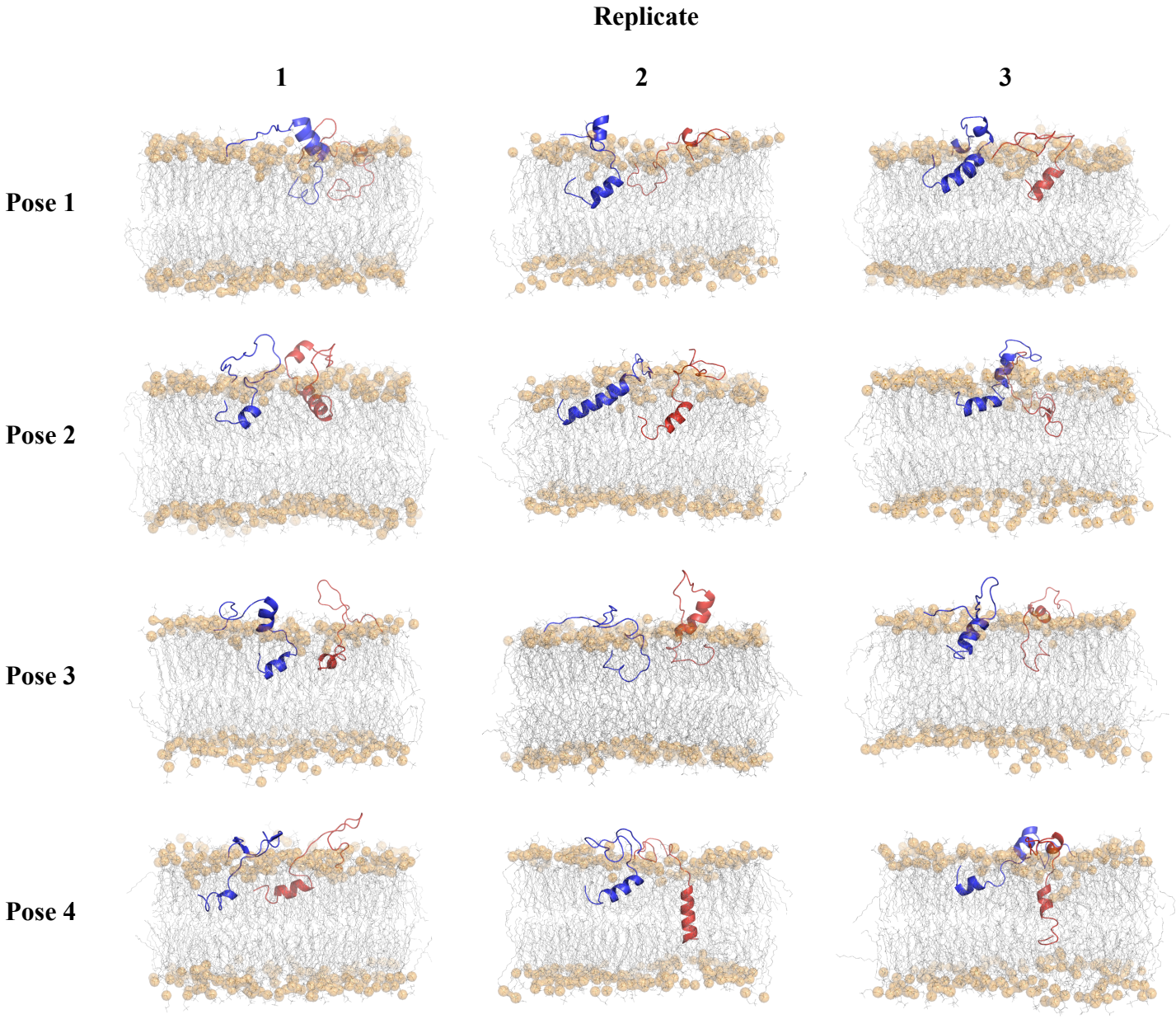

Figure S2. Side-on views of all POPC-CI systems from snapshots at 200 ns. Images are rendered as in Figure S1.

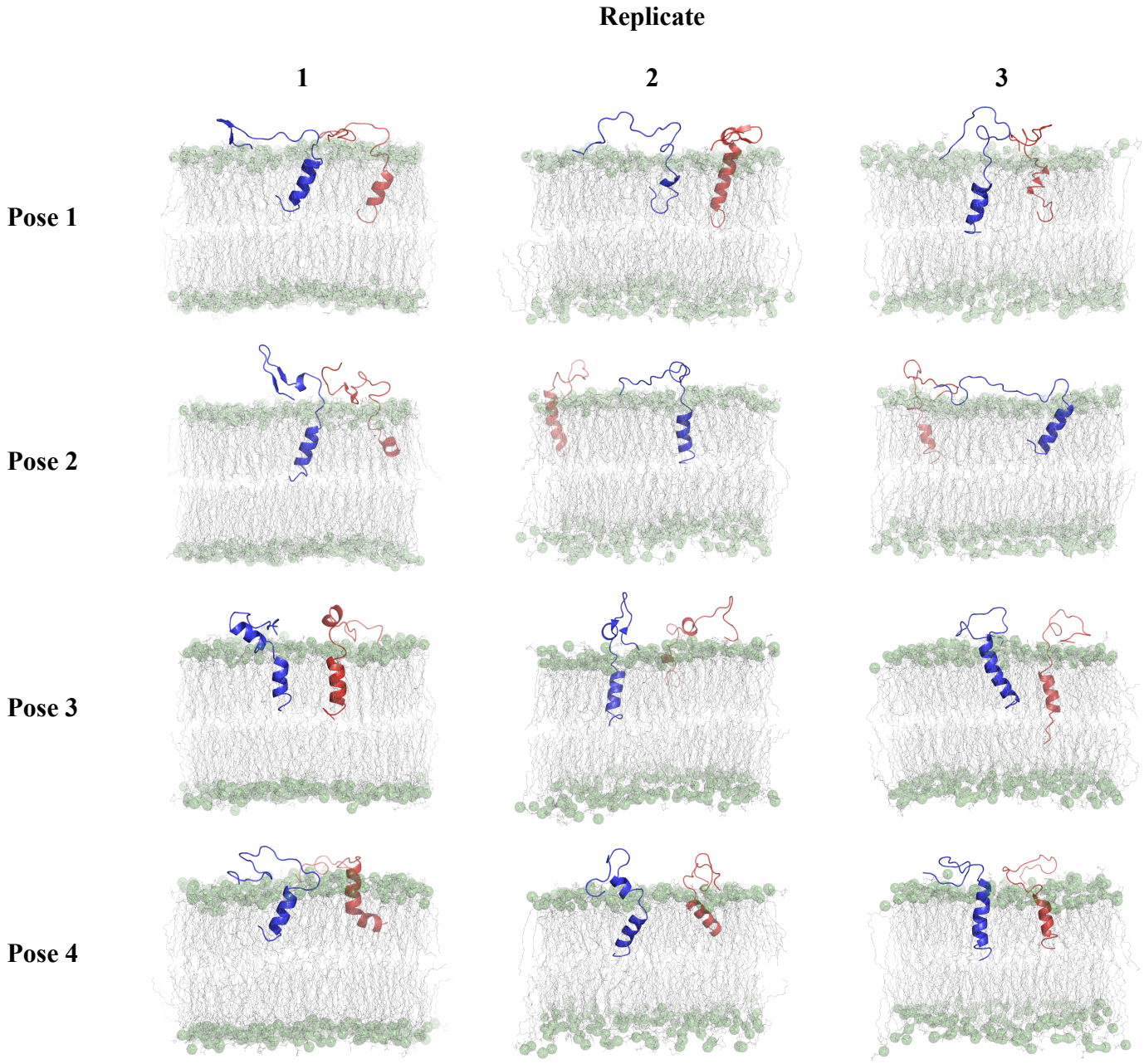

Figure S3. Side-on views of all POPS-CH systems from snapshots at 200 ns. Images are rendered as in Figure S1, with phosphorus atoms shown in green instead of gold.

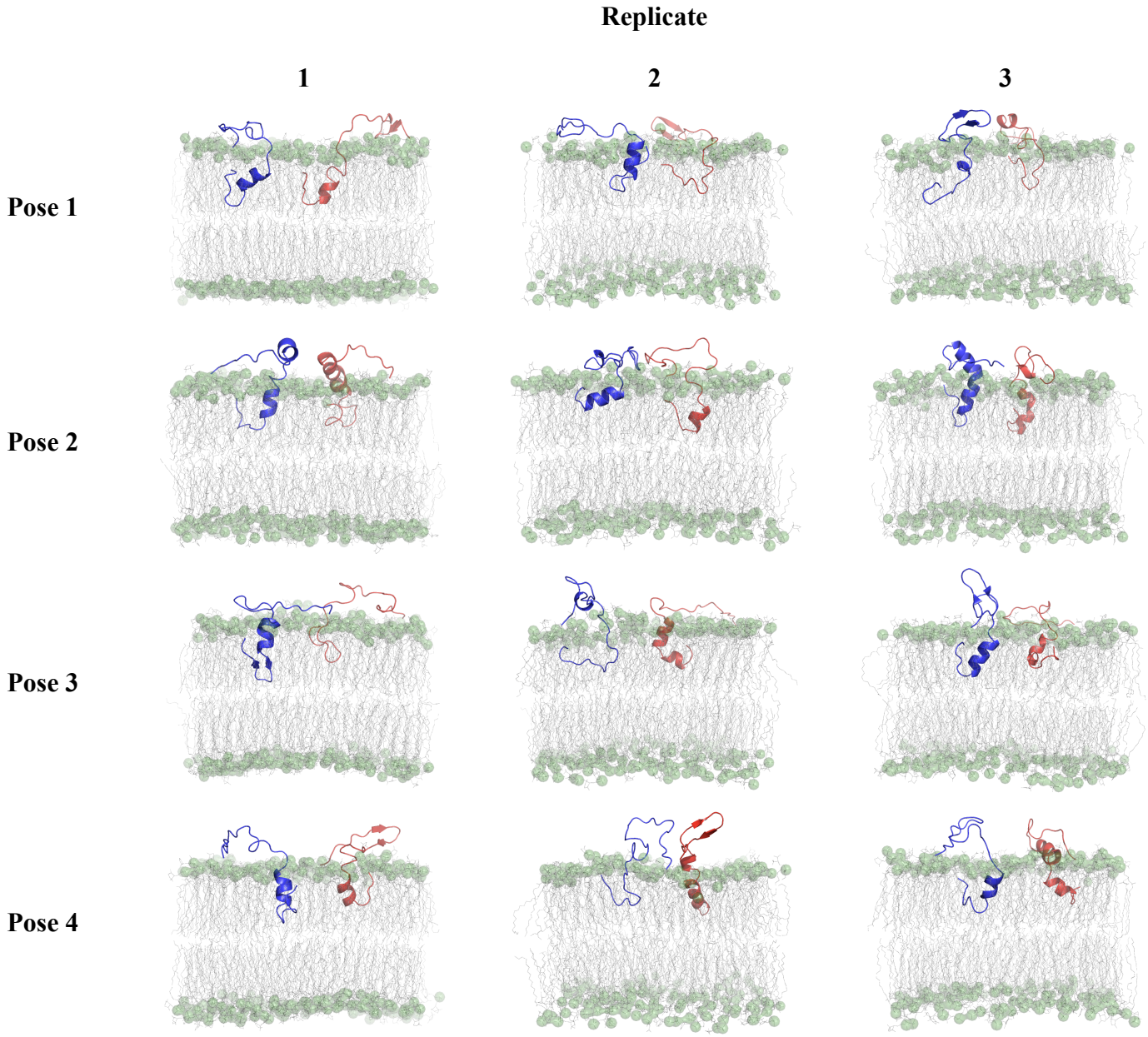

Figure S4. Side-on views of all POPS-CI systems from snapshots at 200 ns. Images are rendered as in Figure S1, with phosphorus atoms shown in green instead of gold.

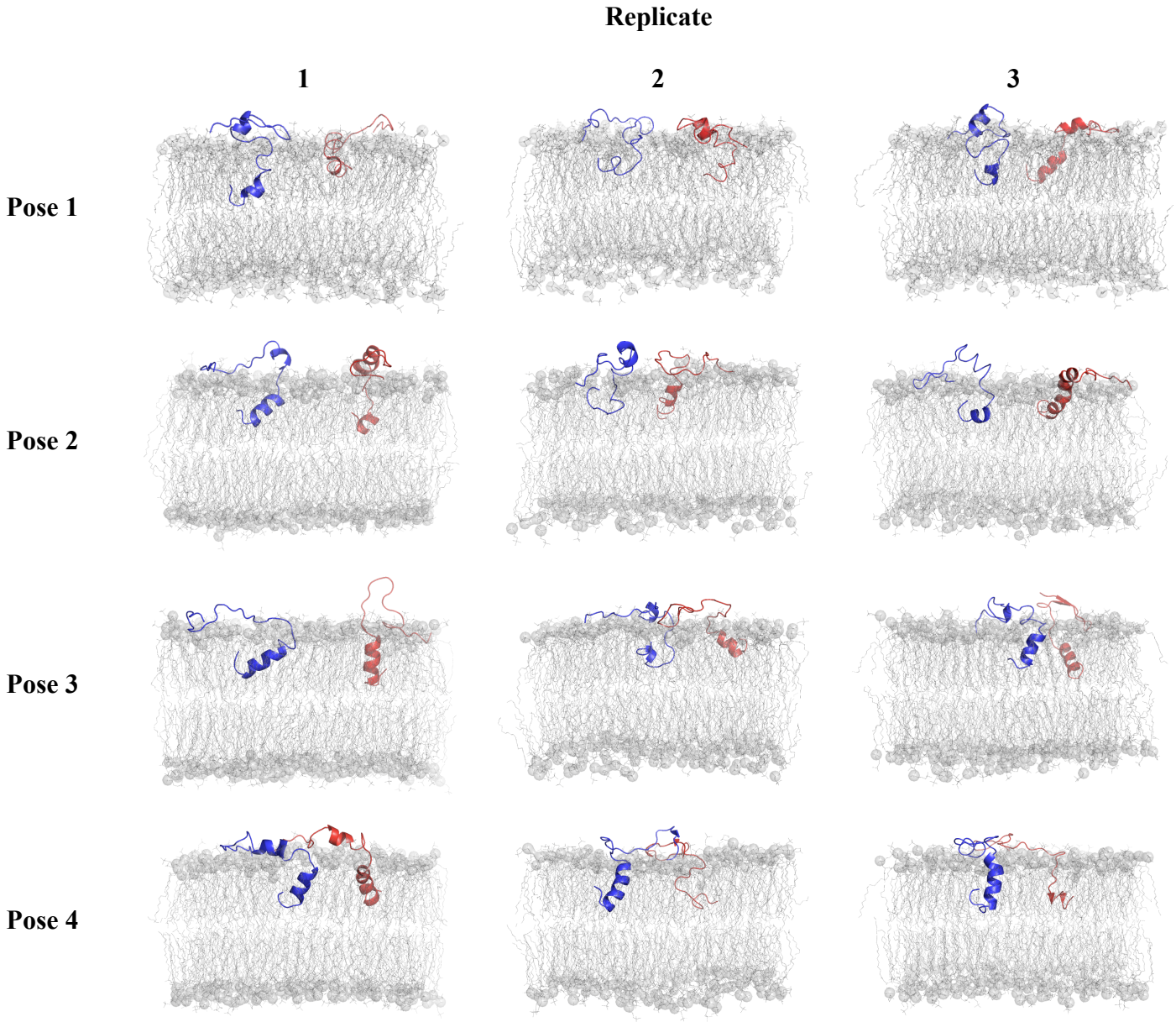

Figure S5. Side-on views of all POPC/POPE-CH systems from snapshots at 200 ns. Images are rendered as in Figure S1, with phosphorus atoms shown in gray instead of gold.

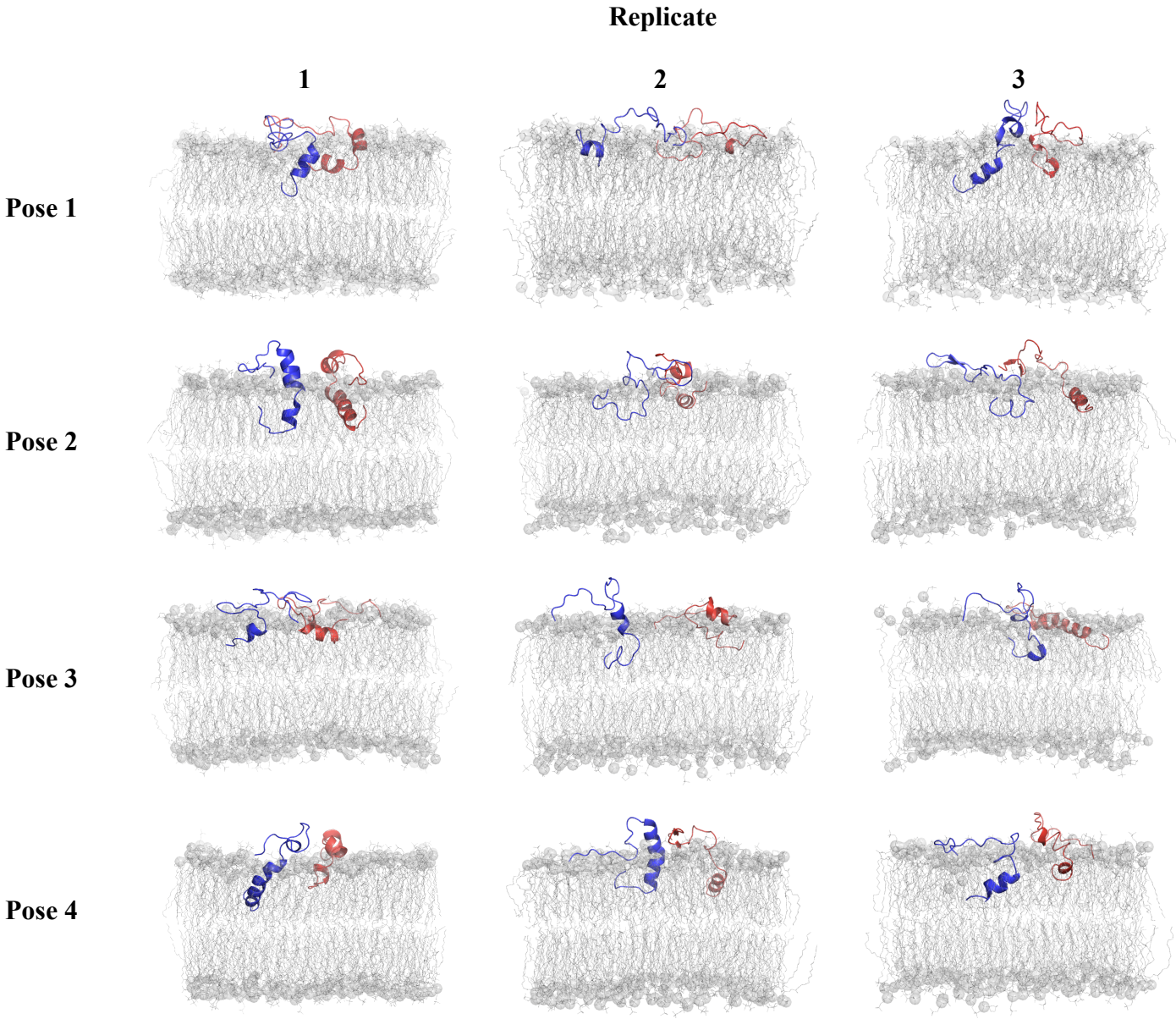

Figure S6. Side-on views of all POPC/POPE-CI systems from snapshots at 200 ns. Images are rendered as in Figure S1, with phosphorus atoms shown in gray instead of gold.

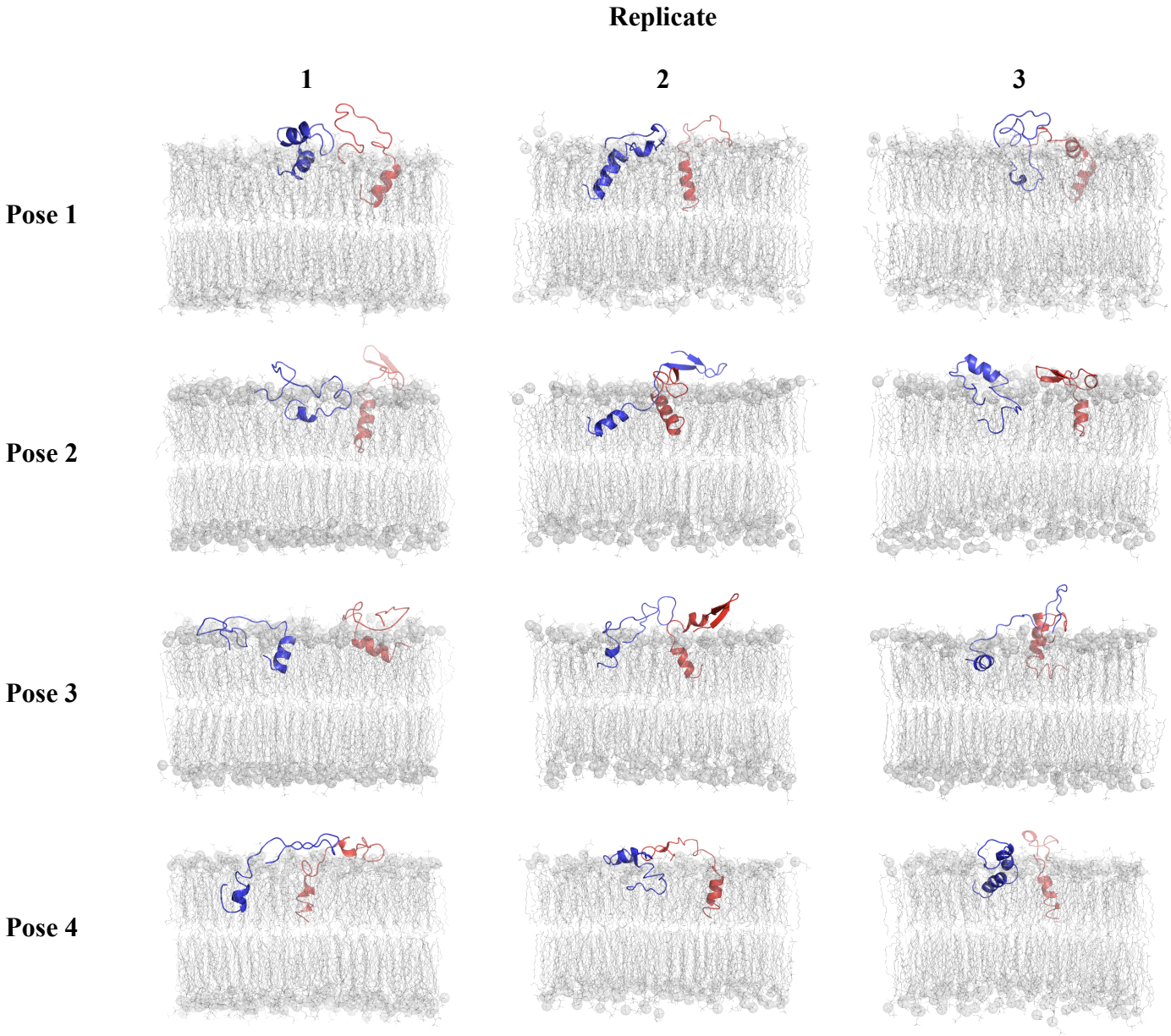

Figure S7. Side-on views of all Raft-CH systems from snapshots at 200 ns. Images are rendered as in Figure S1, with phosphorus atoms shown in gray instead of gold.

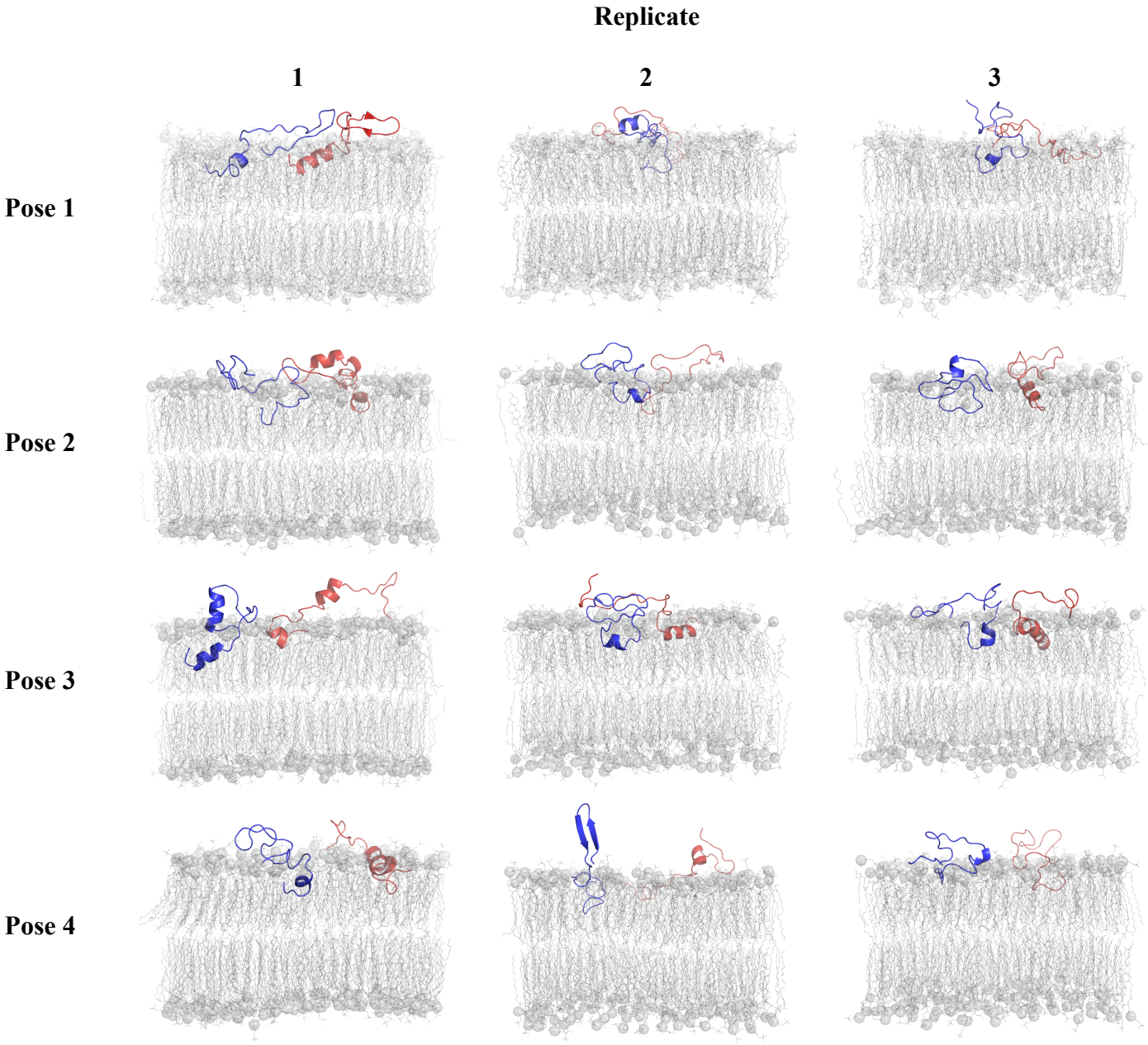

Figure S8. Side-on views of all Raft-CI systems from snapshots at 200 ns. Images are rendered as in Figure S1, with phosphorus atoms shown in gray instead of gold.

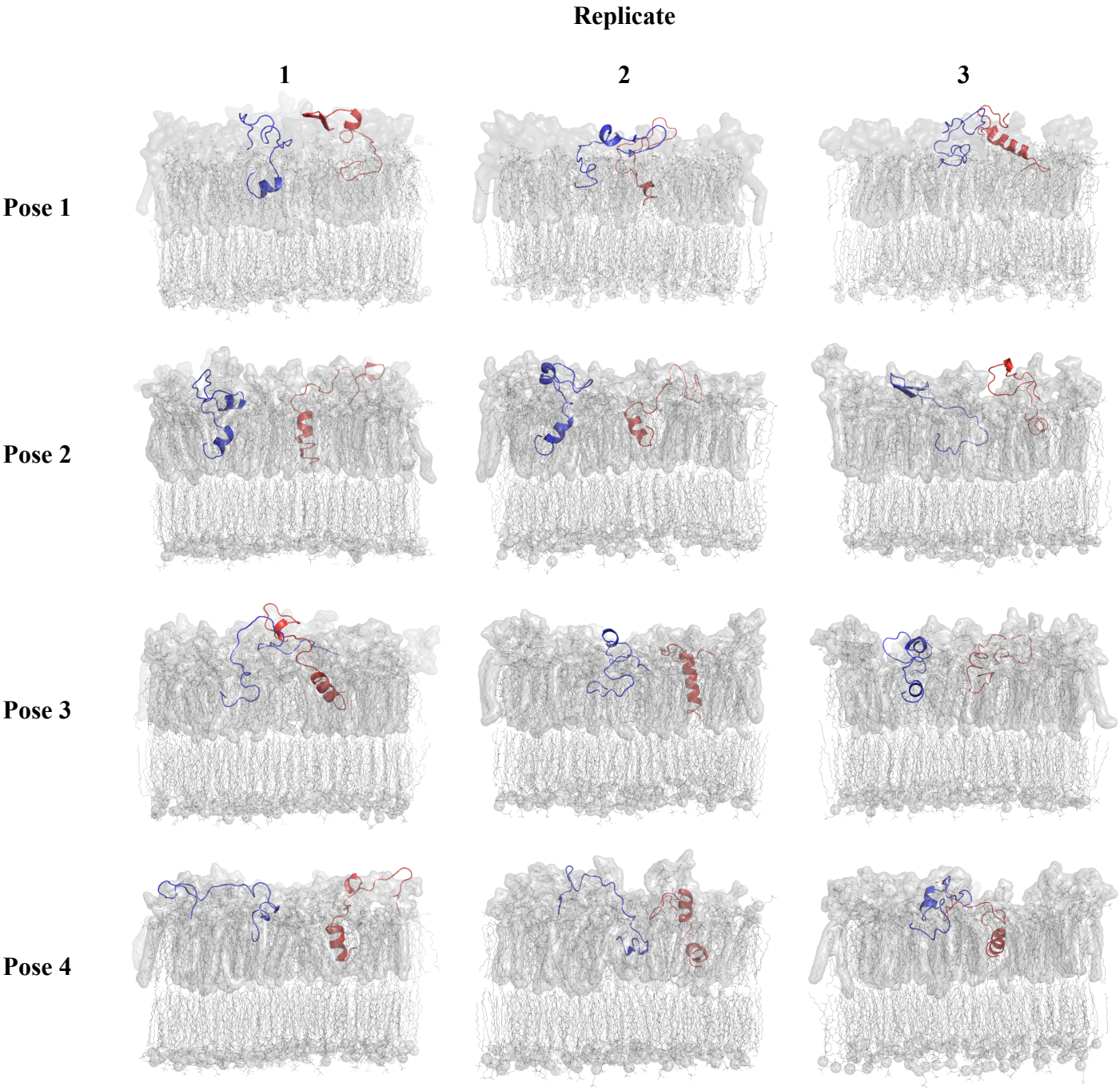

Figure S9. Side-on views of all GM1-Raft-CH systems from snapshots at 200 ns. Images are rendered as in Figure S1, with phosphorus atoms shown in gray instead of gold and GM1 molecules highlighted with translucent surfaces.

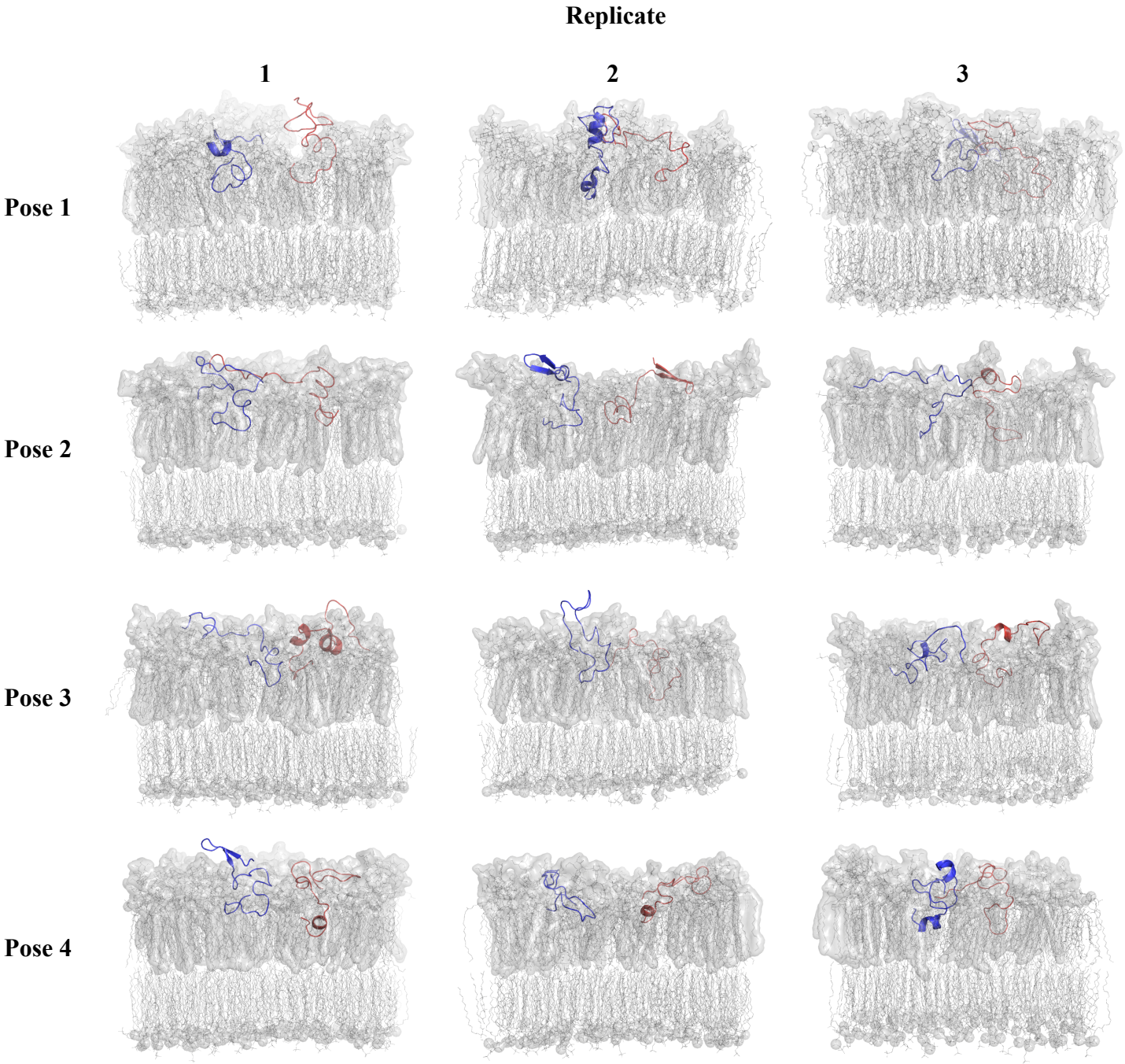

Figure S10. Side-on views of all GM1-Raft-CI systems from snapshots at 200 ns. Images are rendered as in Figure S1, with phosphorus atoms shown in gray instead of gold and GM1 molecules highlighted with translucent surfaces.

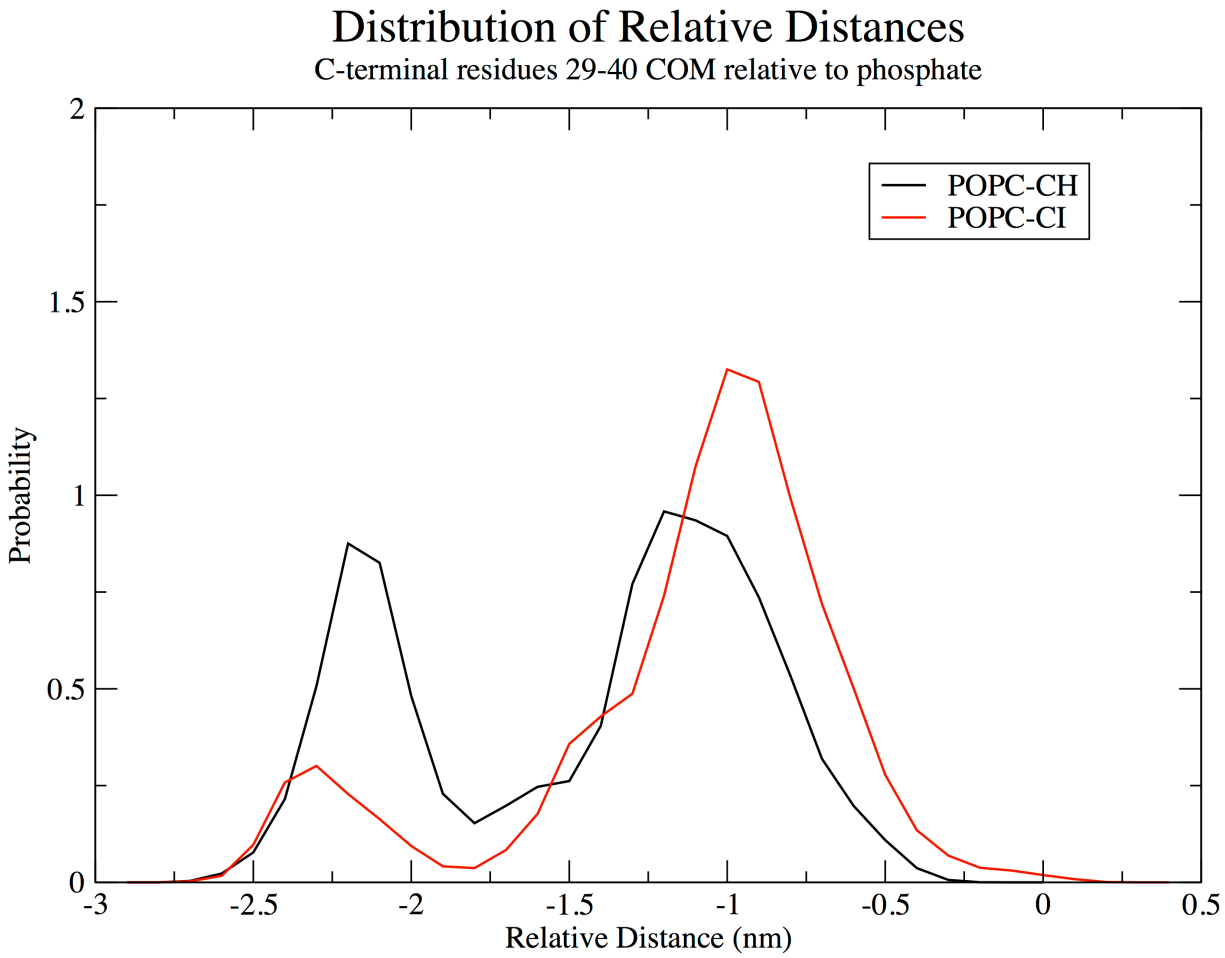

Figure S11. Histogram of positions of C-terminal residues 29-40 relative to phosphate groups in the extracellular leaflet of the POPC membrane.

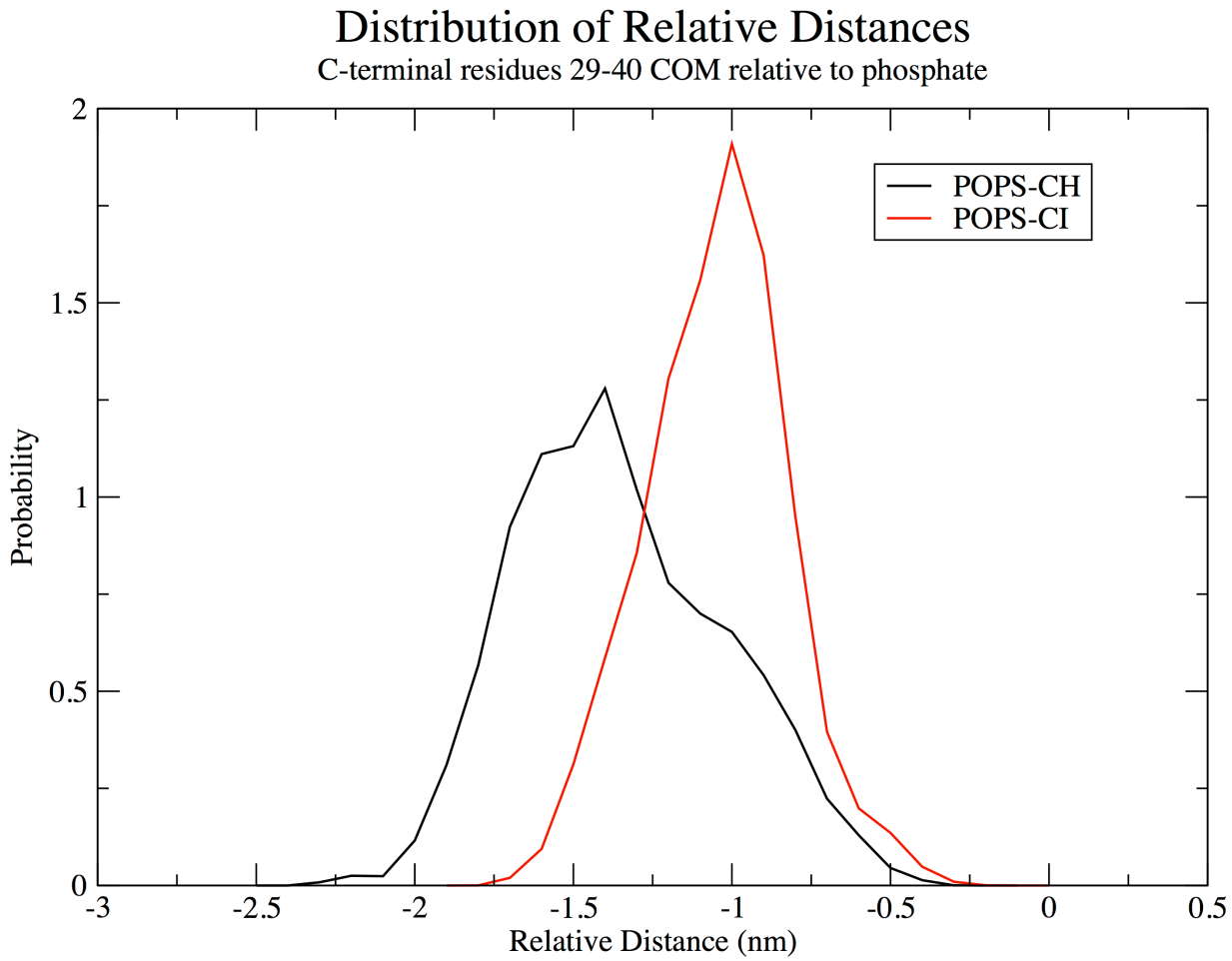

Figure S12. Histogram of positions of C-terminal residues 29-40 relative to phosphate groups in the extracellular leaflet of the POPS membrane.

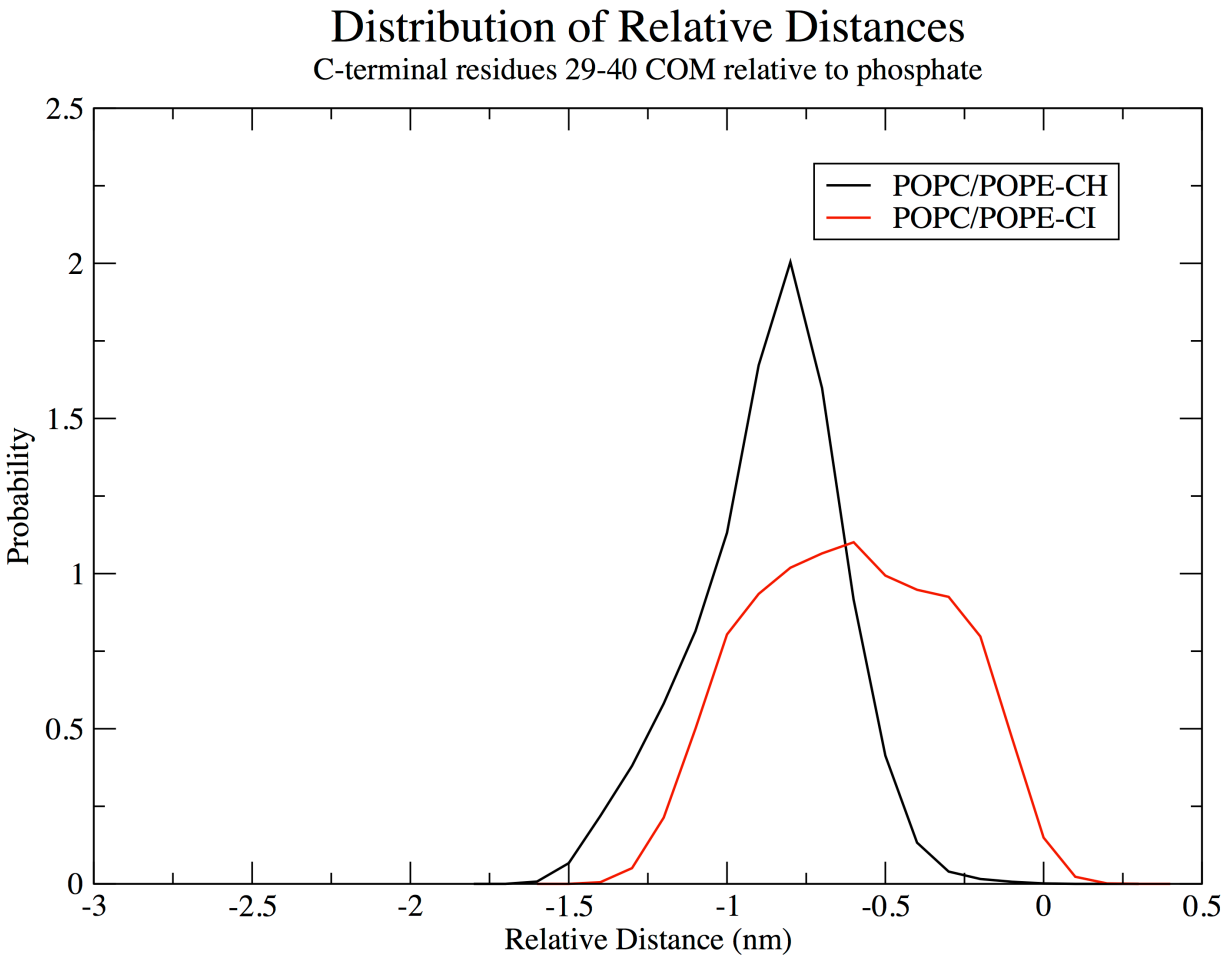

Figure S13. Histogram of positions of C-terminal residues 29-40 relative to phosphate groups in the extracellular leaflet of the POPC-POPE membrane.

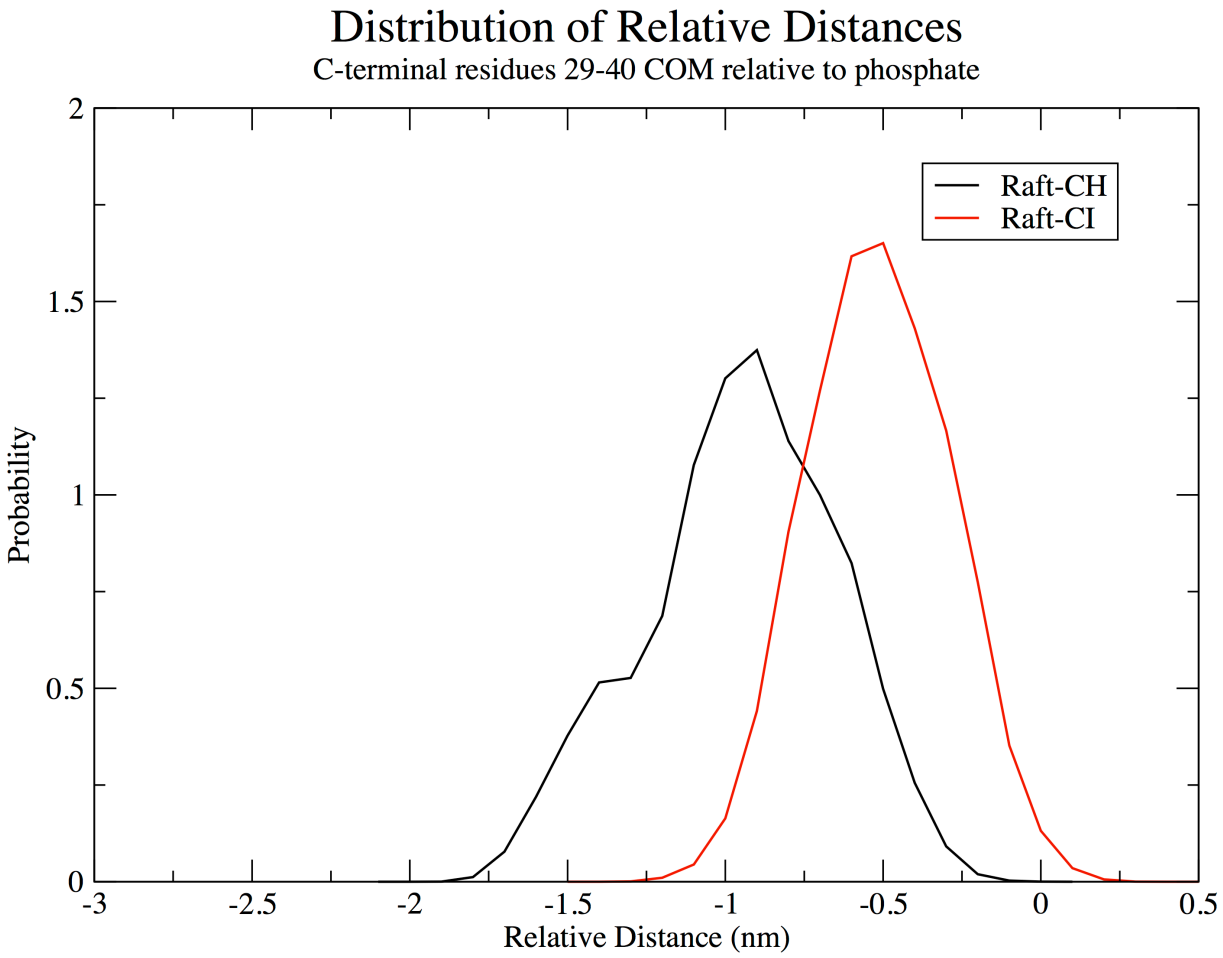

Figure S14. Histogram of positions of C-terminal residues 29-40 relative to phosphate groups in the extracellular leaflet of the Raft membrane.

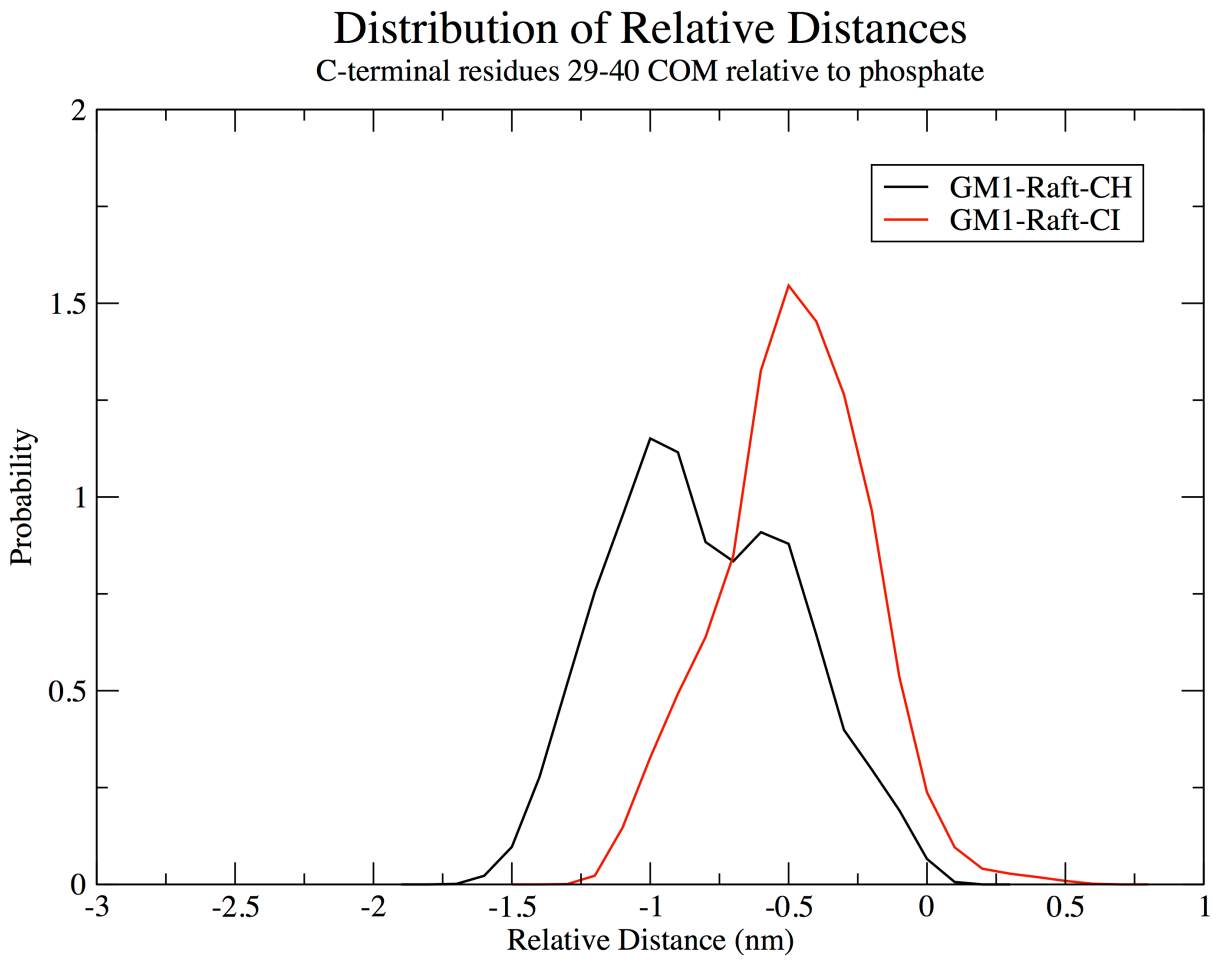

Figure S15. Histogram of positions of C-terminal residues 29-40 relative to phosphate groups in the extracellular leaflet of the GM1-Raft membrane.

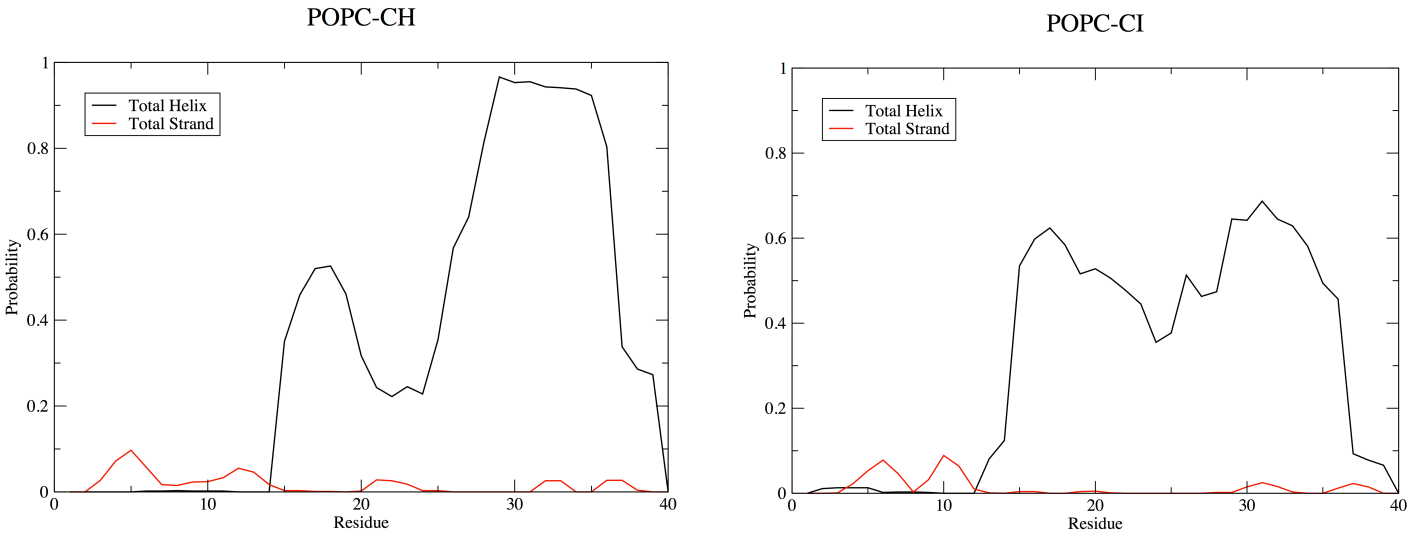

Figure S16. Secondary structure probabilities for POPC systems. Results are averaged over all simulations in all sets.

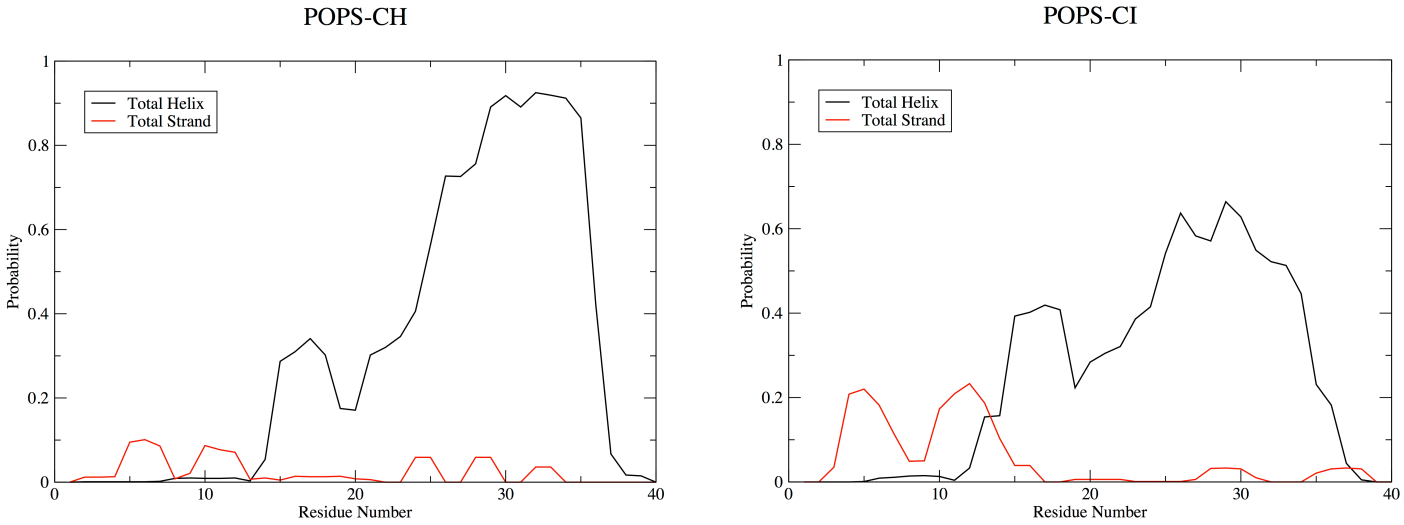

Figure S17. Secondary structure probabilities for POPS systems. Results are averaged over all simulations in all sets.

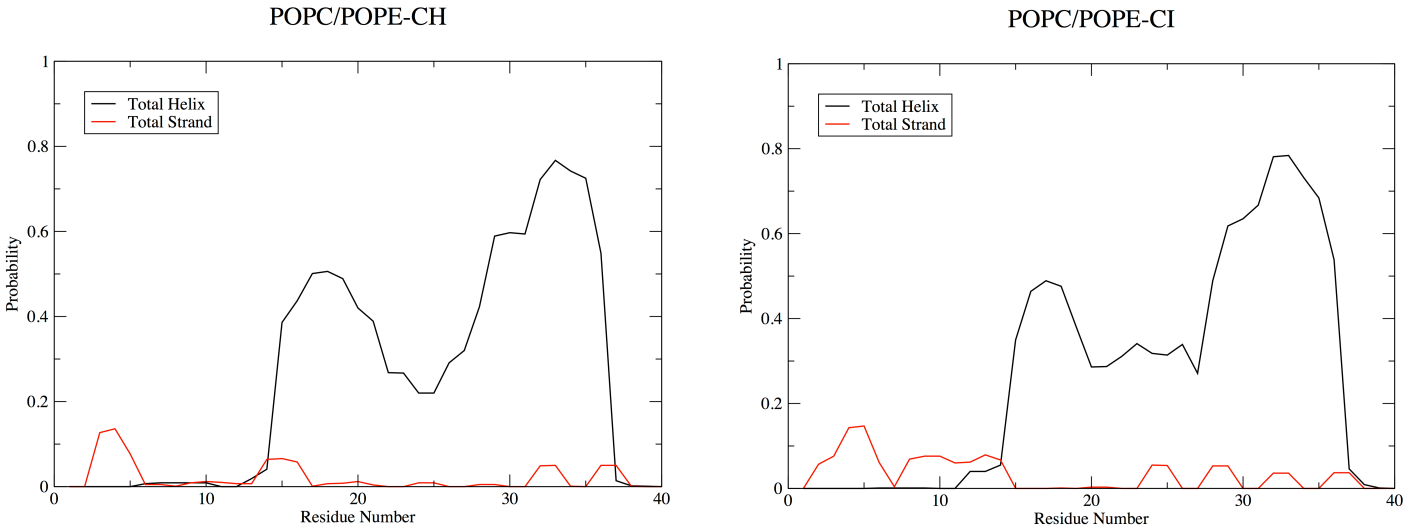

Figure S18. Secondary structure probabilities for POPC-POPE systems. Results are averaged over all simulations in all sets.

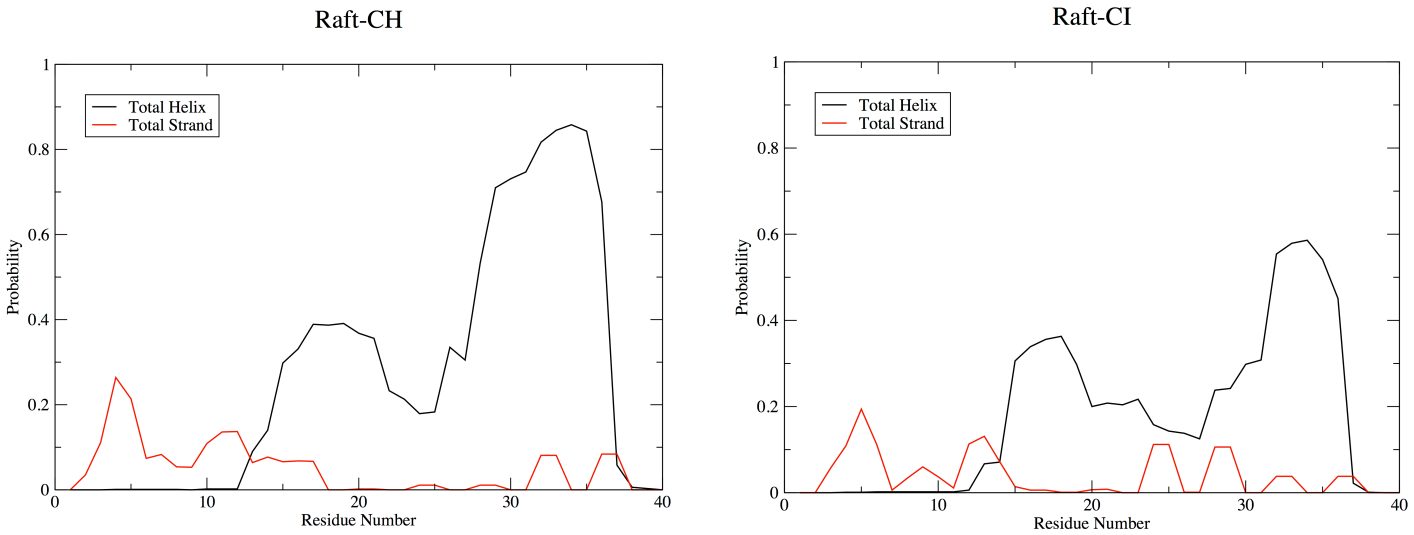

Figure S19. Secondary structure probabilities for Raft systems. Results are averaged over all simulations in all sets.

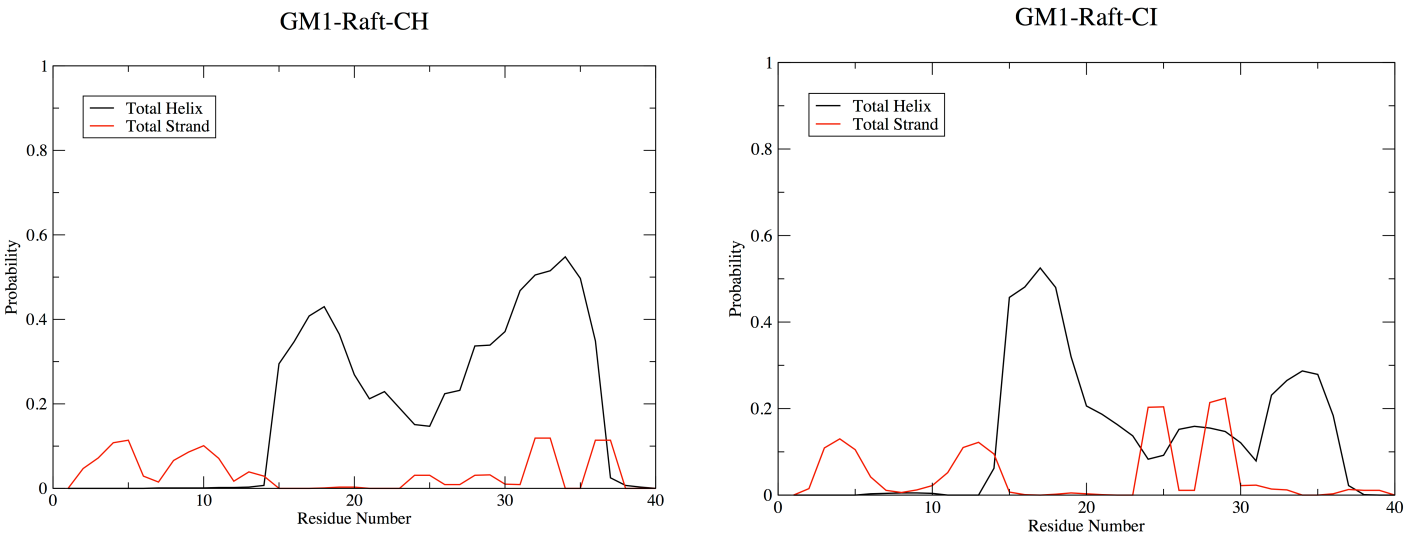

Figure S20. Secondary structure probabilities for GM1-Raft systems. Results are averaged over all simulations in all sets.

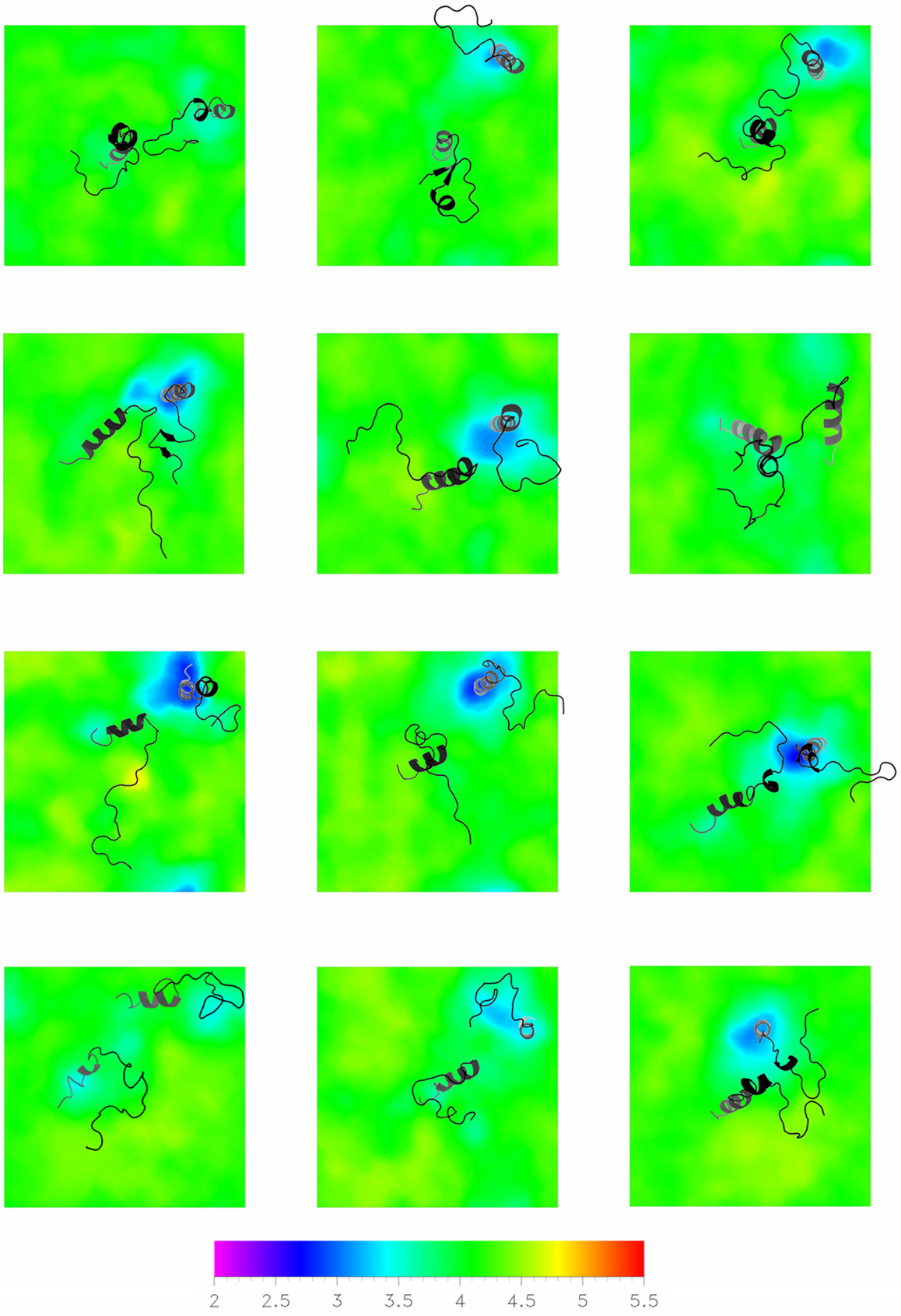

Figure S21. Membrane thickness plots for all systems in the POPC-CH sets. Poses 1 through 4 are shown in each row (top to bottom), with each column representing the three replicates. Thickness data were averaged over the last 50 ns. Peptide configurations were taken from the configuration at 200 ns, and are represented as cartoons with depth indicated by color. Black is nearest (positive z) and gray is furthest away (within the membrane, negative z). The legend represents thickness in nm.

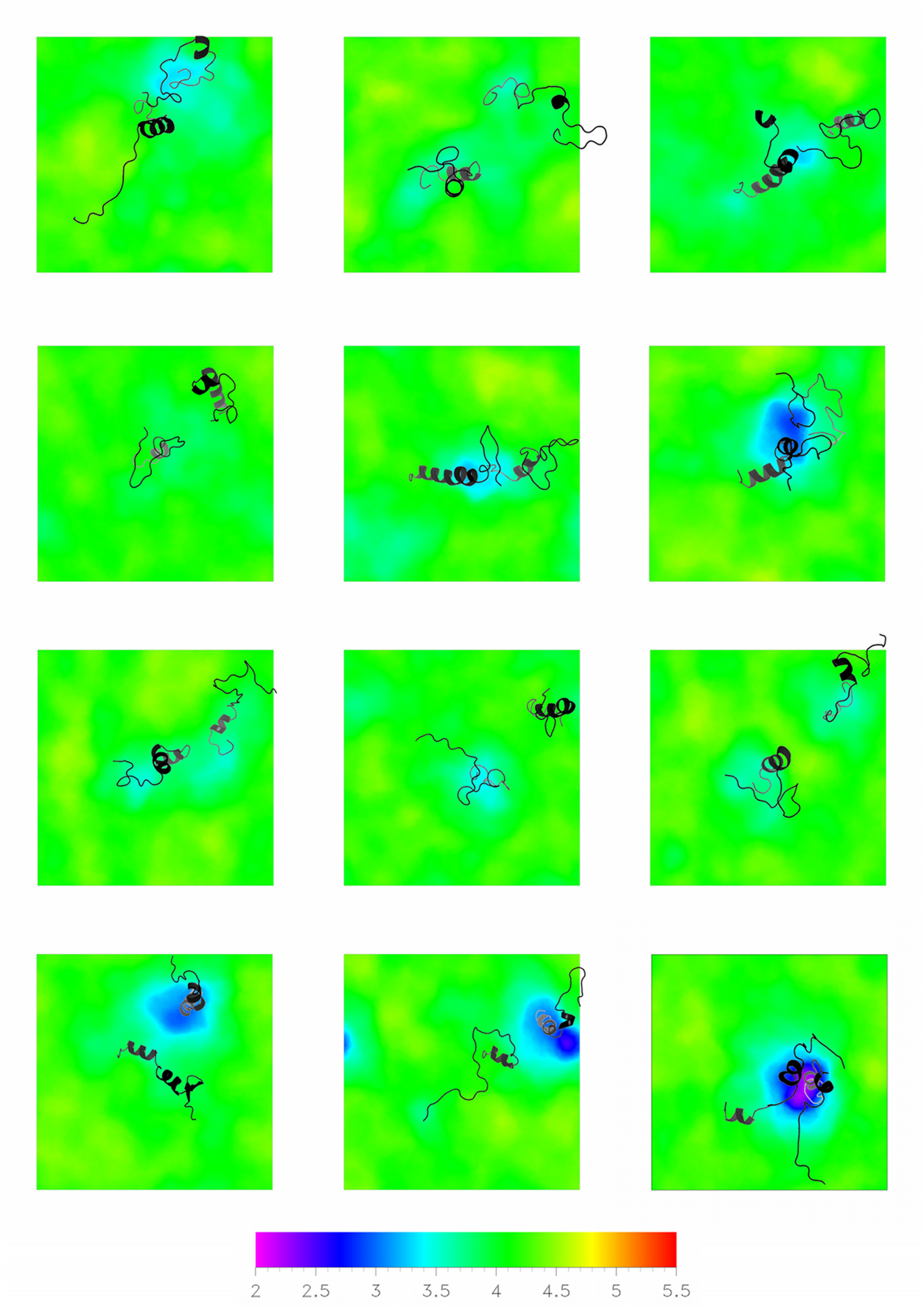

Figure S22. Membrane thickness plots for all systems in the POPC-CI sets. Images are organized and rendered as in Figure S21.

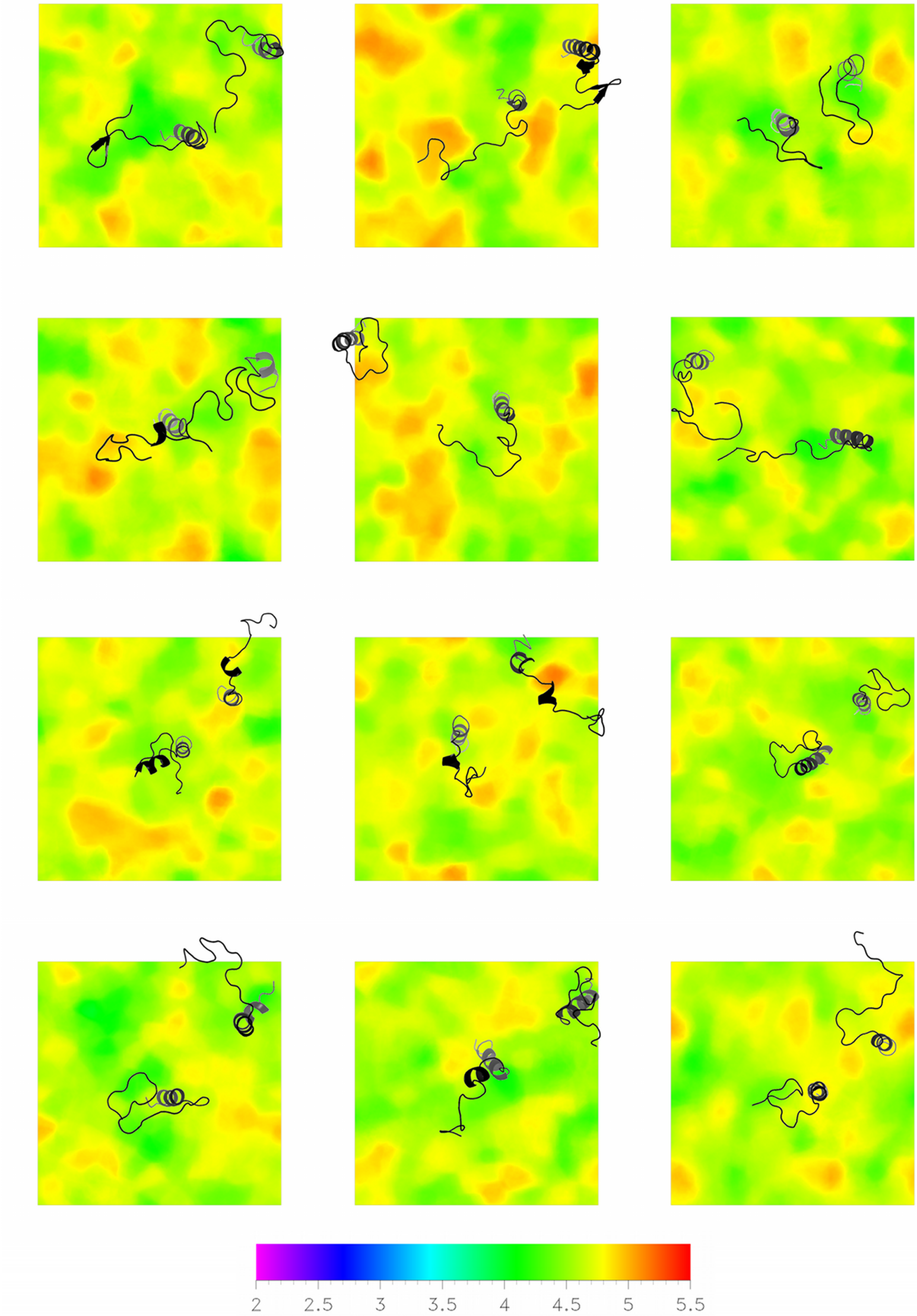

Figure S23. Membrane thickness plots for all systems in the POPS-CH sets. Images are organized and rendered as in Figure S21.

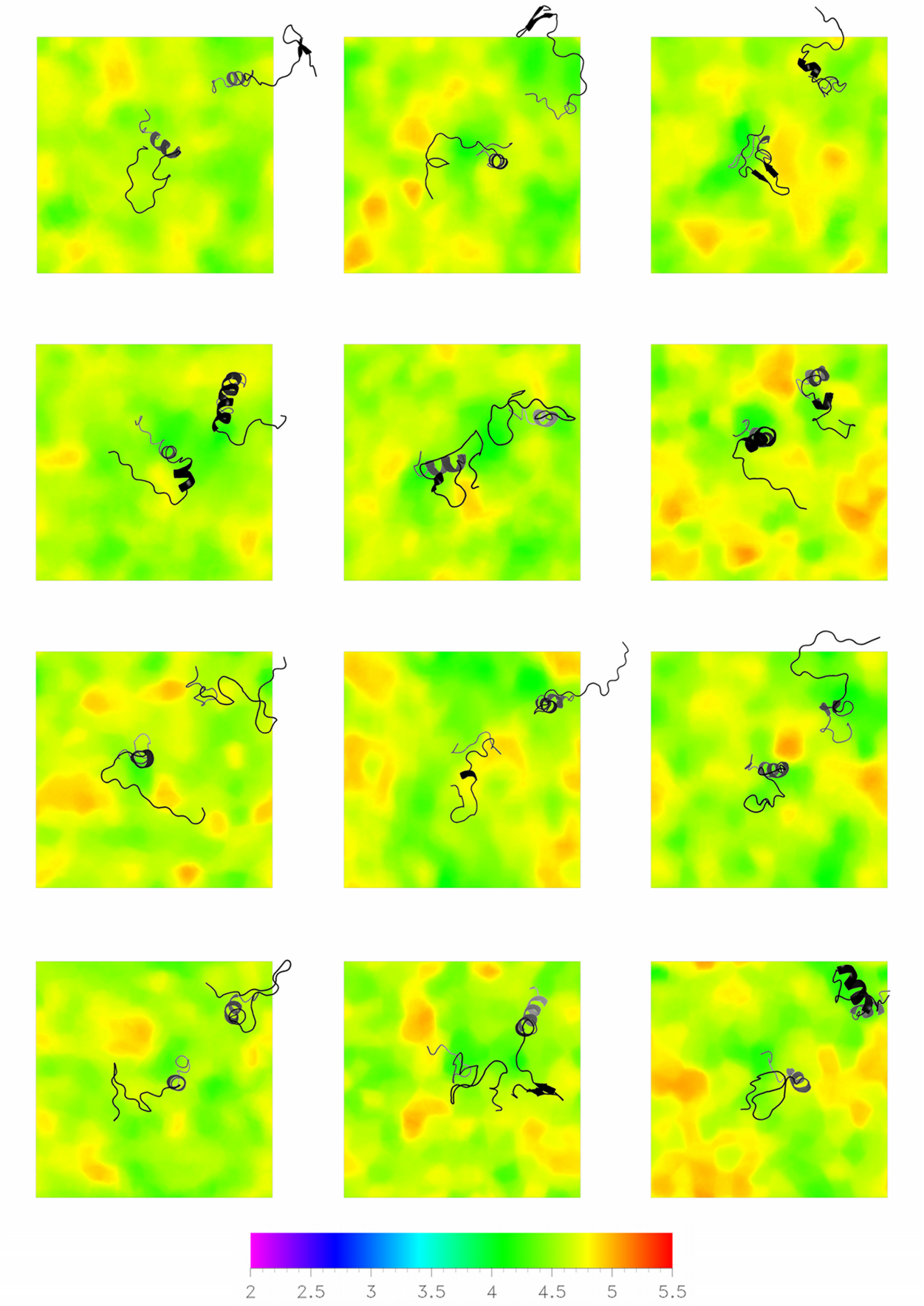

Figure S24. Membrane thickness plots for all systems in the POPS-CI sets. Images are organized and rendered as in Figure S21.

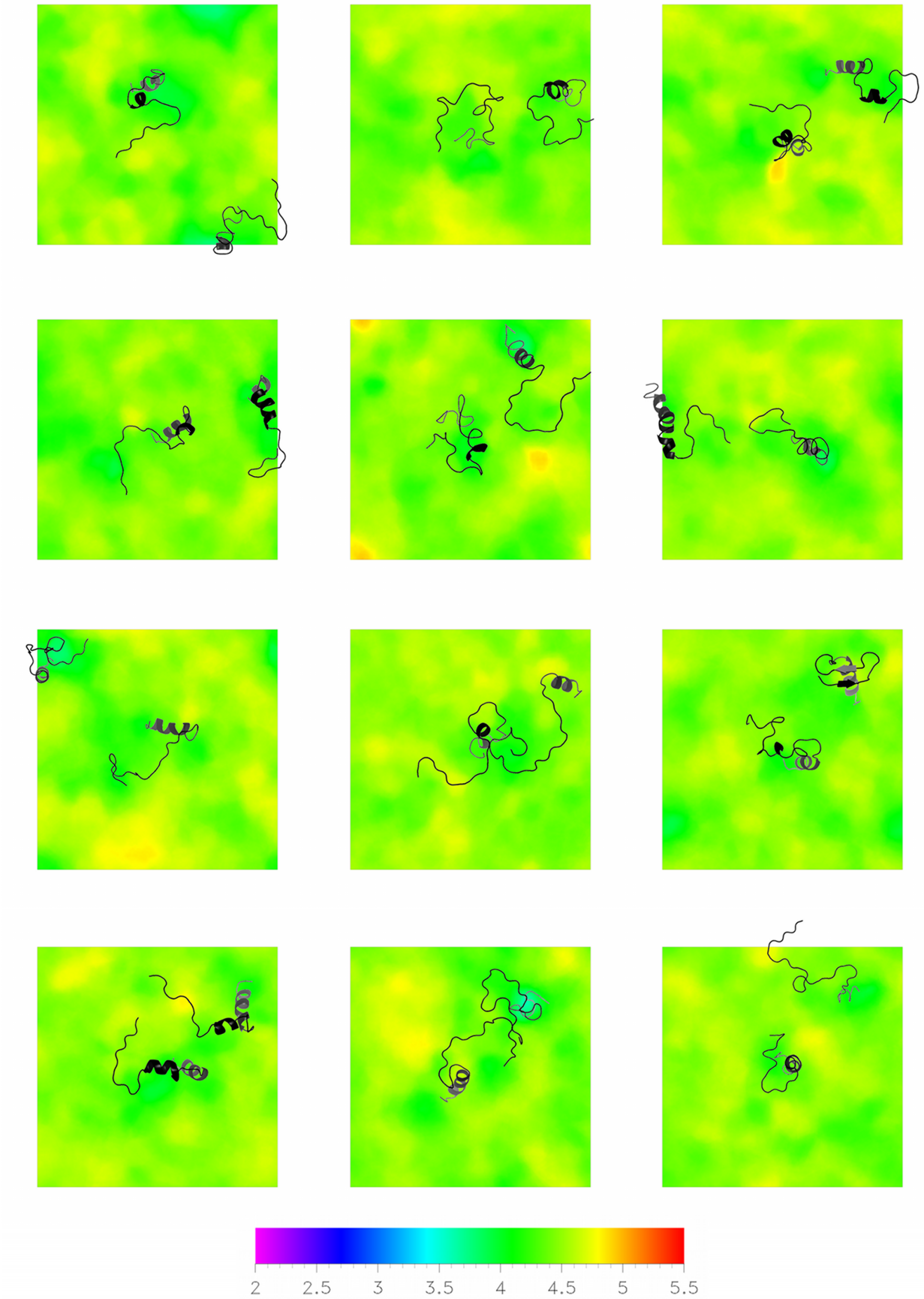

Figure S25. Membrane thickness plots for all systems in the POPC/POPE-CH sets. Images are organized and rendered as in Figure S21.

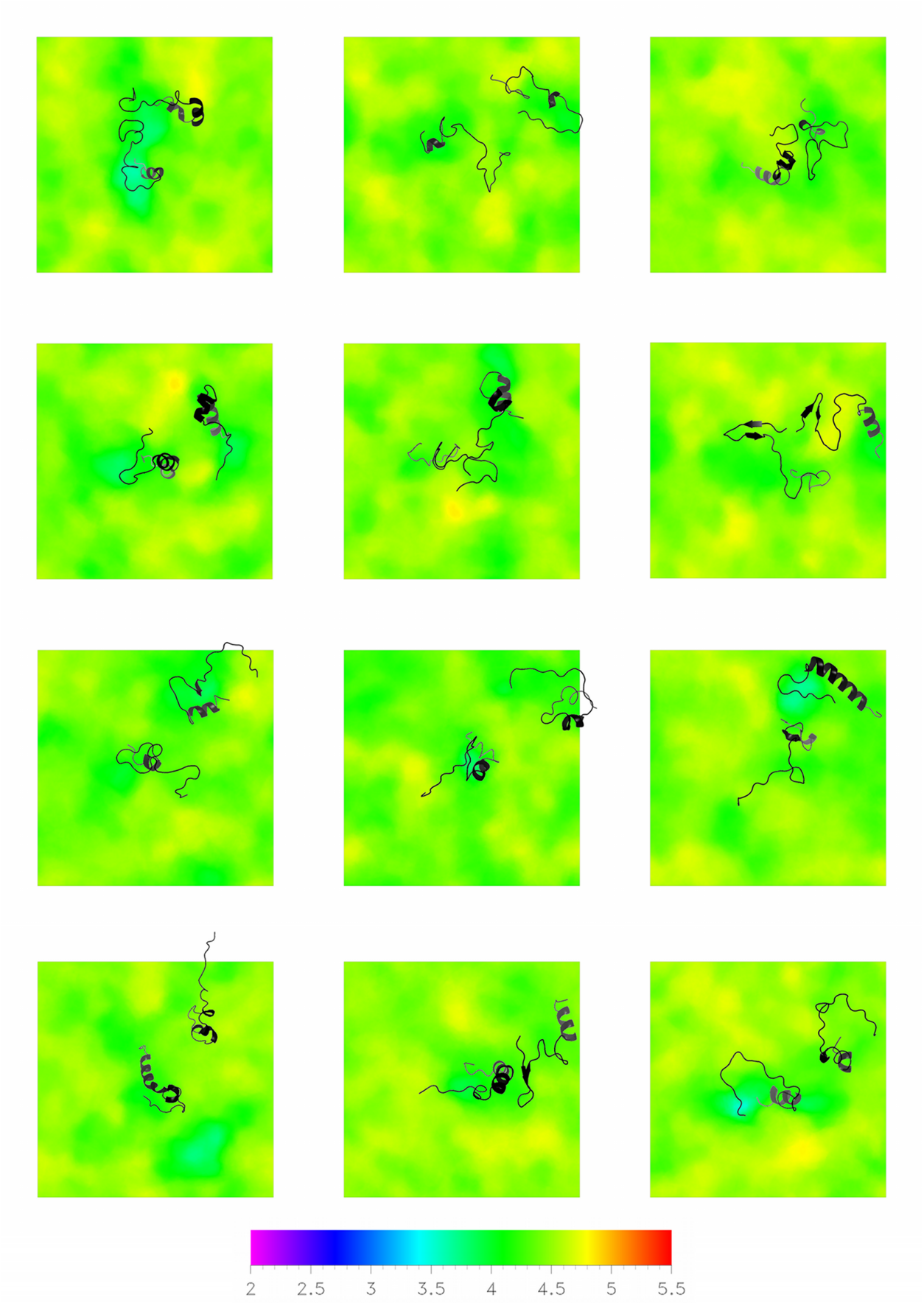

Figure S26. Membrane thickness plots for all systems in the POPC/POPE-CI sets. Images are organized and rendered as in Figure S21.

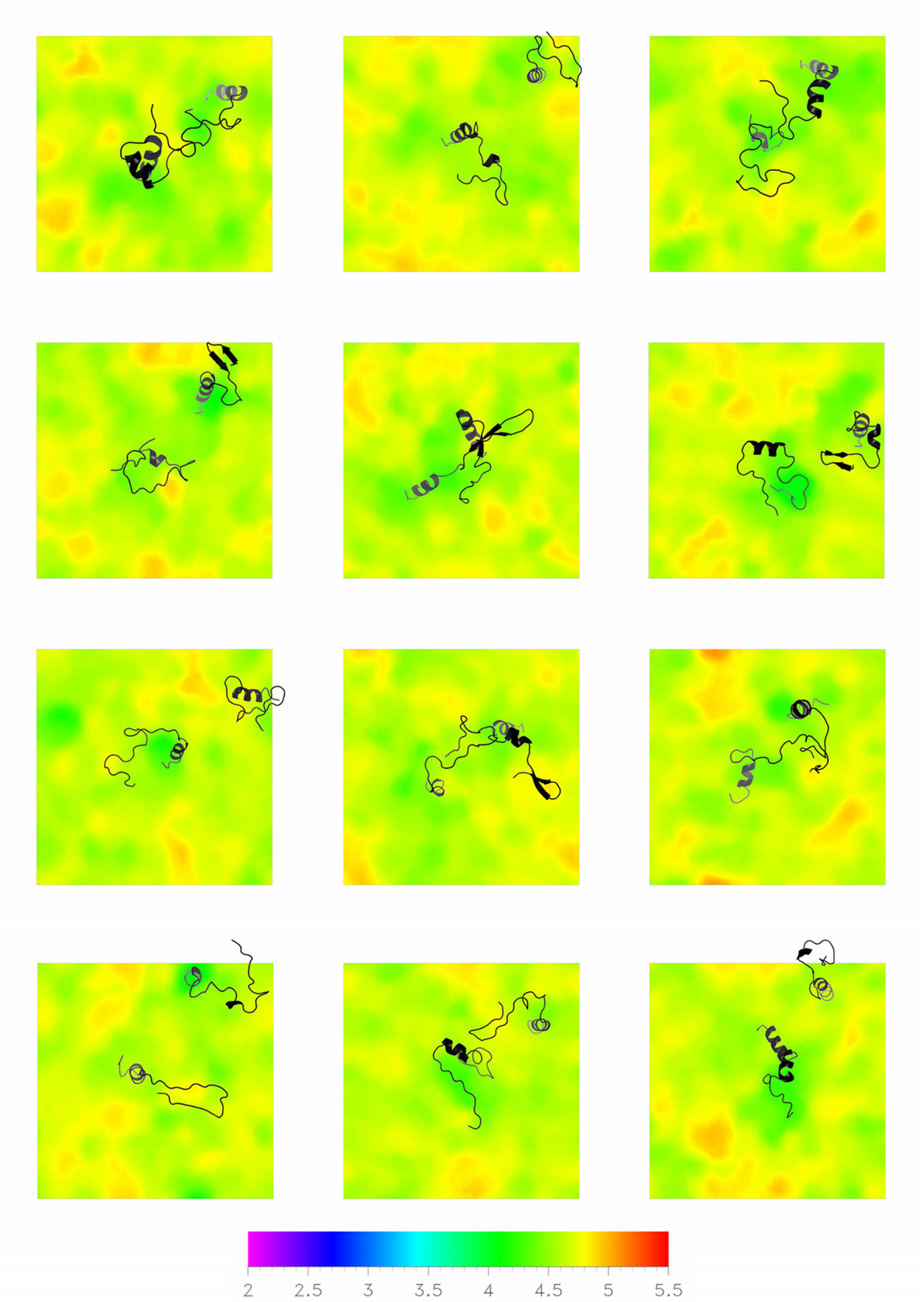

Figure S27. Membrane thickness plots for all systems in the Raft-CH sets. Images are organized and rendered as in Figure S21.

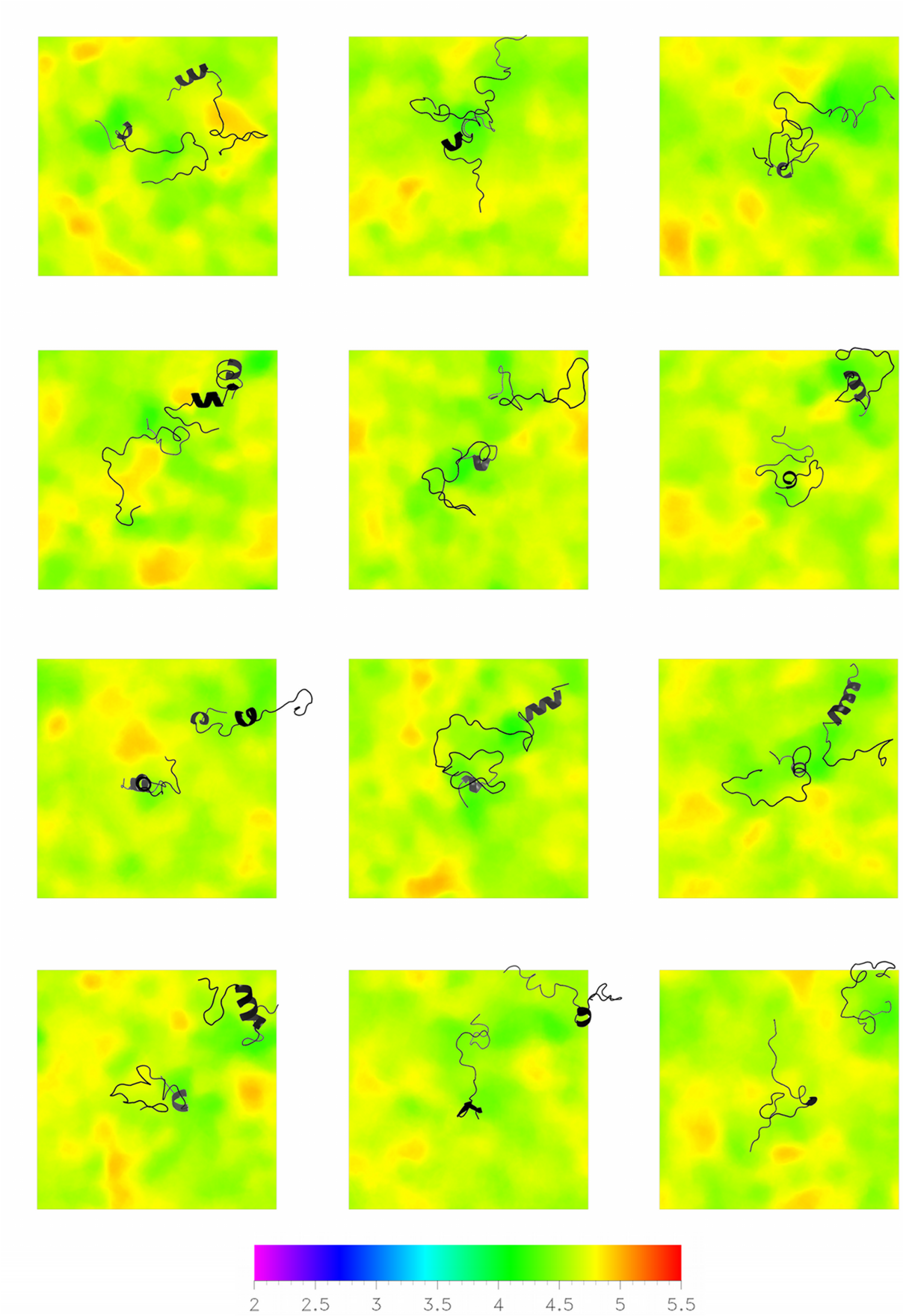

Figure S28. Membrane thickness plots for all systems in the Raft-CI sets. Images are organized and rendered as in Figure S21.

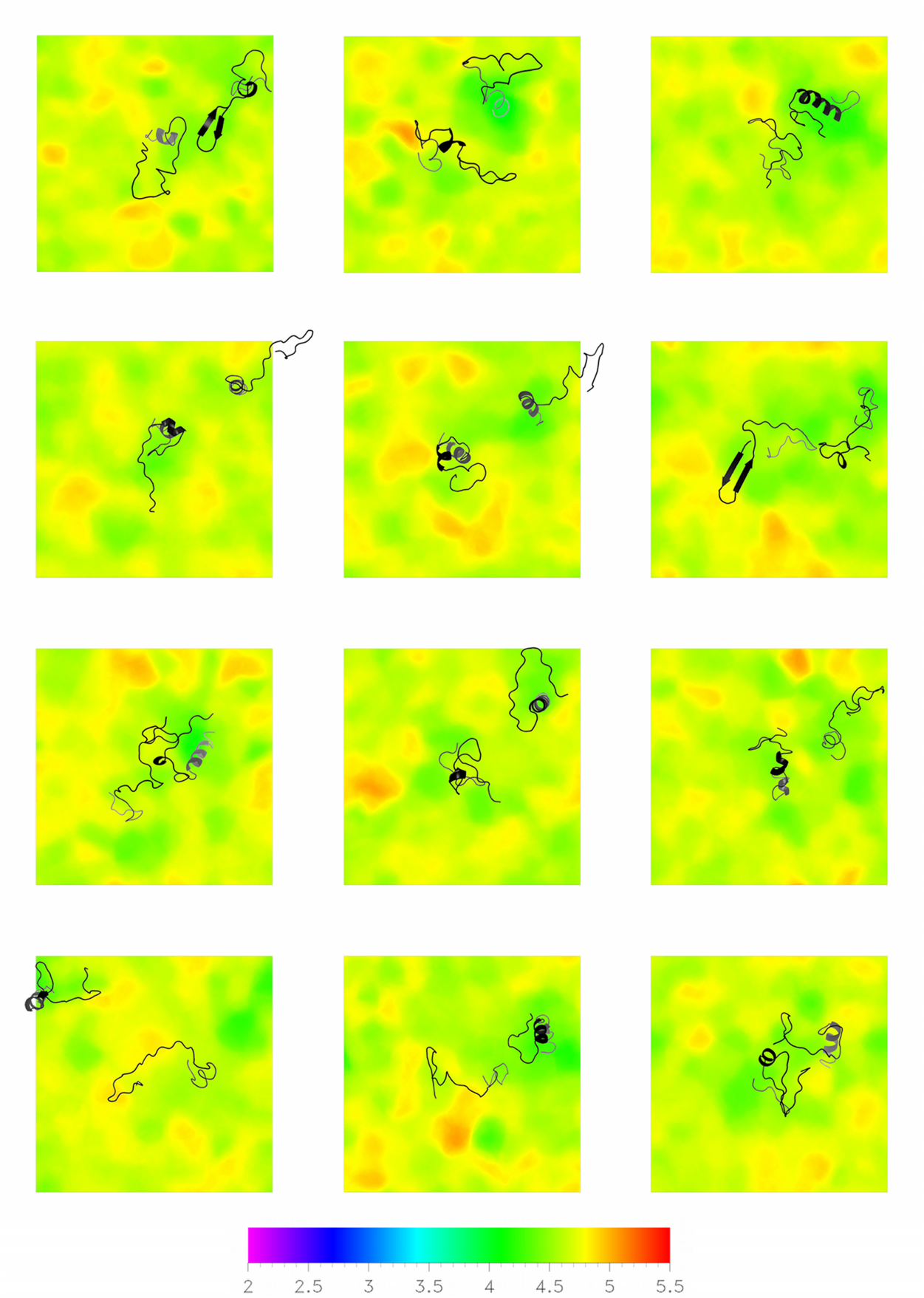

Figure S29. Membrane thickness plots for all systems in the GM1-Raft-CH sets. Images are organized and rendered as in Figure S21.

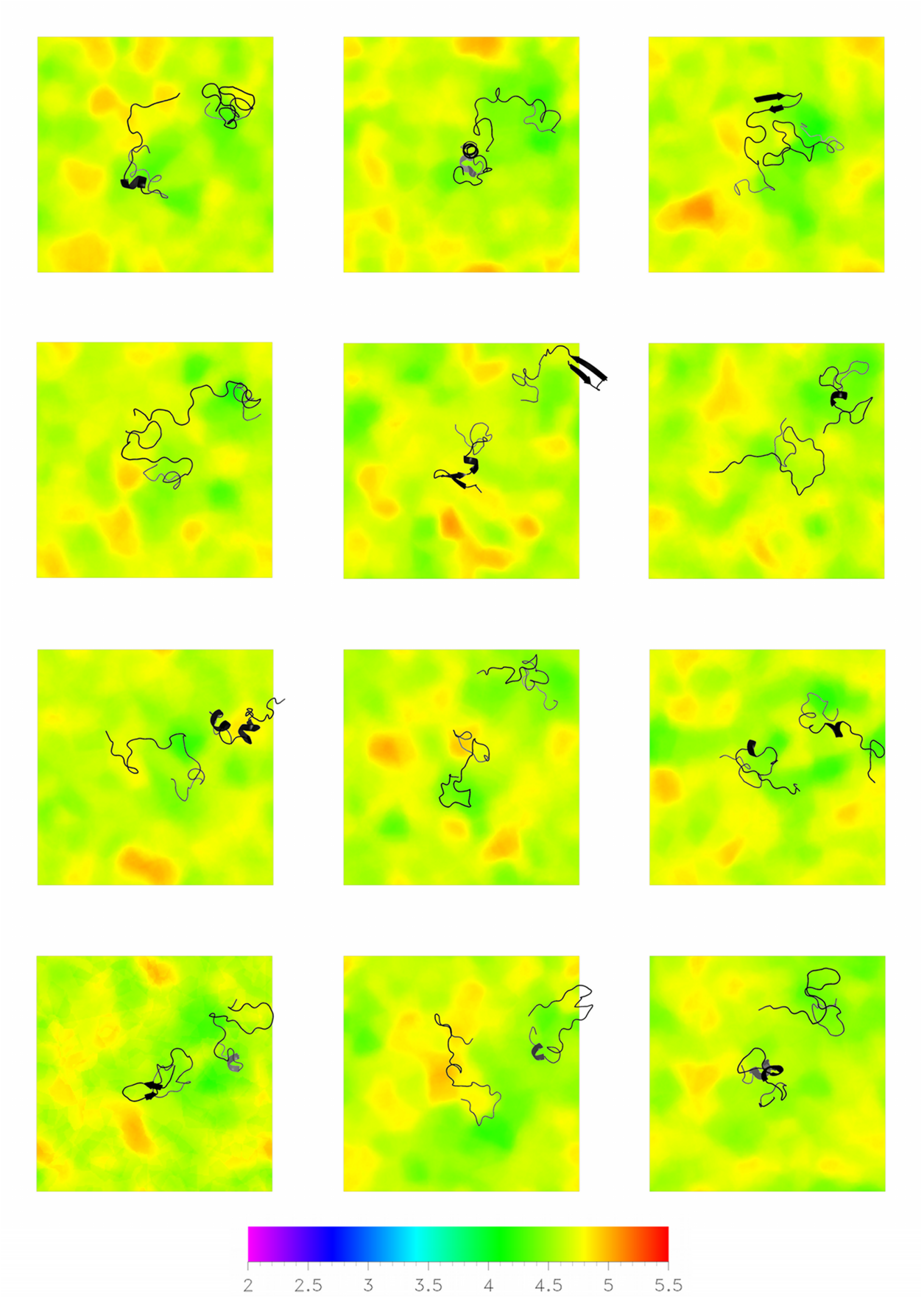

Figure S30. Membrane thickness plots for all systems in the GM1-Raft-CI sets. Images are organized and rendered as in Figure S21.