

Supporting Information

Claws, Disorder, and Conformational Dynamics of the C-terminal Region of Human Desmoplakin

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Overview

This document provides the detailed results of the analysis suite described in the Methods section of the main text, as applied to each of our simulation systems. Each trajectory has been analyzed in terms of (a) Cy_*^{R} , (b) Cy^{R} , (c) SASA of S2849, (d) SASA of R2834, (e) the S2849.....R2834 distance, (f) GSK3 steric clash scores, (g) inter-residue contact maps, and (h) the distribution of peptide backbone torsion angles (ϕ, ψ).

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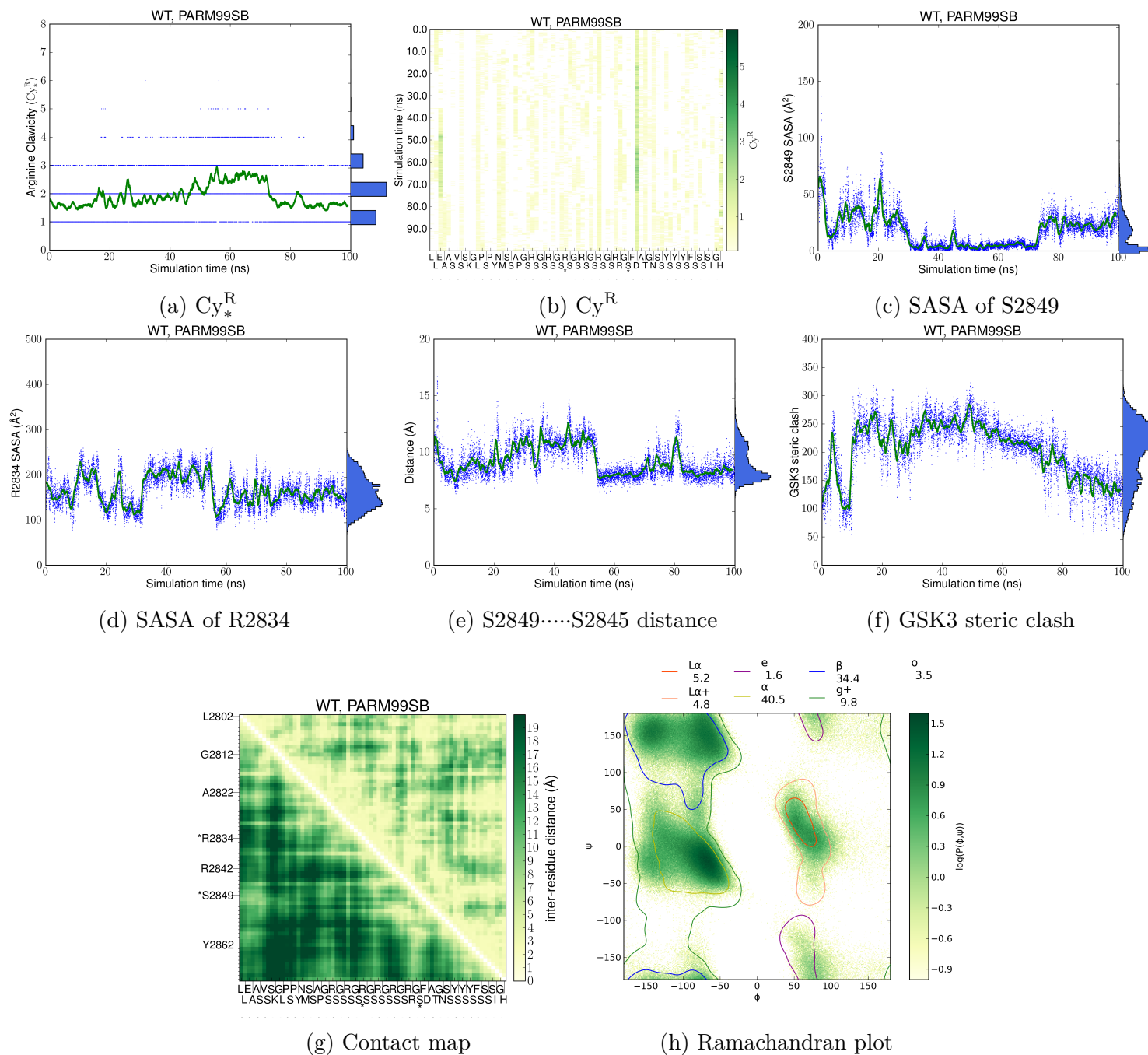


Figure S1: Behavior of **WT_PARM99SB**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

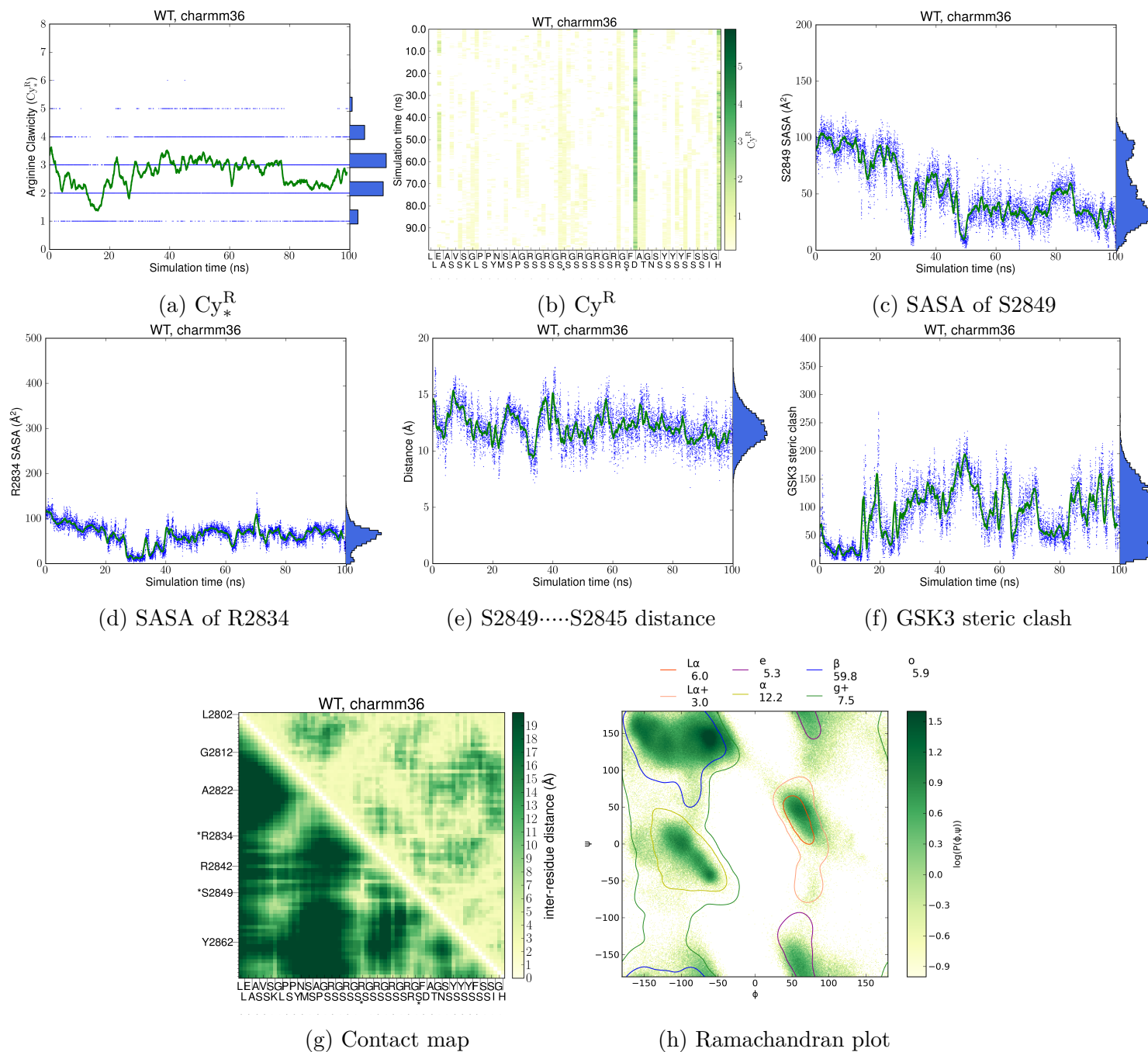


Figure S2: Behavior of **WT_CHARM36**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

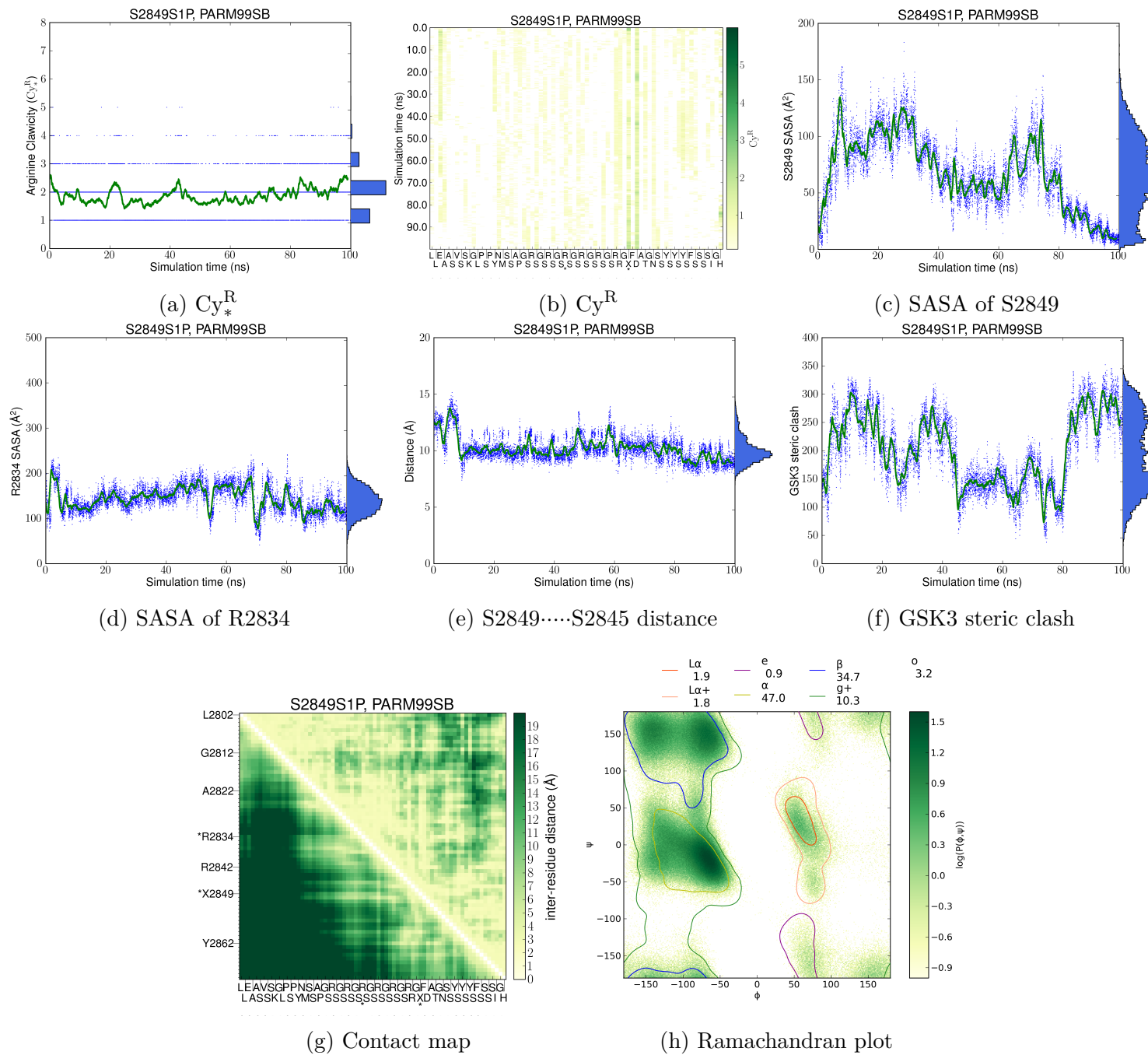


Figure S3: Behavior of **S2849S1P_PARM99SB**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

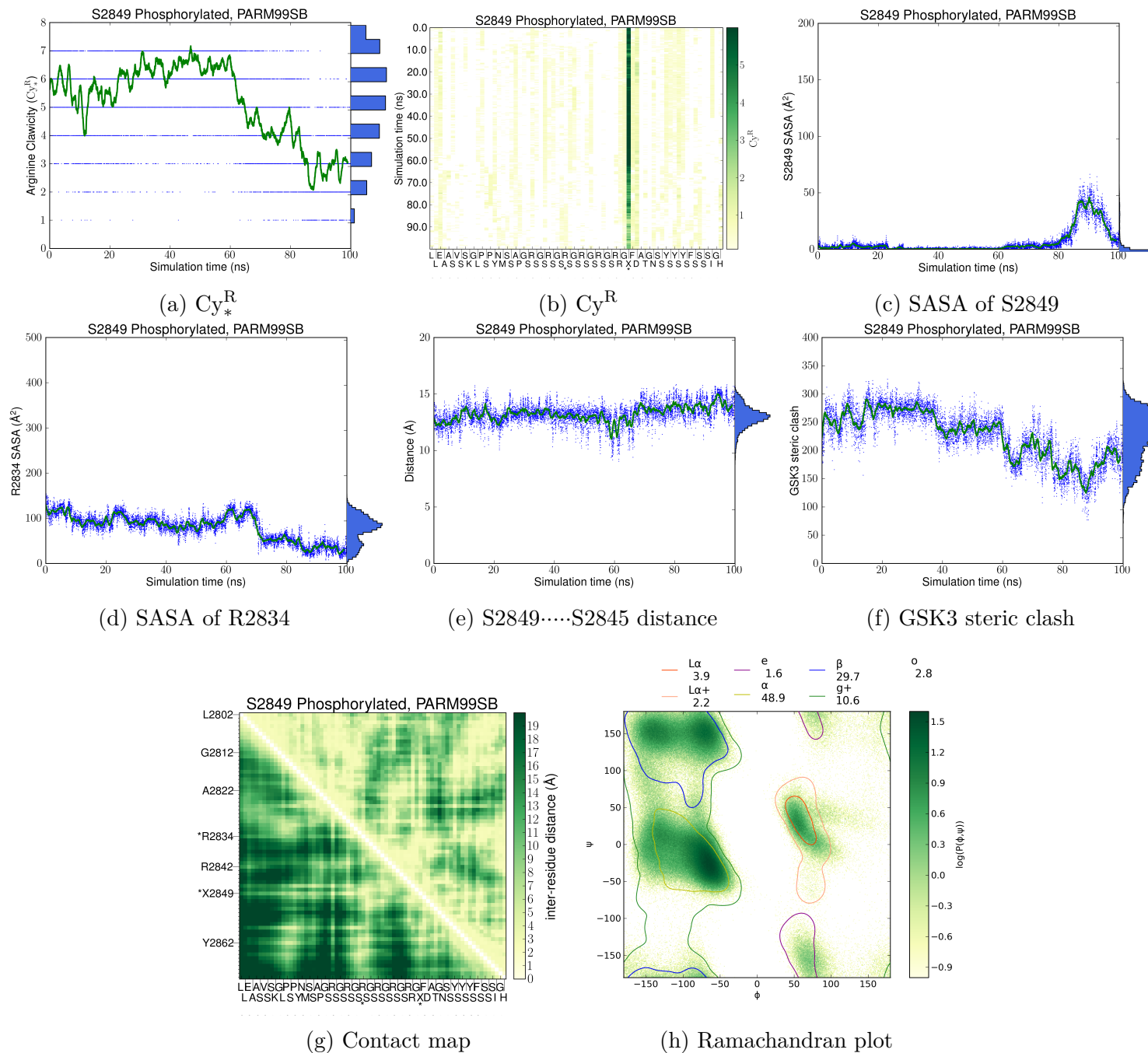


Figure S4: Behavior of **S2849S2P_PARM99SB**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

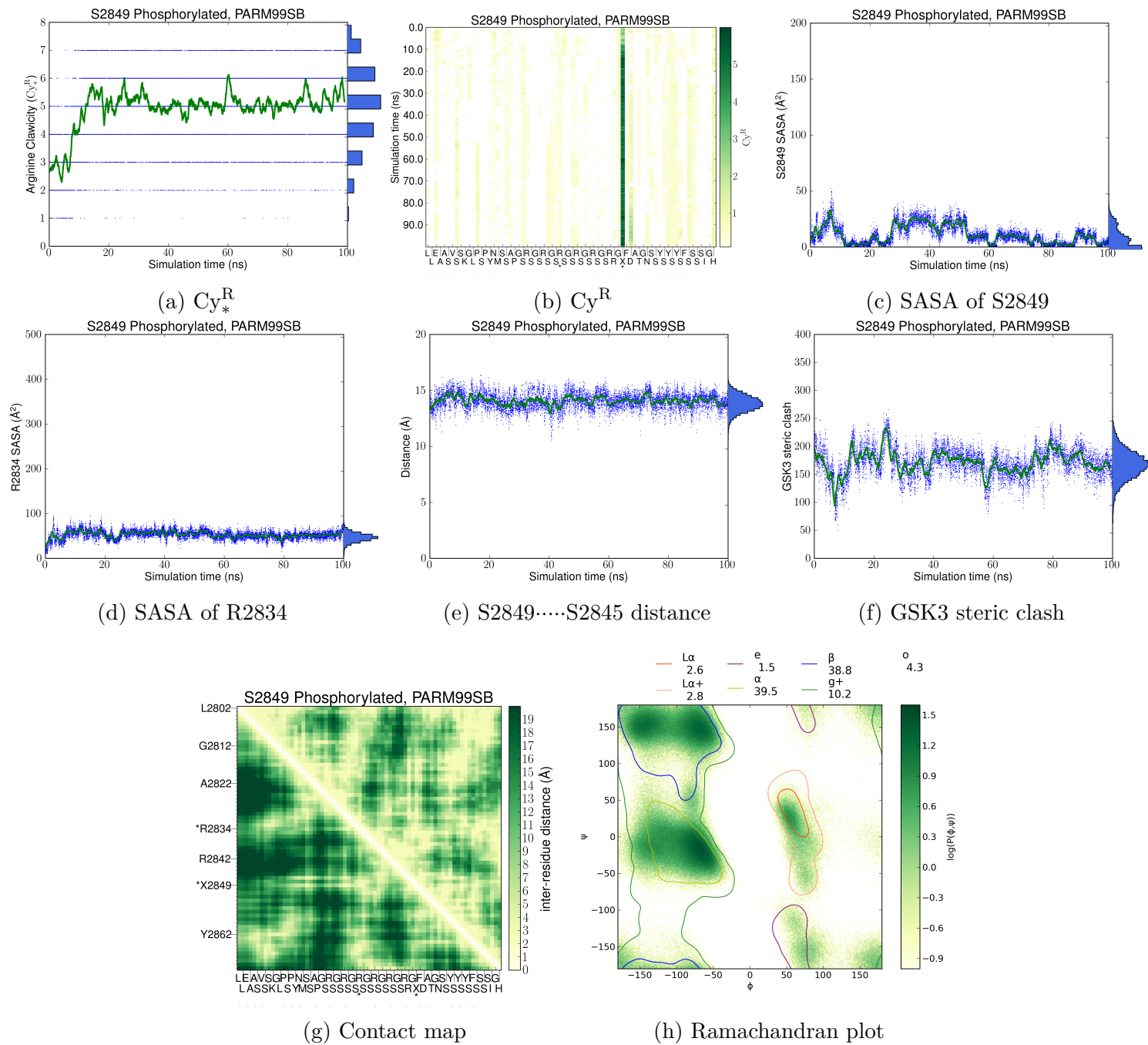


Figure S5: Behavior of **S2849S2P_PARM99SB_cycle2**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

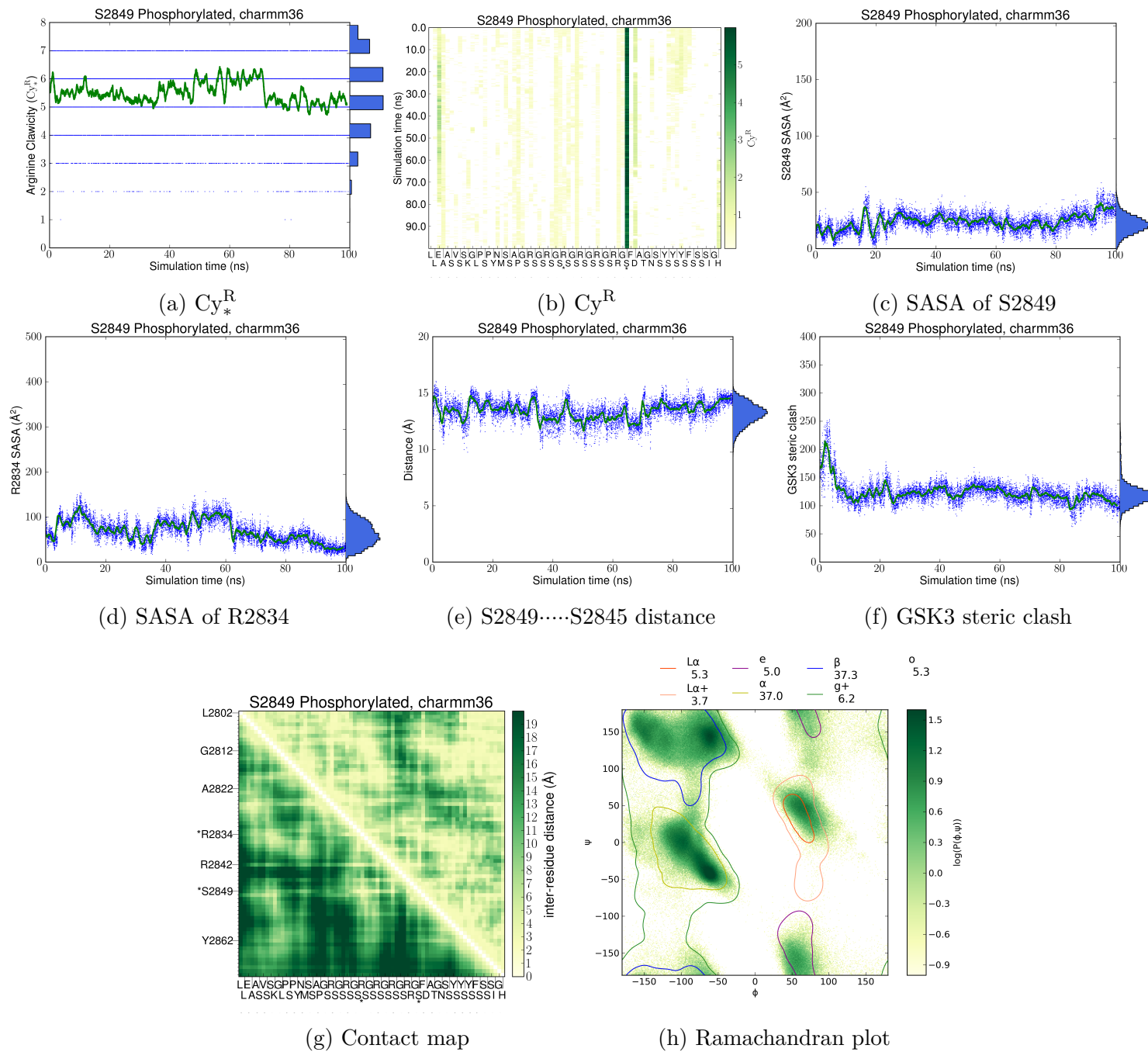


Figure S6: Behavior of **S2849S2P_CHARM36**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

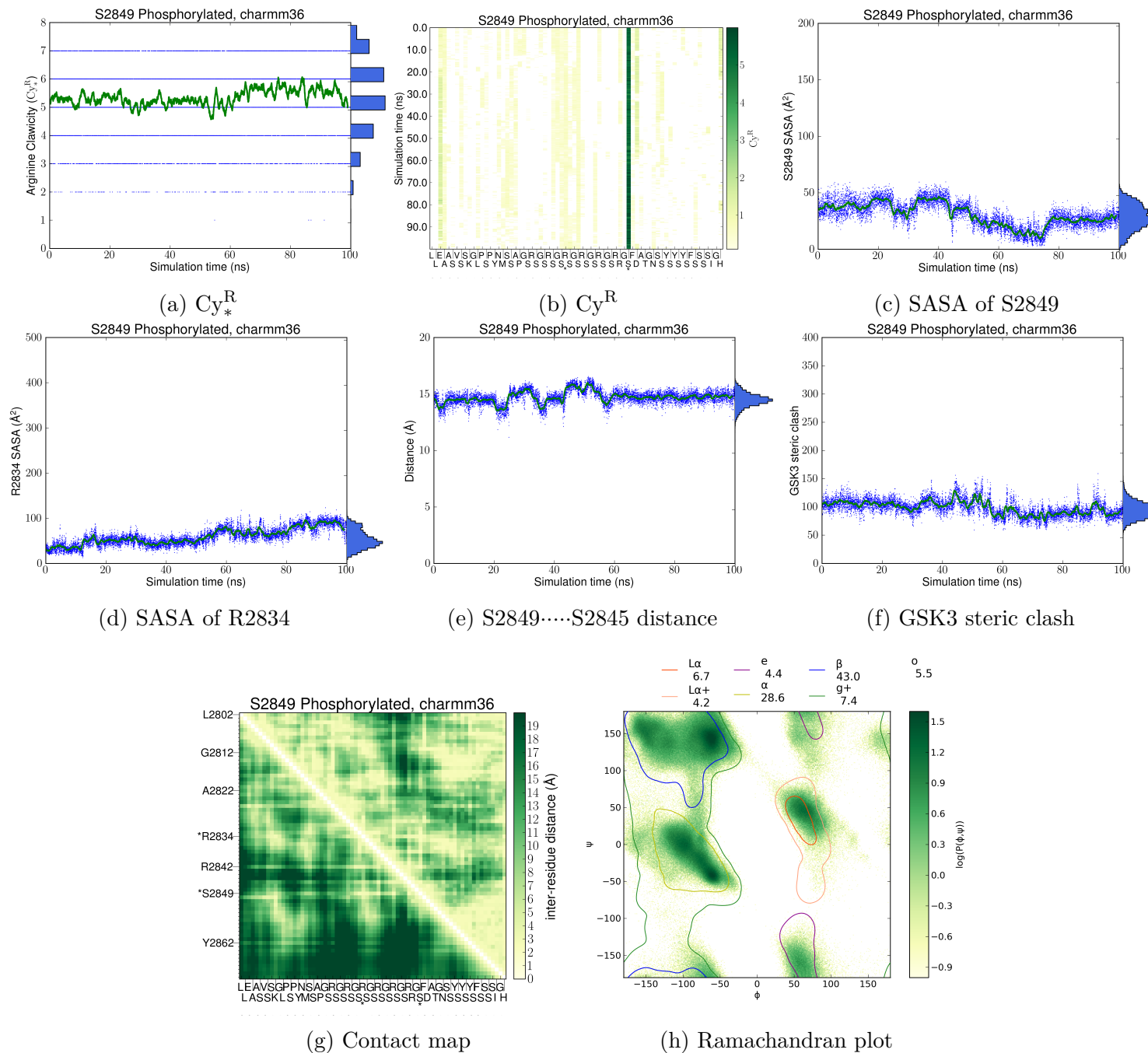


Figure S7: Behavior of **S2849S2P_CHARM36_cycle2**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

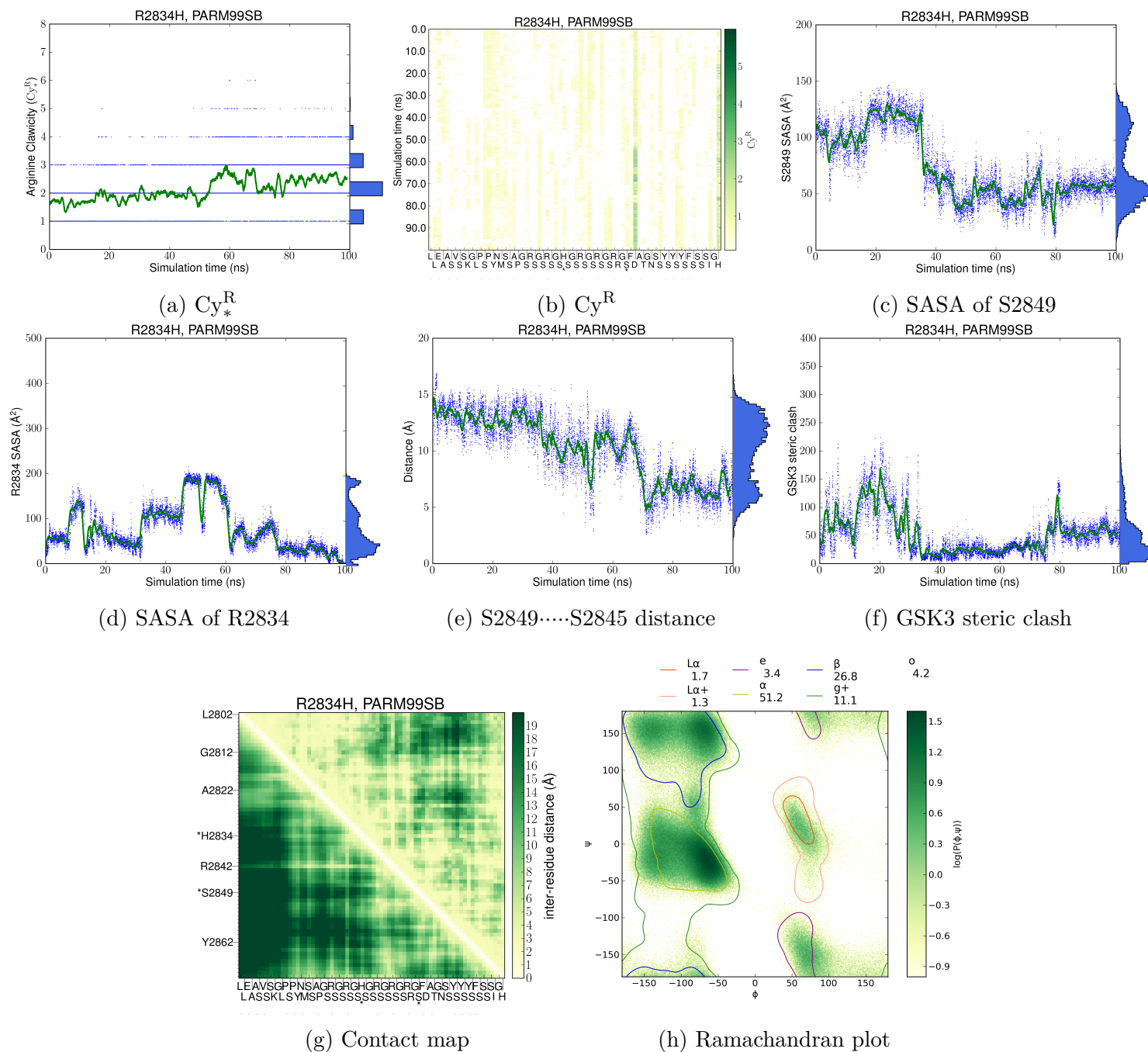


Figure S8: Behavior of **R2834H_PARM99SB**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

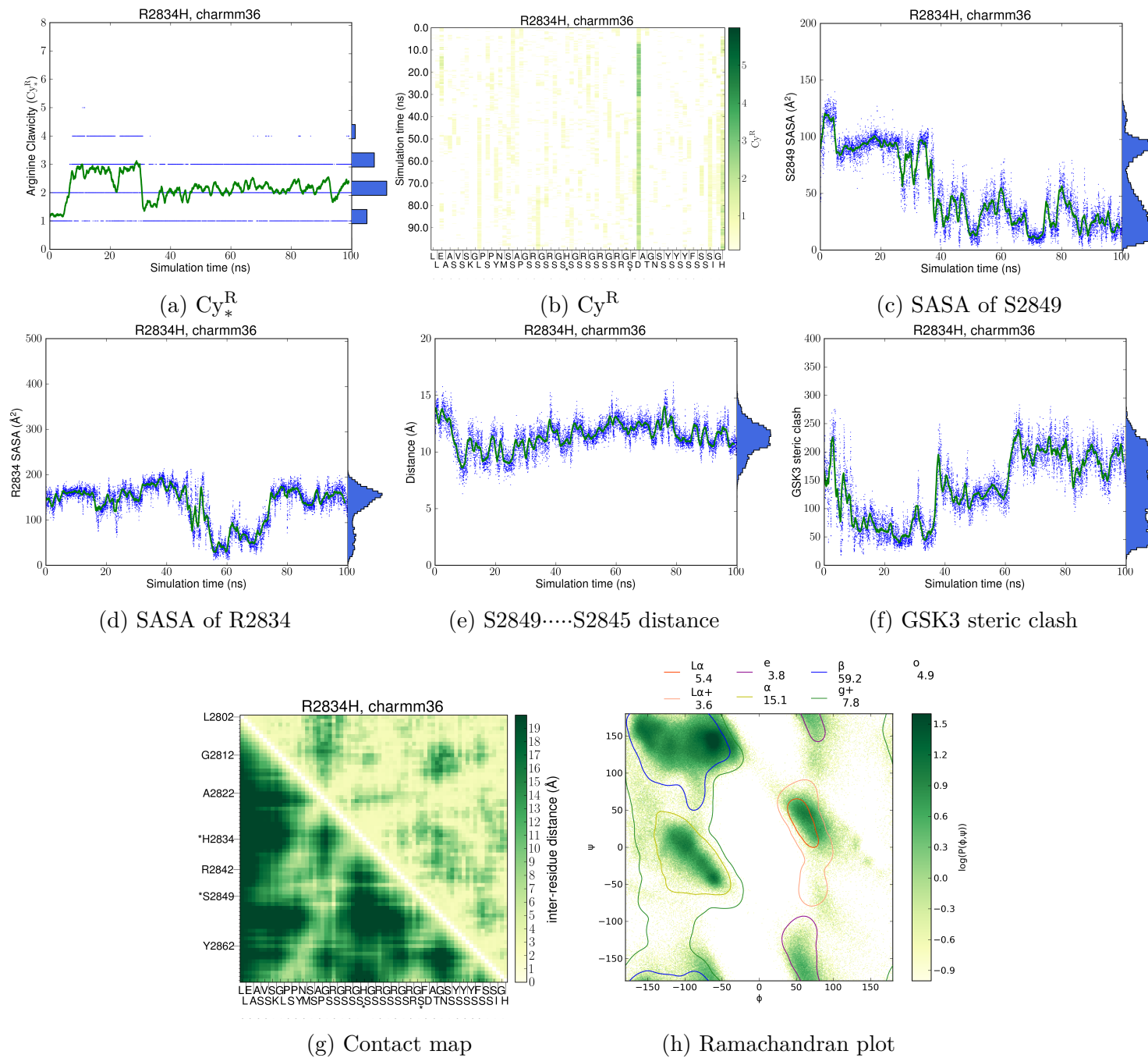


Figure S9: Behavior of **R2834H_CHARMM36**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

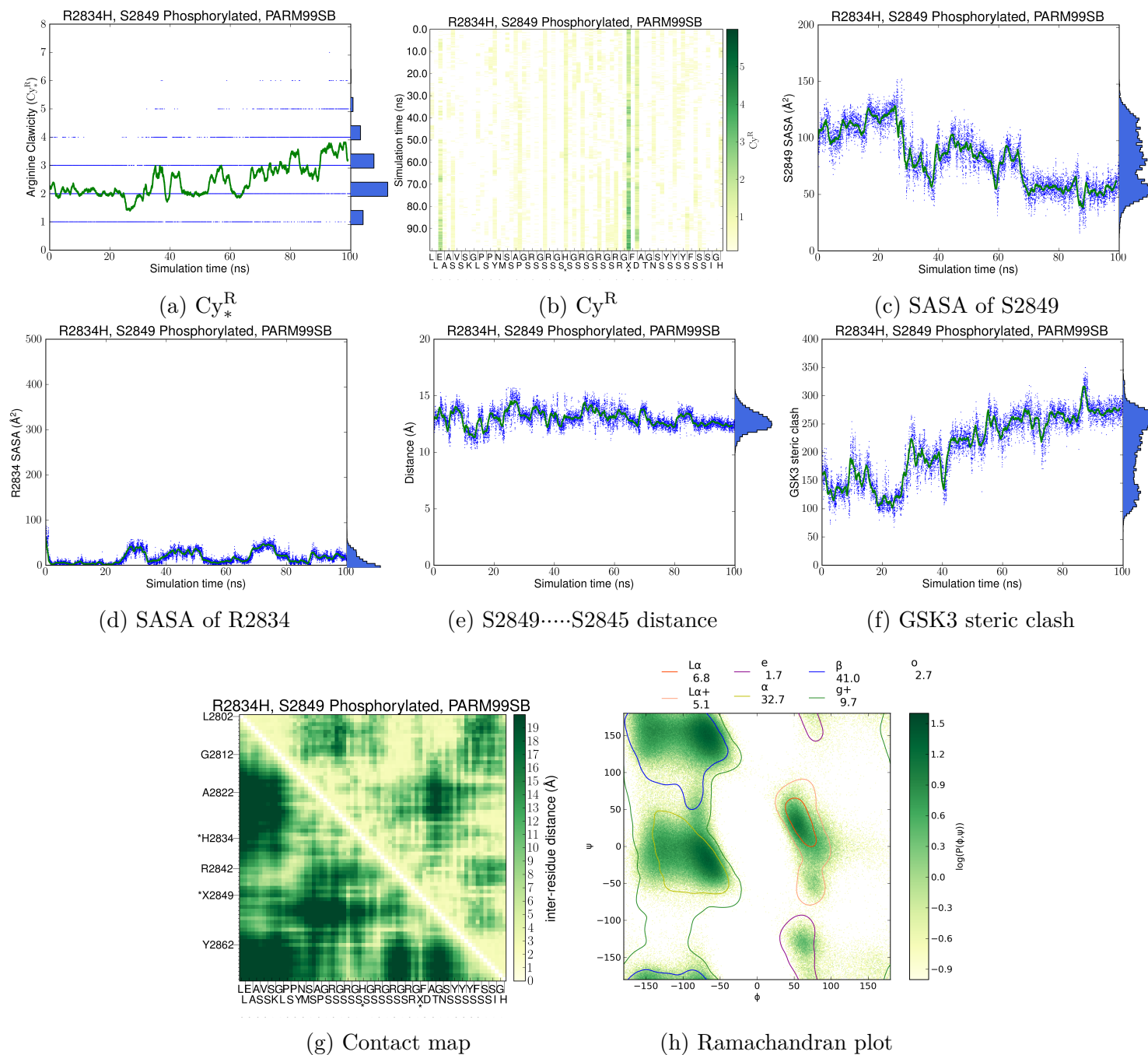


Figure S10: Behavior of **R2834H_S2849S2P_PARM99SB**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

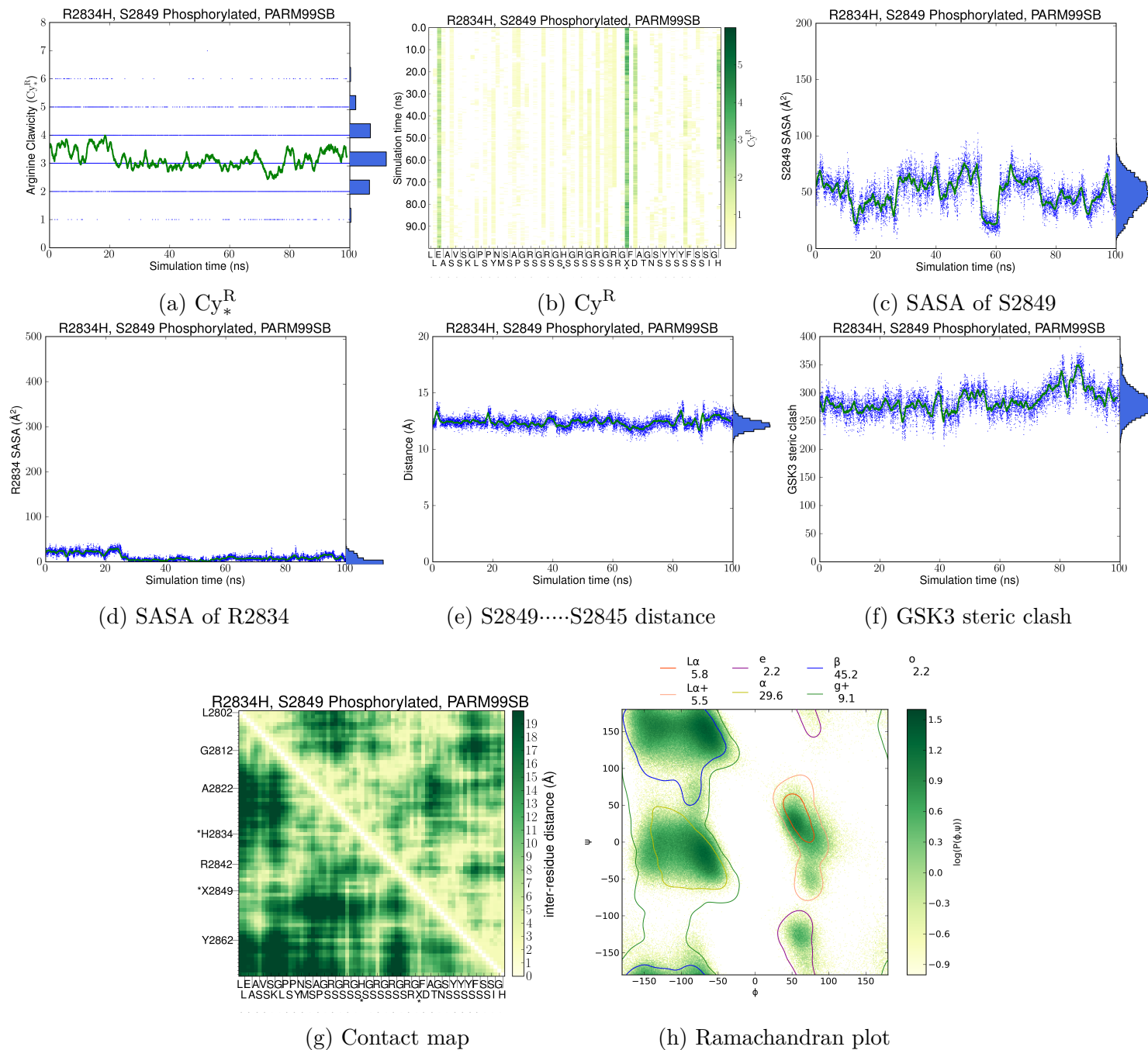


Figure S11: Behavior of **R2834H_S2849S2P_PARM99SB_cycle2**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

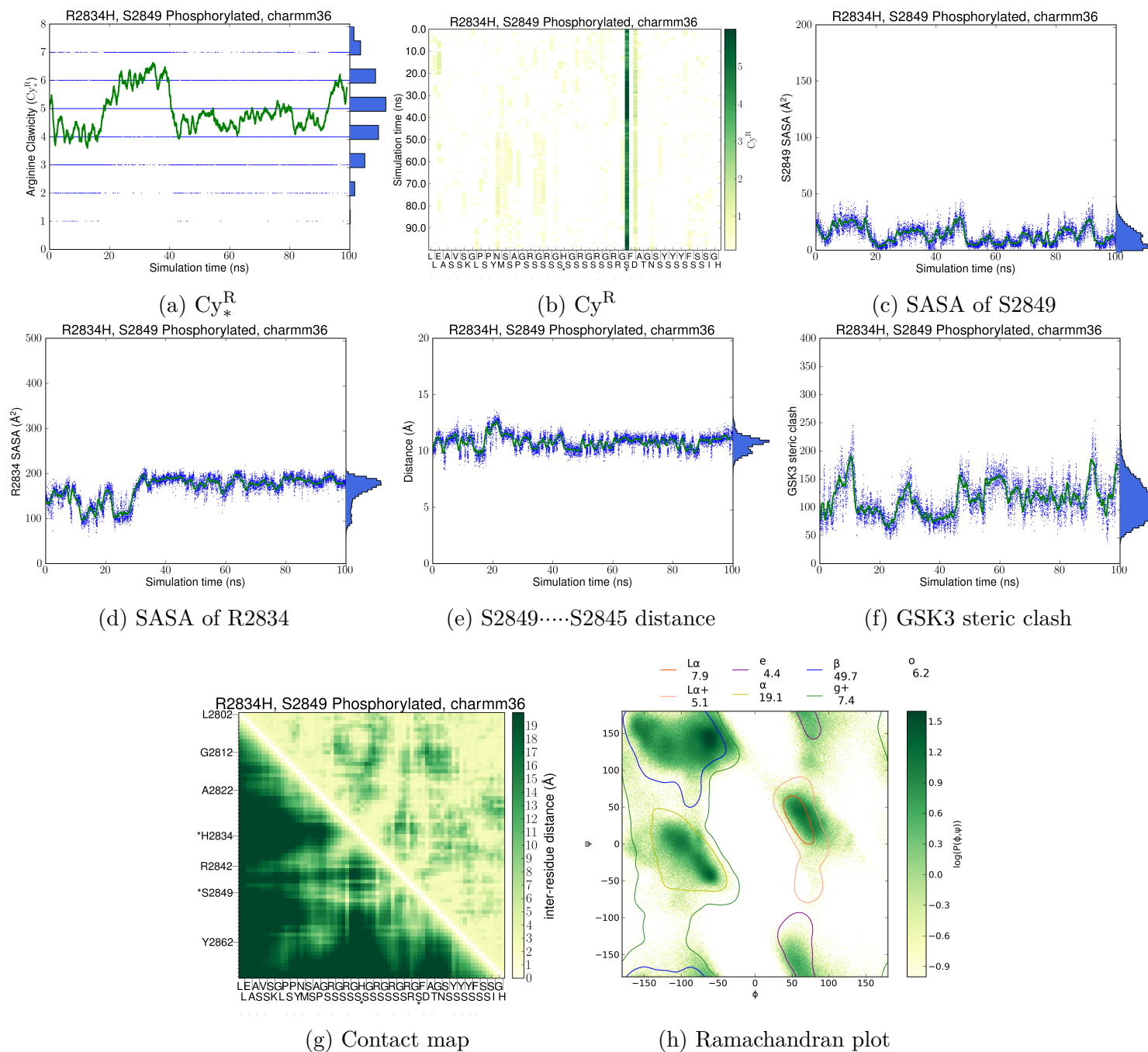


Figure S12: Behavior of **R2834H_S2849S2P_CHARM36**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

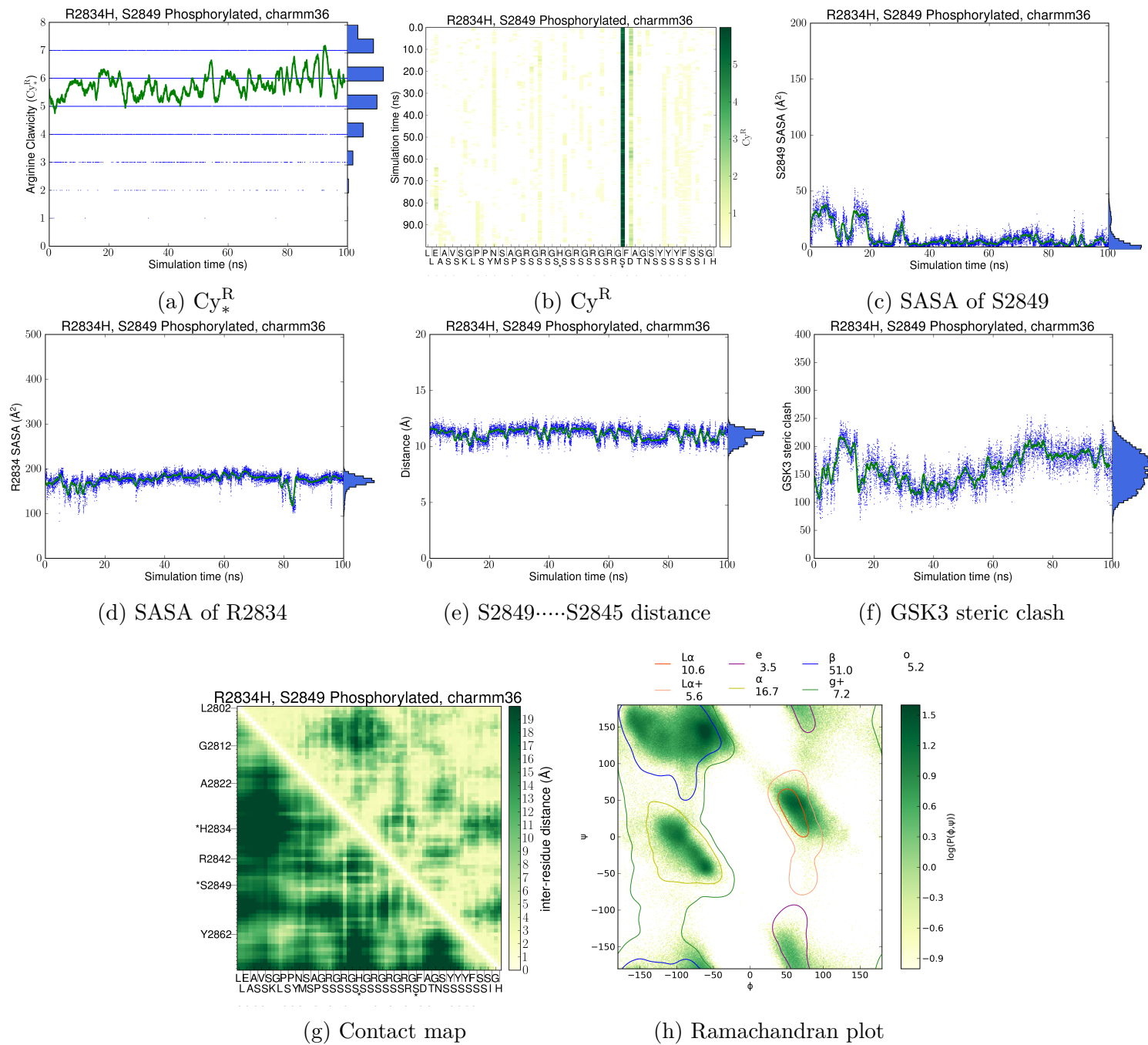


Figure S13: Behavior of **R2834H_S2849S2P_CHARMM36_cycle2**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

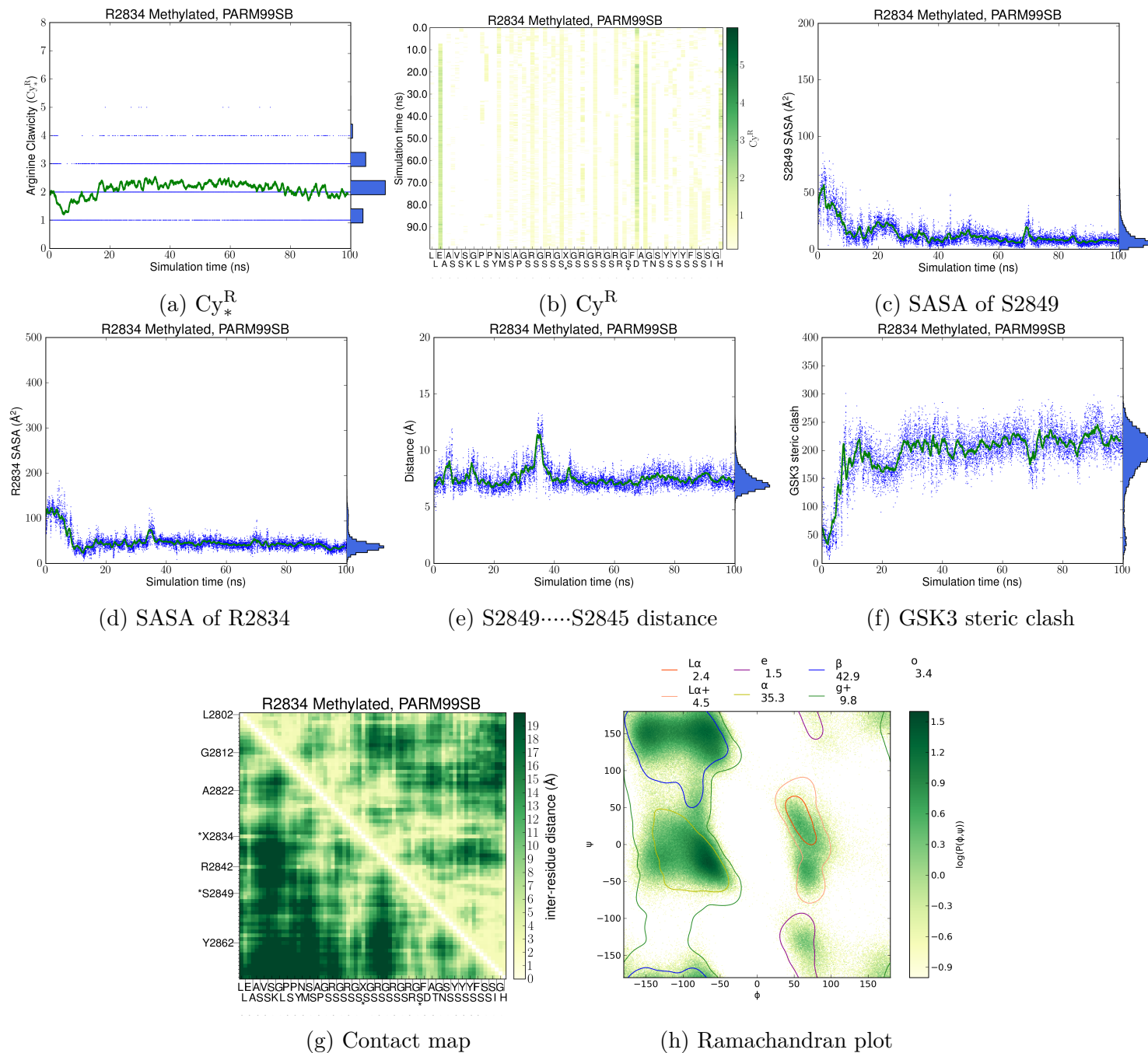


Figure S14: Behavior of **R2834MeMe_PARM99SB**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

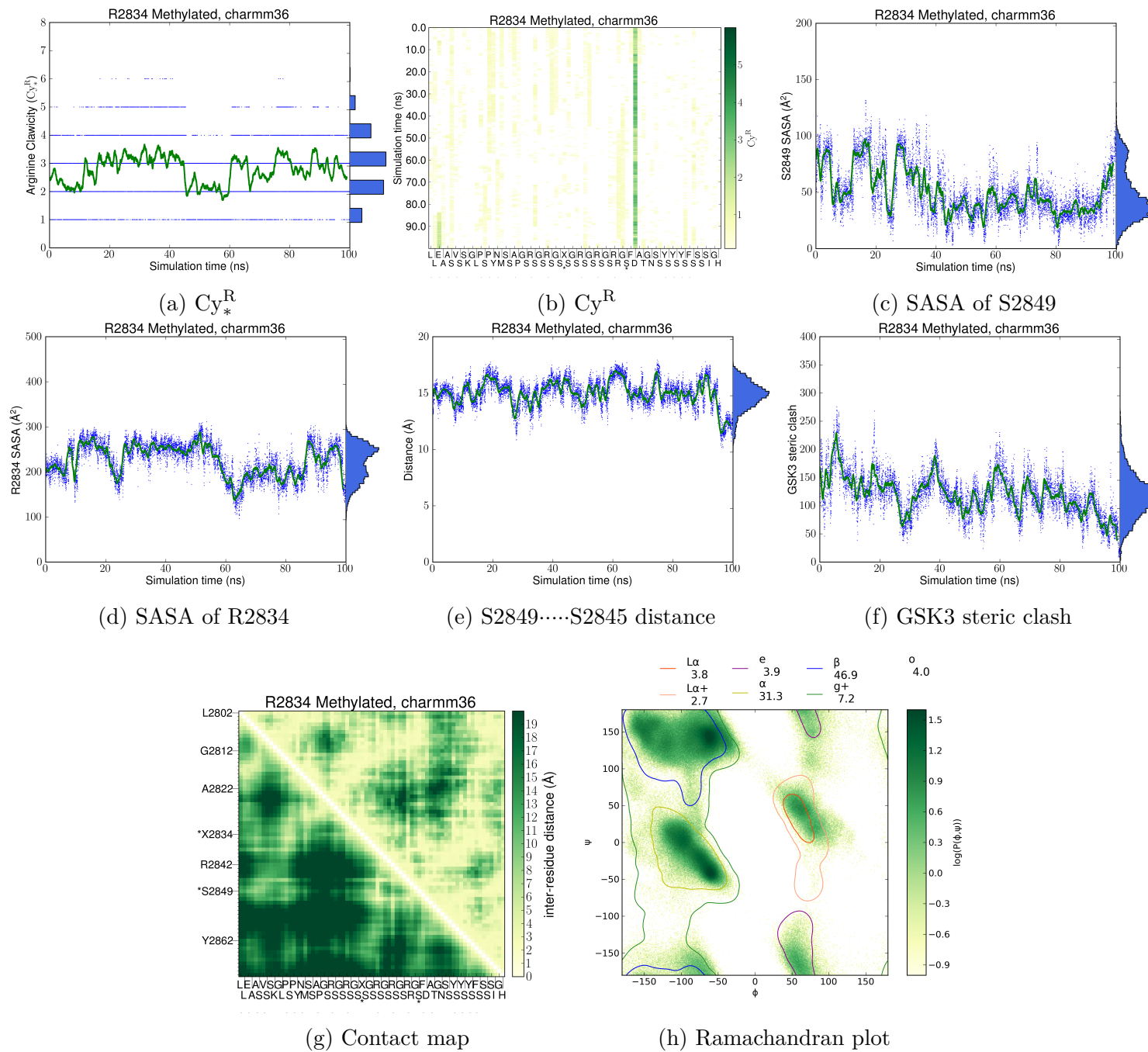


Figure S15: Behavior of **R2834MeMe_CHARMM36**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

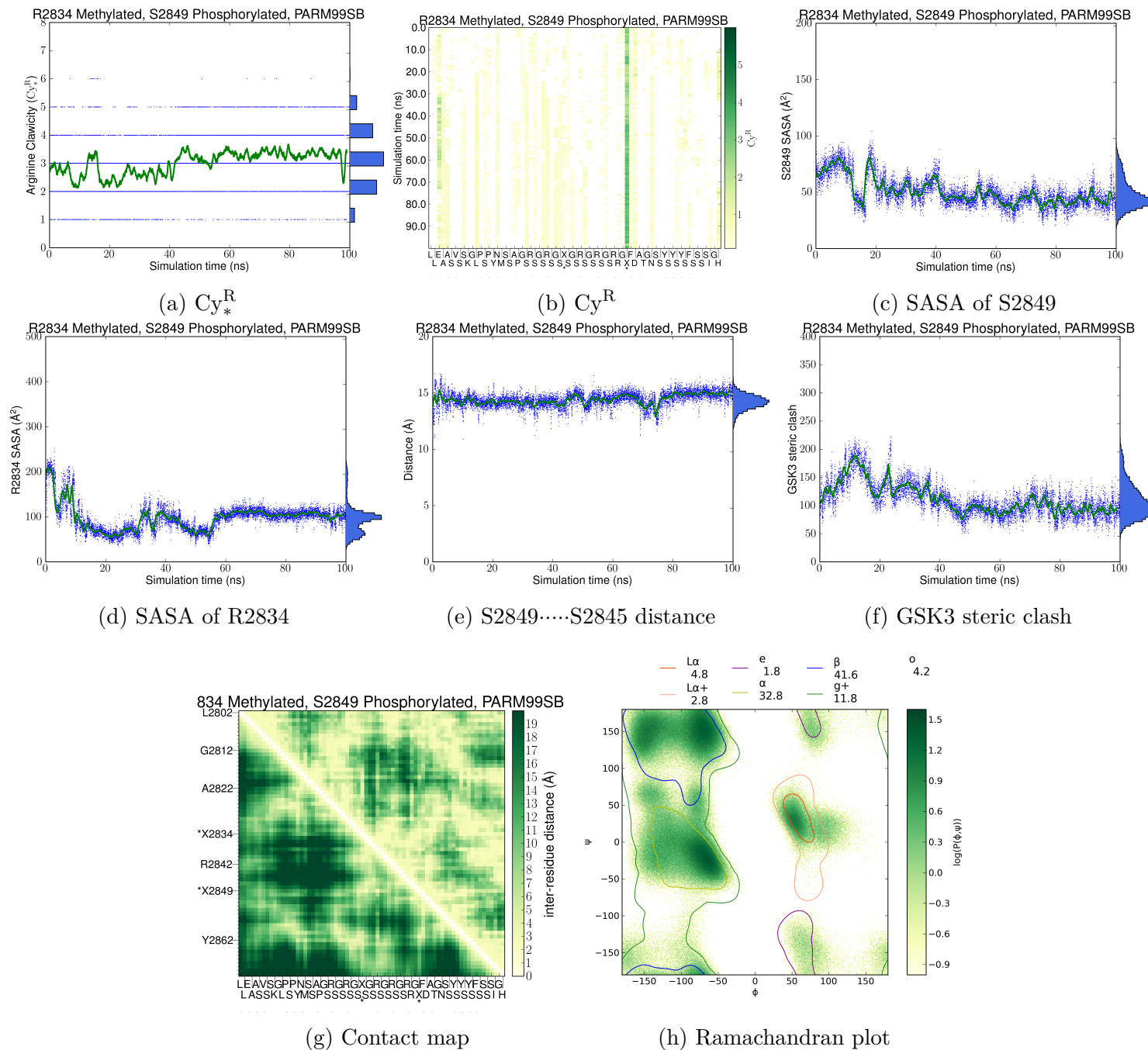


Figure S16: Behavior of **R2834MeMe_S2849S2P_PARM99SB**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

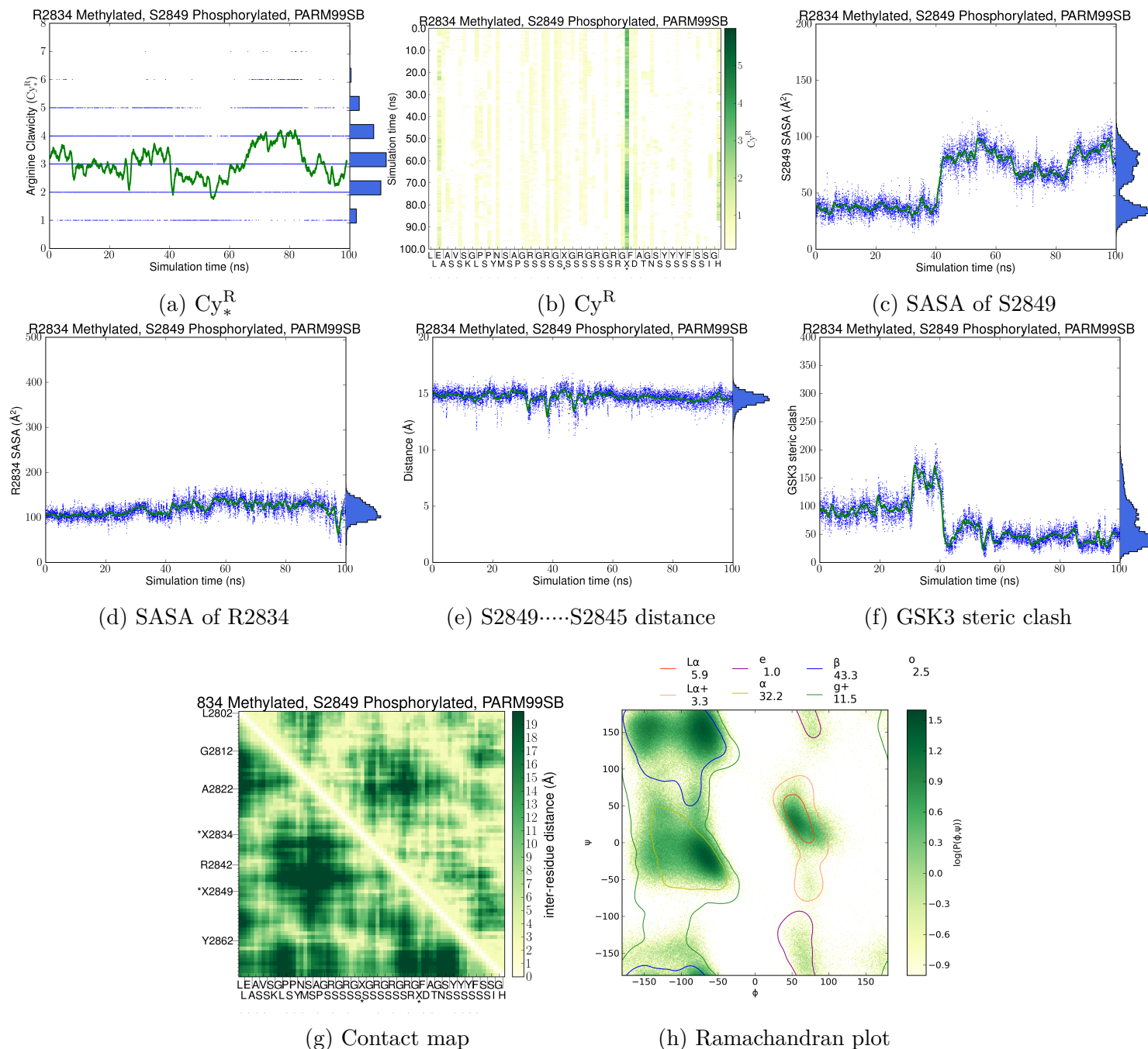


Figure S17: Behavior of **R2834MeMe_S2849S2P_PARM99SB_cycle2**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

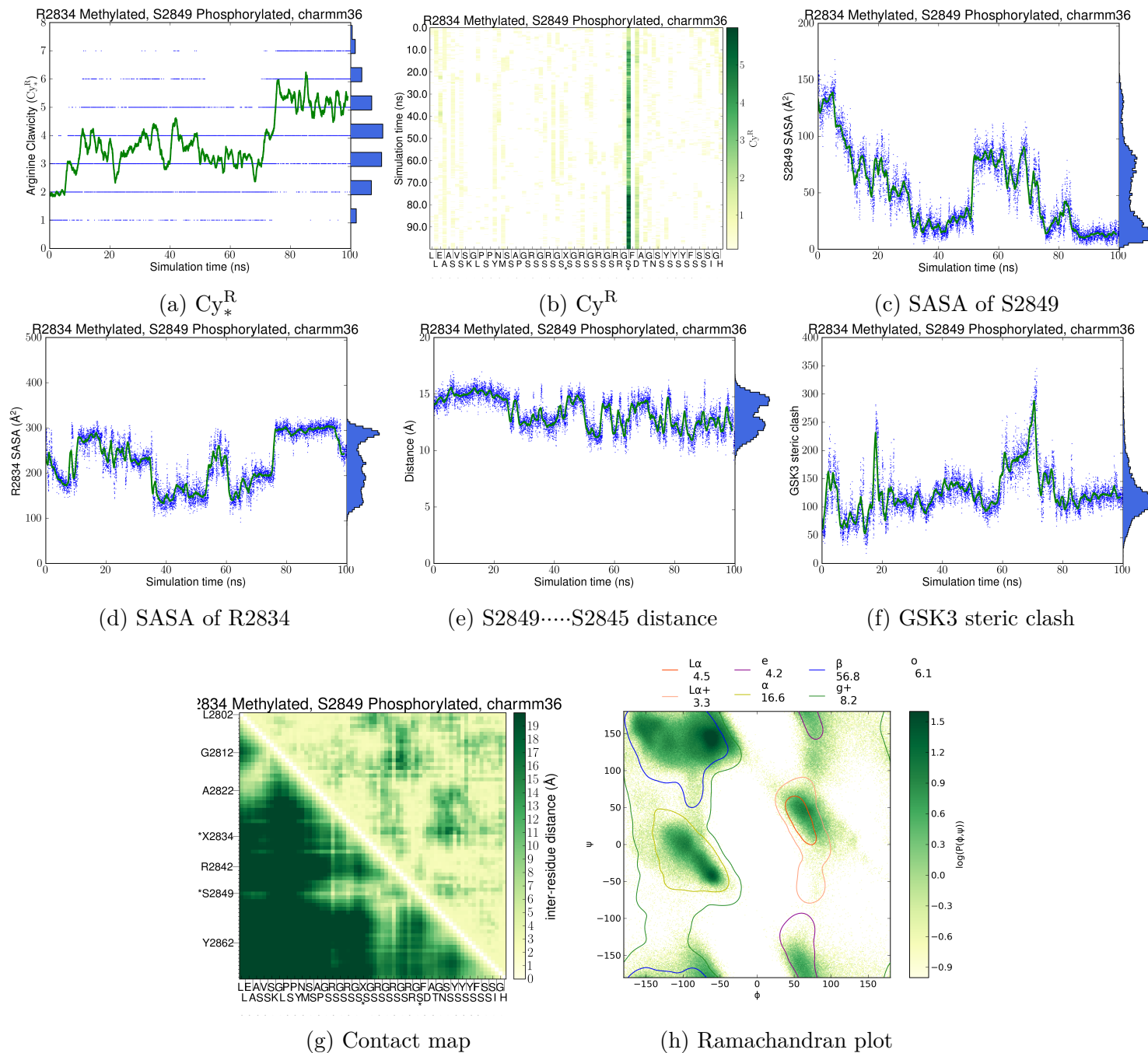


Figure S18: Behavior of **R2834MeMe_S2849S2P_CHARMM36**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.

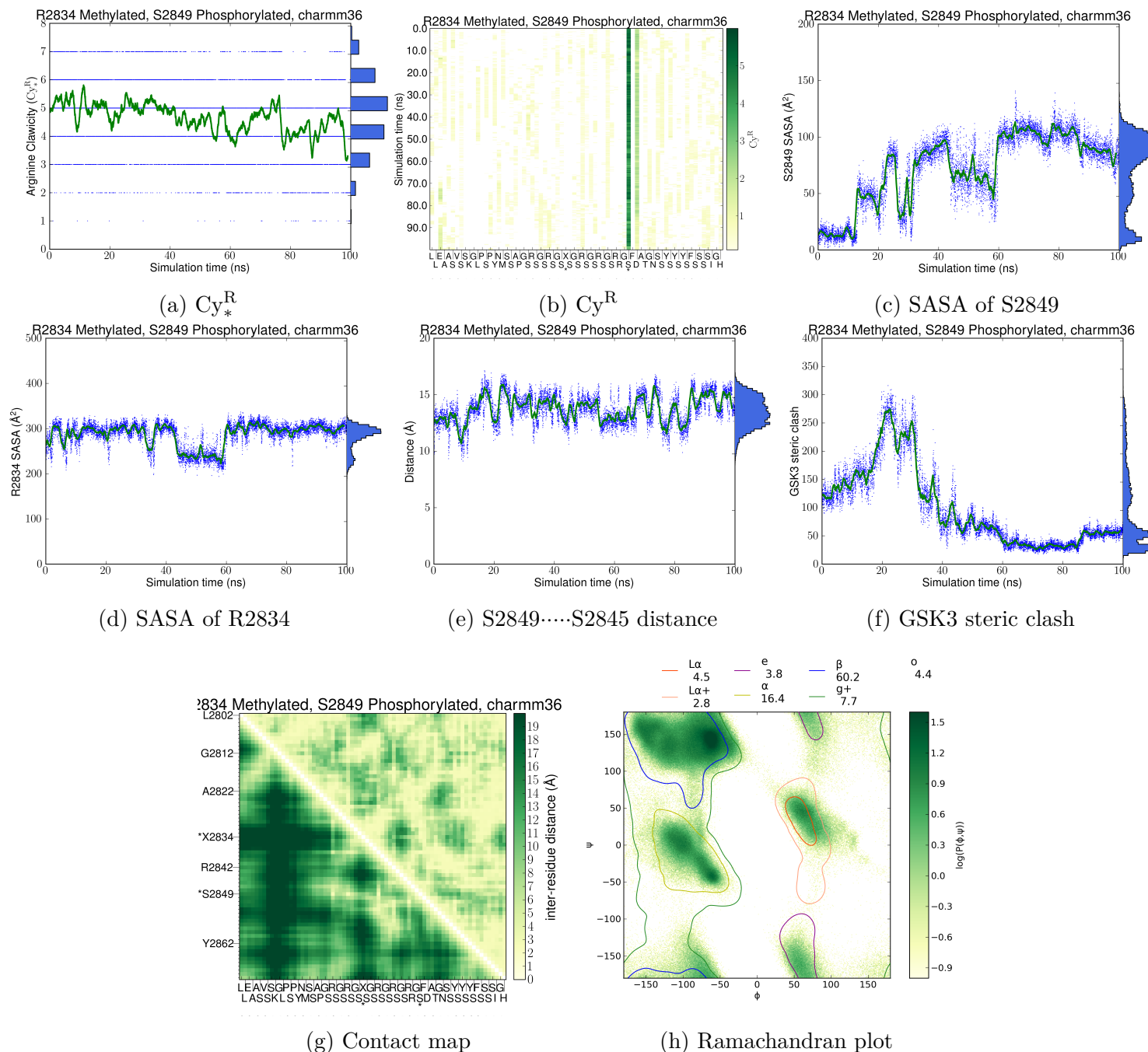


Figure S19: Behavior of **R2834MeMe_S2849S2P_CHARMM36_cycle2**: Time-series plots mark each observation as a blue point and contain a 1-ns running average as a green trace, and the marginal distributions are shown on the right axis, in each of panels a, c, d, e, and f.