Supplementary information to: From polymer to proteins: effect of side chains and broken symmetry in the formation of secondary structures within a Wang-Landau approach

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Supplementary material to the paper by Skrbic *et al.*

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I. PHASE DIAGRAMS OF P MODEL

In Figure 1 we report results obtained from Wang-Landau method applied to model P that are then used to draw the phase diagram (see Figure 2). These include both the specific heat per monomer $C_v(T)/(Nk_B)$ and the reduced mean-square radius of gyration $\langle R^2(T)\rangle/N\sigma^2$ as a function of the reduced temperature k_bT/ϵ. In Figure 2 the phase

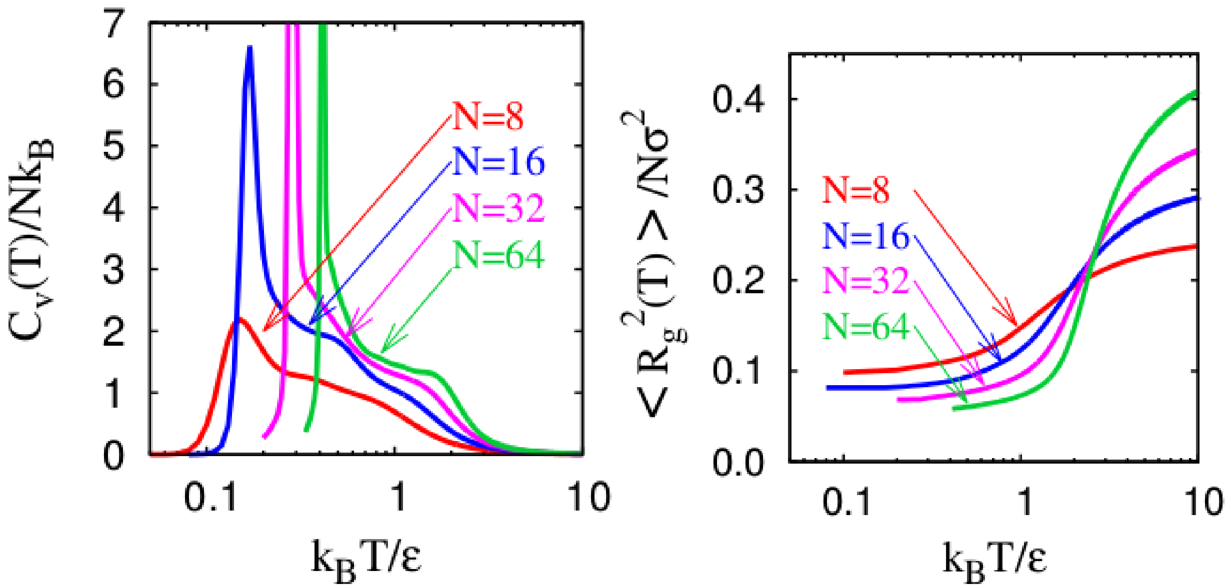

FIG. 1. Left panel. The specific heat per monomer $C_v(T)/(Nk_B)$ as a function of the reduced temperature k_bT/ϵ for the P model with $N = 8, 16, 32, 64$. Right panel. The reduced mean-square radius of gyration $\langle R^2(T)\rangle/N\sigma^2$ as a function of the reduced temperature k_bT/ϵ under the same canditions.

diagram of the P model in the reduced temperature k_BT/ϵ vs interaction range R_c plane is depicted for $N = 50$. Upon cooling from a coil configuration, one finds first a transition to a globule, and then a transition to a crystal. The two transitions merge below $R_c \approx 6$ Åto become a direct coil-crystal transition in agreement with the results by Taylor *et al.* At larger interaction ranges, the crystal structure becomes less definite more similar to a spherical globule as one could expect on a physical ground.

II. TEMPERATURE DEPENDENCE OF THE CORRELATION FUNCTIONS FOR THE OPSC MODEL

The three correlation functions (tangent-tangent, normal-normal, and binormal-binormal) of the OPSC model are plotted as a function of the sequence separation and of the reduced temperature k_BT/ϵ in Fig. 3. The transition from exponential to oscillating behavior upon cooling below a critical temperature line is evident in all three cases.

TABLE I. Comparison between the ground state energies obtained from the microcanonical Wang-Landau and the canonical replica exchange.

$\lambda = 1.05$	N	$-E_{\mathrm{gs}}^{\mathrm{WL}}$	$-E_{\mathrm{gs}}^{\mathrm{RE}}$
	3	1	–
	4	3	–
	5	5	–
	6	7	–
	7	10	–
	8	12	12
	9	15	–
	10	18	–
	12	23	–
	16	34	34
	20	46	–
	32	86	84
	64	205	197
	128	451	–
	256	945	–
$\lambda = 1.3$	N	$-E_{\mathrm{gs}}^{\mathrm{WL}}$	$-E_{\mathrm{gs}}^{\mathrm{RE}}$
	3	1	–
	4	3	–
	5	5	–
	6	8	–
	7	11	–
	8	13	13
	9	16	–
	10	19	–
	12	27	–
	16	40	40
	20	55	–
	32	103	102
	64	240	237
	128	529	–
	256	1113	–
$\lambda = 1.5$	N	$-E_{\mathrm{gs}}^{\mathrm{WL}}$	$-E_{\mathrm{gs}}^{\mathrm{RE}}$
	3	1	–
	4	3	–
	5	6	–
	6	10	–
	7	13	–
	8	17	17
	9	21	–
	10	25	–
	12	34	–
	16	54	54
	20	73	–
	32	139	139
	64	322	330
	128	690	–
	256	1450	–

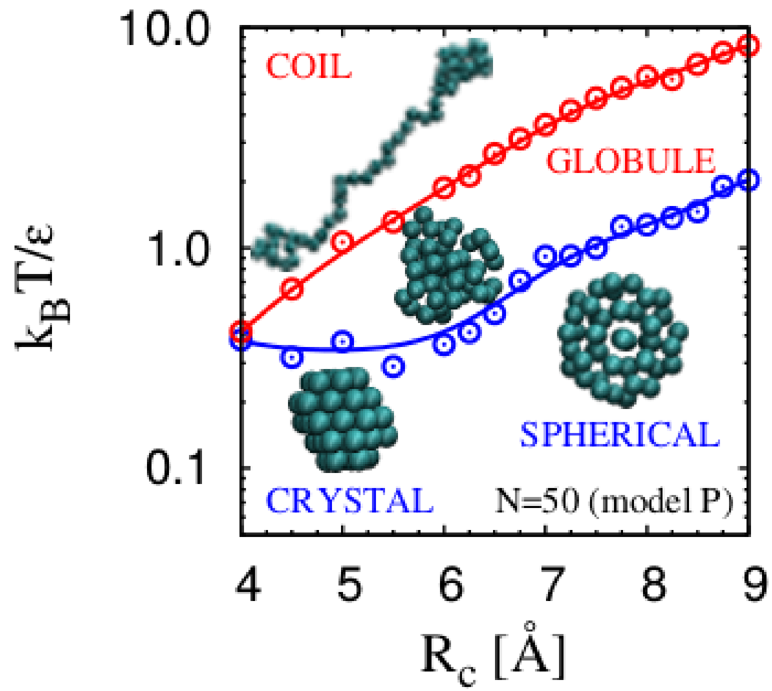

FIG. 2. Phase diagram of the P model in the reduced temperature $k_B T/\epsilon$ vs interaction range R_c plane for $N = 50$.

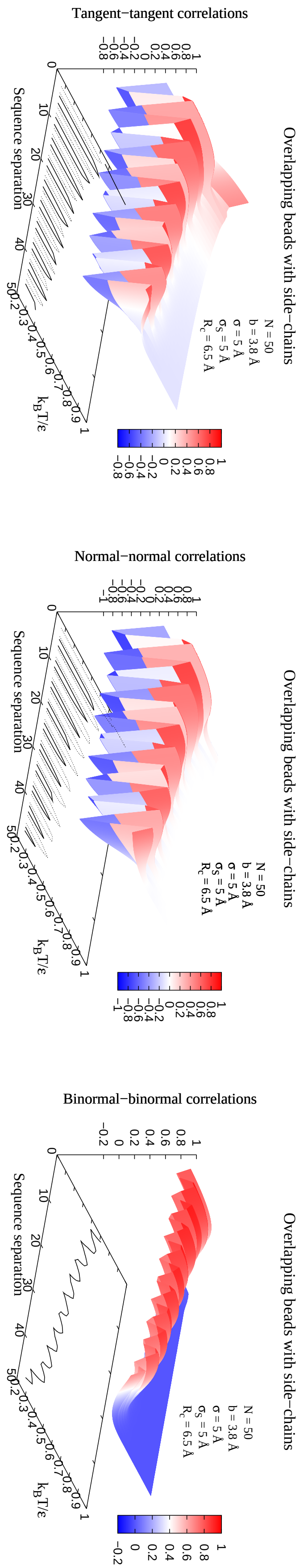

FIG. 3. Three dimensional plot of the tangent-tangent, normal-normal, and binormal-binormal correlation functions as a function of the sequence separation and the reduced temperature k_BT/ϵ.