SUPPORTING INFORMATION.

DPD Simulation of Protein Conformations: from α-helices to β-structures.

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Table S1. Conservative parameters a_{ij} applied to interactions between beads of different types (kT/R_c) and the models of residues, composed of 1 to 3 beads each. B1,B2,B3 denote the bead type, r12 and r23 are the distances between the beads reduced by R_c.

Short-range conservative repulsion parameters, a_{IJ}/kT

	W	S	H	T
W	50.			
S	55	50		
H	50	58	50	
T	63	58	58	50

Skeletal harmonic bonds, $E_b(r)=½K(r-r_e)^2$

1-2: $K = 160\ kT/R_c^2$ $r_e = 0.6\ R_c$

1-3: $K = 80\ kT/R_c^2$ $r_e = 1.2\ R_c$

Volumes, bead types, and bond length for peptide residues

AA	Vol A^3 (a)	*B1*	r_{12}/R_c	*B2*	r_{23}/R_c	B3
Ile	166.1	S	1.05	T		
Phe	189.7	S	0.6	T	0.6	T
Val	138.8	S	0.8	T		
Leu	168.0	S	1.05	T		
Met	165.2	S	1.05	T		
Ala	87.8	T				
Gly	59.9	S				
Tyr	191.2	S	0.8	T	0.6	H
Pro	123.3	S	0.6	T	(b)	
Thr	118.3	S	0.6	H		
Ser	91.7	S	0.4	H		
Glu	140.9	S	0.8	H		
Asn	120.1	S	0.6	H		
Gln	145.1	S	0.85	H	(c)	
Asp	115.4	S	0.5	H	(c)	
Lys	172.7	S	0.5	T	0.7	S
Lys+	172.7	S	0.5	T	0.7	H+

Morse bonds, $E_M(r) = K_M [1-\exp(\alpha (r - r_e)^2]$

	αR_c^2	r_e/R_c	r_M/R_c
Model A, 1-3[(d)]	8.0	0.6	2.5
Model A, 1-5	8.0	0.6	3.0
Model B	8.0	0.6	3.0

(a) "consensus" volumes from ref [26]

(b) due to small alanine volume it is modeled as a single hydrophobic bead

(c) charge –1 assigned to the H bead at pH=7 (deprotonated form); Type H and charge +1 assigned to Lys in the protonated form (see charge profiles, Figure 4).

(d) K_M parameter varied, see text

Table S2. Charges of dissociating residues used in DPD simulations of triblock polypeptide at pH=4 and pH=7

		pH= 4		pH= 7	
RESIDUE	pKa	average charge calculated	smeared charge assumed	average charge calculated	smeared charge assumed
D (-)	4.5	-0.24	0	-1.00	-1
E (-)	4.6	-0.20	0	-1.00	-1
Y (-)	9.7	-2.00E-06	0	-2.00E-03	0
H (+)	6.2	0.99	1	0.14	0
N (+)	8.2	1.00	1	0.94	1
K (+)	10.4	1.00	1	1.00	1
R (+)	12.5	1.00	1	1.00	1

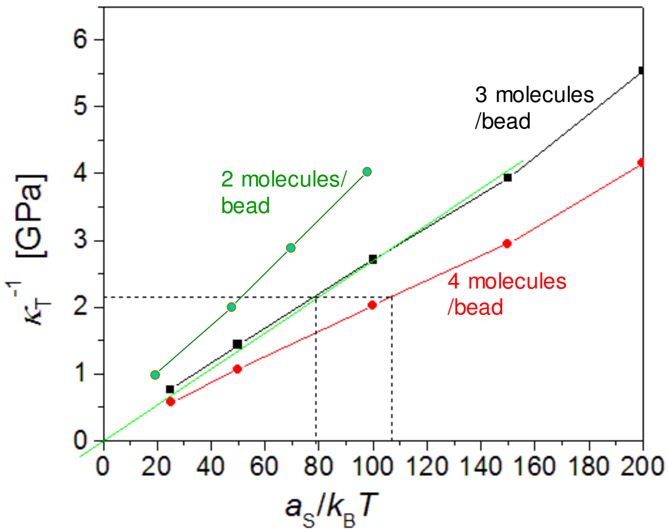

Figure S1. The dependence of the inverse compressibility in a system of soft monomeric beads on the repulsive parameter for $n_B = 2$, $n_B = 3$ and $n_B = 4$ at $\rho^* = 3$. Interpolating the experimental value onto the reference curve, we obtain $a_W = 50.5kT$ at $n_B=2$.

Description of DPD simulations

Non-bonded beads i and j interact via a soft conservative repulsive force, a random thermal force, and a velocity-dependent drag force: $\vec{F}_{ij} = \vec{F}_{ij}^{(C)} + \vec{F}_{ij}^{(R)} + \vec{F}_{ij}^{(D)}$. We applied a standard form of the conservative force, which decays linearly with the distance between the beads r_{ij}, with the cutoff potential radius of action equal to R_c: $\vec{F}_{ij}^{(C)} = a_{ij}(r_{ij} / R_c - 1)(\mathbf{r}_{ij} / r_{ij})$, if $r_{ij} < R_c$; and $\vec{F}_{ij}^{(C)} = 0$, if $r_{ij} \geq R_c$. R_c is effectively the bead diameter and is equal for all quasi-particles in the system; $\mathbf{r}_{ij}$ is the vector between i-th and j-th particles. a_{ij} is the matrix of the conservative repulsion parameters specific for the particular i–j pair; these "mismatch" parameters are linked to the Flory-Huggins parameters[41] and are responsible for structure formation in conventional DFP models of complex fluids. The bond between the neighboring skeleton beads ("S" beads) is modeled as harmonic $E_b(r) = \frac{1}{2}K(r - r_e)^2$ with $r_e = 0.6R_c$ (10) and $K = 80\ kT/R_c^2$. Sidechains were bonded to the skeleton beads also by harmonic bonds with $K = 160\ kT/R_c^2$ and length varied depending on the effective aminoacid volumes.[26] The dimensionless reduced density of beads in the system was set to $\rho R_c^3 = 3$, common for aqueous solutions.[52] The random force, which accounts for thermal fluctuations, is taken to be proportional to the conservative force that is also acting along the vector between the bead centers: $\boldsymbol{F}_{ij}^{(R)}(r_{ij}) = \sigma w^R r_{ij} \theta_{ij}(t) \mathbf{r}_{ij}$, where $\theta_{ij}(t)$ is a randomly fluctuating in time variable with Gaussian statistics and σ scales the magnitude of the force. The drag force is velocity-dependent: $\boldsymbol{F}_{ij}^{(D)}(\mathbf{r}_{ij}, \mathbf{v}_{ij}) = -\gamma w^D(r_{ij})(\mathbf{r}_{ij*}\mathbf{v}_{ij})$, where, $\mathbf{v}_{ij} = \mathbf{v}_j - \mathbf{v}_i$, $\mathbf{v}_i$ and $\mathbf{v}_j$ are the current velocities of the particles and γ is the friction coefficient. We invoke the the fluctuation dissipation theorem to establish the relationship between the drag and random force parameters $w^D(r) = [w^R(r)]^2$. σ and γ are therefore related as $\sigma^2 = 2\gamma kT$ with γ fitted to the diffusion coefficient of pure water (γ=4.2) so as to preserve correct hydrodynamics. Electrostatic interactions between charged beads are accounted for with the "smeared charge" model of Groot[42] recently applied to biosystems.[9] Within this model, the charge is distributed as a symmetric cloud of linearly decreasing density centered at the bead position.

The majority of simulations were performed in $20\times20\times20R_c^3$ cubic box containing 24,000 particles over 400,000 steps with timestep of 0.02 (about 0.07 ps). Statistics were collected over the last 300,000 steps. Block-polypeptide simulations were performed in $24\times24\times24\ R_c^3$ box, and simulation length was 600,000 steps (about 50 ns). Initially, all beads were assigned random positions. Then the energy of the system was minimized by steepest descent algorithm with Hamiltonian that included only short-range repulsion and harmonic bond potentials (electrostatic and Morse interactions were omitted in this step). After this, velocities were assigned according to the Boltzmann distribution and DPD simulation was started. This procedure prevented DPD simulation from divergence, but did not produce any secondary structure in the initial DPD configuration. The temperature was maintained by velocity scaling for the first 100 000 steps, and naturally, from the balance of random and drag forces, afterwards.