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Supplemental Information

Thermodynamics of Conformational Transitions in a Disordered Protein Backbone Model

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Thermodynamics of conformational transitions in a disordered protein backbone model

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1 SUPPLEMENTARY INFORMATION

Table S1: Conformational entropy as a function of the number of glycine residues in oligoglycine. Entropy units are cal/mol/K. Entropy was calculated using the QHA (S^{QHA}), BQH (S^{BQH}), and MIE (S^{MIE}) methods. $S^{\mathrm{MIE}}_{\mathrm{res}}$ is estimated from the distributions of ϕ-ψ dihedrals within each residue, while ignoring inter-residue MI terms. S^{MIE}_1, S^{MIE}_2 and S^{MIE}_3 are the first, second, and third order MIE approximations of the full dihedral conformational entropy, respectively. $S^{\mathrm{MIE,fit}}_2$ and $S^{\mathrm{MIE,fit}}_3$ are the asymptotes of least squares, hyperbolic fits of S^{MIE}_2 and S^{MIE}_3 as functions of time. $t^{\mathrm{MIE,fit}}_2$ and $t^{\mathrm{MIE,fit}}_3$ are the simulation times (μs) required to converge S^{MIE}_2 and S^{MIE}_3, respectively, to within 1 cal/mol/K of their asymptotes. To estimate statistical uncertainty, simulation trajectories of each oligoglycine were split into five contiguous blocks and the standard deviation of each entropy estimate was calculated across the blocks. These are reported in parentheses. Slopes were estimated from linear least squares fits, which yielded $R^2 \geq 0.99$ for all entropy estimates.

Num.	S^{QHA}	S^{BQH}	S^{MIE}_1	$S^{\mathrm{MIE}}_{\mathrm{res}}$	S^{MIE}_2	$S^{\mathrm{MIE,fit}}_2$	S^{MIE}_3	$S^{\mathrm{MIE,fit}}_3$	$t^{\mathrm{MIE,fit}}_2$	$t^{\mathrm{MIE,fit}}_3$
3	16.48 (0.06)	15.26 (0.05)	15.28 (0.05)	13.99 (0.04)	13.35 (0.06)	13.63 (0.11)	12.84	13.46	0.14	0.23
4	22.01 (0.09)	20.38 (0.07)	20.42 (0.06)	18.68 (0.05)	17.87 (0.10)	18.27 (0.10)	17.02	17.92	0.29	0.57
5	27.56 (0.05)	25.55 (0.05)	25.62 (0.05)	23.41 (0.04)	22.45 (0.10)	22.70 (0.27)	21.29	22.23	0.48	1.15
10	55.44 (0.11)	51.54 (0.10)	51.73 (0.10)	47.00 (0.13)	42.83 (0.26)	45.06 (0.59)	32.45	42.41	2.35	9.77
15	83.27 (0.13)	77.78 (0.27)	78.14 (0.23)	71.00 (0.28)	63.03 (0.99)	68.07 (2.14)	29.76	59.73	5.92	34.64
Slope	5.57	5.21	5.24	4.75	4.12	4.52	1.43	3.86		

Table S2: MIE conformational entropy estimates (cal/mol/K) of Gly_{15} as a function of end-to-end distance (R). Separate implicit solvent simulations were performed with the end-to-end distance of Gly_{15} constrained to eight different values of R with a harmonic potential. Each simulation trajectory was split into five blocks and the standard deviation of the entropy across the blocks is reported in parentheses.

R (Å)	S_1^{MIE}	S_{res}^{MIE}	$S_2^{MIE,fit}$	$S_3^{MIE,fit}$	$t_2^{MIE,fit}(\mu s)$	$t_3^{MIE,fit}(\mu s)$
5	77.55 (0.03)	69.43 (0.06)	67.08 (0.27)	63.01	5.20	28.39
10	77.57 (0.05)	69.37 (0.07)	66.97 (0.12)	62.87	5.21	28.29
15	77.65 (0.05)	69.51 (0.10)	67.12 (0.21)	63.11	5.16	28.31
20	77.69 (0.04)	69.64 (0.04)	67.49 (0.11)	63.63	5.14	27.95
25	77.81 (0.02)	69.98 (0.05)	68.08 (0.15)	64.51	5.13	27.80
30	77.73 (0.03)	70.22 (0.05)	68.40 (0.09)	65.05	5.11	27.80
35	77.30 (0.04)	70.29 (0.05)	68.56 (0.15)	65.40	5.06	27.51
40	76.31 (0.06)	70.05 (0.05)	67.90 (0.12)	64.79	5.00	27.07

Table S3: MIE conformational entropy estimates (cal/mol/K) of Gly_{15} as a function of radius of gyration (R_g). Implicit solvent simulations of Gly_{15} with constrained end-to-end distances were partitioned by $R_g \pm 0.5$ Å. Trajectories at each R_g were split into five blocks and the standard deviation of each entropy estimate across the blocks is reported in parentheses

R_g (Å)	S_1^{MIE}	S_{res}^{MIE}	$S_2^{MIE,fit}$	$S_3^{MIE,fit}$	$t_2^{MIE,fit}(\mu s)$	$t_3^{MIE,fit}(\mu s)$
6	76.75 (0.06)	68.20 (0.10)	64.46 (0.41)	59.06	5.18	28.17
7	77.36 (0.22)	69.23 (0.34)	67.22 (0.93)	63.05	5.07	27.28
8	77.70 (0.29)	69.79 (0.58)	68.09 (1.11)	63.47	4.90	26.61
9	77.74 (0.31)	69.89 (0.46)	68.03 (1.06)	63.37	4.97	27.05
10	77.70 (0.21)	70.04 (0.30)	68.20 (0.67)	63.69	5.02	27.08
11	77.47 (0.18)	70.16 (0.21)	68.46 (0.27)	64.57	5.08	27.31
12	76.99 (0.33)	70.19 (0.26)	68.42 (0.45)	64.94	5.07	27.18
13	76.05 (0.37)	69.83 (0.27)	67.59 (0.34)	63.53	5.10	27.27

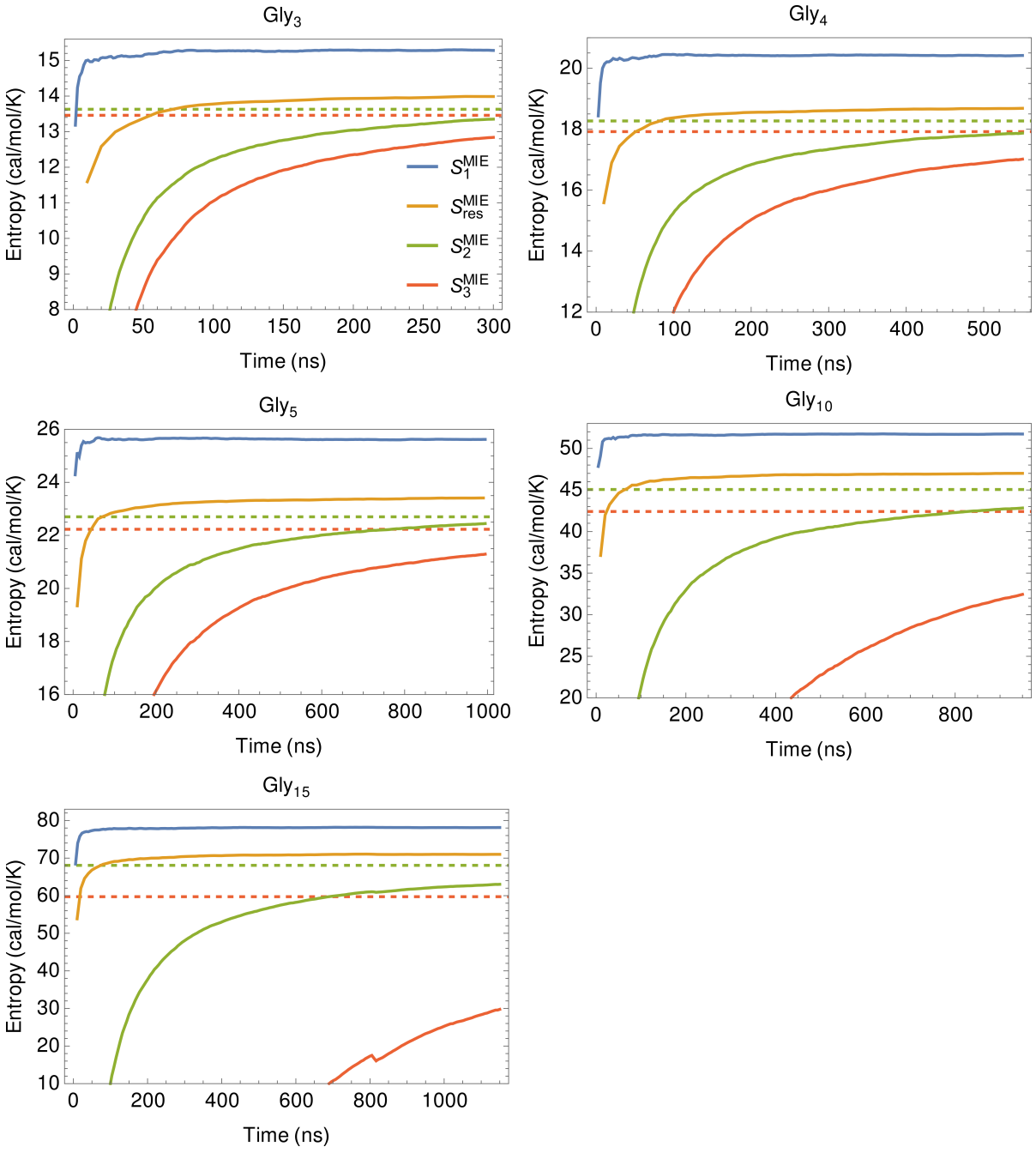

Figure S1: Trajectories of MIE conformational entropy estimates with respect to time. One-dimensional, independent entropy was calculated from the probability distribution for each backbone dihedral angle using the Boltzmann entropy expression. The dashed lines indicate the asymptotes, $S_2^{\mathrm{MIE,fit}}$ and $S_3^{\mathrm{MIE,fit}}$, calculated from the hyperbolic fits of the S_2^{MIE} and S_3^{MIE} trajectories, respectively, and are colored accordingly.