

Supplementary Material

Table S1: Backbone dihedral angles of pA₄ averaged over the trajectory as a function of conformation (see Figure 11): 0–5 ns (IA), 6–17 ns (IIA), 18–25 ns (IB), and 25–40 ns (IIB). (N1–N5 taken from ref. 11).

peptid e		ϕ_1	ψ_1	ϕ_2	ψ_2	ϕ_3	ψ_3	ϕ_4	ψ_4	ϕ_5	ψ_5
IA		69	-109	-103	-4	-146	80	78	-48	-114.8	137
IIA		67	-119	-90	9	-129	-125	-80	-30	-117	143
IB		69	-111	-102	-3	-146	79	80	-49	-115	137
IIB		68	-119	-91	9	-130	-124	-80	-30	-118	143
N1		75	-73	-50	-53	-153	-66	-90	-16	-151	81
N2		75	34	-179	-68	-115	-55	-139	19	-172	68
N3		75	-67	-61	-78	-105	-75	-110	6	-147	71
N4		75	-78	-62	-65	-144	104	65	15	-171	61
N5		75	-142	-57	131	50	65	70	141	50	70

Table S2: N–C' distances of pA₄ structures averaged over the trajectory as a function of conformation (see Figure 11): 0–5 ns (IA), 6–17 ns (IIA), 18–25 ns (IB), and 25–40 ns (IIB). (N1–N5 taken from ref. 11).

peptide	d(Ala3N–Ala5C') (Å)	d(Ala3C'–Ala5N) (Å)
IA	4.05	3.16
IIA	4.04	3.39
IB	4.10	3.19
IIB	4.05	3.39
N1	4.75	3.61
N2	5.03	3.79
N3	4.98	3.70
N4	4.74	3.28
