

Supplementary Tables 1: Martini CG Bonded Interaction Parameters for Diphenylalanine (FF).

Bonds				
A	B	Type	d (nm)	K (kJ nm ⁻² mol ⁻¹)
Backbone – Backbone				
P5	P5	1	0.35	1250
Backbone - Side Chain				
P5	SC5	1	0.31	7500

Constraints			
A	B	Type	d (nm)
Side Chain - Side Chain			
SC5	SC5	1	0.27

Angles					
A	B	C	Type	θ (degrees)	K (kJ mol ⁻¹)
Backbone - Backbone - Side Chain					
P5	P5	SC5	2	100	25
Backbone - Side Chain - Side Chain					
P5	SC5	SC5	2	150	50

Dihedrals						
A	B	C	D	Type	θ (degrees)	K (kJ mol ⁻¹)
Backbone - Side Chain - Side Chain - Side Chain						
P5	SC5	SC5	SC5	2	0	50

Supplementary Tables 2: Martini CG Bonded Interaction Parameters for phenylalanine-asparagine-phenylalanine (FNF).

Bonds				
A	B	Type	d (nm)	K (kJ nm ⁻² mol ⁻¹)
Backbone - Backbone				
P5	P5	1	0.35	1250
Backbone - Side Chain				
P5	SC5	1	0.31	7500
P5	P5	1	0.32	5000

Constraints			
A	B	Type	d (nm)
Side Chain - Side Chain			
SC5	SC5	1	0.27

Angles					
A	B	C	Type	θ (degrees)	K (kJ mol ⁻¹)
Backbone - Backbone - Backbone					
P5	P5	P5	2	127	25
Backbone - Backbone - Side Chain					
P5	P5	SC5	2	100	25
P5	P5	P5	2	100	25
Backbone - Side Chain - Side Chain					
P5	SC5	SC5	2	150	50

Dihedrals						
A	B	C	D	Type	θ (degrees)	K (kJ mol ⁻¹)
Backbone - Side Chain - Side Chain - Side Chain						
P5	SC5	SC5	SC5	2	0	50

Supplementary Table 3: System details: Concentrations, box sizes and particle counts.

Peptide Concentration		Initial Box Size (nm)	Peptide Count			Water & Antifreeze Count		Total Particle Count
Net (peptides/nm ³)	Relative		FF	FNF	Total	WF	W	
0.1	0%	16.59	500	0	500	3800	29218	33518
	10%		450	50	500		29031	33331
	20%		400	100	500		28903	33203
	30%		350	150	500		28901	33201
	40%		300	200	500		28997	33297
	50%		250	250	500		28831	33131
	60%		200	300	500		28732	33032
	70%		150	350	500		28714	33014
	80%		100	400	500		28657	32957
	90%		50	450	500		28664	32964
	100%		0	500	500		28704	33004
0.15	0%	14.77	500	0	500	2700	19805	23005
	10%		450	50	500		19583	22783
	20%		400	100	500		19611	22811
	30%		350	150	500		19583	22783
	40%		300	200	500		19526	22726
	50%		250	250	500		19467	22667
	60%		200	300	500		19328	22528
	70%		150	350	500		19400	22600
	80%		100	400	500		19260	22460
	90%		50	450	500		19306	22506
	100%		0	500	500		19213	22413
0.2	0%	13.56	500	0	500	2100	14895	17495
	10%		450	50	500		12512	15112
	20%		400	100	500		14691	17291
	30%		350	150	500		14626	17226
	40%		300	200	500		14542	17142
	50%		250	250	500		14489	17089
	60%		200	300	500		14475	17075
	70%		150	350	500		14487	17087
	80%		100	400	500		14446	17046
	90%		50	450	500		14432	17032
	100%		0	500	500		14358	16958
0.25	0%	12.66	500	0	500	1700	11626	13826

	10%		450	50	500		11581	13781
	20%		400	100	500		11549	13749
	30%		350	150	500		11490	13690
	40%		300	200	500		11425	13625
	50%		250	250	500		11347	13547
	60%		200	300	500		11364	13564
	70%		150	350	500		11192	13392
	80%		100	400	500		11260	13460
	90%		50	450	500		11107	13307
	100%		0	500	500		11093	13293
0.3	0%	11.97	500	0	500	1400	9622	11522
	10%		450	50	500		9479	11379
	20%		400	100	500		9425	11325
	30%		350	150	500		9390	11290
	40%		300	200	500		9343	11243
	50%		250	250	500		9257	11157
	60%		200	300	500		9230	11130
	70%		150	350	500		9161	11061
	80%		100	400	500		9096	10996
	90%		50	450	500		9105	11005
	100%		0	500	500		8985	10885