

Supplementary materials:

Table S1. β -strand, β -turn, PPII and coil probabilities at 298 K of the amino acid residues defined at least twice in the K3 sequence.

β -strand	N21	N24	F22	F30	L23	L39	L40	V27	V37	S28	S33	D34	D38
trans-K3	10%	14%	12%	19%	15%	12%	10%	18%	14%	9%	11%	9%	20%
cis-K3	10%	20%	14%	1%	20%	13%	10%	6%	19%	5%	2%	8%	23%

β -turn	N21	N24	F22	F30	L23	L39	L40	V27	V37	S28	S33	D34	D38
trans-K3	1%	37%	13%	1%	29%	27%	21%	19%	30%	12%	11%	15%	22%
cis-K3	1%	15%	19%	1%	25%	20%	9%	27%	16%	22%	21%	24%	17%

PPII	N21	N24	F22	F30	L23	L39	L40	V27	V37	S28	S33	D34	D38
trans-K3	35%	6%	10%	20%	12%	12%	22%	13%	8%	9%	2%	12%	12%
cis-K3	33%	11%	6%	12%	12%	12%	30%	12%	11%	7%	14%	15%	13%

Coil	N21	N24	F22	F30	L23	L39	L40	V27	V37	S28	S33	D34	D38
trans-K3	55%	42%	66%	61%	44%	44%	44%	49%	44%	70%	76%	63%	42%
cis-K3	56%	53%	61%	86%	43%	56%	51%	55%	53%	66%	62%	52%	46%

Figure S1: The β -strand probability of each residue at 298 K using the four independent time intervals: 2-22 ns, 22-42 ns, 22-62 ns and 22-82 ns. (a) cis-K3 peptide, (b) trans-K3 peptide.

Figure S2: The time-averaged (22-82 ns) solvent accessible surface of each amino acid at 298 K using (a) all atoms, (b) the side-chain atoms, (c) the main-chain atoms.

Figure S3: Probability distribution of the number of side-chain - side-chain atomic contacts within the Ser28-Gly29-Phe30-His31-Pro32-Ser33 loop region in trans- and cis-K3 peptides.

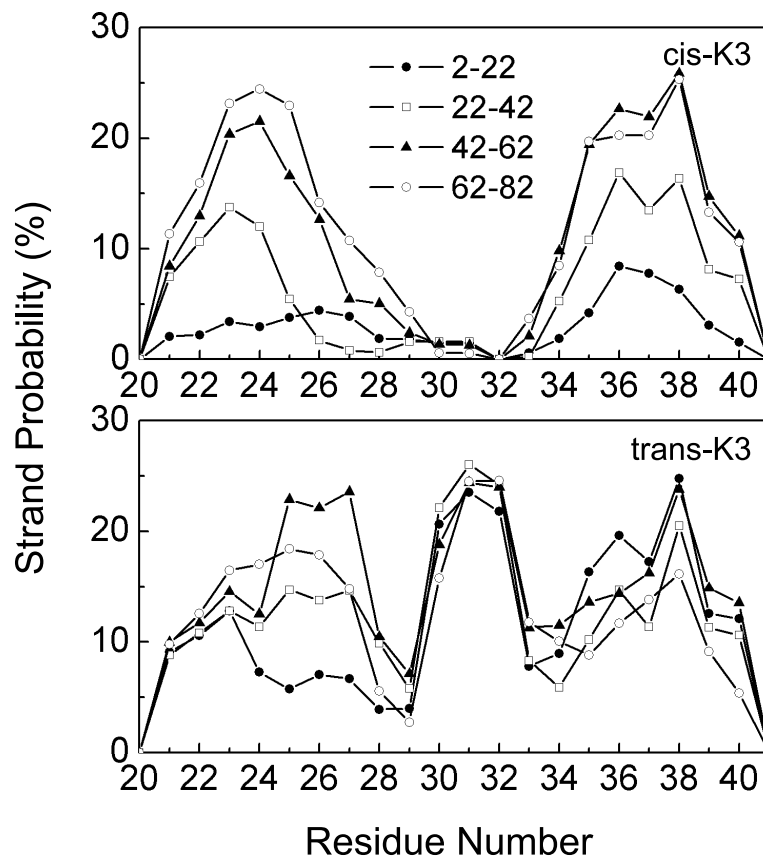


Figure S1

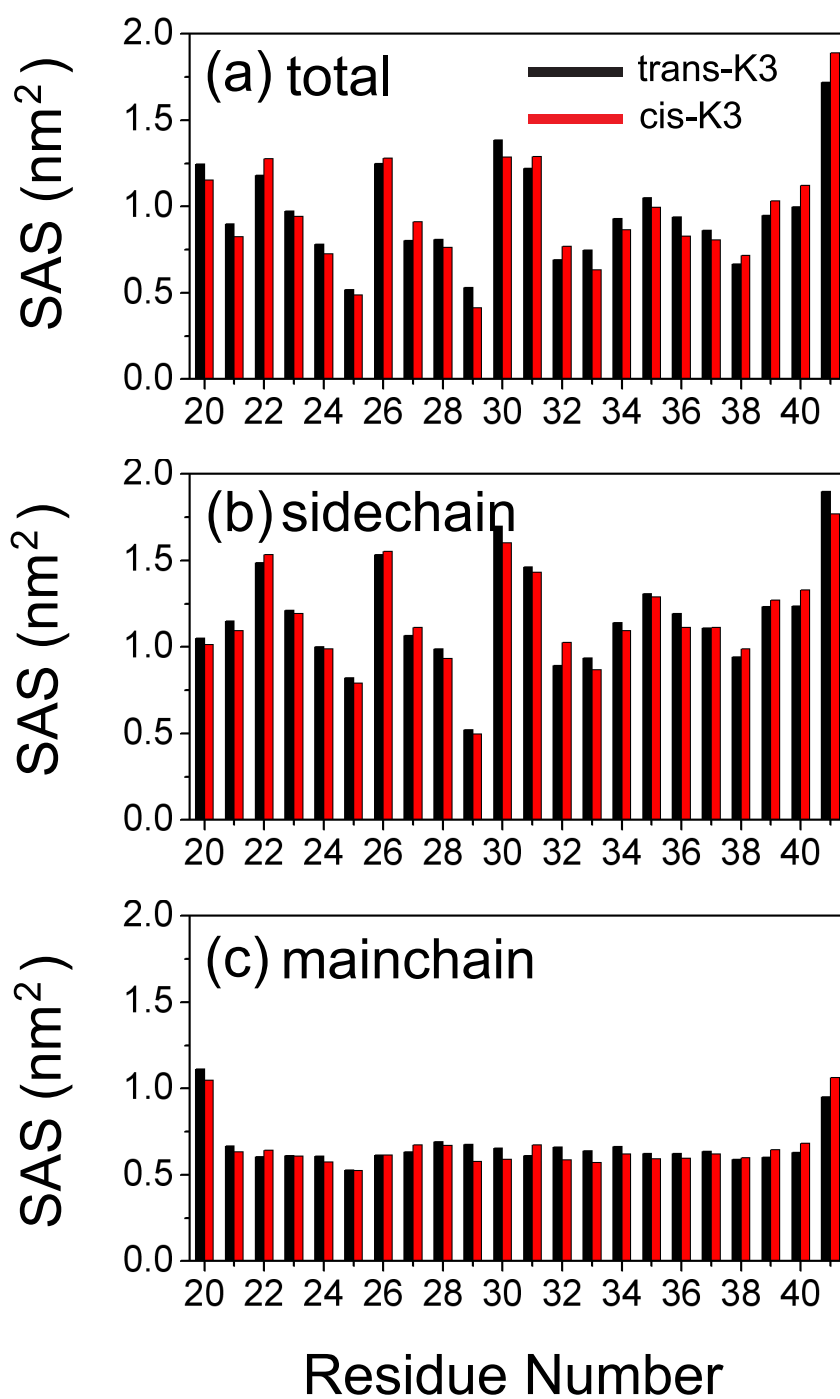


Figure S2

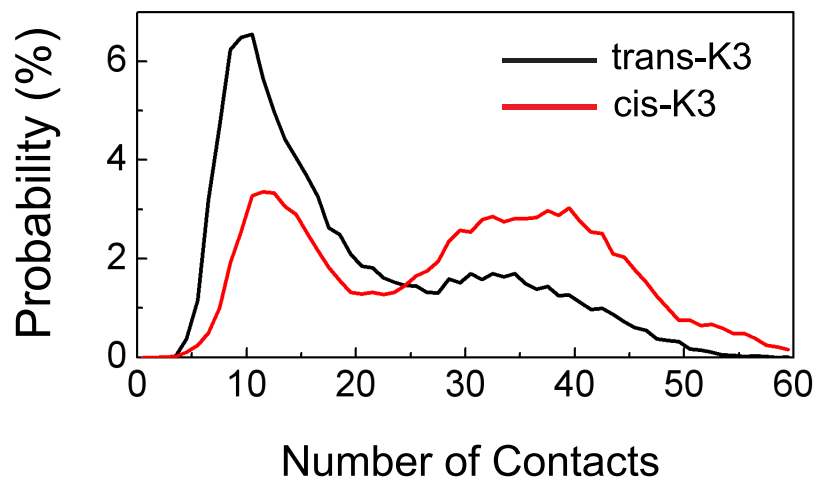


Figure S3