

Statistics for the structures of **4** and **10** overlayed in Figures 4 and 6, respectively

	Peptide 10	Peptide 4
Bond stretching energy (kcal/mole)	3.32 ± 0.13	2.60 ± 0.21
Angle bending energy (kcal/mole)	17.39 ± 1.25	15.18 ± 1.36
Torsional energy (kcal/mole)	17.27 ± 0.94	14.28 ± 1.30
Out of plane bending energy (kcal/mole)	0.15 ± 0.07	0.16 ± 0.07
1-4 Van der Waals energy (kcal/mole)	8.39 ± 0.34	7.23 ± 0.44
Van der Waals energy (kcal/mole)	-28.54 ± 1.78	-18.24 ± 1.77
1-4 Electrostatic energy ((kcal/mole)	28.81 ± 0.68	19.31 ± 0.63
Electrostatic energy (kcal/mole)	-32.37 ± 0.90	-22.46 ± 1.56
Fixed distance range energy (kcal/mole)	0.15 ± 0.11	0.69 ± 0.41
Total energy (kcal/mole)	12.88 ± 2.99	18.78 ± 3.92
Back bone RMSD (Å)	1.36 ± 0.57	0.72 ± 0.34
Heavy atom RMSD (Å)	1.69 ± 0.57	2.23 ± 0.52

