Suppl. Table 1. Statistics of final simulated annealing structures of the sp-E1 synthetic peptide.

A. Constraints used		
Distance restraints		
Intra-residue		0
Sequential		86
Medium rage		53
Total distance restraints		139
Dihedral angle constraints		
Phi angles		21
Psi angles		20
B. Statistics for the final X-PLOR structures		
Number of structures in the final set		27
X-PLOR energy (kcal.mol^{-1})		-70.0 ± 8.4
NOE violations		
Number > 0.5 Å		none
R.m.s. deviation (Å)		0.116 ± 0.005
Dihedral angle violations		
Number > 5°		none
R.m.s. deviation (deg)		0.36 ± 0.30
Deviation from idealized covalent geometry		
Angles (deg.)		0.80 ± 0.03
Impropers (deg.)		0.281 ± 0.014
Bonds (Å)		0.0050 ± 0.0001
R.m.s. deviation (Å)		
Backbone (C', Cα, N)	helix segment 175-185	0.24 ± 0.08
	all residues	2.89 ± 1.01
All heavy atoms	helix segment 175-185	1.17 ± 0.22
	all residues	3.92 ± 0.93
Ramachandran data[a] (on 569 residues)		
Residues in most favoured regions (%)		95.8
Residues in allowed regions (%)		4.2
Residues in generously allowed regions (%)		0
Residues in disallowed regions (%)		0

[a]From PROCHECK (Laskowski *et al* 1993 J Appl Cryst 26, 285-291).