Table S1

Summary of structural constraints and structure statistics	
Experimental restraints	
Distance restraints	2721
Intra-residue (|i-j| = 0)	686
Sequential (|i-j| = 1)	415
Medium-range (2 ≤ |i-j| ≤ 5)	135
Long-range (|i-j| > 5)	682
Ambiguous	803
Total	
Dihedral angle restraints (φ/ψ)	124
Restraints statistics[†]	
RMS of distance violations (Å)	0.1363 ± 0.0293
RMS of dihedral violations (°)	4.6516 ± 0.7490
Structural quality[†]	
Ramachandran statistics[¶]	
Most favoured regions (%)	89
Allowed regions (%)	8
Disallowed regions (%)	3
Coordinates precision*	
All backbone atoms (Å)	0.32 ± 0.1
All heavy atoms (Å)	0.67 ± 0.008

[†] Average values and standard deviations over the 10 lowest-energy conformers

[¶] Percentage of residues in the Ramachandran plot regions determined by MOLPROBITY [51]

* Average root mean square deviation (RMSD) over the 10 lowest-energy conformers' atomic coordinates with respect to the average structure.