Supplementary Table 1.

Structural statistics for the ensemble of 20 lowest target function ADWX-1 structures.

NOE distance restraints	505	
Intraresidue		292
Sequential		118
Medium range		38
Long range		57
Hydrogen bonds	22	
Dihedral angle restraints	45	
backbone		21
side chains		24
Disulfide bond restraints	18	
Target function ($Å^2$)	0.91 +/- 0.012	
AMBER energy (kcal/mol)	-1154.17 +/- 10.73	
Maximum upper limit violations (Å)	0.17 +/- 0.00	
Maximum lower limit violations (Å)	0.06 +/- 0.01	
Maximum van der waals violations (Å)	0.29 +/- 0.00	
Maximum torsion angle violations (Å)	1.68 +/- 0.13	
RMSD of residues 1-37 (Å) [a]		
Backbone	0.23 +/- 0.10	
Heavy Atoms	0.75 +/- 0.10	
Ramachandran analysis [b]		
% residues in most favored regions	80.9	
% residues in additional allowed regions	15.2	
% residues in generously allowed regions	4.0	
% residues in disallowed regions	0.0	

[a] RMSD values from MOLMOL. [b] Data from PROCHECK-NMR.