Figure legend for Supplementary Materials

Figure S1. Effective energy (potential energy plus solvation free energy) as well as the C_α RMSD with respect to the native state as a function of the folding path during the second iteration.

Figure S2. Representative conformations (a-d) along the path in Figure S1. The N-terminal is in blue and the C-terminal is in red.

Figure S3. Effective energy (potential energy plus solvation free energy) as well as the C_α RMSD with respect to the native state as a function of the folding path during the third iteration.

Figure S4. Representative conformations (a-d) along the path in Figure S3. The N-terminal is in blue and the C-terminal is in red.

Table S1. Potential energy component and the solvation free energy for the conformations at last two steps, step 40 and step 41 of the fourth iteration. The unit is Kcal/mol.

Supplementary Materials

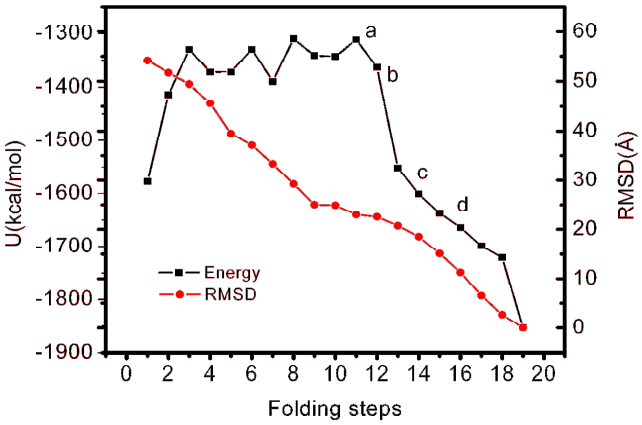

Figure S1

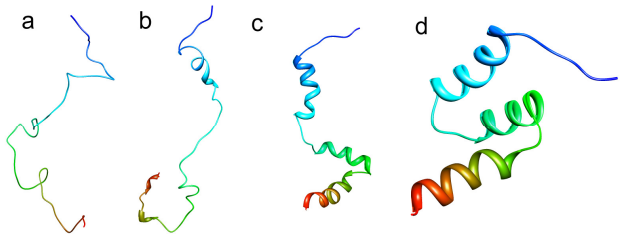

Figure S2

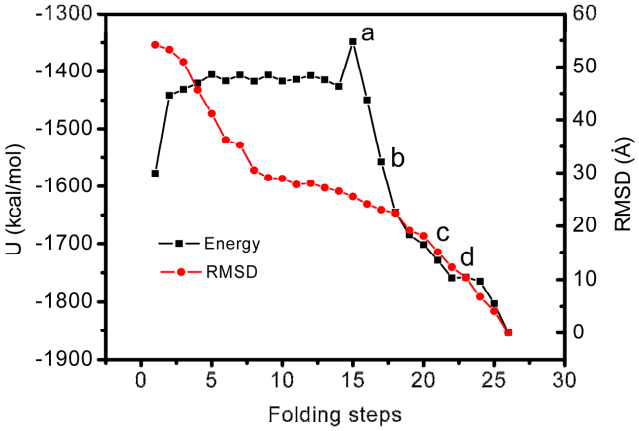
-1300
-1400
-1500
-1600
-1700
-1800
-1900
U (kcal/mol)
60
50
40
30
20
10
0
RMSD (Å)
0
5
10
15
20
25
30
Folding steps
a
b
c
d
Energy
RMSD

Figure S3

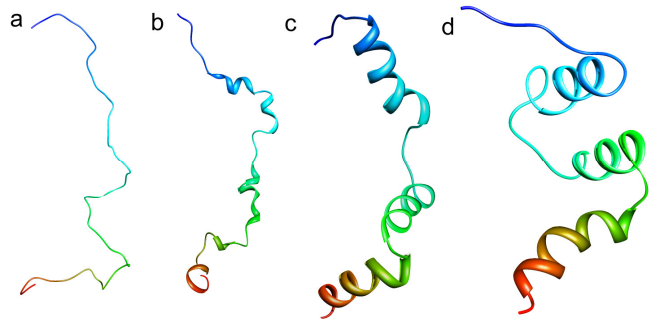

Figure S4

Table S1. Potential energy component and the solvation free energy for the conformations at last two steps, step 40 and step 41 of the fourth iteration. (The unit is Kcal/mol.)

	Step 40	Step 41
Bond	11.36	10.06
Angle	66.23	56.85
Dihedral	48.84	46.55
Improper Dihedral	12.55	9.37
VDW	-371.03	-428.54
Electrostatic	-913.64	-932.07
Solvation	-643.23	-615.83
Total	-1788.92	-1853.62