

SUPPLEMENTARY TABLE S1. STRUCTURE STATISTICS
OF THE ENERGY-MINIMIZED FAMILY OF CONFORMERS
OF $\Delta 76$ Tb1-C-Grx1

NOE upper distance restraints

| | |
|--|-----------------|
| Total | 1909 |
| Intraresidue (i=j) | 553 |
| Sequential ($ i-j =1$) | 499 |
| Medium range ($1 < i-j \leq 5$) | 325 |
| Long range ($ i-j > 5$) | 532 |
| TALOS-derived dihedral restraints | 191 |
| Residual NOE violations ^a | |
| Number ≥ 0.2 Å | 1.2 ± 1.0 |
| Maximum (Å) | 0.22 ± 0.20 |
| Deviation from idealized geometry ^a | |
| Bond lengths (Å) | 0.014 |
| Bond angles (°) | 1.9 |
| Ensemble rmsd ^b (Å) | |
| Backbone (78–182) | 0.54 ± 0.12 |
| All heavy atoms | 1.07 ± 0.09 |
| Ramachandran plot statistics (%) ^c | |
| Most favored regions | 90.7 |
| Additionally allowed regions | 8.8 |
| Generously allowed regions | 0.4 |
| Disallowed regions | 0.2 |

^aThe average values for the 20 energy-minimized structures with the lowest CYANA-target function values and the standard deviation among them are reported.

^brmsd values were calculated with MOLMOL.

^cDetermined by Procheck.