

Supplementary Table S1: Summary of conformational constraints and statistics for the 20 accepted NMR structures of the Pan3 zinc finger domain

Structural constraints

Intra-residue	317
Sequential	239
Medium-range ($2 \leq i-j \leq 4$)	230
Long-range ($ i-j > 4$)	149
Dihedral angle constraints	8
TALOS constraints	62
Distance constraints for 4 hydrogen bonds	8
Zinc co-ordination constraints	10
Total	1023

Statistics for accepted structures

Statistics parameter (\pm SD)	
RMS deviation for distance constraints	$0.0082\text{\AA} \pm 0.0005\text{\AA}$
RMS deviation for dihedral constraints	$0.390^\circ \pm 0.021^\circ$
Mean CNS energy term ($\text{kcal mol}^{-1} \pm$ SD)	
E (overall)	69.29 ± 2.12
E (van der Waals)	29.49 ± 1.34
E (distance constraints)	4.81 ± 0.53
E (dihedral and TALOS constraints)	1.30 ± 0.14
RMS deviations from the ideal geometry (\pm SD)	
Bond lengths	$0.0019 \text{\AA} \pm 0.0005 \text{\AA}$
Bond angles	$0.392^\circ \pm 0.0028^\circ$
Improper angles	$0.250^\circ \pm 0.011^\circ$
Average atomic RMSD from the mean structure (\pm SD)	
Residues 4-35 (N, C α , C atoms)	$0.193 \text{\AA} \pm 0.061 \text{\AA}$
Residues 4-35 (all heavy atoms)	$0.780 \text{\AA} \pm 0.076 \text{\AA}$