Supplementary material for Marvin and Hellinga (2001) *Proc. Natl. Acad. Sci. USA* **98** (9), 4955–4960. (10.1073/pnas.091083898)

Table 5. Detailed descriptions of the designs: Dihedrals and lengths

Site	Residue	$\chi 1$	$\chi 2$	κ	N–Zn bond length
A1	$H63_{II}$	47.3	−84.1	−178.1	2.883
	$H66_{II}$	−66.8	−94.3	172.2	2.155
	$H340_{I}$	−58.6	−135.7	−34.8	2.671
A2	$H63_{II}$	51.4	−87.3	−179.2	2.030
	$H66_{II}$	−58.9	−97.5	166.5	2.373
	$H155_{I}$	−60.6	85.7	174.5	2.508
B1	$H42_{II}$	−172.2	−98.7	160.1	2.392
	$H44_{II}$	65.5	−93.2	168.1	2.272
	$H341_{I}$	−61.3	94.3	−167.7	2.776
B2	$H48_{II}$	−61.9	−70.2	−153.8	2.003
	$H69_{II}$	167.5	−106.1	−12.6	2.234
	$H338_{I}$	−75.1	−77.9	−163.9	2.223

All sites are designed to coordinate Zn through the histidine N_ε, except for A1: $H340_I$ and B1: $H69_{II}$, which coordinate through N_δ. χ angles reported in degrees. N–Zn bond length reported in Å. $\chi 1$ defined as dihedral of N-C_α-C_β-C_γ. $\chi 2$ defined as dihedral of C_α-C_β-C_γ-C_δ. κ defined as dihedral of C_γ-C_δ-N_ε-Zn (C_β-C_γ-N_δ-Zn for A1: $H340_I$ and B1: $H69_{II}$). All dihedrals are within 30° of the observed rotamers for histidine [Lovell, S.C., Word, M. J., Richardson, J. S. & Richardson, D. C. (2000) *Proteins* **40,** 389-408]. Subscripts I and II refer to the domain in which the residue is located (see Fig. 1).