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Supporting Material

Folding Simulations of a De Novo Designed Protein with βαβFold

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Supplementary Information

TABLE S1 Protein fragments studied in this work

Protein	Description	PDB	Residue range	Length	Detection method
NTL9	N-terminal domain of ribosomal protein L9	1CQU	Met1-Ala39	39	NMR
CI2	Chymotrypsin inhibitor 2	2CI2	Leu20-Gly83	64	X-Ray
E3BD F166W	*Bacillus stearothermophilus* peripheral subunit binding domain F166W mutant	1W4E	Asn126-Gly170	45	NMR
BBL H166W	*Escherichia coli* 2-oxoglutarate dehydrogenase peripheral subunit binding domain H166W mutant	2BTH	Gln126-Ala170	45	NMR
DS119	Designed peptide with a β-α-β structure	2KI0	Gln4-Asp36	33	NMR
Psbd41	Peripheral subunit-binding domain of pyruvate dehydrogenase multi-enzyme complex	2PDD	Ala3-Ala43	41	NMR
HP36	Headpiece subdomain of chicken villin	1VII	Met41-Phe76	36	NMR
BBL	*Escherichia coli* 2-oxoglutarate dehydrogenase peripheral subunit binding domain	1BBL	Leu12-Leu48	37	NMR
SH3	Sarcoma homology 3 domain	1FMK	Thr85-Asp141	57	X-Ray
Protein L	IgG-binding domain of protein L	2PTL	Val18-Gly78	61	NMR

FIGURE S1 The change of the solvent accessible surface area of the hydrophobic core in the all atom simulation.

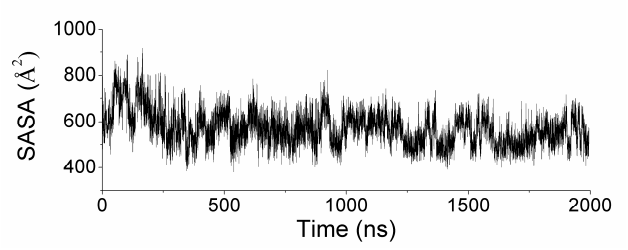

FIGURE S2 Distance between the indole rings of W9 and W34.

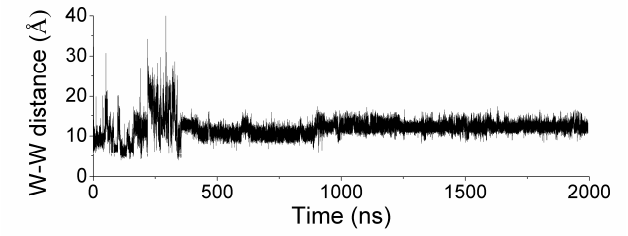

FIGURE S3 A typical folding trajectory from coarse-grained simulations under transition temperature. The total native contacts were decomposed into contacts inside the α-helix (*Helix*), contacts between the N-terminal β-strand and the α-helix (*N-Beta*), contacts between the C-terminal β-strand and the α-helix (*C-Beta*), and contacts between the N- and C-terminal *β*-strands (*Beta-Sheet*). The dot line indicates the folding transition.