Biophysical Journal, Volume 96

Supporting Material

Macromolecular crowding modulates folding mechanism of α/β protein apoflavodoxin

Dirar Homouz, Loren Stagg, Pernilla Wittung-Stafshede, and Margaret S. Cheung

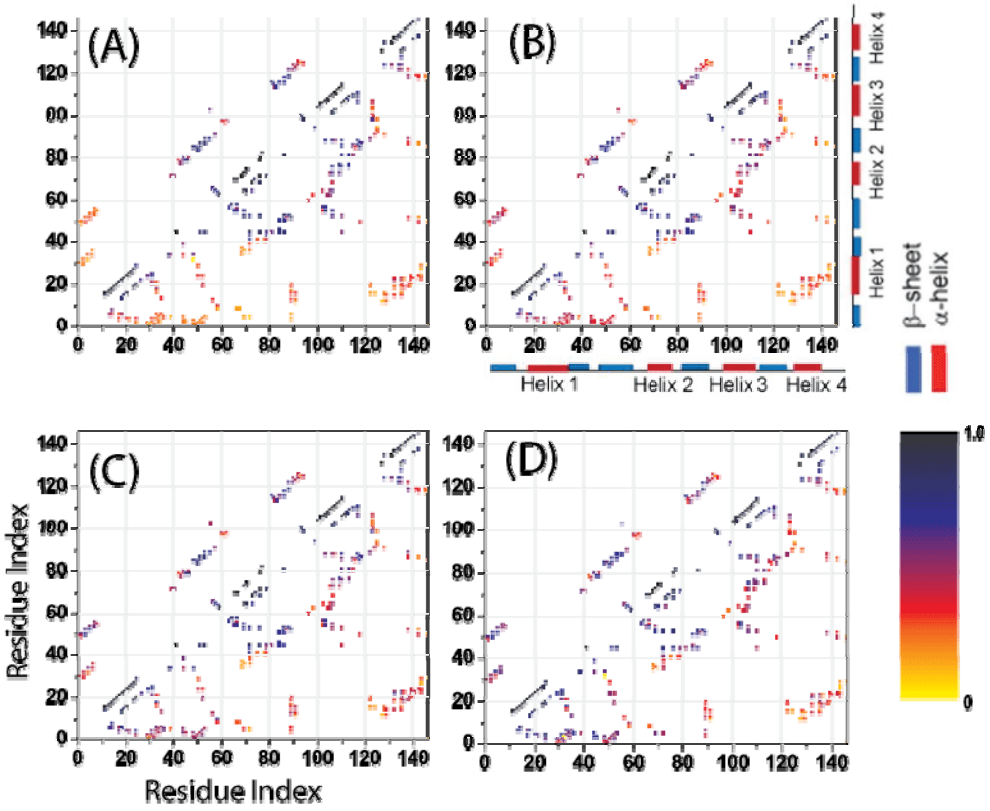
Supplement Materials

Table S1: The ensemble-averaged radius of gyration, R_g, of unfolded states at 400K in the presence of crowding agents, computed by WHAM (See Method sections for details). Small dumbbell* is a spherocylindrical crowder with the equivalent volume as a one Ficoll 70.

ϕ_c	R_g (in unit of σ)
bulk	10.08 ± 0.01
25% (Ficoll 70)	9.72±0.01
40% (Ficoll 70)	7.11±0.01
40% (dumbbell)	4.53±0.2
40% (small dumbbell*)	4.49±0.3

Figure S1: Probability of contact map formation of the transition state at different crowding conditions at 360K: (A) bulk, (B) ϕ_c (Ficoll 70)=25%, (C) ϕ_c (Ficoll 70)=40%, and (D) ϕ_c (dumbbell)=40%. Elements in the upper triangles are probability of native contact formation between backbone hydrogen bonds and the lower triangles ones are native contact formation between side chain beads. Both axes are shown by residue indices. Probability of contact formation is shown in color.

Figure S1


(A)
(B)
(C)
(D)
Helix 1
Helix 2
Helix 3
Helix 4
β–sheet
α-helix
1.0
0
Residue Index
Residue Index