Supporting Information

Studies of Cytochrome c-551 Unfolding Using Fluorescence Correlation Spectroscopy and Other Biophysical Techniques.

PallabiSil[#], SimantaSarani Paul[#], Eva Di Silvio[!], Carlo Travaglini-Allocatelli[!], Krishnananda Chattopadhyay*

*Structural Biology and Bioinformatics Division

CSIR-Indian Institute of Chemical Biology

4 Raja S. C. Mallick Road

Kolkata 700032, INDIA

011913324995843

krish@iicb.res.in

[!] Department of Biochemical Sciences

University of Rome “La Sapienza”

P.le A. Moro, 5 - 00185

Rome, Italy

# Equal contribution

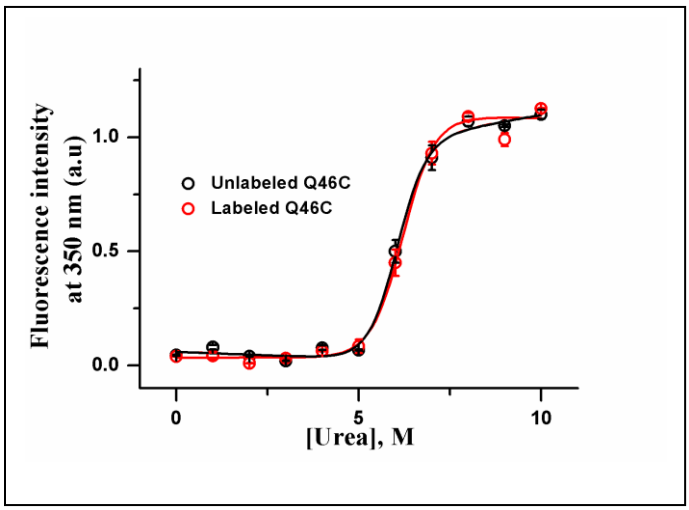

Figure S1: Urea induced unfolding transition of the labeled and unlabeled Q46C as monitored by typtophan fluorescence. For both labeled and unlabeled proteins, the data are fit using a two state unfolding transition model with C_m 6.20 and 6.09 respectively. This result clearly suggests that the labeling of the proteins did not significantly change the stability.

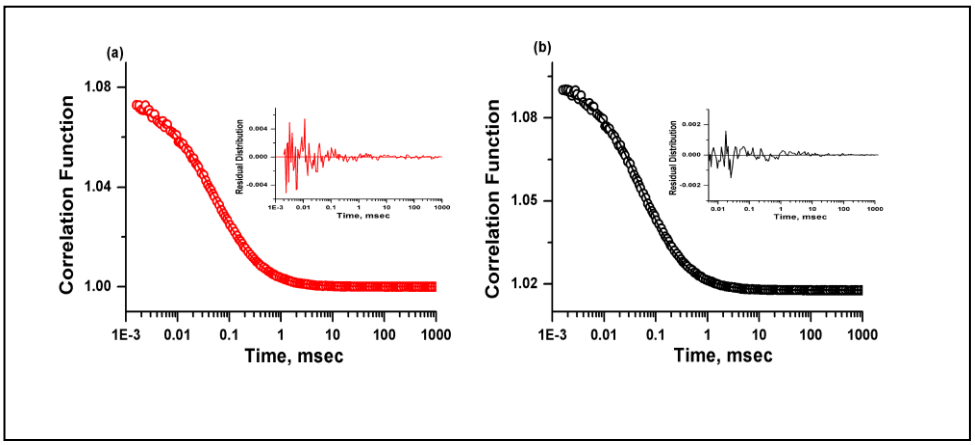

Figure S2: (a) and (b), the correlation functions of K33TMR and V5TMR respectively in their native state. The lines through the data are fit using one diffusion one exponential model. The goodness of their fits were determined using the randomness of the residual distributions (shown in the inset).

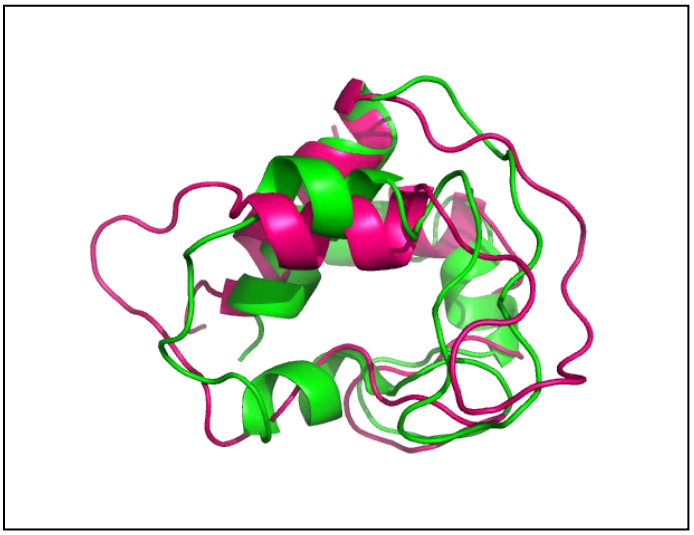

Figure S3: Overlay between the crysal structures of WT cytc551 (represented by pink color) and end structure of MD simulation of WT cytc551 (green color) in aqueous solvent. The end simulation figure indicates that the un-restrained structure of WT cytc551, in aqueous solvent is marginally bigger compare to restrained crystal structure.