The Proteolysis Adaptor NblA Binds to the N-terminus of β-phycocyanin: Implications in the Mechanism of Phycobilisome Degradation

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Supplementary Data

(Supplementary Table S1 and Supplementary Figures S1-S3)

Table S1 Strains, plasmids, and oligonucleotides

Strains, plasmids, or oligonucleotides	**Description**	**Source of reference**
Strains		
Synechococcus 2973	Wild-type fast growing cyanobacterium	(Yu et al. 2015)
Synechococcus 2973 Δ*nblA*	Fast growing cyanobacterium with *nblA* deleted	(Yu et al. 2015)
DH5αMCR *E. coli*	Background strain	
Transformed pET21a/ NblA$_{2973}$_His$_7$	*E. coli* transformed with expression vector carrying *nblA*$_{2973}$_*His7*	This reference
Plasmids		
pET21a	Expression vector containing multiple cloning sites	
pET21a/ NblA$_{2973}$_His$_7$	Vector for expression of *nblA*$_{2973}$_*His*$_7$	This reference
Oligonucleotides[a]		
# nbl1: NblA.TEV.His.F	AGATATACATatgctcccccctctccccg	
# nbl2: pET21a.R	gggggagcatATGTATATCTCCTTCTTAAAGTTAAAC	
# nbl3: pET21a.F	GAGAACCTGTACTTCCAGGGCAGTAGTCACCACCACCACCACCAC	
# nbl4: NblA.TEV.His.R	ACTACTGCCCTGGAAGTACAGGTTCTCacttccttggcgaatcatgC	

[a] Oligonucleotides read in 5’ to 3’ direction.

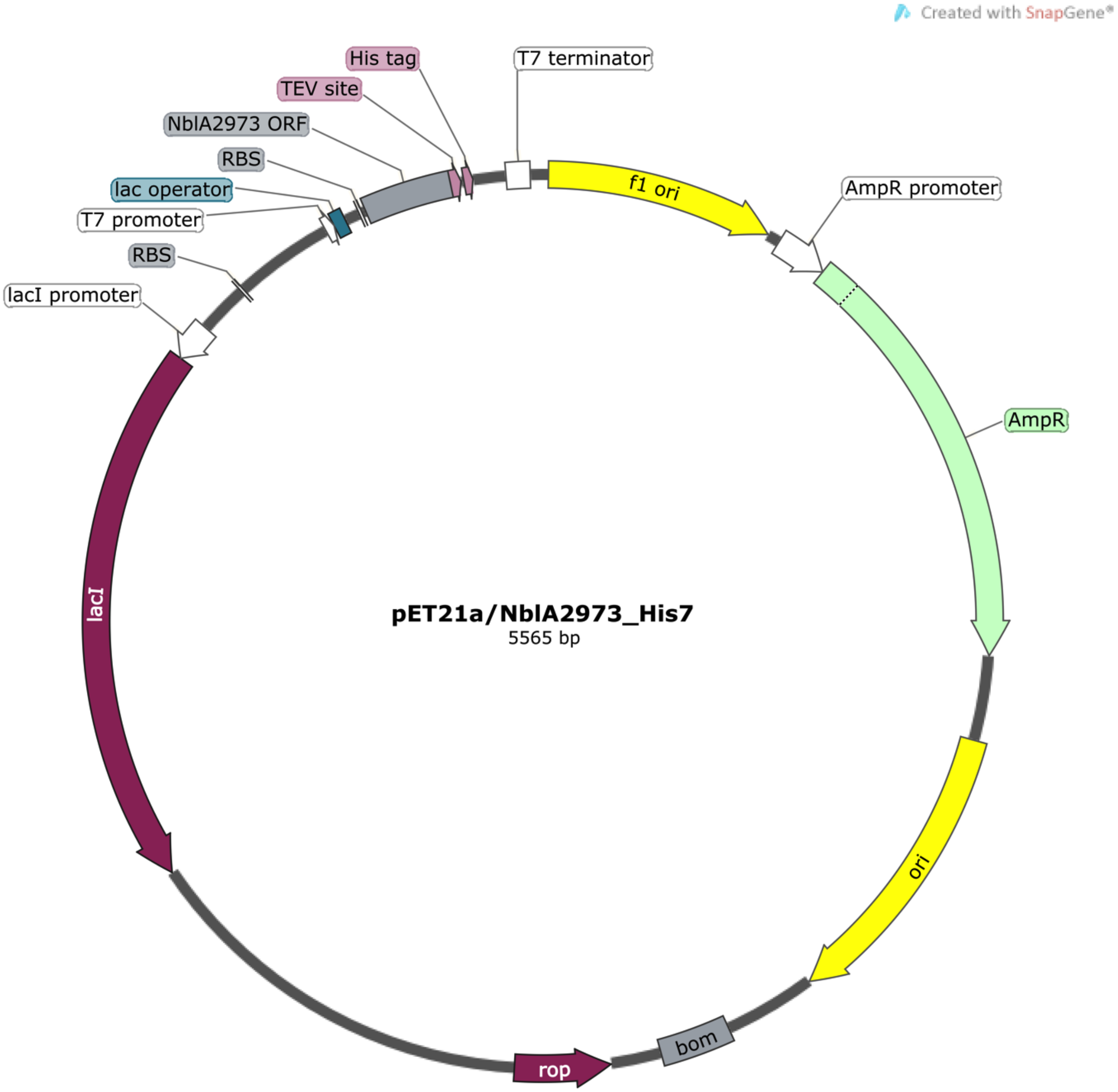

Fig S1 Plasmid map of the overexpression of the $\text{NblA}_{2973}\text{\_His}_7$ strain

ORF of *nblA* was appended with a C-terminal TEV and His tag in the pET21a expression vector. The T7 promoter was used to overexpress *nblA*.

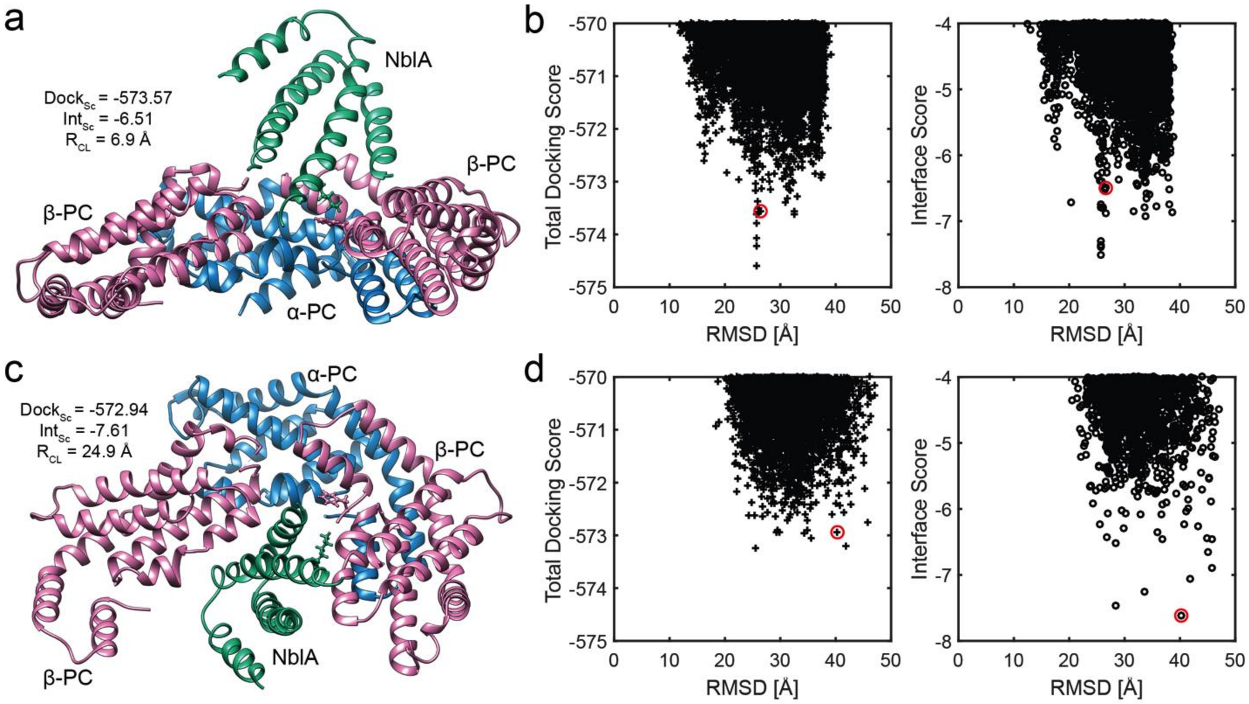

Fig S2 Docking results of an NblA dimer globally docked to α-PC/β-PC monomer from initial orientation I

a Best globally docked pose sorted by lowest cross-linking distance [R$_{CL}$] between residue K^{52} of NblA (green) and residue T^{2} of β-PC (pink) after extracting the top ten scoring structures from 100,000 docked poses from initial orientation I. Total docking score [Dock$_{Sc}$] and interface score [Int$_{Sc}$] are also reported for the pose in addition to cross-linking distance [R$_{CL}$]. **b** Total docking score for the 100,000 globally docked poses vs. RMSD [Å] from initial orientation I, and Interface score for the 100,000 globally docked poses vs. RMSD [Å] from initial orientation I. The location of the best globally docked pose from orientation I is circled in red on both plots. **c** Best globally docked pose sorted by lowest cross-linking distance [R$_{CL}$] between residue K^{52} of NblA (green) and residue T^{2} of β-PC (pink) after extracting the top ten scoring structures from 100,000 docked poses from initial orientation II. Total docking score [Dock$_{Sc}$] and interface score [Int$_{Sc}$] are also reported for the pose in addition to cross-linking distance [R$_{CL}$]. **d** Total docking score for the 100,000 globally docked poses vs. RMSD [Å] from initial orientation II, and Interface score for the 100,000 globally docked poses vs. RMSD [Å] from initial orientation II. The location of the best globally docked pose from orientation II is circled in red on both plots.

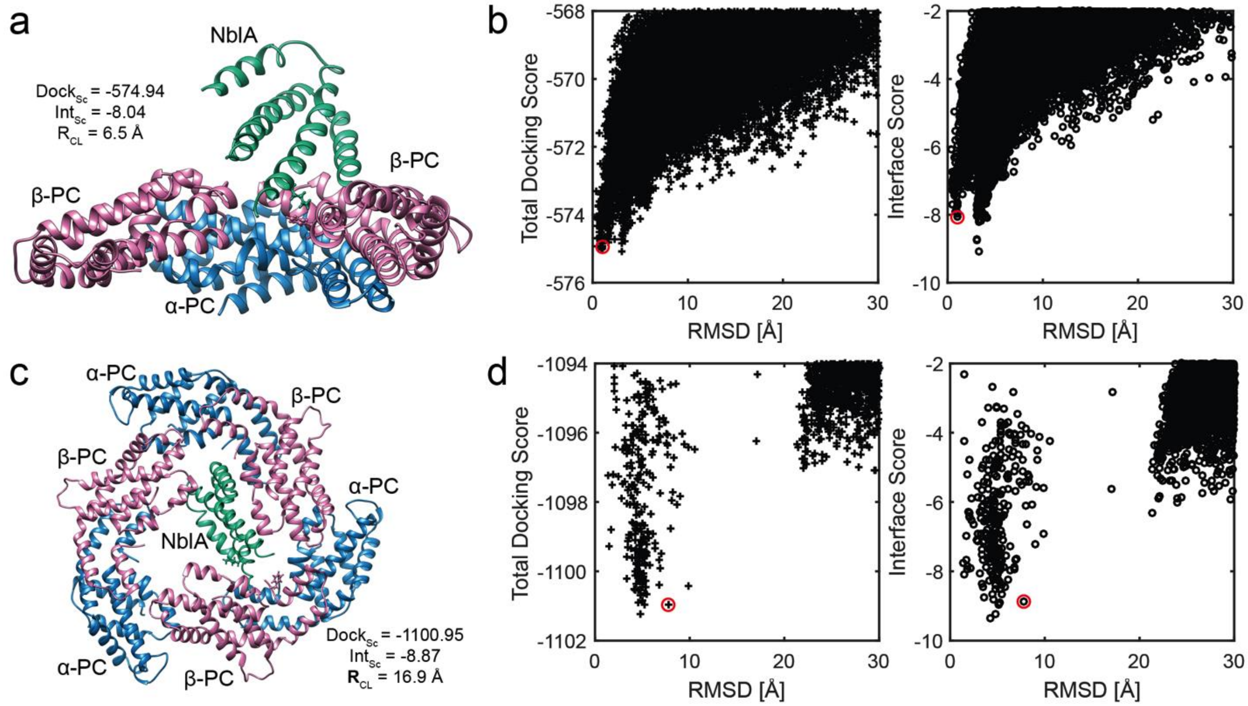

Fig S3 Docking results of an NblA dimer globally docked to α-PC/β-PC monomer from initial orientation II

a Best locally docked pose sorted by lowest cross-linking distance [R_{CL}] between residue K^{52} of NblA (green) and residue T^{2} of β-PC (pink) after extracting the top ten scoring structures from 25,000 docked poses from initial orientation I. Total docking score [Dock_{Sc}] and interface score [Int_{Sc}] are also reported for the pose in addition to cross-linking distance [R_{CL}]. **b** Total docking score for the 25,000 locally docked poses vs. RMSD [Å] from initial orientation I, and Interface score for the 25,000 locally docked poses vs. RMSD [Å] from initial orientation I. The location of the best locally docked pose from orientation I is circled in red on both plots. **c** Best locally docked pose sorted by lowest cross-linking distance [R_{CL}] between residue K^{52} of NblA (green) and residue T^{2} of β-PC (pink) after extracting the top ten scoring structures from 25,000 docked poses from initial orientation II. Total docking score [Dock_{Sc}] and interface score [Int_{Sc}] are also reported for the pose in addition to cross-linking distance [R_{CL}]. **d** Total docking score for the 25,000 locally docked poses vs. RMSD [Å] from initial orientation II, and Interface score for the 25,000 locally docked poses vs. RMSD [Å] from initial orientation II. The location of the best locally docked pose from orientation II is circled in red on both plots.