NMR structure and binding studies of PqqD, a chaperone required in the biosynthesis of the bacterial dehydrogenase cofactor pyrroloquinoline quinone

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Figure S1. The PqqD portion of MePqqCD was identified using an alignment of nine species, two of which were natural fusions. 'MexCD_(Q49150)' represents MePqqCD. The pink/purple arrow identifies the linker region and PqqC enzyme portion of the fusion, and the purple/blue, PqqD. The Uniprot identifiers are enclosed in parentheses and the alignment was completed using Clustal Omega (http://www.uniprot.org/ and http://www.ebi.ac.uk/Tools/msa/clustalo/, respectively).

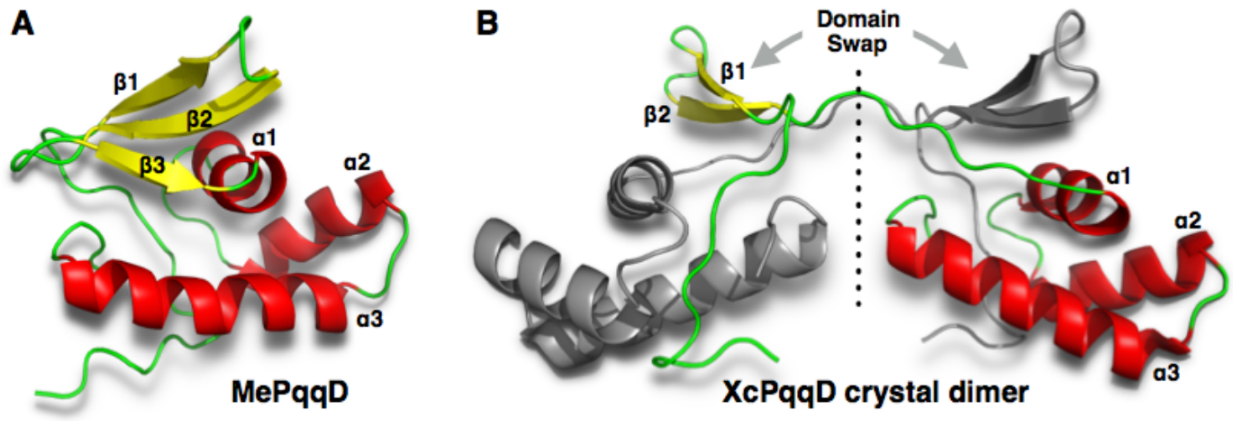

Figure S2. The PqqD structure. (A) The MePqqD monomeric NMR solution structure. (B) The XcPqqD dimeric crystal structure showing that the domain swapped β-hairpins occupy a similar position in the MePqqD monomer.

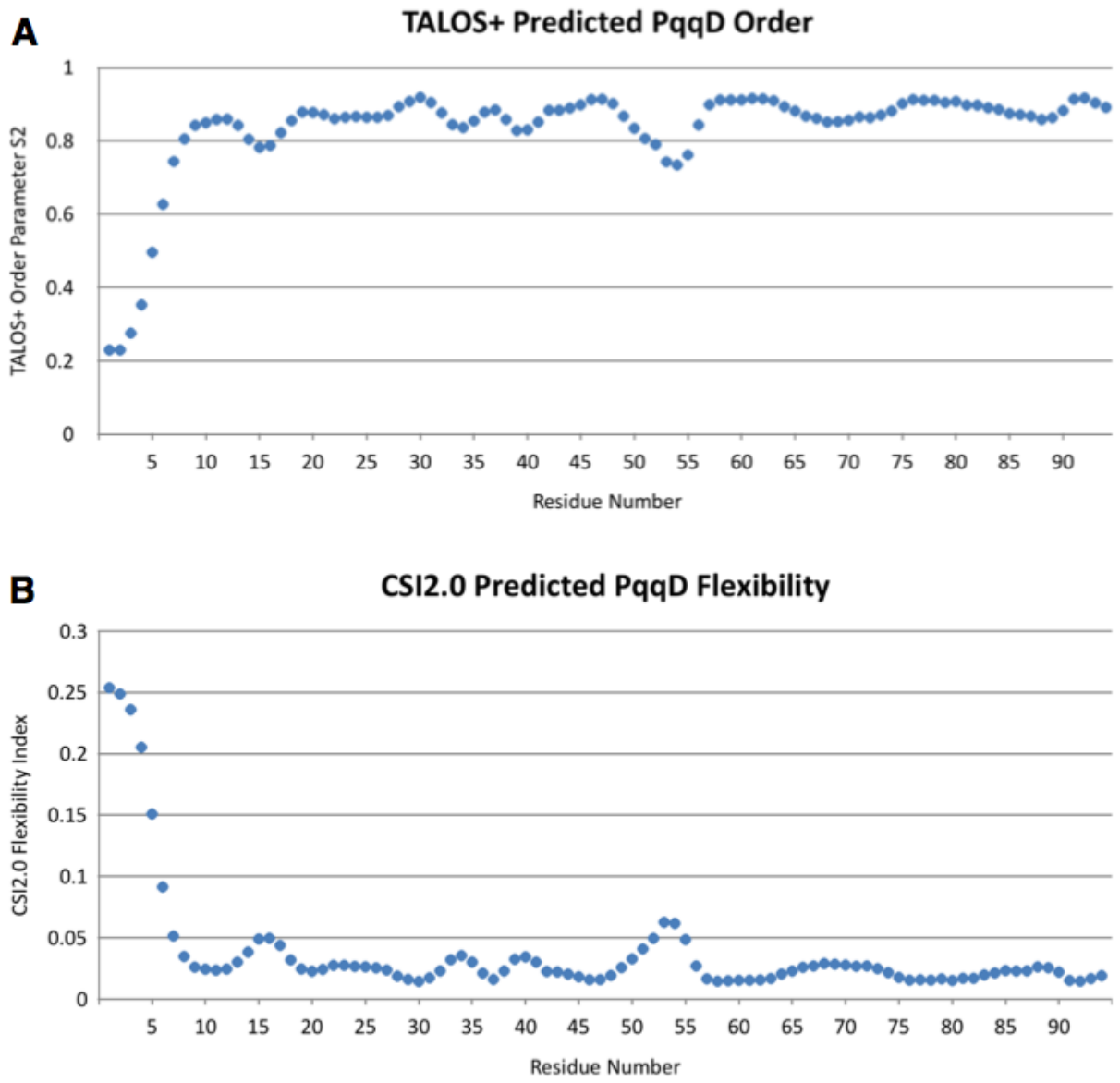

Figure S3. Structural order and flexibility by residue number as predicted by TALOS+ (A) and CSI2.0 (B).

K.p.p. PqqC ⇔ *Methylobacterium extorquens* PqqCD ⇔ *K.p.p.* PqqD alignments identifying the linker region

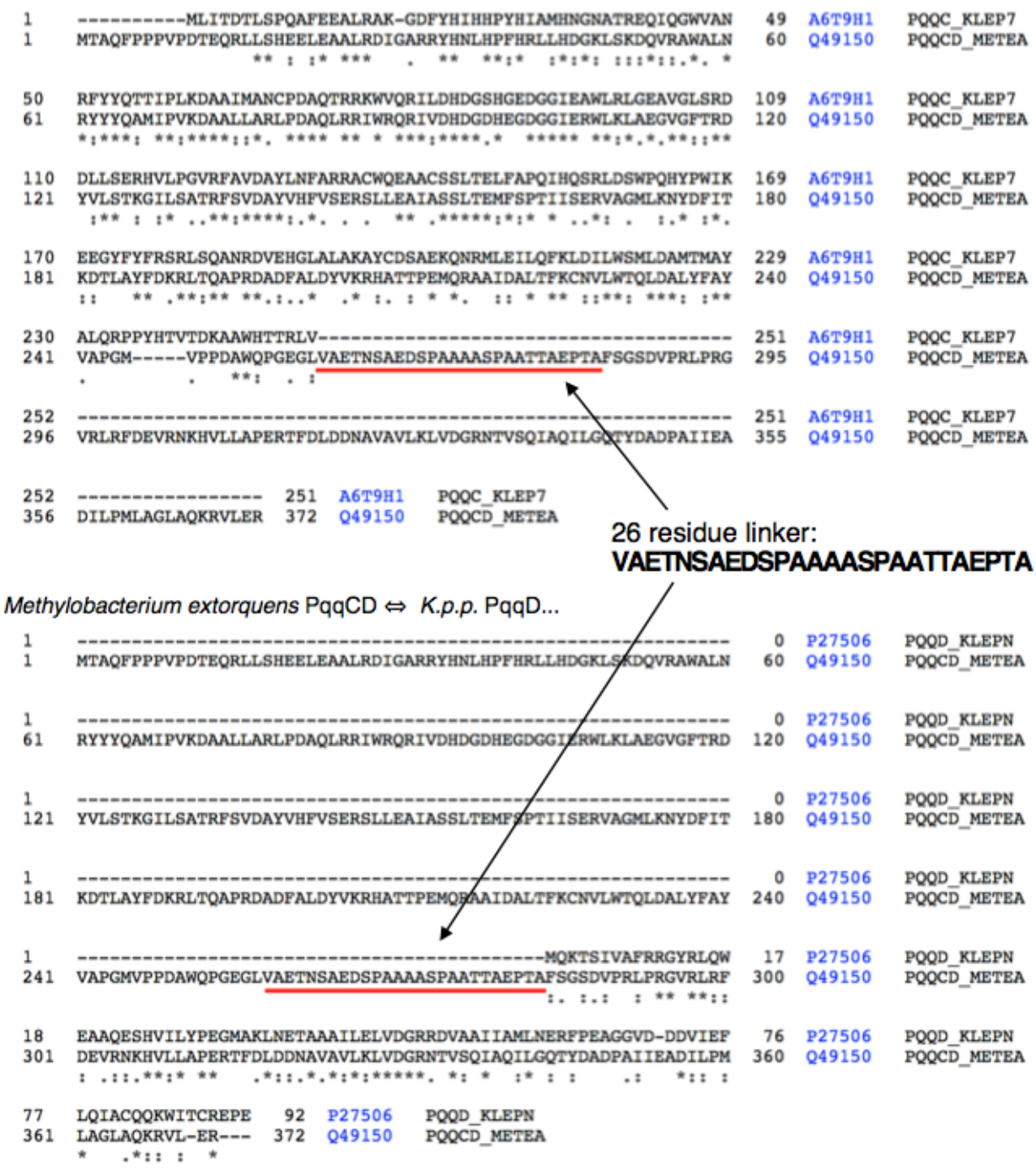

Figure S4. The linker region in MePqqCD was identified using an alignment of MePqqCD and *Klebsiella pneumoniae* PqqC and D.