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

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ALIGNMENT OVERLAP REGION		
From full CLUSTAL 0(1.2.3) multiple sequence alignment		
PpD_(B1JDZ9)	MSFDRKQVPNWRPGYRFQY	19
AcD_(P07781)	MNKEQFDLNLVPTWRQGYRFQF	22
KpD_(B5XX59)	MQKTSIVAFRRGYRLQW	17
AvD_(C1DEW6)	MSETTLNDIPQLRRGFRFOW	20
GoD_(Q9L3B1)	MTEAPHVVAEGTVLSFARGHRLQH	24
RpD_(Q6N8F4)	MAPRRISVSETCRPVLPRHARLKF	24
MexCD_(Q49150)	VAPGMVPPDAWQPGEGLVAETNSAEDSPAAAASPAATTAEPTAFSGSDVPRLPRGVRLRF	300
MspDE_(J7QTJ2)	MSEAQAARFVIGPDSRPAFTRYARLHE	27
XcD_(Q8P6M8)	MSTISRDSCPALRAGVRLQH	20
	*::	
PpD_(B1JDZ9)	EPAQKGHVLLYPEGMIKLNDSASLIGGLIDGKRDVNAIITELEQQFPG-VPEVADDIEQF	78
AcD_(P07781)	EPAQNGFVILYPEGMIKLNESAGAIGQYIDGQQNVSAIIAQLKQKFGD-ISEIDQDVVDY	81
KpD_(B5XX59)	EAAQESHVILYPEGMAKLNETAAAILELVDGRRDVAAIIAMLNERFPE-AGGVDDDVVEF	76
AvD_(C1DEW6)	EPAQNCHVLLYPEGMVKLNDSAAAILGQVDGDRSIAAIVAALRERFPE-SDGIEEDVLEF	79
GoD_(Q9L3B1)	DRVRDVWIVQAPEKAFVVEGAAPHILRLLDGKRSVGEIIQQLAIEFSAPREVIAKDVLAL	84
RpD_(Q6N8F4)	DDTRQRWVILAPERVLAPDEIAVEILQLCDGACDVAAIIDALAAKYTADRAEIGRDVMAM	84
MexCD_(Q49150)	DEVRNKHVLLAPERTFDLDDNAVAVLKLVDGRNTVSQIAQILGQTYDADPAIIEADILPM	360
MspDE_(J7QTJ2) XcD_(Q8P6M8)	DRARSRTVILAPERAYELDPIGLIVLRAIDGATRLADLCARLAQQYSAPLDVITRDVTAL	87 80
ACD_(Q8P6M8)	DRARDQWVLLAPERVVELDDIALVVAQRYDGTQSLAQIAQTLAAEFDADASEIETDVIEL : .:. :: ** : : ** : : *:	OU
PpD_(B1JDZ9)	MEVARGEHWITLA	91
AcD_(P07781)	MLVAKQQHWIDLV	94
KpD_(B5XX59)	LQIACQQKWITCREPE	92
AvD_(C1DEW6)	LEVARERSWIELH	92
GoD_(Q9L3B1)	LSELTEKNVLHT	96
RpD_(Q6N8F4)	LQDLADKGFLTEARETAP	102
MexCD_(Q49150)	LAGLAQKRVLER	372
MspDE_(J7QTJ2)	LQGLADKRLLRDGTDKFAPPPPSAFATSIAPFAGGPAGLLAELTHRCPLQCPYCSNPLEL	147
XcD_(Q8P6M8)	TTTLHQKRLLRL	92
	. :	

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).

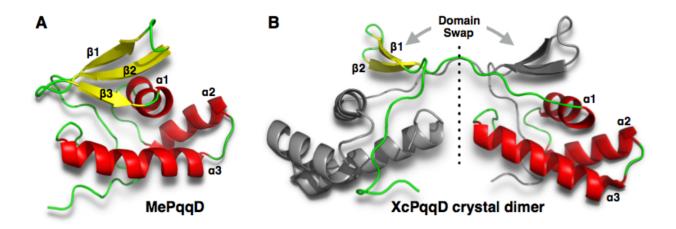
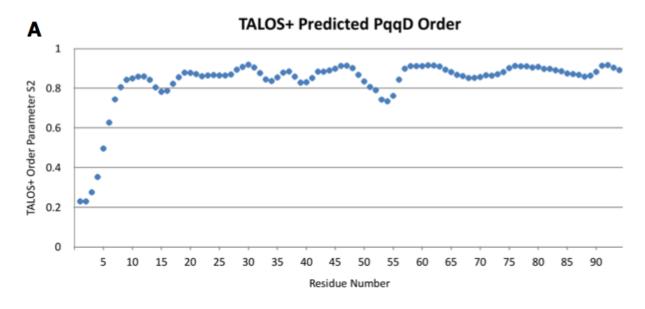


Figure S2. The PqqD structure. (A) The MePqqD monomeric NMR solution structure. (B) The XcPqqD dimeric crystal structure showing that the domain swapped β -hairpins occupy a similar position in the MePqqD monomer.



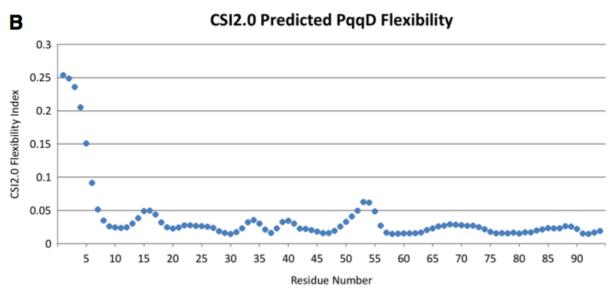


Figure S3. Structural order and flexibility by residue number as predicted by TALOS+ (A) and CSI2.0 (B).

K.p.p. PqqC \Leftrightarrow Methylobacterium extorquens PqqCD \Leftrightarrow K.p.p. PqqD alignments identifying the linker region

K.p.p. PqqC ⇔ Methylobacterium extorquens PqqCD...

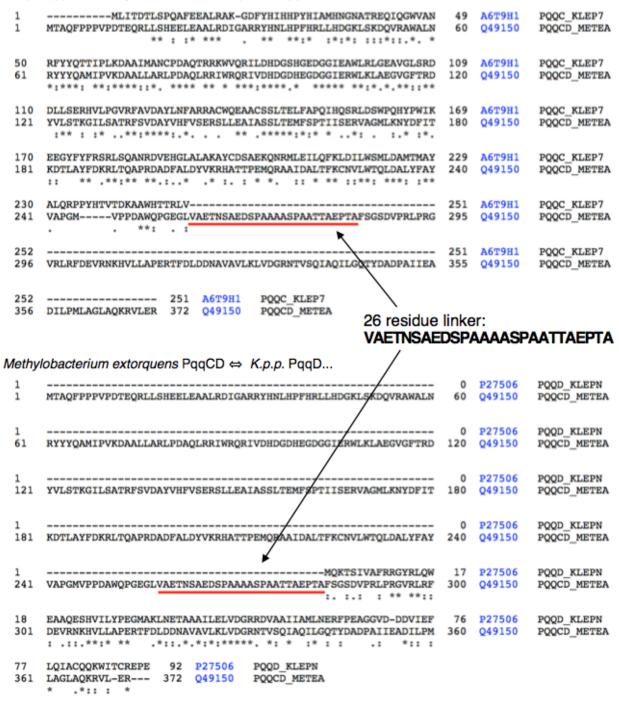


Figure S4. The linker region in MePqqCD was identified using an alignment of MePqqCD and *Klebsiella pneumoniae* PqqC and D.