Supplementary Materials

Structure and dynamics of the first archaeal parvulin reveal a new functionally important loop in parvulin-type prolyl isomerases

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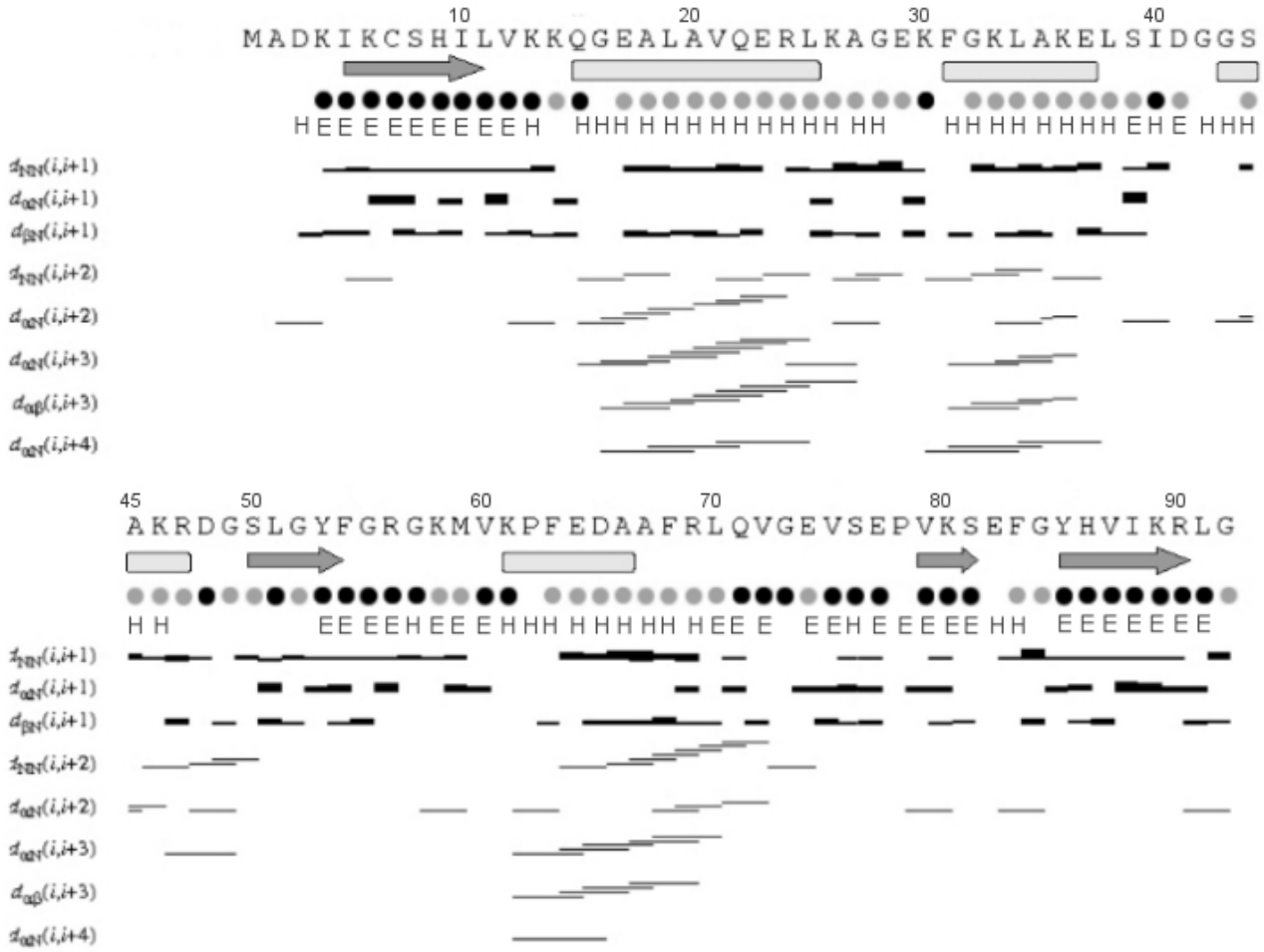

Figure S10: Short and medium range NOE connectivities observed in ^{15}N-edited 3D NOESY-HSQC spectrum. Positions of secondary structure elements in PinA are denoted as black arrows (β-sheets) and gray bars (α-helices). Values of $^{2}\boldsymbol{J}_{N(i)C\alpha(i-1)}$ couplings are shown as black (bigger than -7.2Hz) and gray (less than -7.2Hz) circles (Ding & Gronenborn, 2004) taking the sign of coupling into account (Kozminski et al., 2005). Please note that scalar $^{2}\boldsymbol{J}_{N(i)C\alpha(i-1)}$ couplings correlate with ψ backbone torsion angles of their preceding residues. Predictions originating from the TALOS+ software for 40 residues are indicated as 'H' (helix) or 'E' (extended), respectively.

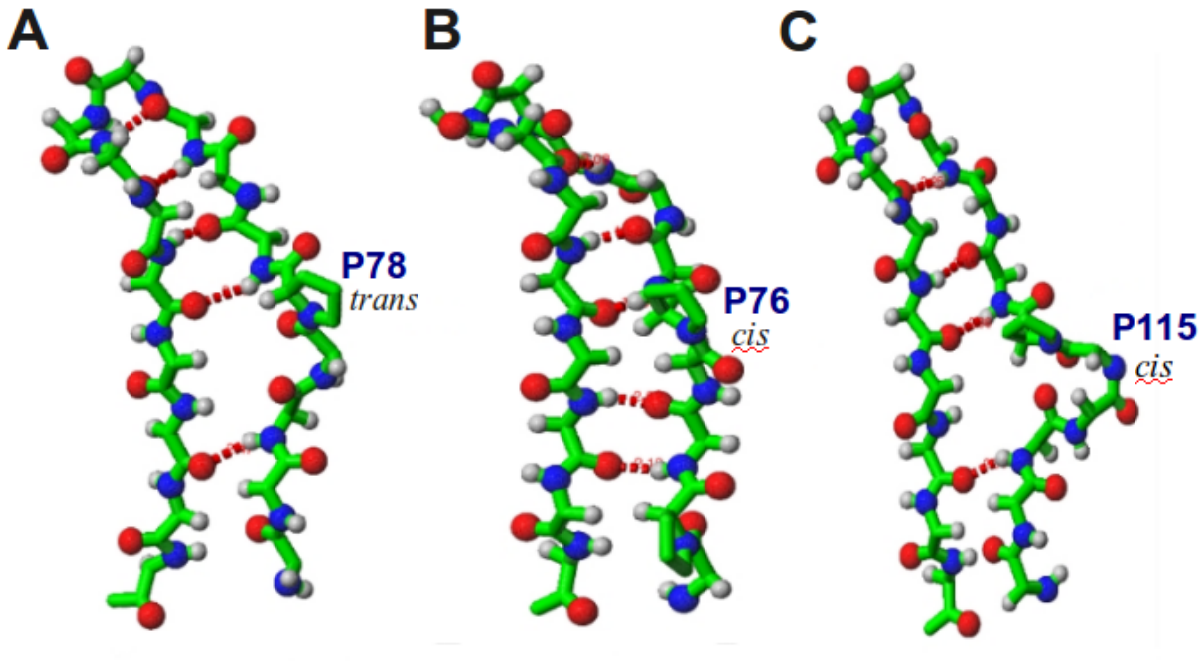

Figure S11: Conformation of a conserved Xaa-Pro motif in different parvulins. Conformation and hydrogen bonding network between the third and fourth beta-strands are shown for **(A)** *C. symbiosum* PinA (PDB 2RQS), **(B)** *E. coli* Par10 (PDB 1JNS) and **(C)** *H. sapiens* Par14 (PDB 1EQ3). The conserved Xaa-proline at the beginning of the third beta-strand shows *trans* conformation in *C. symbiosum* PinA. However, the Gly76-Pro77 bond in *E. coli* Par10 as well as the Pro114-Pro115 bond in human Par14 exhibit *cis* conformation, which was additionally confirmed by chemical shift analysis (Shen & Bax, 2010).

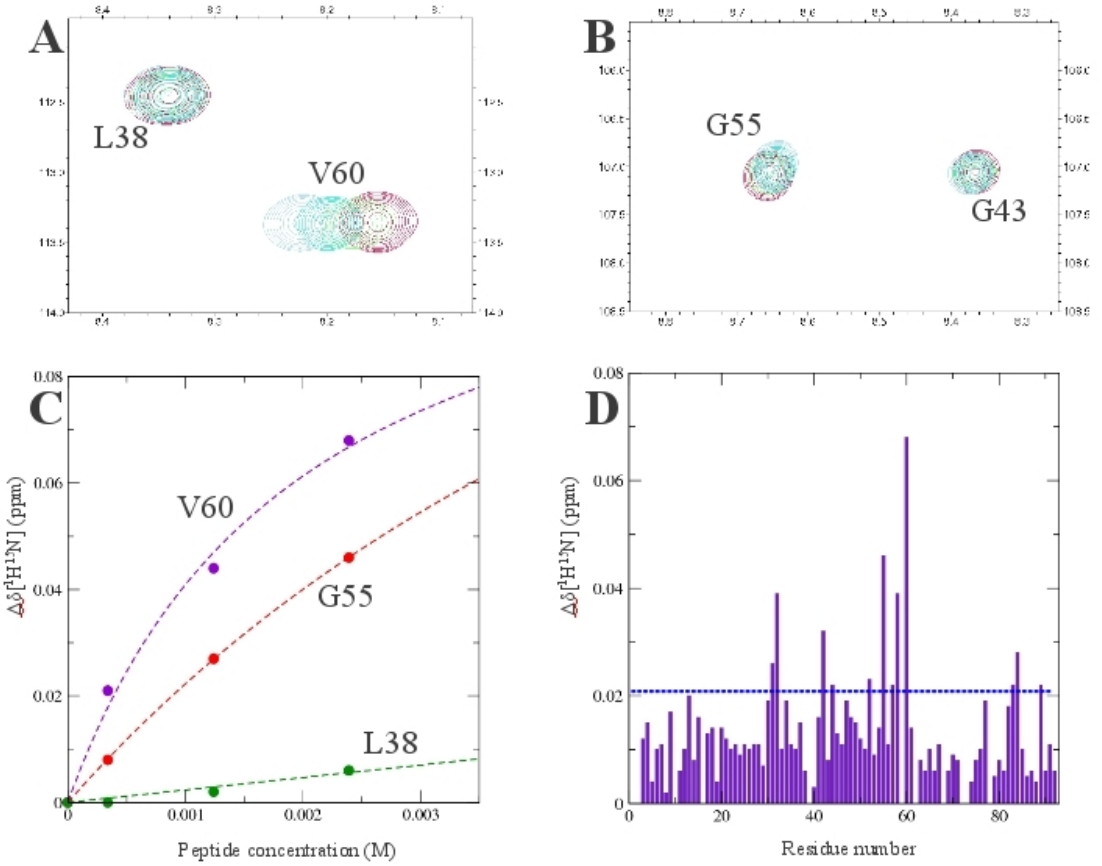

Figure S12: Binding of the peptide HQSPWHH to PinA from *C. symbiosum*. **(A, B)** Part of ^{1}H-^{15}N HSQC spectra demonstrating chemical shifts after the addition of peptide. Cross peaks for **(A)** Val60 and **(B)** Gly55 are shown. Protein/peptide ratios were 1:0, 1:1, 1:4 and 1:8 shown in red, orange, yellow and green, respectively. **(C)** Best fit of chemical shift perturbations for Leu38, Gly55 and Val60. **(D)** Chemical shift perturbations in PinA upon binding to the peptide HQSPWHH at 283 K. The threshold of 0.022 ppm is indicated by a blue line.

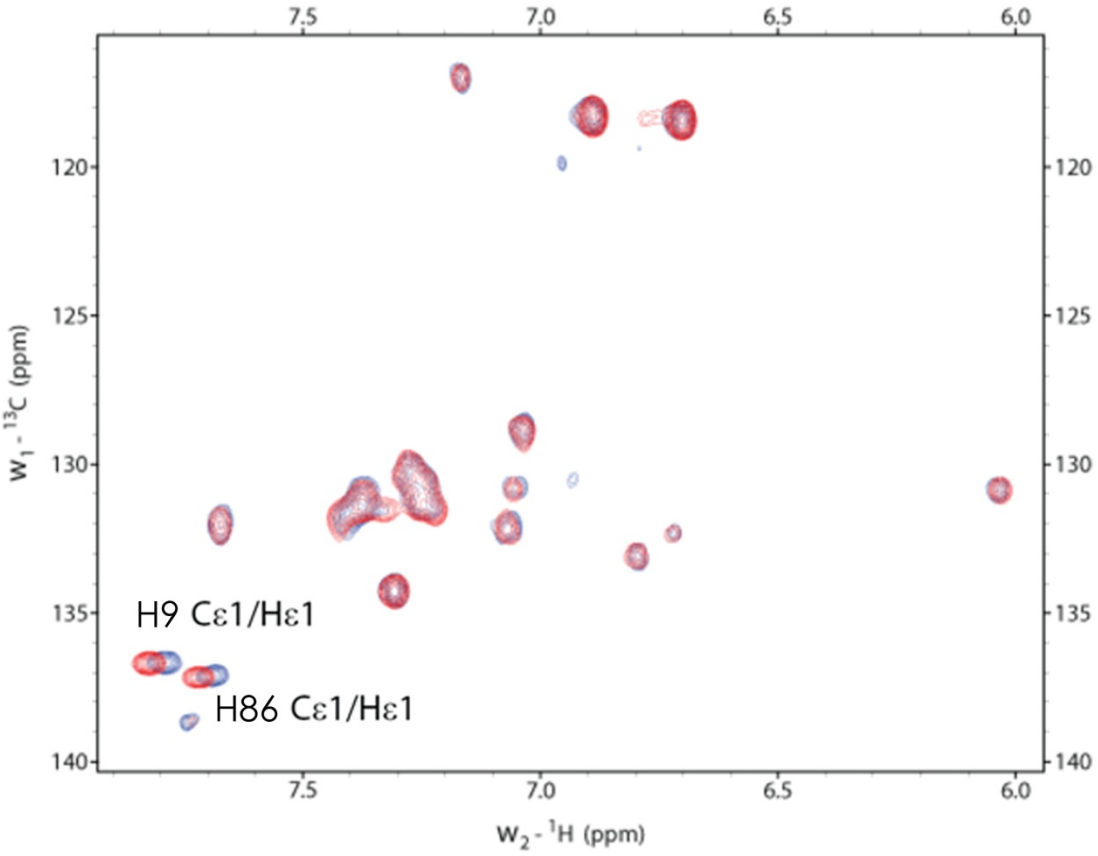

Figure S13: Titration of the PinA protein with the peptides selected by phage display was also monitored with ^{1}H-^{13}C correlation spectra. Only for the best binding peptide HQSPWHH chemical shift changes for the Cε1/Hε1 correlation of the two conserved histidines, His9 and His86, could be observed.

Supplementary table 1: Peptide sequences found after screening a phage displayed 7-mer peptide library using PinA as bait

7-mer motifs	Remarks
HKRPRNN (5x)*	Besides the HQSPWHH peptide, HKRPRNN was also tested for HSQC titrations. This peptide however only gave minor chemical shift perturbations and was not investigated further. * These peptides have been identified multiple times. ** According to the manufacturer of the 7-mer library (NEB), this is a target-unrelated peptide that might obscure whole panning procedures. It occurred only once during our screening, proving the selection to be effective.
HQSPWHH (3x)*	
APSPMIW	
WDPSQMR	
SLHSRPN	
TIEQHPP	
VYLTGPS	
LDRANVF	
NQLTTLN	
SHTIRML	
YVHQQRH	
TMCIYCT	
GLCCSRL	
HAIYPRH**	