Supplementary Information

Methionine in a protein hydrophobic core drives tight interactions required for assembly of spider silk

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Supplementary Tables

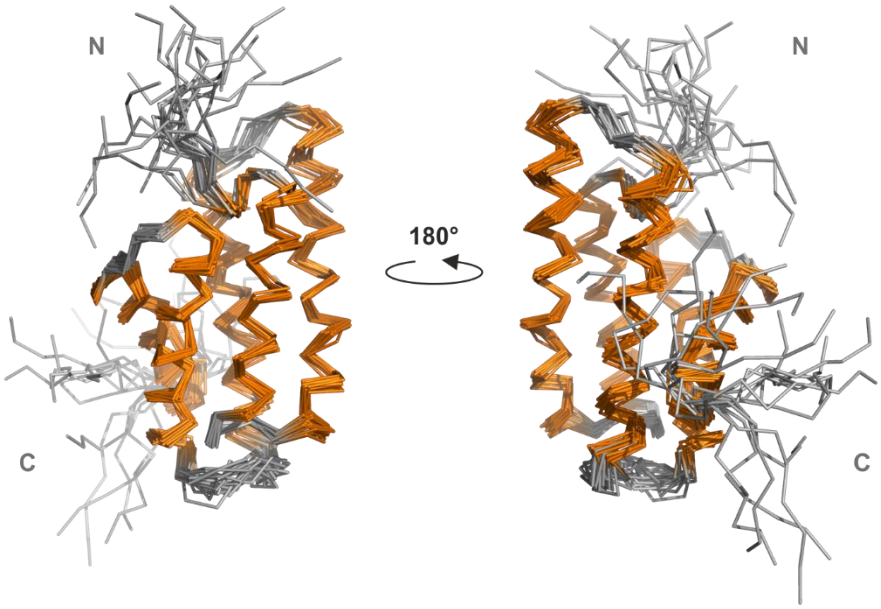
Supplementary Table 1: Structural statistics for the NMR solution structure of L6-NTD

Conformational restricting restraints	
Total NOE distance restraints	1673
intraresidue $\|i = j\|$	448
sequential $\|i - j\| = 1$	463
medium-range $1 < \|i - j\| < 5$	347
long-range $\|i - j\| \geq 5$	415
Dihedral angle restraints (Talos-N)	216
No. of restraint per residue	14.4
No. of long-range restraints per residue	3.2
Residual restraint violations[a]	
Average no. of distance violations per structure	
0.1-0.2 Å	6.95
0.2-0.5 Å	0
>0.5 Å	1
Average no. of dihedral angle violations per structure	
1-10°	4.4
>10°	0
Model quality (ordered residues)[a]	
RMSD backbone atoms (Å)	2.9
RMSD heavy atoms (Å)	2.9
RMSD bond lengths (Å)	0.02
RMSD bond angles (°)	0.25
MolProbity Ramachandran statistics[a]	
Most favored regions	98.4
Allowed regions	1.6
Disallowed regions	0
Global quality scores (raw/Z score)[a]	
Verify3D	0.39
Prosall	0.84
PROCHECK (φ-ψ)	0.47
PROCHECK (all)	-0.11
MolProbity clash score	2.80
Model contents	
Ordered residue ranges (HetNOE > 0.6)	0-60, 63-82, 90-108, 110-129
Total no. of residues	137
BMRB accession number	27683
PDB ID code	6QJY

[a] calculated using Protein Structure Validation Software 1.5 for using ordered residues (HetNOE > 0.6). Average distance violations were calculated using the sum over r^{-6}

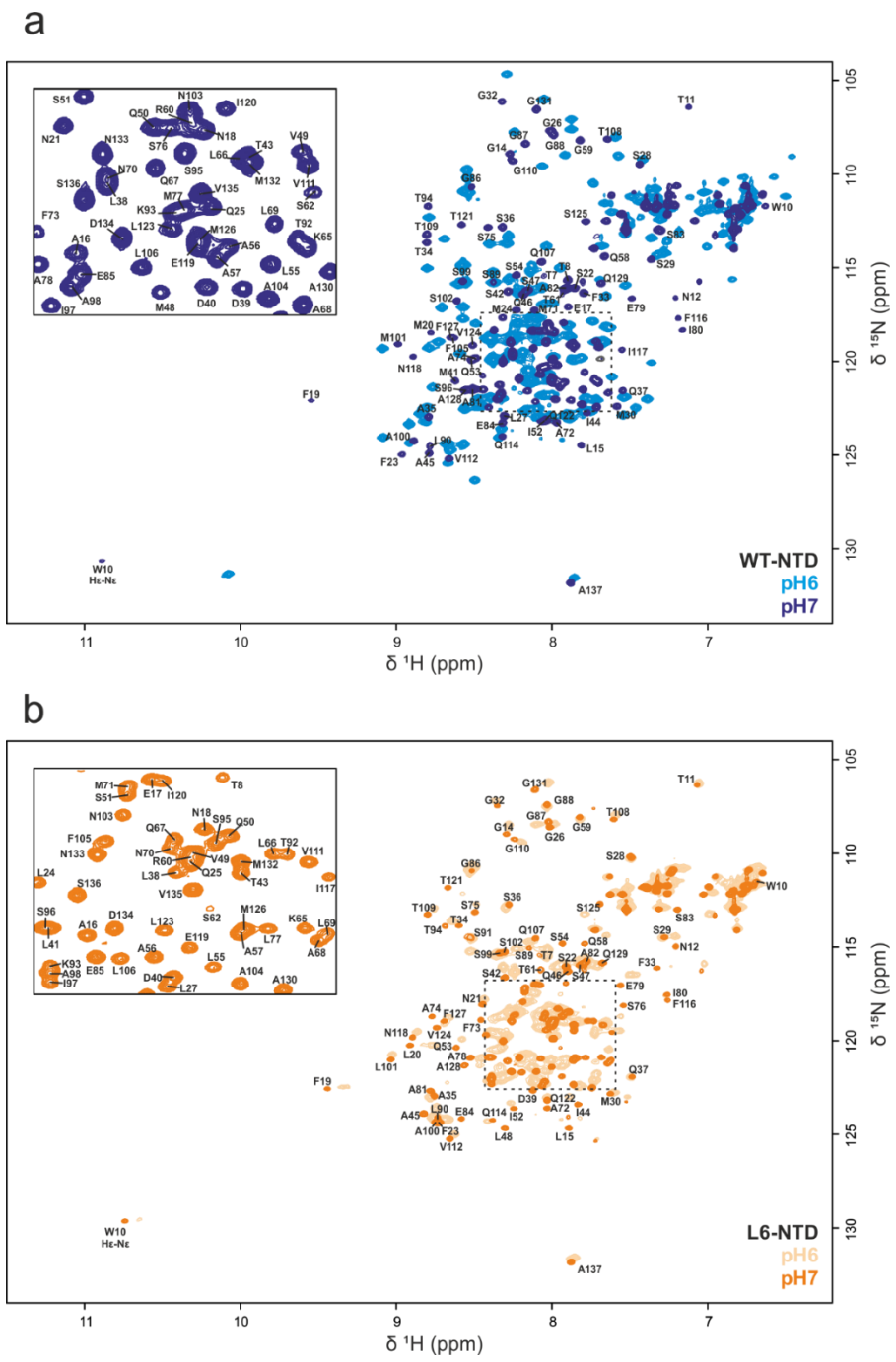
Supplementary Figures

Supplementary Figure 1



Structure bundle of L6-NTD determined by solution NMR spectroscopy. Alignment of the 20 lowest-energy conformers shown as backbone trace. The backbone heavy atom RMSD for the NMR structure bundle is 1.2 Å. Helices are highlighted orange. N- and C-terminus are indicated.

Supplementary Figure 2



^{1}H, ^{15}N-HSQC NMR spectra of WT-NTD and L6-NTD. (**a**) Spectra of WT-NTD recorded in pH 7.0 and 200 mM ionic strength (blue) and in pH 6.0 and 8 mM ionic strength (cyan). (**b**) Spectra of L6-NTD recorded in pH 7.0 and 200 mM ionic strength (orange) and in pH 6.0 and 8 mM ionic strength (light orange). Assignments for the spectra recorded under monomer conditions (pH 7.0) are indicated (source data are provided in the BMRB; entry 18262: WT-NTD; entry 27683: L6-NTD).