Supplementary material
for

A conserved charged single alpha helix with a putative steric role in paraspeckle formation

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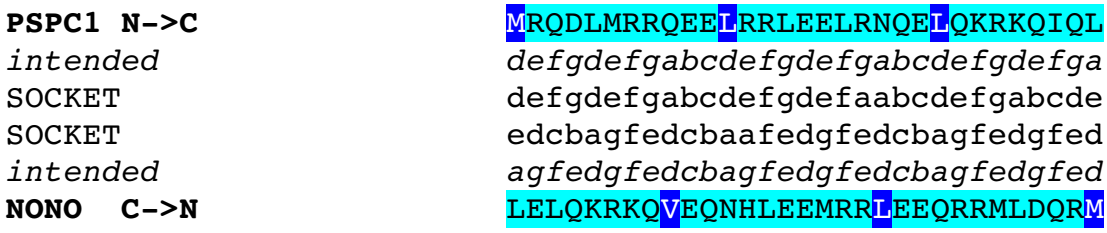


Figure S1.
Intended residue pairings in the core segment of the modeled extended coiled coil region. Charavcteristic hydrophobic residues in the hendecad repeat are highlighted. Residues shown: PSPC1_HUMAN: 320-350, NONO_HUMAN: 312-342

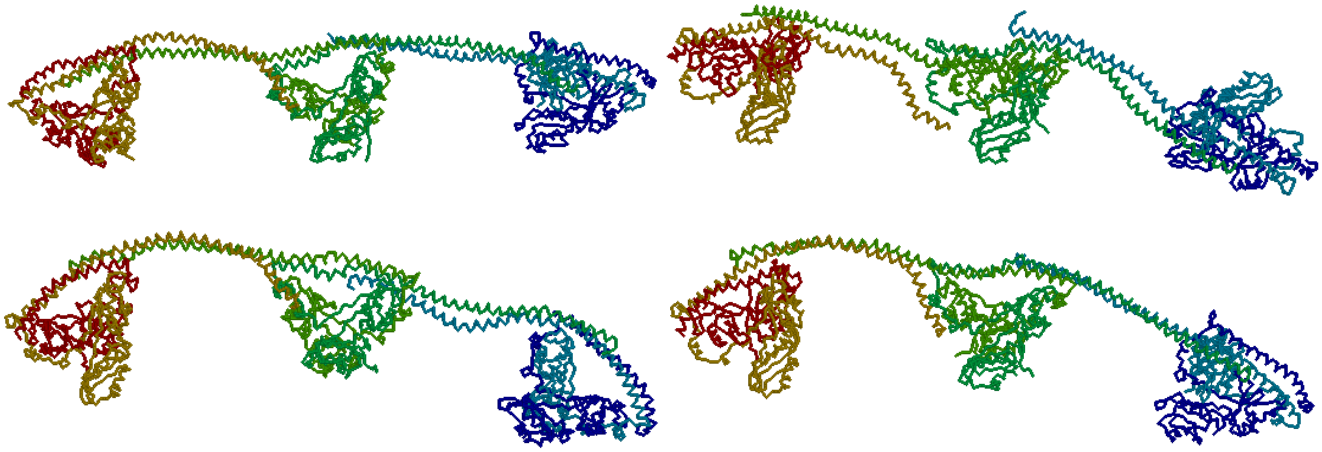
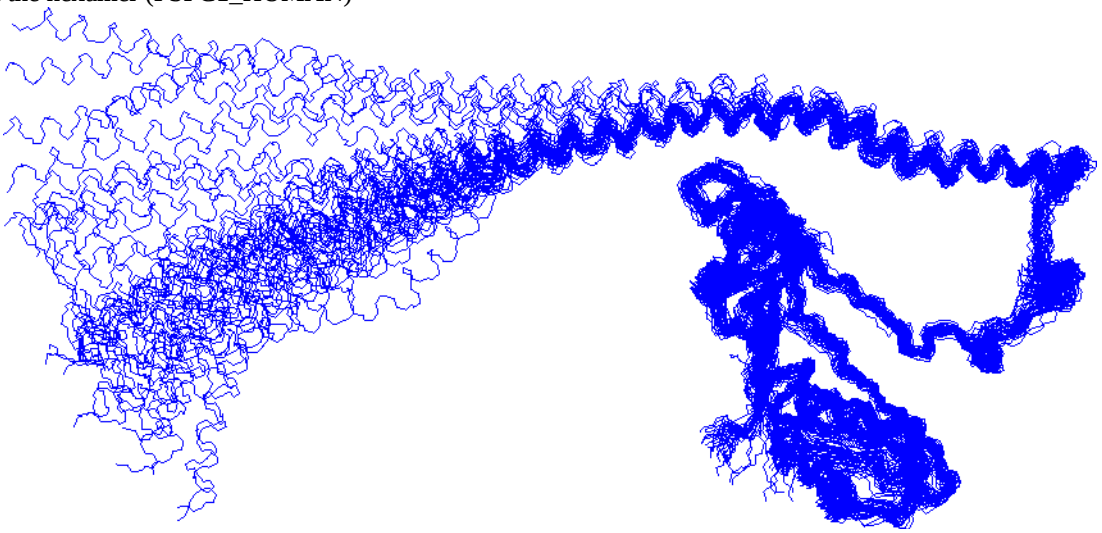


Figure S2.
Snapshots of the 20 ns MD simulation of the hexameric model, from top left, clockwise: 5 ns, 10 ns, 15 ns , 20 ns. The AMBER99SB-ILDN force field was used with the GBSA method for implicit solvent modeling. Born radii were calculated with the OBC method. The hexameric model was energy minimized to the 500 kJ/mol/nm force limit. To relax the structure and particularly the side chains in the modeled coiled coil region, 10 rounds of alternating MD runs with and without position-restrained backbone atoms were performed. These simulations were performed at 100 K for 100 ps with a step size of 0.1 fs. The production run lasted for 20 ns at 298 K with a step size of 0.1 fs.
Cα trace shown, coloring according to chains. The extended coiled coil regions are highly flexible allowing different relative orientations of the core dimers. The CSAH segments make contacts with the neighboring core dimers.
Note that the structures neither contain the disordered N- and C-termini nor the NEAT1 lncRNA required for paraspeckle formation, thus the results of the simulation might not reflect physiologically relevant states/conformations.
Figures prepared with RasMol (openrasmol.org).

Chain C in the hexamer (PSPC1_HUMAN)



Chain D in the hexamer (NONO_HUMAN)

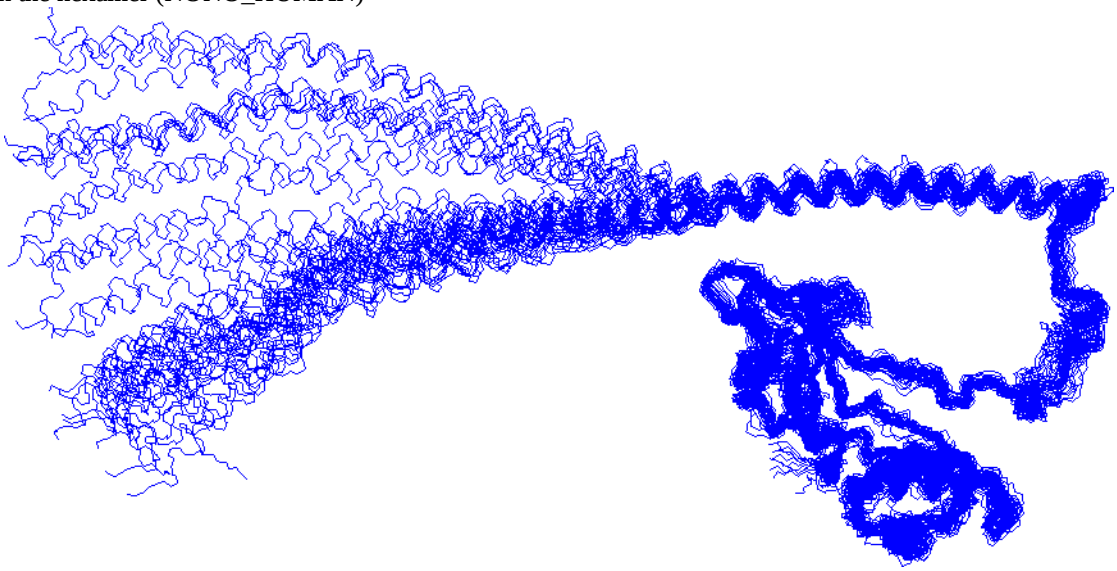


Figure S3. Fitted snapshots of the 20 ns MD simulation for chains C (PSPC1, top) and D (NONO, bottom). Fit was performed for residues 66-320 for chain C (backbone RMSD 2.06 ± 0.61 Å for the fitted part and 4.72 ± 2.14 Å overall) and 66-304 for chain D (backbone RMSD 1.92 ± 0.49 Å for the fitted part and 5.38 ± 2.80 Å overall), corresponding to the range of residues in the 3SDE structure. This 'core' remains stable during the simulation but the extended coiled coil/CSAH segment adopts different orientations while remaining helical (see also Supplementary Table S4). Figures prepared with MOLMOL (Koradi et al. (1996) J. Mol. Graph. 14, 51-55).