SUPPORTING INFORMATION FOR:

Localization of Zn^{2+} ions affects the structural folding and mechanics of Nereis virens Nvjp-1

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The following files are included:

Table S1. Secondary Structure Propensity (%) for Figure 3a.

Secondary Structure	Initial	A	B	C
Coil	9.7	42.7	40.2	35.4
Helix	9.4	5.2	6.7	4.8

Table S2. SASA (nm^2) for Figure 3b.

A	B	C
260.957 ± 0.281	253.710 ± 1.725	259.840 ± 1.481

Table S3. Final Number of MC bonds for Figure 3c.

Amino Acid	A-initial	A	B-initial	B	C-initial	C
Asp	3	24±0	3	32±0	3	23±0
Gly	7	2±0	18	3±0	7	0±0
His	21	11±0	19	13±0	20	10±0
Total Coordinated Amino Acids	40	42±0	53	56±0	40	40±0

Table S4. Hydrogen bonds for Figure 3d.

Initial	A	B	C
47	42.3±4.6	45.3±5.8	48±6.2

Files included:

Dir: Structures
- 1.1. File: nvjp.pdb (Initial PDB structure from Chou et al.[14])
- 1.2. File: simA-final-remd.pdb (final lowest energy pdb of simulation A)
- 1.3. File: simB-final-remd.pdb (final lowest energy pdb of simulation B)
- 1.4. File: simC-final-remd.pdb (final lowest energy pdb of simulation C)

Dir: REMD
1. Dir: Simulation
   - 1.1. Dir: Structure_name
     - 1.1.1. File: clone_reps.vmd (from NAMD replica exchange distribution files)
     - 1.1.2. File: replica_util.vmd (from NAMD replica exchange distribution files)
     - 1.1.3. File: replica.namd (from NAMD replica exchange distribution files)
     - 1.1.4. File: show_replicas.namd (from NAMD replica exchange distribution files)
     - 1.1.5. Dir: md
       - 1.1.5.1. Dir: output (where output of replicas are saved)
       - 1.1.5.2. File: createjobs.sh (file to automatically create job files sequentially, useful if cluster has a time limit)
       - 1.1.5.3. File: fold_nvjp.conf (from NAMD replica exchange distribution files, sets number of websites, sets temperature range, sets number of runs)
       - 1.1.5.4. File: jobx.conf (restarts REMD simulations)
       - 1.1.5.5. File: nvjp_base.namd (sets base NAMD parameters including time step, box size, force field, parameter file, ensemble)
       - 1.1.5.6. File: par_all27_prot_na.prm (from CHARMM force field files)
       - 1.1.5.7. File: readme.md (overview of files)
       - 1.1.5.8. File: sort.sh (sort simulation files to bring all replicas in folder 0 (350 K) to same folder
       - 1.1.5.9. File: submit.sh (submit multiple jobs sequentially, useful if cluster has a time limit)
2. Dir: Analysis
   - 2.1. File: mc.tcl; calculates number of metal-coordinate bonds (from https://www.ks.uiuc.edu/Research/vmd/script_library/scripts/metal_environment/)
   - 2.2. File: sasa.tcl; calculates SASA from VMD (from https://www.ks.uiuc.edu/Research/vmd/mailing_list/vmd-l/18670.html)

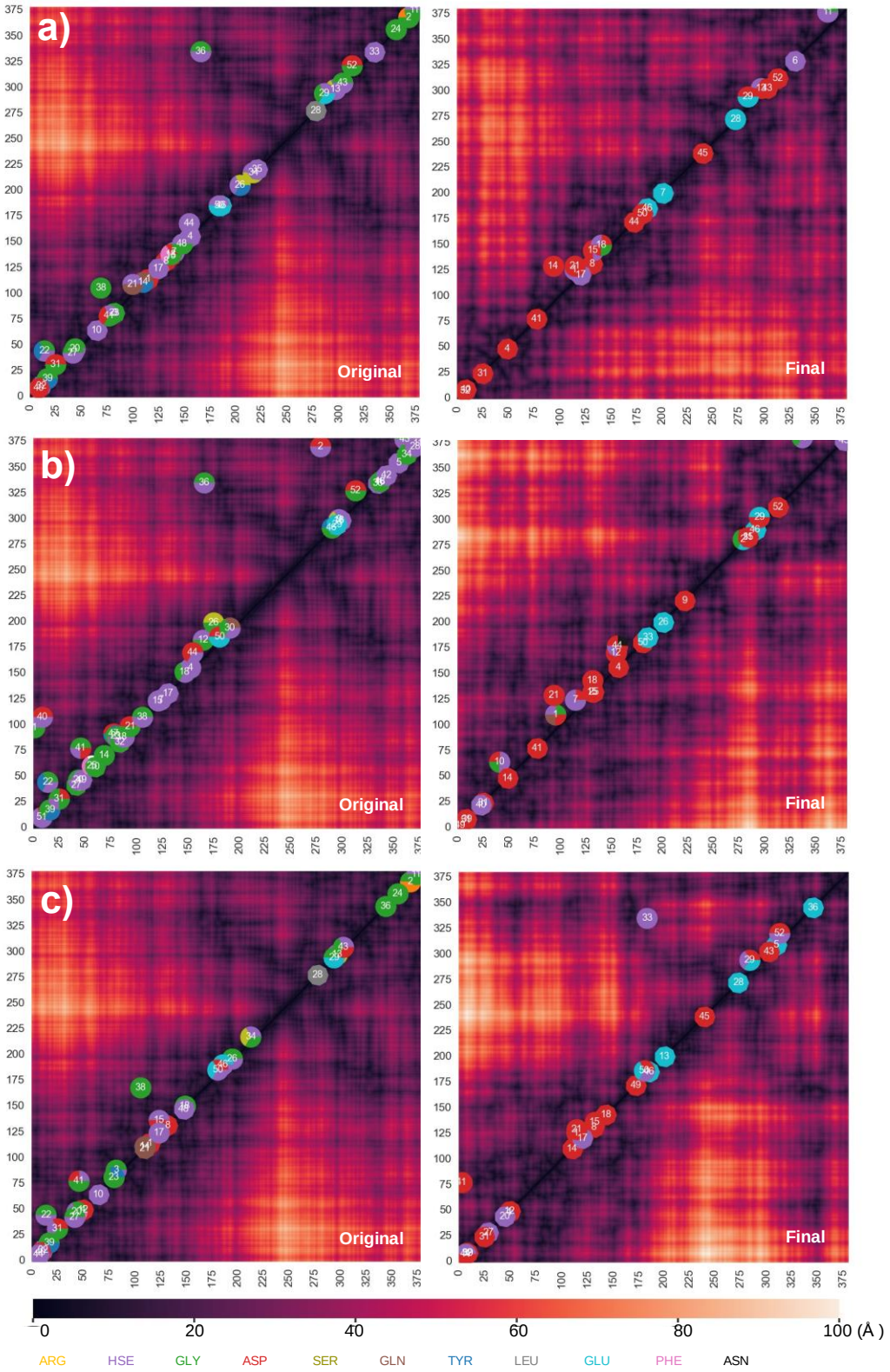

Figure S1. Contact map showing initial coordination and final coordination geometries of simulations A, B, and C. Contact maps for the original starting condition and final representative protein structure after REMD simulations are shown. The circles represent the position of the metal ions, and the indices are used to visualize where the metal ion stays or moves during the simulation. Metal ions are colored by the coordinating residues in the binding pocket.

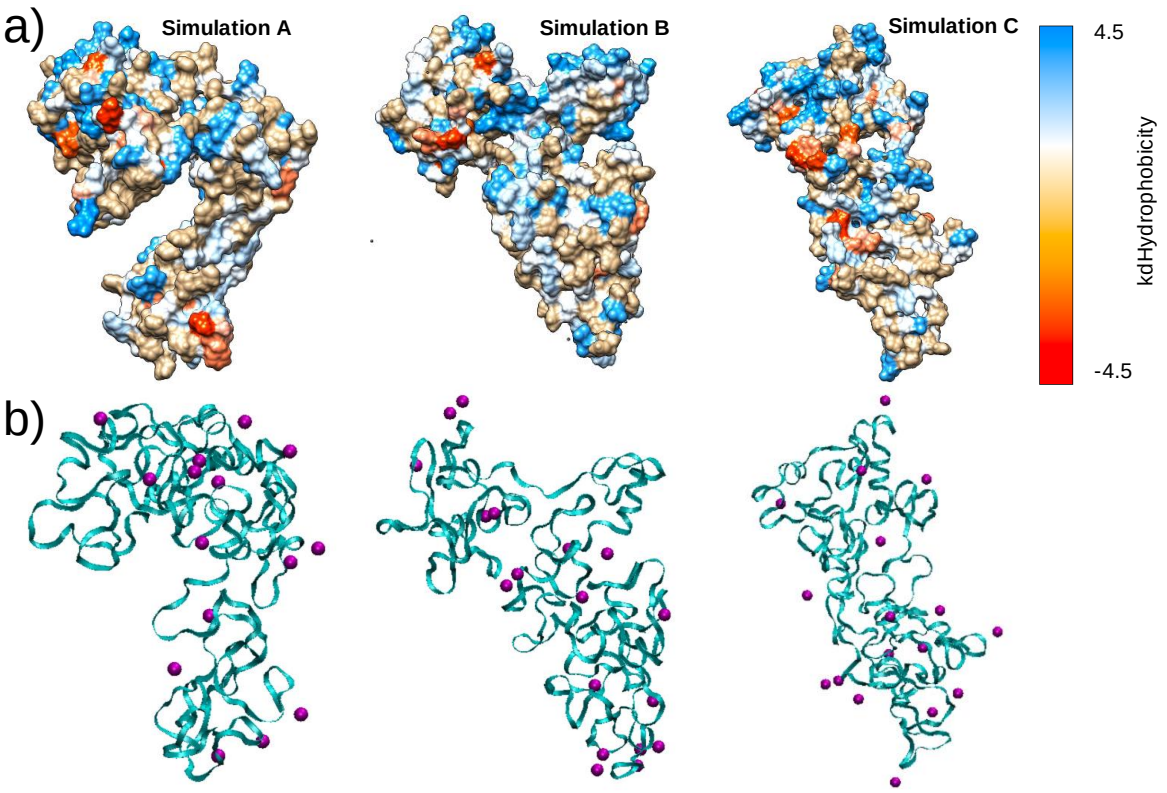

Figure S2. Surface characterization of Nvjp-1 proteins to suggest intermolecular crosslinking between proteins. a) The Kyte-Doolittle scale in Chimera is used to assess the hydrophobicity of the surface. In each protein, there are several hydrophobic or hydrophilic regions that may participate in intermolecular crosslinking. b) Several Zn^{2+} ions remain coordinated to the surface of the protein, even though they do not participate directly in internal intramolecular loadbearing interactions. These surface Zn^{2+} ions can serve as potential intermolecular crosslinking sites.

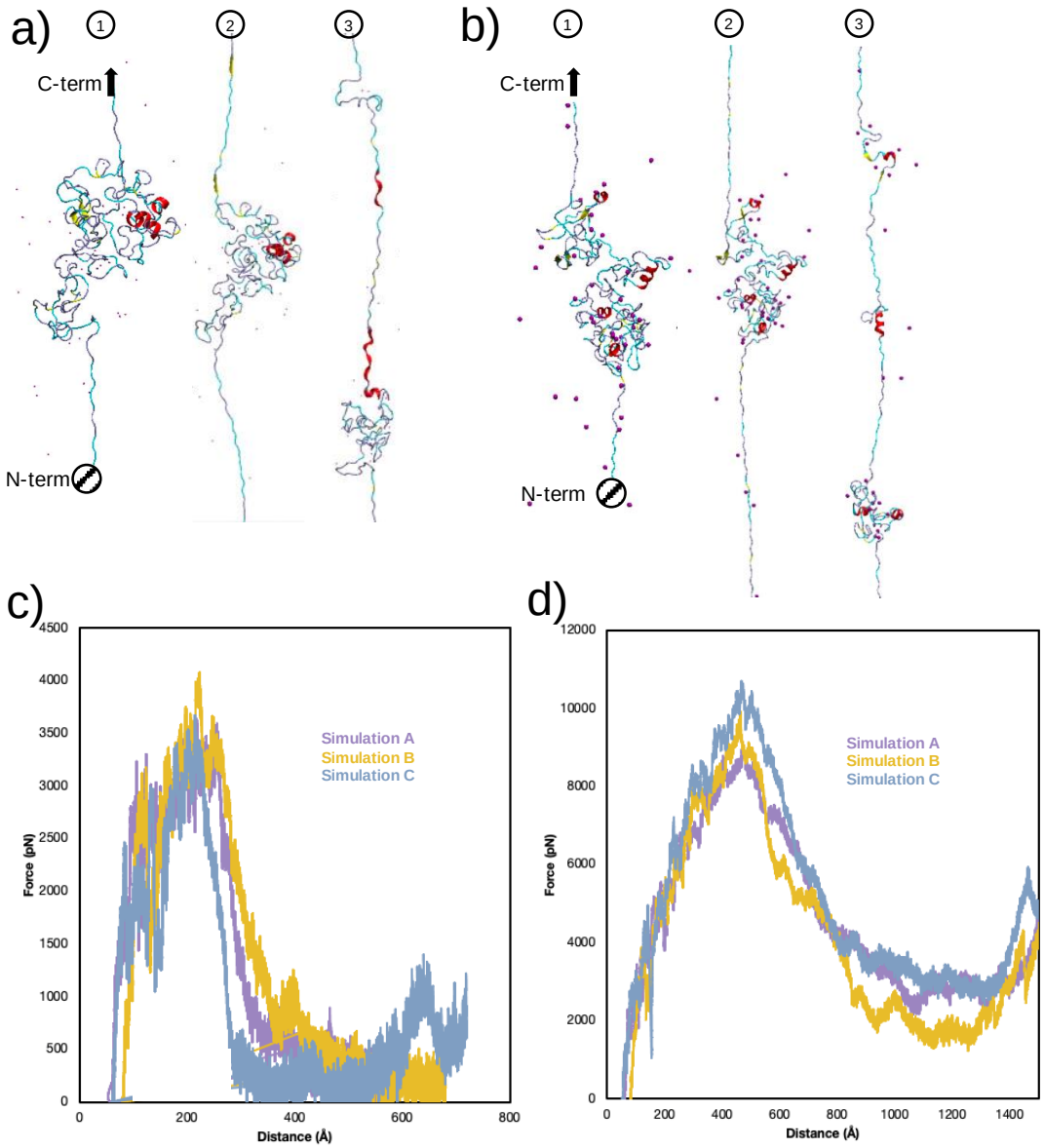

Figure S3. Steered molecular dynamics of Nvjp-1 proteins. Screenshots of Nvjp-1 proteins show how the protein deforms for a) simulation A and b) simulation B. Numbered circles correspond to the deformation snapshots in **Figure 5a**. SMD pulling tests for the three models at c) 0.2 m/s and d) 20 m/s.