

**NMR STRUCTURE OF THE N-TERMINAL COILED COIL DOMAIN OF THE ANDES
HANTAVIRUS NUCLEOCAPSID PROTEIN**

Yu Wang,^{1#} Daniel M. Boudreaux,^{2#} D. Fernando Estrada,¹ Chet W. Egan,¹ Stephen C. St. Jeor,²
and Roberto N. De Guzman^{1*}

Department of Molecular Biosciences¹, University of Kansas, Lawrence, KS 66045 USA, and
Department of Microbiology and Immunology², University of Nevada, Reno, NV 89557 USA

Running head: Andes hantavirus nucleocapsid coiled coil

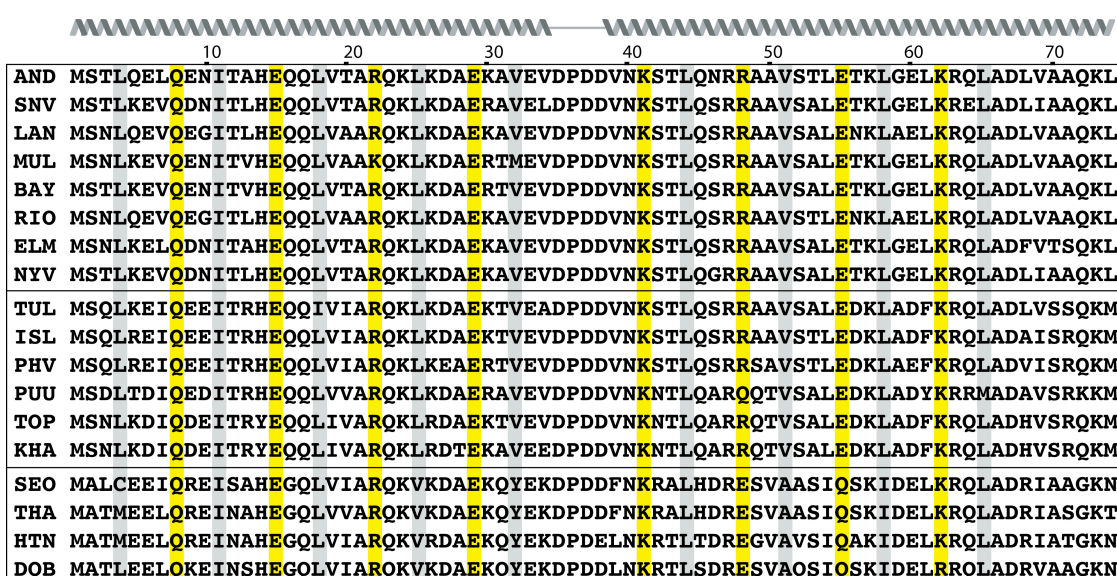


Fig. S1. Sequence alignment of hantavirus nucleocapsid N¹⁻⁷⁴ coiled coil domain with the conserved hydrophobic (gray) and polar (yellow) heptads highlighted. The sequences are arranged according to hantaviral species that cause: **(top)** HCPS (Hantavirus CardioPulmonary Syndrome), **(middle)** non-pathogenic or mild form of HFRS (Hemorrhagic Fever with Renal Syndrome) and **(bottom)** severe form of HFRS. The hantavirus species are: AND, Andes; SNV, Sin Nombre; LAN, Laguna Negra; MUL, Muleshoe; BAY, Bayou; RIO, Rio Mamore; ELM, El Moro Canyon; NYV, New York; TUL, Tula; ISL, Isla Vista; PHV, Prospect Hill; PUU, Puumala; TOP, Topografov; KHA, Khabarovsk; SEO, Seoul; THA, Thailand; HTN, Hantaan; DOB, Dobrava.

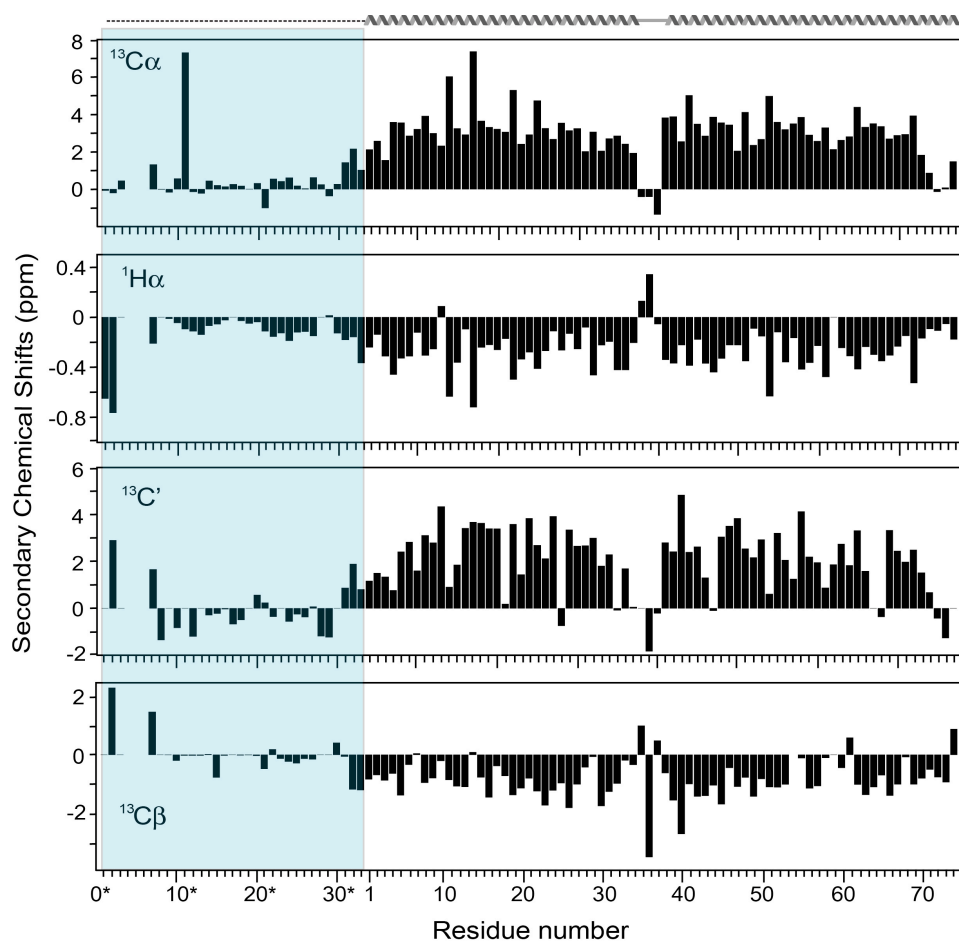


Fig. S2. Secondary C^α , H^α , C' , and C^β chemical shifts show that the first 33 residues (shaded), which are the His-tag from pET151, lack secondary structure whereas the Andes virus N^{1-74} region consists of two α -helices.

Table S1. Structural statistics for 20 NMR structures of Andes virus N¹⁻⁷⁴ coiled coil domain.

Total unambiguous distance restraints	1432
Intraresidue (i,i)	92
Sequential (i, i+1)	361
Medium Range (2<= i-j <=4)	700
Long Range (i-j > 4)	279
Hydrogen bond restraints (19 hydrogen bonds)	38
Total dihedral angle restraints	135
Phi	73
Psi	62
RMS difference from mean structure	
Backbone atoms (N,C ^α ,C ^γ) (Å)	0.21
All heavy atoms (C,N,O) (Å)	0.53
Violation analysis	
Max distance violation (Å)	0.27
Max dihedral angle violation (°)	3.2
Energies	
mean AMBER energy (kcal mol ⁻¹)	-3861
mean restraint energy (kcal mol ⁻¹)	117
Ramachandran plot	
Most favorable region	91.4%
Additionally allowed regions	8.2%
Generously allowed regions	0.4%
Disallowed regions	0.1%

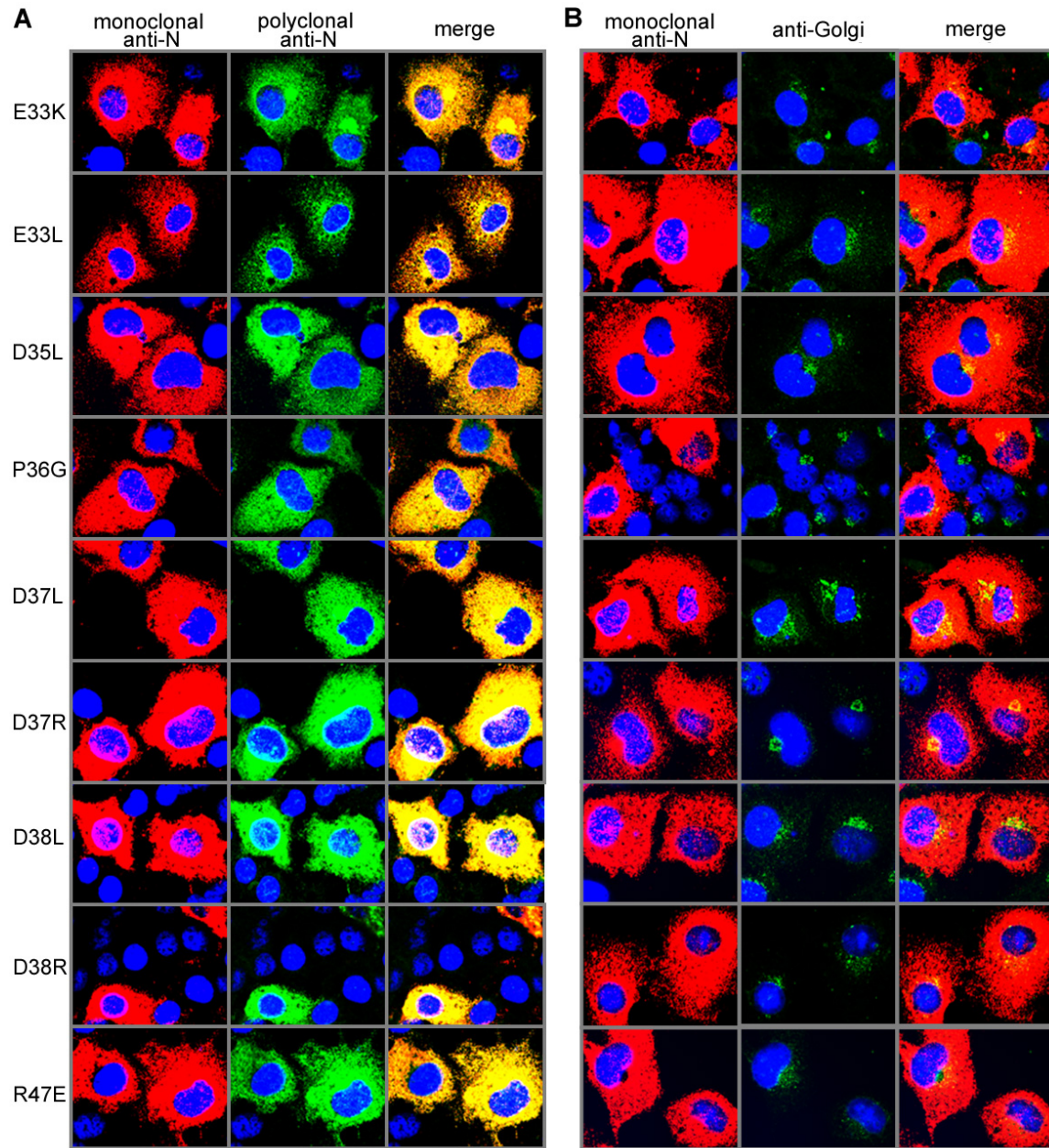


Fig. S3. Immunocytochemistry of full length N protein with mutations in the N¹⁻⁷⁴ coiled coil domain. Cos-7 cells were transfected with wild type and mutant N protein, and doubly stained with **(A)** monoclonal and polyclonal anti-N antibodies, and **(B)** monoclonal anti-N and Golgi-specific antibodies. The anti-N monoclonal antibody was AB34757 from Abcam (Cambridge, Mass.).