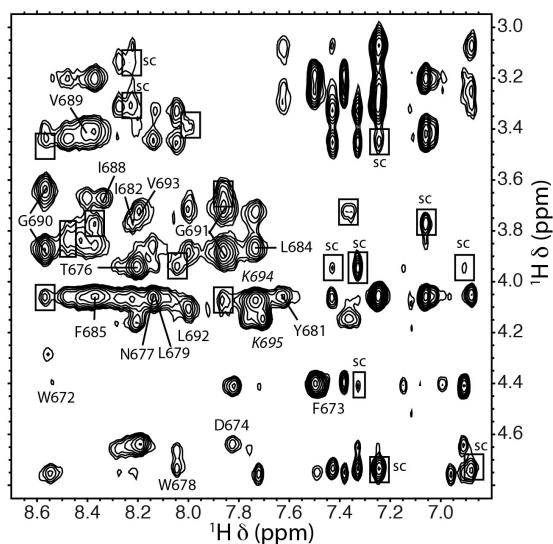


## **Supplemental Data**

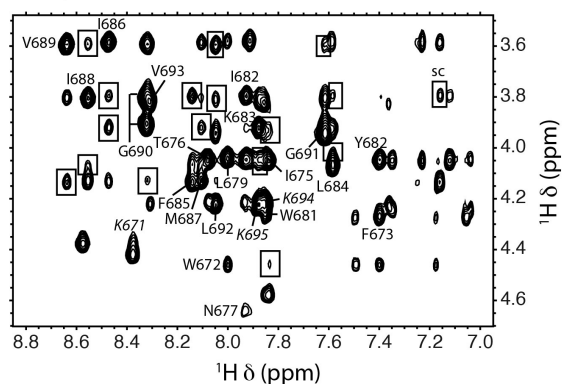
### **The Atomic Structure of the HIV-1 gp41 Transmembrane Domain and its Connection to the Immunogenic Membrane-proximal External Region.**

Beatriz Apellániz, Edurne Rujas, Soraya Serrano, Koldo Morante, Kouhei Tsumoto, José M. M. Caaveiro, M. Ángeles Jiménez, and José L. Nieva

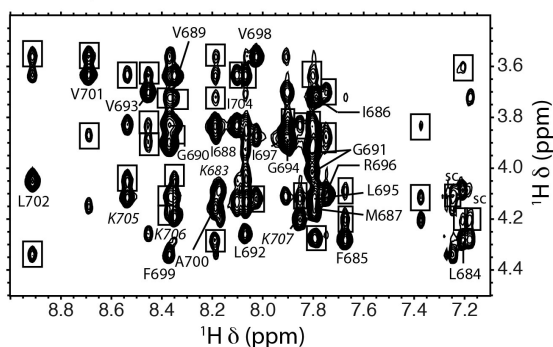
(A) CpreTM, DPC



(B) CpreTM, HFIP

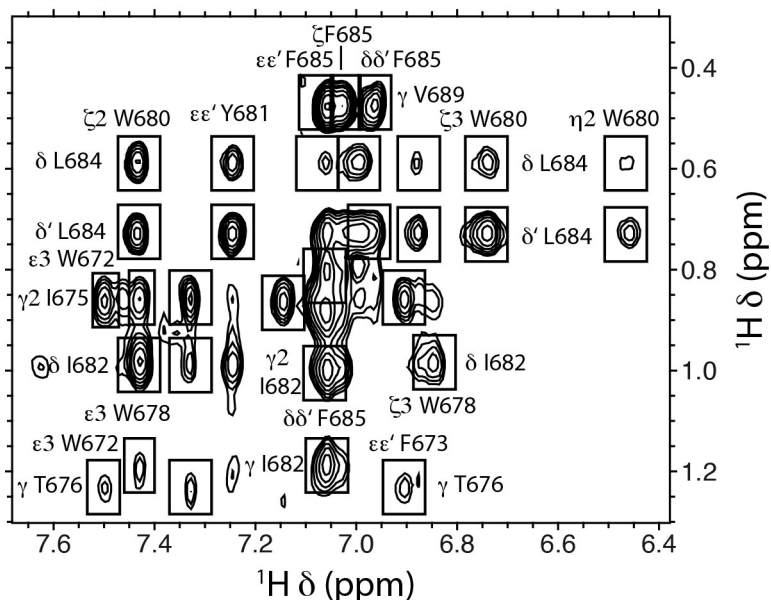


(C) TMDp, HFIP

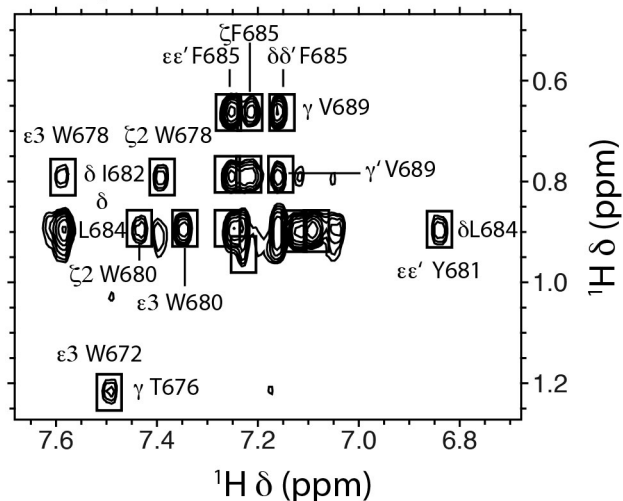


**Selected regions of the 2D  $^1\text{H}, ^1\text{H}$ -NOESY spectra (I)** recorded for CpreTM in 20 mM DPC (A) and in 25 % HFIP (B), and for TMDp in 25 % HFIP (C) at pH 7.0 and 25°C. The intra-residual  $\text{d}\alpha\text{N}(i,i)$  NOEs are labelled, and the medium-range non-sequential NOEs are boxed. ‘sc’ indicates the cross-peaks corresponding to non-sequential NOEs involving side chain protons. All the other non-sequential cross-peaks are  $\text{d}\alpha\text{N}(i,i+2)$ ,  $\text{d}\alpha\text{N}(i,i+3)$ , or  $\text{d}\alpha\text{N}(i,i+4)$ .

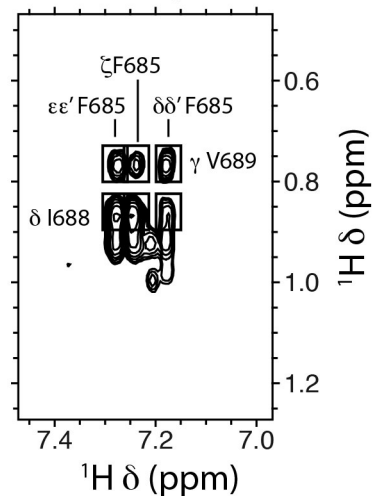
### (A) CpreTM, DPC



### (B) CpreTM, HFIP



### (C) TMDp, HFIP



**Selected regions of the 2D  $^1\text{H}$ ,  $^1\text{H}$ -NOESY spectra (II)** recorded for CpreTM in 20 mM DPC (A) and in 25 % HFIP (B), and for TMDp in 25 % HFIP (C) at pH 7.0 and 25°C showing NOEs involving aromatic protons. The medium-range non-sequential NOEs are boxed and labelled, except for those in crowded regions.