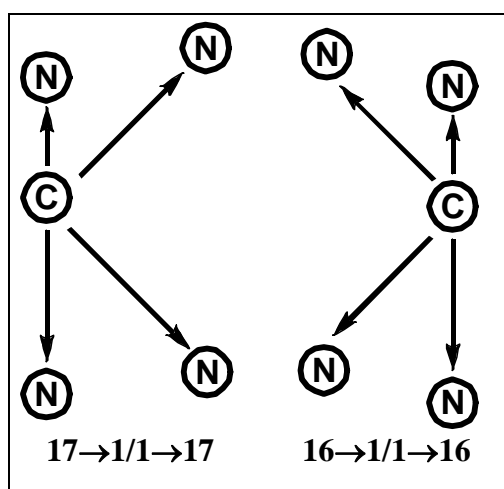


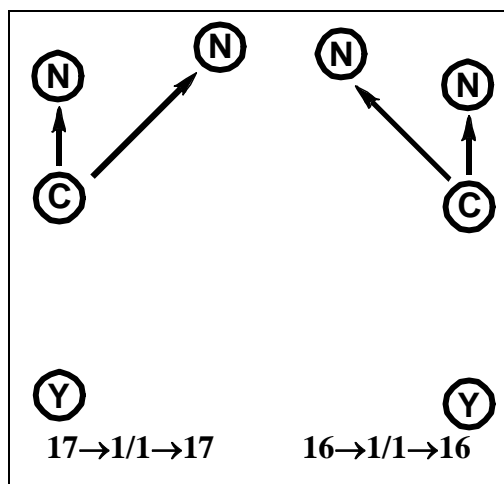
Supporting Information for “Major Antiparallel and Minor Parallel β Sheet Populations Detected in the Membrane-Associated Human Immunodeficiency Virus Fusion Peptide” by S. Schmick and D. Weliky

$(\Delta S/S_0)^{exp} + \sigma^{exp}$ in parentheses				
Dephasing time (ms)	HFP-NC	HFP-P	HFP-A	HFP-AP
2.2	0.019 (.013)	0.027 (.013)	0.012 (.023)	0.017 (.028)
8.2	0.056 (.020)	0.053 (.013)	0.077 (.036)	0.055 (.026)
16.2	0.071 (.020)	0.061 (.015)	0.107 (.021)	0.128 (.022)
24.2	0.077 (.023)	0.108 (.013)	0.202 (.026)	0.219 (.016)
32.2	0.086 (.017)	0.087 (.018)	0.244 (.025)	0.265 (.020)
40.2	0.093 (.018)	0.126 (.023)	0.306 (.031)	0.294 (.023)
48.2	0.089 (.028)	0.162 (.025)	0.325 (.060)	0.344 (.020)

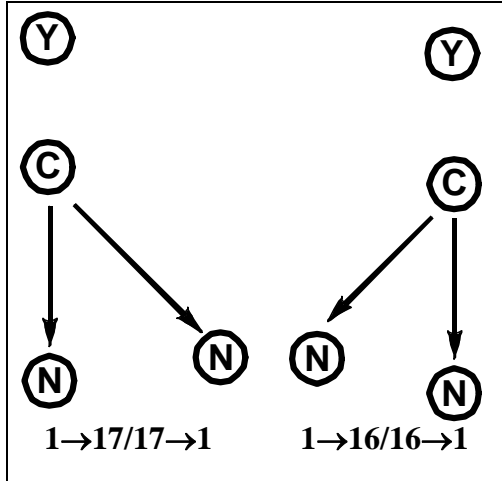
Spin geometries and associated calculated $\gamma_{1uv}^{lab}(\tau)$ for specific t , u , and v in the fully constrained model or calculated $\gamma_{1t_1t_2uv}^{lab}(\tau)$ for specific t_1 , t_2 , u , and v in the unconstrained model. In each spin geometry schematic, N or C respectively denote a labeled ^{15}N nucleus or a labeled ^{13}CO nucleus, and Y denotes either: (1) a ^{13}CO HFP; (2) a X registry not detected by the labeling schemes of the HFP-P, HFP-A, or HFP-AP samples; or (3) any other registry with $r_{CN} > 7 \text{ \AA}$ for the labeled ^{13}CO and the labeled ^{15}Ns . These latter r_{CN} s are not detected in the REDOR experiments. Each arrow denotes ^{13}CO - ^{15}N dipolar coupling considered in the simulation. For unconstrained model geometries, the top/middle strand registry is at the top of the schematic and the middle/bottom strand registry is at the bottom of the schematic. When more than one spin geometries are shown, each $\gamma(\tau)$ is the average for the displayed geometries.



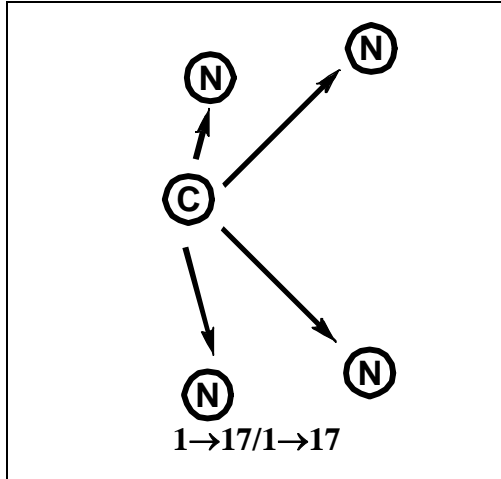
τ (ms)	$\gamma_{1uv}^{lab}(\tau)$	t	u	v
2.2	0.9889	2	2	4
8.2	0.8599	2	3	4
16.2	0.5566			
24.2	0.2791			
32.2	0.1326			
40.2	0.0885			
48.2	0.0725			



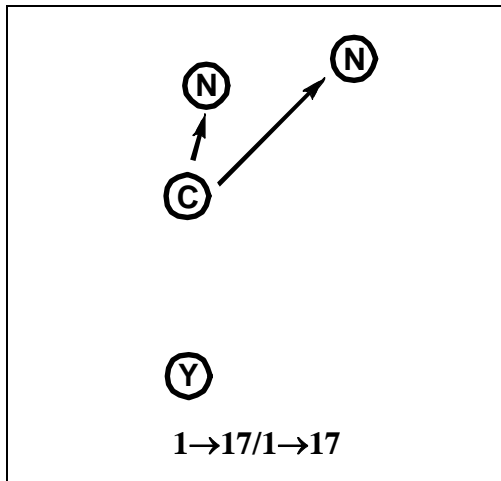
τ (ms)	$\gamma_{1uv}^{lab}(\tau)$	t	u	v
2.2	0.9907	2	2	2
8.2	0.8805	2	3	2
16.2	0.5972			
24.2	0.2859			
32.2	0.0698			
40.2	-0.0082			
48.2	0.0112			



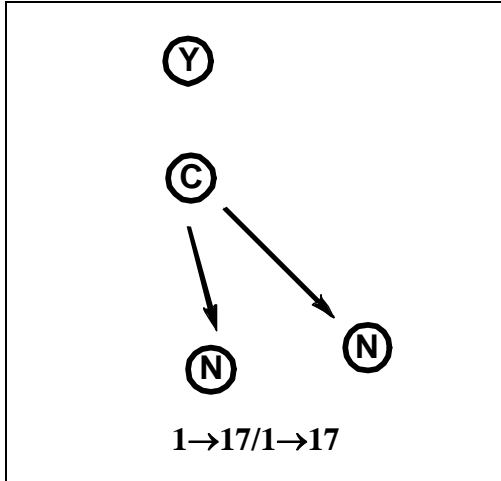
τ (ms)	$\gamma_{1uv}^{lab}(\tau)$	t	u	v
2.2	0.9982	2	2	3
8.2	0.9754	2	3	3
16.2	0.9075			
24.2	0.8044			
32.2	0.6779			
40.2	0.5417			
48.2	0.4092			



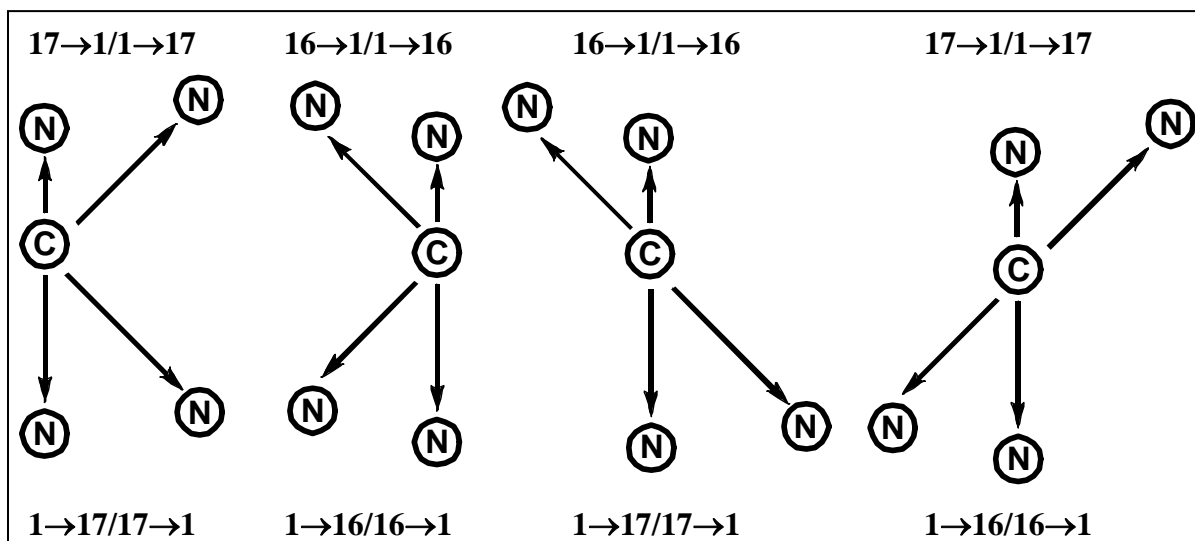
τ (ms)	$\gamma_{tuv}^{lab}(\tau)$	t	u	v
2.2	0.9903	1	1	4
8.2	0.8770	1	3	4
16.2	0.6043			
24.2	0.3394			
32.2	0.1782			
40.2	0.1094			
48.2	0.0782			



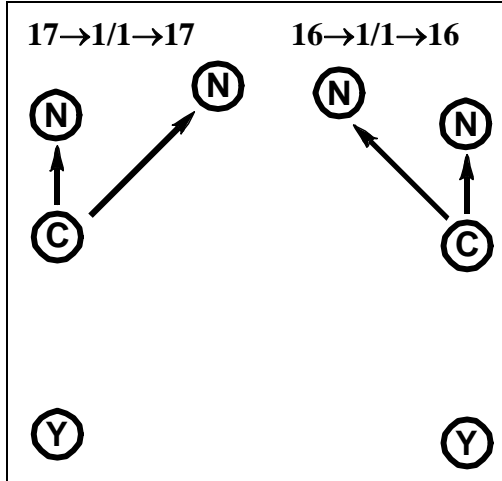
τ (ms)	$\gamma_{tuv}^{lab}(\tau)$	t	u	v
2.2	0.9933	1	1	2
8.2	0.9134	1	3	2
16.2	0.6961			
24.2	0.4263			
32.2	0.1902			
40.2	0.0436			
48.2	-0.0055			



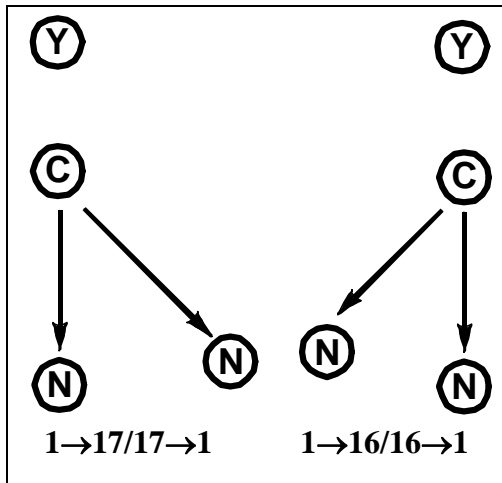
τ (ms)	$\gamma_{tuv}^{lab}(\tau)$	t	u	v
2.2	0.9979	1	1	3
8.2	0.9717	1	3	3
16.2	0.8941			
24.2	0.7773			
32.2	0.6364			
40.2	0.4883			
48.2	0.3488			



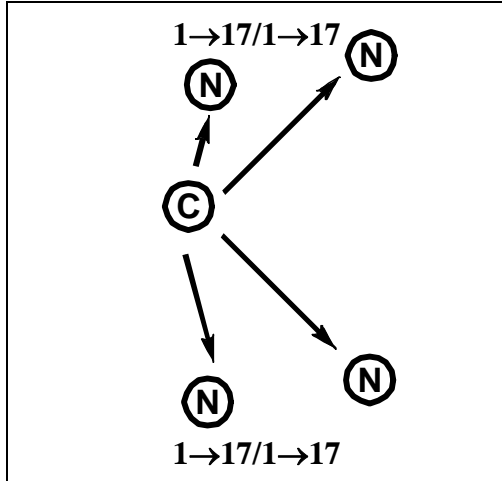
τ (ms)	$\gamma_{1t_1 t_2 uv}^{lab}(\tau)$	t_1	t_2	u	v
2.2	0.9889	2	2	2	4
8.2	0.8605	2	2	3	4
16.2	0.5582				
24.2	0.2806				
32.2	0.1318				
40.2	0.0847				
48.2	0.0681				



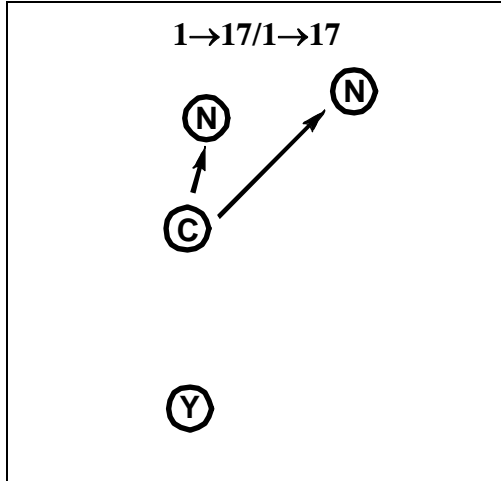
τ (ms)	$\gamma_{1t_1t_2uv}^{lab}(\tau)$	t_1	t_2	u	v
2.2	0.9907	2	2	2	2
8.2	0.8805	2	2	3	2
16.2	0.5972	2	1	2	2
24.2	0.2859	2	1	2	4
32.2	0.0698	2	3	2	2
40.2	-0.0082	2	3	2	4
48.2	0.0112	2	3	3	2
		2	3	3	4



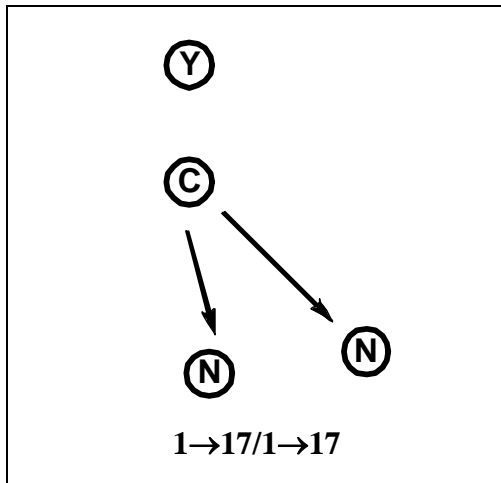
τ (ms)	$\gamma_{1t_1t_2uv}^{lab}(\tau)$	t_1	t_2	u	v
2.2	0.9982	2	2	2	3
8.2	0.9754	2	2	3	3
16.2	0.9075	1	2	2	3
24.2	0.8044	1	2	2	4
32.2	0.6779	3	2	2	3
40.2	0.5417	3	2	2	4
48.2	0.4092	3	2	3	3
		3	2	3	4



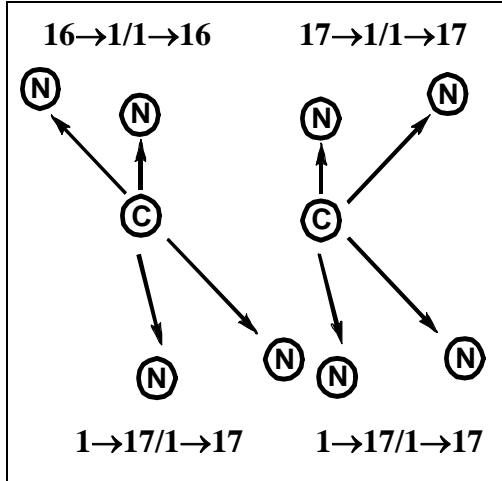
τ (ms)	$\gamma_{1t_1t_2uv}^{lab}(\tau)$	t_1	t_2	u	v
2.2	0.9903	1	1	1	4
8.2	0.8770	1	1	3	4
16.2	0.6043				
24.2	0.3394				
32.2	0.1782				
40.2	0.1094				
48.2	0.0782				



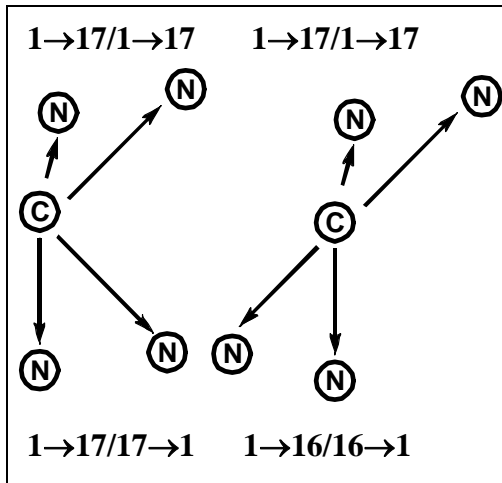
τ (ms)	$\gamma_{1t_1t_2uv}^{lab}(\tau)$	t_1	t_2	u	v
2.2	0.9933	1	1	1	2
8.2	0.9134	1	1	3	2
16.2	0.6961	1	2	1	2
24.2	0.4263	1	2	1	4
32.2	0.1902	1	3	1	2
40.2	0.0436	1	3	1	4
48.2	-0.0055	1	3	3	2
		1	3	3	4



τ (ms)	$\gamma_{1t_1t_2uv}^{lab}(\tau)$	t_1	t_2	u	v
2.2	0.9979	1	1	1	3
8.2	0.9717	1	1	3	3
16.2	0.8941	2	1	1	3
24.2	0.7773	2	1	1	4
32.2	0.6364	3	1	1	3
40.2	0.4883	3	1	1	4
48.2	0.3488	3	1	3	3
		3	1	3	4



τ (ms)	$\gamma_{1t_1t_2uv}^{lab}(\tau)$	t_1	t_2	u	v
2.2	0.9903	2	1	3	4
8.2	0.8766				
16.2	0.5998				
24.2	0.3263				
32.2	0.1591				
40.2	0.0937				
48.2	0.0712				



τ (ms)	$\gamma_{1t_1t_2uv}^{lab}(\tau)$	t_1	t_2	u	v
2.2	0.9904	1	2	3	4
8.2	0.8782				
16.2	0.6061				
24.2	0.3389				
32.2	0.1753				
40.2	0.1079				
48.2	0.0805				