

Supplementary Table 1 NMR chemical shifts of the Vpr-(52–96) protein in 30% C²H₃CN/70% water at 303 K, pH 3, calibrated to water
 Chemical shifts at 2 mM concentration might not be exactly the same as those observed in heteronuclear experiments. This is due to a slight difference in acetonitrile concentration.

Residues	¹⁵ N	NH	αH	βH	Others
D52		7.81	4.31	2.89, 2.94	
T53	114.18	8.33	4.16	3.93	γCH ₃ 0.97
W54		7.93	4.47	3.22	2H 7.21; 4H 7.45; 5H 6.94; 6H 7.09; 7H 7.36; NH 9.97
T55	114.38	7.98	4.05	4.15	γCH ₃ 1.2
G56		7.9	3.84		
V57	121.22	7.86	3.7	2.19	γCH ₃ 0.98
E58		8.08	3.92	2.03, 2.14	γCH ₂ 2.48, 2.4
A59	120.64	7.91	4.03	1.46	
L60		7.75	4.06	1.81	γCH ₂ 1.71; δCH ₃ 0.86
I61	119.25	8.17	3.52	1.92	γCH ₂ 1.05, 1.79; γCH ₃ 0.89; δCH ₃ 0.81
R62		7.71	4.06	1.91	γCH ₂ 1.61; δCH ₂ 3.14; NH 7.15
I63	119.84	7.92	3.78	2.01	γCH ₂ 1.19, 1.78; γCH ₃ 1.69; δCH ₃ 0.85
L64	120.11	8.37	4	1.9	γH 1.46
Q65		8.56	3.87	1.98	γCH ₂ 2.26, 2.53; δNH ₂ 6.9, 6.5
Q66		7.95	4.1	2.18, 2.27	γCH ₂ 2.39, 2.52; δNH ₂ 7.08, 6.56
L67	119.02	8.27	4.09	2.01	δCH ₃ 0.91
L68	119.25	8.22	4	1.85	γH 1.6; δCH ₃ 0.93
F69	118.49	8.18	4.34	3.24, 3.29	2.6H 7.25; 3.5H 7.3
I70		8.21	3.69	1.96	γCH ₂ 1.28, 1.78; γCH ₃ 0.86; δCH ₃ 0.88
H71	117.29	8.08	4.18	2.83, 2.95	4H 6.31; 2H 8.42
F72	117.08	8.1	4.32	3.17	2.6H 7.25; 3.5H 7.3
R73		7.94	4.02	1.69, 1.73	γCH ₂ 1.48; δCH ₂ 3.27; NH 7.09
I74		7.83	3.96	1.82	γCH ₂ 1.16; γCH ₃ 0.85; δCH ₃ 0.79
G75	110.09	7.99	3.88, 3.81		
C76		7.79	4.37	2.82	

R77		8.01	4.19	1.53, 1.6	γCH_2 1.7, 1.77; δCH_2 3.12; NH 7.13
H78		8.23	4.66	3.12, 3.25	4H 7.28; 2H 8.58
S79		8.08	4.39	3.78, 3.83	
R80		8.27	4.32	1.62 1.73	γCH_2 1.84; δCH_2 3.14; NH 7.15
I81		7.9	4.1	1.82	γCH_2 1.17; γCH_3 0.89; δCH_3 0.84
G82	111.68	8.14	3.84	3.92	
I83		7.72	4.1	1.82	γCH_2 1.14, 1.43; γCH_3 0.88; δCH_3 0.82
I84		7.91	4.05		γCH_2 1.15; γCH_3 0.93; δCH_3 0.86
Q85		8.17	4.23	2.31	γCH_2 2.03; δNH_2 6.68, 7.32
Q86		8.17	4.23	2.31	γCH_2 2.03; δNH_2 6.77, 7.41
R87		8.16	4.23	1.73, 1.81	γCH_2 1.61; δCH_2 3.15; NH 7.11
R88		7.93	4.35	1.73; 1.84	γCH_2 1.6; δCH_2 3.13; NH 7.13
T89	114.34	7.94	4.31	4.17	γCH_3 1.17
R90		8.2	4.3	1.73, 1.84	γCH_2 1.6; δCH_2 3.15; NH 7.12
N91		8.28	4.63	2.72, 2.78	
G92		8.19	3.88		
A93	122.92	7.99	4.32	1.37	
S94		8.04	4.39	3.81	
K95	122.56	8.12	4.38	1.65, 1.42	γCH_2 1.74; δCH_2 1.87; ϵCH_2 2.95; ϵNH_3 7.4
S96		8.08	3.88	3.81	