Supporting Information For

HIV-1 Capsid Function is Regulated by Dynamics: Quantitative Atomic-Resolution Insights by Integrating Magic-Angle-Spinning NMR, QM/MM, and MD

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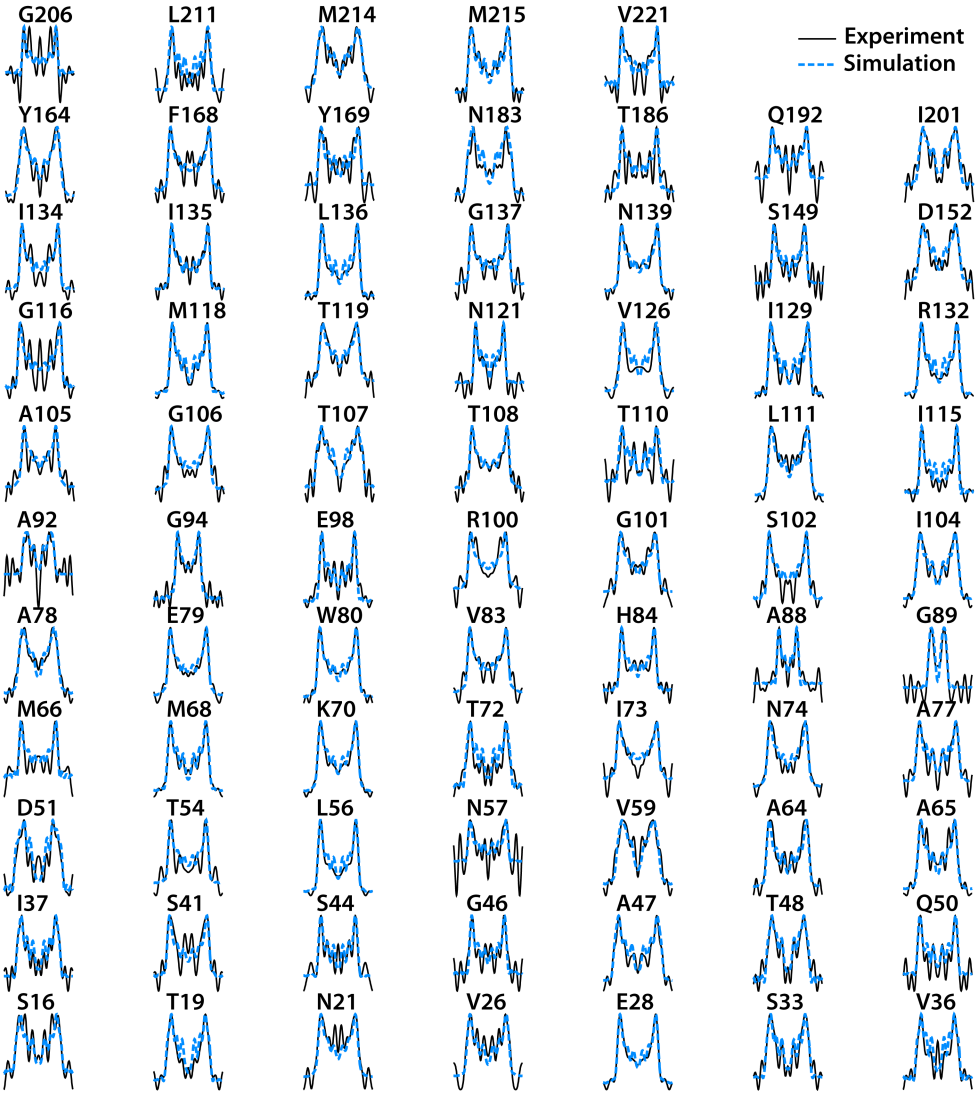

Figure S1. Experimental (solid black lines) and simulated (dashed blue lines) ^{15}N CSA lineshapes for different residues in tubular assemblies of CA HXB2 extracted from the $R8_1^3$-RNCSA 3D spectra, recorded at the magnetic field of 21.1 T and the MAS frequency of 14 kHz.

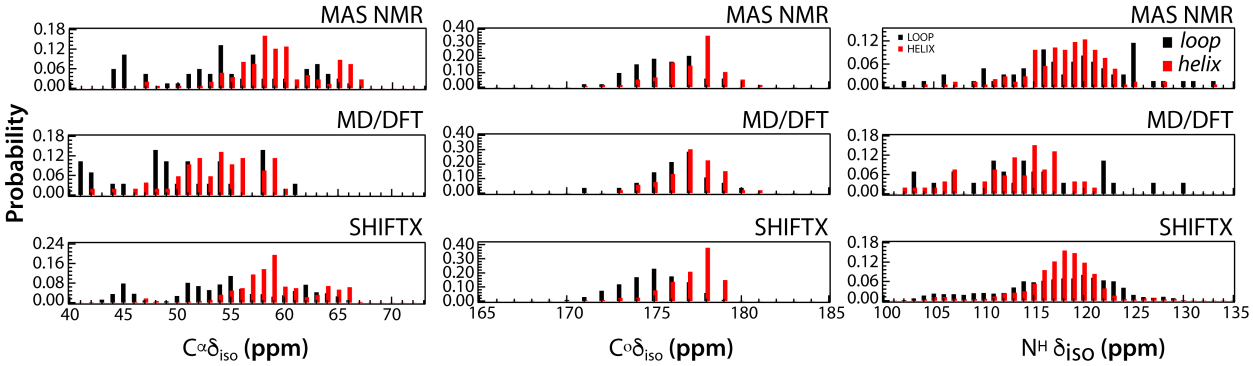

Figure S2. Distribution plots for the isotropic $^{13}C^{\alpha}$ (left), $^{13}C^{o}$ (middle), and $^{15}N^{H}$ (right) chemical shifts in HIV-1 CA assemblies. Top: experimental MAS NMR; middle, calculated from MD/DFT; bottom, calculated by SHIFTX as the averaged values over the MD trajectory. The distributions for helical regions are shown in red, for loops- in black.

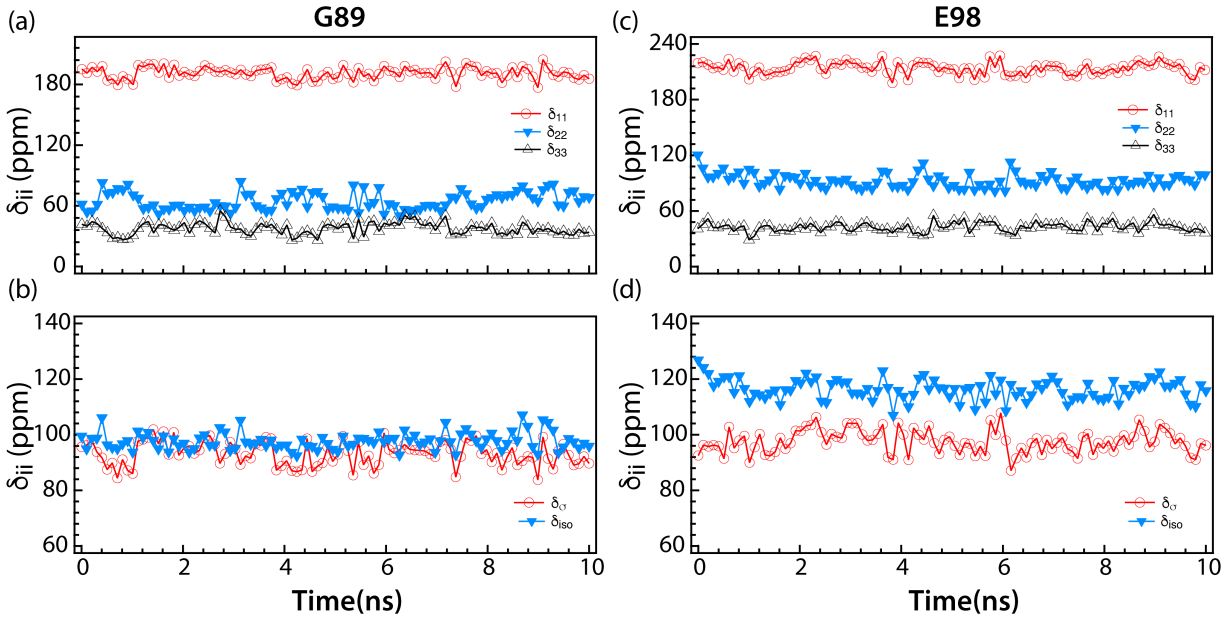

Figure S3. Principal components of ^{15}N CSA tensor, δ_{ii}, δ_{σ}, and δ_{iso}, calculated along the MD trajectory, for selected CA residues: G89 (a, c) and E98 (b, d). For the calculations, 100 frames were used from the first 10 ns of the 100-ns MD trajectory.

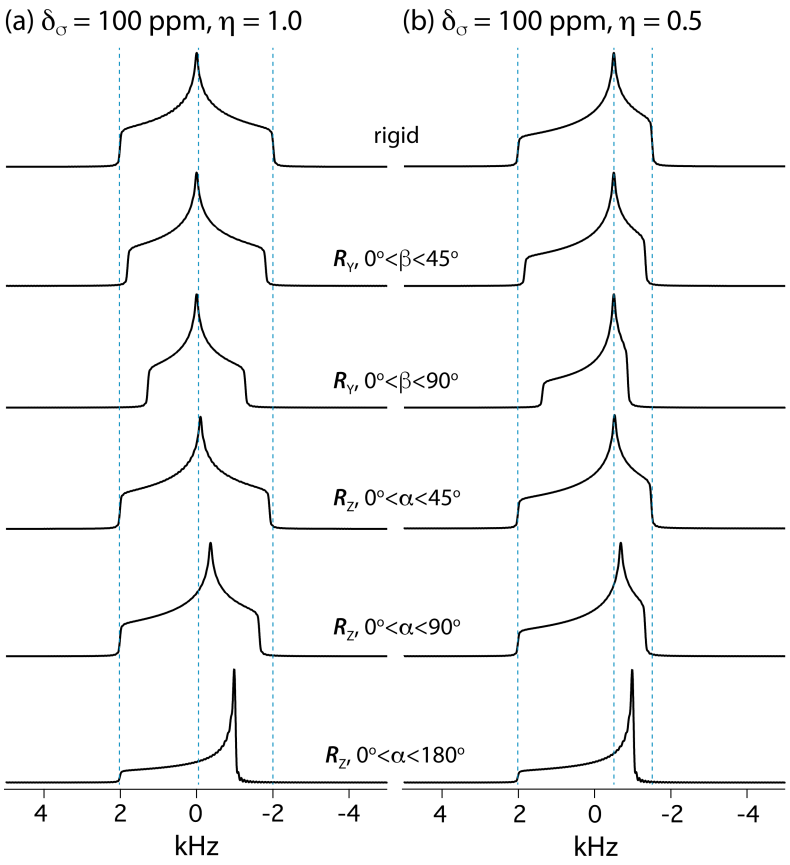

Figure S4. Simulated rigid and motionally reduced ^{15}N CSA line shapes for the sites with the following CSA NMR parameters: (a) δ_σ = 100 ppm and η = 1.0; (b) δ_σ = 100 ppm and η = 0.5. The Euler angles are indicated next to each line shape.

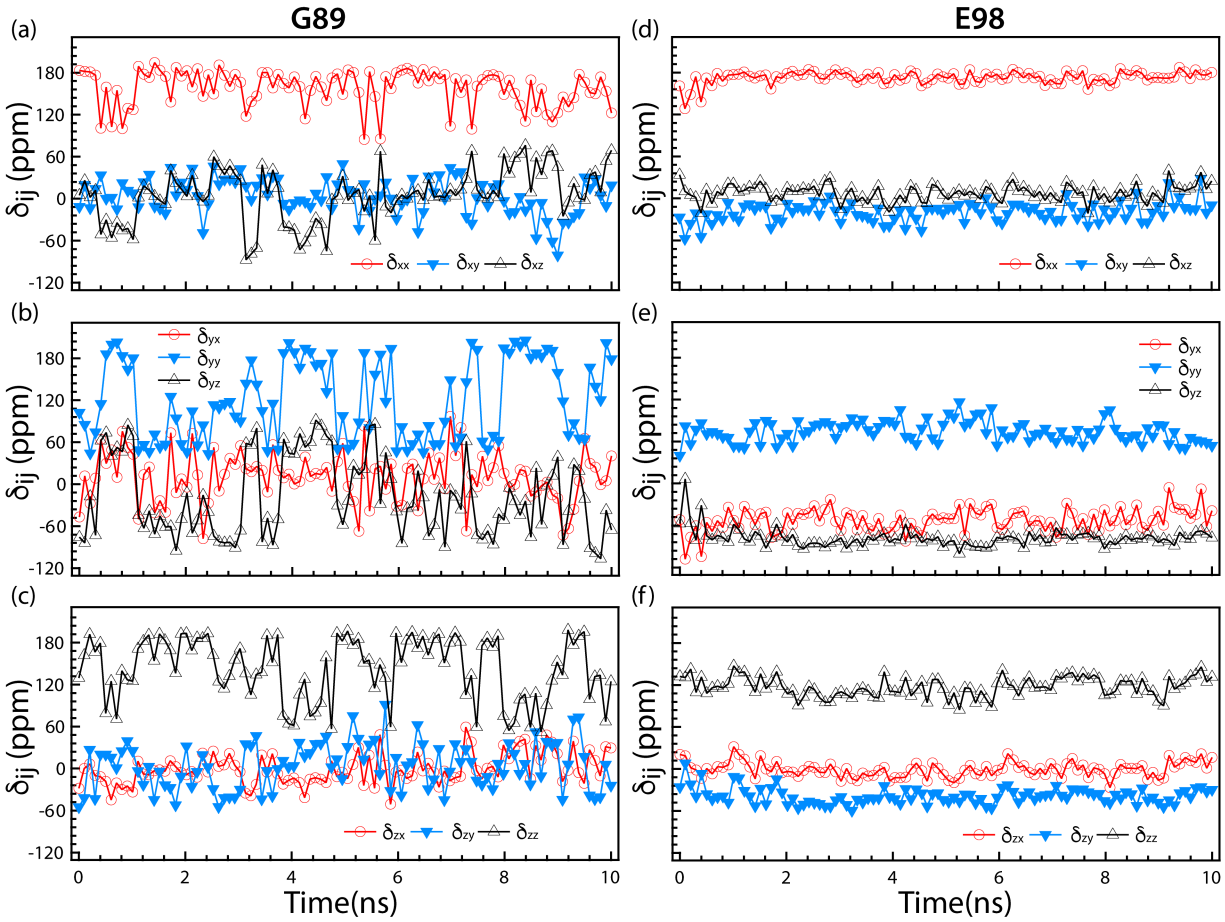

Figure S5. Individual components of ^{15}N CSA tensor δ_{ij} (molecular fixed frame representation), calculated along the MD trajectory, for selected CA residues: G89 (a-c) and E98 (d-f). For the calculations, 100 frames were used from the first 10 ns of the 100-ns MD trajectory.

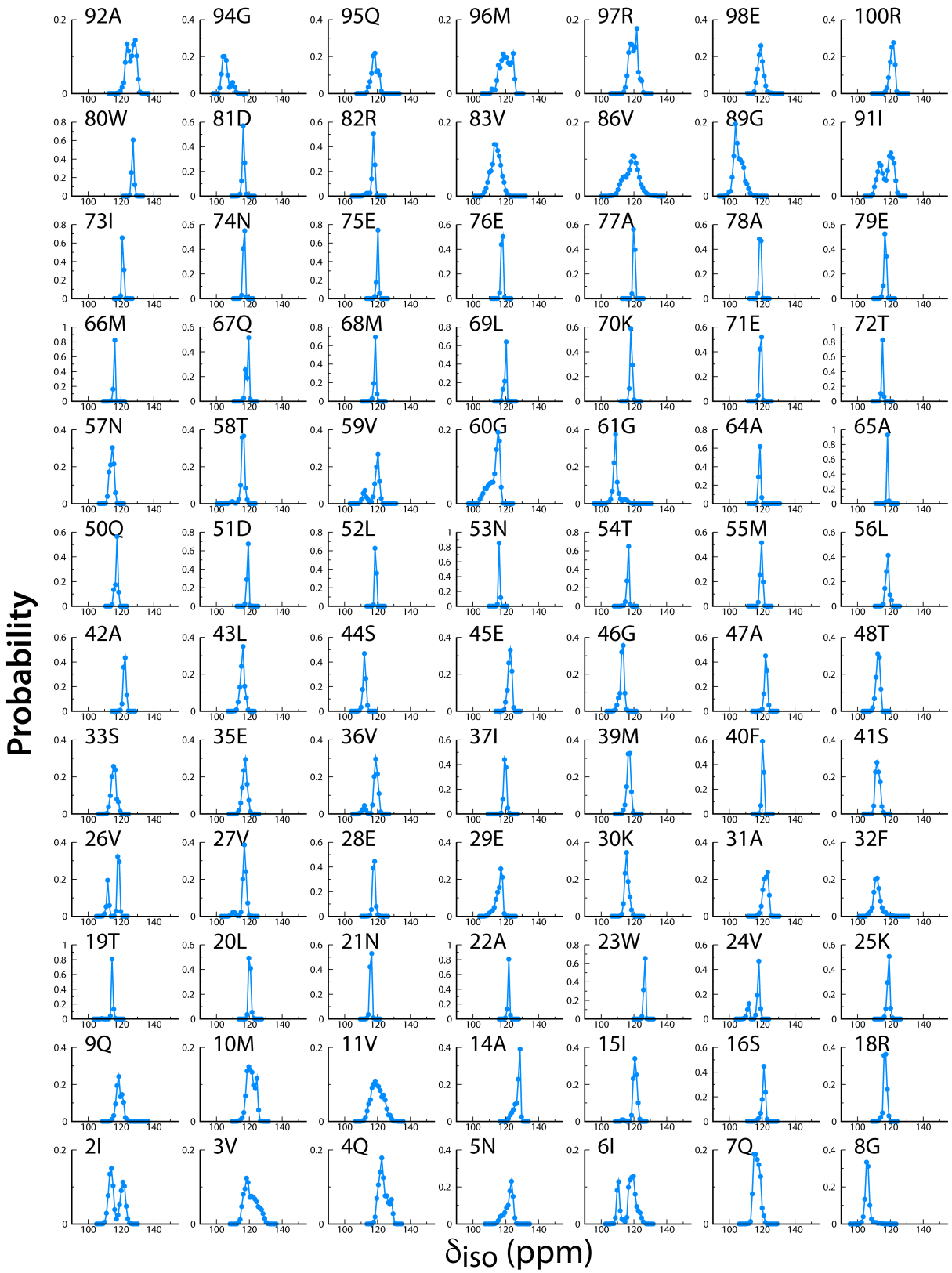

Figure S6. Probability distributions of ^{15}N isotropic chemical shifts of HIV-1 CA calculated by Shiftx based on 5000 frames extracted from 100 ns MD simulation.

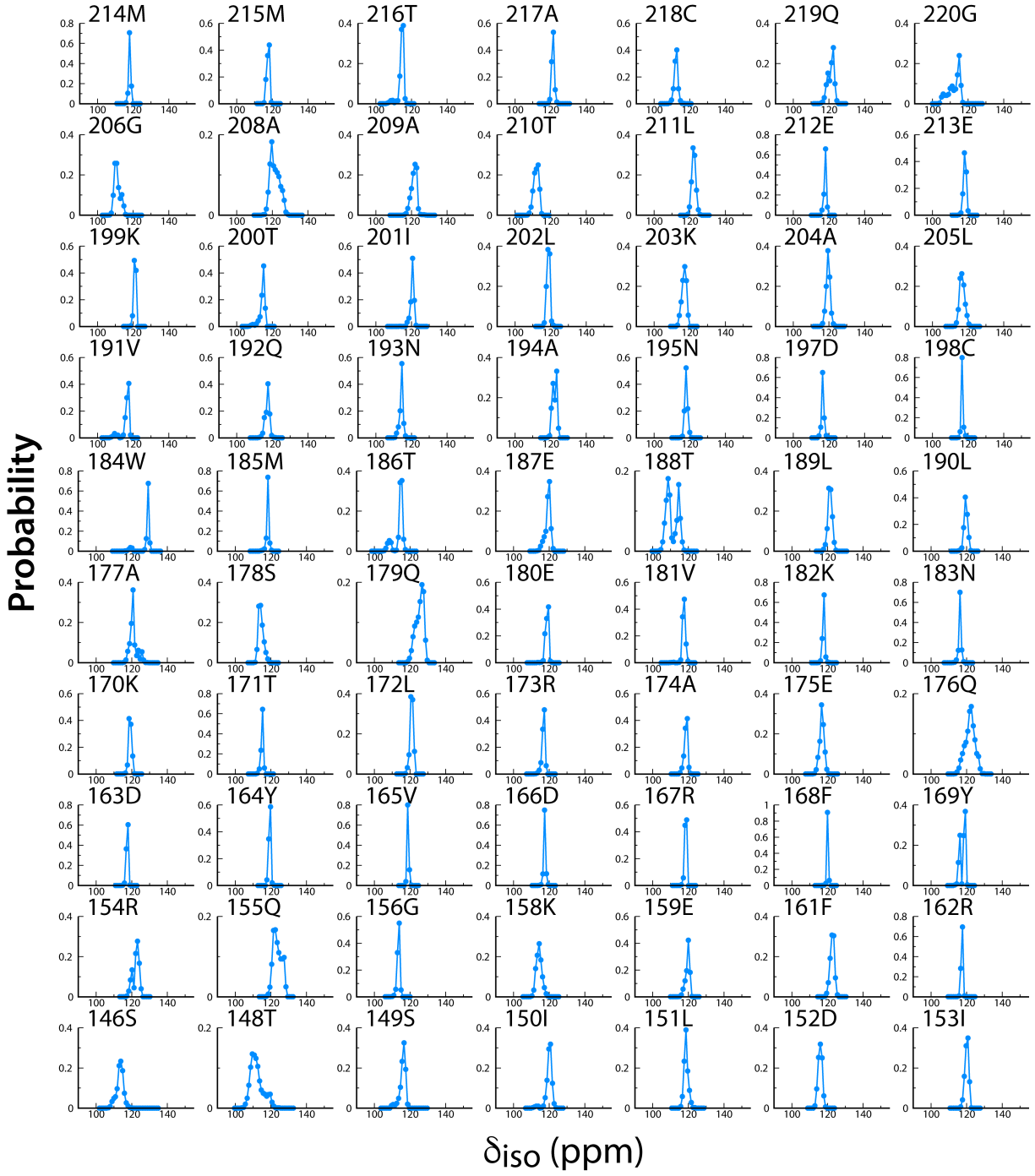

Figure S6. (con'd) Probability distributions of ^{15}N isotropic chemical shifts of HIV-1 CA calculated by Shiftx based on 5000 frames extracted from 100 ns MD simulation.

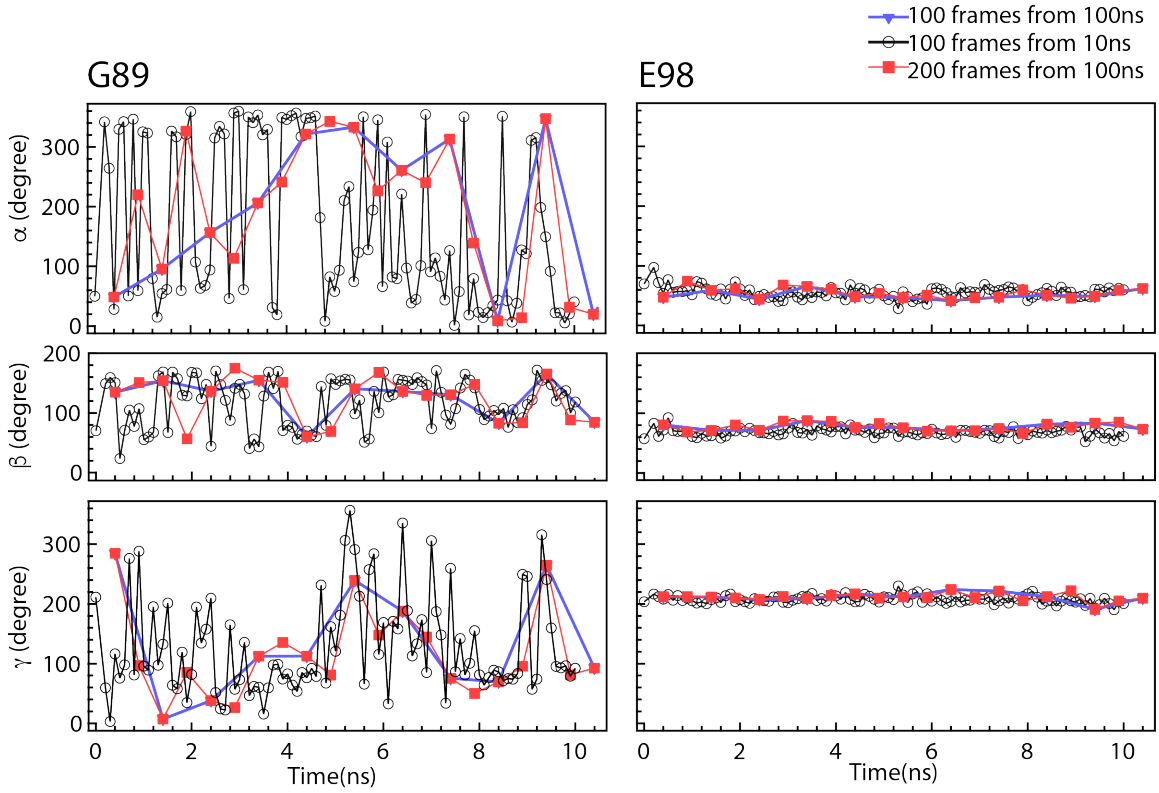

Figure S7. Euler angles of the ^{15}N CSA tensors for G89 and E98 residues of CA, calculated by MD/DFT with different sampling schedules: 200 frames from 100-ns MD trajectory, red; 100 frames from 100-ns MD trajectory, blue; 100 frames from the first 10 ns of the 100-ns MD trajectory, black. The corresponding ^{15}N CSA parameters for G89 are: δ_σ = 28.92 ppm, η_σ = 0.11; δ_σ = 23.28 ppm, η_σ = 0.10; δ_σ = 23.75 ppm, η_σ = 0.12. The corresponding ^{15}N CSA parameters for E98 are: δ_σ = 93.83 ppm, η_σ = 0.52; δ_σ = 93.00 ppm, η_σ = 0.53; δ_σ = 92.94 ppm, η_σ = 0.54.

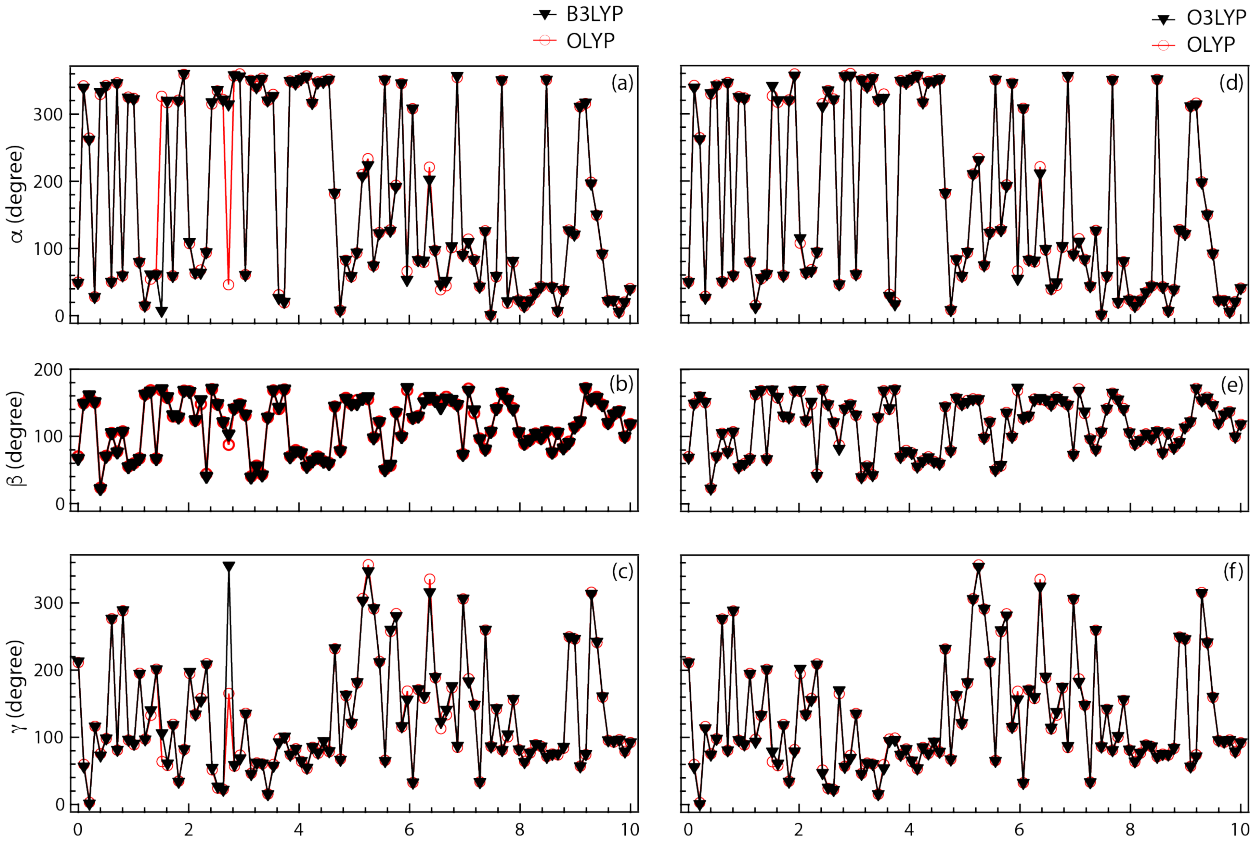

Figure S8. Euler angles of the ^{15}N CSA tensors for G89 residue in the molecular frame along the MD trajectory, calculated using (a-c) B3LYP and OLYP functionals (black and red symbols, respectively), and (d-f) O3LYP and OLYP functionals (black and red symbols, respectively). The angles were calculated using δ_σ = 25.63, 23.75, and 24.66 ppm for B3LYP, OLYP, and O3LYP, respectively. Note that the differences are small for δ_σ computed with the three functionals. For the calculations, 100 frames were used from the first 10 ns of the 100-ns MD trajectory.