

**SUPPORTING INFORMATION**

**Hybrid All-Atom/Coarse-Grained Simulations of Proteins by  
Direct Coupling of CHARMM and PRIMO Force Fields**

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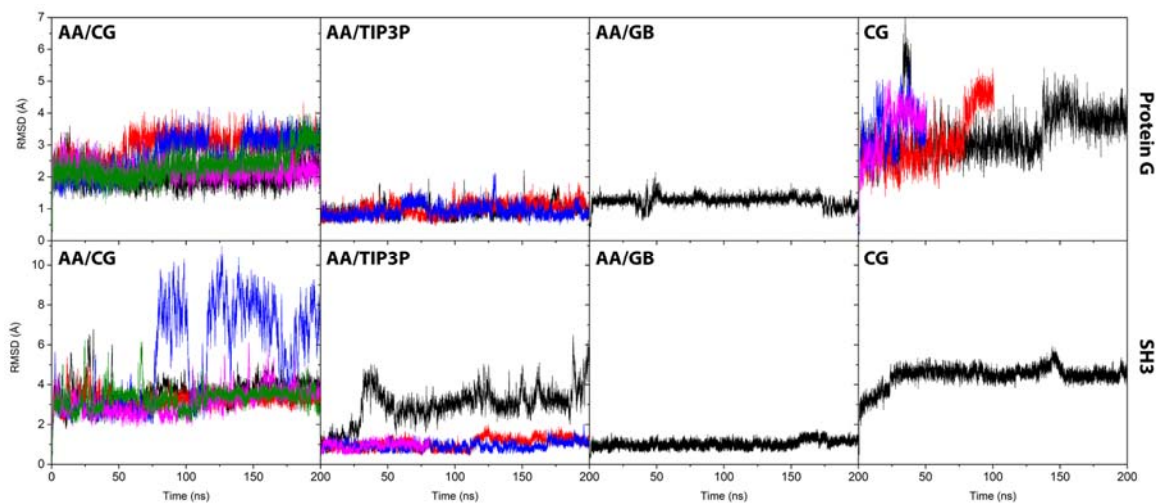
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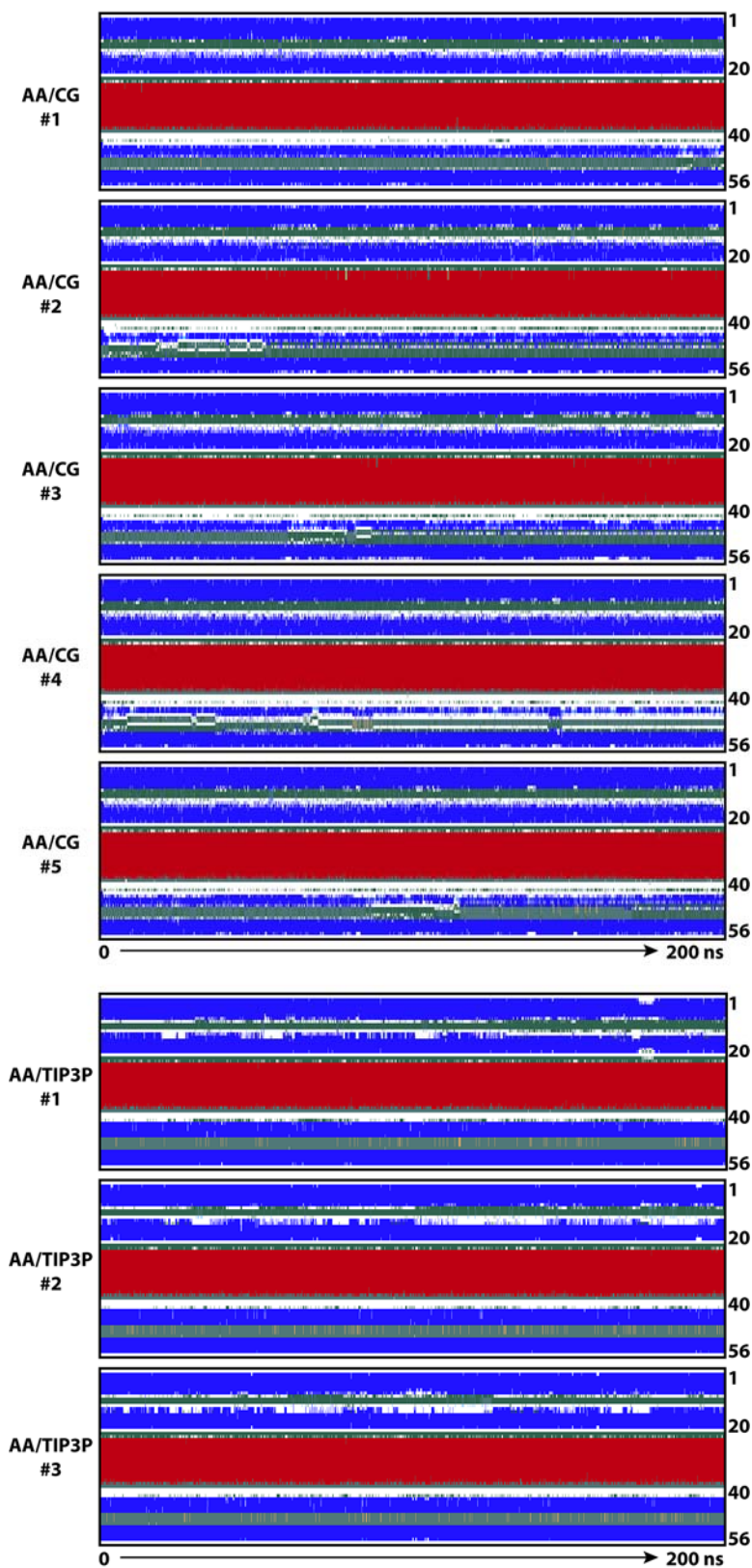
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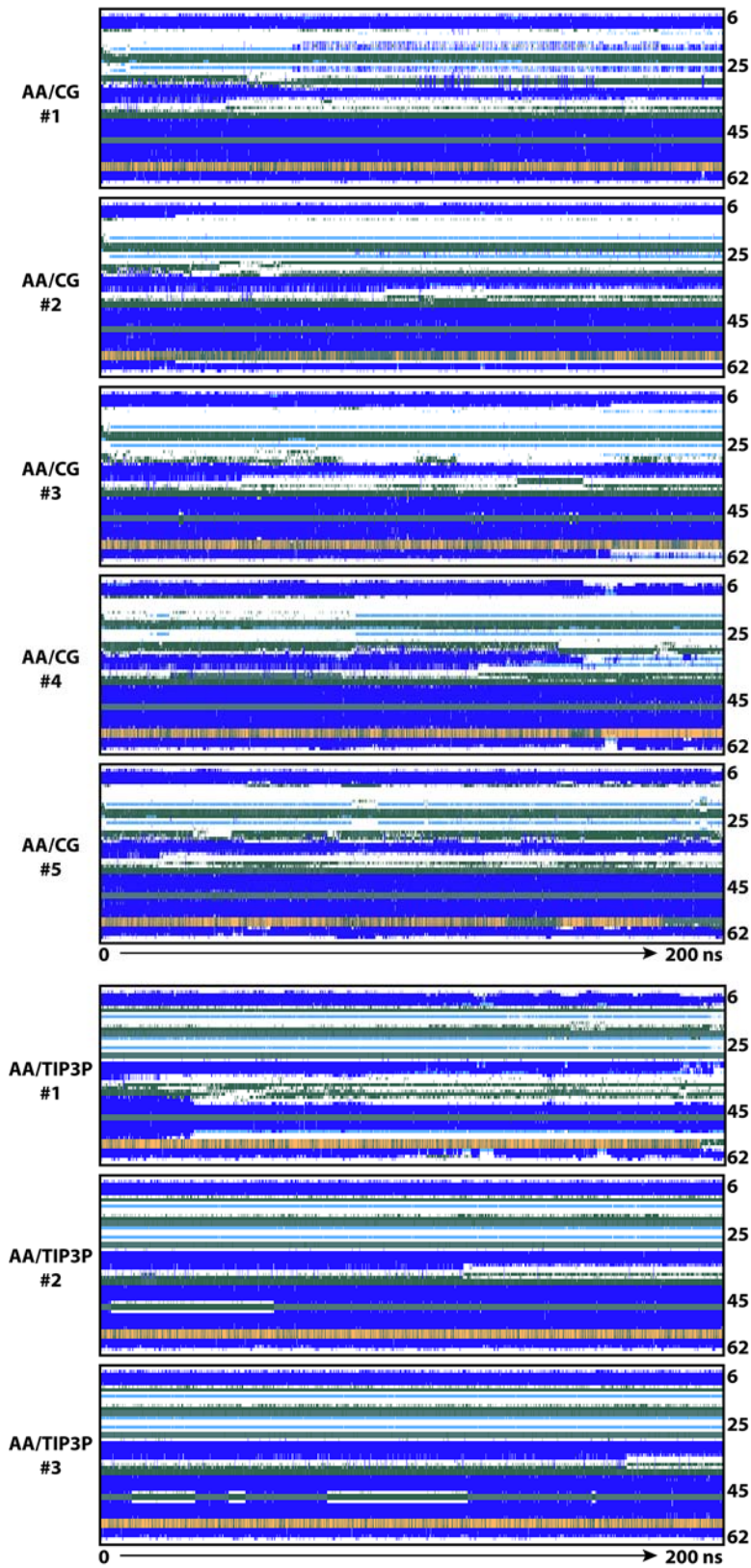
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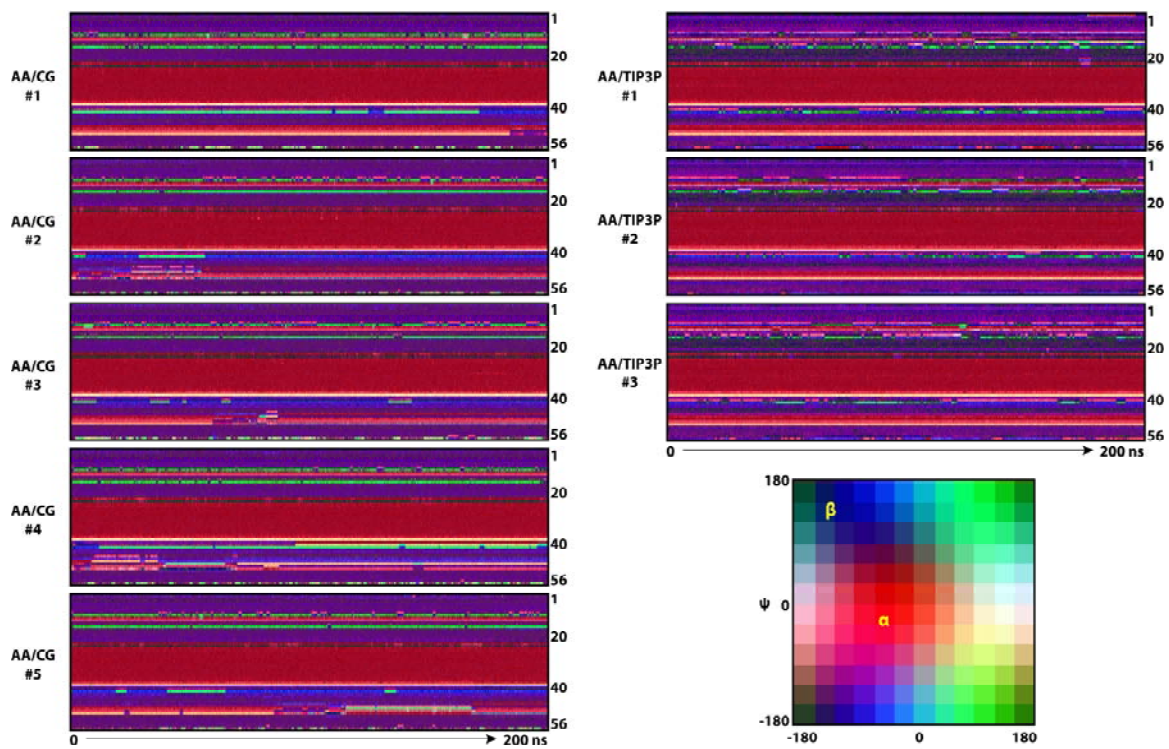
**Figure S1:** Time evolution of  $C_{\alpha}$  root-mean-squared-deviation (RMSD) with respect to the experimental structure for protein G (PDB code: 3GB1, top), and the SH3 domain (PDB code: 1SHG, bottom) with the hybrid AA/CG model (AA/CG), fully atomistic simulations with explicit solvent (AA/TIP3P), AA/GBMV (AA/GB), or coarse-grained simulations using the PRIMO force field (CG). Different colored lines represent simulation replicates.



**Figure S2:** Time evolution of secondary structure for protein G based on DSSP analysis for AA/CG and AA/TIP3P simulations ( $\alpha$ -helix: red;  $\beta$ -sheet: blue/light blue; orange:  $3^{10}$ -helix; turn: grey; bend: dark green).

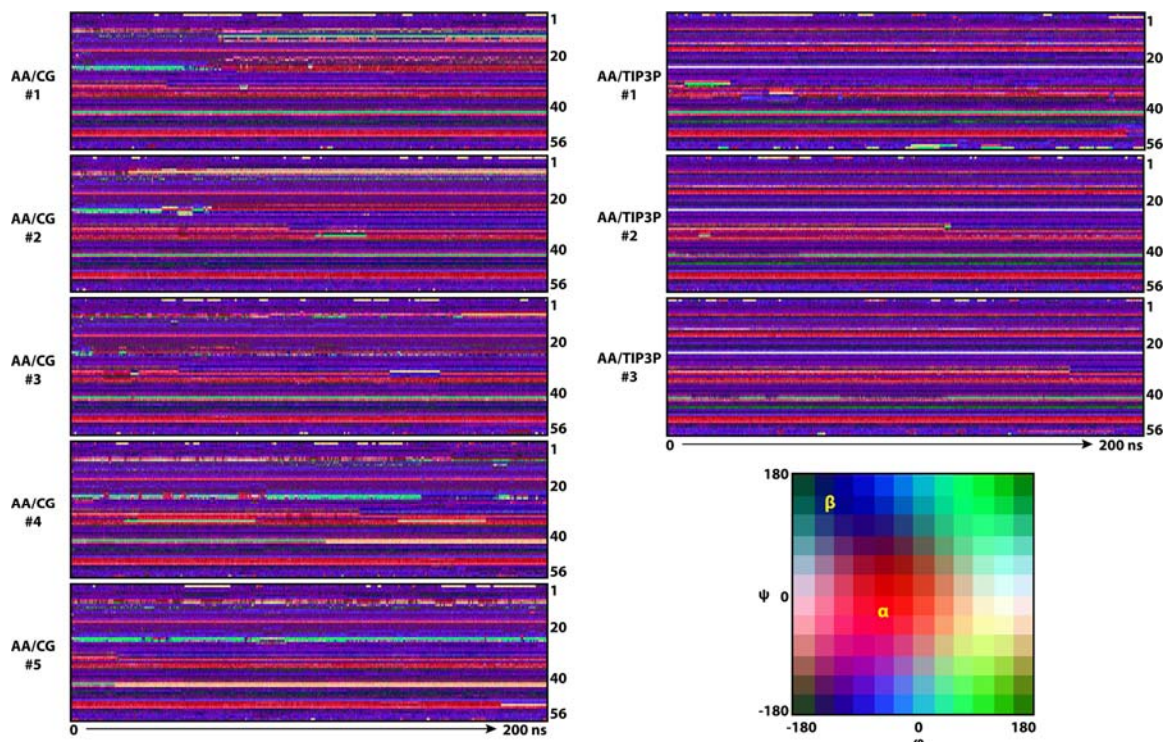


**Figure S3:** Time evolution of secondary structure for SH3 domain based on DSSP analysis for AA/CG and AA/TIP3P simulations (colors as in Fig. S2).

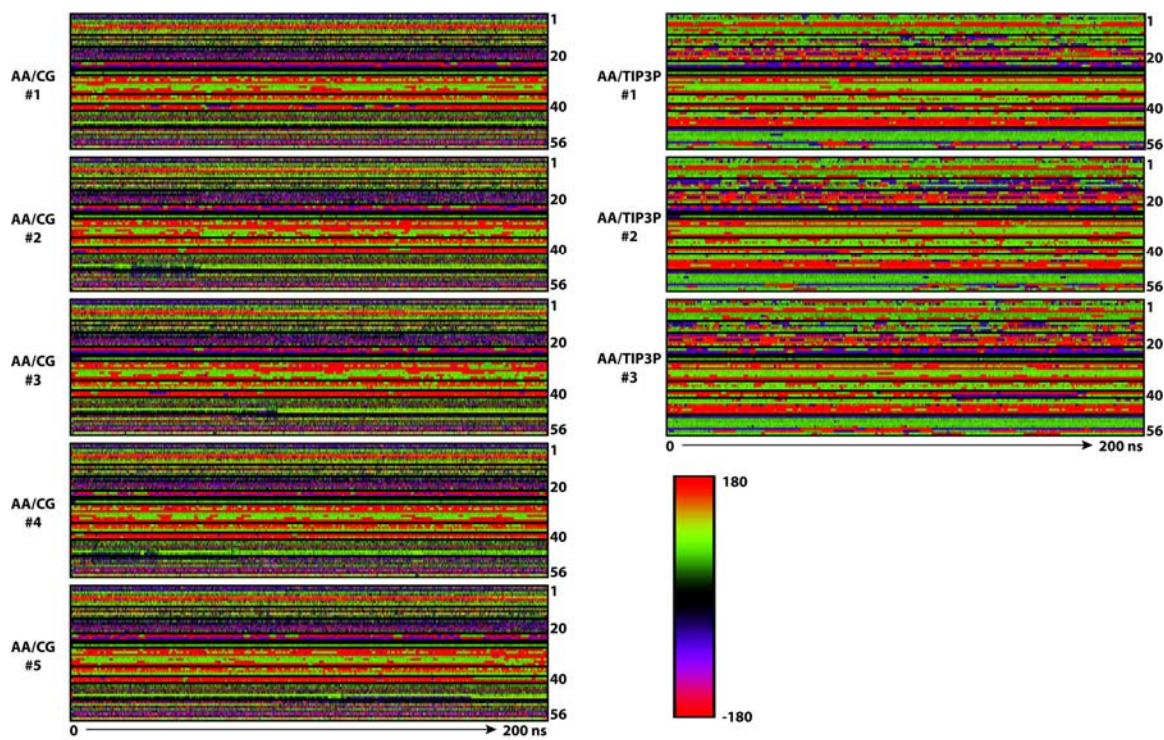


**Figure S4:** Time evolution of  $\phi/\psi$  backbone torsion angles for protein G in AA/CG and AA/TIP3P simulations according to color diagram.

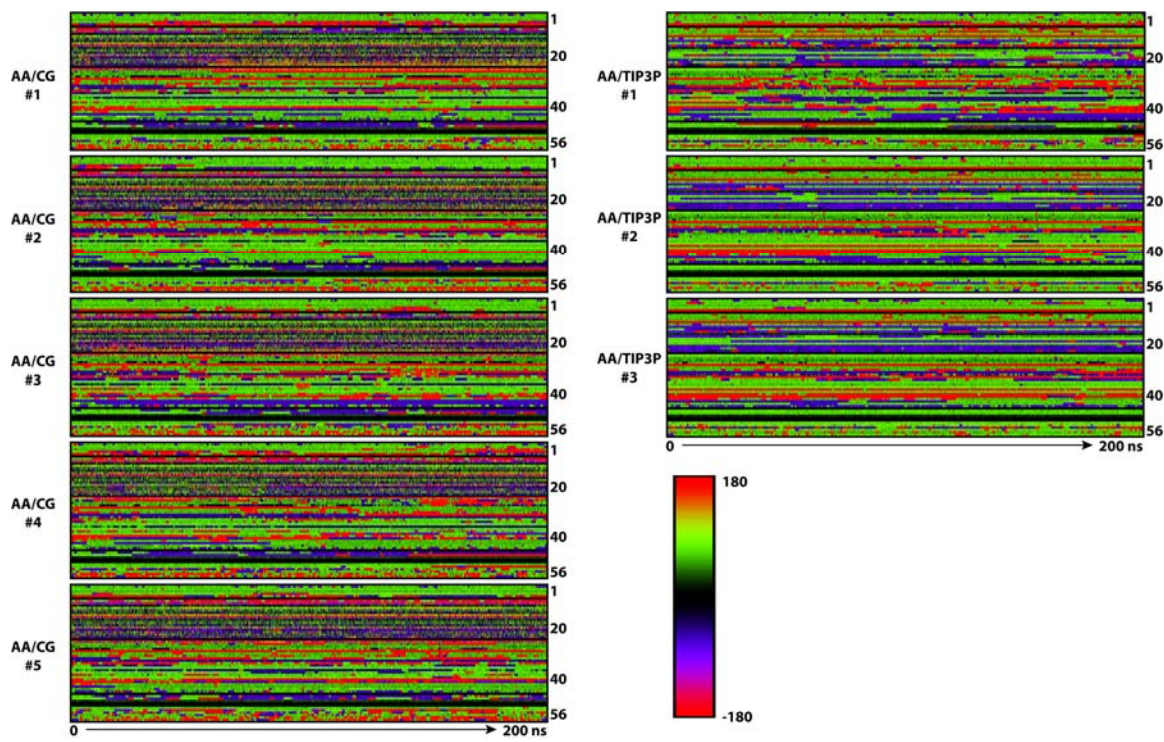




**Figure S5:** Time evolution of  $\phi/\psi$  backbone torsion angles for SH3 domain in AA/CG and AA/TIP3P simulations according to color diagram.



**Figure S6:** Time evolution of  $\chi_1$  side chain torsion angles for protein G in AA/CG and AA/TIP3P simulations according to color diagram.



**Figure S7:** Time evolution of  $\chi_1$  side chain torsion angles for SH3 domain in AA/CG and AA/TIP3P simulations according to color diagram.