SUPPORTING INFORMATION – APPENDIX

Coarse-Grained Simulations Complemented by Atomistic Molecular Dynamics Provide New Insights into Folding of Human Telomeric G-Quadruplexes

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This appendix contains graphs of time evolution of various order parameters (collective variables, CVs) for all MD simulations in this study (see Main text Table 1 for the list of simulations).

FIGURES

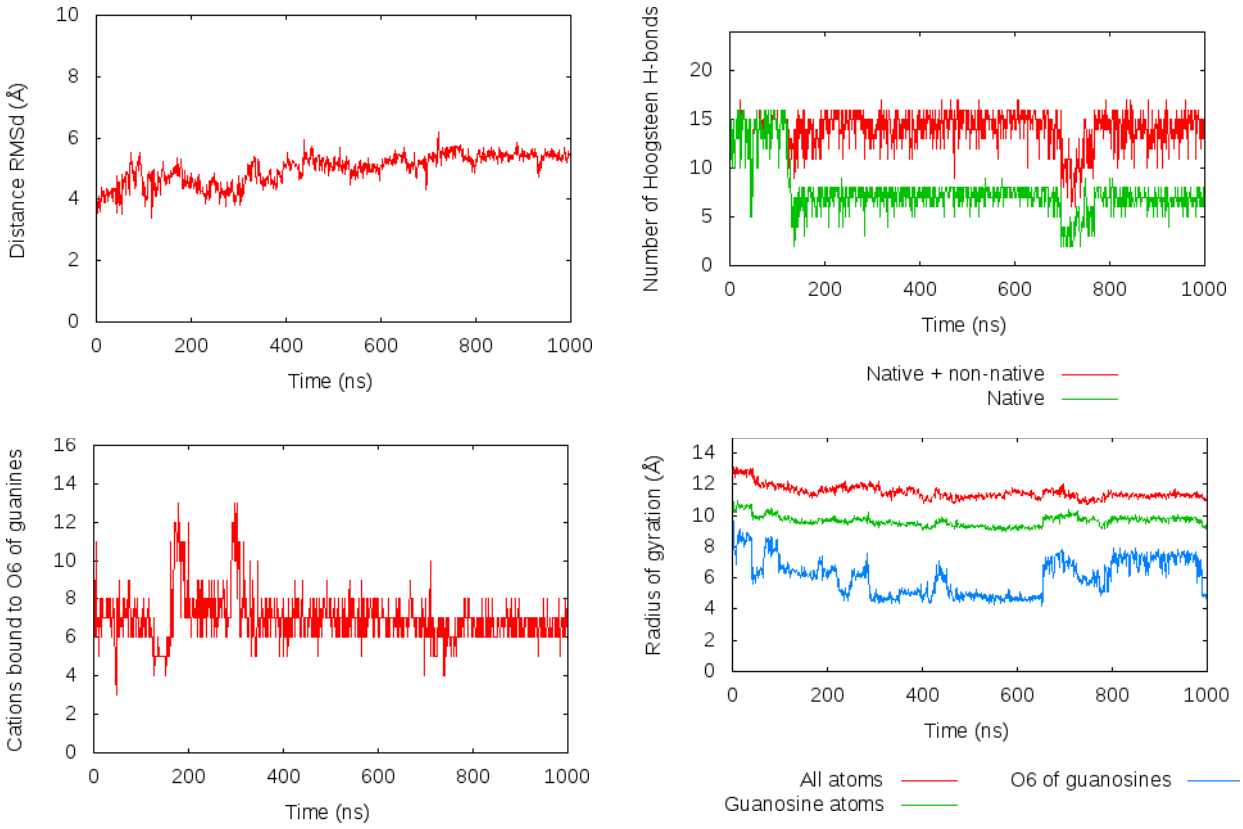

Figure SA1. Evolution of seven CVs in the simulation 1KF1-**A**. Top left: C4′ distance RMSd with respect to the native structure 1KF1. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

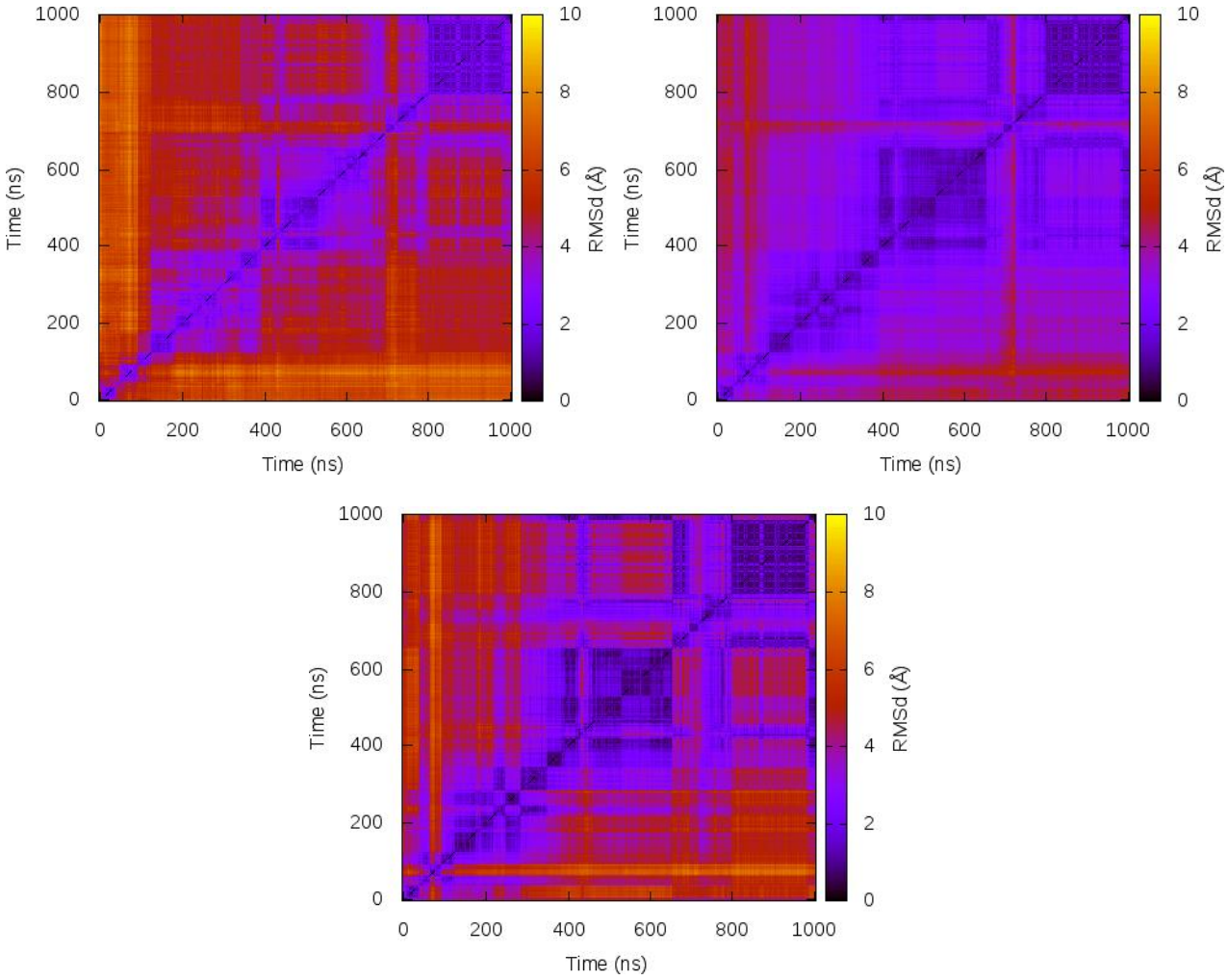

Figure SA2. 2D RMSd plots of structures in the simulation 1KF1-**A**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

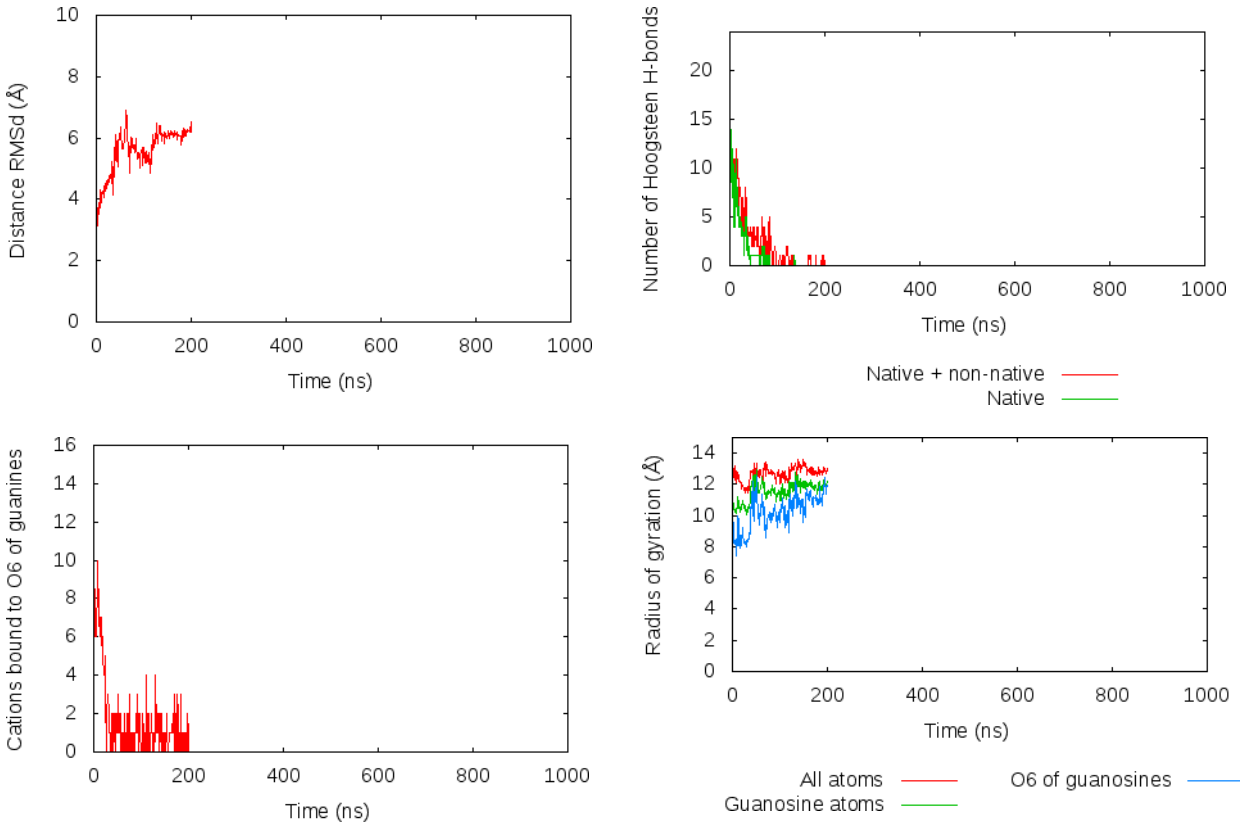

Figure SA3. Evolution of seven CVs in the simulation 1KF1-**B**. Top left: C4′ distance RMSd with respect to the native structure 1KF1. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

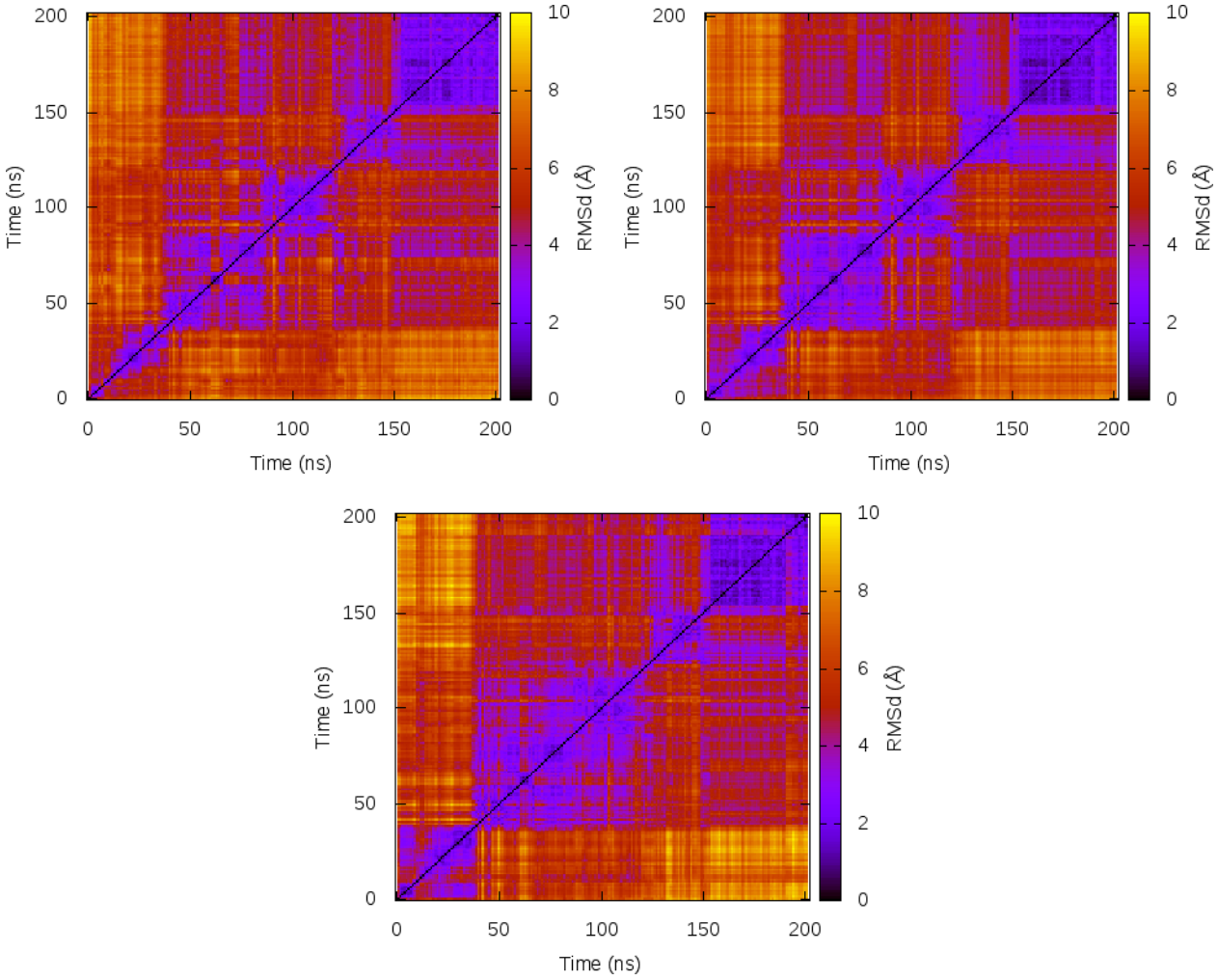

Figure SA4. 2D RMSd plots of structures in the simulation 1KF1-**B**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

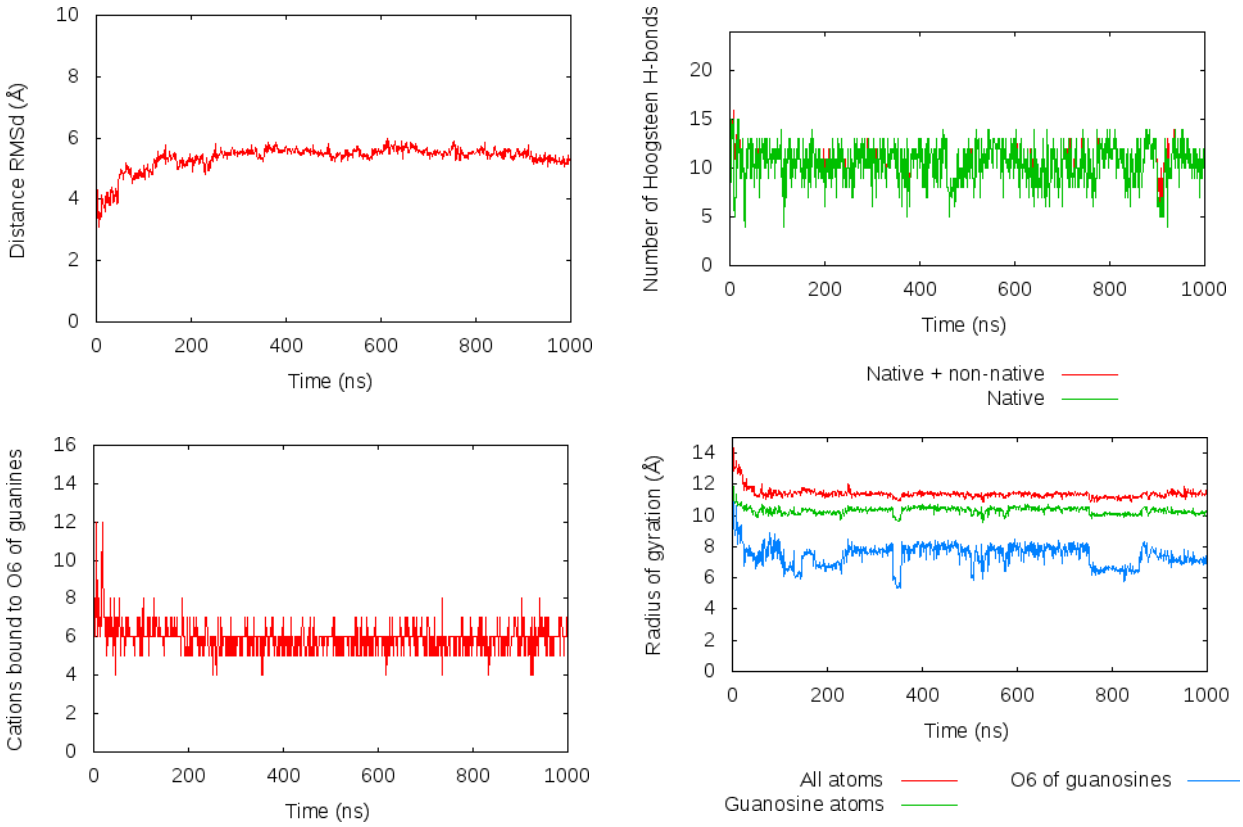

Figure SA5. Evolution of seven CVs in the simulation 1KF1-**C**. Top left: C4′ distance RMSd with respect to the native structure 1KF1. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

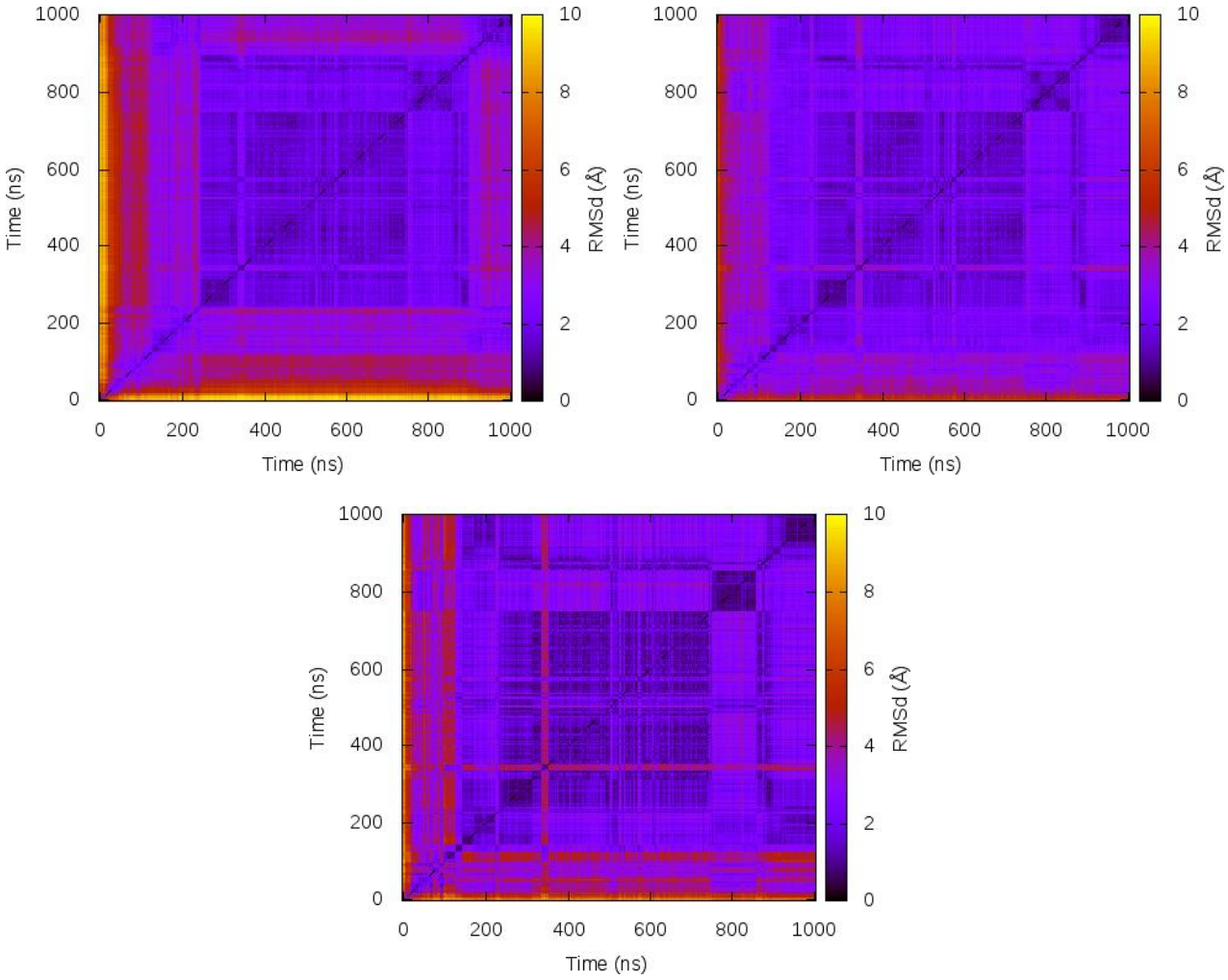

Figure SA6. 2D RMSd plots of structures in the simulation 1KF1-**C**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

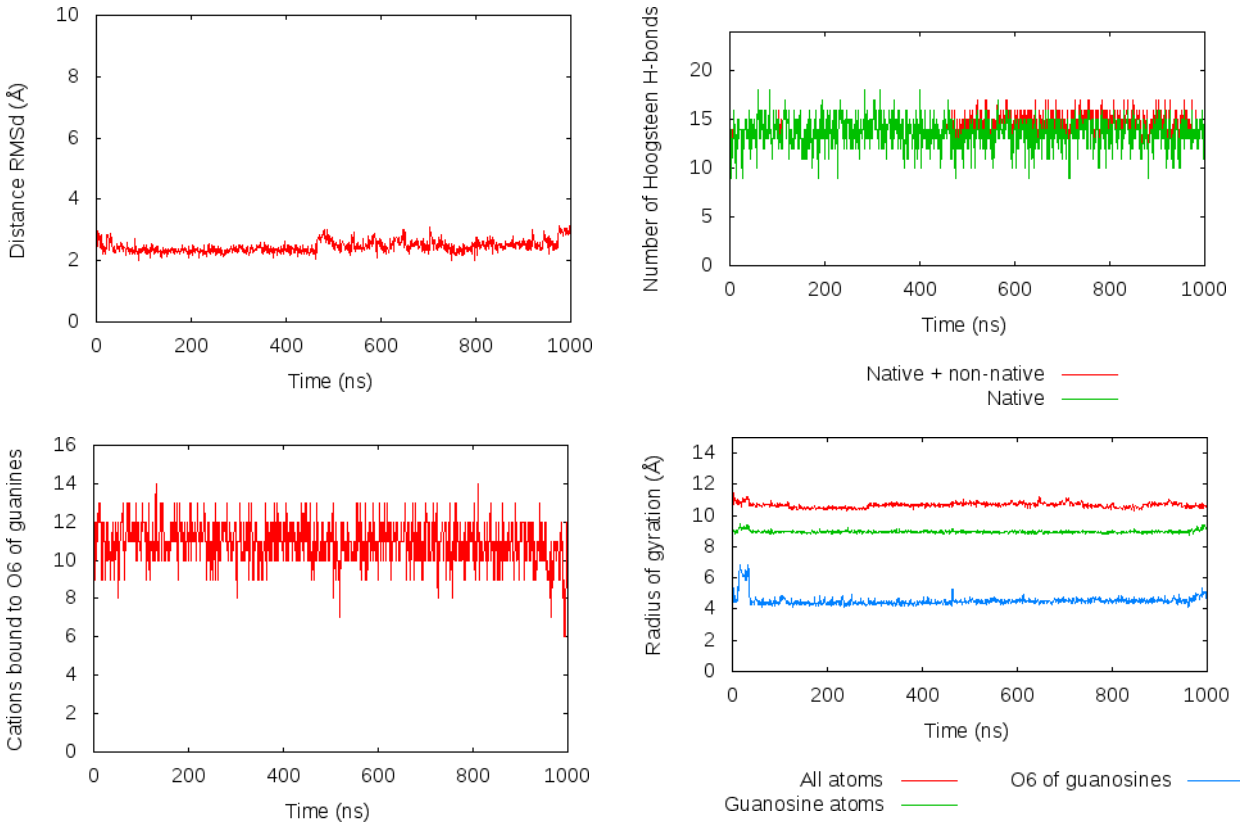

Figure SA7. Evolution of seven CVs in the simulation 143D-**A**. Top left: C4′ distance RMSd with respect to the native structure 143D. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

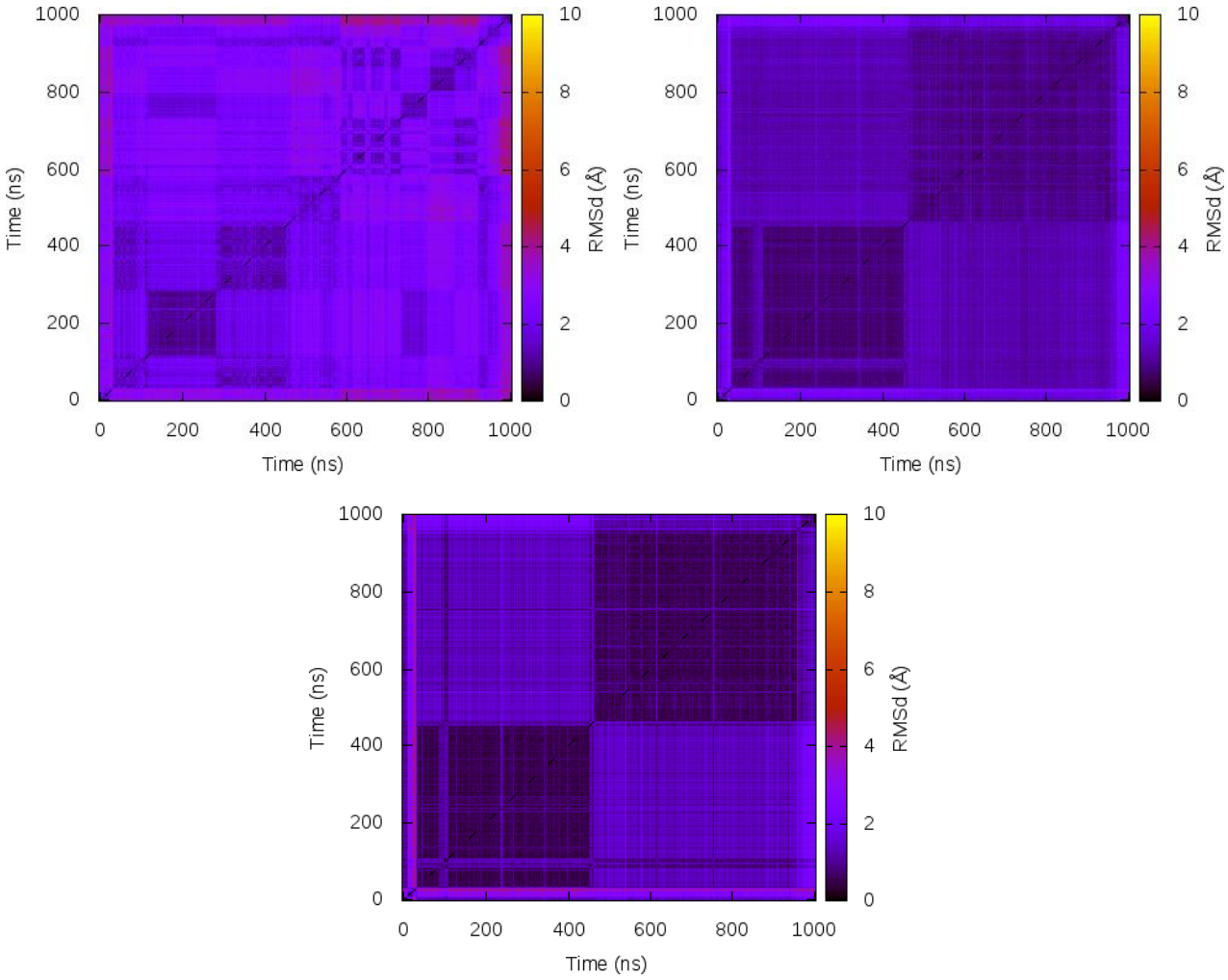

Figure SA8. 2D RMSd plots of structures in the simulation 143D-**A**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

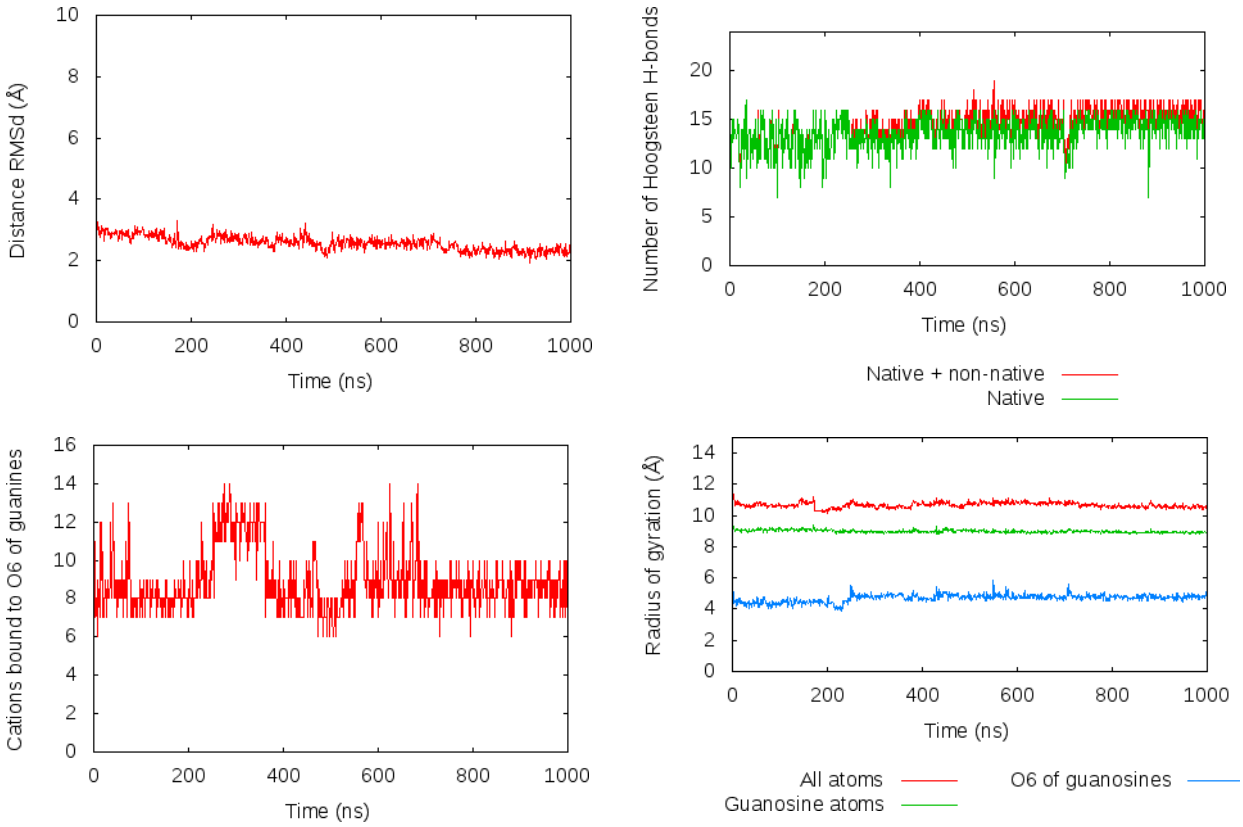

Figure SA9. Evolution of seven CVs in the simulation 143D-**B**. Top left: C4′ distance RMSd with respect to the native structure 143D. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

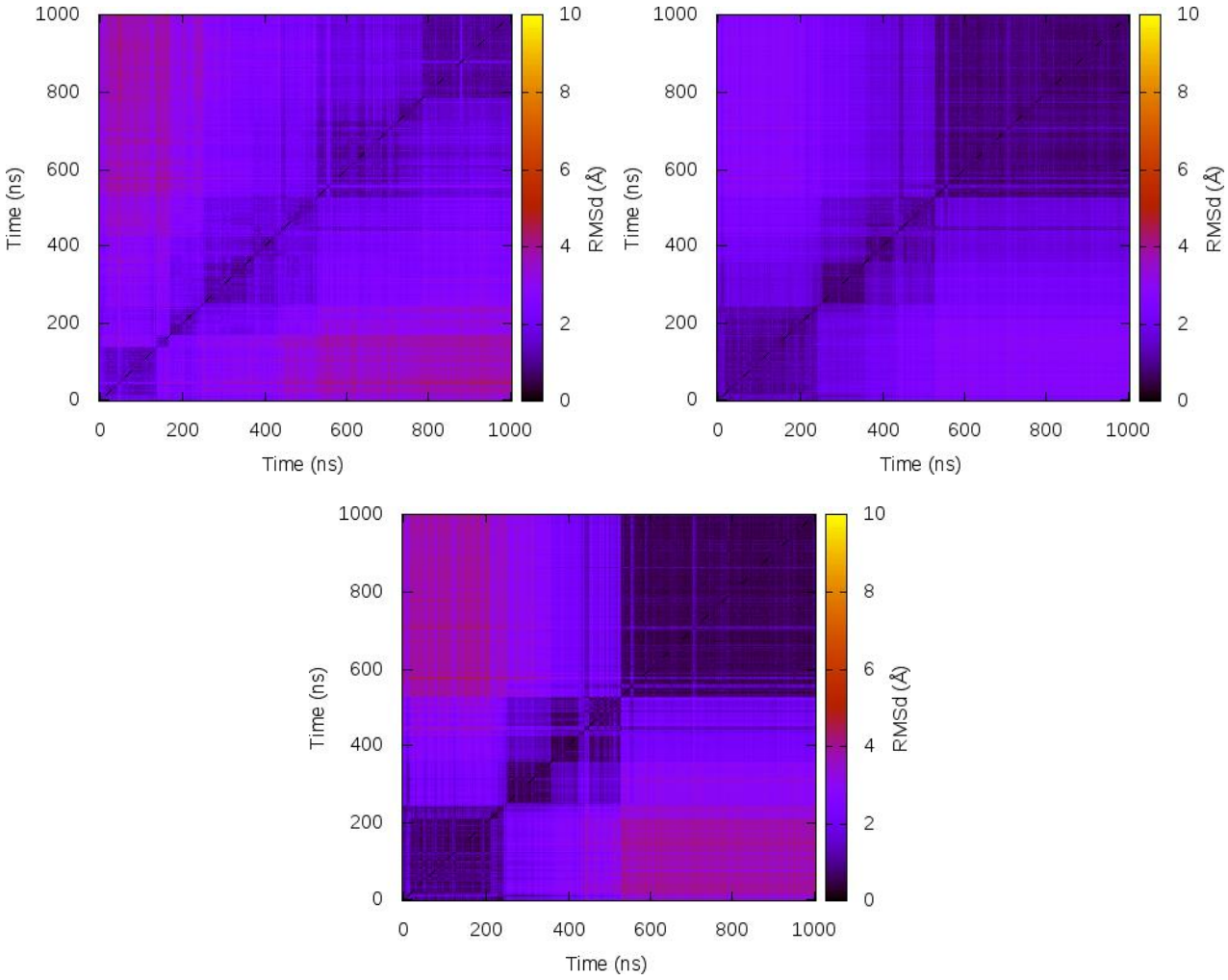

Figure SA10. 2D RMSd plots of structures in the simulation 143D-**B**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

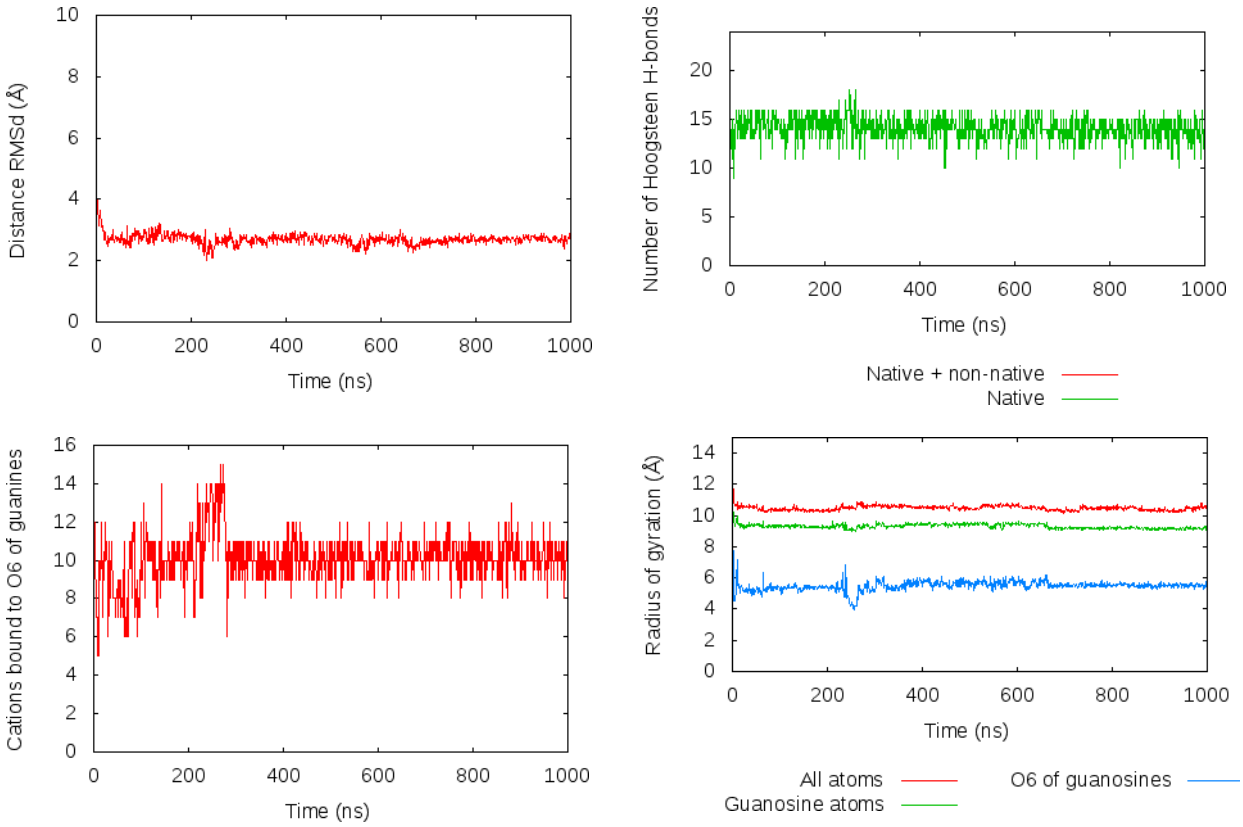

Figure SA11. Evolution of seven CVs in the simulation 143D-**C**. Top left: C4′ distance RMSd with respect to the native structure 143D. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

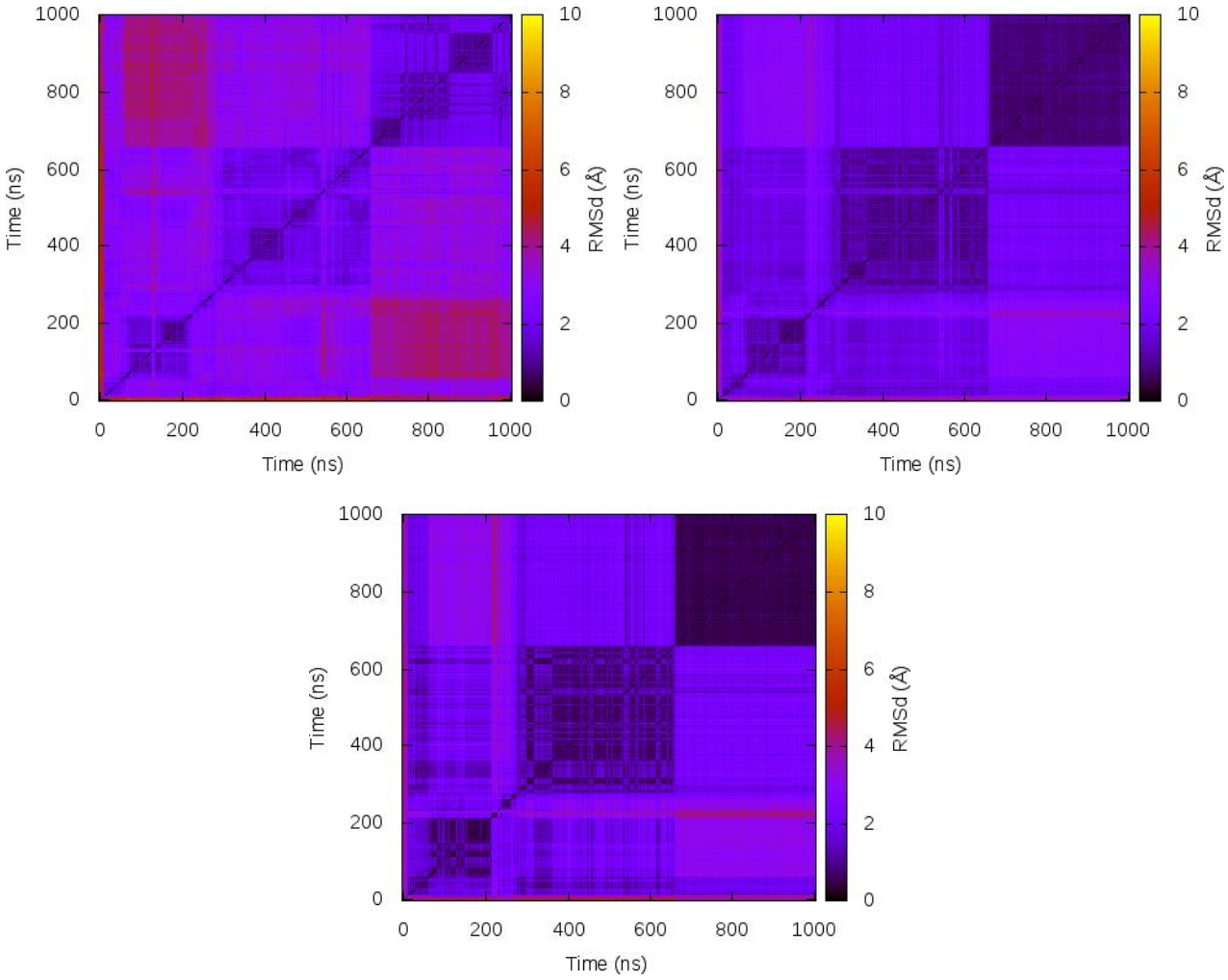

Figure SA12. 2D RMSd plots of structures in the simulation 143D-**C**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

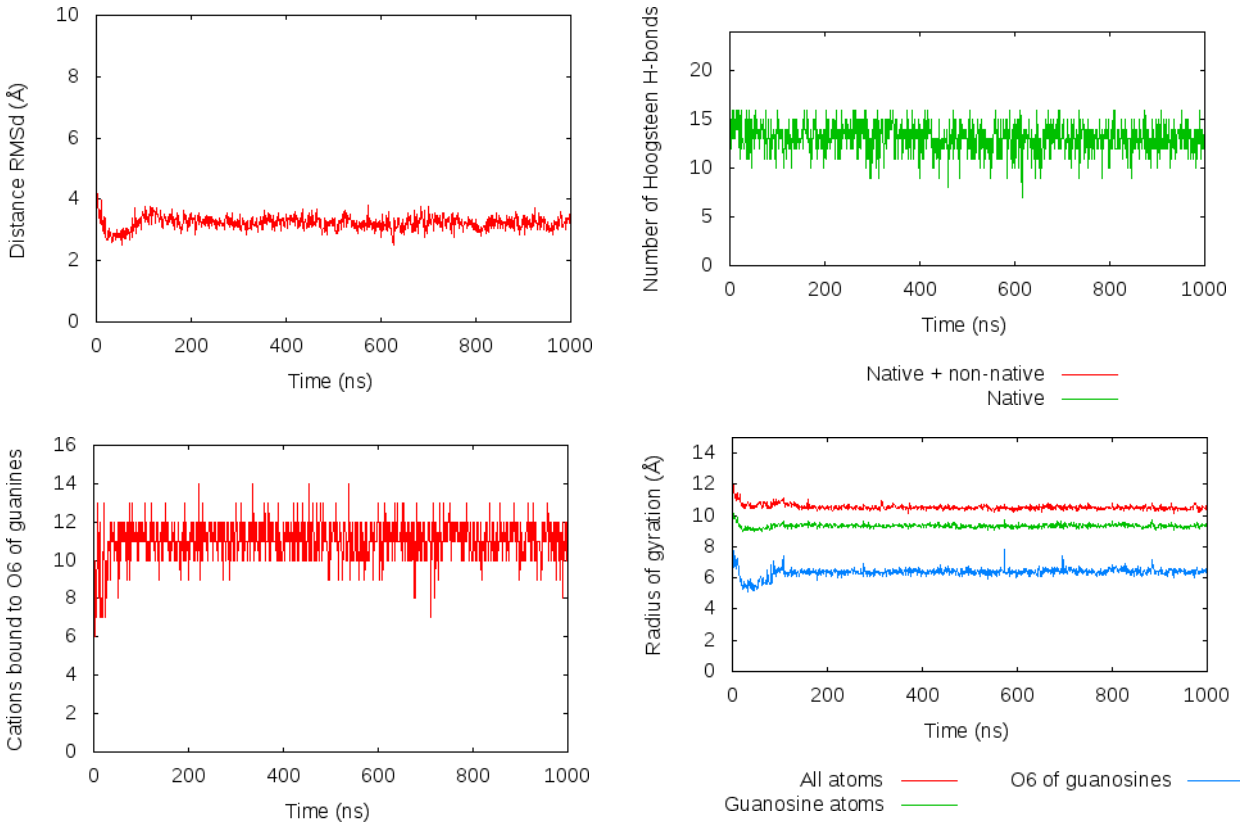

Figure SA13. Evolution of seven CVs in the simulation 143D-**D**. Top left: C4′ distance RMSd with respect to the native structure 143D. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

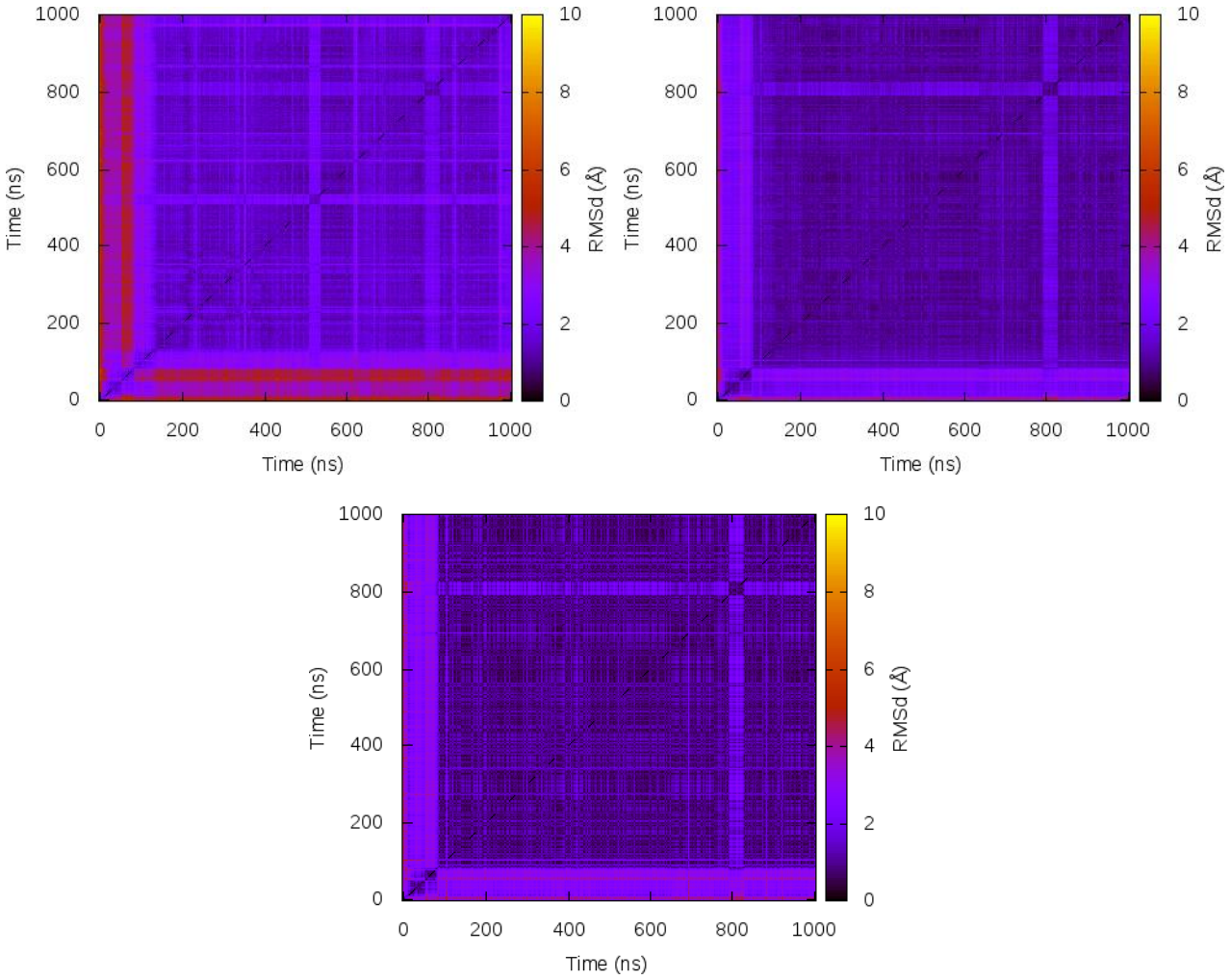

Figure SA14. 2D RMSd plots of structures in the simulation 143D-**D**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

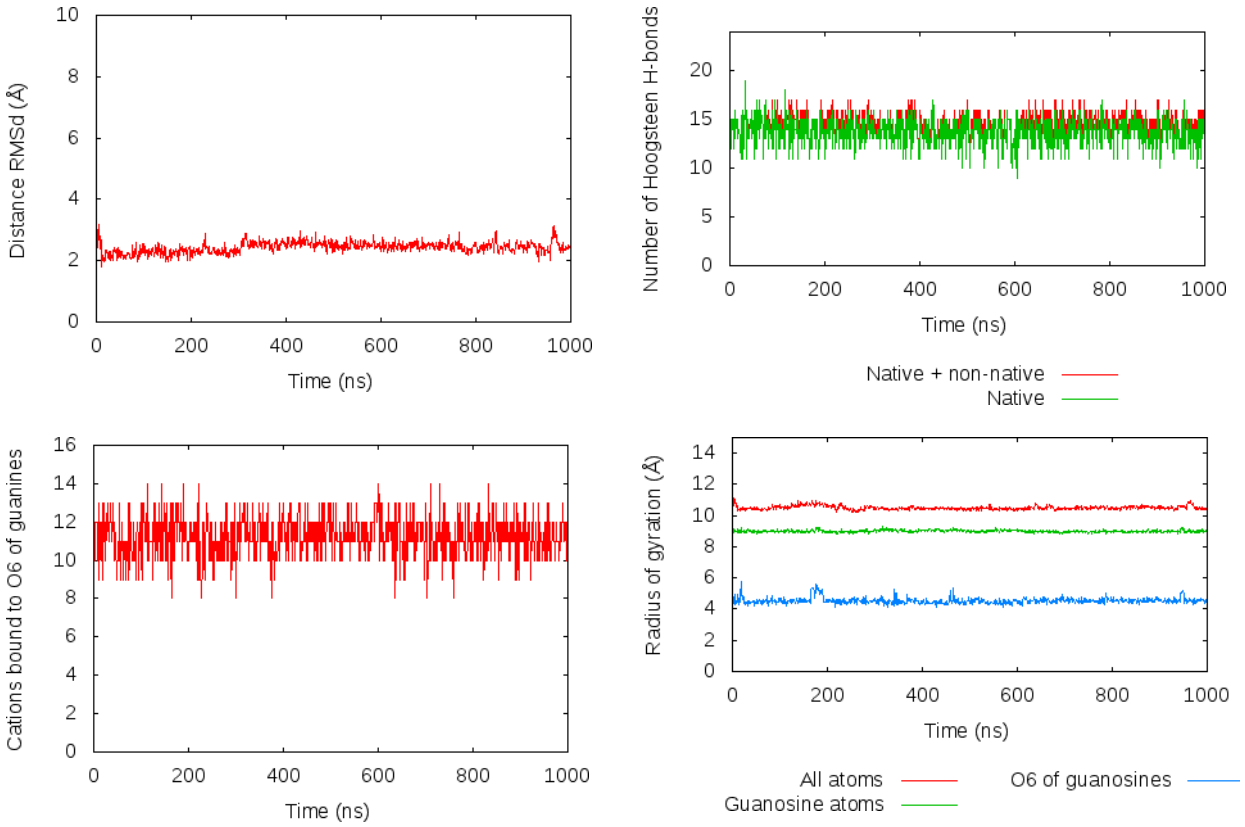

Figure SA15. Evolution of seven CVs in the simulation 143D-**E**. Top left: C4′ distance RMSd with respect to the native structure 143D. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

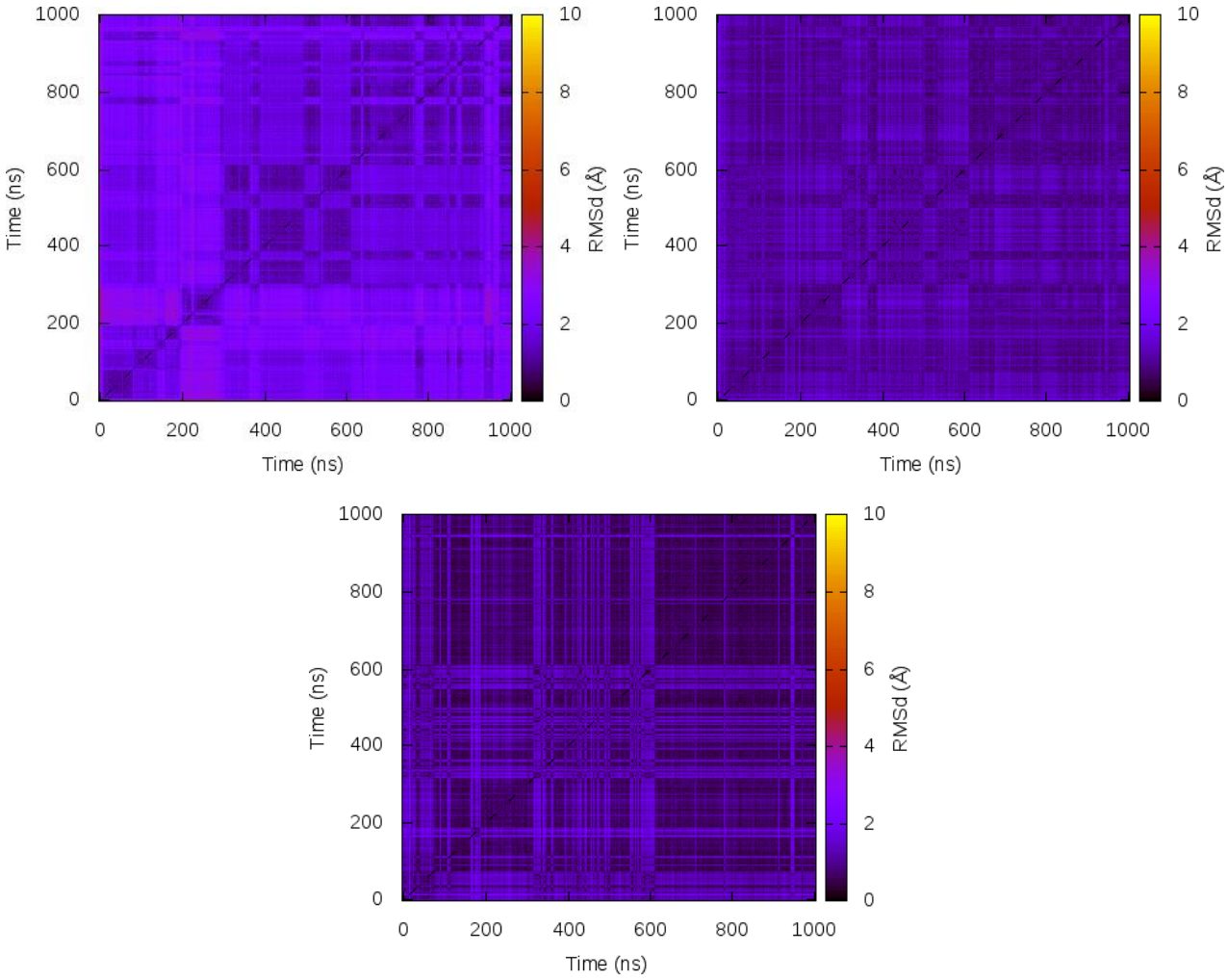

Figure SA16. 2D RMSd plots of structures in the simulation 143D-**E**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

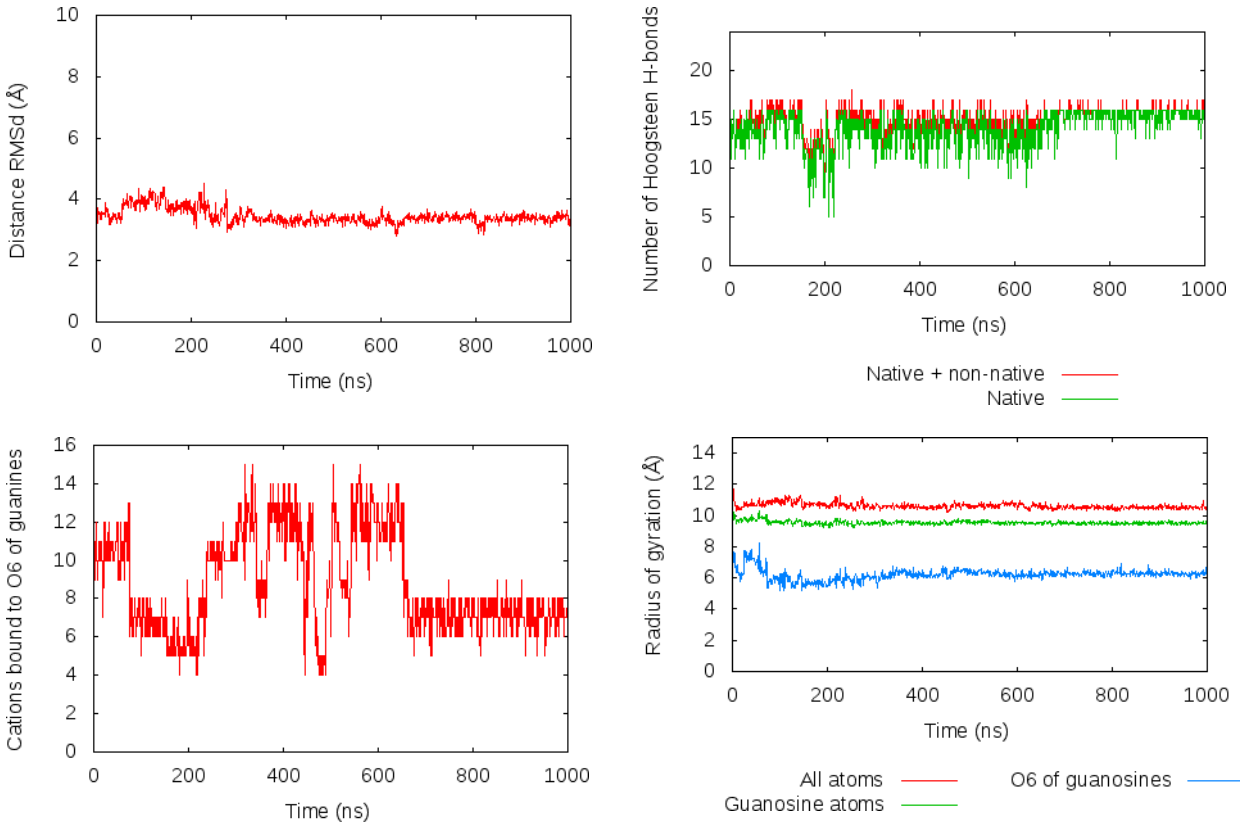

Figure SA17. Evolution of seven CVs in the simulation 143D-**F**. Top left: C4′ distance RMSd with respect to the native structure 143D. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

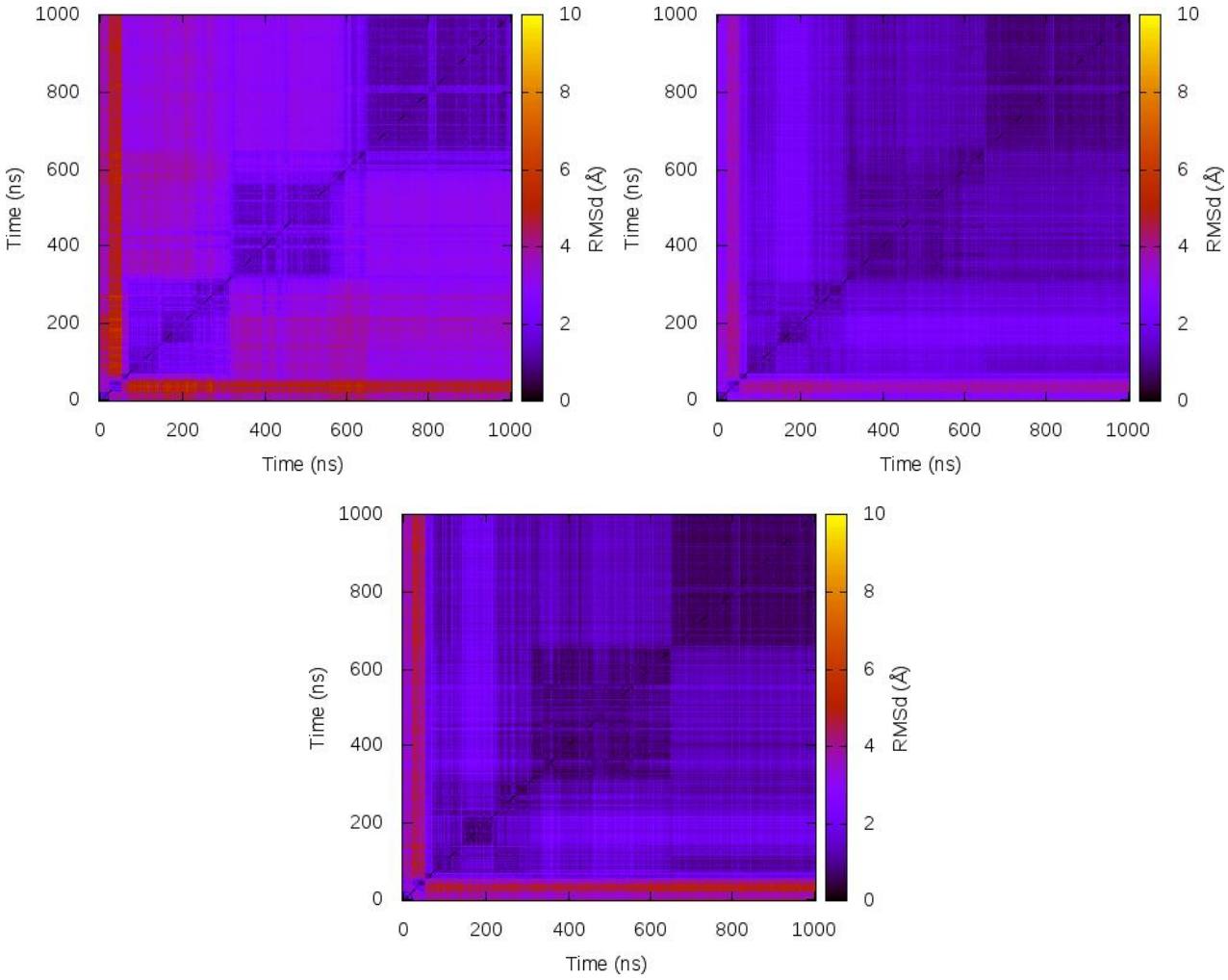

Figure SA18. 2D RMSd plots of structures in the simulation 143D-**F**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

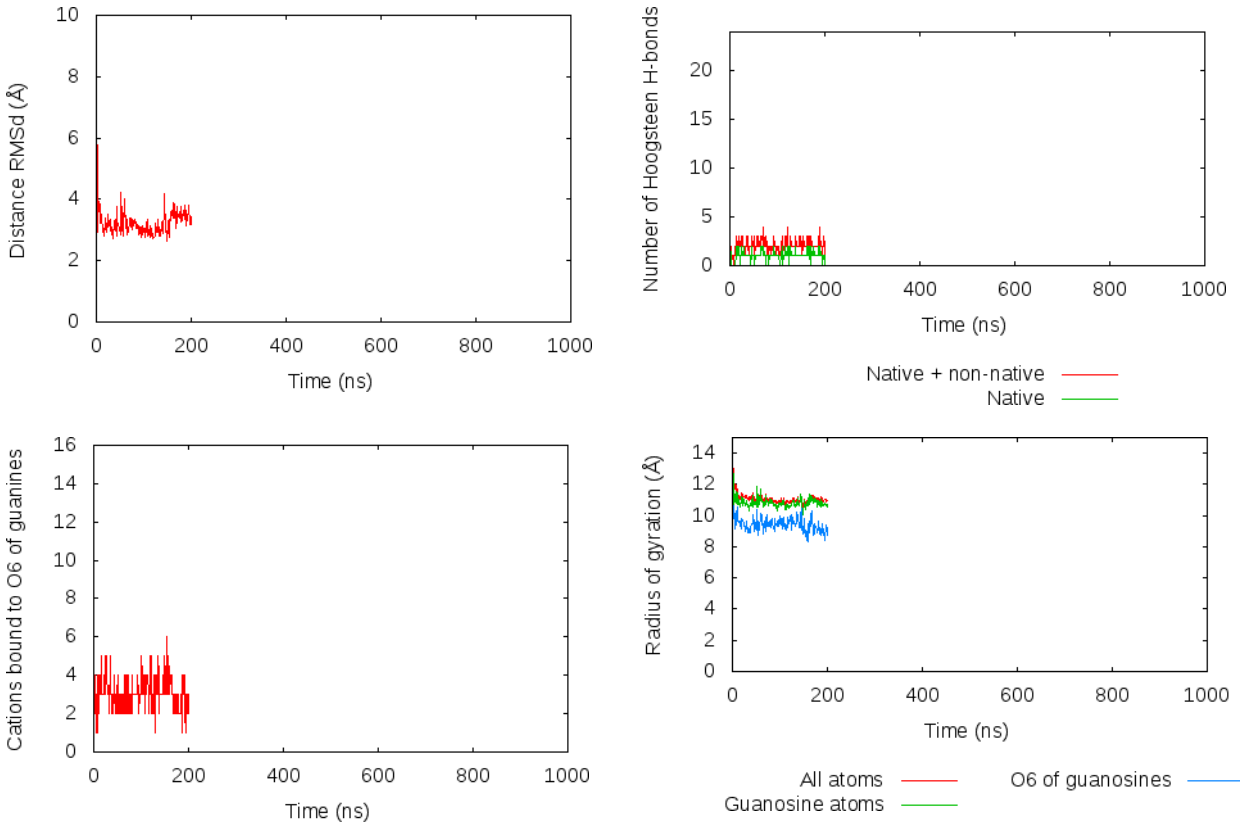

Figure SA19. Evolution of seven CVs in the simulation 143D-**G**. Top left: C4′ distance RMSd with respect to the native structure 143D. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

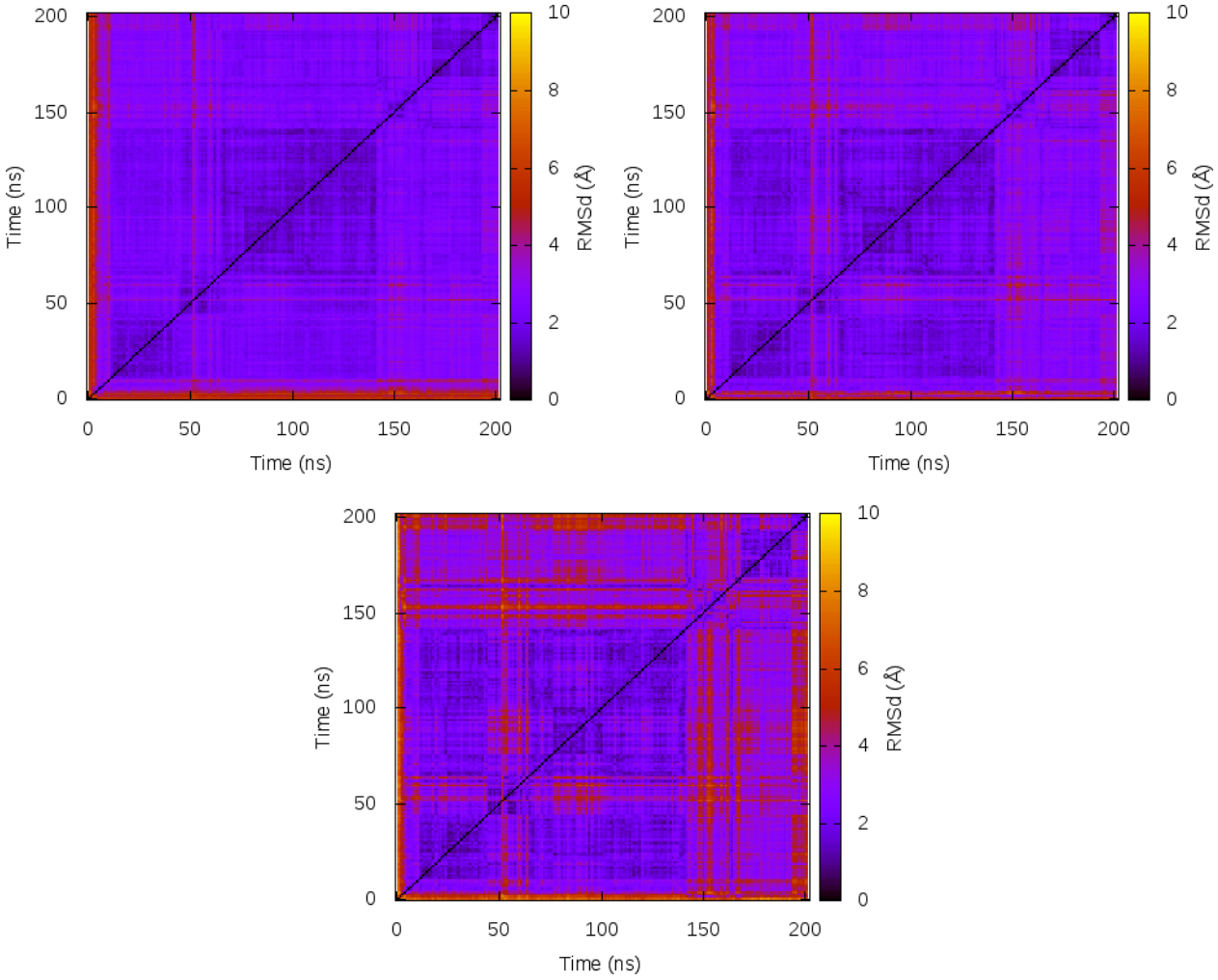

Figure SA20. 2D RMSd plots of structures in the simulation 143D-**G**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

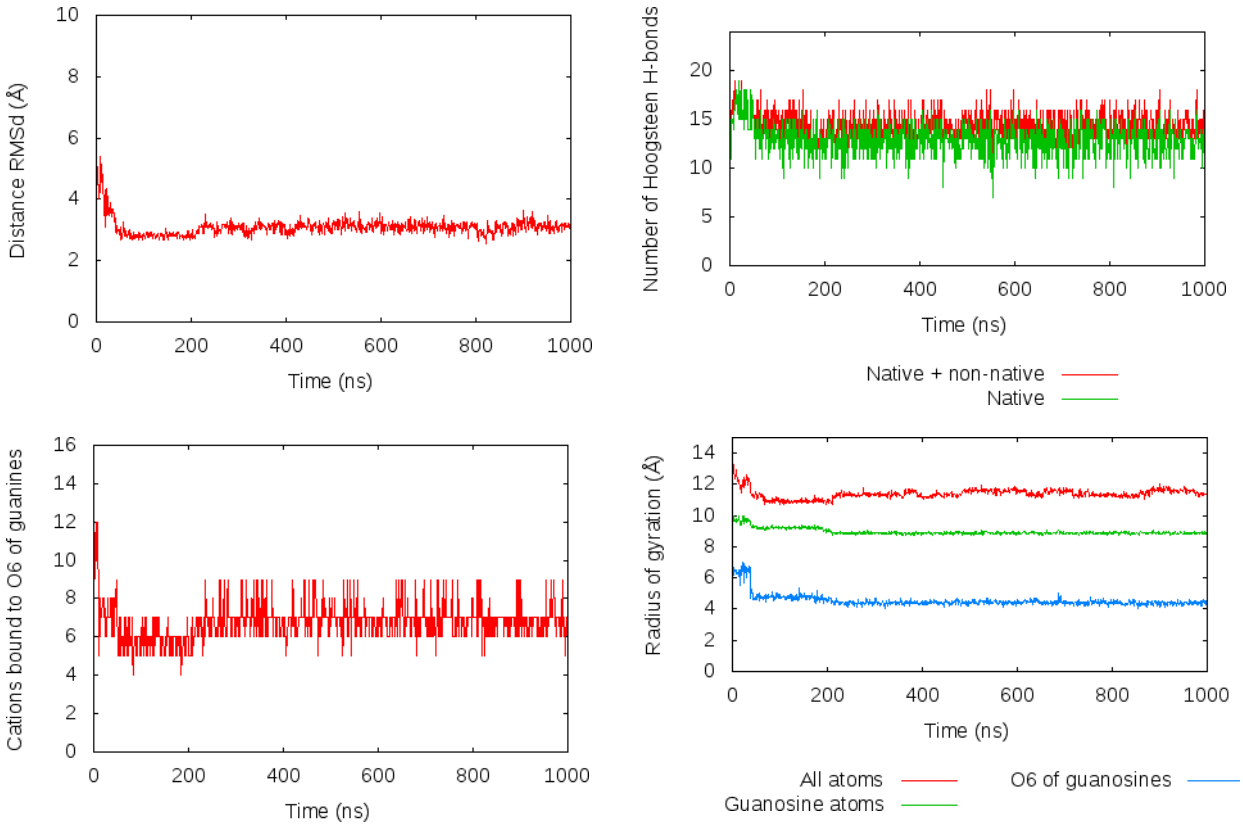

Figure SA21. Evolution of seven CVs in the simulation 2JSM-**A**. Top left: C4′ distance RMSd with respect to the native structure 2JSM. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

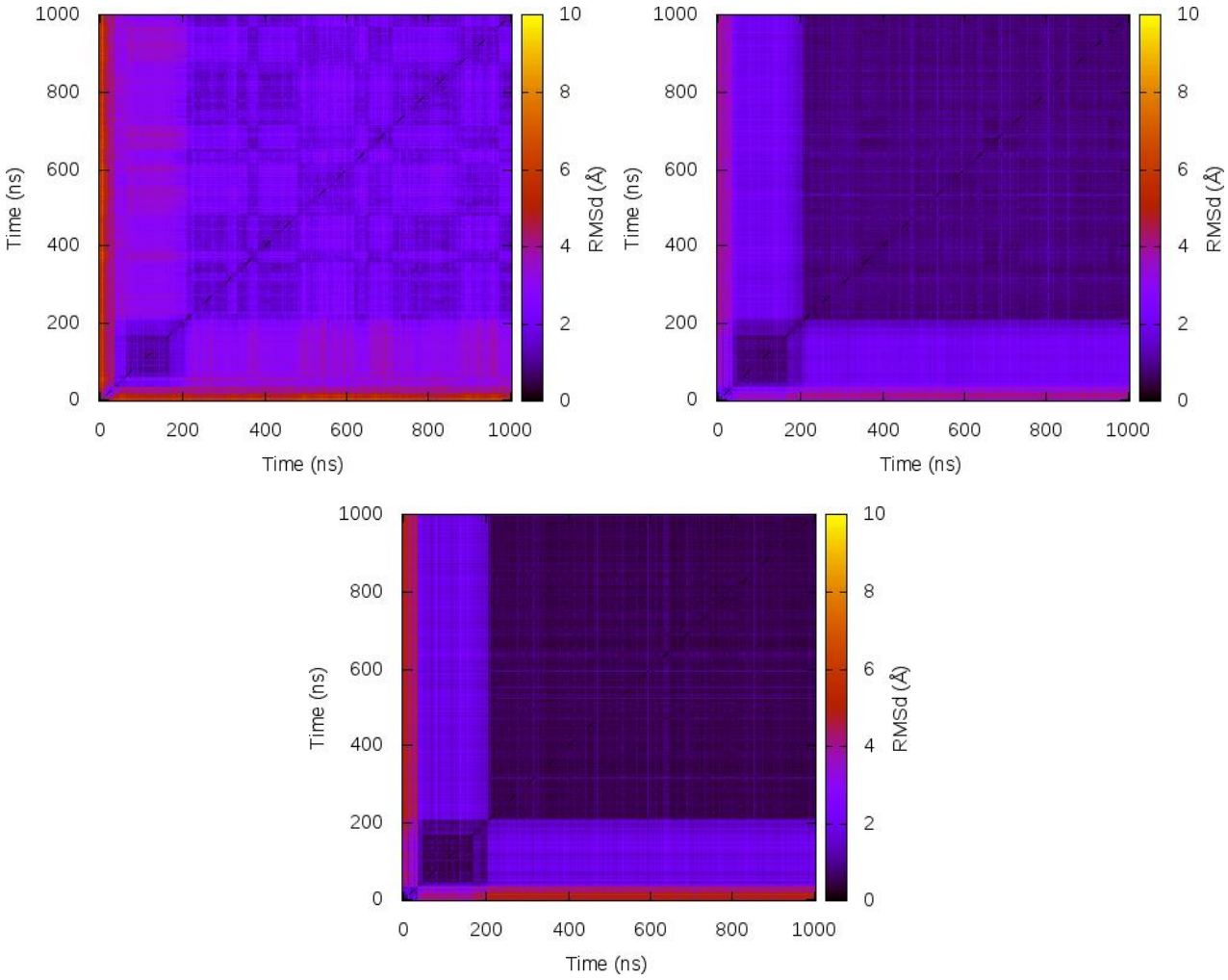

Figure SA22. 2D RMSd plots of structures in the simulation 2JSM-**A**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

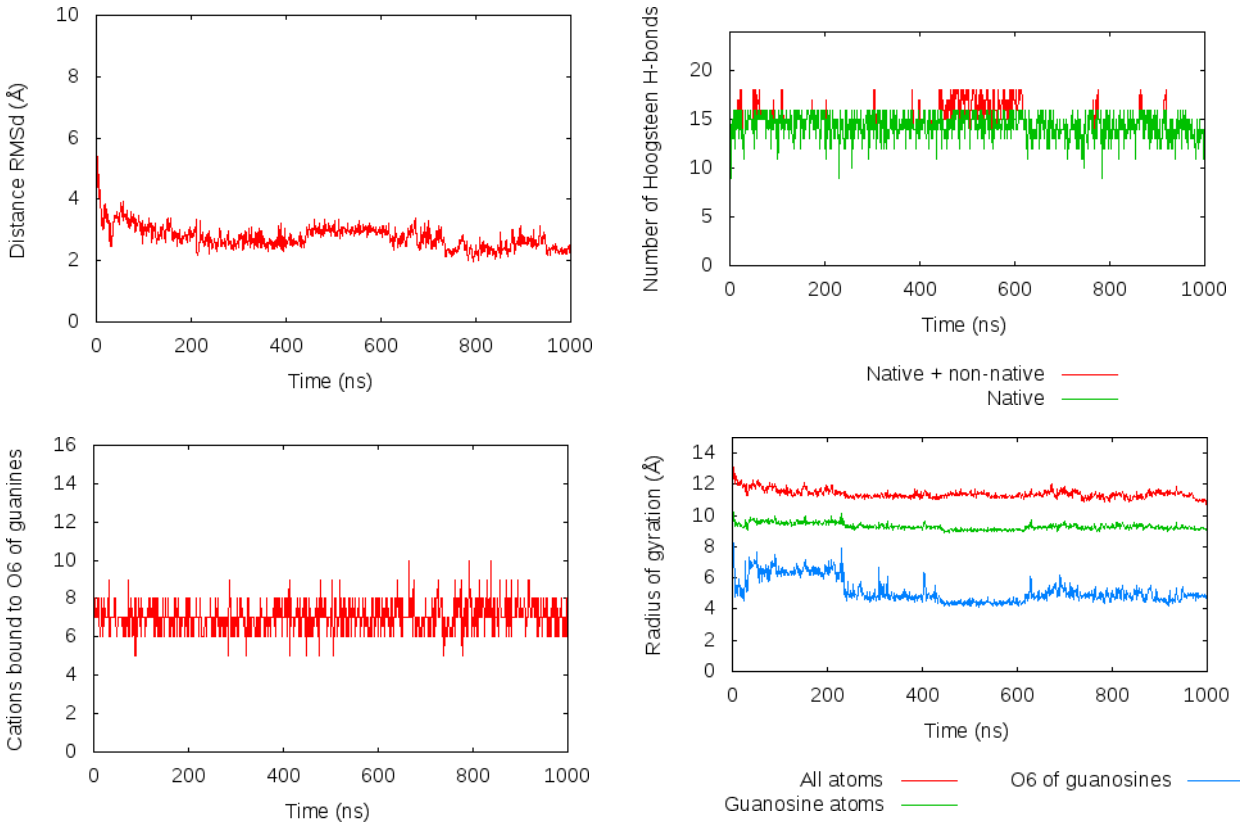

Figure SA23. Evolution of seven CVs in the simulation 2JSM-**B**. Top left: C4′ distance RMSd with respect to the native structure 2JSM. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

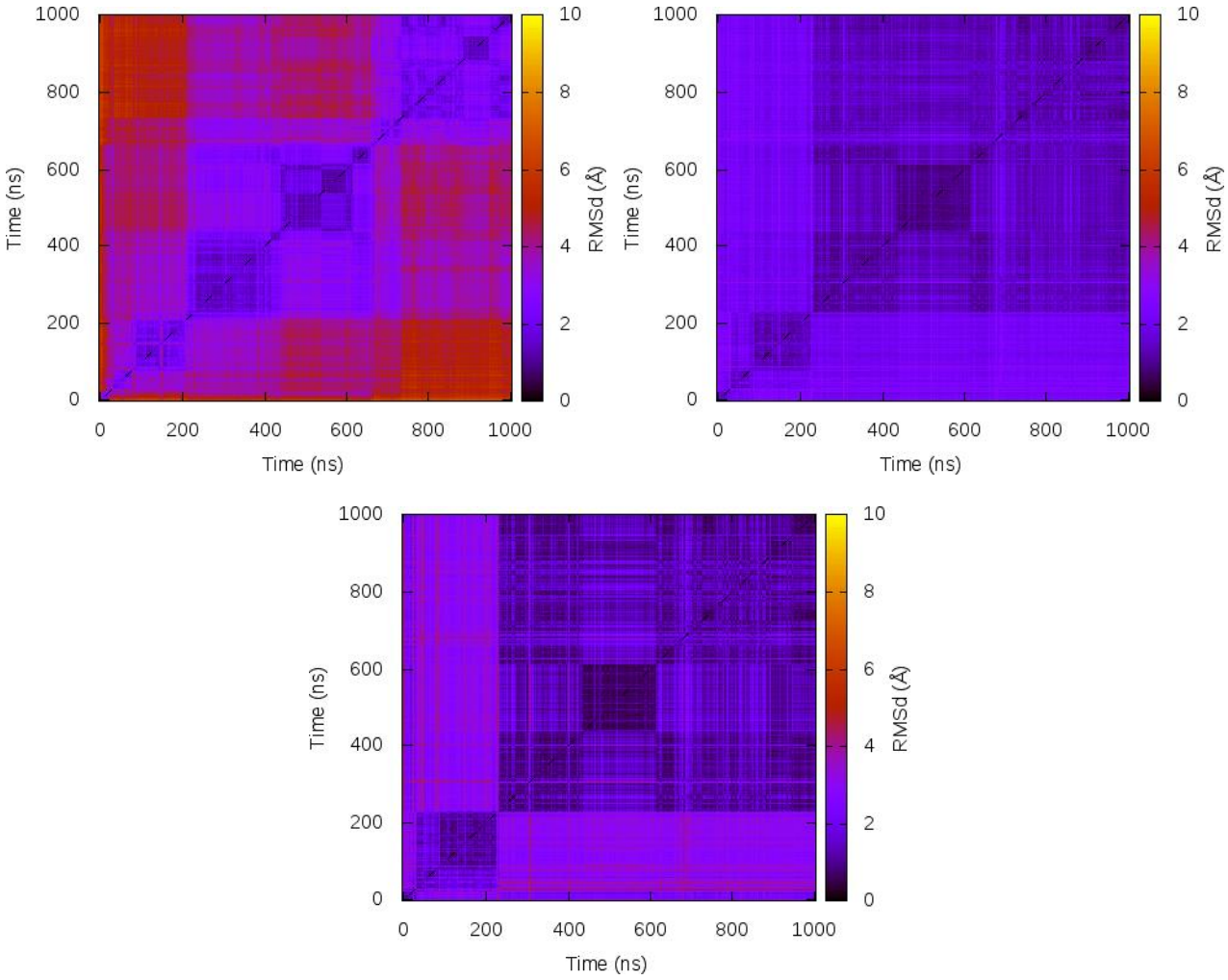

Figure SA24. 2D RMSd plots of structures in the simulation 2JSM-**B**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

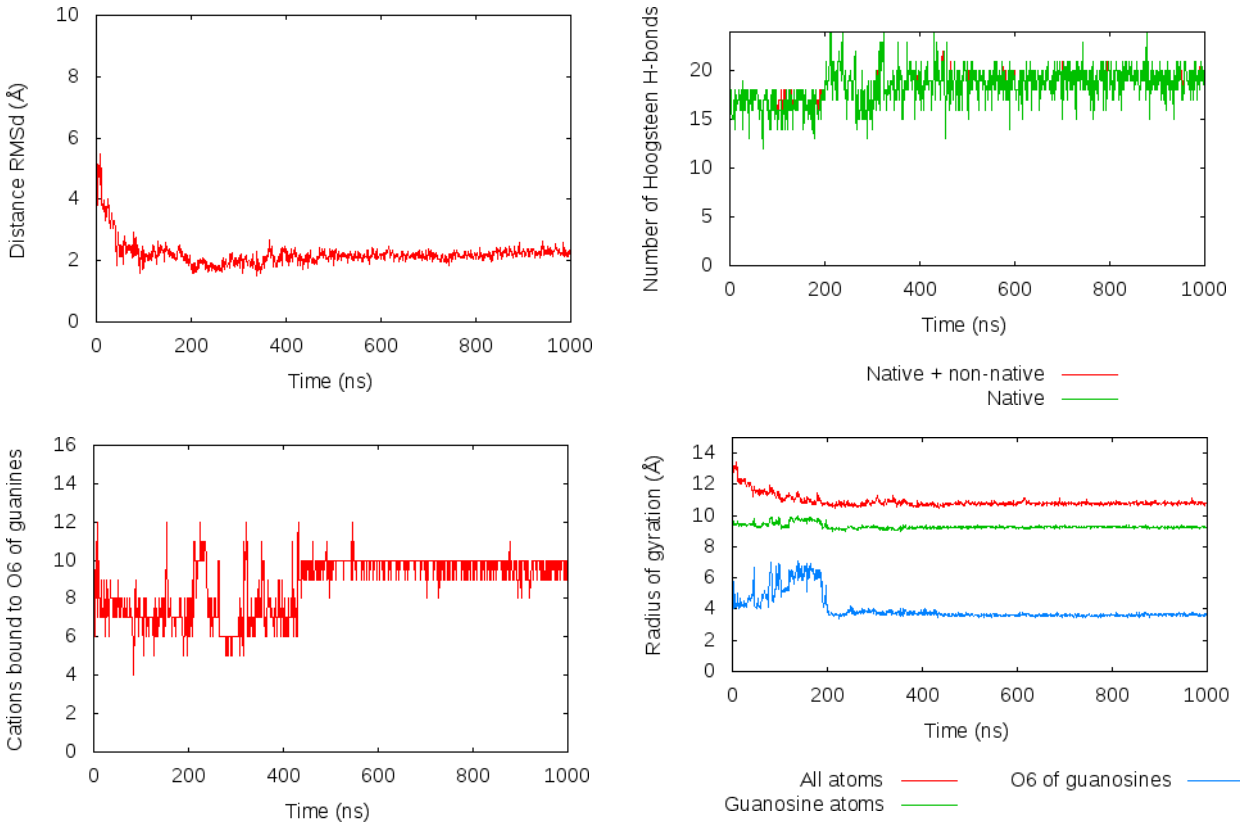

Figure SA25. Evolution of seven CVs in the simulation 2JSM-**C**. Top left: C4′ distance RMSd with respect to the native structure 2JSM. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

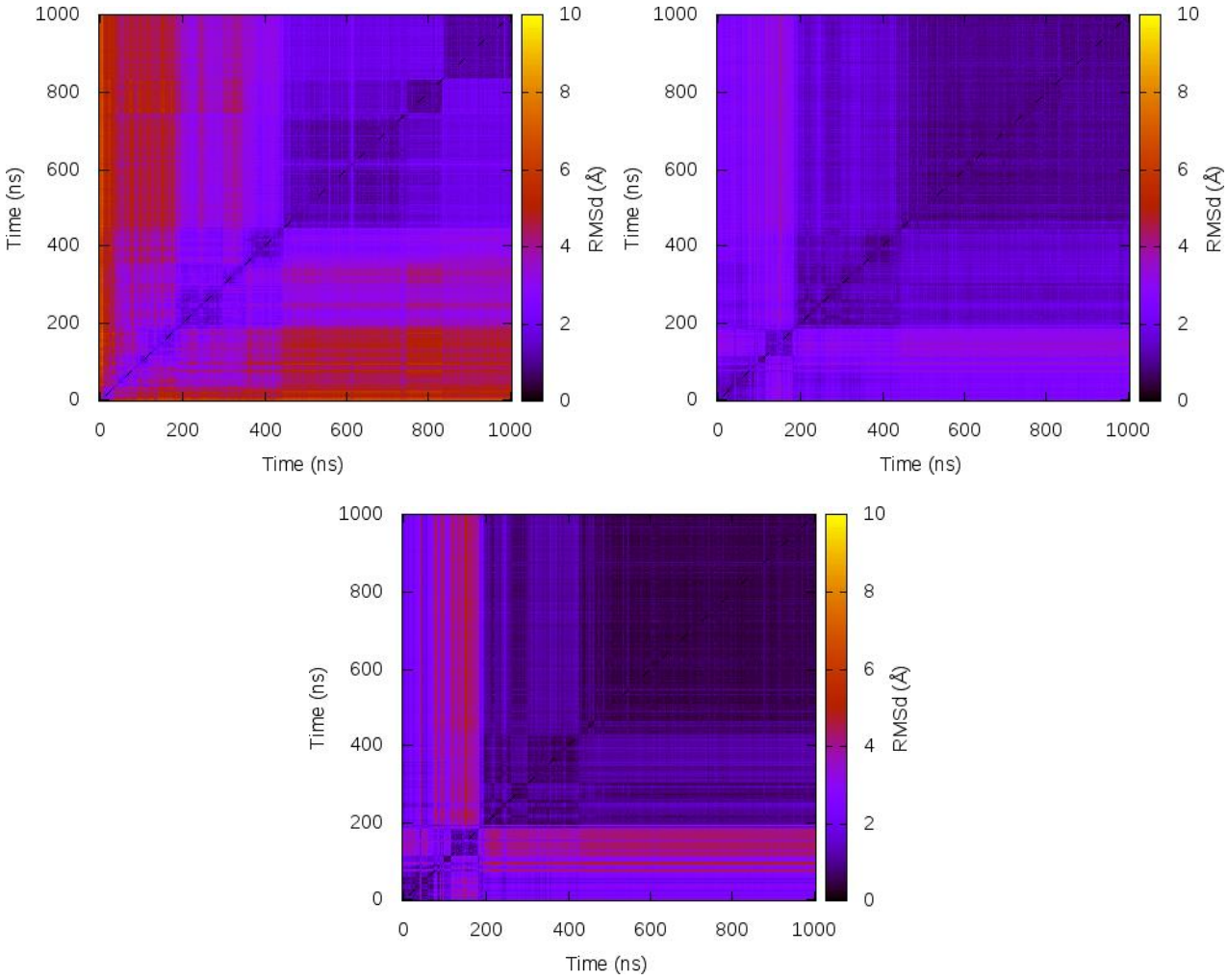

Figure SA26. 2D RMSd plots of structures in the simulation 2JSM-**C**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

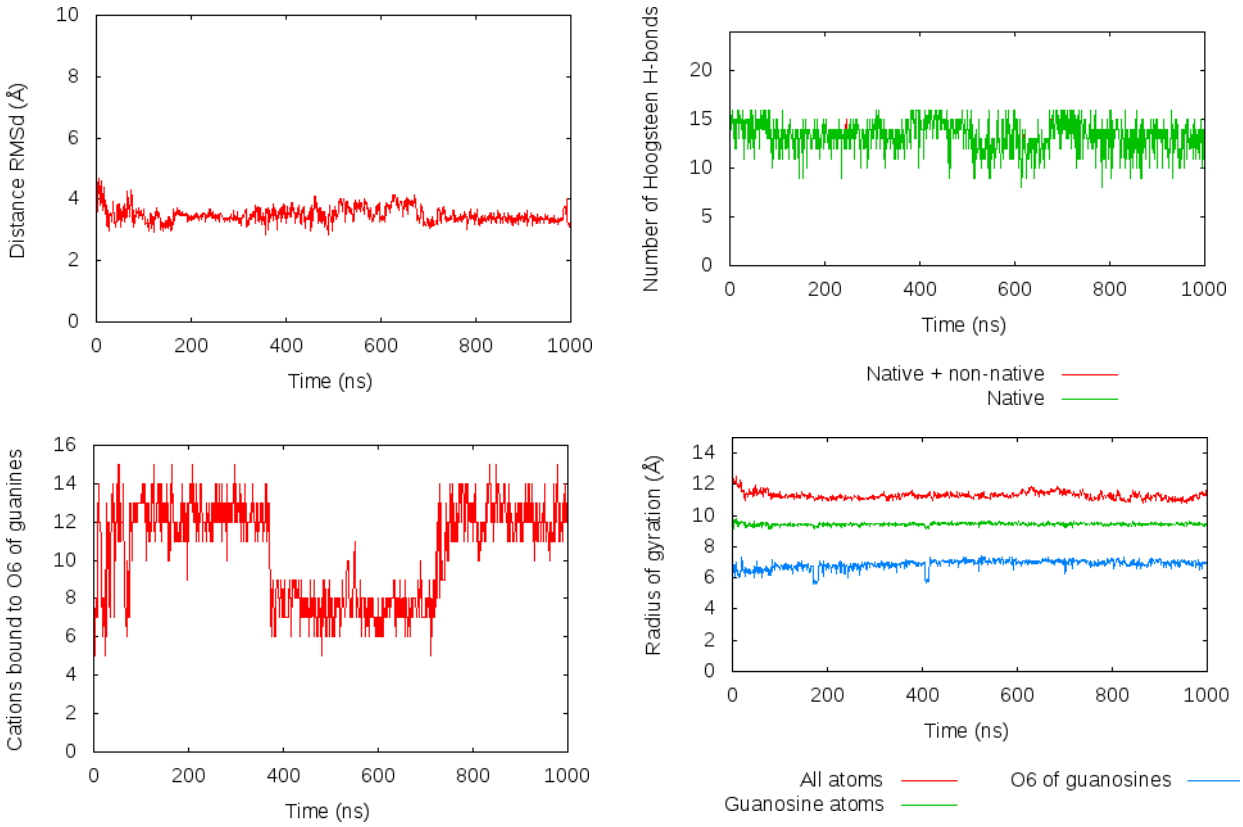

Figure SA27. Evolution of seven CVs in the simulation 2JSM-**D**. Top left: C4′ distance RMSd with respect to the native structure 2JSM. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

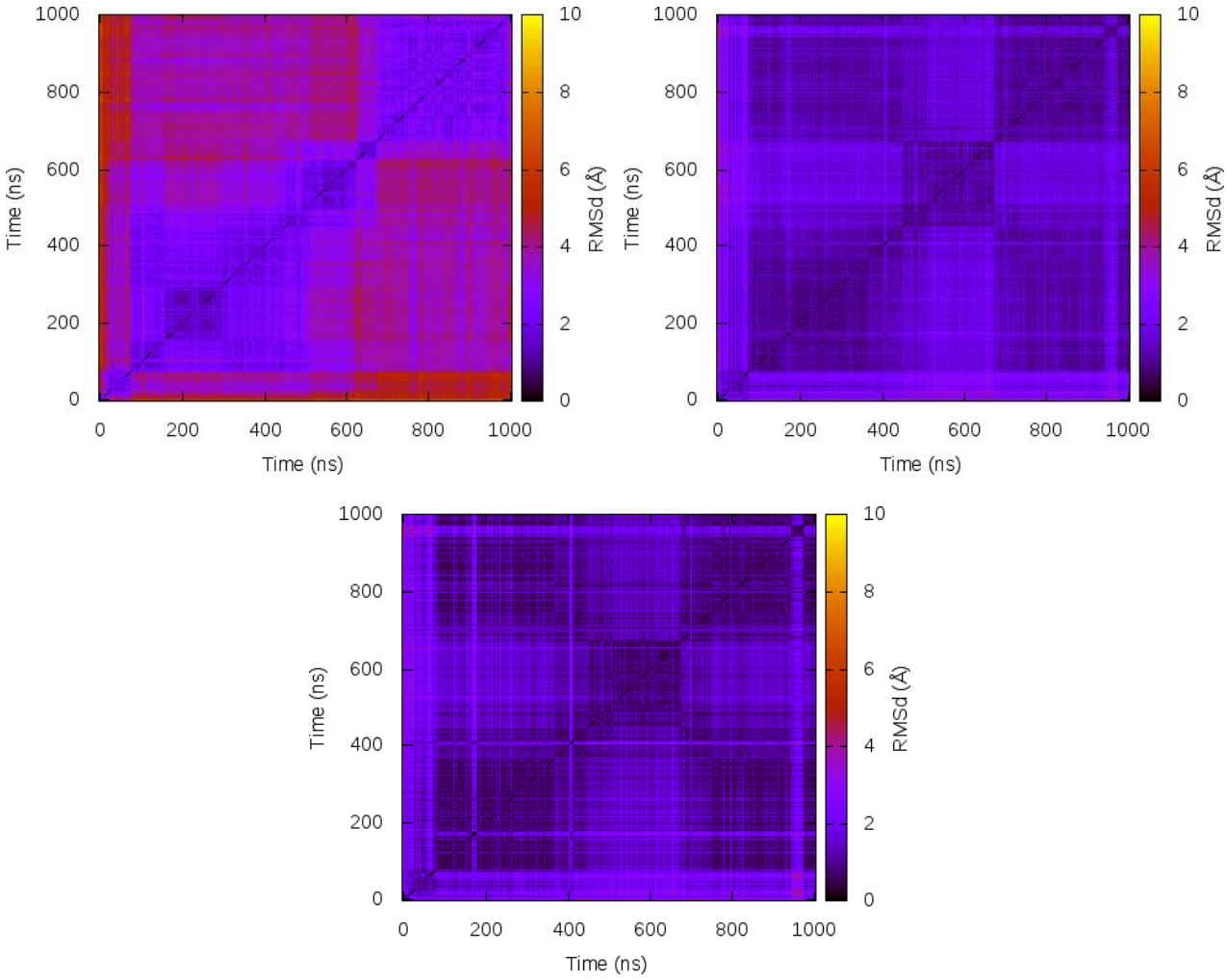

Figure SA28. 2D RMSd plots of structures in the simulation 2JSM-**D**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

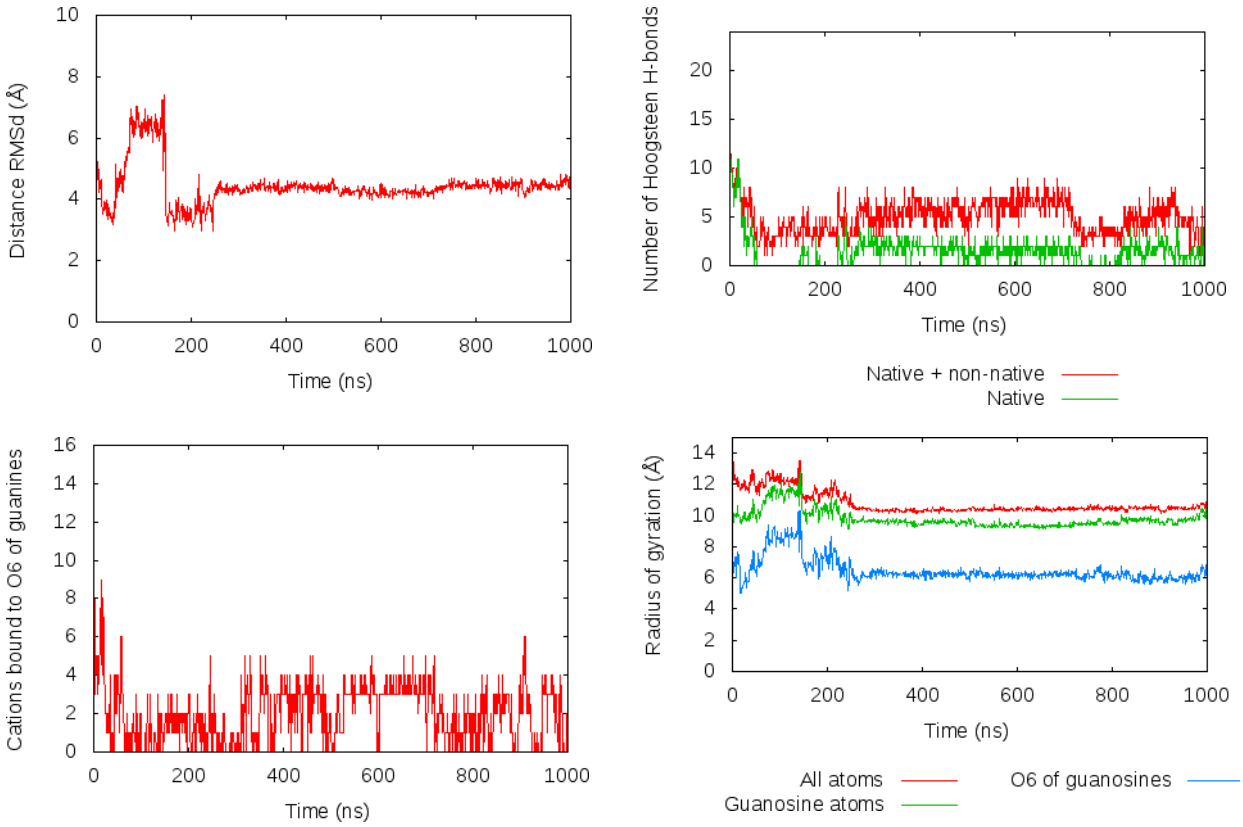

Figure SA29. Evolution of seven CVs in the simulation 2JSM-**E**. Top left: C4′ distance RMSd with respect to the native structure 2JSM. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

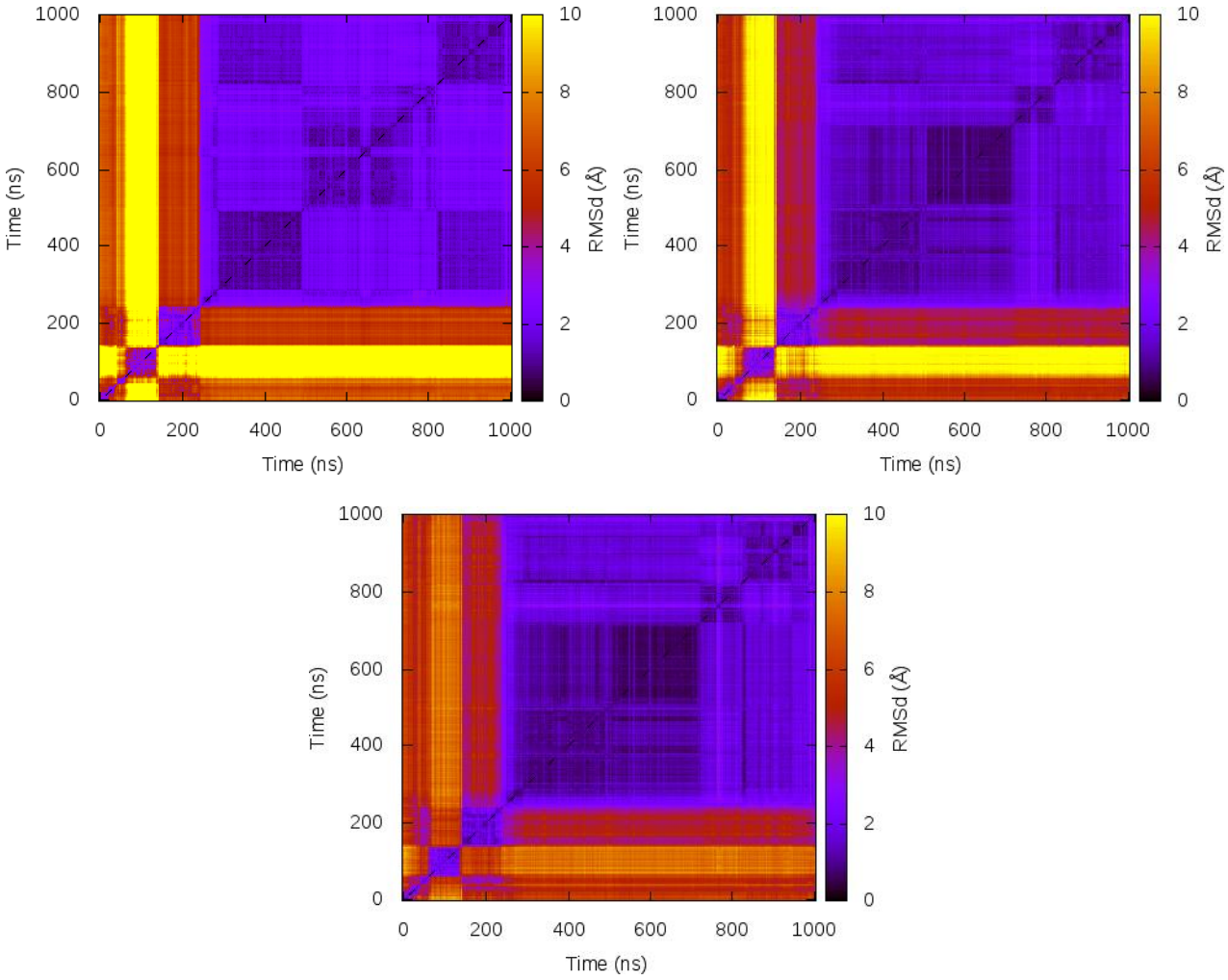

Figure SA30. 2D RMSd plots of structures in the simulation 2JSM-**E**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

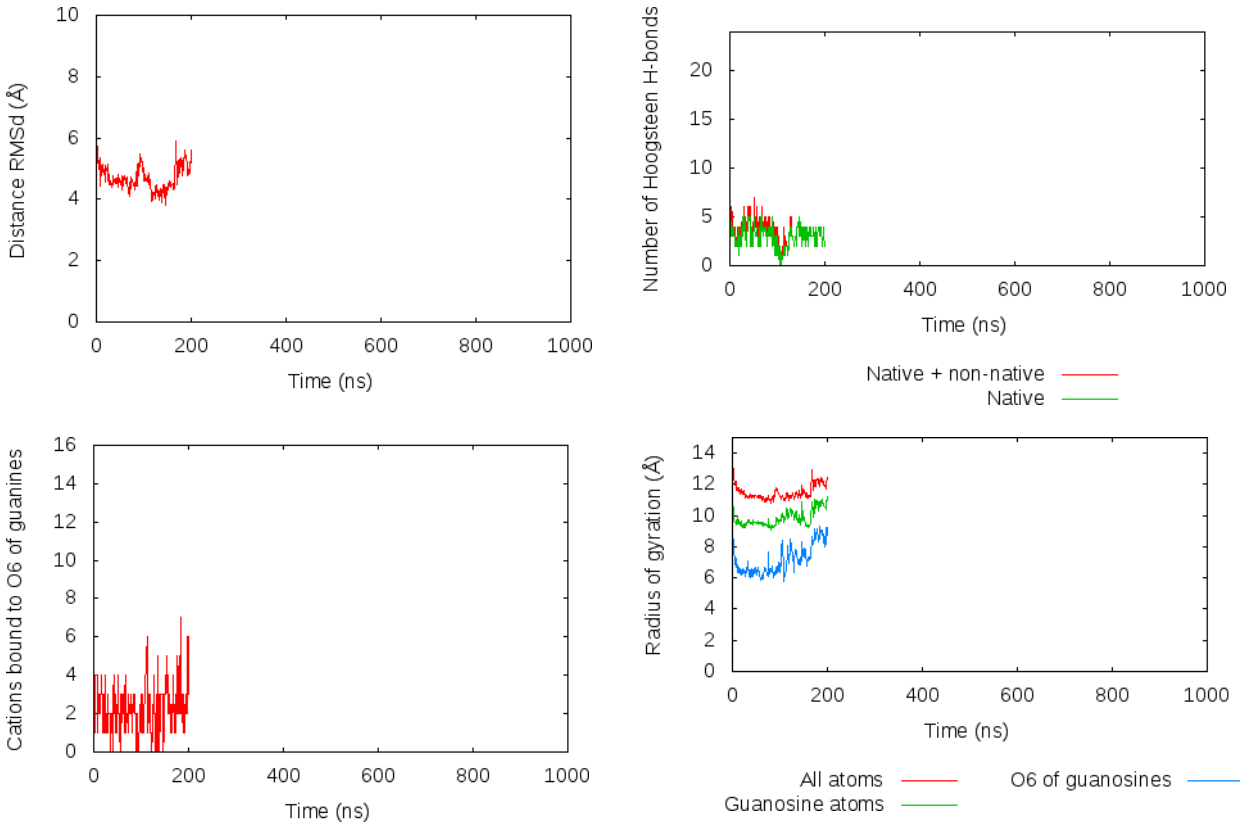

Figure SA31. Evolution of seven CVs in the simulation 2JSM-**F**. Top left: C4′ distance RMSd with respect to the native structure 2JSM. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

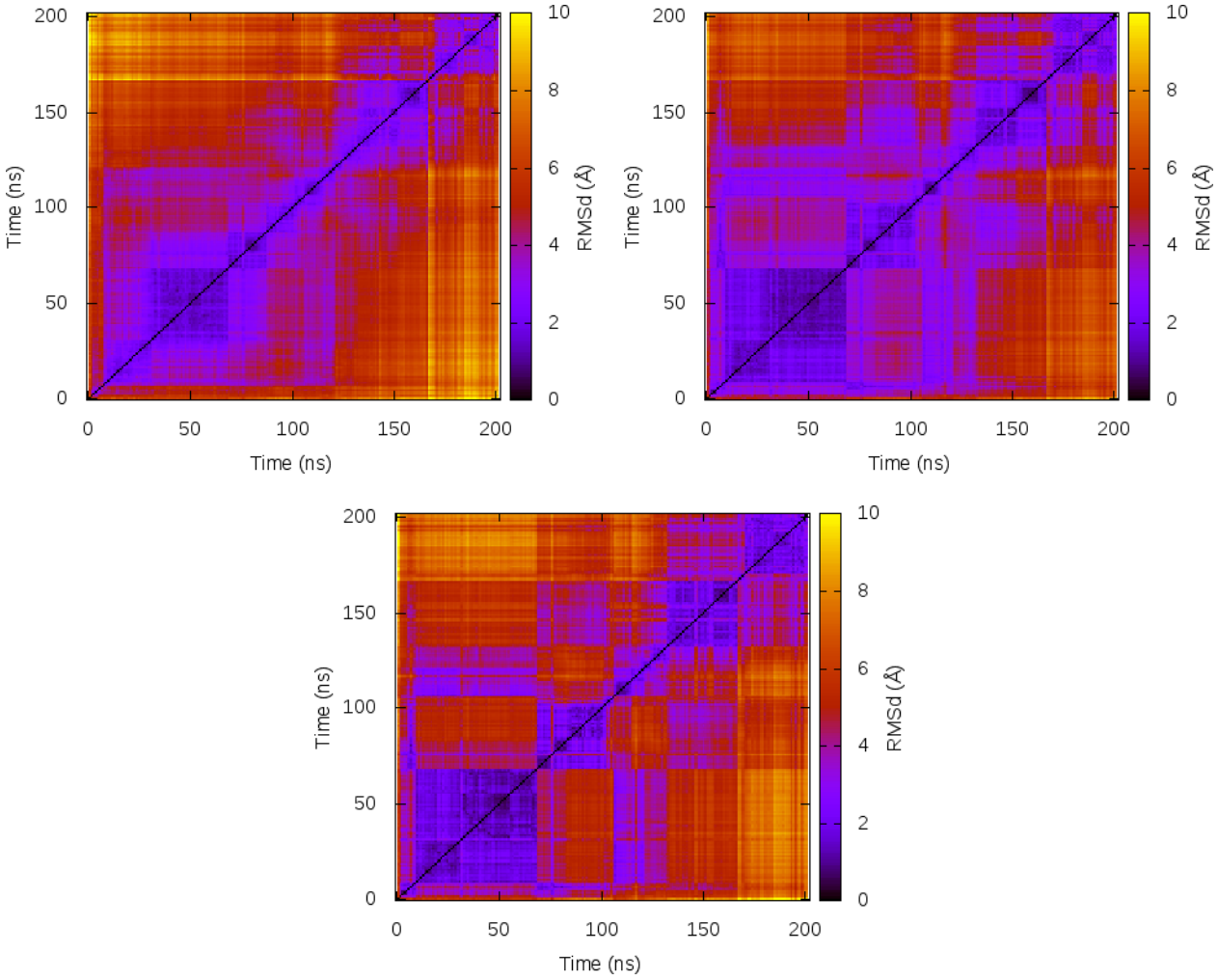

Figure SA32. 2D RMSd plots of structures in the simulation 2JSM-**F**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

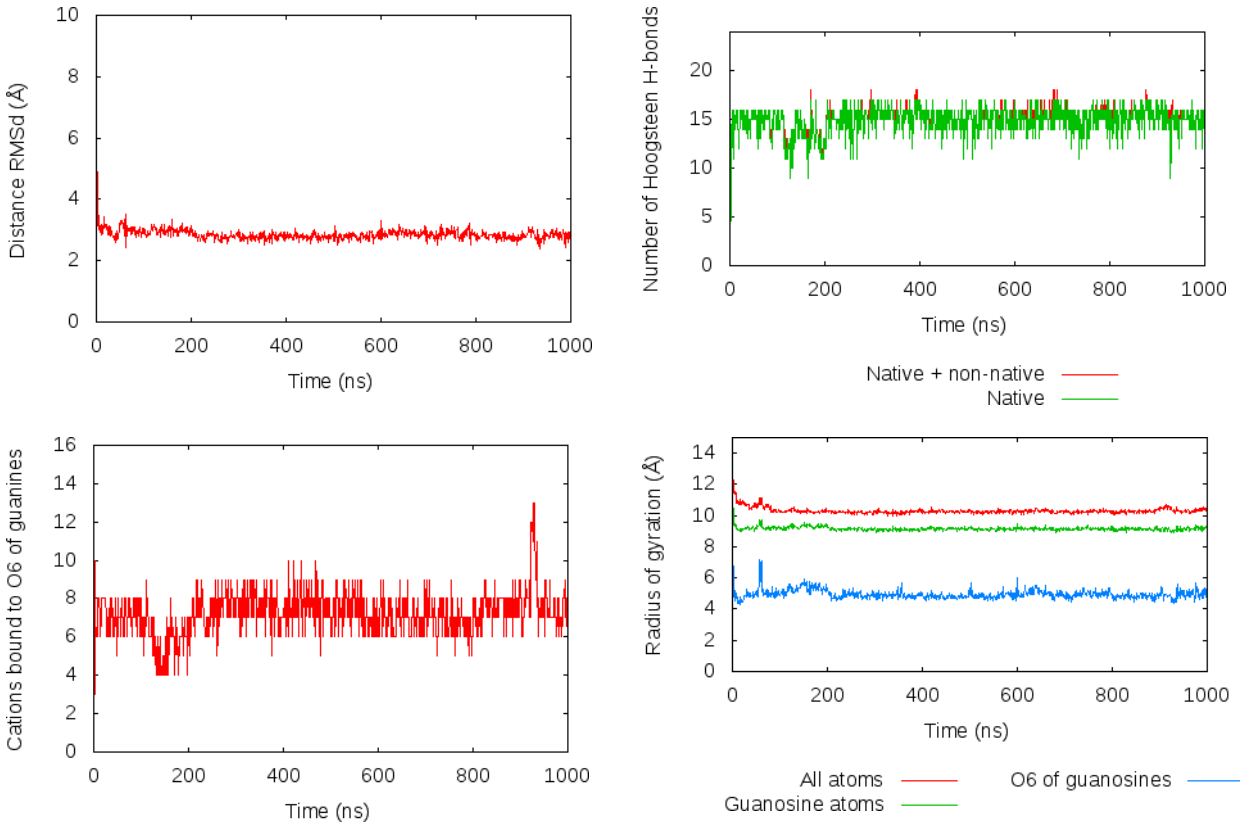

Figure SA33. Evolution of seven CVs in the simulation 2KF8-**A**. Top left: C4′ distance RMSd with respect to the native structure 2KF8. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

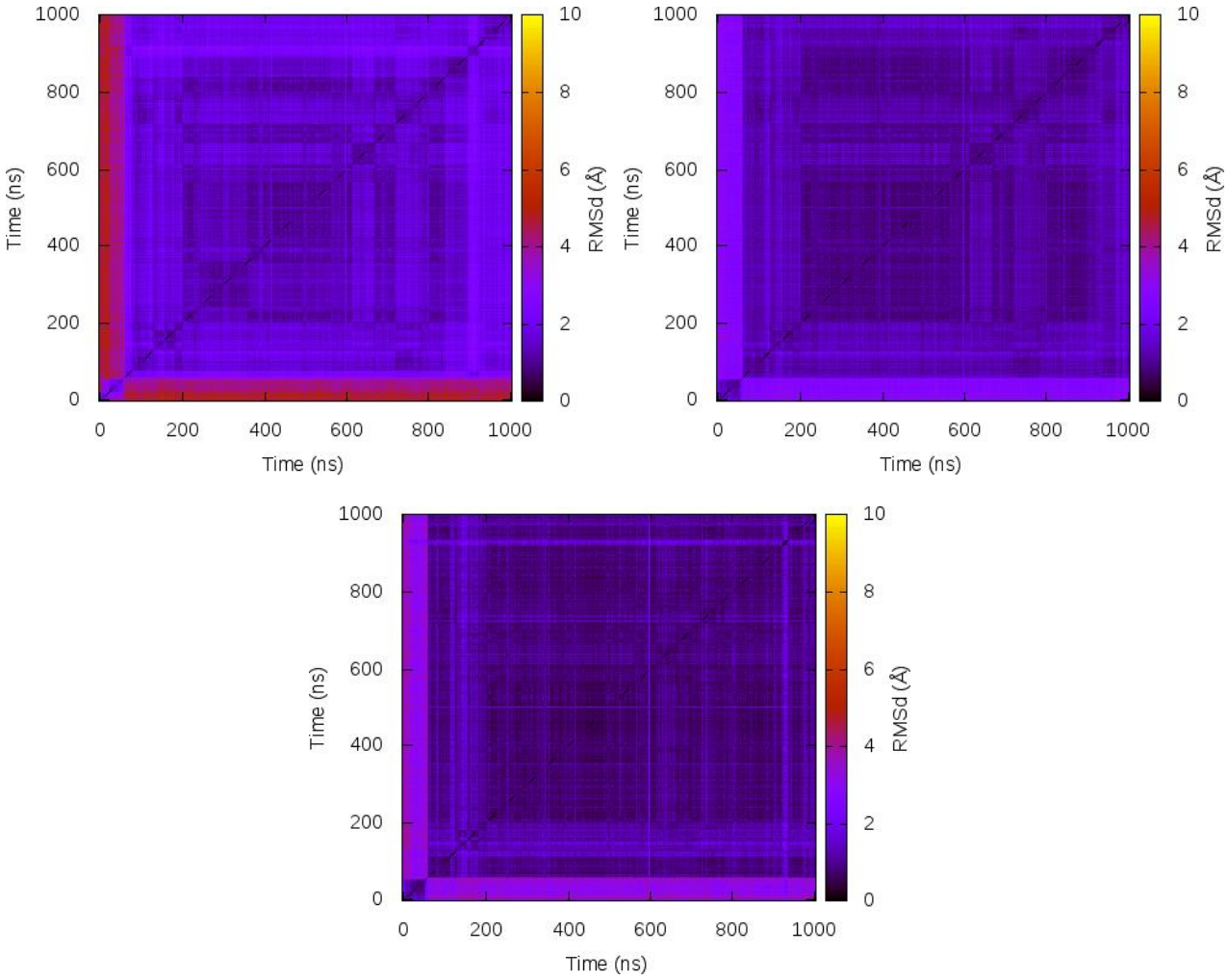

Figure SA34. 2D RMSd plots of structures in the simulation 2KF8-**A**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

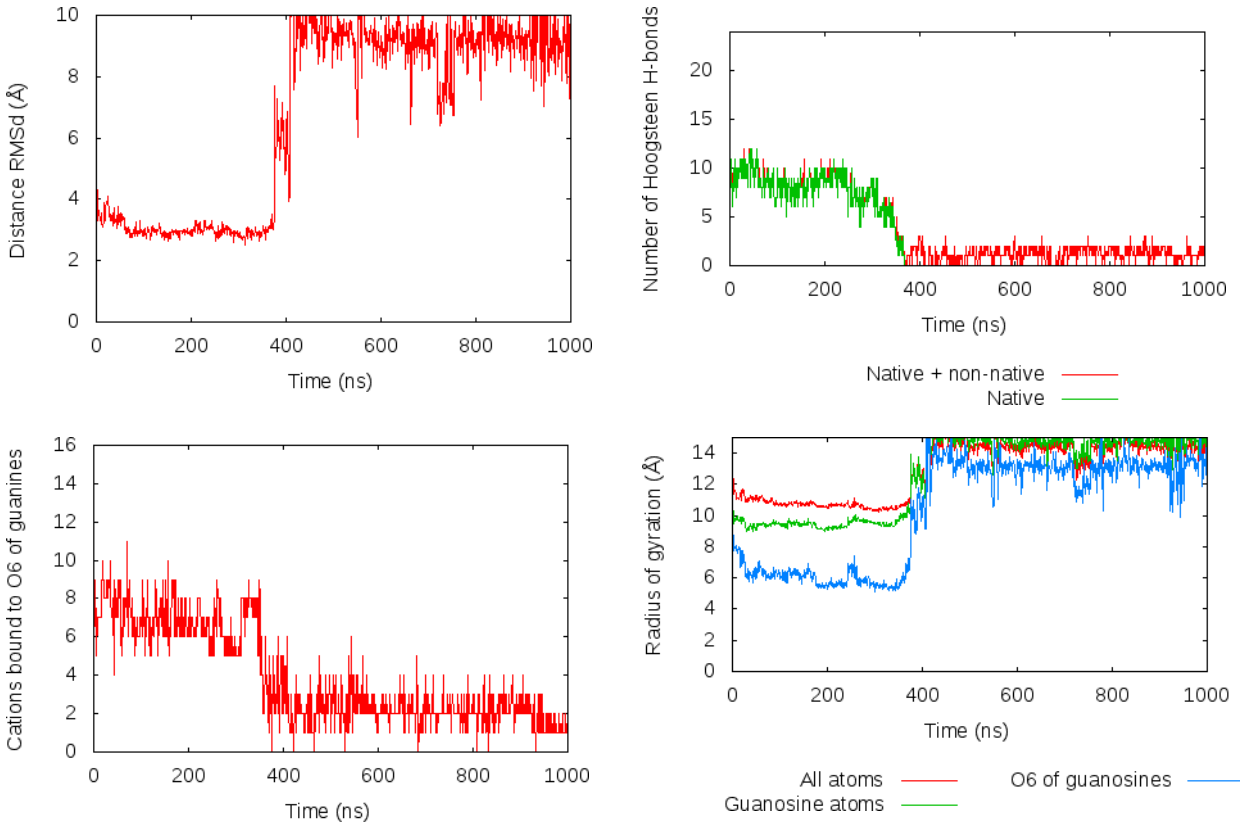

Figure SA35. Evolution of seven CVs in the simulation 2KF8-**B**. Top left: C4′ distance RMSd with respect to the native structure 2KF8. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

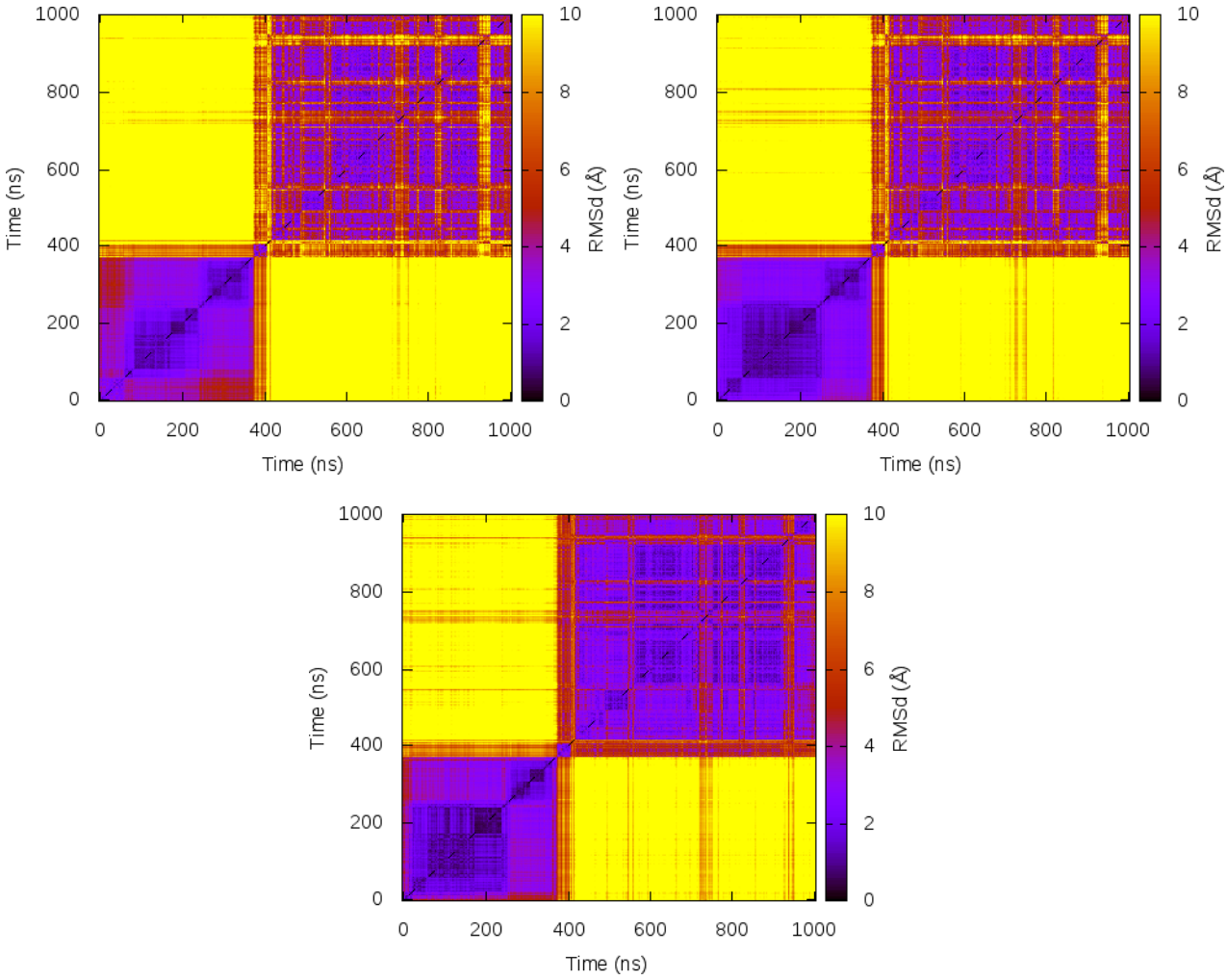

Figure SA36. 2D RMSd plots of structures in the simulation 2KF8-**B**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

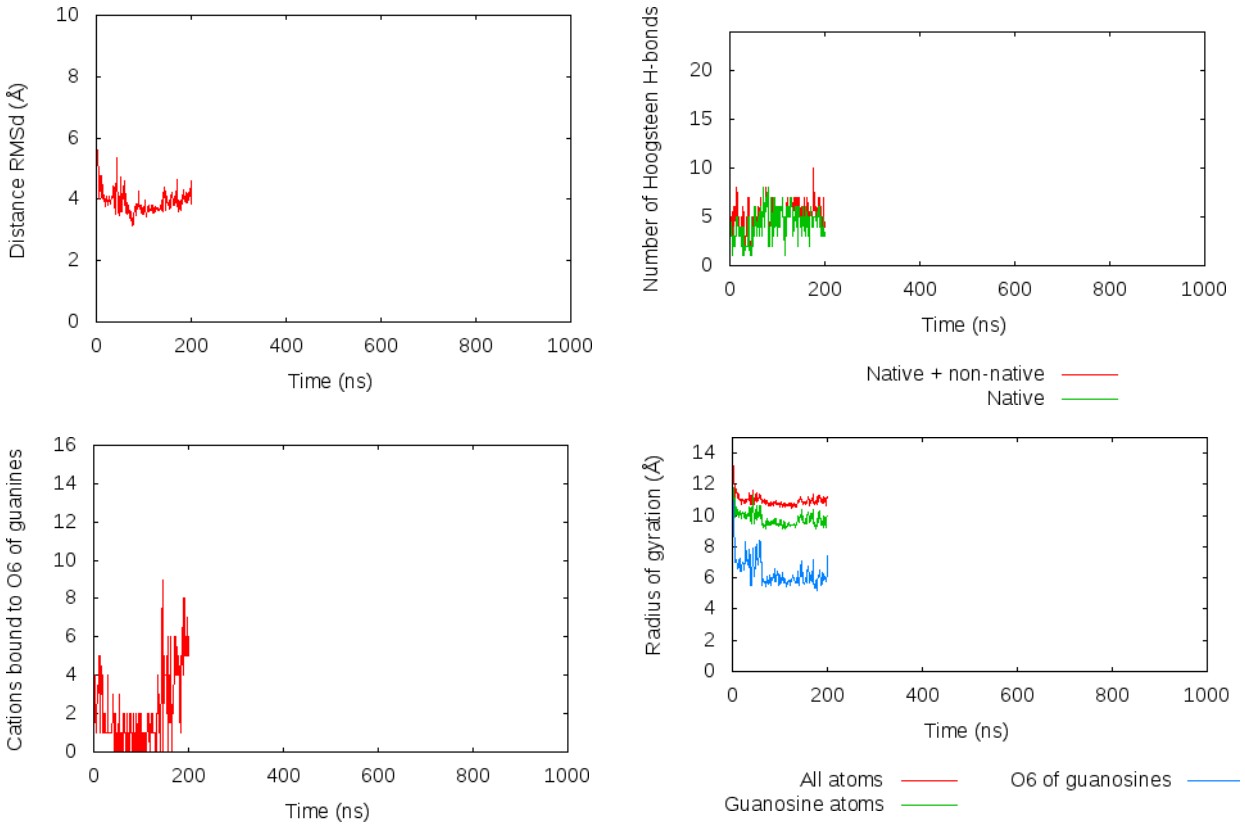

Figure SA37. Evolution of seven CVs in the simulation 2KF8-**C**. Top left: C4′ distance RMSd with respect to the native structure 2KF8. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

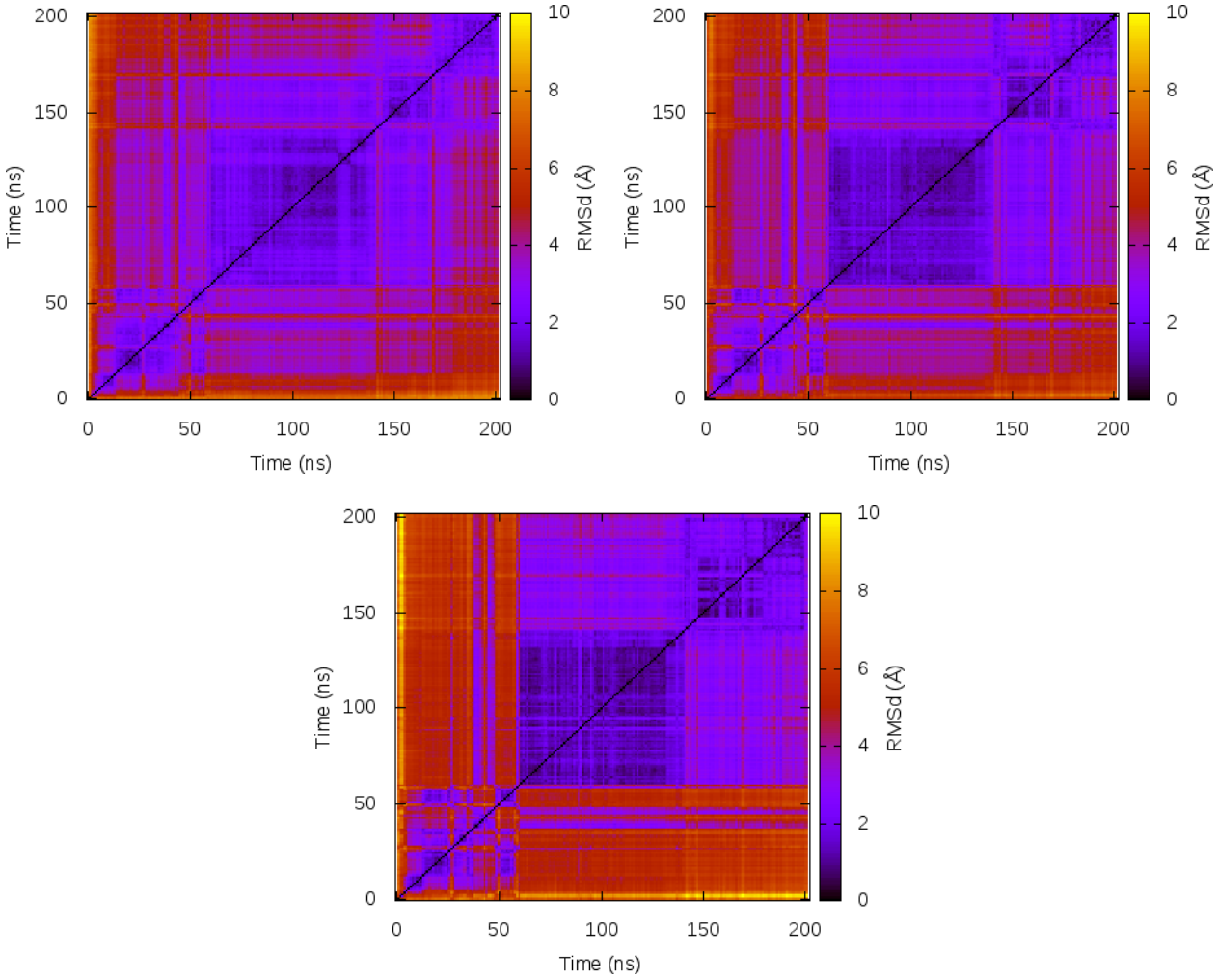

Figure SA38. 2D RMSd plots of structures in the simulation 2KF8-**C**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

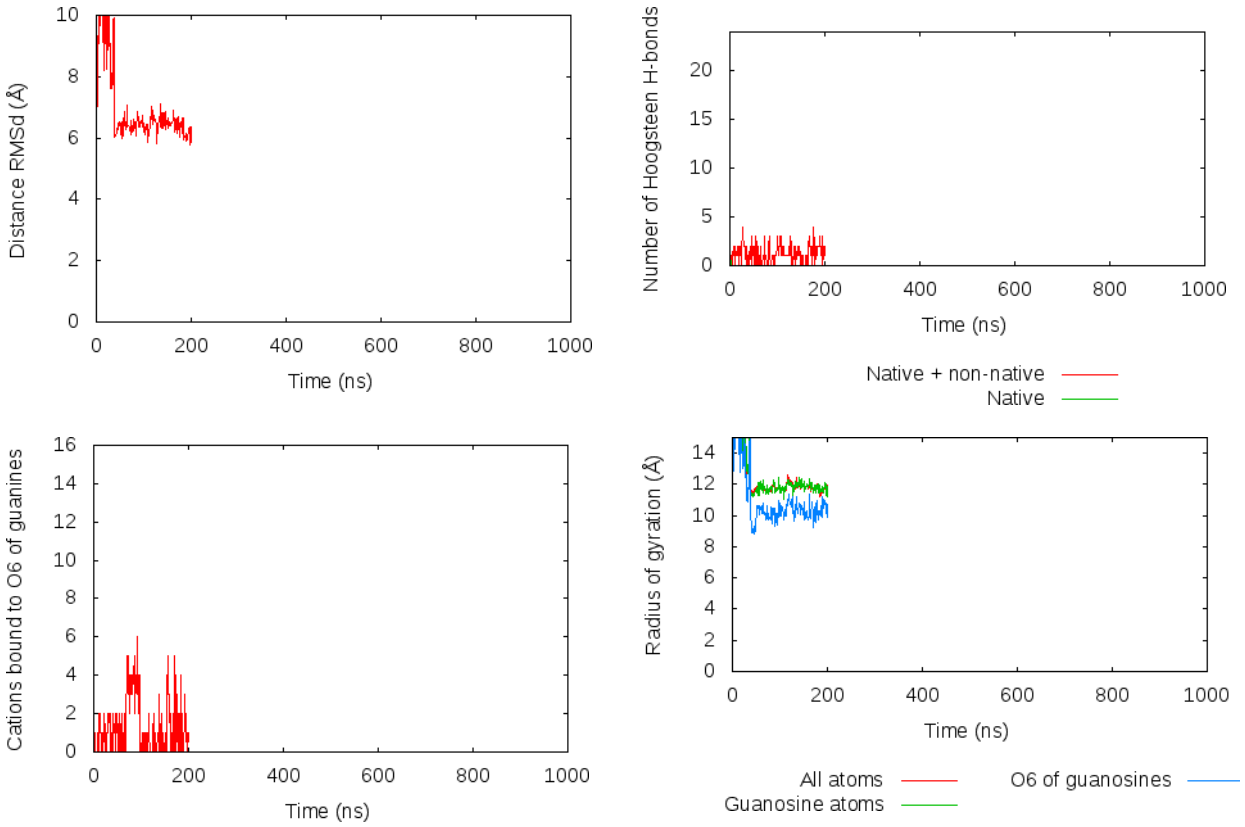

Figure SA39. Evolution of seven CVs in the simulation 2KF8-**D**. Top left: C4′ distance RMSd with respect to the native structure 2KF8. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Bottom left: Total number of cation-G(O6) contacts. Bottom right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only.

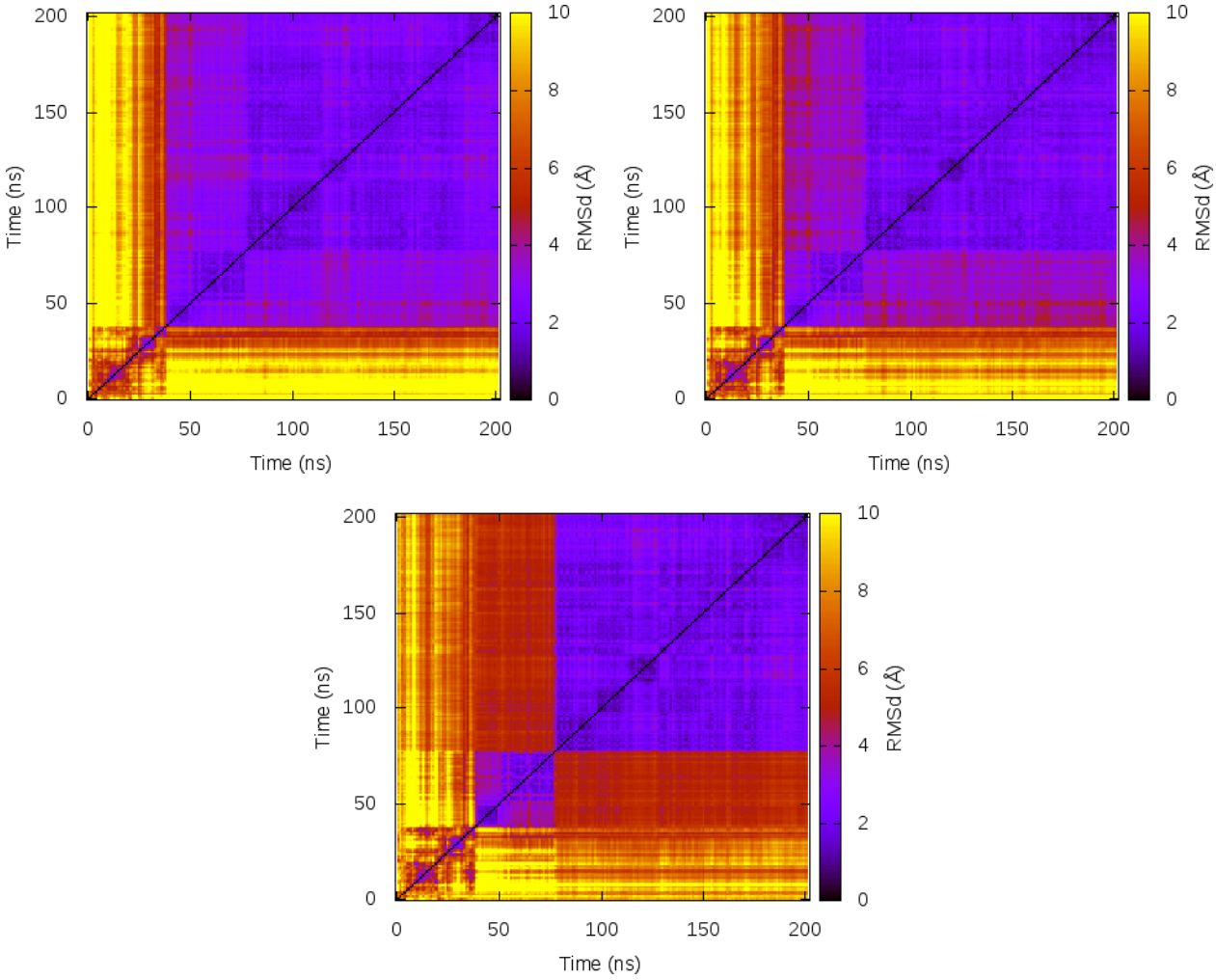

Figure SA40. 2D RMSd plots of structures in the simulation 2KF8-**D**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

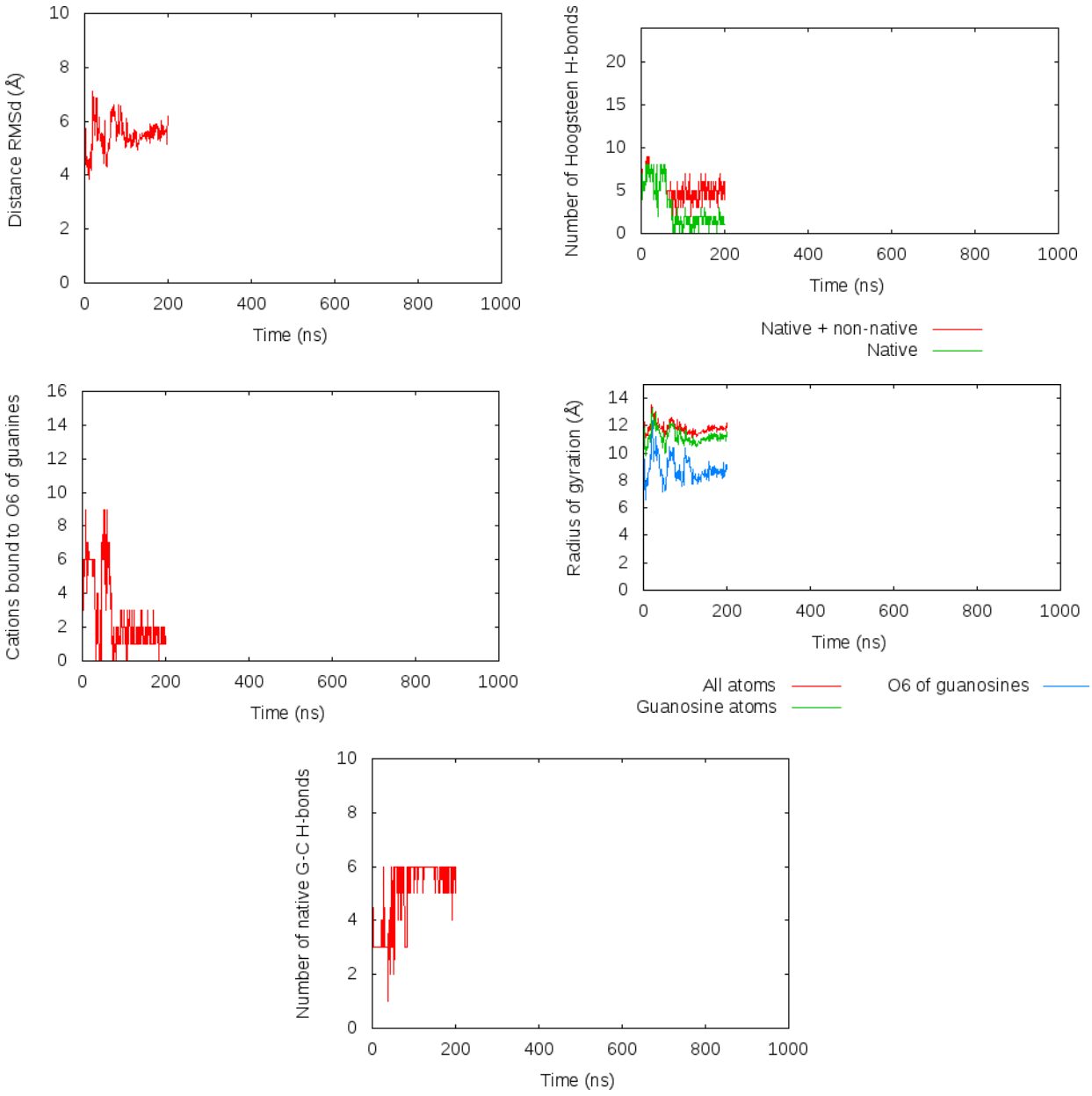

Figure SA41. Evolution of eight CVs in the simulation 2KM3-**A**. Top left: C4′ distance RMSd with respect to the native structure 2KM3. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Middle left: Total number of cation-G(O6) contacts. Middle right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only. Bottom: Total number of native *c*WW G-C hydrogen bonds.

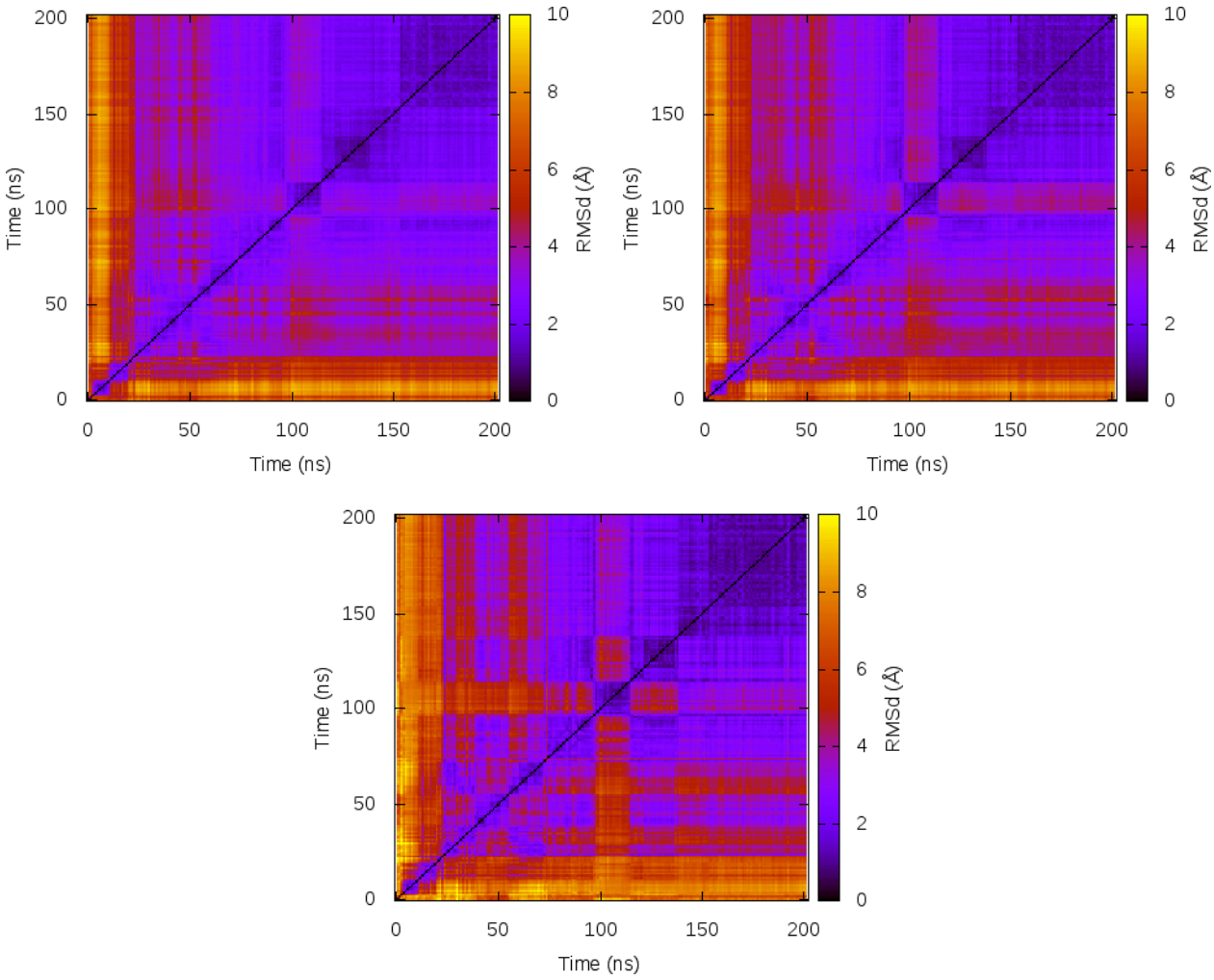

Figure SA42. 2D RMSd plots of structures in the simulation 2KM3-**A**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

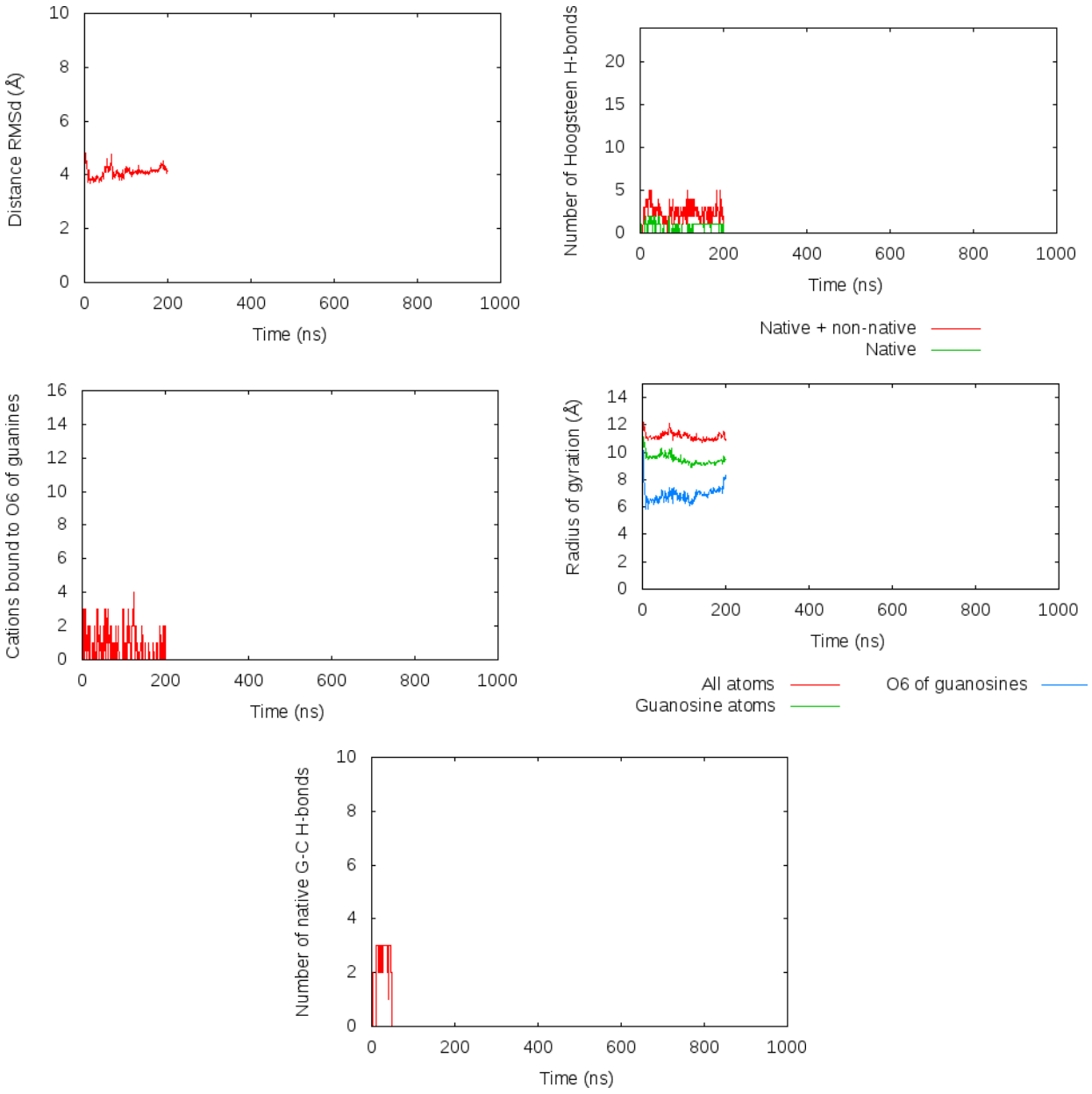

Figure SA43. Evolution of eight CVs in the simulation 2KM3-**B**. Top left: C4′ distance RMSd with respect to the native structure 2KM3. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Middle left: Total number of cation-G(O6) contacts. Middle right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only. Bottom: Total number of native *c*WW G-C hydrogen bonds.

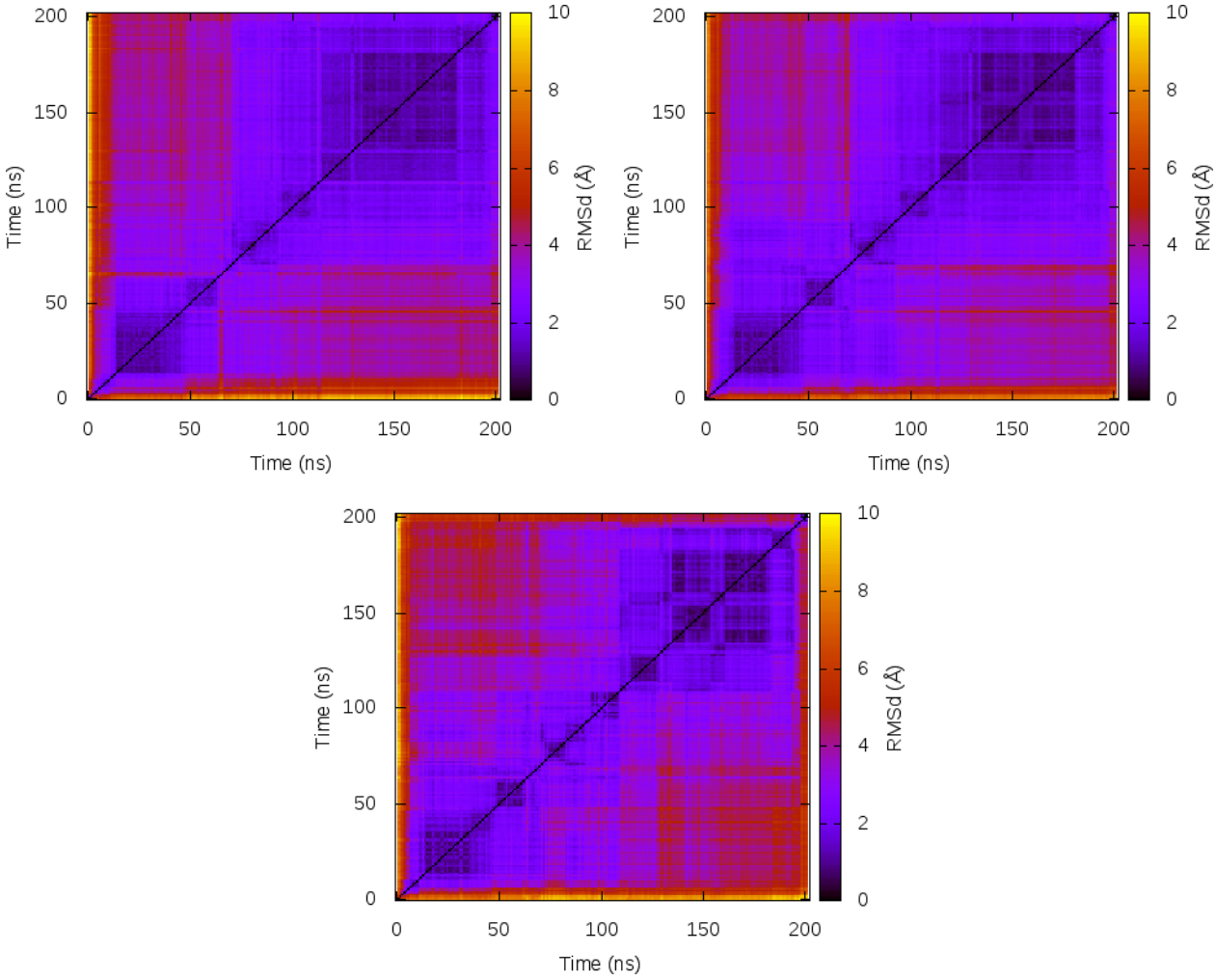

Figure SA44. 2D RMSd plots of structures in the simulation 2KM3-**B**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

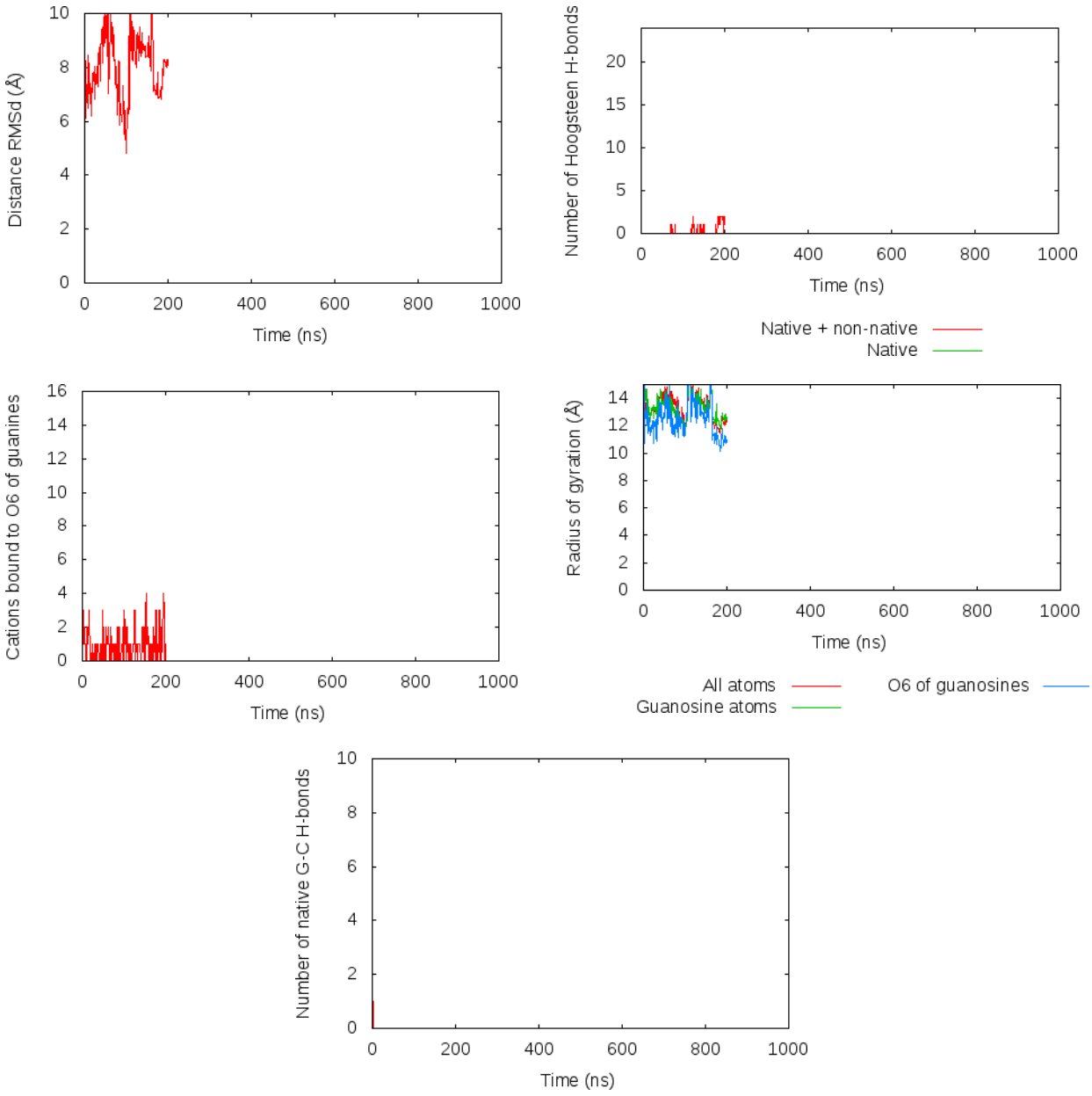

Figure SA45. Evolution of eight CVs in the simulation 2KM3-**C**. Top left: C4′ distance RMSd with respect to the native structure 2KM3. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Middle left: Total number of cation-G(O6) contacts. Middle right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only. Bottom: Total number of native *c*WW G-C hydrogen bonds.

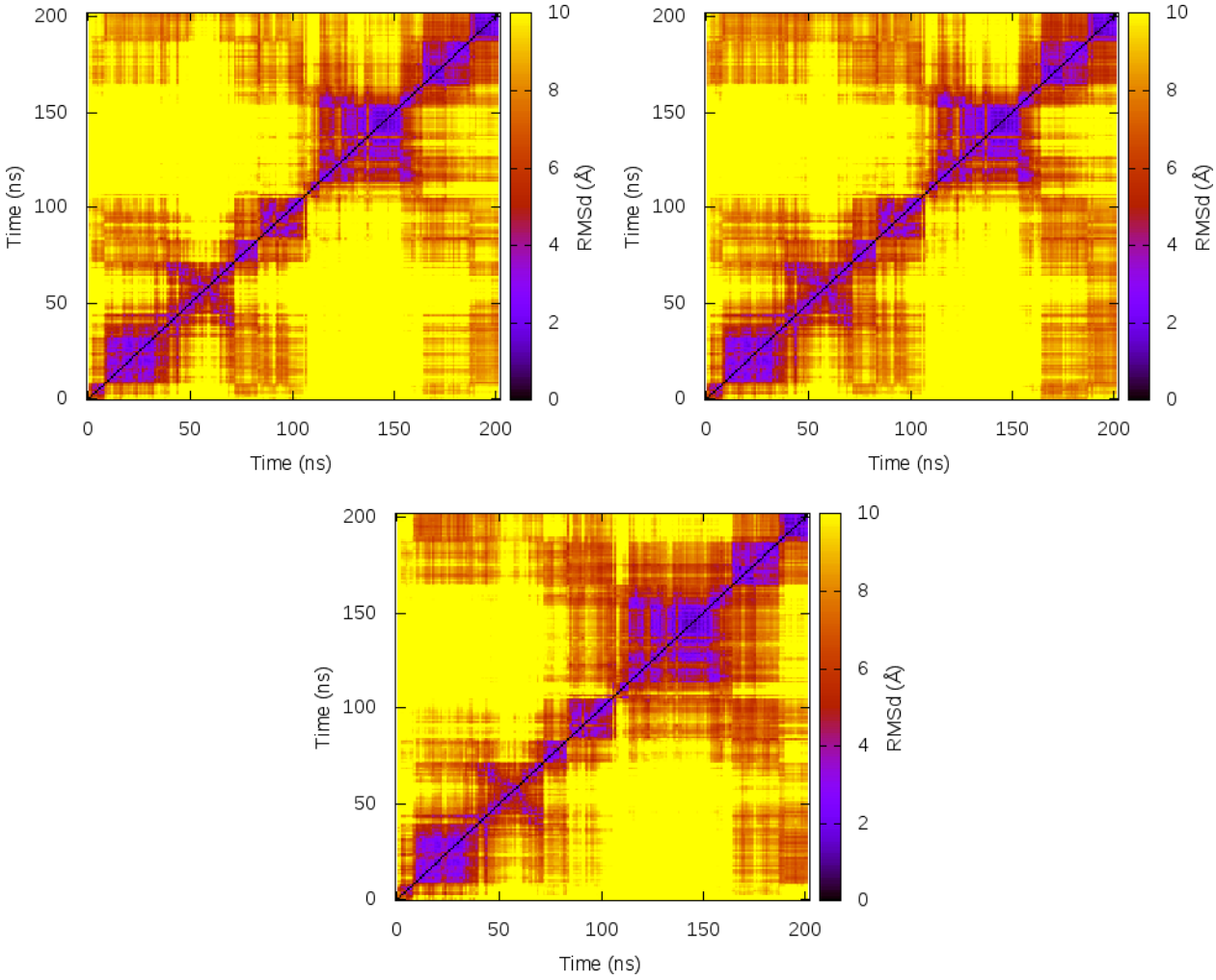

Figure SA46. 2D RMSd plots of structures in the simulation 2KM3-**C**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

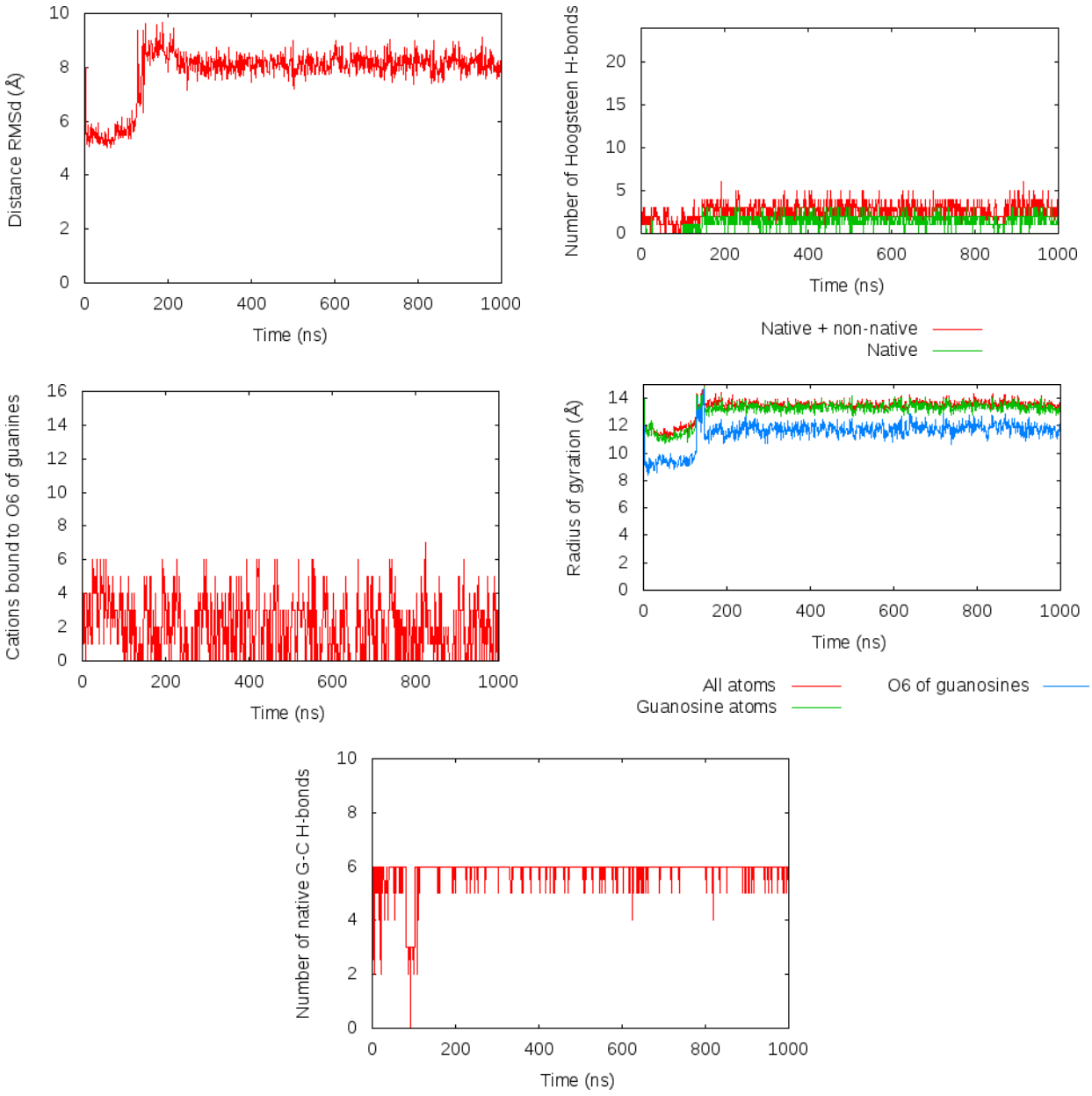

Figure SA47. Evolution of eight CVs in the simulation 2KM3-**D**. Top left: C4′ distance RMSd with respect to the native structure 2KM3. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Middle left: Total number of cation-G(O6) contacts. Middle right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only. Bottom: Total number of native *c*WW G-C hydrogen bonds.

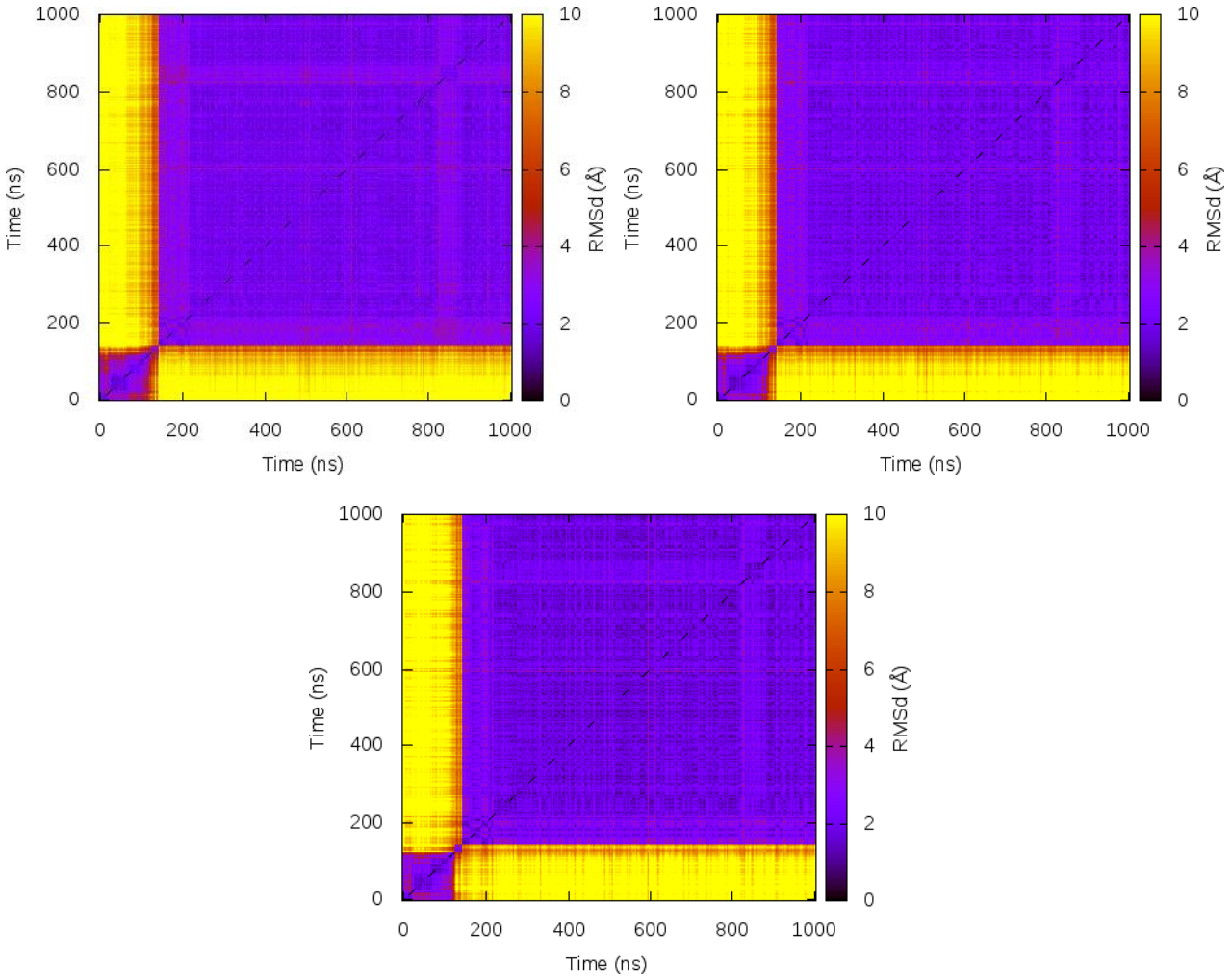

Figure SA48. 2D RMSd plots of structures in the simulation 2KM3-**D**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.

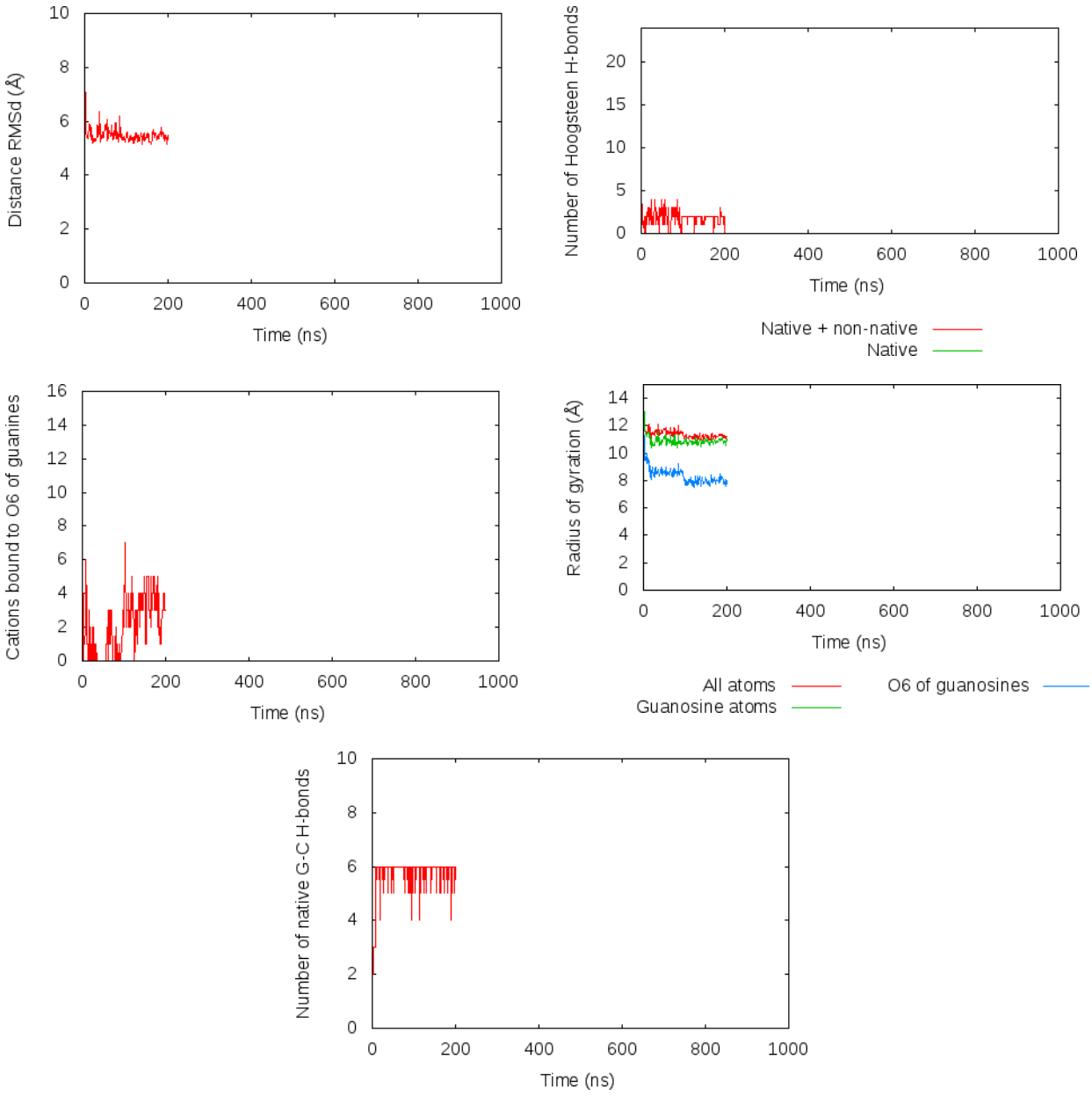

Figure SA49. Evolution of eight CVs in the simulation 2KM3-**E**. Top left: C4′ distance RMSd with respect to the native structure 2KM3. Top right: Total number of native *c*WH G-G hydrogen bonds and total number of all *c*WH G-G hydrogen bonds. Middle left: Total number of cation-G(O6) contacts. Middle right: Radius of gyration of all atoms, all guanosine atoms, and G(O6) atoms only. Bottom: Total number of native *c*WW G-C hydrogen bonds.

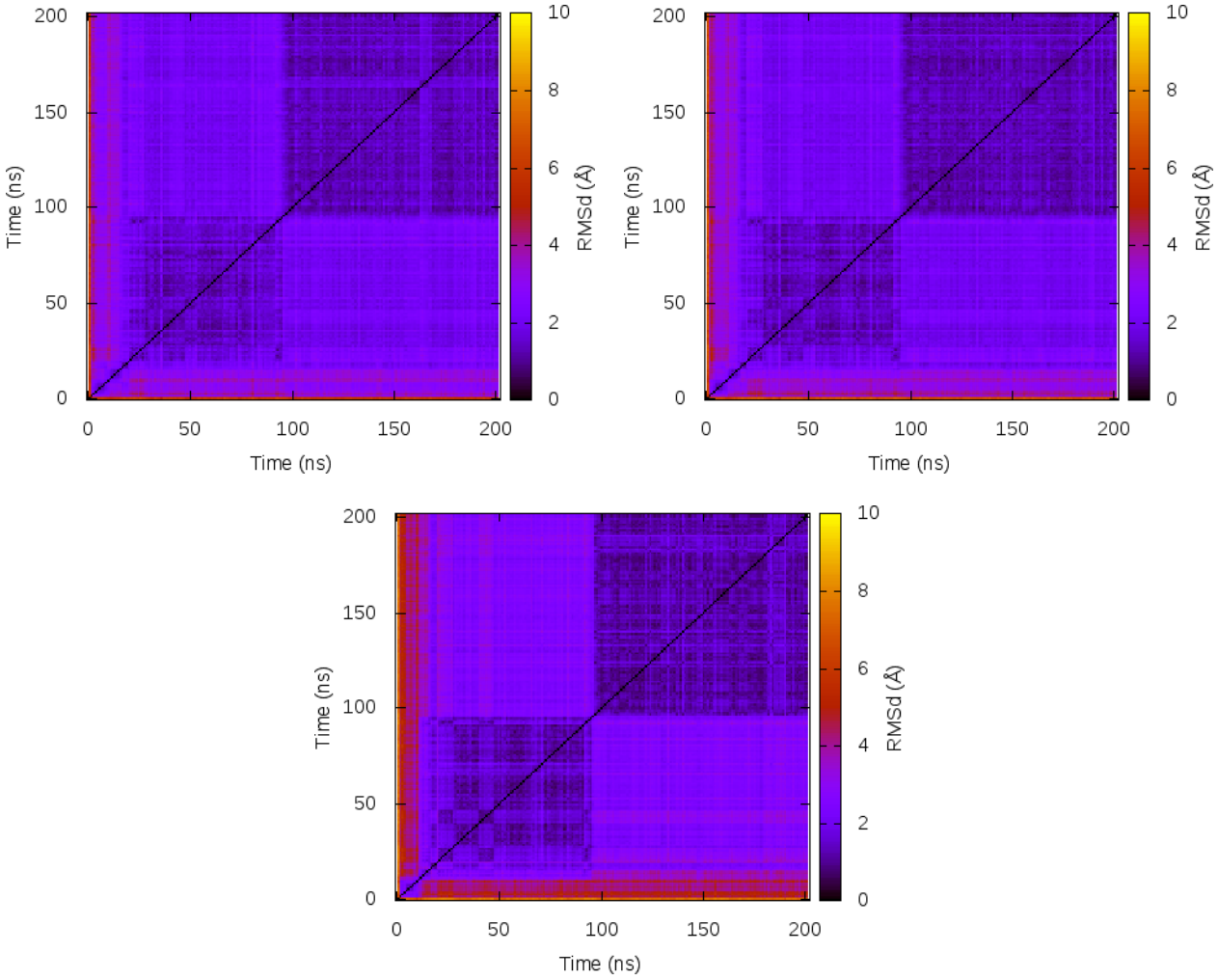

Figure SA50. 2D RMSd plots of structures in the simulation 2KM3-**E**. Top left: All-atom mass-weighted RMSd. Top right: All-guanosines-all-atom mass-weighted RMSd. Bottom: All-guanosines O6 RMSd.