

Supporting Information: Cross-Correlated Motions in Azidolysozyme

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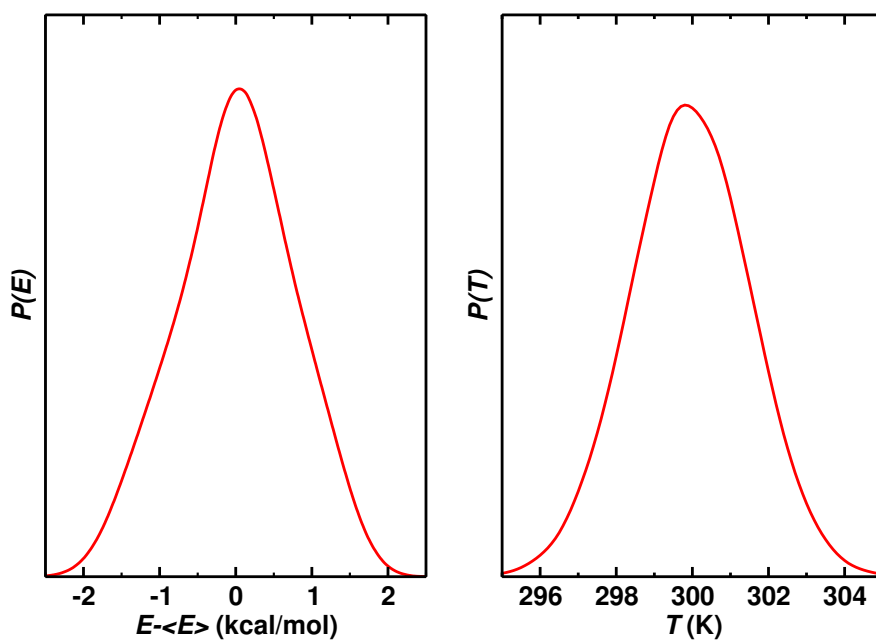


Figure S1: Energy conservation (left panel) and temperature distribution (right panel) from 2 ns RKHS-based NVE simulations of modified lysozyme at position Ala92.

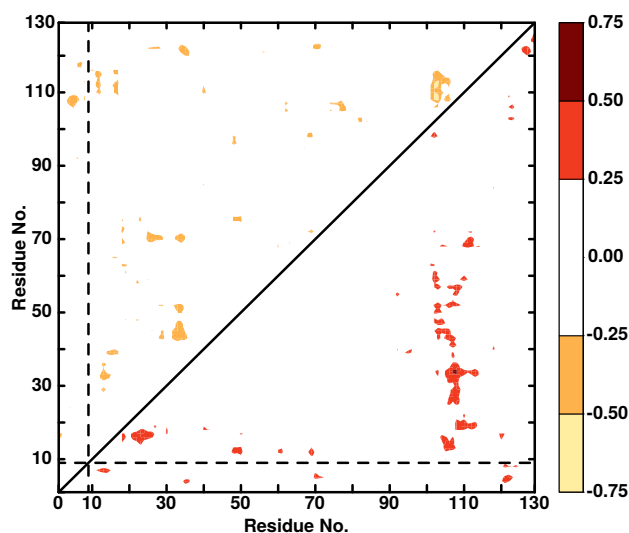


Figure S2: Δ DCCM between WT and Ala9N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

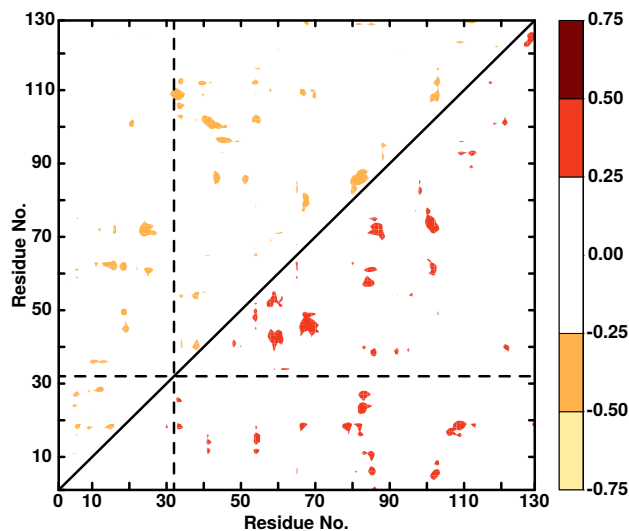


Figure S3: Δ DCCM between WT and Ala32N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

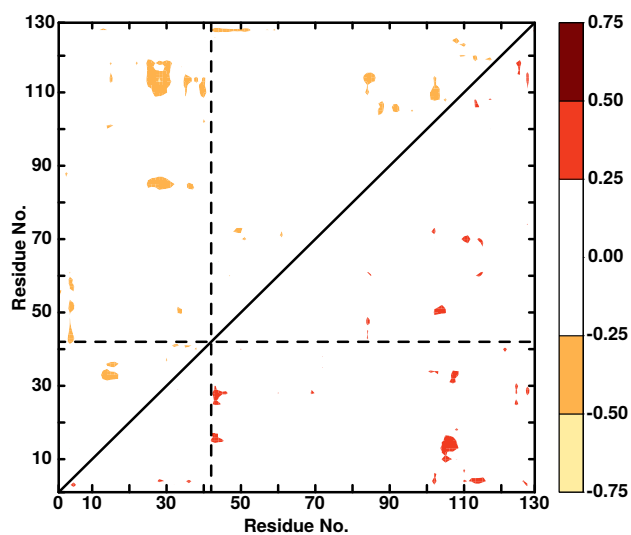


Figure S4: Δ DCCM between WT and Ala42N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

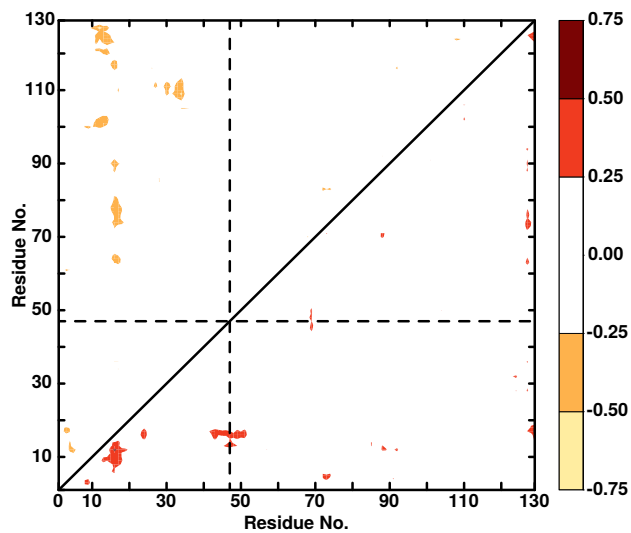


Figure S5: Δ DCCM between WT and Ala47N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

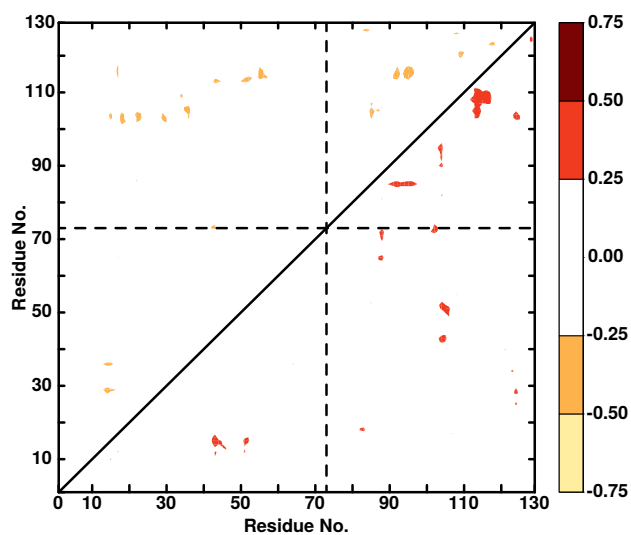


Figure S6: Δ DCCM between WT and Ala73N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

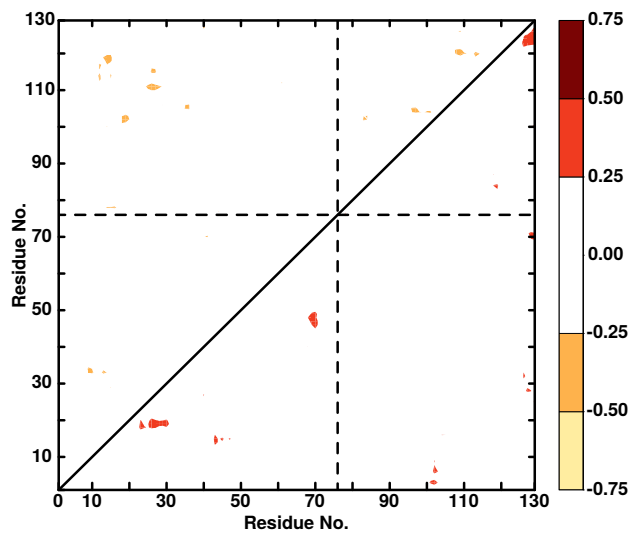


Figure S7: Δ DCCM between WT and Ala76N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

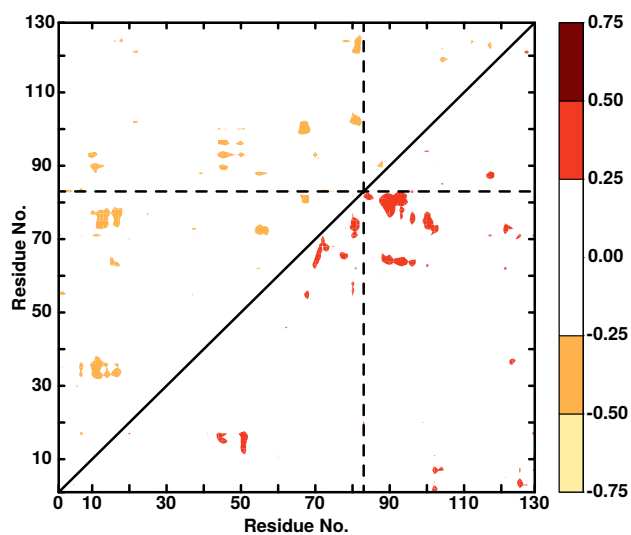


Figure S8: Δ DCCM between WT and Ala83N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

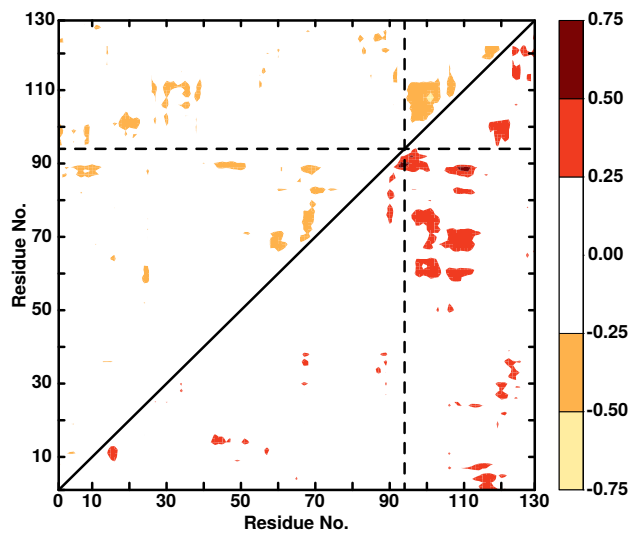


Figure S9: Δ DCCM between WT and Ala94N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

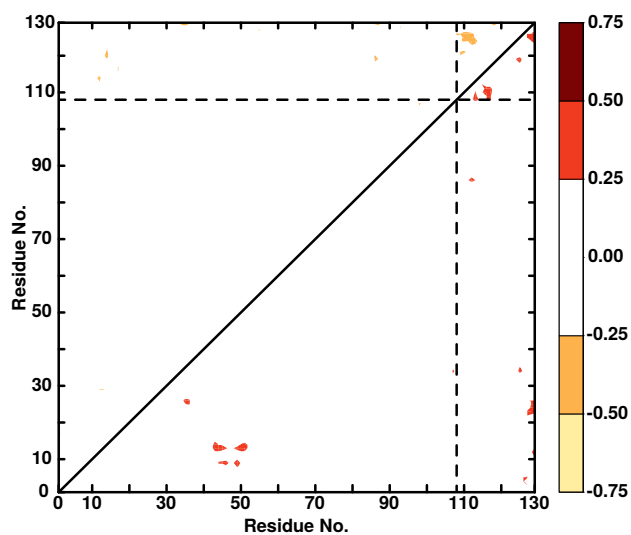


Figure S10: Δ DCCM between WT and Ala108N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

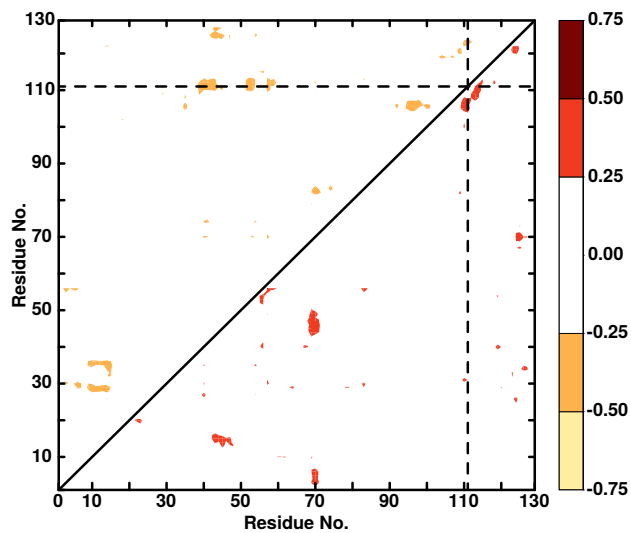


Figure S11: Δ DCCM between WT and Ala111N₃. Positive differences are in the lower right triangle, negative differences in the upper left triangle. Only differences with an absolute value greater than 0.25 are displayed.

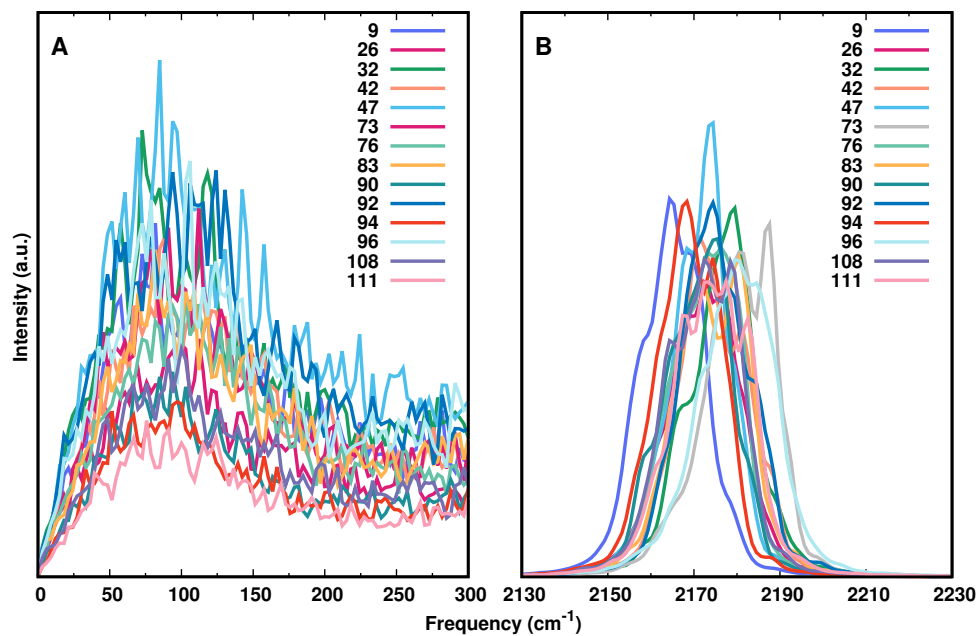


Figure S12: IR spectrum obtained from Fourier Transform of the dipole moment auto-correlation function of protein (panel A) and -N₃ label (panel B) for all AlaN₃ modifications. The labels in each panel refer to the alanine residue that carries the -N₃ moiety.

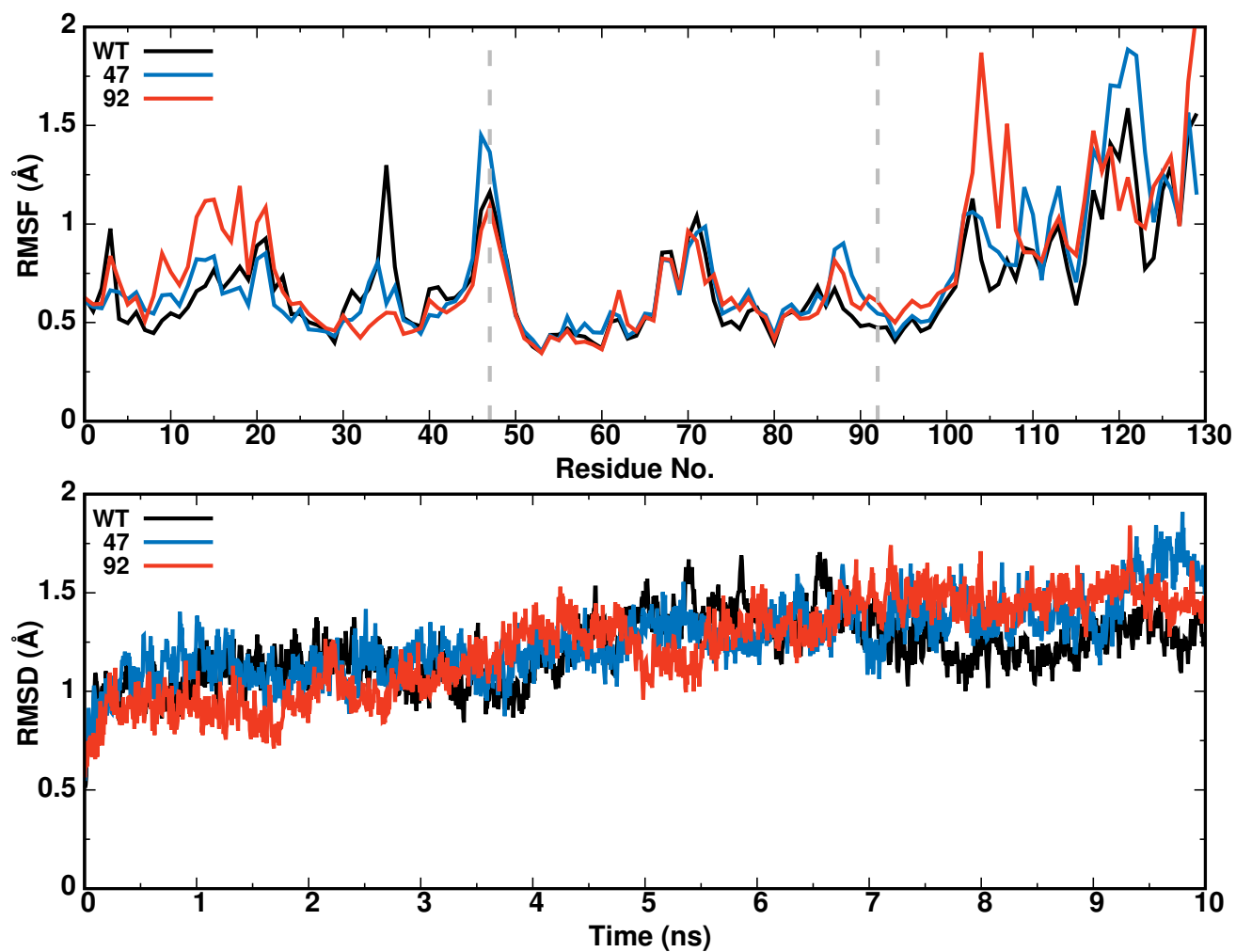


Figure S13: Root mean squared fluctuations (top) and root mean squared deviation (bottom) for the C_{α} atoms of the WT, Ala47N₃ and Ala92N₃ protein from 10 ns RKHS-based simulations. The dashed lines in top panel show the positions of the modified Ala residues.

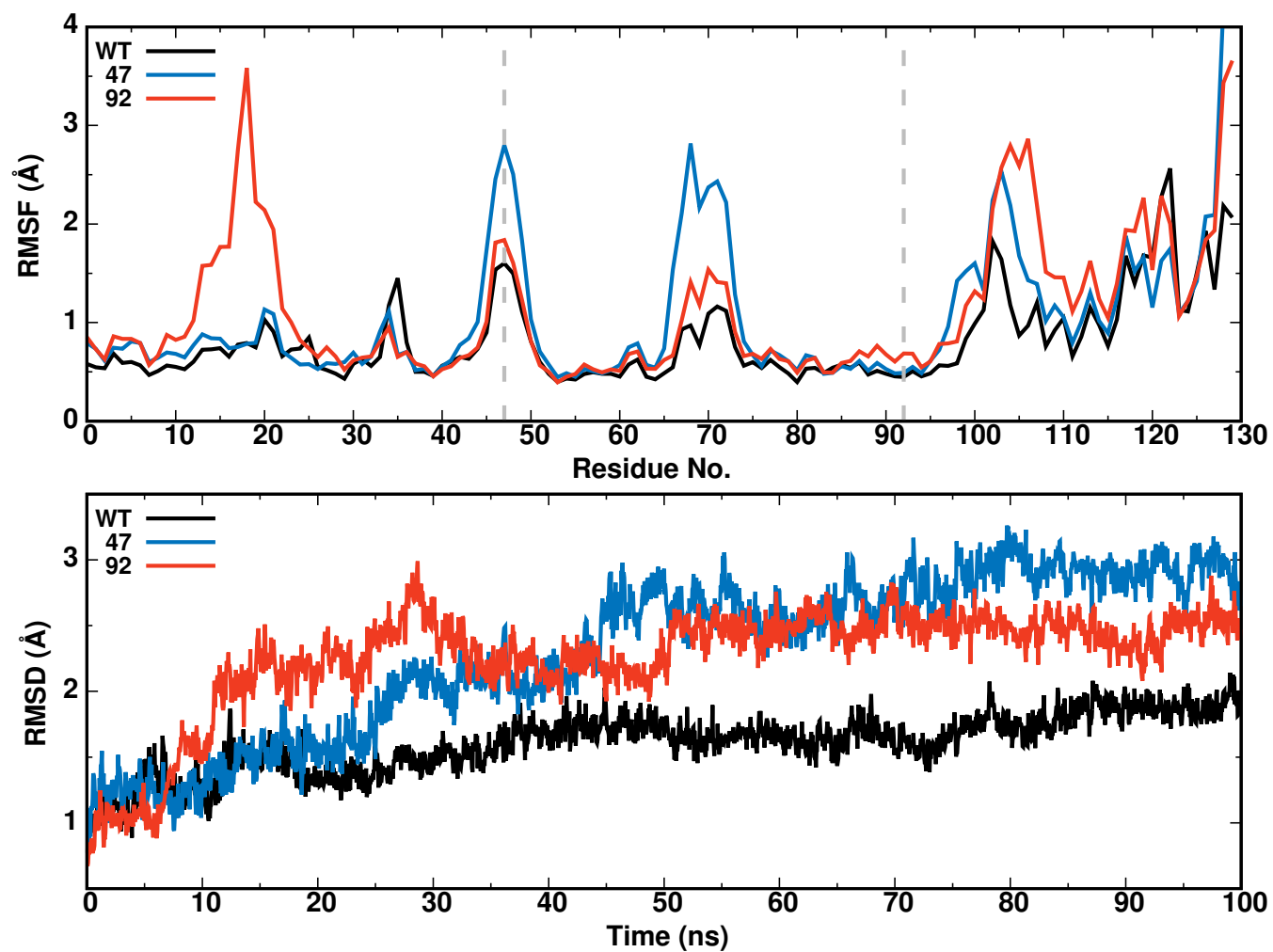


Figure S14: Root mean squared fluctuations (top) and root mean squared deviation (bottom) for the C_{α} atoms of the WT, Ala47N₃ and Ala92N₃ protein from 100 ns conventional force field simulations. The dashed lines in top panel show the positions of the modified Ala residues.

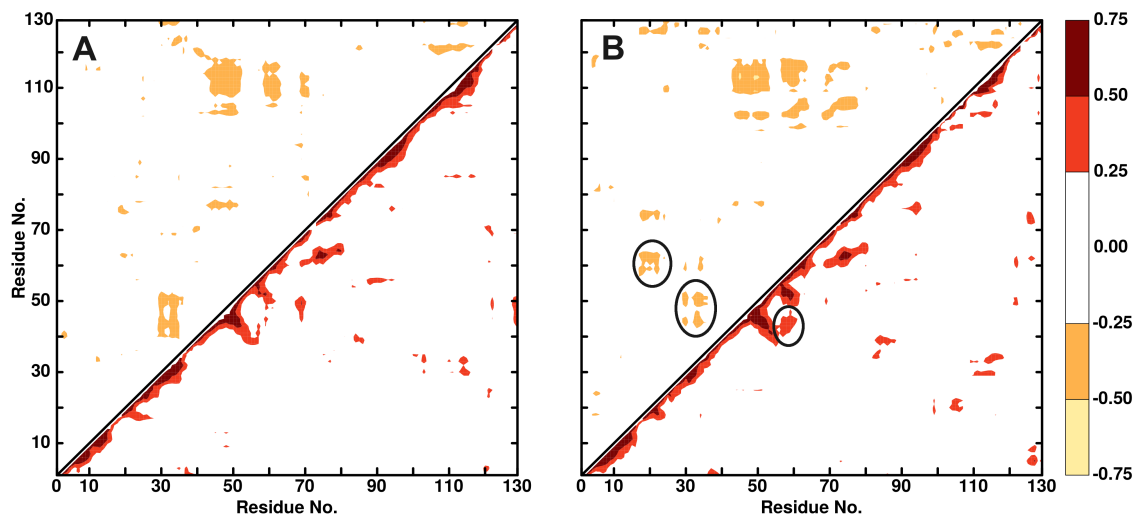


Figure S15: DCCM maps for WT lysozyme from A) 10 ns and B) 100 ns conventional force field simulations. Positive correlations are in the lower right triangle, negative correlations in the upper left triangle. Only correlation coefficients with an absolute value greater than 0.25 are displayed. Notable differences are encircled in panel B.

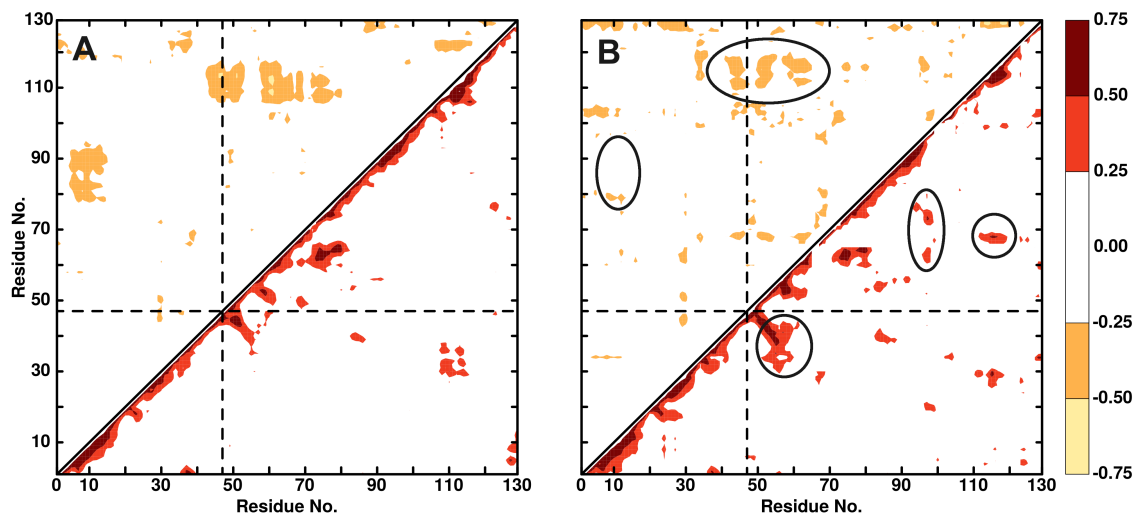


Figure S16: DCCM maps for Ala47N₃ from A) 10 ns RKHS-based and B) 100 ns conventional force field simulations. Positive correlations are in the lower right triangle, negative correlations in the upper left triangle. Only correlation coefficients with an absolute value greater than 0.25 are displayed. Notable differences are encircled in panel B.

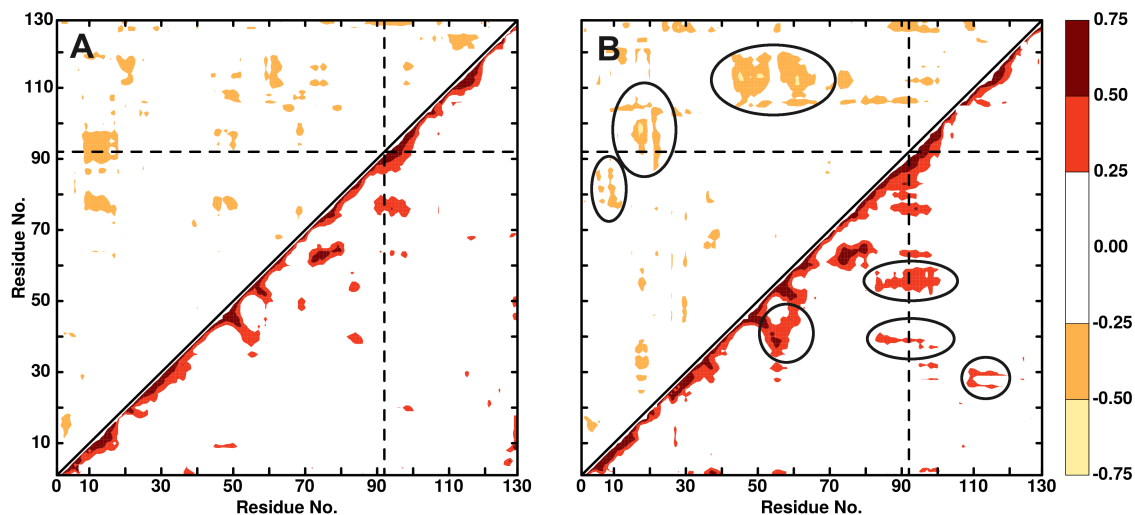


Figure S17: DCCM maps for Ala92N₃ from A) 10 ns RKHS-based and B) 100 ns conventional force field simulations. Positive correlations are in the lower right triangle, negative correlations in the upper left triangle. Only correlation coefficients with an absolute value greater than 0.25 are displayed. Notable differences are encircled in panel B.