

Figure 1: WW

MD Data

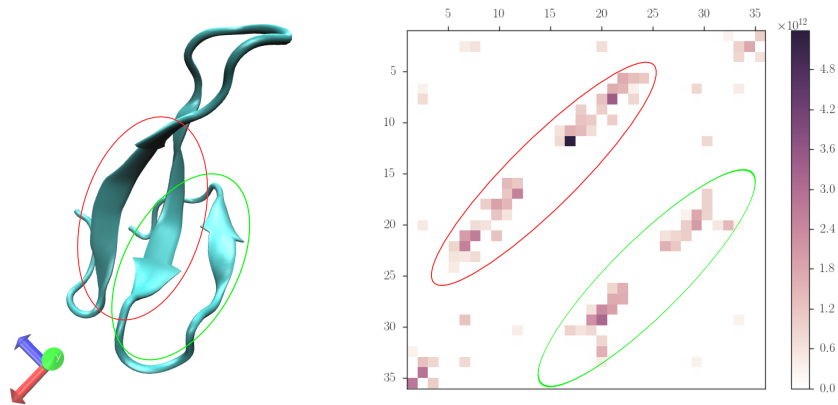


Figure 2: Polar contact transition rates between residues.

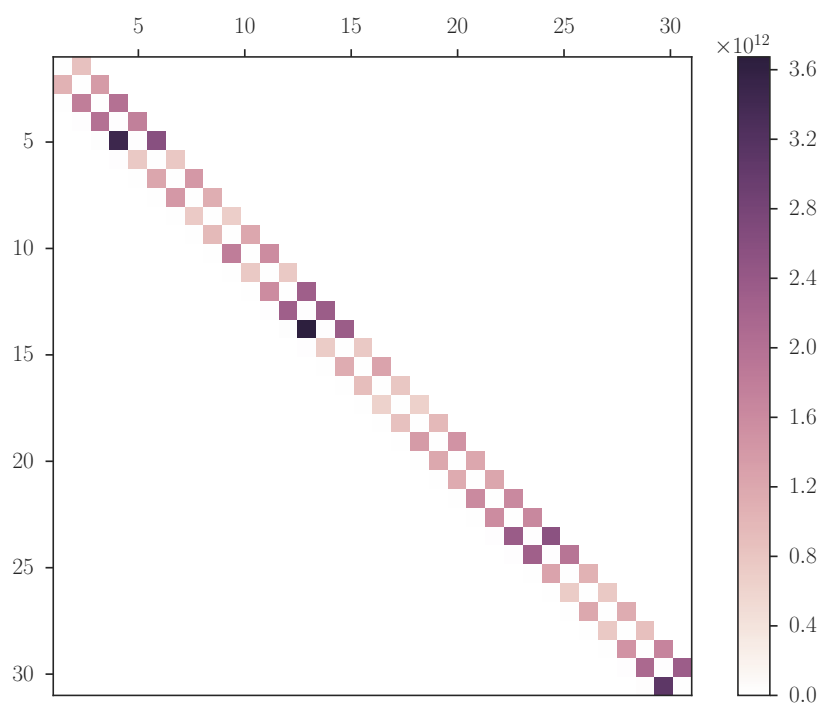


Figure 3: Backbone transition rates matrix

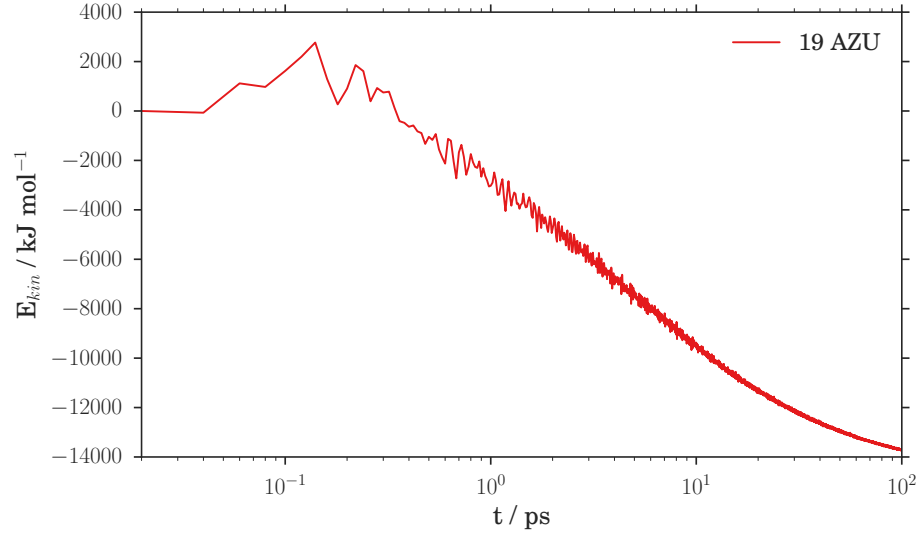


Figure 4: Kinetic energy of the heated residuum AZU 19.

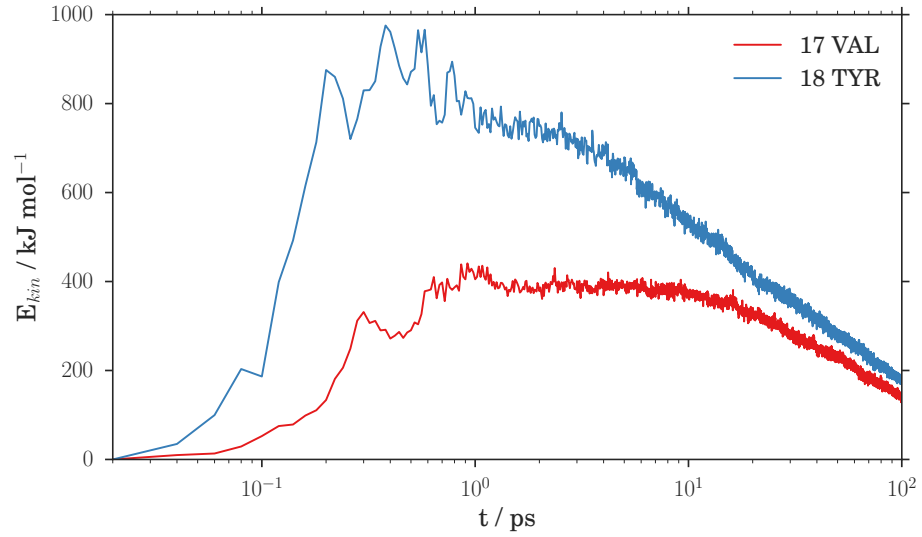


Figure 5: Kinetic energy of residues 17 and 18 obtained from MD simulations. Heated residue is AZU 19.

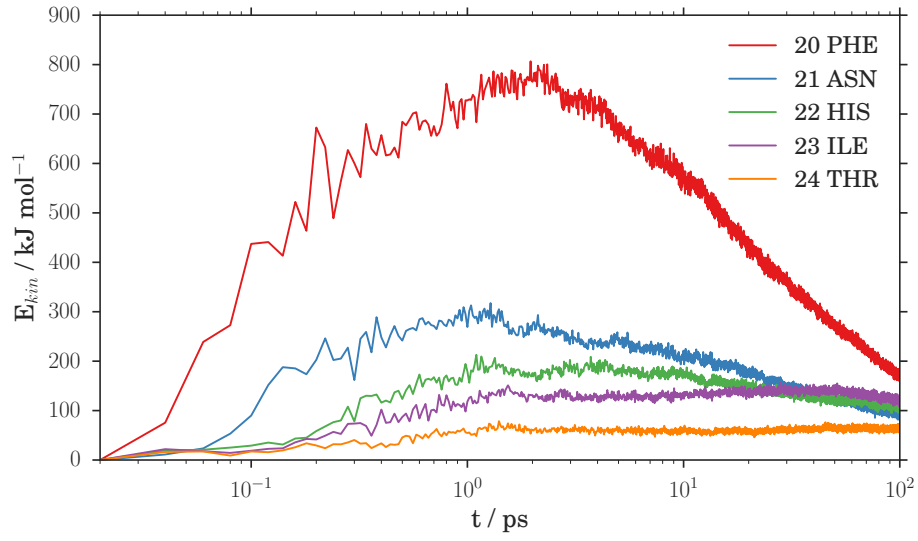


Figure 6: Kinetic energy of residues 20 to 24 obtained from MD simulations.

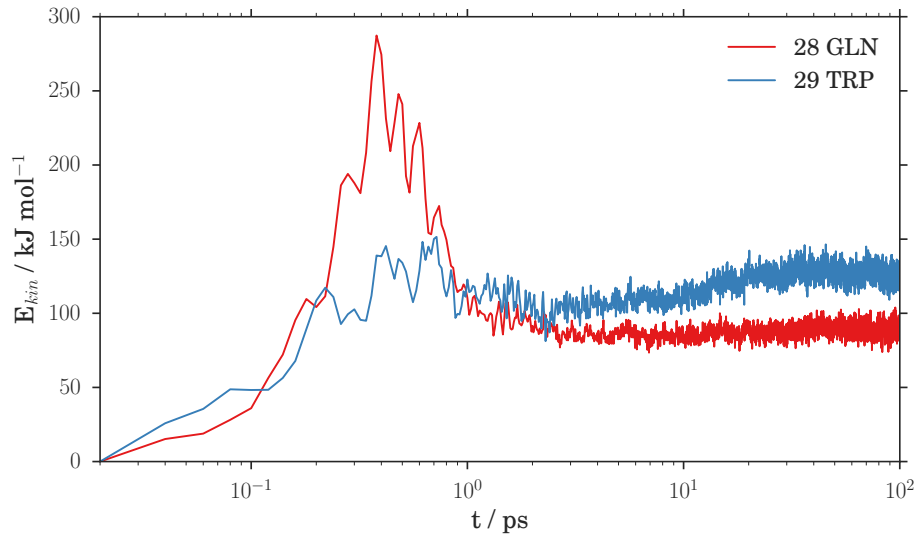


Figure 7: Kinetic energy of residues 28 and 29, of which 28 is in polar contact with 19 AZU.

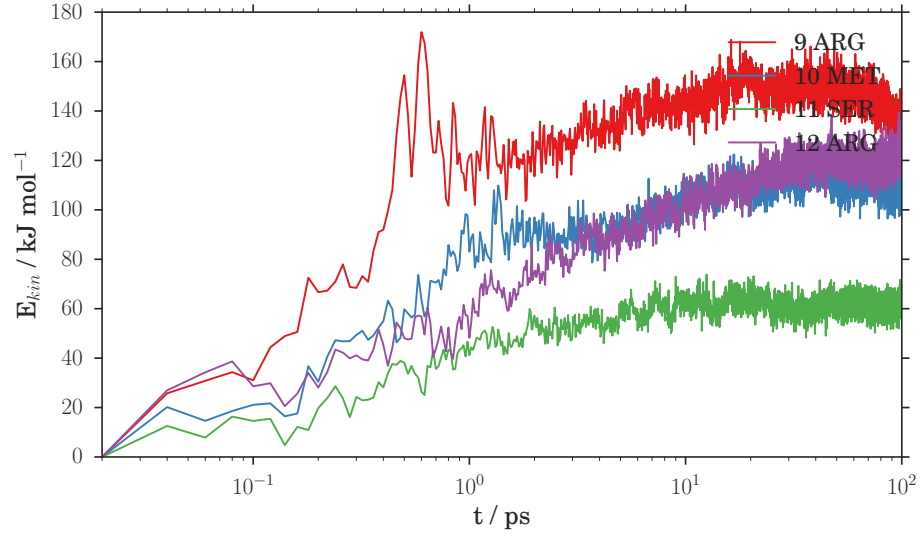


Figure 8: Kinetic energy of residues 9 to 12 of which 9 ARG is in polar contact with 18 TYR and 20 PHE.

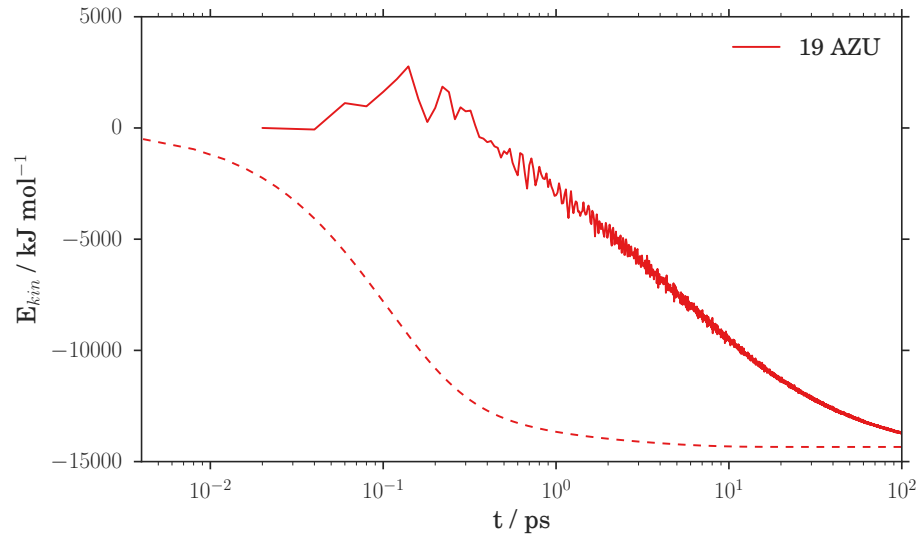


Figure 9: Comparison to MEQ simulation for heated residue 19 AZU.

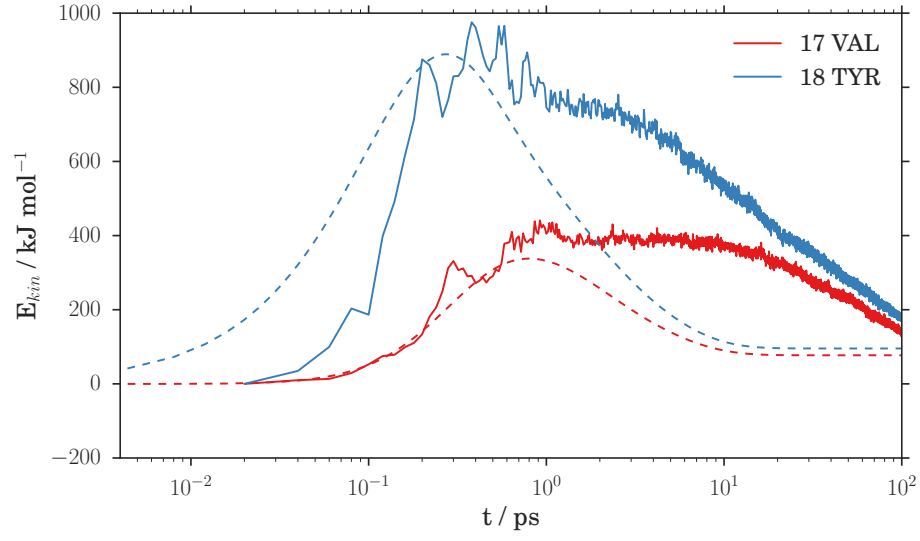


Figure 10: Comparison to MEQ simulation data for residues 17 and 18.

