Supporting information

Studying the mechanism of phase separation in aqueous solutions of globular proteins via molecular dynamics computer simulations

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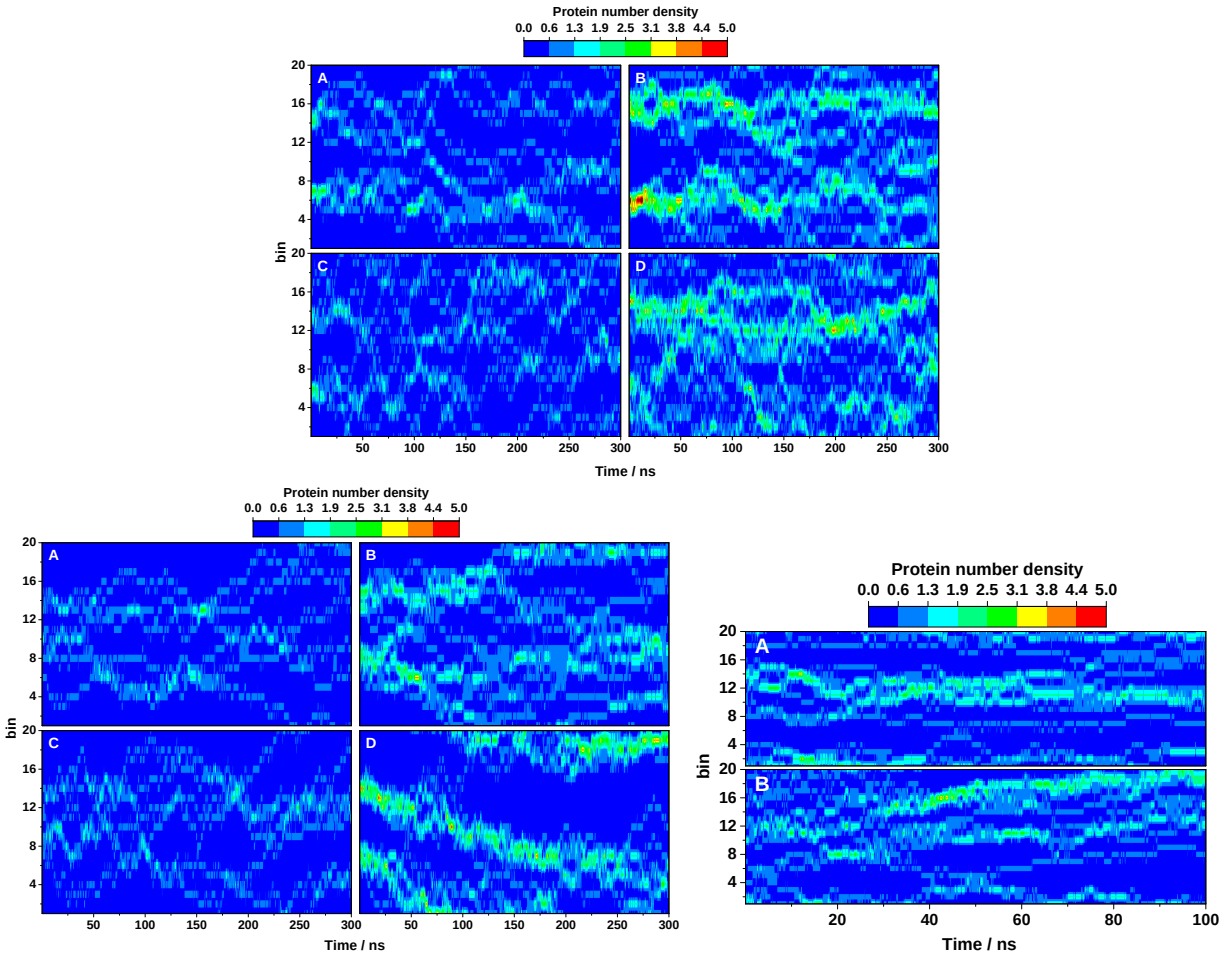

Figure S1: Density fluctuations of proteins in the y-axis direction. HEWL (top line) at 42 mg/mL (A at 267 K, C at 300 K) and 93 mg/mL (B at 267 K and D at 300 K). T4 WT* (bottom left) at 45 mg/mL (A at 267 K and C at 300 K) and 90 mg/mL (B at 267 K and D at 300 K). γ-D crystallin (bottom right) at 100 mg/mL (A at 300 K and B at 320 K).

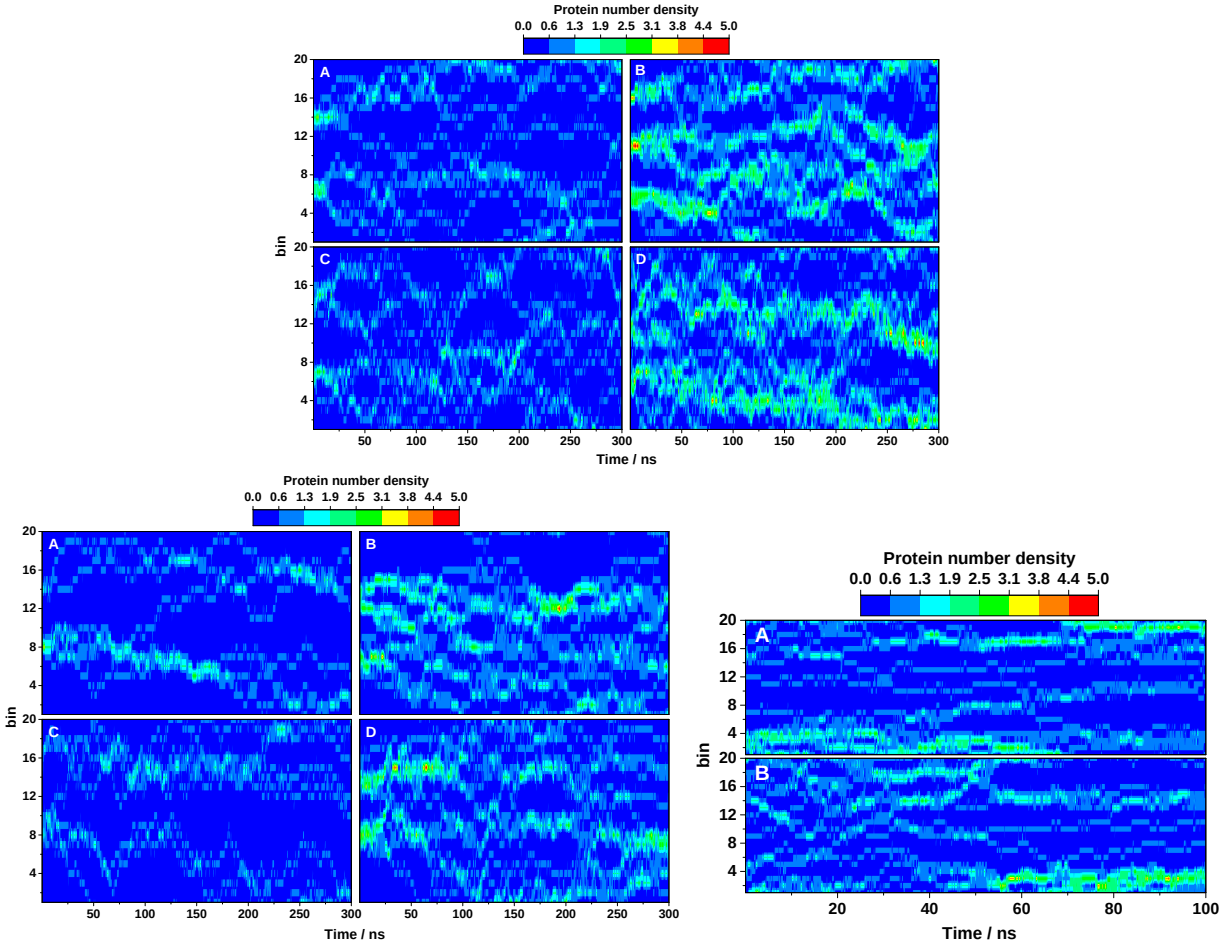

Figure S2: Density fluctuations of proteins in the z-axis direction. HEWL (top line) at 42 mg/mL (A at 267 K, C at 300 K) and 93 mg/mL (B at 267 K and D at 300 K). T4 WT* (bottom left) at 45 mg/mL (A at 267 K and C at 300 K) and 90 mg/mL (B at 267 K and D at 300 K). γ-D crystallin (bottom right) at 100 mg/mL (A at 300 K and B at 320 K).

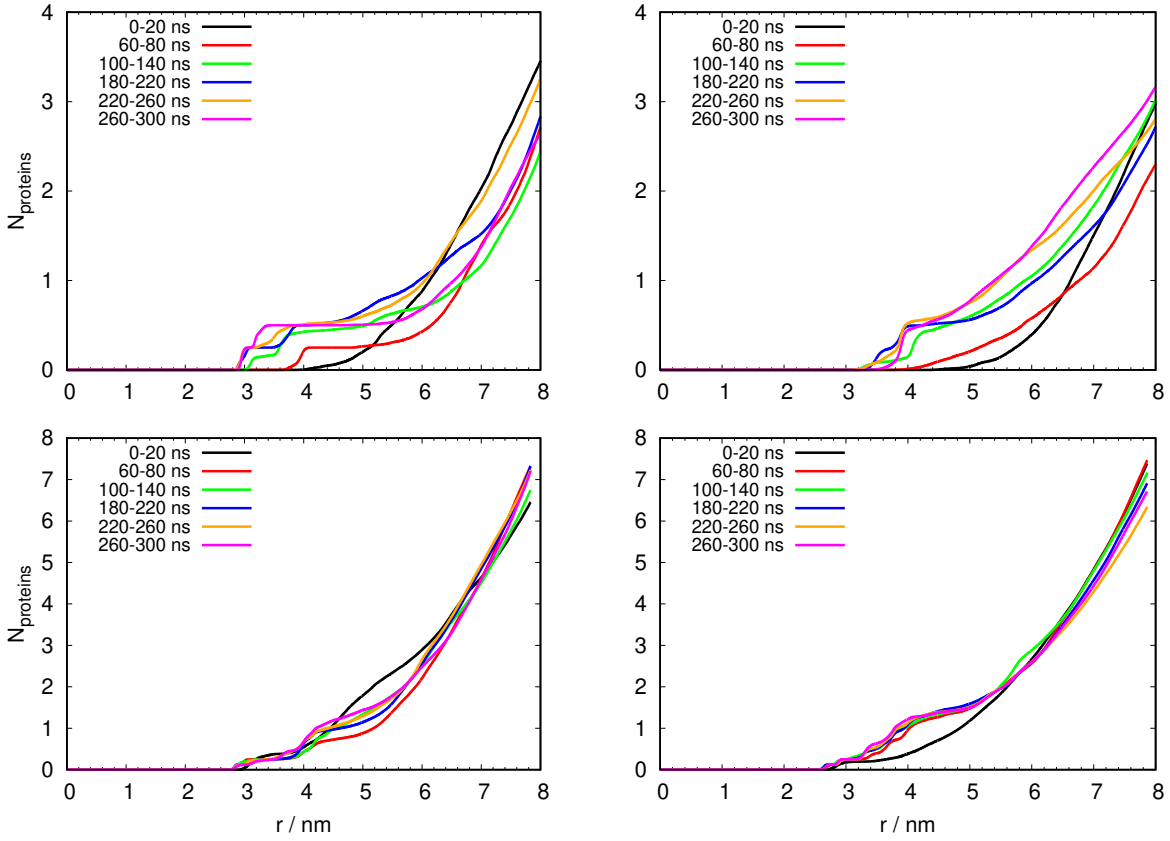

Figure S3: The number of protein molecules at different times of the simulation in the vicinity of HEWL molecule at 42 mg/mL (top left 267 K and top right 300 K) and 93 mg/mL (bottom left 267 K and bottom right 300 K)

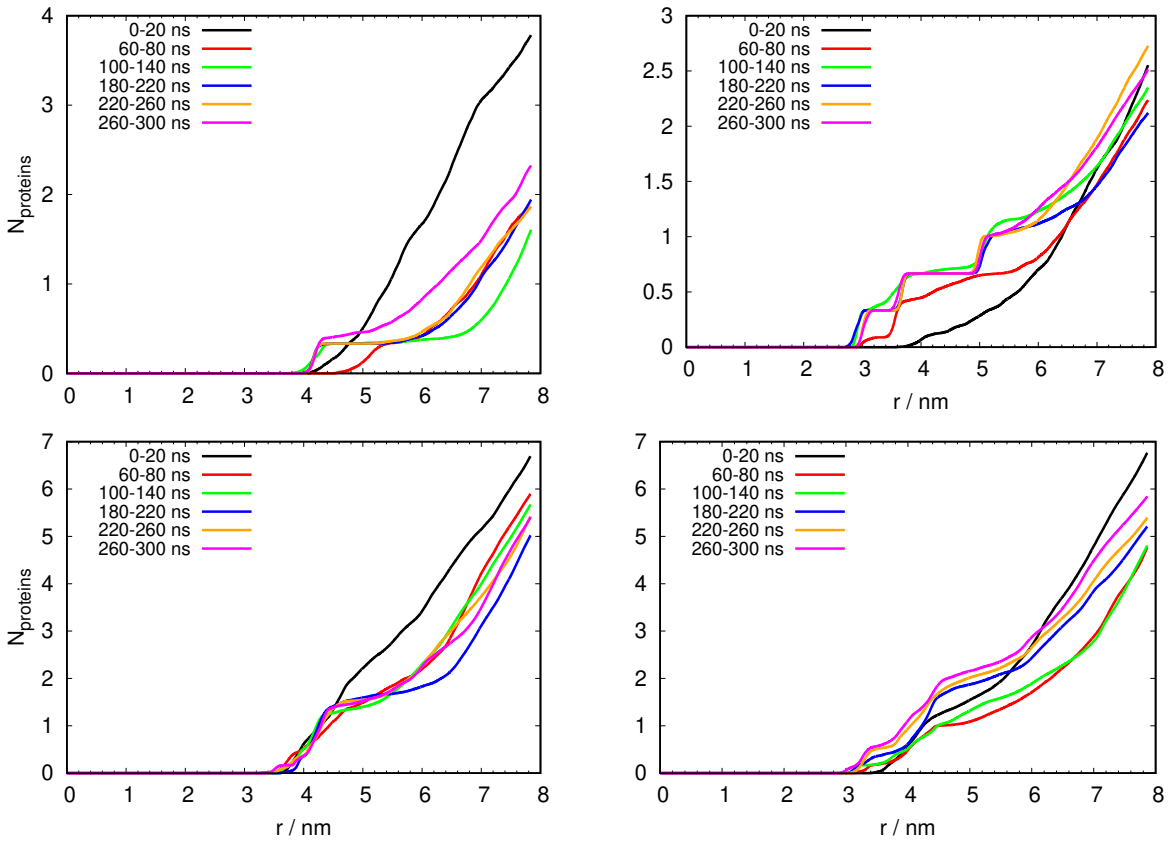

Figure S4: The number of protein molecules at different times of the simulation in the vicinity of T4 WT* molecule at 45 mg/mL (top left 267 K and top right 300 K) and 90 mg/mL (bottom left 267 K and bottom right 300 K).

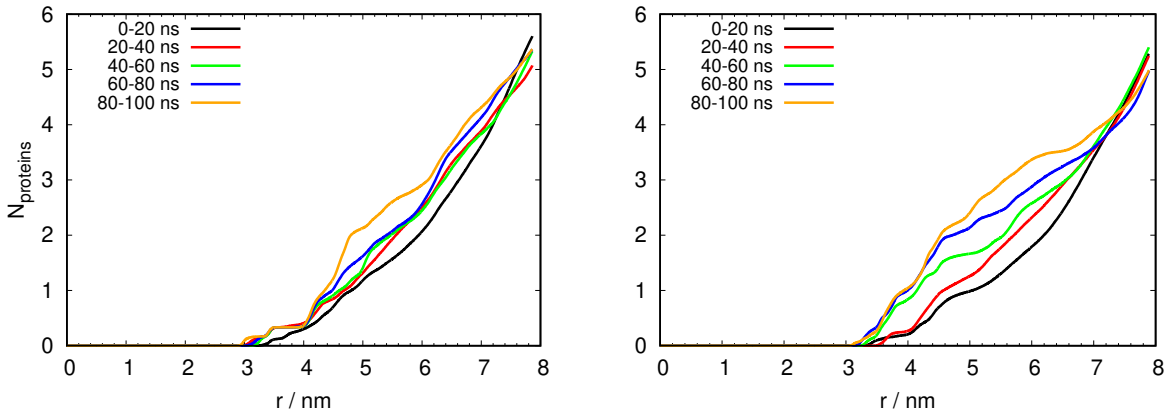

Figure S5: The number of protein molecules at different times of the simulation in the vicinity of γ-D crystallin molecule at 100 mg/mL (left 300 K and right 320 K).

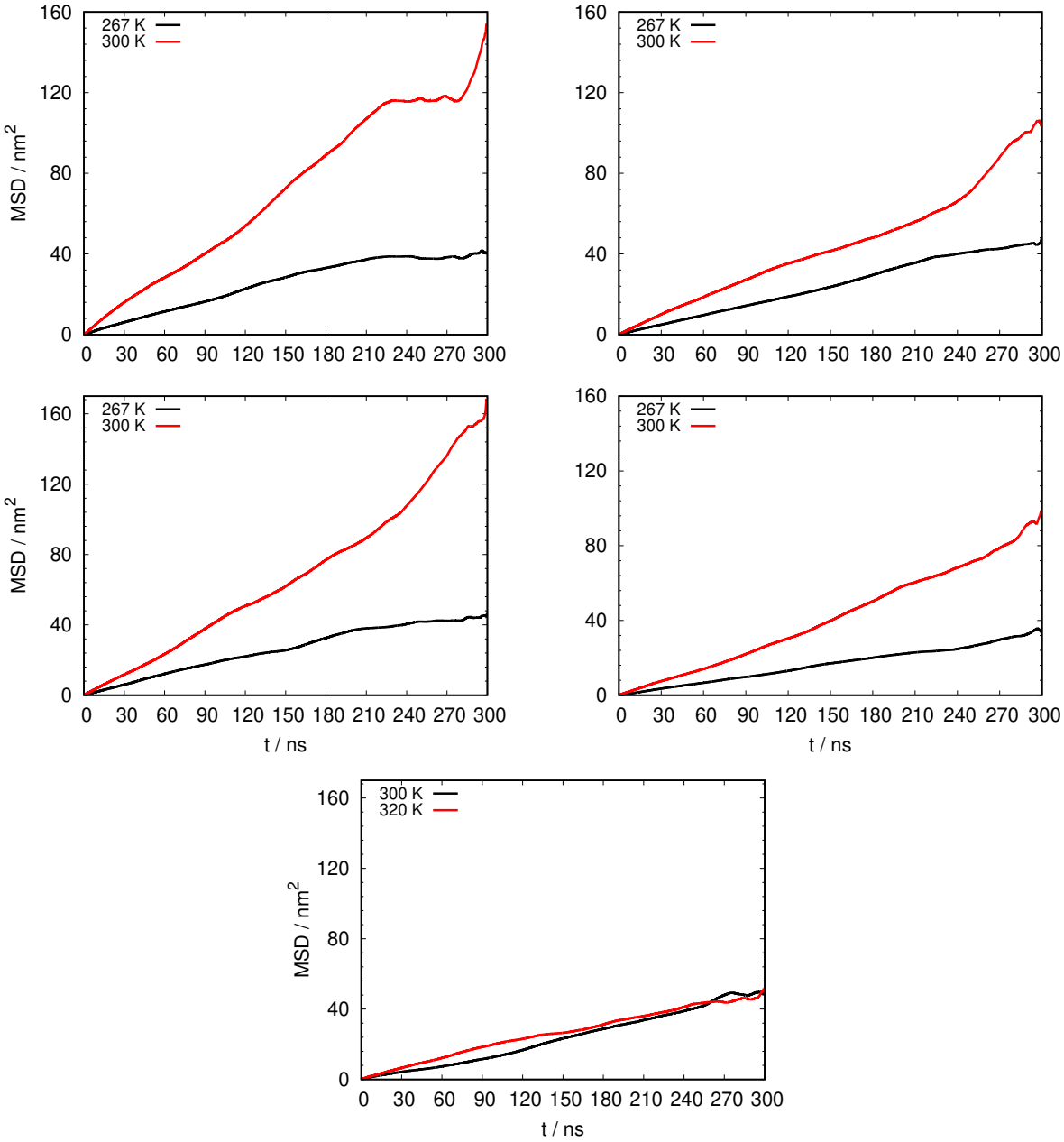

Figure S6: Mean square displacement of proteins at different temperatures. HEWL at 42 mg/mL (top left) and 93 mg/mL (top right). T4 WT* at 45 mg/mL (middle left) and at 90 mg/mL (middle right). γ-D crystallin at 100 mg/mL (bottom).

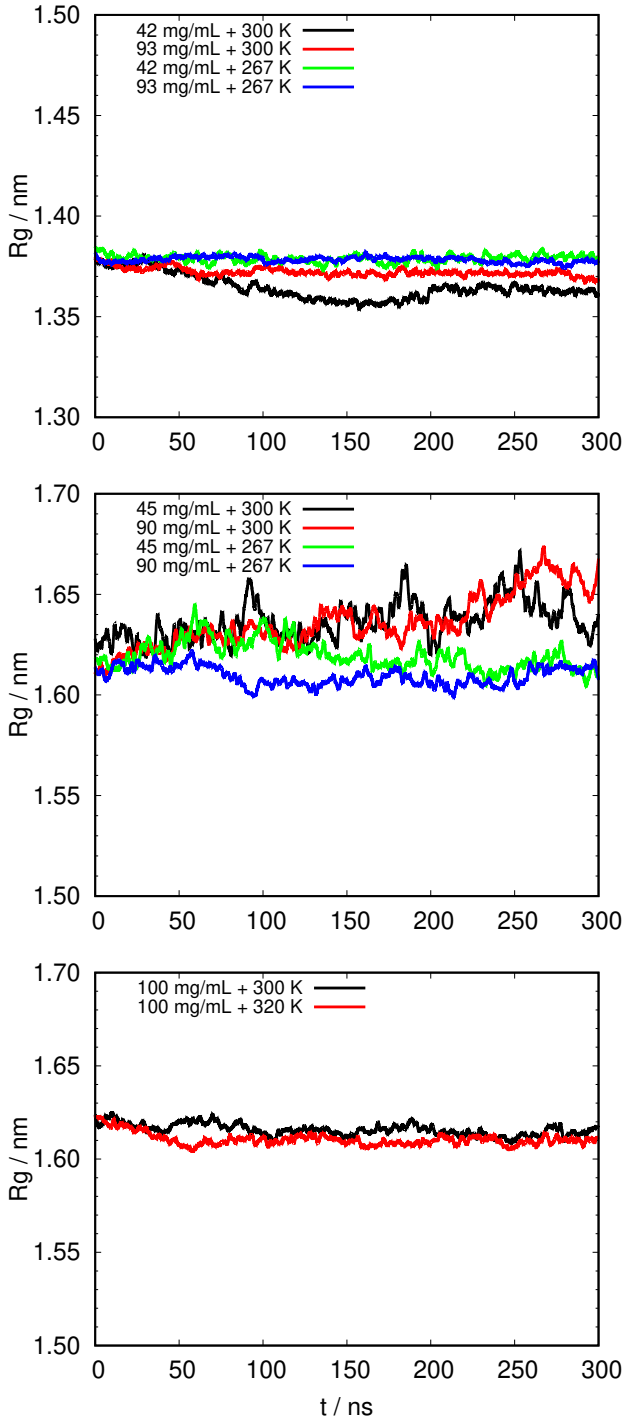

Figure S7: The radius of gyration of HEWL (top), T4 WT* lysozyme (middle) and of γ-D crystallin (bottom).

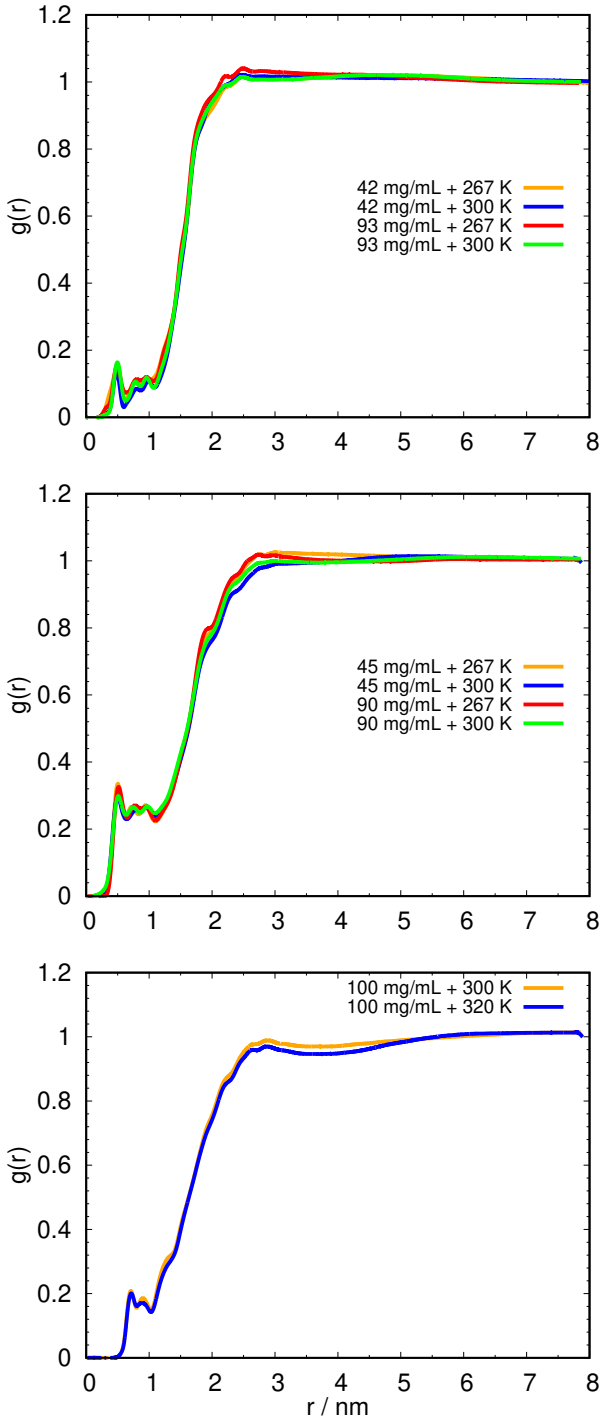

Figure S8: The water oxygen - protein center of mass pair distribution functions for HEWL (top), T4 WT* lysozyme (middle) and γ-D crystallin (bottom).

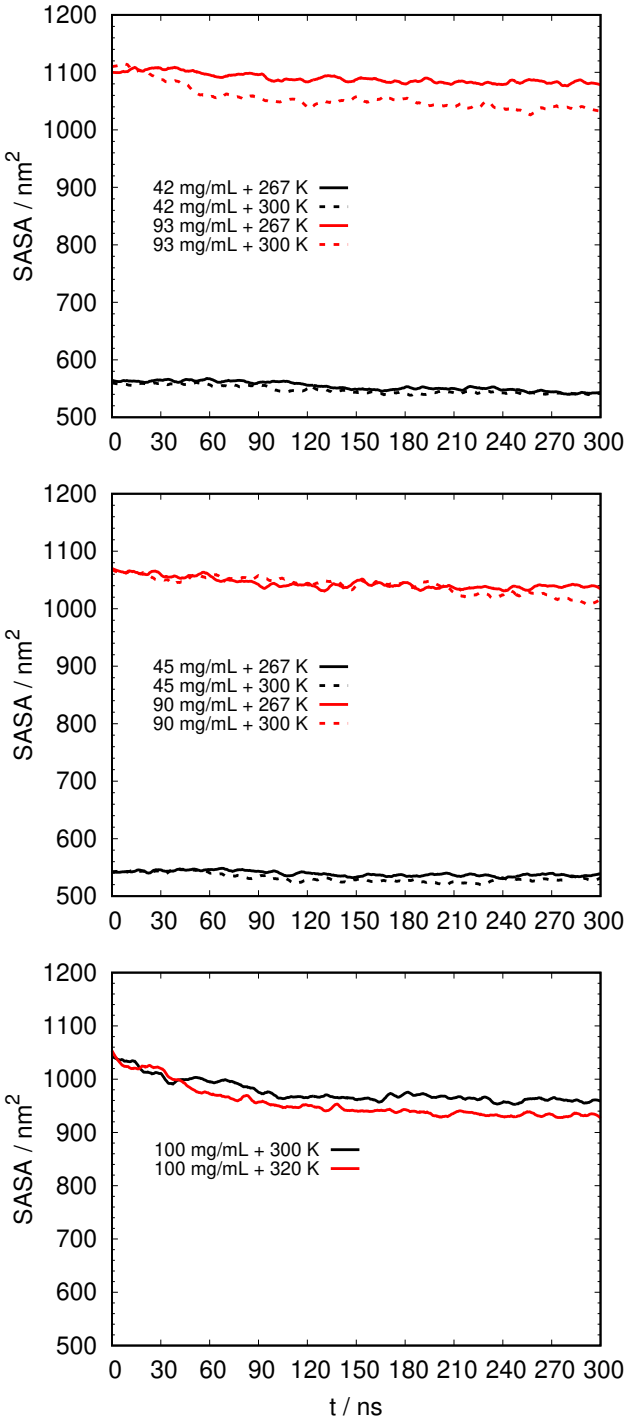

Figure S9: Solvent accessible surface area (SASA) for HEWL (top), T4 WT* lysozyme (middle) and γ-D crystallin (bottom).

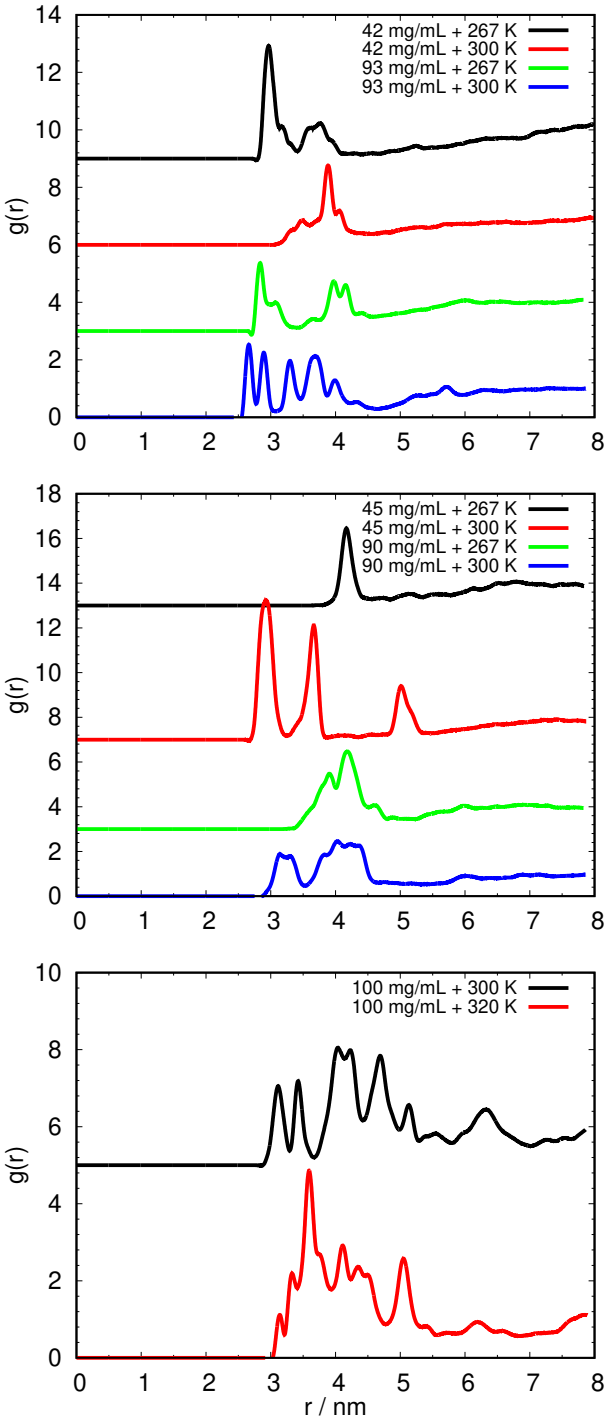

Figure S10: Protein-protein pair distribution functions for HEWL (top), T4 WT* lysozyme (middle) and γ-D crystallin (bottom). Plots are shifted vertically for clarity.

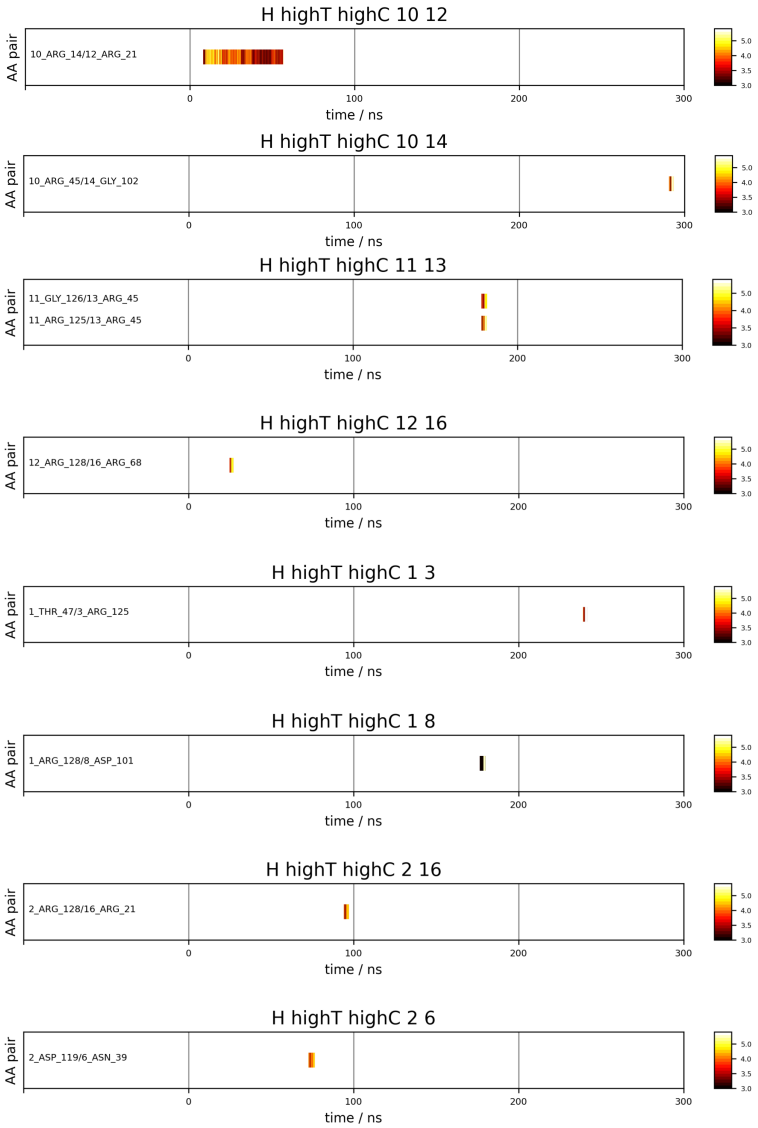

Figure S11: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 93 mg mL^{-1} of HEWL at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space

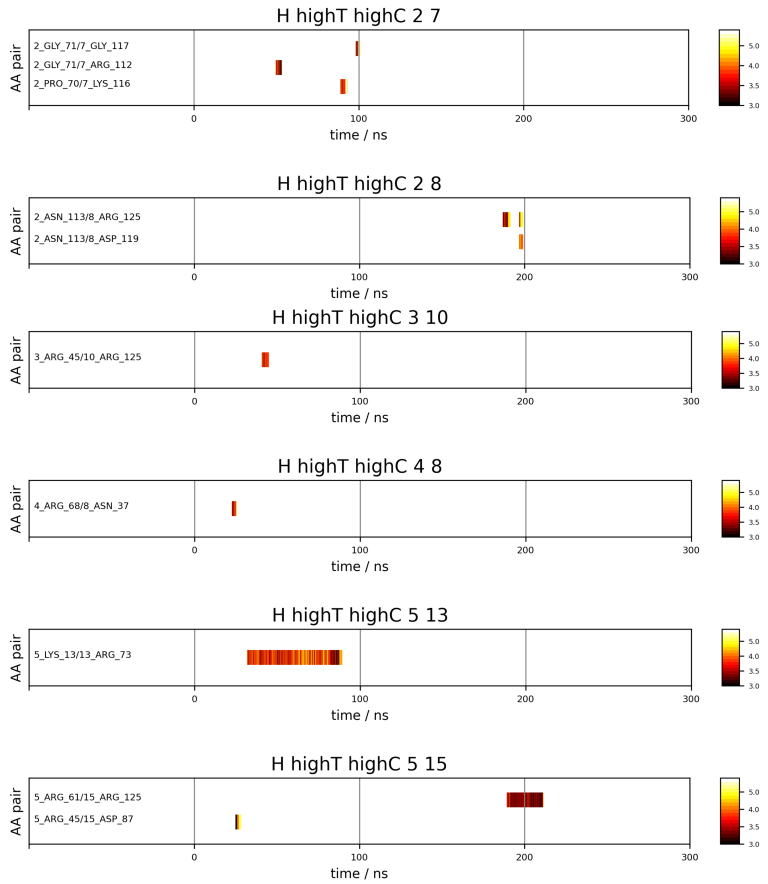

Figure S12: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 93 mg mL^{-1} of HEWL at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

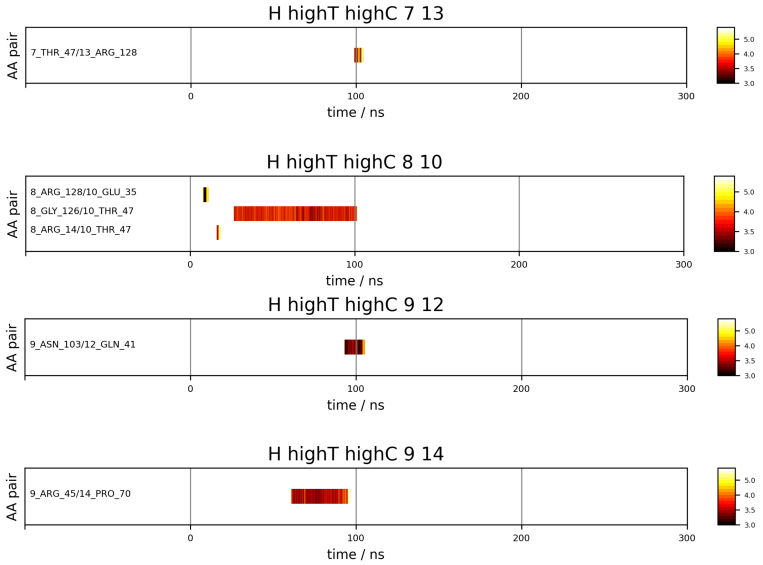

Figure S13: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 93 mg mL^{-1} of HEWL at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

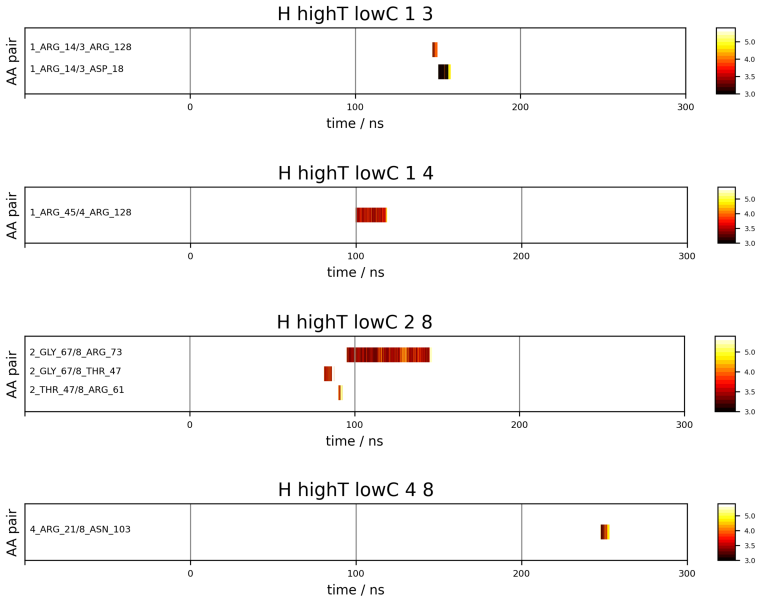

Figure S14: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 42 mg mL^{-1} of HEWL at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

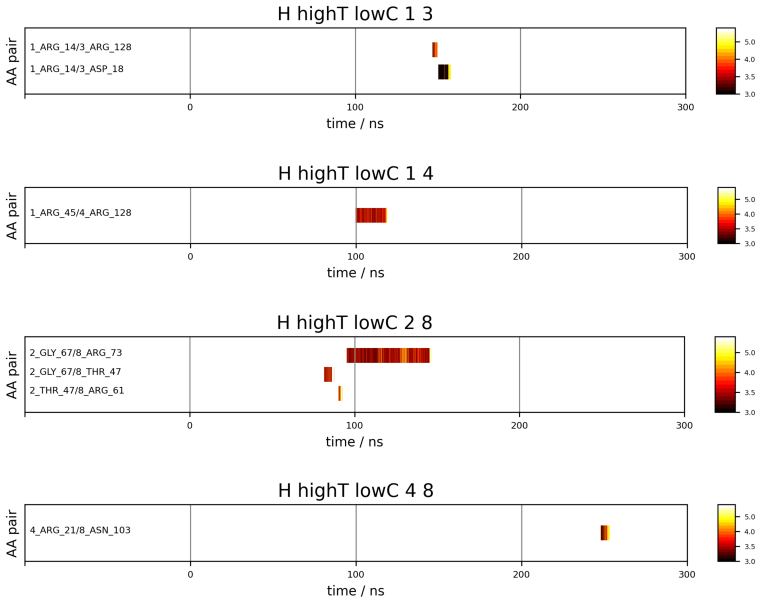

Figure S15: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 42 mg mL^{-1} of HEWL at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

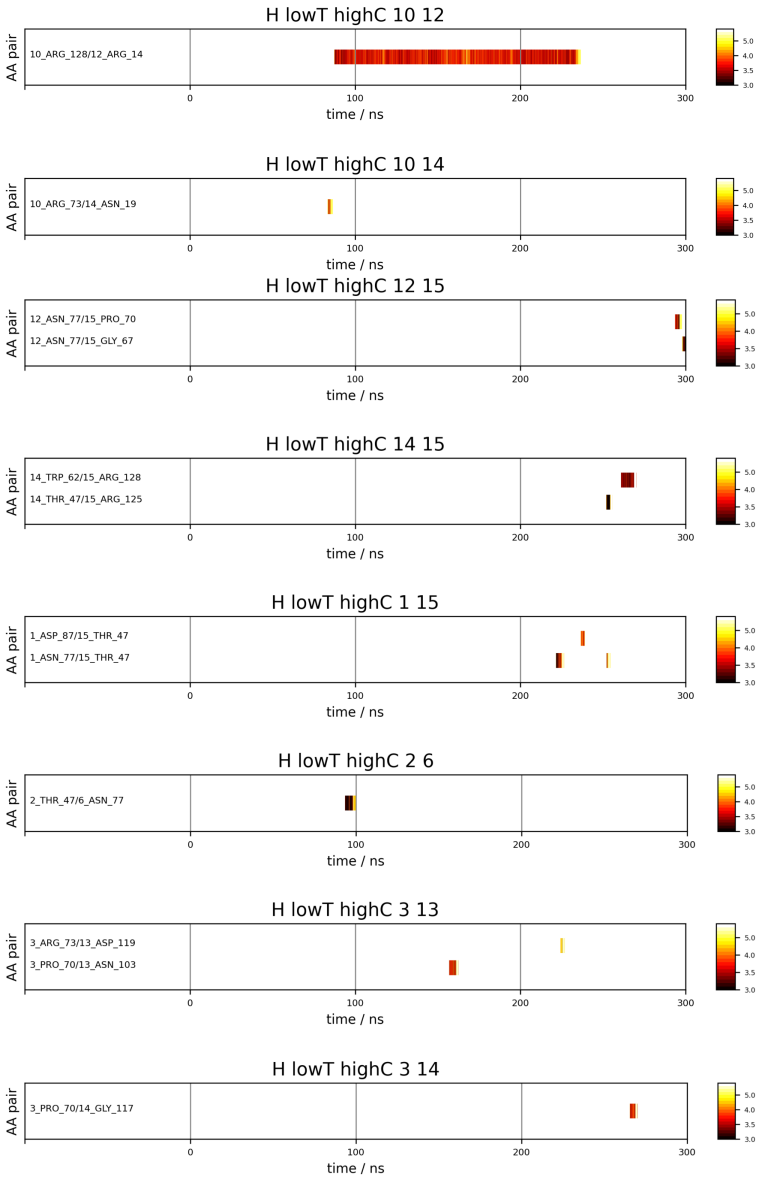

Figure S16: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 93 mg mL^{-1} of HEWL at 267 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

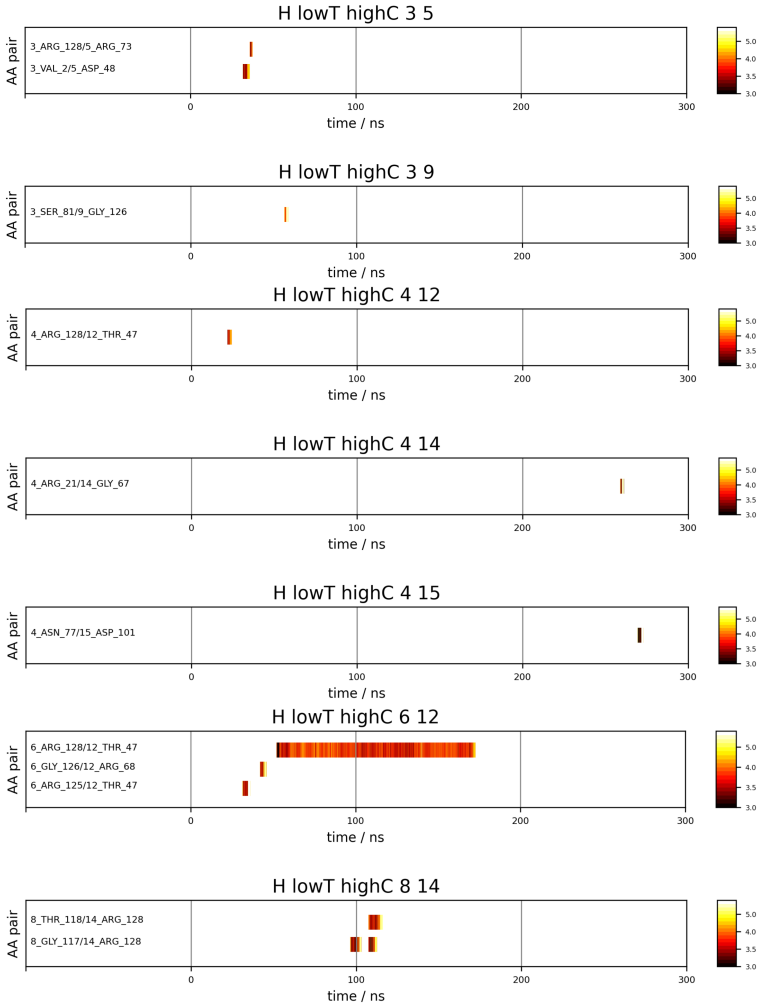

Figure S17: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 93 mg mL^{-1} of HEWL at 267 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

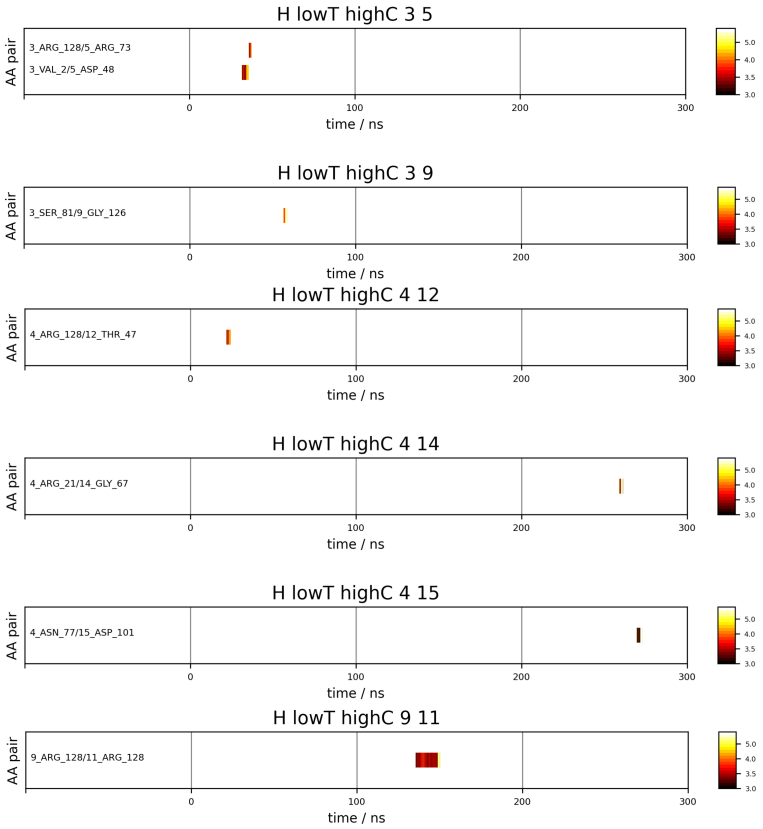

Figure S18: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 93 mg mL^{-1} of HEWL at 267 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

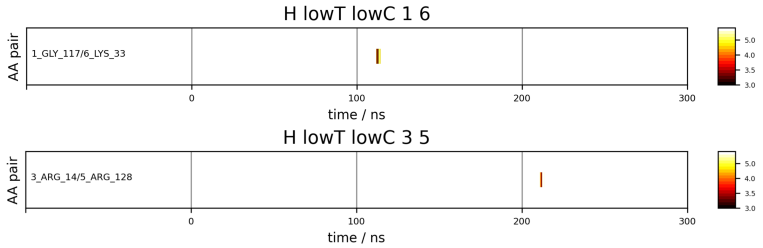

Figure S19: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of HEWL molecules in the solution comprising of 42 mg mL^{-1} of HEWL at 267 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

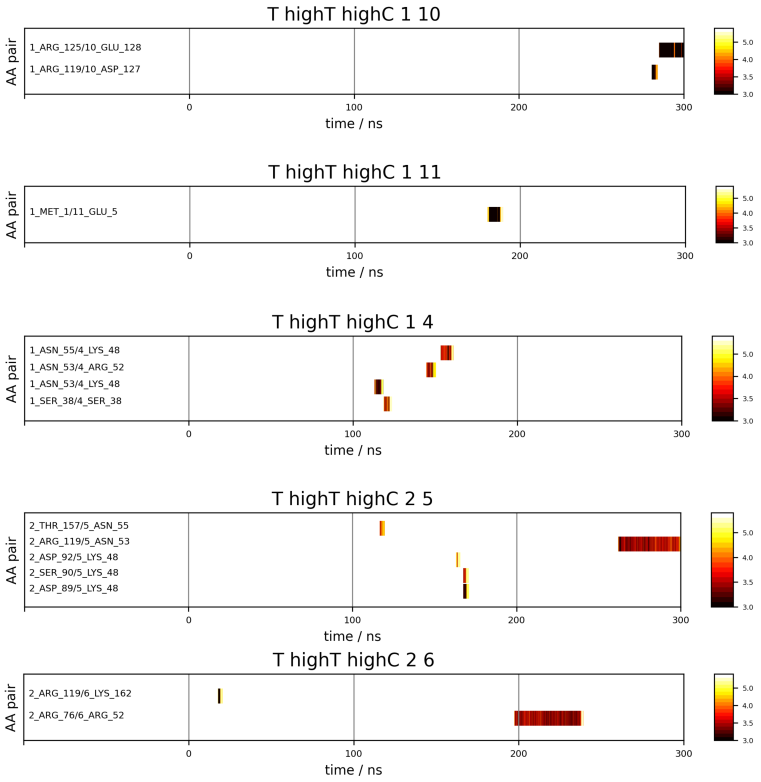

Figure S20: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 90 mg mL^{-1} of T4 WT* at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

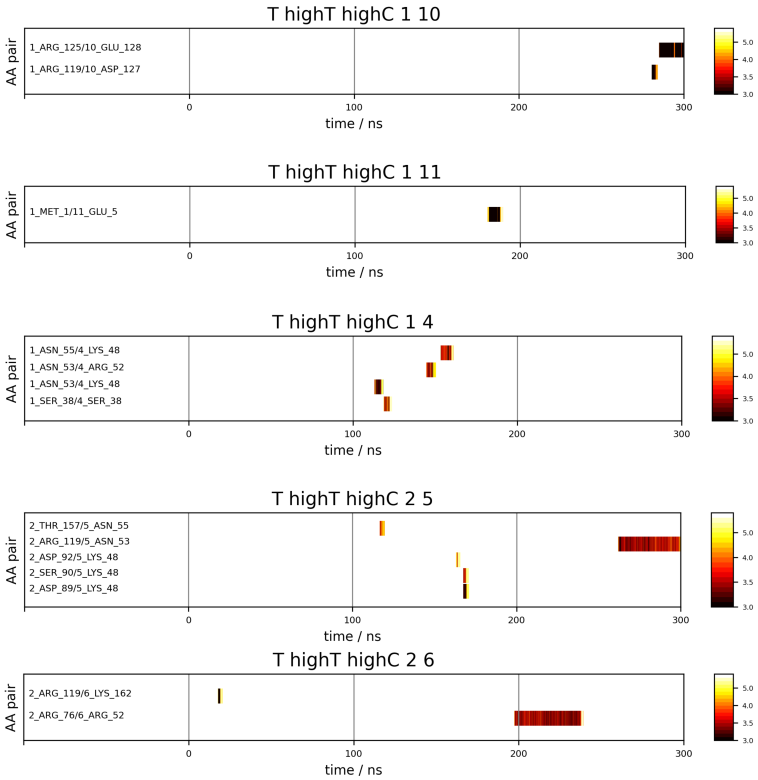

Figure S21: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 90 mg mL^{-1} of T4 WT* at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

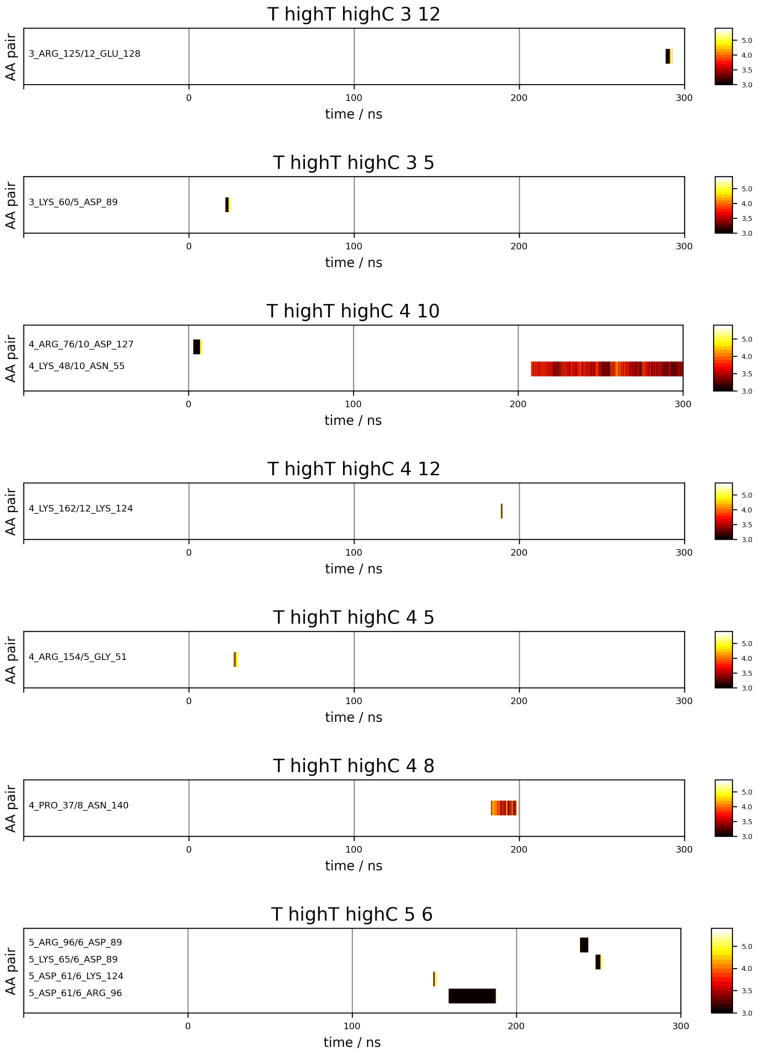

Figure S22: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 90 mg mL^{-1} of T4 WT* at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

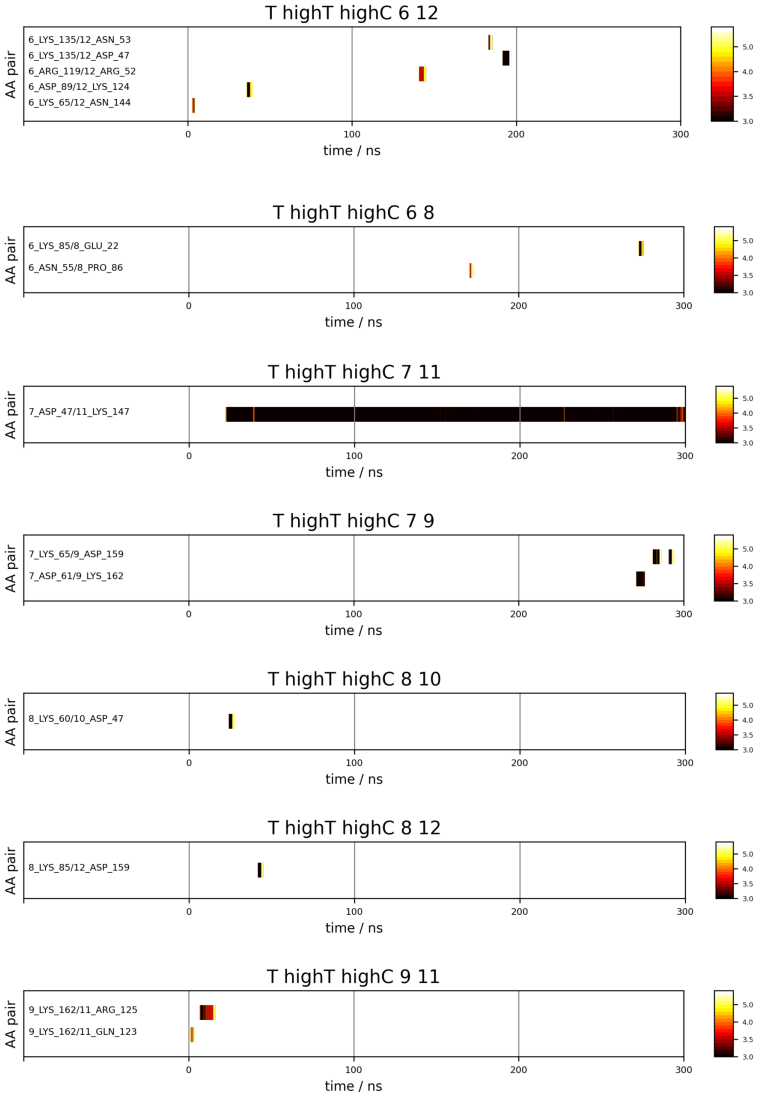

Figure S23: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 90 mg mL^{-1} of T4 WT* at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

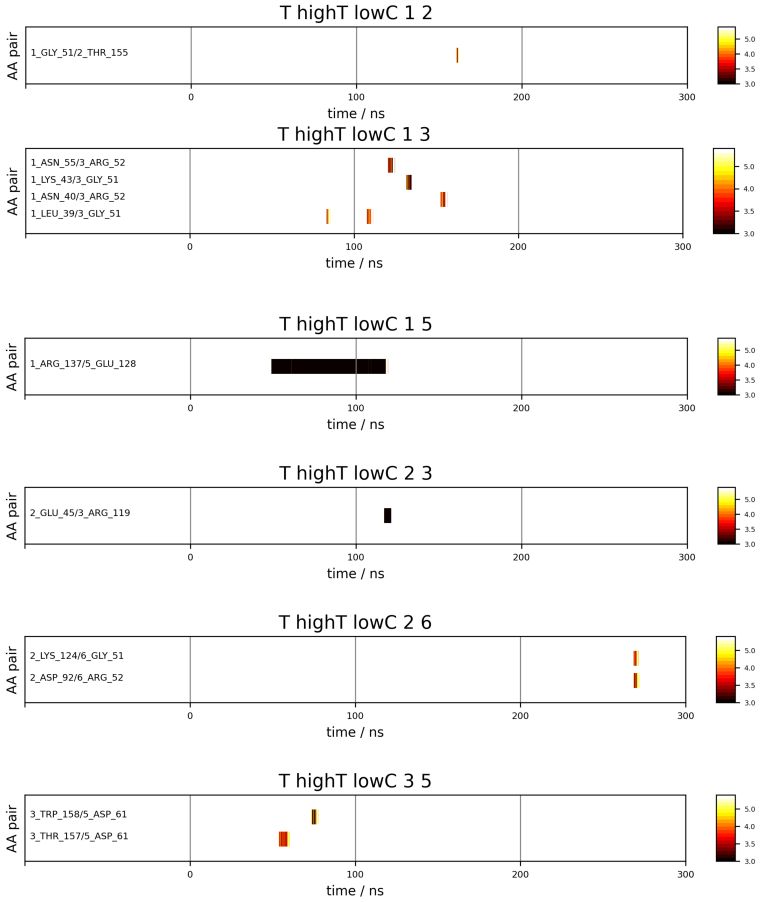

Figure S24: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 45 mg mL^{-1} of T4 WT* at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

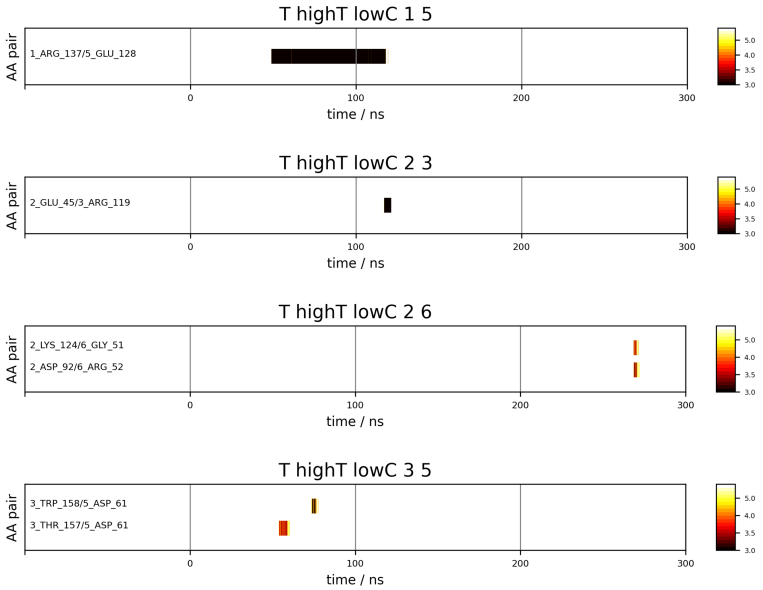

Figure S25: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 45 mg mL^{-1} of T4 WT* at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

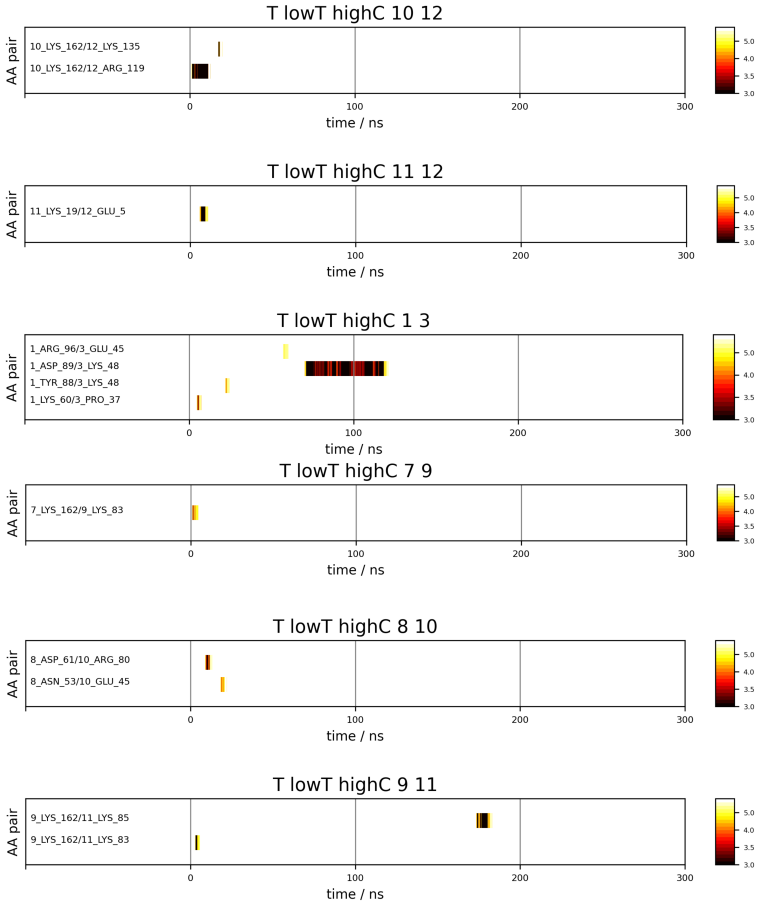

Figure S26: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 90 mg mL^{-1} of T4 WT* at 267 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

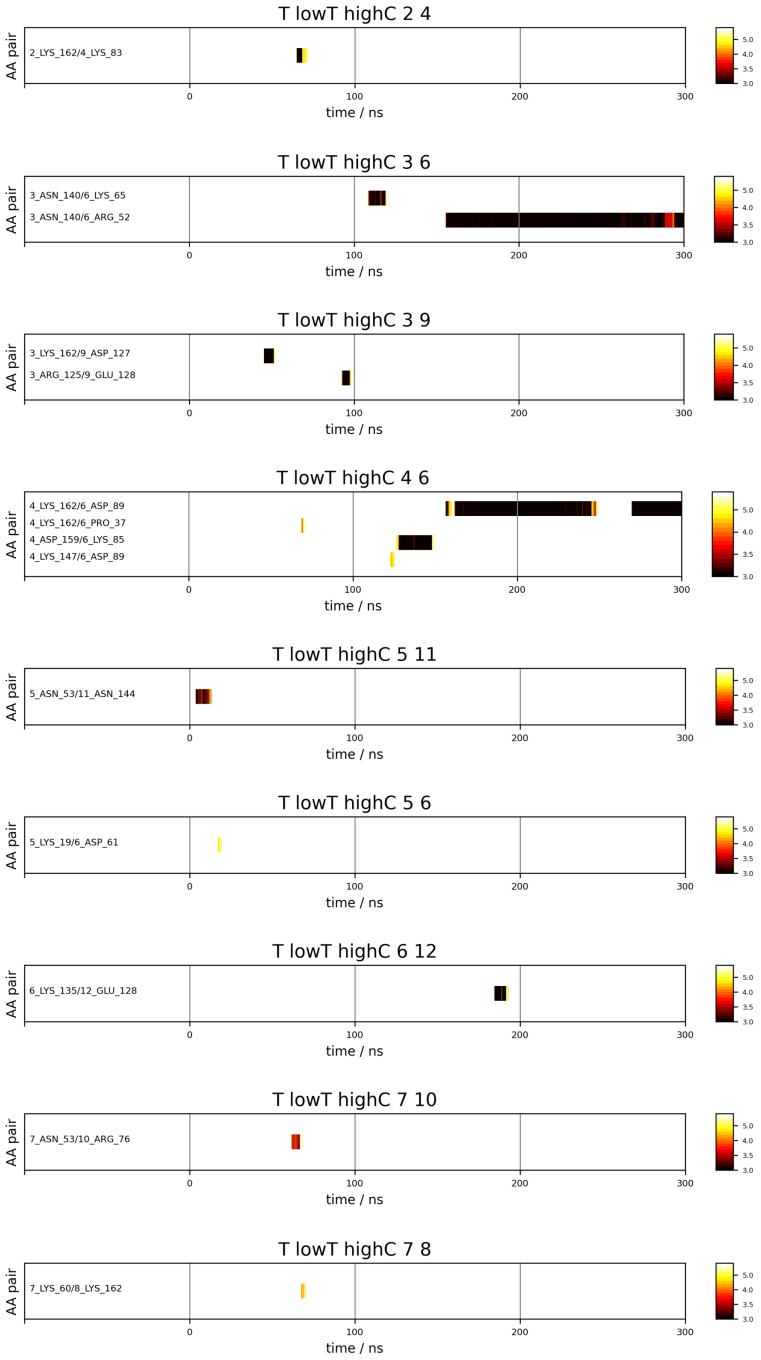

Figure S27: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 90 mg mL^{-1} of T4 WT* at 267 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

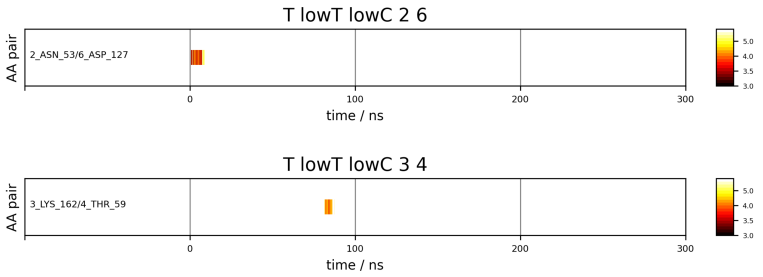

Figure S28: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of T4 WT* molecules in the solution comprising of 45 mg mL^{-1} of T4 WT* at 267 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

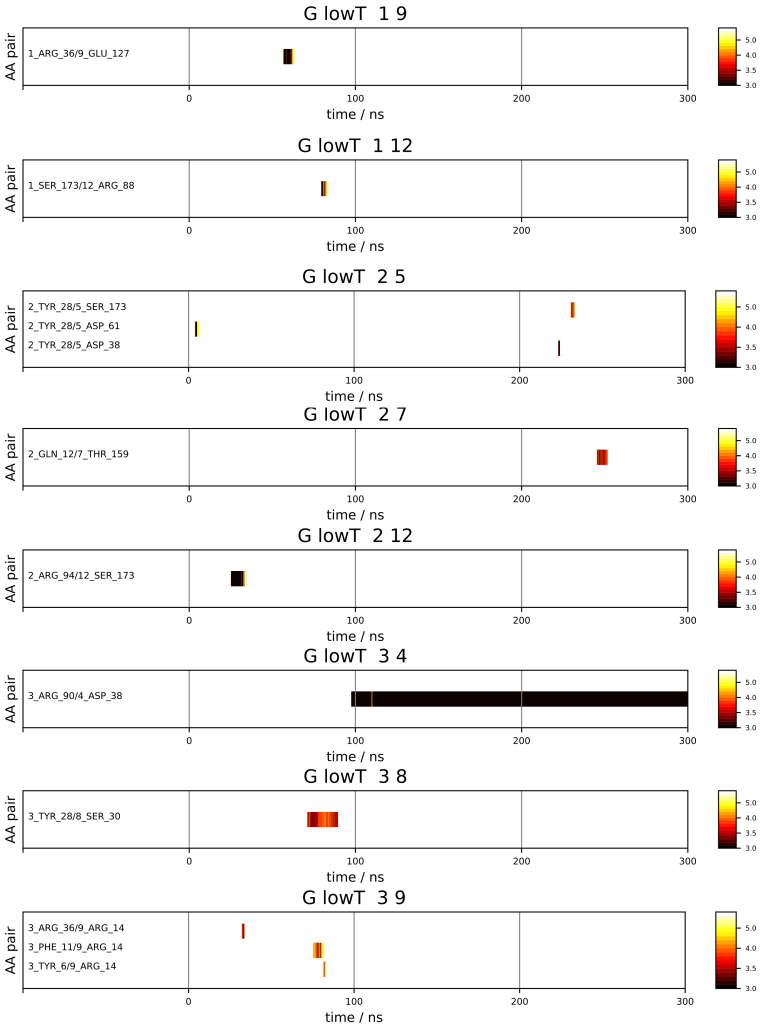

Figure S29: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of γ-D crystallin molecules in the solution comprising of 100 mg mL^{-1} of γ-D crystallin at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

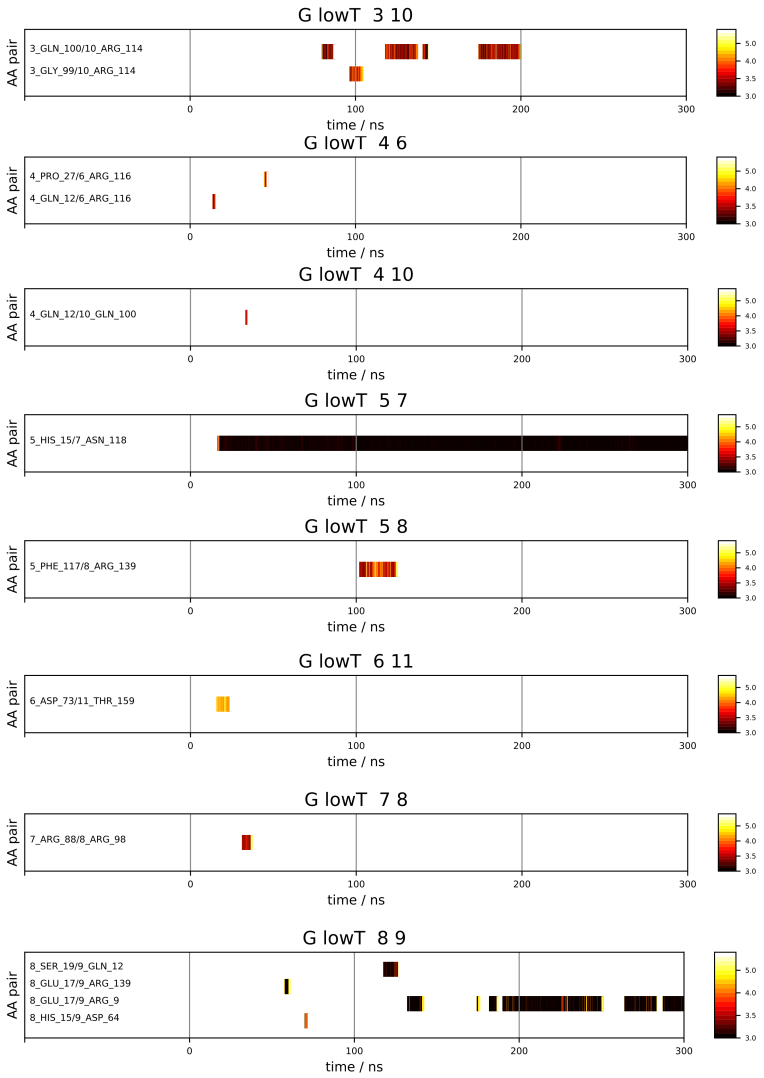

Figure S30: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of γ-D crystallin molecules in the solution comprising of 100 mg mL^{-1} of γ-D crystallin at 300 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

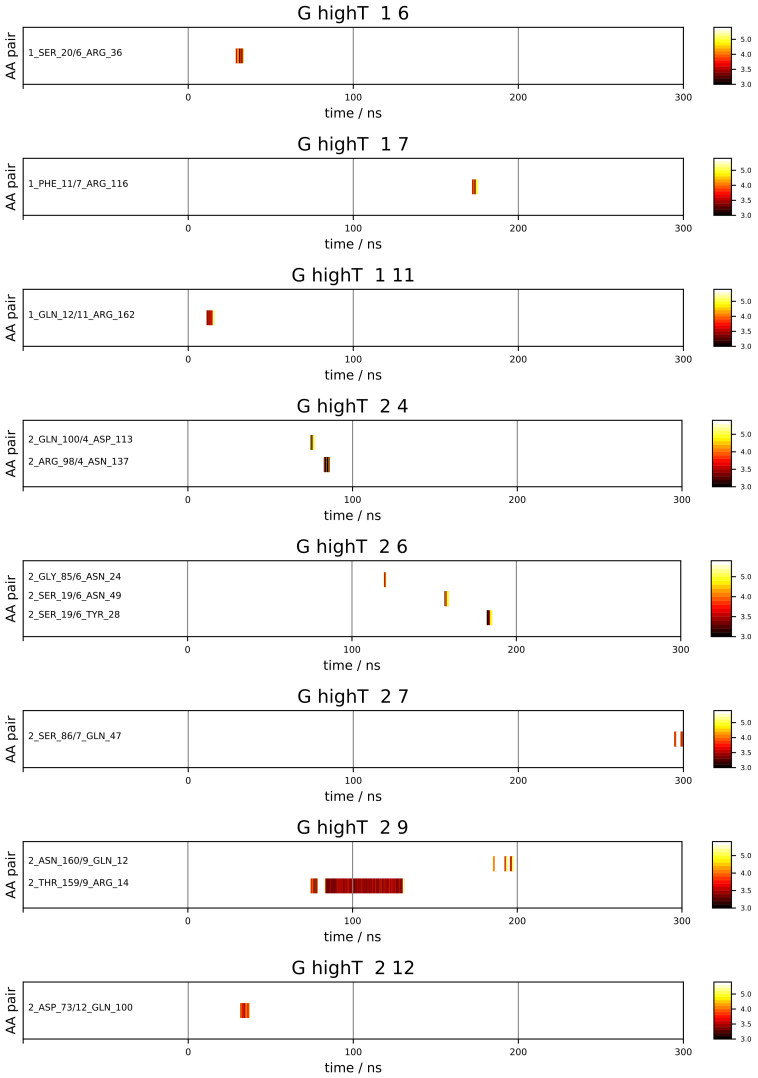

Figure S31: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of γ-D crystallin molecules in the solution comprising of 100 mg mL^{-1} of γ-D crystallin at 320 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

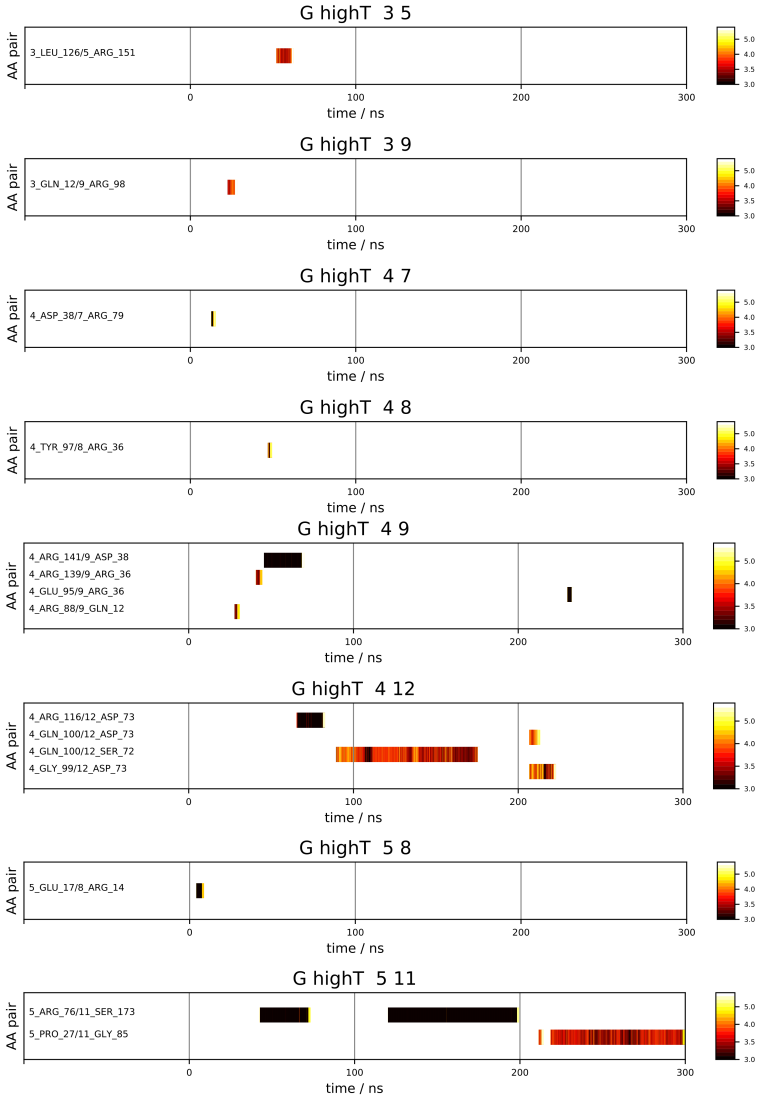

Figure S32: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of γ-D crystallin molecules in the solution comprising of 100 mg mL^{-1} of γ-D crystallin at 320 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.

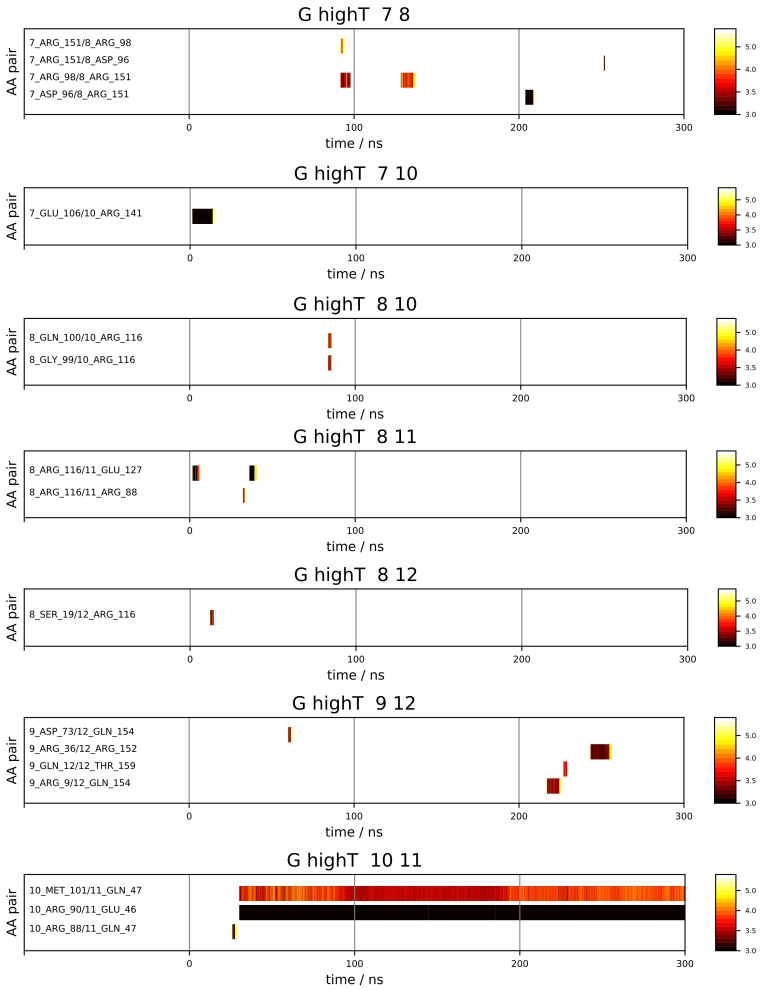

Figure S33: Time evolution of residue-residue contacts that appear within 6 Å between different pairs of γ-D crystallin molecules in the solution comprising of 100 mg mL^{-1} of γ-D crystallin at 320 K. The shortest distance (here in Å) between the residue pairs is represented with a heat map on the right. Distances above 6 Å are plotted as white space.