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Dual-resolution modeling demonstrates greater conformational heterogeneity of CENP-A/H4 dimer than that of H3/H4 HAIQING ZHAO, University of Maryland — Centromere protein A (CENP-A) is a centromere-specific H3 histone variant and shares only about 50% amino acid sequence identity with the canonical H3 protein. CENP-A is required for packaging the centromere and for the proper separation of chromosomes during mitosis. Despite their discrete functions, previously reported crystal structures of the CENP-A/H4 and H3/H4 dimers reveal surprising similarity. In this work, we characterize the structure and dynamics of CENP-A/H4 and H3/H4 dimers with a dual-resolution approach, using both all-atom and coarse-grained (CG) molecular dynamics (MD) simulations. Interestingly, the histone dimer containing CENP-A is more structurally variable than the canonical H3 dimer. Furthermore, our calculations revealed significant conformational distinctions between the interface profiles of CENP-A/H4 and H3/H4. In addition, the presence of the CENP-A-specific chaperone HJURP dramatically reduced the conformational heterogeneity of CENP-A/H4. Overall, these results are in general agreement with the available experimental data and provide new dynamic insights into the mechanisms underpinning the chaperone-mediated assembly of CENP-A nucleosomes *in vivo*.

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