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Supplemental information

**Molecular dynamics simulations reveal subtle consequences of H3K9
and H3K27 tri-methylation on chromatin constituents**

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Supporting Information for “Molecular Dynamics Simulations Reveal Subtle Consequences of H3K9 and H3K27 tri-methylation on Chromatin Constituents”

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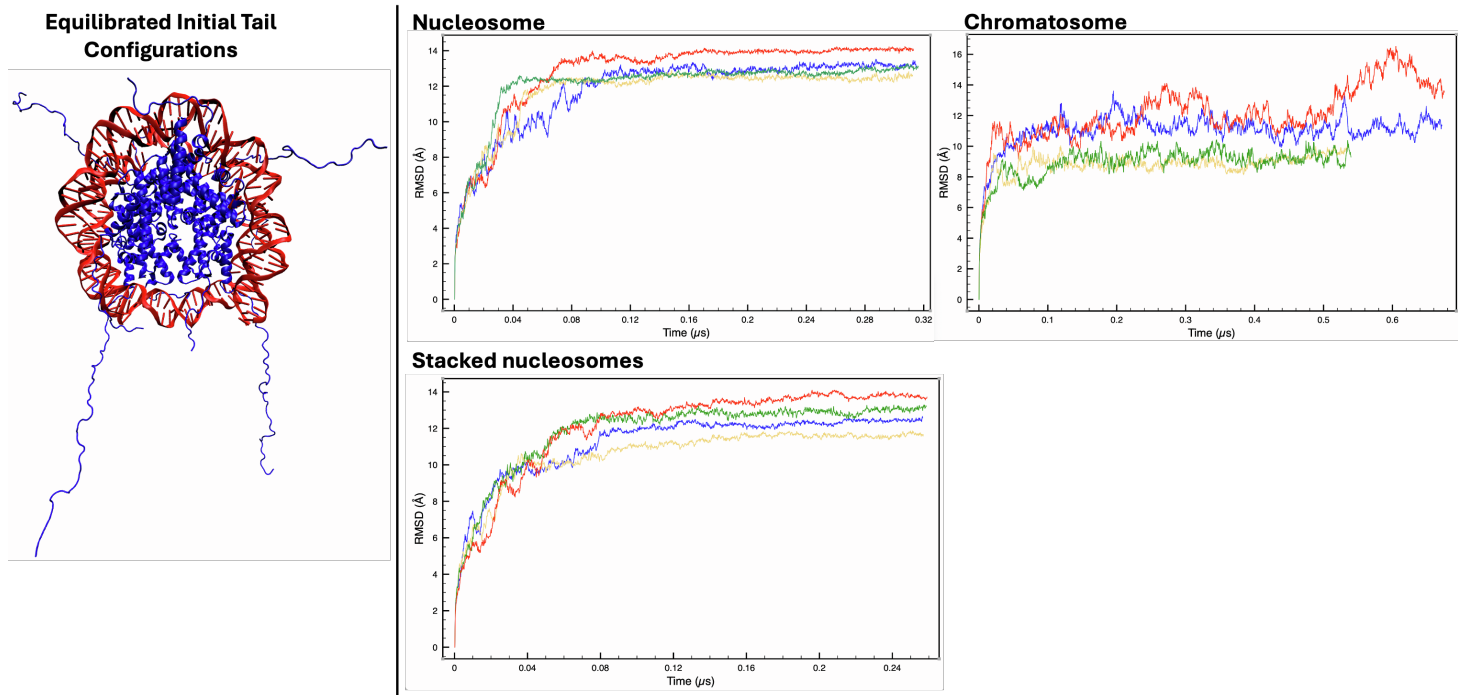


Figure S1. Initial tail configurations used in simulations of nucleosomes, chromosomes, and stacked nucleosomes to test effect of initial structure on overall results.

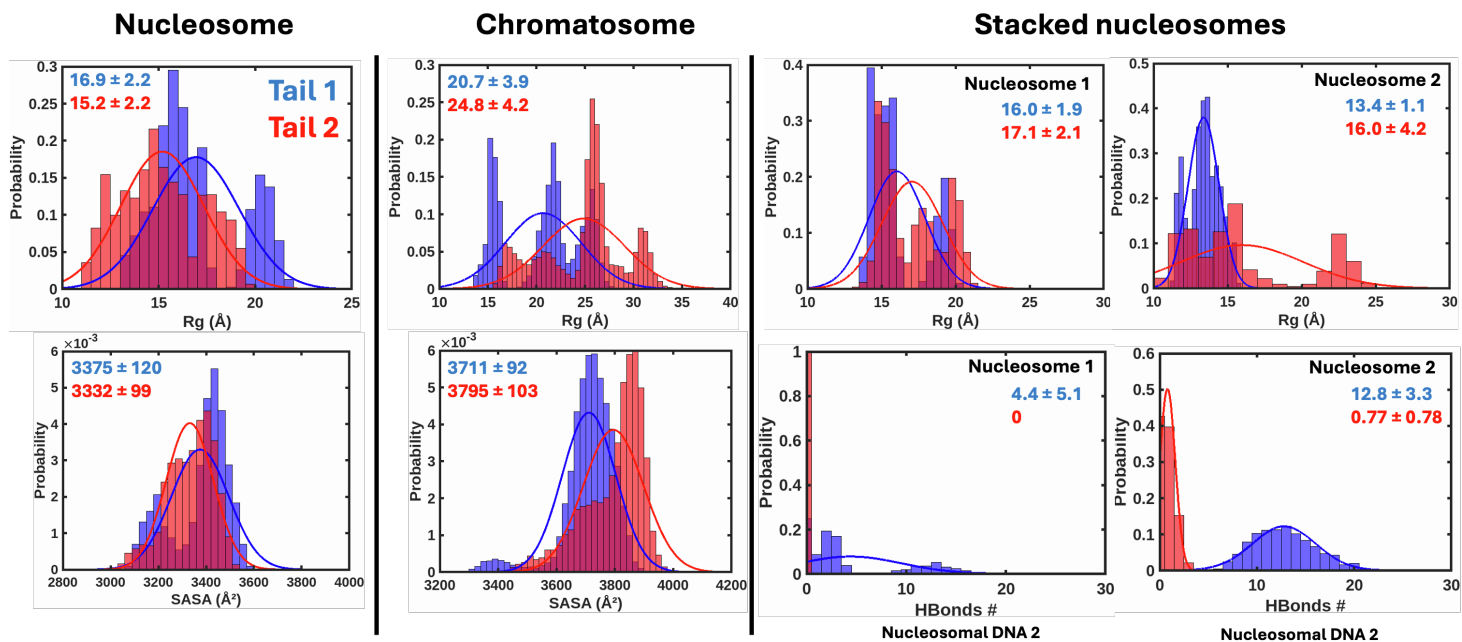


Figure S2. Comparison of behavior of native H3 Tail 1 versus Tail 2 in the nucleosome, chromosome, and stacked nucleosome systems when starting from extended tail configurations.

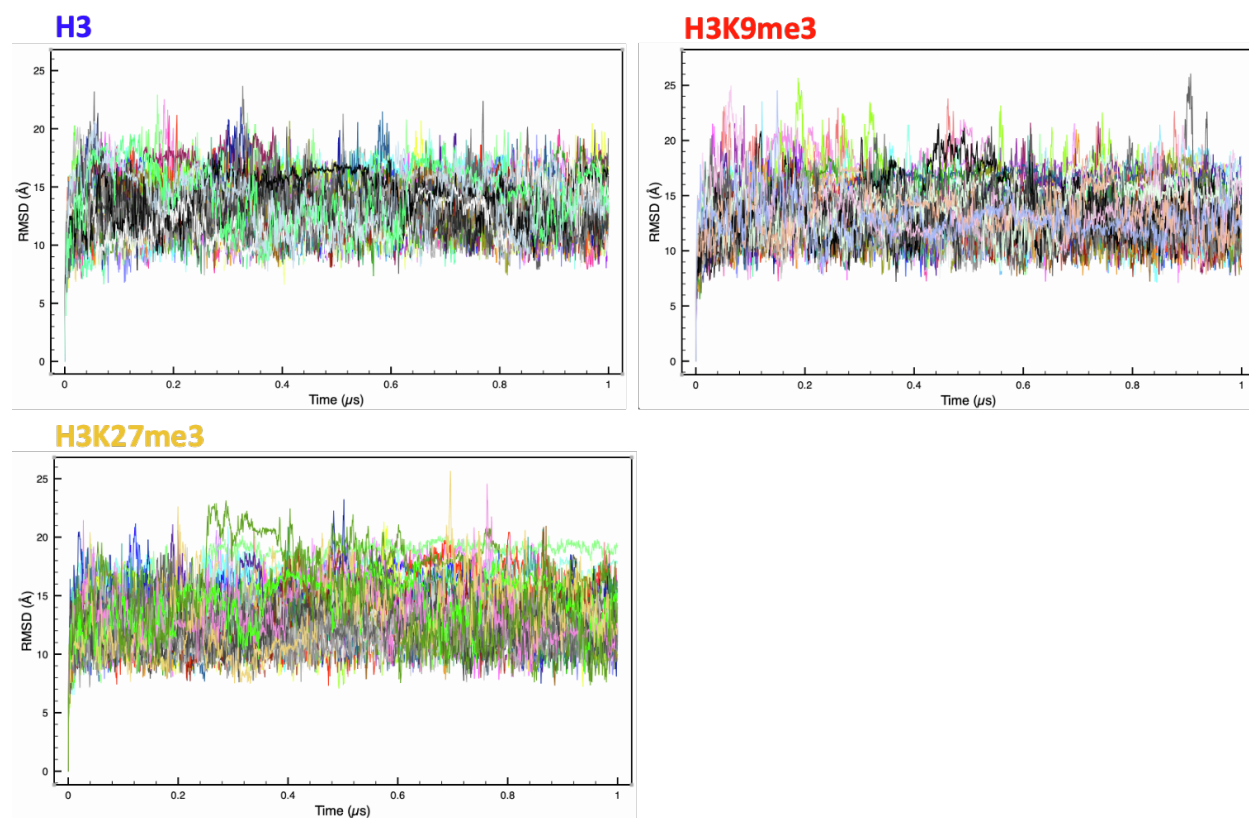


Figure S3. RMSD for the 50 replicas of native H3 tail and the K9me3 and K27me3 H3 tails.

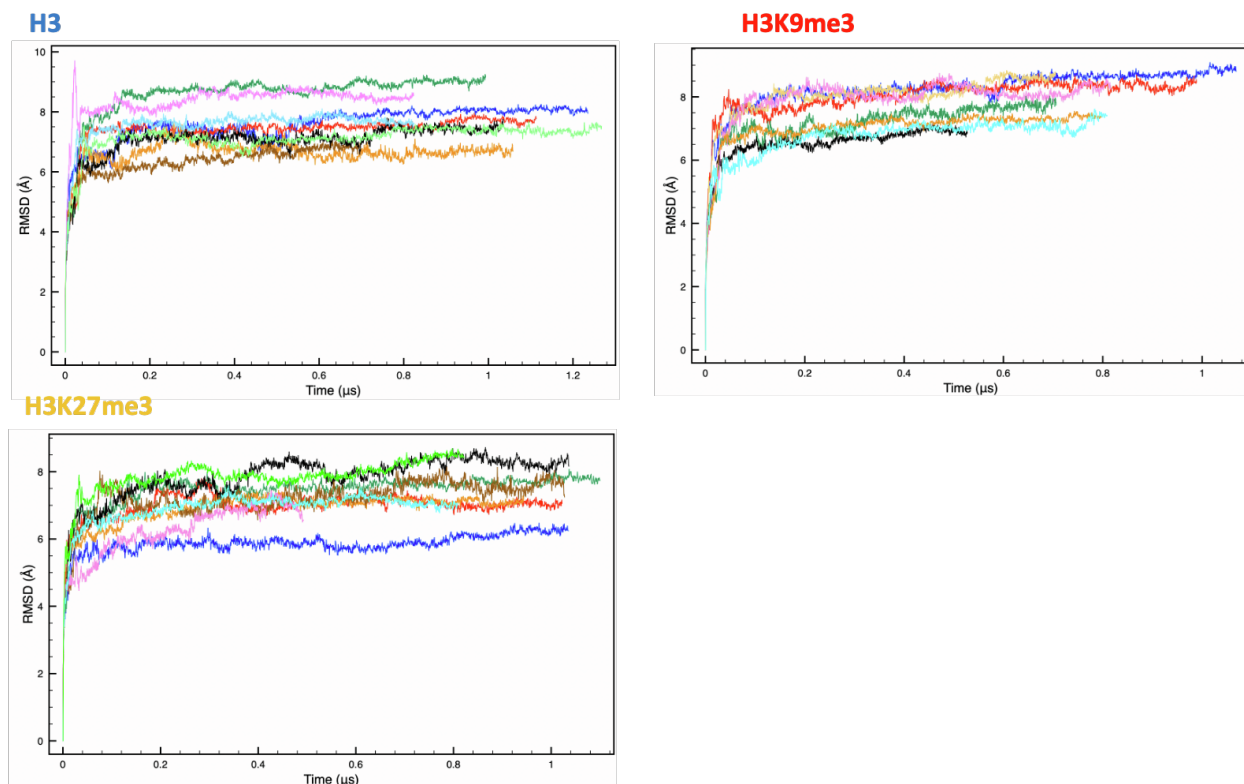


Figure S4. RMSD for the 9 replicas of the nucleosome with native H3 tails and the K9me3 and K27me3 H3 tails.

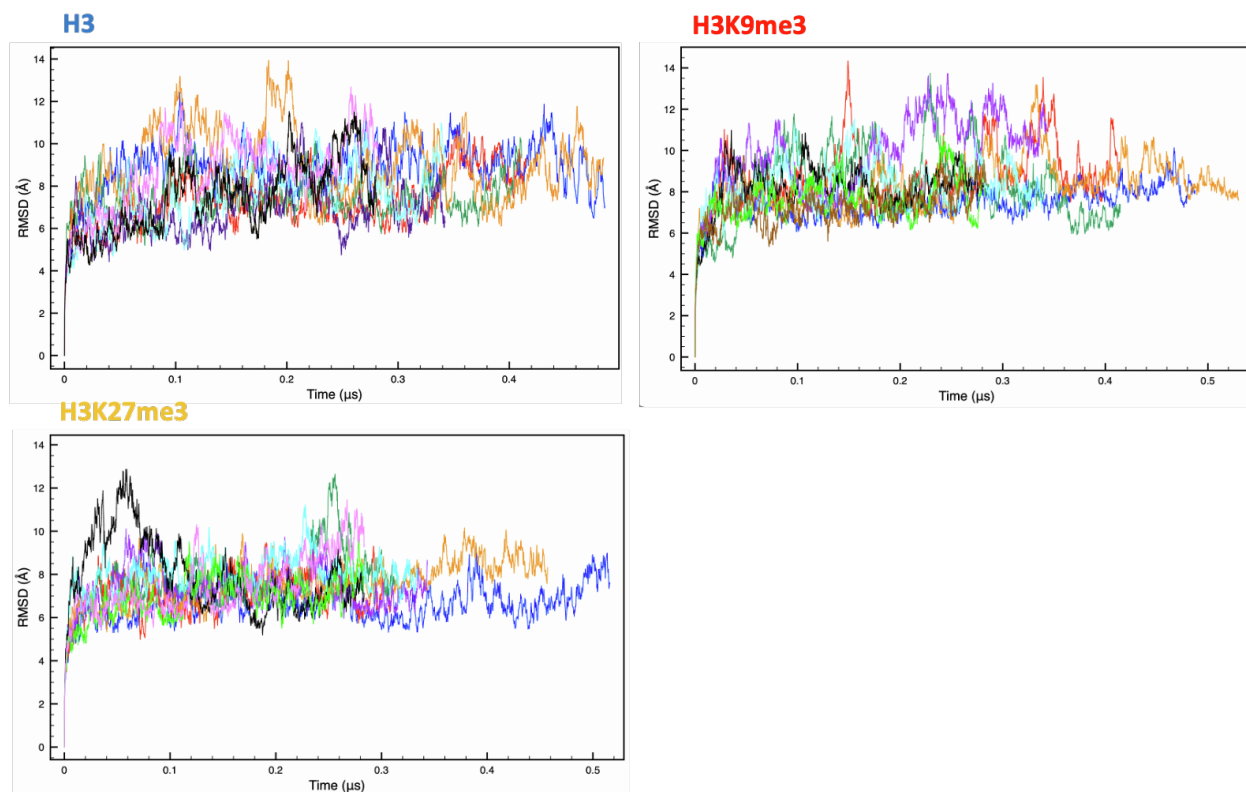
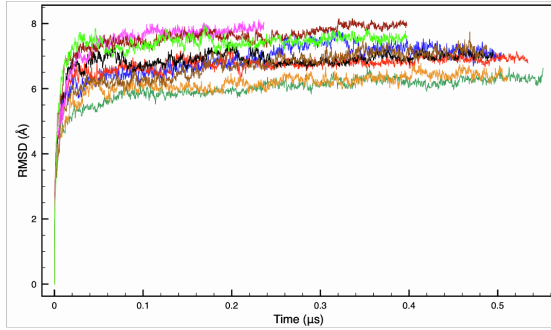


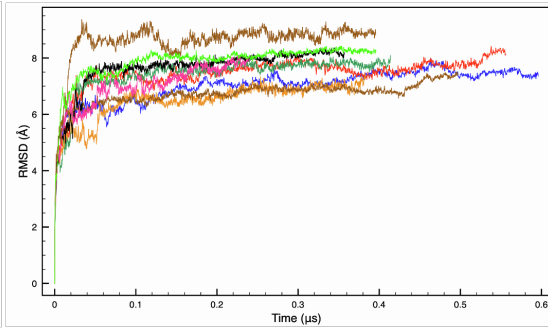
Figure S5. RMSD for the 9 replicas of chromosomes with native H3 tails and with K9me3 and K27me3 H3 tails.

Stacked nucleosomes

H3



H3K9me3



H3K27me3

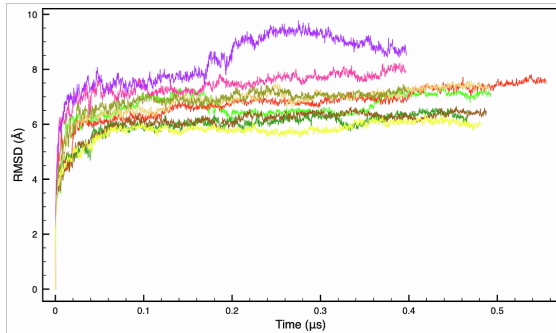


Figure S6. RMSD for the 9 replicas of two stacked nucleosomes with native H3 tails and with K9me3 and K27me3 H3 tails.

Table S1. p-values for Student's test comparing compaction properties of the native H3 versus K9 and K27 methylated H3.

Chromatosome					Nucleosome					Stacked Nucleosomes				
System 1	System 2	Property	p-value	NULL hypothesis	System 1	System 2	Property	p-value	NULL hypothesis	System 1	System 2	Property	p-value	NULL hypothesis
Native	K9me3	Entry-Exit	0.95	not rejected	Native	K9me3	Tail1			Native	K9me3	Rg (tail1; nuc1)	7.68E-39	rejected
Native	K27me3	Entry-Exit	2.81E-04	rejected	Native	K27me3	Rg	0.00E+00	rejected	Native	K27me3	Rg (tail1; nuc1)	1.65E-08	rejected
Native	K9me3	Beta angle	0	rejected	Native	K27me3	Rg	0.00E+00	rejected	Native	K9me3	Rg (tail2; nuc1)	0.00E+00	rejected
Native	K27me3	Beta angle	2.37E-25	rejected	Native	K9me3	SASA	0	rejected	Native	K27me3	Rg (tail2; nuc1)	4.87E-50	rejected
					Native	K27me3	SASA	0	rejected	Native	K9me3	Rg (tail1; nuc2)	0.00E+00	rejected
Native	K9me3	Rg	0	rejected	Native	K9me3	HBond	1.63E-05	rejected	Native	K27me3	Rg (tail1; nuc2)	0.00E+00	rejected
Native	K27me3	Rg	0	rejected	Native	K27me3	HBond	5.58E-78	rejected	Native	K9me3	Rg (tail2; nuc2)	2.61E-126	rejected
Native	K9me3	SASA	0	rejected	Native	K9me3	End-to-End	0.00E+00	rejected	Native	K27me3	Rg (tail2; nuc2)	5.01E-28	rejected
					Native	K27me3	End-to-End	0.00E+00	rejected					
Native	K27me3	SASA	0	rejected						Native	K9me3	Hbonds (tail1;nuc2;DNAnuc2)	2.92E-08	rejected
										Native	K27me3	Hbonds (tail1;nuc2;DNAnuc2)	1.64E-214	rejected
Native	K9me3	Hbonds	4.69E-176	rejected						Native	K9me3	Hbonds (tail2;nuc2;DNAnuc1)	0.00E+00	rejected
Native	K27me3	Hbonds	1.29E-12	rejected	Native	K9me3	Rg	9.60E-50	rejected	Native	K27me3	Hbonds (tail2;nuc2;DNAnuc1)	0.00E+00	rejected
					Native	K27me3	Rg	0.00E+00	rejected	Native	K9me3	Hbonds (tail2;nuc2;DNAnuc2)	0.00E+00	rejected
					Native	K9me3	SASA	0.00E+00	rejected	Native	K27me3	Hbonds (tail2;nuc2;DNAnuc2)	0.00E+00	rejected
Native	K9me3	Rg	2.41E-87	rejected	Native	K27me3	SASA	0.00E+00	rejected					
Native	K27me3	Rg	0	rejected	Native	K9me3	HBond	1.66E-31	rejected					
Native	K9me3	SASA	0	rejected	Native	K27me3	HBond	8.3003e-322	rejected					
Native	K9me3	SASA	0	rejected	Native	K9me3	End-to-End	2.80E-101	rejected					
Native	K27me3	Hbonds	9.56E-06	rejected	Native	K27me3	End-to-End	0	rejected					

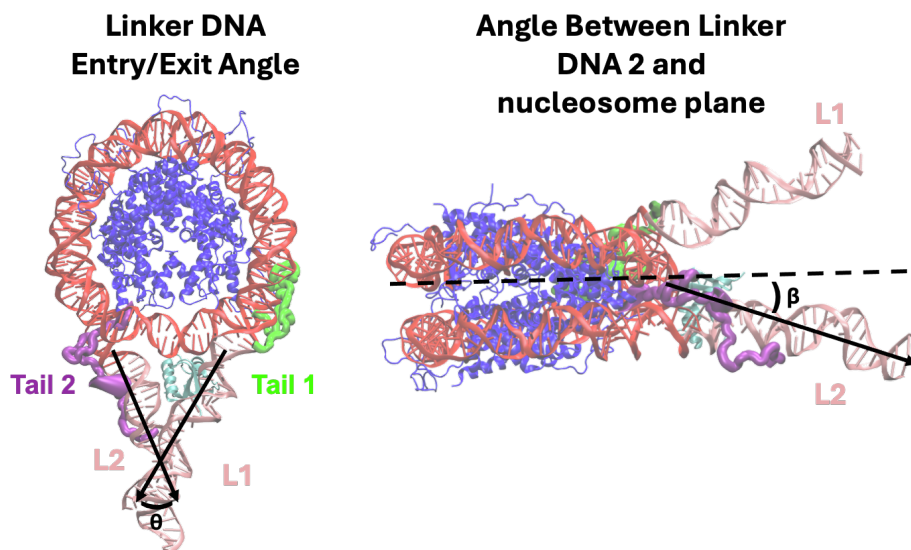


Figure S7. Sketch showing the calculation of the linker DNA entry/exit angle and β angle.

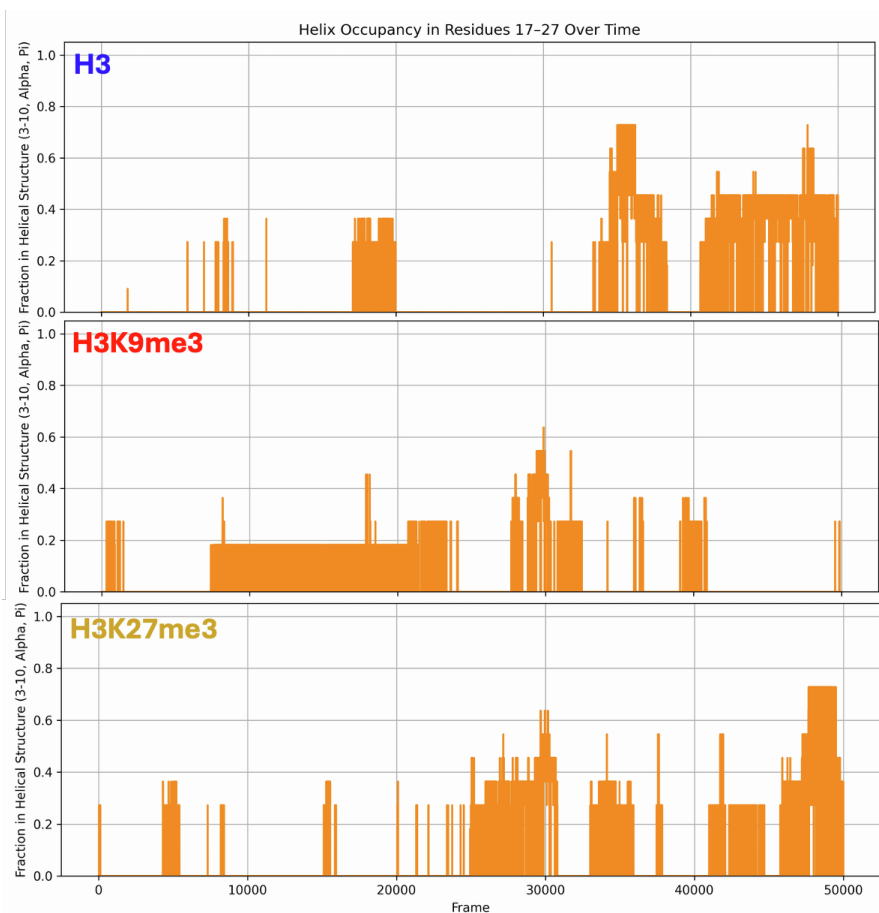


Figure S8. Alpha helix content across a single trajectory for native and methylated H3 tails. We determine the fraction of residues 17 to 27 that are in helix conformation across each frame of a single trajectory.

Table S2. Probability of secondary structure motifs of residues 17 to 27 of native and methylated isolated H3 tails across the 50 MD replicas.

H3residue #	Alpha helix	3--10	Pi	Turn	Bend	Extended	Bridge
17	0.3716	0.0206	0	0.1036	0.1043	0.0077	0.0153
18	0.4236	0.0385	0	0.1043	0.155	0.0077	0.0096
19	0.4283	0.0439	0	0.0939	0.107	0.0082	0.021
20	0.4336	0.0382	0	0.1063	0.1011	0.0067	0.0076
21	0.3692	0.0239	0	0.1206	0.1674	0.0096	0.0035
22	0.3142	0.0124	0	0.0745	0.2171	0.0139	0.0202
23	0.4293	0.028	0	0.1196	0.1656	0.0137	0.0072
24	0.415	0.0291	0	0.125	0.1671	0.0068	0.0032
25	0.3728	0.0355	0	0.1323	0.1233	0.0029	0.0084
26	0.3227	0.0306	0	0.1512	0.1536	0.0097	0.0134
27	0.2279	0.0218	0	0.1964	0.2156	0.0165	0.0172
H3K9me3 residue #	Alpha helix	3--10	Pi	Turn	Bend	Extended	Bridge
17	0.4358	0.0258	0	0.0935	0.0744	0.0126	0.0166
18	0.4763	0.0297	0	0.0999	0.1011	0.014	0.0158
19	0.499	0.0352	0.0001	0.0968	0.0787	0.0099	0.0133
20	0.4888	0.028	0.0001	0.1209	0.0933	0.0053	0.0038
21	0.432	0.026	0.0001	0.1273	0.1514	0.004	0.0056
22	0.3724	0.018	0	0.0965	0.1922	0.006	0.0095
23	0.4254	0.0269	0.0001	0.1661	0.1361	0.0068	0.0057
24	0.3965	0.0257	0.0001	0.1318	0.1581	0.0064	0.0089
25	0.338	0.0307	0.0001	0.1321	0.1301	0.0035	0.0064
26	0.2766	0.0277	0	0.1529	0.1574	0.0047	0.0086
27	0.1797	0.0213	0	0.2239	0.2311	0.0152	0.0164
H3K27me3 residue #	Alpha helix	3--10	Pi	Turn	Bend	Extended	Bridge
17	0.4092	0.0265	0	0.1083	0.0856	0.0213	0.0129
18	0.4475	0.0346	0	0.1008	0.1322	0.0226	0.0128
19	0.4577	0.0464	0	0.1026	0.0954	0.006	0.0115
20	0.4648	0.0373	0	0.1278	0.1023	0.0049	0.0092
21	0.4019	0.0278	0	0.1293	0.1618	0.0124	0.007
22	0.3474	0.0143	0	0.0685	0.1708	0.0256	0.0229
23	0.3526	0.0337	0	0.1345	0.1557	0.0257	0.0132
24	0.3038	0.0367	0	0.1548	0.1741	0.0104	0.014
25	0.2352	0.0364	0	0.1597	0.1497	0.0059	0.0182
26	0.1709	0.0151	0	0.1163	0.2295	0.0099	0.0089
27	0.0889	0.0051	0	0.1642	0.3022	0.0155	0.0092

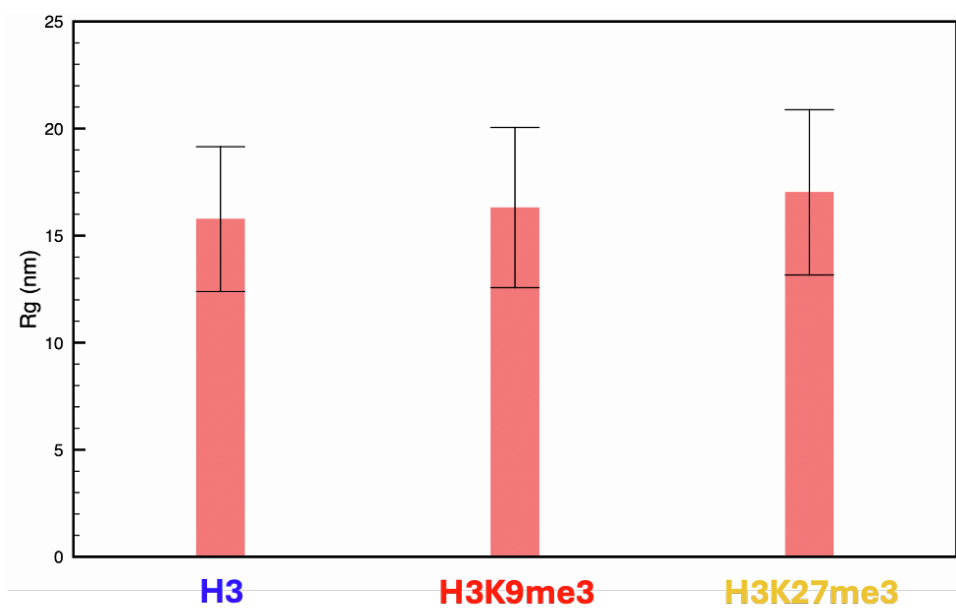
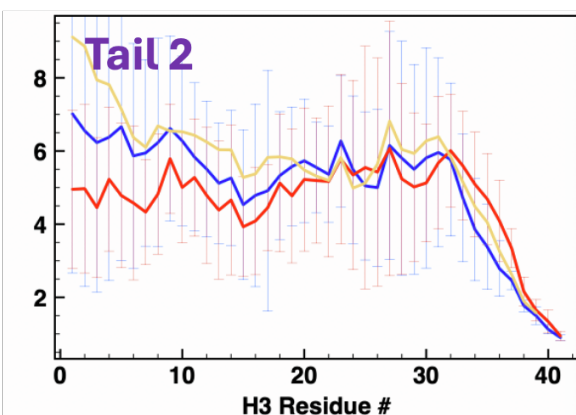
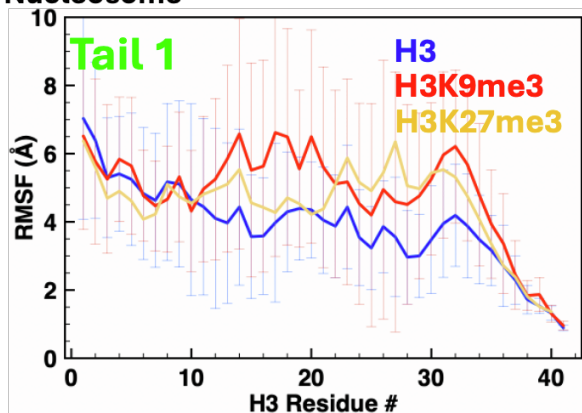
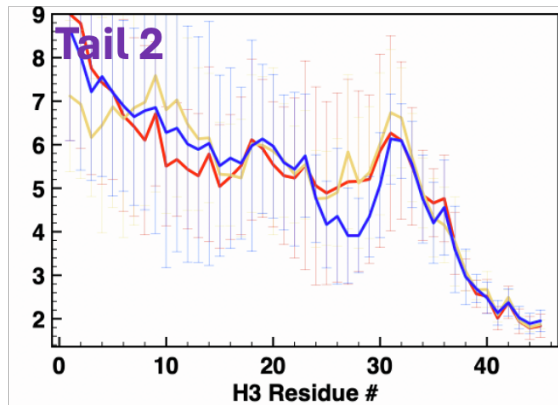
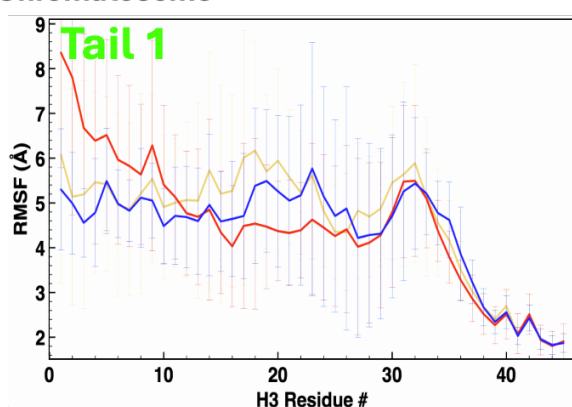


Figure S9. Average Rg for isolated H3 tails in native form and methylated on K9 or K27.

Nucleosome



Chromatosome



Stacked nucleosome

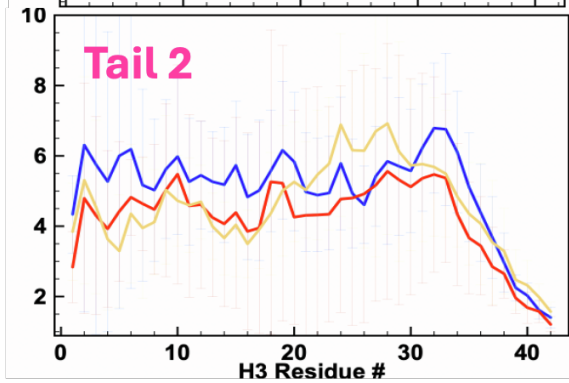
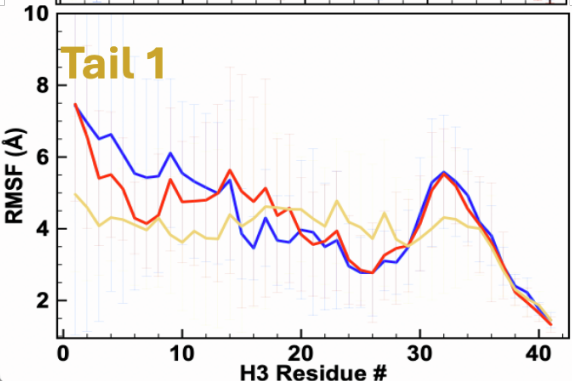
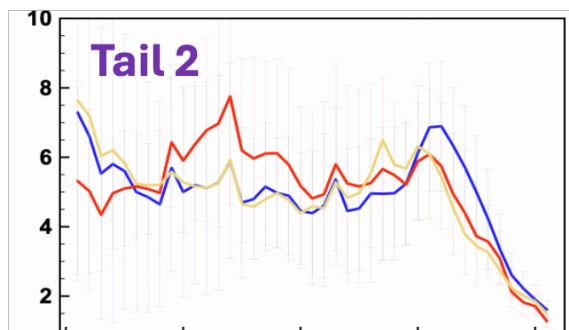
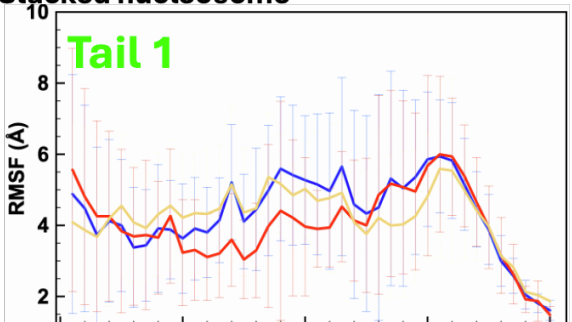
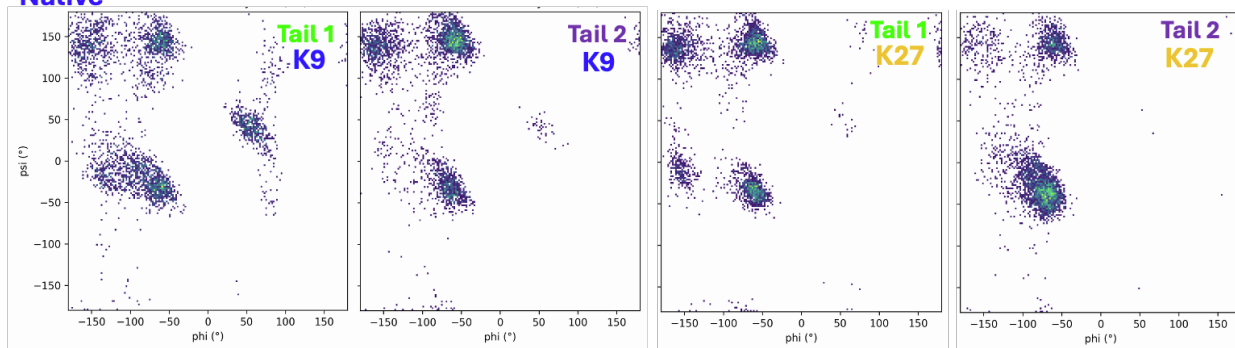


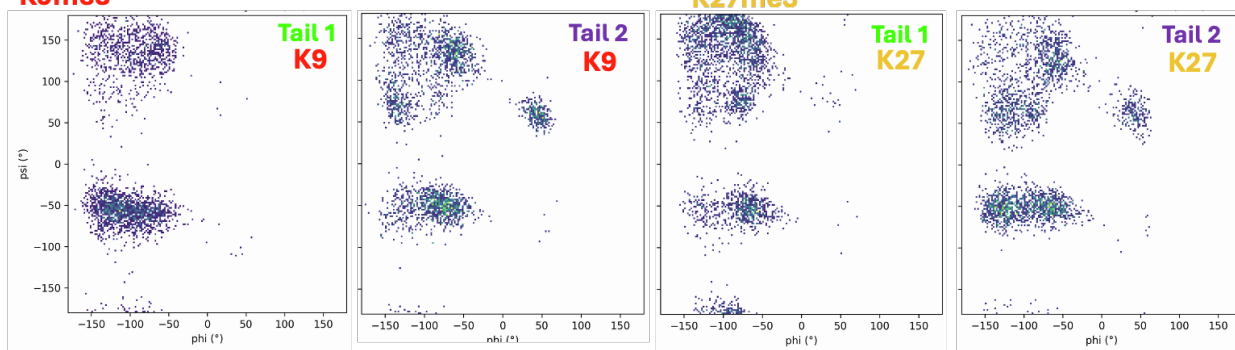
Figure S10. Average RMSF calculated for 6 replicas for the nucleosome, chromatosome, and stacked nucleosome systems.

Nucleosome

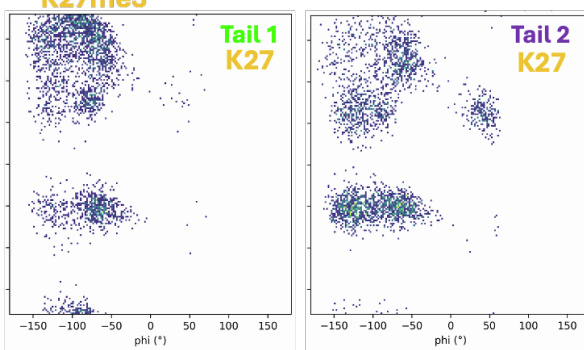
Native



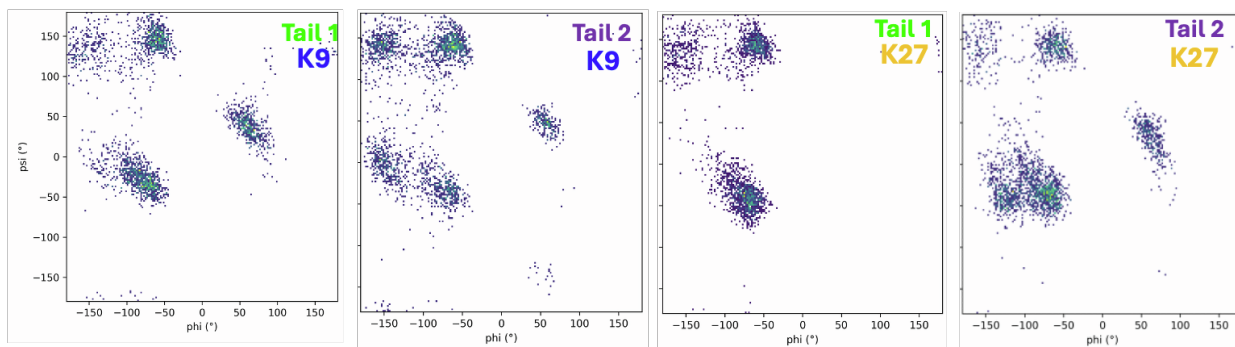
K9me3



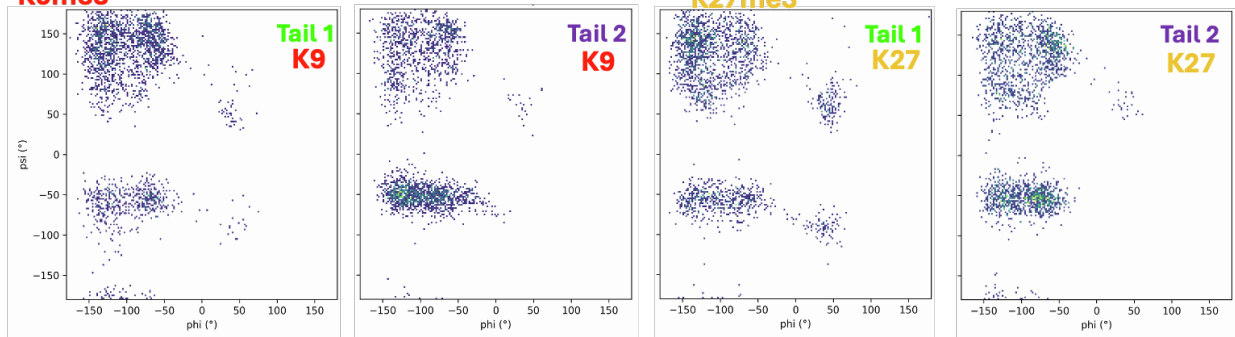
K27me3



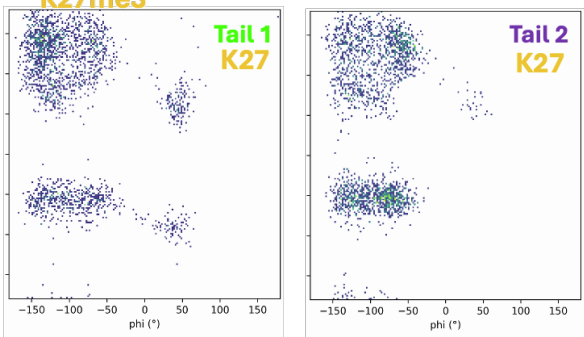
Chromatosome



K9me3



K27me3



Stacked Nucleosomes

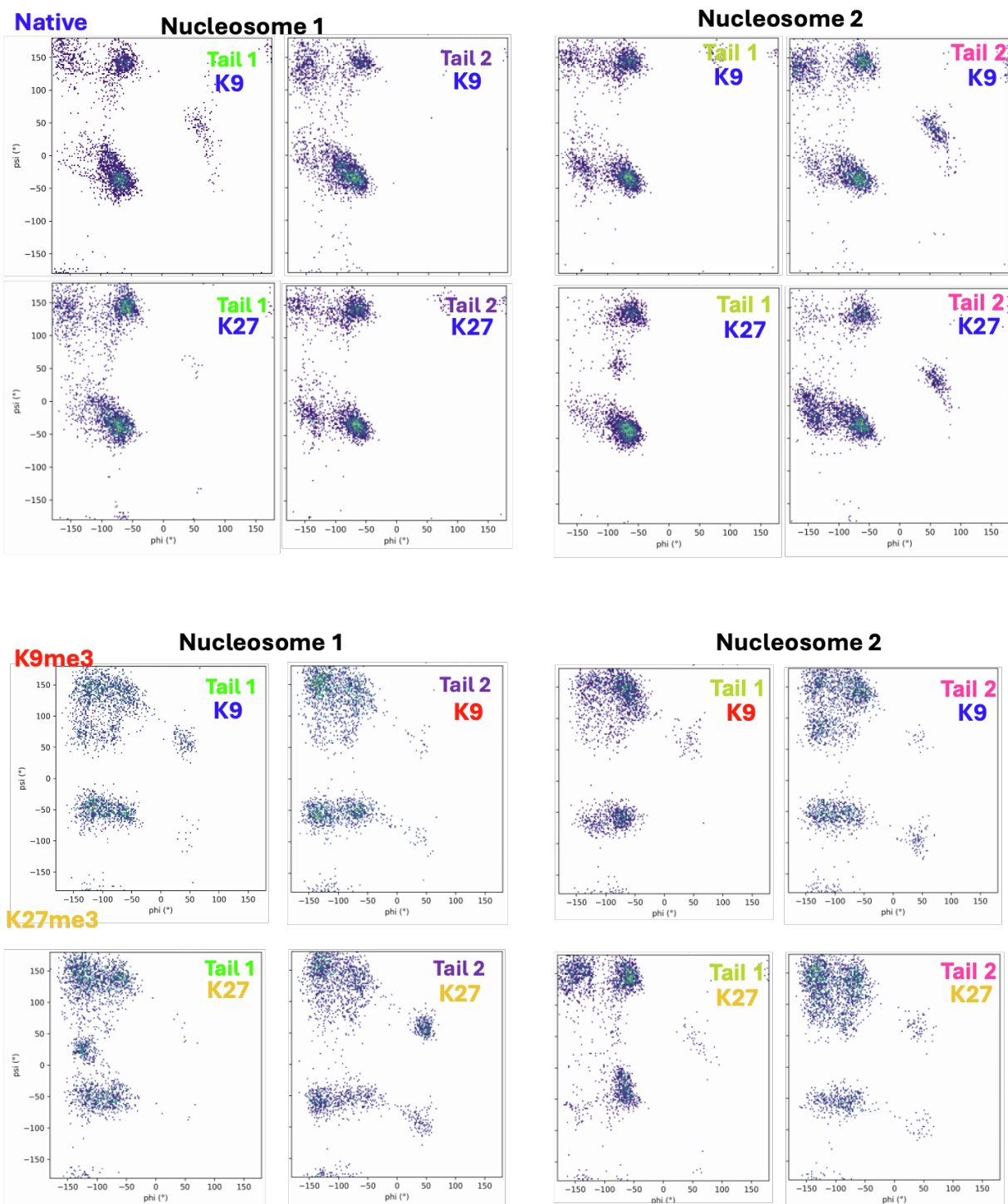


Figure S11. Ramachandran plots for residues K9 and K27 in the in the nucleosome, chromatosome, and stacked nucleosomes with native and K9me3 and K27me3 H3 tails.

Chromosome

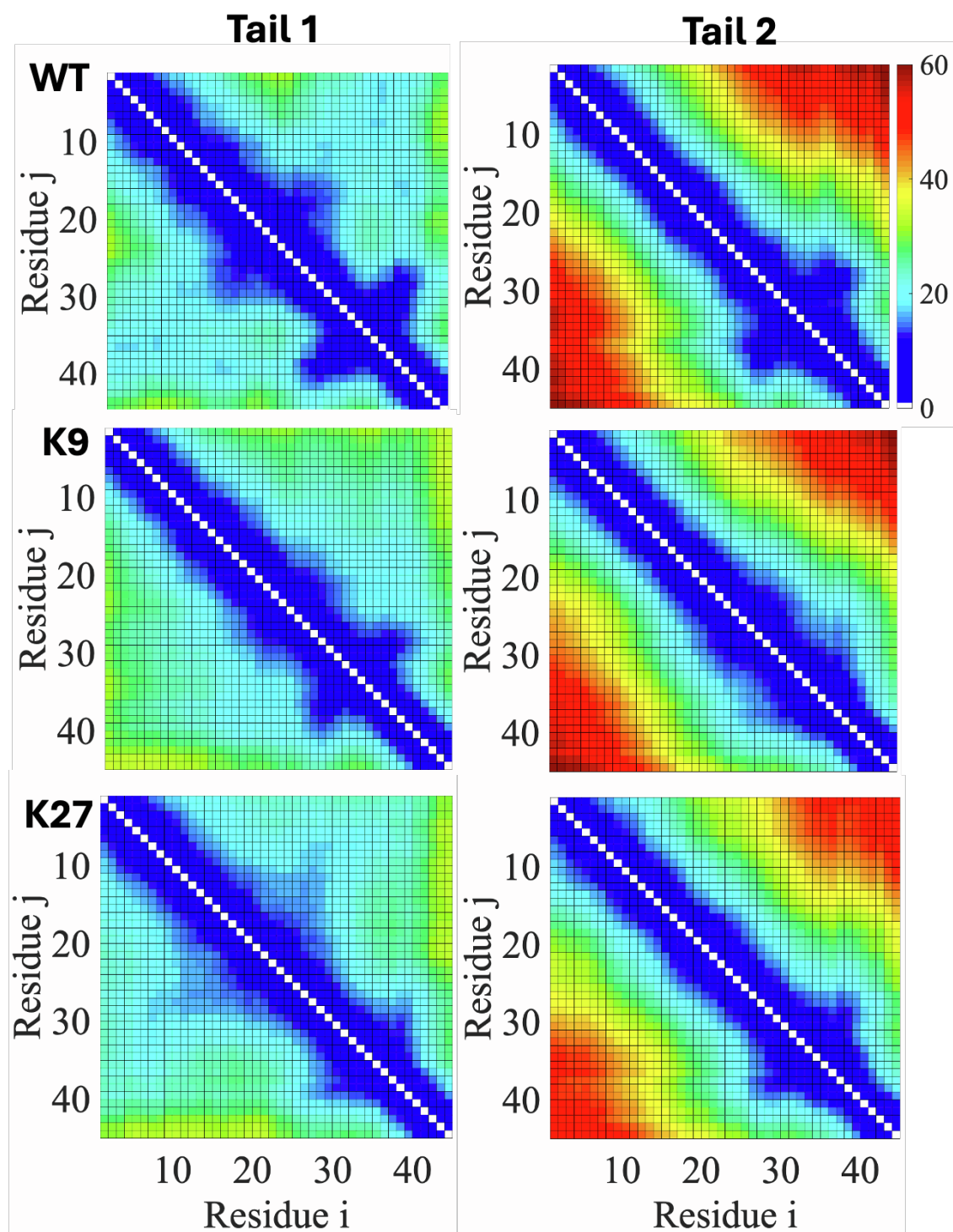


Figure S12. Contact matrices depicting $C\alpha$ - $C\alpha$ distances across all residues for the Tail1 and Tail2 of native and methylated chromosomes.

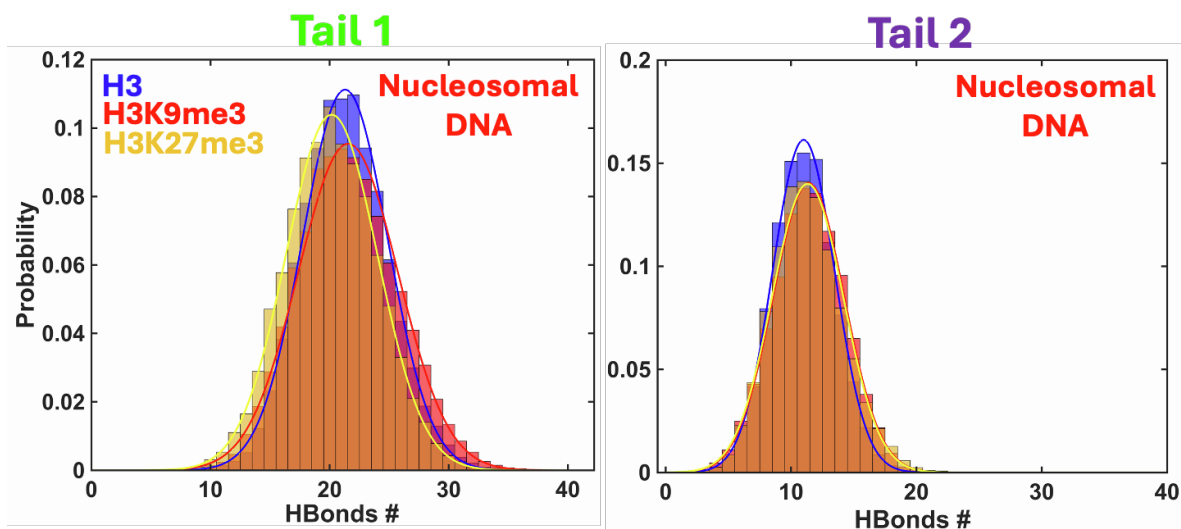


Figure S13. Number of hydrogen bonds (HBonds) between the tail 1 or tail 2 and the nucleosomal DNA of the chromosome.

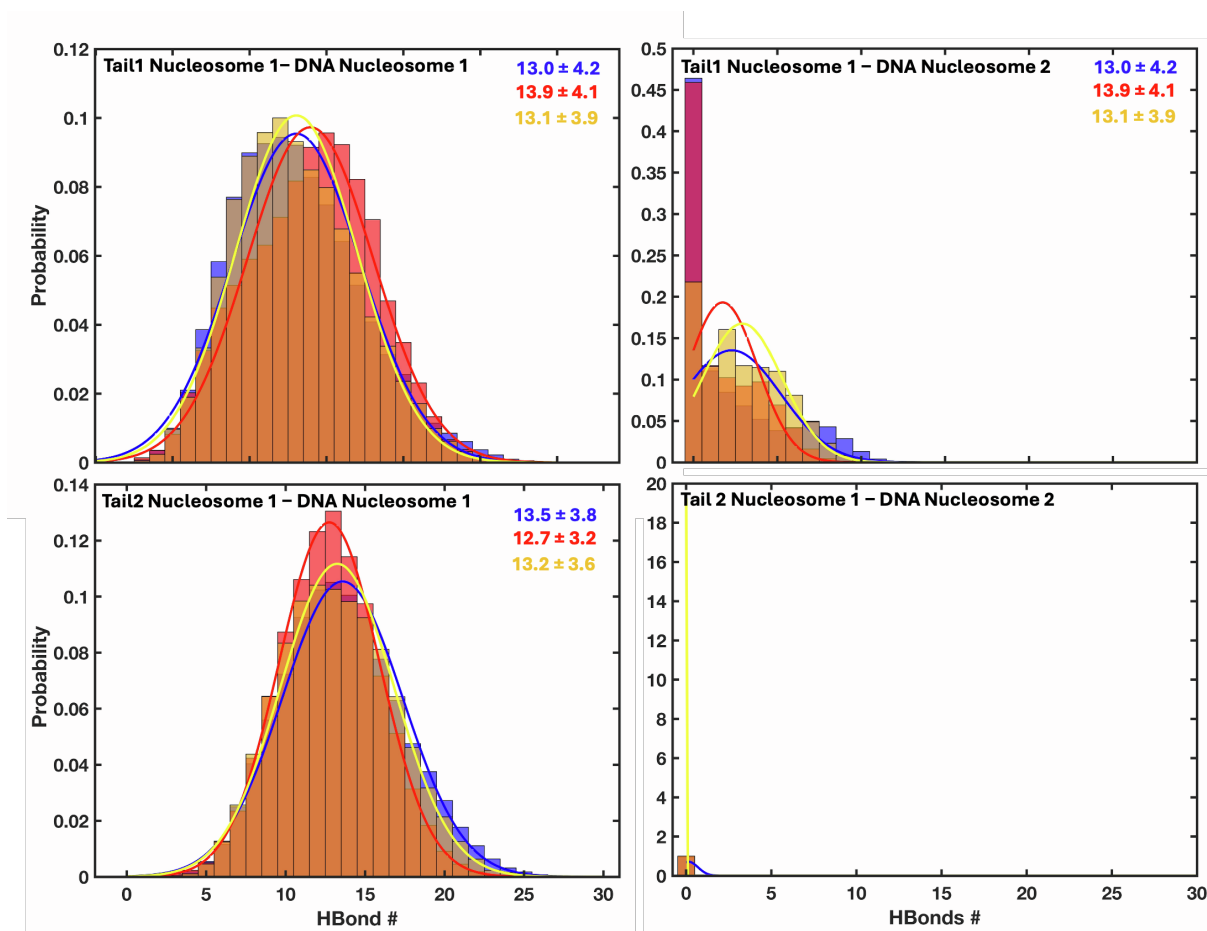


Figure S14. Number of hydrogen bonds (HBonds) between the tail 1 or tail 2 of nucleosome 1 of the stacked nucleosome system and the nucleosomal DNA of nucleosome 1 and nucleosome 2.