**Supplementary Table 1: Comparison between 20 ns [Ref. 19] and 100 ns nucleosome trajectories**

<table>
<thead>
<tr>
<th></th>
<th>20 ns</th>
<th>100 ns</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intact nucleosome simulation</td>
<td></td>
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</tr>
<tr>
<td>Backbone RMSD</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H3(1)</td>
<td>~ 1.2 Å</td>
<td>1.31 ± 0.13 Å</td>
</tr>
<tr>
<td>H3(2)</td>
<td></td>
<td>1.32 ± 0.13 Å</td>
</tr>
<tr>
<td>H4(1)</td>
<td>~ 0.8 Å</td>
<td>1.32 ± 0.16 Å</td>
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<tr>
<td>H4(2)</td>
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<td>1.15 ± 0.19 Å</td>
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<tr>
<td>H2A(1)</td>
<td>~ 2.1 Å</td>
<td>1.41 ± 0.16 Å</td>
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<tr>
<td>H2A(2)</td>
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<td>1.50 ± 0.19 Å</td>
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<tr>
<td>H2B(1)</td>
<td>~ 0.9 Å</td>
<td>1.56 ± 0.24 Å</td>
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<tr>
<td>H2B(2)</td>
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<td>1.37 ± 0.17 Å</td>
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<tr>
<td>Conservation of protein secondary</td>
<td>x</td>
<td>α-helices formation in H3 and H2B tail during simulation</td>
</tr>
<tr>
<td>structure</td>
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</tr>
<tr>
<td>DNA RMSD</td>
<td>~ 2.5 Å</td>
<td>3.2 ± 0.17 Å</td>
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<tr>
<td>DNA backbone conformation</td>
<td>B1 type</td>
<td>B1 type</td>
</tr>
<tr>
<td>Tail-truncated simulations</td>
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<tr>
<td>Structural changes in the H2A2α3</td>
<td>x</td>
<td>Structural changes in the sidechain hydrogen bonding Arg81 and Arg88 are observed in H3 and H2A tail-truncated simulations</td>
</tr>
<tr>
<td>domain</td>
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<tr>
<td>Change of interaction between the H2A docking domain and contact residues</td>
<td>x</td>
<td>Interaction changes observed in H3 and H2A tail-truncated simulations.</td>
</tr>
</tbody>
</table>