<table>
<thead>
<tr>
<th>Simulation</th>
<th>Proteins</th>
<th>Duration (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>tal-sol-AT</td>
<td>F0-F1-F2-F3 (loop-res: 134-172; simulation in aqueous solution)</td>
<td>2x100</td>
</tr>
<tr>
<td>tal-h2F0-CG</td>
<td>F0-F1-F2-F3 (loop-res: 134-172/helix-res:154-167; conformation derived from the tal-sol-AT simulations)</td>
<td>5x1500</td>
</tr>
<tr>
<td>tal-h2F0pc-CG</td>
<td>F0-F1-F2-F3 (loop-res: 134-172/helix-res:154-167; conformation derived from the tal-sol-AT simulations)</td>
<td>5x1500</td>
</tr>
<tr>
<td>tal-lF0F1-CG</td>
<td>F0-F1-F2-F3 (loop-res: 134-172; conformation derived from the tal-sol-AT simulations)</td>
<td>5x1500</td>
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<tr>
<td>tal-l25-CG</td>
<td>F0-F1-F2-F3 (loop-res: 134-172; harmonically restrained 25 kJ/mol/Å²)</td>
<td>5x1000</td>
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<tr>
<td>tal-l50-CG</td>
<td>F0-F1-F2-F3 (loop-res: 134-172; harmonic restrained 50 kJ/mol/Å²)</td>
<td>5x1000</td>
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<tr>
<td>tal-l4E-CG</td>
<td>F0-F1-F2-F3 (loop-res: 134-172 [4E])</td>
<td>5x1000</td>
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<tr>
<td>tal-lK324D-CG</td>
<td>F0-F1-F2-F3 (loop-res: 134-172 [K324D])</td>
<td>5x1000</td>
</tr>
<tr>
<td>tal-h2F0-AT</td>
<td>F0-F1-F2-F3 (loop-res: 134-172/helix-res:154-167)</td>
<td>3x45</td>
</tr>
</tbody>
</table>

In all simulations a POPC/POPG bilayer (ratio 3:2) was used, with the exception of the tal-h2F0pc-CG where a POPC bilayer was used.