Table S3. Sizes of simulated systems.

<table>
<thead>
<tr>
<th>System</th>
<th>With Ca^{2+}</th>
<th>Without Ca^{2+}</th>
<th>Number of atoms</th>
<th>Number of counterions (Na^+)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMBER</td>
<td>28,951</td>
<td>31,382</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>CHARMM</td>
<td>31,750</td>
<td>31,382</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>GROMOS</td>
<td>34,627</td>
<td>28,559</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>Crystal mimic</td>
<td>586,592</td>
<td></td>
<td>88</td>
<td></td>
</tr>
<tr>
<td>Glycosylated</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Full glycosylation</td>
<td>88,194</td>
<td></td>
<td>14</td>
<td></td>
</tr>
<tr>
<td>Minimal glycosylation</td>
<td>65,078</td>
<td></td>
<td>8</td>
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</tr>
</tbody>
</table>