Developing a computational model that accurately reproduces the structural features of a dinucleoside monophosphate unit within B-DNA

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Electronic Supplementary Information (ESI)

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<td></td>
</tr>
<tr>
<td></td>
<td>170.4</td>
<td>172.2</td>
<td>171.3</td>
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<tr>
<td>(P^3)</td>
<td>174.4 180.6</td>
<td>167.3 157.8</td>
<td>173.0 166.2</td>
<td>144–190(^c)</td>
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<tr>
<td></td>
<td>176.7</td>
<td>167.0</td>
<td>173.5</td>
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\(^a\) See Figure 2 for definitions of backbone torsion angles. \(^b\) See Ref. 113. \(^c\) See Ref. 72. \(^d\) Due to SCF convergence issues, structures were obtained using M06-2X-optimized structures as input rather than the standard HyperChem-generated structures.
Table ESI–4: Comparison of the 6-31G(d,p) and 6-31+G(d,p) backbone torsion angles (°), pseudorotation phase angles (P, °) and the angle between nucleobase planes (φ, °) for the 5′–GT–3′ sequence calculated in the gas-phase and water with M06-2X for the anionic and counterion phosphate models, as well as the average value (Exp.) and standard deviation (SD) obtained from experiment.

<table>
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<tr>
<th></th>
<th>Anionic 6-31+G(d,p)</th>
<th>Anionic 6-31G(d,p)</th>
<th>Counterion 6-31+G(d,p)</th>
<th>Counterion 6-31G(d,p)</th>
<th>Exp.  (^b)</th>
<th>SD  (^b)</th>
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<td>150.2</td>
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<td>167.2</td>
<td>162.6</td>
<td>162.4</td>
<td>202.8</td>
<td>154.4</td>
<td>160.3</td>
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<tr>
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<td>279.4</td>
<td>272.6</td>
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<td>276.6</td>
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<td>49.1</td>
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\(^a\)See Figure 2 for definitions of backbone torsion angles. \(^b\)See Ref. 113. \(^c\)See Ref. 72.