



**Figure 3a, b.** Wedge-roll values for the various base-pair steps in crystal structures of (a) octamer d(GGCCGGCC) in A-form and (b) dodecamer d(CGCGAATTCGCG) in B-form (native). '+' The reported values<sup>2</sup>. ' $\Delta$ ' The values calculated using equation (13). The root-mean-square deviations between the calculated and the reported values are  $0.28^\circ$  and  $0.36^\circ$  for the A-DNA and B-DNA structures respectively. ' $\diamond$ ' The values calculated using the approximation  $\Theta_R = \Theta_{y2} - \Theta_{y1}$ , large deviations from the reported values are seen in this case.

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