

23. STRUCTURAL ANALYSIS AND CLASSIFICATION

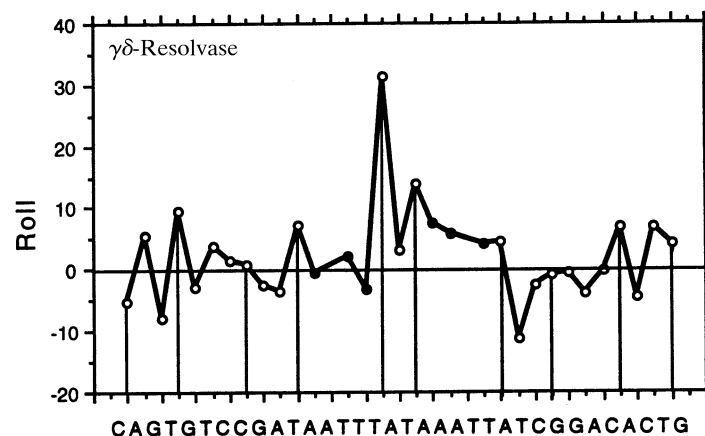
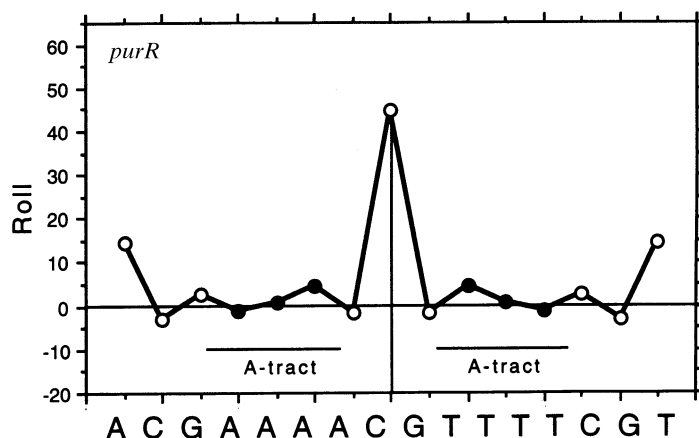
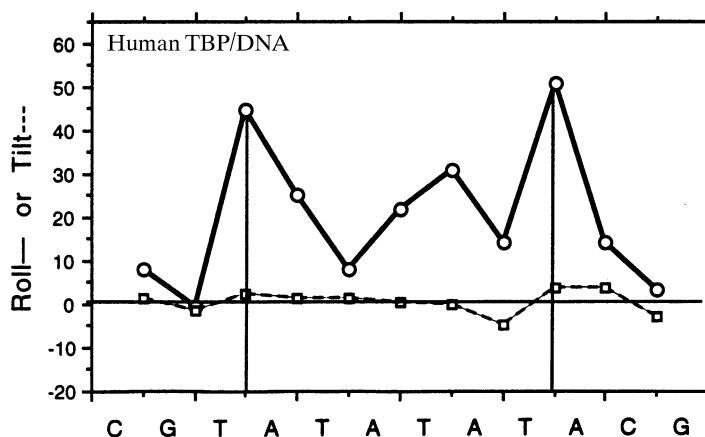
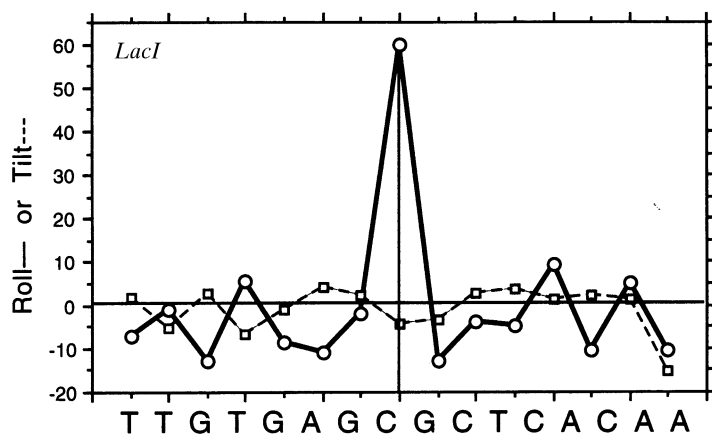


Fig. 23.3.4.6. Roll-angle plots for sequence-specific DNA–protein complexes with *lacI* (top) and *purR* (bottom). In each case, bending occurs via localized roll at a C–G step. Other steps of the sequence have random rolls of ca 10° or less. Note that, as with IHF, A-tracts are especially straight and unbent. Dashed lines in the *lacI* plot demonstrate the unimportance of tilt in production of helix bending.

Fig. 23.3.4.7. Bending via roll at T–A steps in TBP or the TATA-binding protein (top) and in  $\gamma\delta$ -resolvase (bottom). Note that not every T–A step in TBP or  $\gamma\delta$ -resolvase is necessarily bent. Note also in  $\gamma\delta$ -resolvase that C–A = T–G steps, which in proteins such as CAP are used to generate sharp roll bends, here, frequently, are local roll maxima, even though they contribute little to the overall bending. They have a bending potential that is not used in this particular setting.

Table 23.3.4.2. Sequence-dependent differential deformability in B-DNA. II. The Minor Canon

These generalizations are illustrated by Fig. 23.3.4.9, and are justified at greater length by El Hassan & Calladine (1997) and Dickerson (1998a,b,c).

(6) Heterogeneous steps ending in A: C–A, T–A and G–A

Steps ending in adenine, aside from A–A, tend to display (a) negative correlation between slide and roll, and between twist and roll, and (b) positive correlation between slide and twist.

(7) Purine–pyrimidine steps

R–Y steps display, on average, a systematic preference for negative slide and for twist below 36°.

(8) Relative step frequencies in sequence-specific protein–DNA complexes

Step A–A is the most common of all, and in 55% of the cases it occurs within A-tracts.

Steps containing only GC base pairs are least common, and seemingly are less compatible with formation of sequence-specific protein complexes.

(9) Local environment and DNA behaviour

Sequence-dependent local helix deformations are quite similar in DNA crystals and in protein–DNA complexes. DNA molecules packed against proteins in their normal biological environment appear to have more in common with DNA packed against other DNA helices in the crystal than with free DNA in solution.