

23. STRUCTURAL ANALYSIS AND CLASSIFICATION

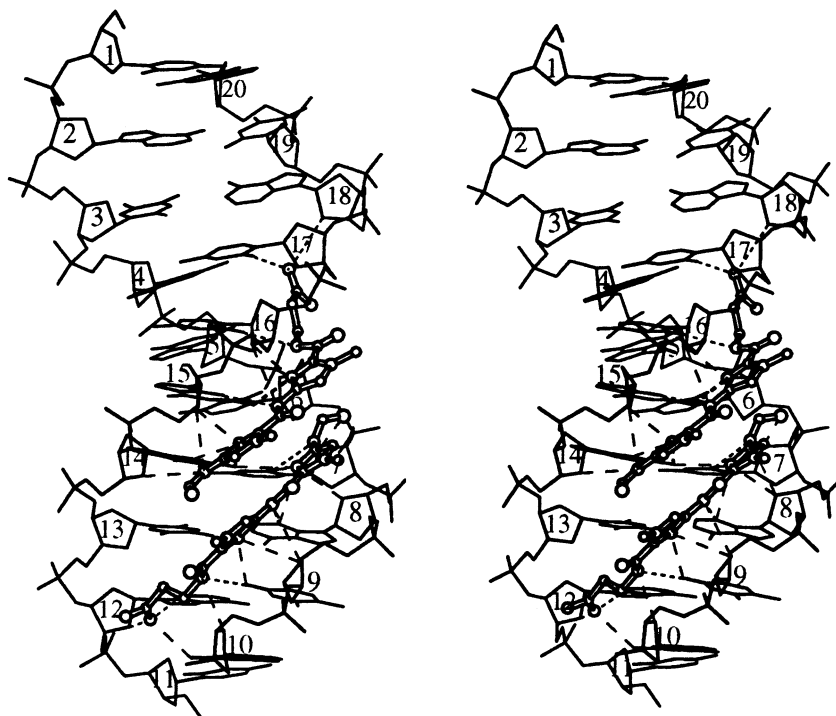
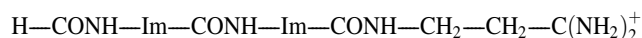


Fig. 23.3.4.4. Structure of the 2:1 complex of a di-imidazole lexitropsin with C-A-T-G-G-C-C-A-T-G (B108). The drug now is represented by



where Im is a five-membered imidazole ring, or again more compactly by  $^0\text{Im}=\text{Im}=\text{Im}^+$ . The uncharged leading amide group, characteristic of distamycins, is identified by  $^0$ . Distamycin itself would be represented in this shorthand notation by  $^0\text{Py}=\text{Py}=\text{Py}=\text{Py}^+$ . Reprinted from B108, copyright (1977), with permission from Excerpta Medica Inc.

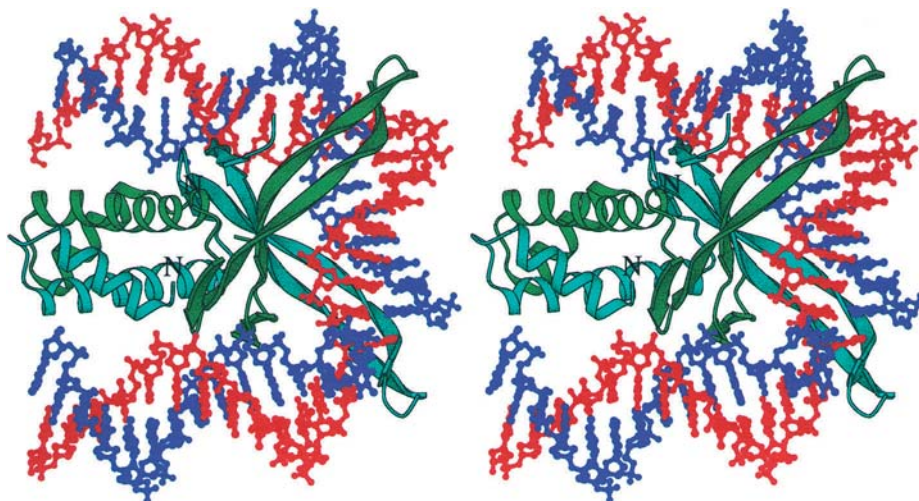


Fig. 23.3.4.5. DNA duplex (red and blue strands) looped around IHF or integration host factor. The two subunits of the IHF duplex are green and turquoise. Two antiparallel loops of protein chain, one from each subunit, insert into the minor groove of B-DNA at the sequence C-A-A-T/A-T-T-G and produce abrupt bends *via* local roll angles of  $60^\circ$ . The two localized bends are additive because they occur one helical turn apart. All other steps have roll angles of  $5^\circ$  or less. The two flanking helix segments pack against the IHF dimer and must be kept straight and unbent. This is accomplished in one of the two segments by an A-tract of sequence C-A-A-A-A-A-G. From Dickerson & Chiu (1997). Coordinates courtesy of P. Rice.