Structural Prediction of A- and B-DNA Duplexes Based on Coordinates of the Phosphorus Atoms

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ABSTRACT The sequence-dependent structure of DNA double helices was studied extensively during the past 10 years. How the backbone structure correlates with the base structure in a duplex conformation is still an important yet open question. Using a set of reduced coordinates and a least-squares fitting procedure, we have developed a method to predict structures for B-DNA duplexes based on coordinates of the phosphorus atoms. This method can be used to predict all-atom structures for both bent and straight molecules. We estimated the accuracies of the predictions by studying a set of 10 oligonucleotides with their structures available from the Protein Data Bank. We used this method to construct a modeled structure for the bacteriophage λ cro operator for which the phosphorus coordinates were known from 3.5-Å resolution crystal data (4CRO).

INTRODUCTION

Since the high-resolution single-crystal data for B-DNA duplexes became available (Wing et al., 1980; Dickerson and Drew, 1981; Fratini et al., 1982), the sequence-dependent structures of DNA has been studied extensively (e.g., Lysov et al., 1979; Calladine, 1982; Kabsch et al., 1982; Tung and Harvey, 1986; Srinivasan et al., 1987; Sarai et al., 1988). Contrary to the traditional view (Watson and Crick, 1953) in which all DNA molecules assume a uniform double-helical conformation regardless of their sequences, structural variations were observed from both crystal (Dickerson and Drew, 1981) and solution (Peck and Wang, 1981; Rhodes and Klug, 1981) data. Intrinsic bending (Wu and Crothers, 1984; Hagerman, 1985) is a classical example of a DNA duplex having a structure that significantly deviates from the canonical B conformation (Arnott and Hukins, 1972) as a direct consequence of the sequence. The sequence-dependent structure of DNA duplexes is a very attractive idea. It provides additional mechanisms for molecular recognition. For example, DNA molecules with little sequence homology may share a similar structural motif that can be recognized by DNA-binding molecules such as protein and drug (Tung and Harvey, 1987).

Because of the involvement of the six torsional angles (α, β, γ, δ, ϵ, ζ; Seeman et al., 1976) plus the flexibility in the sugar ring and the glycosidic angle, the sugar-phosphate backbone of the DNA duplex is generally considered very flexible. Whether there is a direct correlation between the structure of the flexible sugar–phosphate backbone and the structure of the bases is still an open question. However, there are experimental observations that support the notion that the structure of the sugar–phosphate backbone is driven by the structure of the bases in DNA duplexes. For example, narrowed minor groove width is a direct consequence of the large propeller twist angles inherent in the A-tract structure (Nelson et al., 1987). The alternating purine–pyrimidine dimer building blocks in left-handed Z-DNA structures give rise to a zigzag backbone pattern (Rich et al., 1984). A B_{II} type of backbone is associated with large twist angles (Dickerson, 1988). Based on model building studies and analyses of crystal structure data, it was found that both minor groove width and depth are strongly correlated with base-pair (bp) slide (Bhattacharyya and Bansal, 1992). Our unpublished data also show that one can control the minor groove width of B-DNA duplexes by changing the bp parameters (Dickerson et al., 1989) such as twist angle (Ω), roll angle (ρ), and tilt angle (τ). All these results indicate that there is a direct correlation between the structure of the bases and the structure of the backbone in a B-DNA duplex.

There are low-resolution crystal data of DNA duplexes for which the coordinates of the phosphorus atoms are determined. For example, the 7-Å resolution crystal data of the nucleosomal complex (Struck et al., 1992) revealed the structure of the phosphorus atoms of the 146-bp DNA in the complex. The structure of the phosphorus atoms of a 17-bp operator was determined through the 3.5-Å crystal structure of the bacteriophage λ cro protein DNA complex (Brennan et al., 1986). The phosphorus structure of an 18-bp DNA was available from the crystal structure of the HIV-1 reverse transcriptase/DNA complex solved at 7-Å resolution (Jacobo-Molina et al., 1993). In all three complexes, DNA molecules were significantly bent. The 17-bp operator in the cro complex displayed an overall 46° bent, and the 18-bp DNA in the HIV-1 reverse transcriptase/DNA complex has shown an overall 43° bent. In the nucleosome, the 146-bp DNA is wrapped around the histone core in one and one-half turns of the left-handed superhelix. Apparently, the canonical B-conformation cannot be used to model these DNA duplexes adequately. A method to predict base structures of these molecules based on the phosphorus atoms

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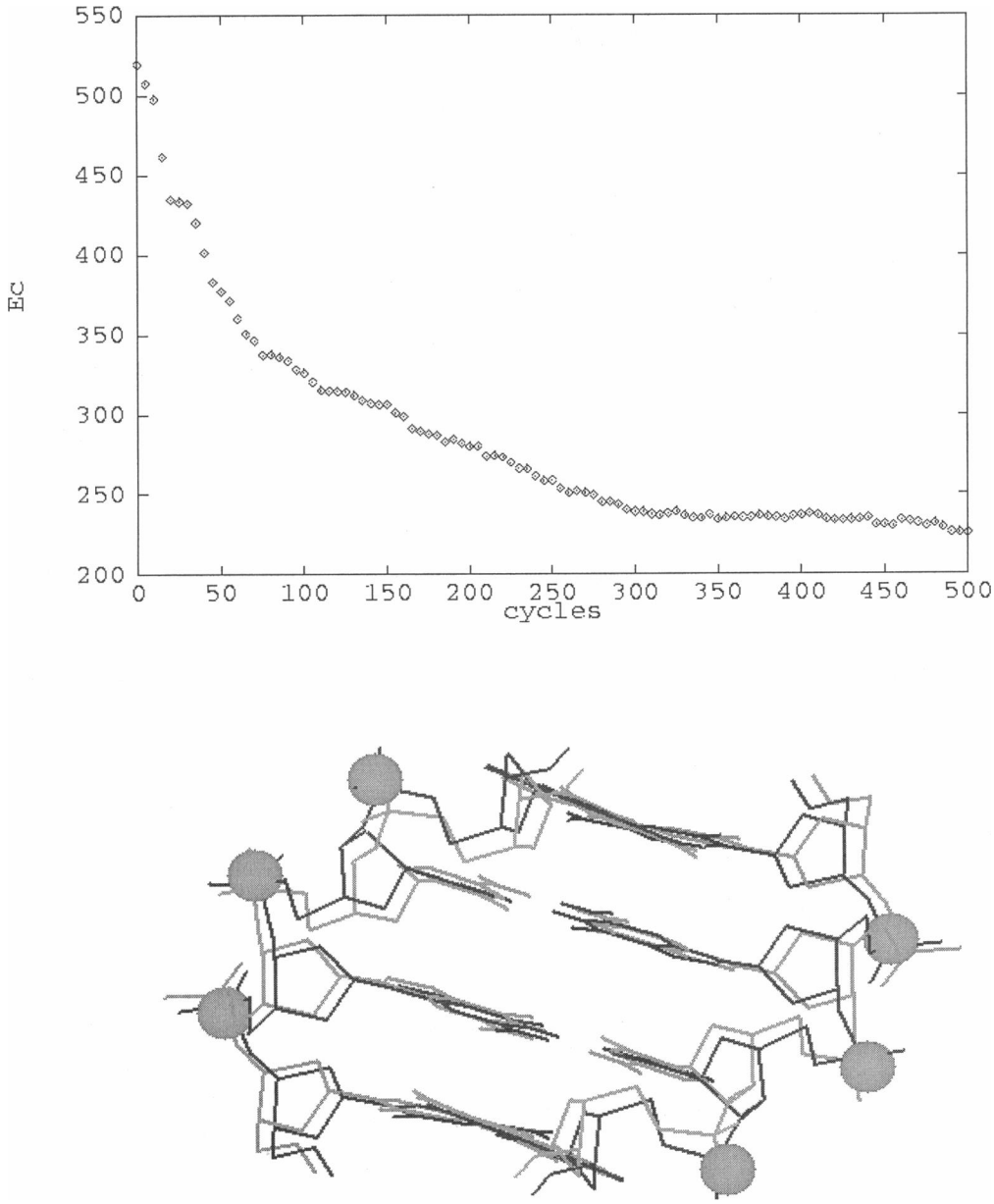

FIGURE 1 Constraint equilibration of a tetramer with a run of 500 cycles of the Metropolis Monte Carlo simulation. The top figure shows the plot of the constraint energy (E_c in kcal/mol) versus cycles of simulation. The initial (*gray*) and the final (*black*) structures of the tetramer are plotted, together with the target phosphorus atoms (*gray spheres*) in the lower part of the figure.

could be very useful in studying the detailed interactions between the DNA and the protein in the complex.

Here, we introduce a computational approach for constructing modeled structures of DNA oligonucleotides in atomic details based on the known coordinates of the phosphorus atoms. This method is first tested on a set of 10 known structures of B-DNA duplexes from the Protein Data Bank (Bernstein et al., 1977). We study the accuracies of the predicted base-and-sugar structures by comparing these structures with the crystal structures. Next, we test the method by constructing the structure of a highly bent 30-bp DNA duplex in the CAP–DNA complex. Finally, this approach is used to predict the structure of the λ cro operator based on the structure of the set of phosphorus atoms as revealed by x-ray crystallography.

MATERIALS AND METHODS

The basic unit used in this approach is a 4-bp duplex (tetramer). The goal is to find the structure of the tetramer with the phosphorus atoms (three consecutive pairs between the four base pairs) match those of the target set. We measure the goodness of fit by calculating the root-mean-square (rms) difference (D_{rms}) between the phosphorus atoms of the tetramer and those

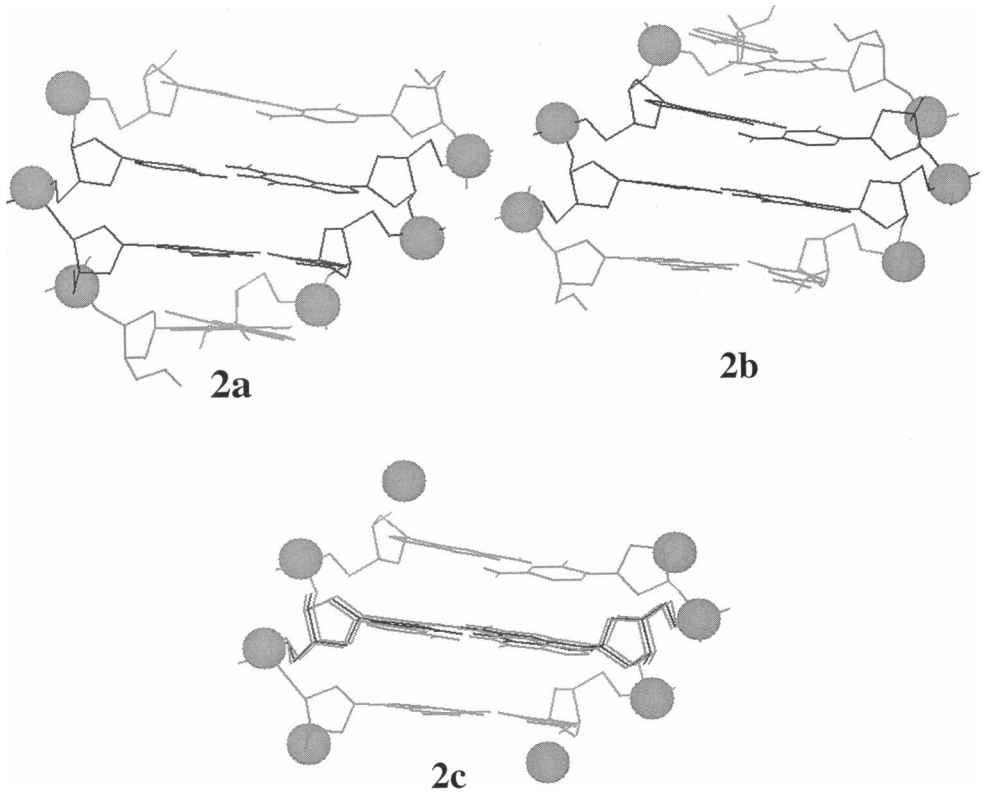

FIGURE 2 Basic fitting procedure. The fitted *n*th tetramer (*stick model*) plus the target phosphorus atoms (*spheres*) are plotted in *a*, and the corresponding $(n + 1)$st tetramer plus the target phosphorus atoms are plotted in *b*. The averaged structure (shown in *c*) of the central bp is deduced from the structure of the third bp of the tetramer in *a* and the structure of the second bp of the tetramer in *b*.

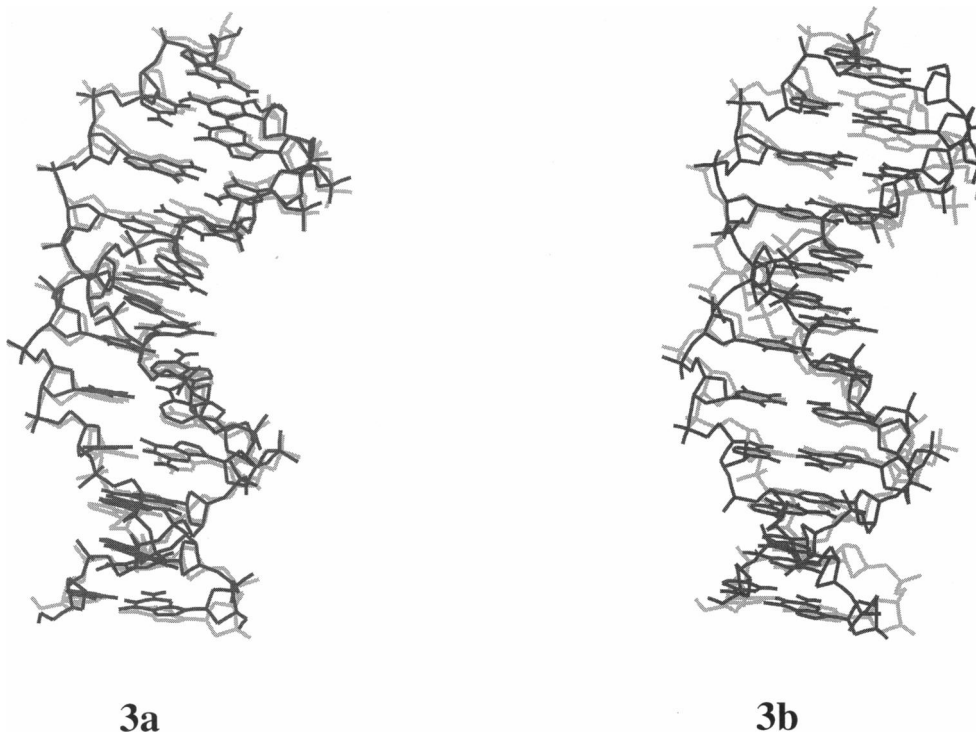

FIGURE 3 Plot of the predicted structure versus the crystal structure of 1BNA. In *a*, the predicted structure (*black*) is plotted against the crystal structure (*gray*). As a comparison, the structure of the dodecamer in a canonical B-conformation (*black*) and the crystal structure (*gray*) are shown in *b*. The D_{rms} is significantly smaller between the two molecules in *a* than that between the two molecules in *b*.

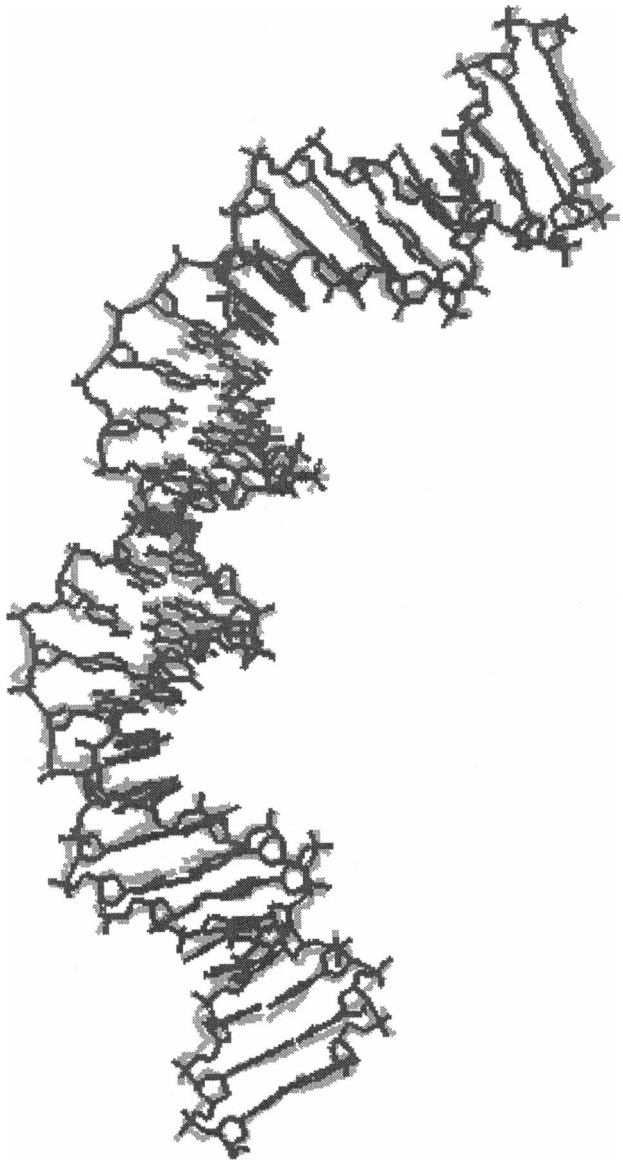

FIGURE 4 Plot of CAP-DNA solved by x-ray crystallography (1CGP, *gray*) and the predicted structure (*black*).

from the target set, using a least-squares superposition method developed by McLachlan (1979). A harmonic constraint energy is introduced as

$$E_c = \frac{1}{2} K_c \sum_{i=1}^{6} (r_i - r_{ti})^2, \quad (1)$$

where $\mathbf{r}_i$ is the coordinate of the ith phosphorus atoms in the tetramer, $\mathbf{r}_{ti}$ is the coordinate of the ith phosphorus atoms in the target set, and K_c is the constraint constant arbitrarily chosen to be 2000 kcal/mol Å^{-2} such that it provides adequate strength for constraining the set of phosphorus atoms to the target set. We model the structure of the tetramer by using a set of reduced coordinates developed in our laboratory (Soumpasis and Tung, 1988; Tung, 1993; Tung et al., 1994). The structure of the tetramer is refined through a short run of Metropolis Monte Carlo simulation (Metropolis et al., 1953) using E_c. During the simulation, all sugar structures (Cremer and Pople, 1975; Garcia and Krumhansl, 1987) are kept at a canonical B-conformation (pseudorotational angle, 160°; out-of-plane distortion, 0.38; glycosidic angle (O1′-C1′-N1/N9-C2/C4), −90°). The orientation (ψ) of the phosphate group (Tung, 1993; O3′(n)-P(n+1)-C5′(n+1)-OM(n+1), where OM is a pseudoatom that lies on the midpoint between the two phosphate oxygens O1P and O2P) is also set to that for the canonical B-conformation (160°). Starting from a canonical B-conformation for all the bases, the structure of the central base pair step (D_x, D_y, D_z, τ, Ω, ρ; Dickerson et al., 1989) plus propeller twist angles (ω) of the central two base pairs are allowed to relax during the simulation. The plot of E_c versus cycles of a Monte Carlo run from a typical simulation is shown at

TABLE 1 Angles for 1BNA

bp Step	Crystal	FITPP	Trifonov's
Twist angles (Ω)			
1	34.9	33.9	29.8
2	38.9	32.9	40.0
3	28.3	32.7	29.8
4	34.6	36.6	36.9
5	38.5	36.4	35.9
6	31.2	34.8	31.5
7	35.4	35.8	35.6
8	42.0	40.5	36.9
9	28.0	35.2	29.8
10	42.0	35.4	40.0
11	38.6	33.9	29.8
Correlation with crystal	–	0.44	0.70
Roll angles (ρ)			
1	7.21	−1.90	6.70
2	−3.30	5.30	−5.00
3	5.30	1.90	6.70
4	6.00	3.20	−2.70
5	1.10	4.80	−6.50
6	−6.40	−0.20	2.60
7	0.90	2.00	−6.50
8	2.70	−4.40	−2.70
9	1.90	0.00	6.70
10	−10.00	−5.00	−5.00
11	−0.90	−4.80	6.70
Correlation with crystal	–	0.25	0.34

TABLE 2 Rms differences (in Å) between modeled structures and crystal structures

Molecule	bps	Phosphorus atoms	Sugar atoms	Base atoms
B-DNA oligomers				
1BNA	12	0.19	0.52	0.42
119D	12	0.24	0.57	0.46
126D	10	0.27	0.62	0.55
167D	10	0.19	0.55	0.34
1CGC	10	0.20	0.62	0.43
1D23	10	0.26	0.52	0.46
1D49	10	0.27	0.53	0.46
1D65	12	0.23	0.50	0.41
1D89	12	0.27	0.75	0.55
1D98	12	0.22	0.56	0.45
Average		0.23	0.57	0.45
σ		0.03	0.07	0.06
Other DNA oligomers				
3ANA	10	0.33	0.56	0.50
113D	12	0.32	0.57	0.49

FIGURE 5 Stereo plot of the crystal structure (4CRO, *gray*) and the predicted structure (*black*) of the bacteriophage λ cro operator.

the top of Fig. 1. There are only eight degrees of freedom involved in the simulation of the tetramer structure; a run of a few hundred cycles of simulation is sufficient to bring the phosphorus atoms of the tetramer to the target set. The lower part of Fig. 1 shows the initial tetramer structure (gray lines) and the final tetramer structure (black lines) superimposed upon the target phosphorus atoms (gray spheres) from this particular run. The rms difference between the phosphorus atoms of the initial structure and the target set is 0.52 Å. After 500 cycles of simulation, the rms difference between the final structure and the target set has been reduced to 0.23 Å.

This basic fitting procedure is applied from one end of the molecule, moving one bp at a time, toward the other end of the molecule, as illustrated in Fig. 2. In Fig. 2 *a*, the first set of target phosphorus atoms was plotted as spheres. The fitted tetramer is plotted as a stick model with black for the central two bps and gray for the two bps at the ends. Moving up one bp, we show the corresponding target set of phosphorus atoms and the fitted tetramer in Fig. 2 *b*. We calculate the structure of the middle bp (plotted in black) in Fig. 2 *c* by taking the average of the structure of the same bp in tetramer 1 (the third bp) and that in tetramer 2 (the second bp).

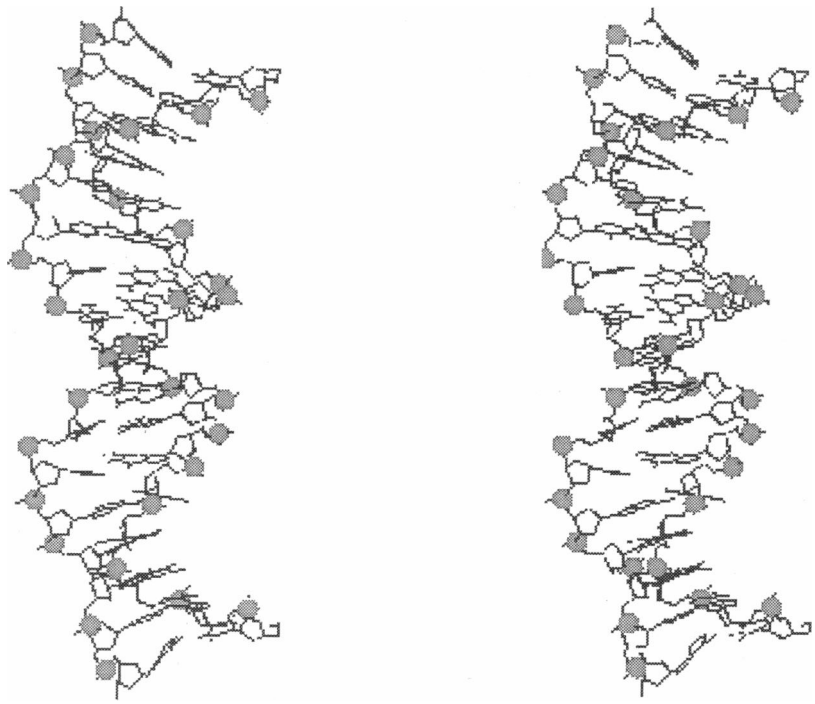

FIGURE 6 Stereo plot of the minimized structure (*black lines*) and the crystal coordinates of the phosphorus atoms (*gray spheres*) of 4CRO. The energy-minimized structure is obtained by running 5000 cycles of constraint minimization, using AMBER starting with the predicted structure.

The structures of the two bps at the extreme of the molecule were taken from the two tetramers that fitted the two sets of phosphorus atoms at the ends of the molecule.

A FORTRAN program (FITPP) has been developed based on the fitting procedure described in the previous paragraphs. FITPP was first tested on a well-known DNA dodecamer (1BNA; Drew et al., 1981). Using the set of crystal coordinates of the phosphorus atoms as input, FITPP calculates the atomic structure of the dodecamer. This fitting procedure is extremely fast. It took 1.1 s CPU time on a SGI INDY workstation to construct the modeled structure for this 12-bp DNA oligomer. Fig. 3 *a* shows the modeled structure (*black*) of the dodecamer superimposed upon the crystal (*gray*) structure. The rms difference between the two sets of phosphorus atoms is 0.19 Å, and the rms differences for the base atoms and the sugar atoms are 0.41 and 0.51 Å, respectively. These numbers are to be compared with 0.75 Å (base atoms), 1.10 Å (sugar atoms), and 1.20 Å (phosphorus atoms) between the dodecamer in a canonical B conformation (*black*) and the crystal structure (Fig. 3 *b*). 1BNA is a slightly bent DNA duplex. By taking into account the structure of the phosphorus atoms, our predicted structure has a significantly lower D_{rms} from the crystal structure than a duplex in a canonical B form.

Table 1 lists twist angles and roll angles of our predicted dodecamer structure together with those for the crystal structure (1BNA) and those according to Trifonov's prediction (Kabsch et al., 1982; Bolshoy et al., 1991). In either case, Trifonov's prediction has a higher correlation with those from the crystal structure than our predicted structure. If one constructs 1BNA structure using parameters (twist, roll, and tilt angles) based on Trifonov's prediction with a sugar-phosphate backbone in a canonical B form, the D_{rms} between the constructed and the crystal structures is 0.74, 1.05, and 1.10 Å, respectively, for base, sugar, and phosphorus atoms. These numbers are compatible with those deduced from the structure in a canonical B form (as discussed in the previous paragraph). This result illustrates an important point that, in terms of similarity, the structural parameter does not map one on one to the structure itself of the molecule.

Another interesting observation is that our prediction of the base structure is more precise (0.41 and 0.51 Å in D_{rms}, respectively) than our prediction of the sugar structure when phosphorus constraints were applied. At first, this result seems to be counterintuitive because sugars are attached to phosphate groups directly whereas bases are connected to phosphate groups through sugars. One would expect bases to be more flexible than sugars if phosphorus atoms were constrained in space. That base pairings should always be maintained in DNA double helices, provides additional constraints (H bonds between the bases in a base pair) on the base structure. With these additional constraints, the base structure is better defined than the sugar structure when phosphorus atoms are constrained to their target coordinates.

To study the accuracy of our prediction procedure, we have randomly selected nine additional B-DNA duplexes besides 1BNA from the Protein Data Bank. For each duplex, a modeled structure was constructed based on the coordinates of the phosphorus atoms in the crystal structure. The rms differences between the modeled structures and the crystal structures for these DNA duplexes are tabulated in Table 2. The averaged D_{rms} for base atoms is 0.45 Å with a standard deviation of 0.06 Å, and the averaged D_{rms} for sugar atoms is 0.57 Å with a standard deviation of 0.07 Å. In all cases, the structures of the bases are better defined than the structures of the sugars, with the known coordinates of the phosphorus atoms as constraints.

Because of the structural similarity between the B and the A conformations (both are built from a monomer bp step), it is relatively straightforward to modify our procedure for predicting structures of DNA oligomers in an A conformation. The rms differences for the predicted and the crystal structures of 3ANA are 0.50, 0.56, and 0.33 Å, respectively, for base, sugar, and phosphorous atoms as shown in Table 2. These numbers are compatible with those for B-DNA oligomers. The procedure was also extended to predict structure of DNA oligomer with mismatches. The rms differences for the predicted and the crystal structures of 113D (with two Gua–Thy mismatches) are 0.49, 0.57, and 0.32 Å, respectively, for base, sugar, and phosphorous atoms as shown in Table 2.

Before applying the procedure to predict the all atoms structure of the highly bent cro operator, we tested it on the DNA duplex in the CAP–DNA complex (1CGP; Schultz et al., 1991). This 30-bp duplex is significantly bent (≈90° overall bending) on binding of the protein. Fig. 4 shows the structure of the modeled duplex superimposed upon the crystal structure. The rms differences between the two structures are 0.31, 0.54, and 0.66 Å, respectively, for phosphorus atoms, base atoms, and sugar atoms. The rms differences between the predicted base and sugar atoms and those in the crystal structure of this highly bent DNA duplex fall within the range for those listed in Table 1. This result indicates that the procedure predicts structures of the highly bent DNA duplexes as well as structures of relatively straight DNA duplexes.

Finally, we ran FITPP to construct an all-atom modeled structure for the DNA operator in the cro–DNA complex based on the low-resolution crystal structure (4CRO). Fig. 5 shows the predicted structure (*black*) superimposed upon the crystal structure (*gray*) in a stereo plot. D_{rms} between the phosphorus atoms of the predicted structure and the crystal structure is 0.37 Å. The predicted structure can be further refined by using any of the existing molecular refinement programs (e.g., AMBER (Weiner et al., 1984), CHARMM (Brooks et al., 1983), and BIOSYM). We use AMBER to refine the structure of the cro operator by running a constraint minimization. A short run (5000 cycles) of constraint minimization has reduced the D_{rms} to 0.15 Å. The energy-minimized structure of the cro operator is plotted in Fig. 6.

CONCLUSION

We have developed a computational approach to predict the structure of B-DNA duplexes by using the known coordinates of the phosphorus atoms as input. Based on a study of a set of 10 oligonucleotides, it was shown that the prediction of the base structure is more precise than the prediction of the sugar structure. We argued that the base pairing provided additional constraints on the base structure. The estimated accuracy of the predicted base structures is ≈0.5 Å. This method can be used to predict structures of highly bent duplexes as well as those of relatively straight duplexes. These results strongly support the notion that the base structure is directly correlated with the structure of the phosphorus atoms in B-DNA duplexes.

Our developed prediction procedure is general. It can be used to predict atomic structures of any B- and A-DNA duplexes with phosphorus coordinates determined from different experimental methods. The procedure is extremely fast; it can be used as part of the structural refinement procedures in x-ray crystallography or nuclear magnetic resonance. We used it to construct a modeled structure for the bacteriophage λ cro operator in the cro–DNA complex. The predicted atomic structure of the operator can be used to study detailed interactions between the sidechains of the cro protein and the DNA.

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