Volume 15 Number 14 1987 Nucleic Acids Research

The structure of poly(dA):poly(dT) in a condensed state and in solution

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Received April 3, 1987; Revised June 16, 1987; Accepted June 25, 1987

ABSTRACT

New X-ray and energetically optimal models of poly(dA):poly(dT) with the hydration spine in the minor groove have been compared with the NMR data in solution (Behling, R.W. and Kearns, D.R. (1986) Biochemistry 25, 3335-3346). These models have been refined to achieve a better fit with the NMR data. The obtained results suggest that the poly(dA):poly(dT) structure in a condensed state is similar to that in solution. The proposed conformations of poly(dA):poly(dT), unlike the classic B form, satisfy virtually all geometrical requirements which follow from the NMR data. Thus, the X-ray and energetically optimal poly(dA):poly(dT) structures (or those with slight modifications) can be considered as credible models of the poly(dA):poly(dT) double helix in solution. One of the features distinguishing these models from the classic B form is a narrowed minor groove.

INTRODUCTION

The poly(dA):poly(dT) structure has been extensively discussed lately. One of the reasons of such an increased interest is the observation that some natural DNAs display bending which has been attributed to structural features of $dA_n:dT_n$ runs (ref. (1) and references cited therein). It has been also noted that there are anomalies in the interaction of some proteins, antibiotics, etc. with poly(dA):poly(dT) and $dA_n:dT_n$ runs of natural DNAs.

Until recently the poly(dA):poly(dT) structure in fibers has been described by the so-called heteronomous DNA model, in which the poly(dA) chain assumes the A-type conformation (C3'-endo sugar) and the poly(dT) chain assumes the B-type conformation (C2'-endo sugar). This model was derived by Arnott et al. (2) from the X-ray diffraction data for the poly(dA):poly(dT) sodium salt. However, the X-ray structure analysis of the poly(dA):poly(dT) calcium salt (3,4) prompted a review of this model. It turned out that the Ca-poly(dA):poly(dT) structure is similar to the classic B form and is characterized by the C2'-endo sugar in both chains, though differs from the B form by a 0.28 nm narrower minor groove of the double helix. The revised

Na-poly(dA):poly(dT) structure proposed by Alexeev et al. (3,4) is close to the Ca-poly(dA):poly(dT) structure and agrees much better with the X-ray fiber diffraction data reported in ref. (2) than the heteronomous DNA model.

The poly(dA):poly(dT) structure in fibers is very similar to the structure of A/T run in the CGCGAATTCGCG dodecamer in crystals (5,6). One of the important features of the dodecamer is a bilayer spine of hydration found in its A/T run in the minor groove (6-8). Water molecules of the first hydration shell are hydrogen-bonded with N3 atoms of adenines and O2 atoms of thymines of adjacent base-pairs, thus bridging bases of the opposite chains of the double helix. Each molecule of the second shell is hydrogen-bonded with two molecules of the first hydration shell.

Energy calculations (9,10) suggest that the distinctive features of the poly(dA):poly(dT) structure in fibers are largely due to the existence of the spine of hydration. The interaction of water molecules with the opposite sugar-phosphate backbones is responsible for the narrowing of the minor groove observed in fibers, while in the absence of the spine of hydration the energetically 'optimal' structures have a wider minor groove. It was shown that the helical repeat value of ~10.0, which is characteristic of poly(dA):poly(dT) in solution (11-13), is due to the spine of hydration (10), whereas without the spine the helical repeat increases to ~10.6, a value characteristic of other sequences (11-14). Energy calculations for poly(dA):poly(dT) have been perfomed by many authors (see, for example, ref. (15)). However, nobody ever took into account the strong influence of the regular water spine in the minor groove which can be assumed in poly(dA):poly(dT) on the basis of the dodecamer structure and other experimental data obtained in a condensed state and in solution (see DISCUSSION).

As for the poly(dA):poly(dT) structure in solution, NMR studies (16,17) have shown that both chains have the sugar puckering of the C2'-endo type. Behling and Kearns (17) obtained the regions of allowed (within the experimental error) values for ten H-H interproton distances as functions of the angles α formed by H-H vectors with the helix axis. Another interesting result was that the distance between the adenine H2 atom (AH2) and the nearest H1' atom of the poly(dT) chain (TH1') was less than 0.45 nm and appeared to be smaller than that from AH2 to the corresponding atom of the poly(dA) chain (AH1'). Behling and Kearns concluded that their results were inconsistent with either the heteronomous model (2), or B' (18) or B (ref. (2) and S. Arnott, unpublished) models, though B' and B are less unacceptable.

From these three structures, the B form provided the closest fit with the NMR data (17).

Here we present a comparison between the poly(dA):poly(dT) structure in fibers and a low-energy structure with the spine of hydration in the minor groove, with the NMR data (17). We have also refined both the experimental and the calculated structures to fit them to the NMR data in solution. In the refined structures some interproton distances were modified by about 0.02 nm. The results suggest that these (experimental and calculated) or slightly refined structures fit the NMR data (17) clearly better than the model of the B-DNA. Therefore our models seem to be the most adequate representations of the poly(dA):poly(dT) structure in solution.

METHODS

We used the X-ray fiber diffraction data of poly(dA):poly(dT) calcium salt (3,4). They show that Ca-poly(dA):poly(dT) is a 10-fold double helix with a pitch of 3.232 nm, the conformation of poly(dA) and poly(dT) chains being identical. We optimized the X-ray diffraction model with the same constraints as in refs. (3,4). The structure parameters used and the optimization procedure are described in ref. (4).

The energy calculations were performed using semi-empirical atom-atom potential functions (see the corresponding parameters in refs. (19,20)). In the present work we calculated the complex of poly(dA):poly(dT) with the hydration spine in the minor groove. The conformations of poly(dA) and poly(dT) chains were optimized independently, though in all cases they proved similar. The calculation procedure has recently been described in detail (10). The winding angle of the polynucleotide was taken to be 36^{o}, which corresponds to a helical repeat of 10.0, as observed for poly(dA):poly(dT) in fibers and in solution.

We refined the structure parameters according to the NMR data (17) by adjusting the corresponding interproton distances to the values obtained from the experimental curves. In the figures of ref. (17) the distances are given on the abscissa and the angles are on the ordinate. We shall consider deviations from the experimental curves (17) only as a difference between the abscissa values, i.e. between the calculated and the nearest experimental interproton distances at a given angle α.

RESULTS

1. Comparison of the Poly(dA):Poly(dT) Structure in Fibers and in Solution

The poly(dA):poly(dT) model derived from the X-ray diffraction data for the calcium salt fibers (3,4) agrees well with 7 out of 10 dependences considered in ref. (17). The H-H distances calculated from the model are within the allowed limits (17) or deviate from them by less than 0.01 nm. Judging by the width of the allowed regions (0.02-0.06 nm) such a deviation is quite acceptable. Moreover, in the Ca-poly(dA):poly(dT) model, unlike the classic B form, the AH2-TH1' distance is less than 0.45 nm and is smaller than AH2-AH1', which is in agreement with the NMR data (17).

At the same time the calculated AH8-AH1' distance is 0.04 nm larger than the largest one following from the NMR experiment, the width of the allowed region being 0.02 nm (17). For the TH1'-TH5m interacting protons the calculated distance also exceeds the maximal experimental one. When the methyl proton is placed so as to provide the closest fit with the NMR data, the deviation of the TH1'-TH5m distance from the nearest experimental value is ~0.04 nm, the allowed region being ~0.06 nm. The AH2-AH2 distance differs most considerably (by ~0.11 nm) from the NMR data (17). These discrepancies could result from the inaccuracy of the model derived from the X-ray data. The traditional Hamilton's test (21) can be used to determine whether the constraints imposed by the NMR data on the optimized model result in a statistically significant disagreement with the diffraction data. Optimization has shown that the AH8-AH1' and TH1'-TH5m distances can approach those obtained from the NMR data without a statistically significant increase of the R-factor ($R = \Sigma |F_{obs} - F_{calc}| / \Sigma F_{obs}$; F_{obs} and F_{calc} are the observed and the calculated X-ray structure amplitudes, respectively) equal to 0.31 for the starting model. At the same time we were unable to construct a model with the AH2-AH2 distance close to 0.32 nm (the NMR value) and a required small angle between the AH2-AH2 vector and the helix axis. These conditions would be satisfied if AH2 atoms were close to the helix axis. However, even at AH2-AH2 distances equal to ~0.34 nm the R-factor increases up to ~0.47 and the sterical properties of the structure become much worse (in particular, the molecules in the unit cell overlap). According to statistical Hamilton's test (21) such models are inferior at the 99.5% level of significance to the model without constraint for the position of AH2 atoms. The same applies to the AH2 atoms in the Na-poly(dA):poly(dT) structure (4).

As a result, we concluded that the poly(dA):poly(dT) model derived from the X-ray diffraction data fits the NMR data, except for the increased

Table 1. H-H interproton distances (nm) and α angles (degrees) formed by H-H vectors with the helix axis for the three poly(dA):poly(dT) models. The differences (ΔL) between the calculated and the experimentally allowed H-H distances were estimated from the plots of ref. (17) at calculated values of α angles.

	1 Ca-poly(dA):poly(dT)		2 Poly(dA):poly(dT)		3 B-DNA	
	H-H /α	ΔL	H-H /α	ΔL	H-H /α	ΔL
AH2 -AH2	0.389/34	0.12	0.401/35	0.13	0.363/21	0.06
AH1'-AH2"	0.239/39	0.00	0.234/40	0.00	0.238/43	0.00
AH8 -AH1'	0.358/ 8	0.03	0.345/ 9	0.02	0.355/ 8	0.03
AH8 -AH2'	0.237/68	0.01	0.240/69	0.01	0.228/77	0.00
AH8 -AH2"	0.243/45	0.01	0.237/47	0.01	0.214/33	0.04
TH1'-TH5m	0.425/32	0.03	0.392/35	0.01	0.405/47	0.07
TH1'-TH2"	0.240/38	0.00	0.234/38	0.00	0.238/43	0.00
TH6 -TH1'	0.350/ 4	0.00	0.345/ 5	0.00	0.353/ 8	0.00
TH6 -TH2'	0.209/63	0.00	0.215/63	0.00	0.197/75	0.04
TH6 -TH2"	0.237/47	0.00	0.234/47	0.00	0.221/37	0.02
AH2 -TH1'	0.364/66		0.364/55		0.508/50	
AH2 -AH1'	0.386/46		0.385/44		0.447/85	

Note: Structures 1 and 2 are slightly refined variants of the X-ray model (No. 1) and the energetically optimal model (No. 2) of poly(dA):poly(dT) allowing for the NMR constraints (17). Atomic coordinates of the classic B form (structure No. 3) were derived by S. Arnott and co-workers (unpublished) from the X-ray data for Li-B-DNA (for structural parameters see ref. (2)). The table lists only the shortest interproton distances. ΔL=0.00 if the calculated values are within the experimentally allowed regions (17). ΔL deviations by something like the half-width of the allowed regions (0.01-0.03 nm), which corresponds to the experimental errors (17), are considered as acceptable.
For structures 1 and 2 AH2-TH1'<AH2-AH1'<0.45 nm which fits the NMR data (17), while for B-DNA this condition is not satisfied. Moreover, the AH8-AH2" and TH6-TH2' distances in structures 1 and 2 provide a better fit with the NMR data than B-DNA. The position of the methyl proton in B-DNA (S. Arnott, unpublished) is not optimal in terms of the NMR data (17) and corresponds to ΔL=0.07 nm for TH1'-TH5m.
The AH2-AH2 distance/angle dependence was obtained by Behling and Kearns (17,24) from relaxation measurements, while the dependences for all the other proton pairs were determined from NOE. The first approach is very sensitive to the geometric model of the structure, and the calculated AH2-AH2 distances in our structures (Nos. 1 and 2) largely deviate from those obtained from the NMR experiment. One of the possible explanations of this disagreement is that H1' protons are situated close to AH2 ones in these structures. The AH2-AH2 and AH2-H1' interactions are of the same order in this case, while the NMR data were interpreted (17,24) to mean that the first ones are dominant.

distance between AH2 protons.

Table 1 lists interproton distances and the angles α formed by H-H vectors with the helix axis for such a slightly refined poly(dA):poly(dT) structure in fibers. It is seen that in this structure, unlike the B form,

AH2-TH1'<AH2-AH1'<0.45 nm, which is consistent with the NMR requirements (17). Moreover, for AH8-AH2" and TH6-TH2' in the B form the ΔL deviations from the experimental values (17) are larger than in our X-ray diffraction model. As it is seen from Table 1, for all other dependences the B form fits the NMR data just as well as structure No.1 (for TH1'-TH5m see the Note to Table 1).

This comparison permits us to conclude that our slightly modified X-ray model agrees with the NMR data (17) clearly better than the classic B form.

2. Comparison of the Energetically Optimal Structure with the NMR Data

A whole family of low-energy poly(dA):poly(dT) conformations with a bilayer spine of hydration in the minor groove has been obtained recently (10). We consider structures with the energies higher than the optimal one by no more than ~0.5 kcal/mol per nucleotide pair, which is comparable with the energy of thermal fluctuations at room temperature. At the winding angle of 36° these structures are characterized by a narrowed minor groove of the double helix (the shortest distance between the phosphorus atoms of the opposite chains is about 0.90-0.95 nm). This family of conformations includes both structures with a large propeller twist ($\sim 18^{\circ}$) and a small negative tilt $\sim -4^{\circ}$, and structures with a small propeller twist $\sim 7^{\circ}$ and a more negative tilt $\sim -12^{\circ}$.

It has been shown (10) that the distinctive features of the obtained structures are largely due to the interaction of DNA with water molecules in the minor groove.

Our analysis has shown that the structures of this family fit better the NMR data (17) than the B form. As an example we have taken a structure from this family with an intermediate propeller twist of 12°, which is slightly preferable by energy and fits somewhat better the NMR data (17). A noticeable deviation from the experimental values is observed only for the distances TH1'-TH5m ($\Delta L \approx 0.03$ nm) and AH2-AH2 ($\Delta L \approx 0.13$ nm). Optimization can decrease the deviation of the TH1'-TH5m distance to a quite acceptable value of 0.01 nm at the expense of the energy increase less than 0.5 kcal/ mol. In this structure the methyl group was oriented so as to favour the formation of a structure-stabilizing hydrophobic contact with the sugar ring CH2 group of the adjacent 5'-nucleotide (see ref. (22)). At the same time, the energy considerably increased when AH2 protons approached the helix axis. Even in the absence of restraints imposed by the existence of the spine of hydration in the minor groove, the decrease of the distance between AH2 protons to ~0.35 nm resulted in a ~6 kcal/mol increase of the polynucleotide energy

Table 2. Cartesian and cylindrical polar coordinates of atoms of a nucleotide pair from the poly(dA):poly(dT) structure represented in Fig. 1A

ATOM	x(nm)	y (nm)	z (nm)	R (nm)	PhI (deg)	ATOM	x (nm)	y(nm)	z (nm)	R (nm)	PhI (deg)
PHOSPHATE (A)						PHOSPHATE (T)					
P	0.096	0.969	0.232	0.974	84.3	P	0.097	-0.977	-0.237	0.982	-84.3
O1P	-0.017	0.974	0.137	0.975	91.0	O1P	-0.016	-0.983	-0.142	0.984	-90.9
O2P	0.171	1.096	0.249	1.109	81.1	O2P	0.172	-1.103	-0.257	1.117	-81.1
O3'	0.045	0.917	0.374	0.918	87.2	O3'	0.045	-0.923	-0.379	0.924	-87.2
O5'	0.197	0.853	0.189	0.875	77.0	O5'	0.198	-0.861	-0.194	0.883	-77.1
SUGAR (A)						SUGAR (T)					
C1'	0.337	0.524	0.088	0.623	57.2	C1'	0.337	-0.535	-0.092	0.632	-57.8
C2'	0.346	0.642	-0.008	0.730	61.7	C2'	0.350	-0.651	0.008	0.739	-61.7
C3'	0.437	0.741	0.066	0.860	59.5	C3'	0.441	-0.748	-0.069	0.868	-59.4
C4'	0.395	0.715	0.211	0.817	61.1	C4'	0.397	-0.724	-0.213	0.825	-61.3
C5'	0.308	0.822	0.275	0.878	69.4	C5'	0.313	-0.834	-0.276	0.891	-69.4
O4'	0.323	0.587	0.214	0.671	61.2	O4'	0.321	-0.599	-0.218	0.680	-61.8
H1'	0.427	0.464	0.079	0.630	47.4	H1'	0.426	-0.474	-0.088	0.638	-48.1
H2'	0.247	0.686	-0.021	0.730	70.1	H2'	0.254	-0.697	0.023	0.741	-70.0
H2"	0.394	0.611	-0.100	0.727	57.2	H2"	0.401	-0.616	0.097	0.735	-56.9
H3'	0.411	0.842	0.038	0.937	64.0	H3'	0.418	-0.849	-0.040	0.946	-63.8
H4'	0.483	0.698	0.271	0.849	55.3	H4'	0.484	-0.705	-0.275	0.855	-55.5
H5'	0.367	0.911	0.291	0.982	68.0	H5'	0.373	-0.924	-0.284	0.996	-68.0
H5"	0.272	0.786	0.370	0.832	70.9	H5"	0.281	-0.804	-0.374	0.851	-70.7
ADENINE						THYMINE					
N1	0.169	0.045	0.013	0.175	14.8	N1	0.218	-0.450	-0.068	0.500	-64.1
C2	0.291	0.096	0.031	0.306	18.2	C2	0.240	-0.316	-0.054	0.396	-52.8
N3	0.326	0.221	0.050	0.394	34.1	O2	0.350	-0.265	-0.060	0.440	-37.1
C4	0.218	0.302	0.050	0.373	54.2	N3	0.127	-0.240	-0.032	0.271	-62.2
C5	0.088	0.264	0.033	0.279	71.6	C4	-0.003	-0.286	-0.024	0.286	-90.6
C6	0.063	0.128	0.014	0.143	63.8	O4	-0.095	-0.208	-0.004	0.230	-114.8
N6	-0.060	0.077	-0.004	0.098	127.8	C5	-0.015	-0.429	-0.040	0.429	-92.1
N7	0.004	0.375	0.038	0.375	89.3	C5m	-0.151	-0.493	-0.033	0.516	-107.0
C8	0.085	0.475	0.058	0.482	79.8	C6	0.093	-0.505	-0.061	0.513	-79.6
N9	0.218	0.438	0.066	0.490	63.5	H3	0.140	-0.141	-0.022	0.199	-45.3
H2	0.371	0.024	0.030	0.372	3.7	H6	0.081	-0.612	-0.073	0.617	-82.4
H16	-0.139	0.138	-0.004	0.196	135.4	H5m1	-0.172	-0.521	0.069	0.549	-108.3
H26	-0.072	-0.021	-0.017	0.075	-163.5	H5m2	-0.225	-0.423	-0.068	0.480	-118.0
H8	0.052	0.577	0.068	0.579	84.8	H5m3	-0.152	-0.581	-0.096	0.601	-104.6

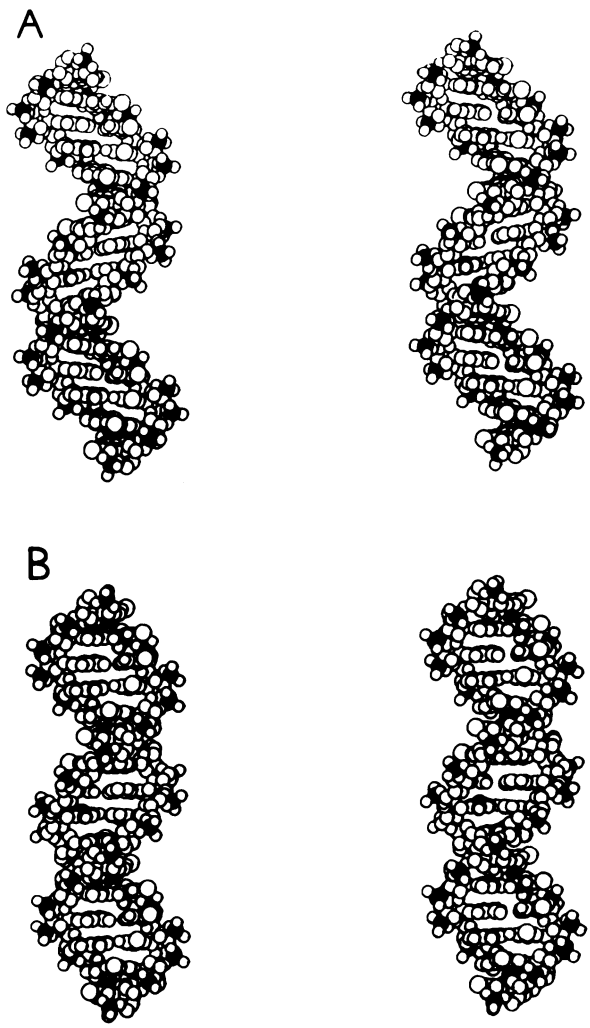

Figure 1. (A) Stereo view of the poly(dA):poly(dT) structure optimized by energy with the NMR constraints assuming the existence of a bilayer spine of hydration in the minor groove and (B) poly(dA):poly(dT) in the classic B form (ref. (2) and S. Arnott, unpublished). Phosphorus atoms are shown by black circles. Our structure has the following parameters: the winding angle of 36°, the helical pitch of 3.29 nm, the sugar conformation of the C2'-endo type, the tilt of -7°, the propeller twist of 12°, the minor groove width of 0.94 nm. This structure is not the only low-energy model fitting the NMR data (17) (see the text for details). The same parameters for the B form are: 36°, 3.37 nm, C2'-endo, 2°, 13°, 1.2 nm (2).

and a strong deoxyribose deformation. If we did not allow such deformation, the energy increased by no less than 10 kcal/mol. The energy increased even more if the interaction of such polynucleotide molecules with water molecules in the minor groove was taken into account.

Therefore, in our model we have not imposed constraints on the positions of AH2 atoms following from NMR experiments (17).

Table 1 lists the interproton distances and deviations from the experimental curves (17) for this structure. Coordinates of atoms are given in Table 2, and Figure 1A presents the projection of the molecule normal to the helix axis. It is seen from Table 1 that the condition AH2-TH1'<AH2-AH1'< <0.45 nm is satisfied for this model as well as for the X-ray model, but not for the B form. Our low-energy model fits the NMR data (17) just as well as the X-ray model (section 1). A still better agreement can be achieved at the expense of some energy increase. However, this would not be expedient to do because of the experimental errors in the NMR data (17) and the limited number of variables characterizing the structure (the same is also true for the X-ray model of poly(dA):poly(dT)).

DISCUSSION

The poly(dA):poly(dT) structure derived from X-ray fiber diffraction and that derived from energy optimization are very similar, both pertaining to the B family. They differ from the classic B form by a narrower (by 0.25-0.3 nm) minor groove of the double helix. In terms of polynucleotide geometry, the narrowing of the minor groove can be due, first of all, to the negative tilt of base pairs, i.e. the direction of the tilt is opposite to that of the A-form DNA. For the X-ray model the tilt is equal to -6° and for the model in Fig. 1A the tilt is equal to -7°. An increased propeller twist of the bases in a pair also contributes to the narrowing of the minor groove, though to a lesser extent (the X-ray model of Ca-poly(dA):poly(dT) and the energetically optimal model both refined to fit the NMR data have propeller twists of 18° and 12°, respectively, and rather close minor groove widths). It can be noted that the AH8-AH1' and TH1'-TH5m distances in the structure with the propeller twist of $\sim 12^{\circ}$ fit the NMR data (17) better than the same distance in the X-ray model. In both models the same tilt was postulated for adenines and thymines while the X-ray data for Na-poly(dA):poly(dT) suggest the possibility of different tilts for adenine and thymine (4). This, however, does not significantly affect the minor groove width.

Energy calculations show (9,10) that the cause of the minor groove narrowing in poly(dA):poly(dT) is the bilayer spine of hydration analogous to that observed in CGCGAATTCGCG crystals (6-8). The existence of such a spine of hydration in poly(dA):poly(dT) fibers seems obvious, taking into account coincidence of the structures derived independently from X-ray diffraction data and from energy optimization (3,4,9,10). It also follows from this coincidence that intermolecular interactions in fibers weakly affect the Ca-poly(dA):poly(dT) structure. This fact, as well as the coincidence of helical repeats of the poly(dA):poly(dT) double helix in fibers and in solution (11-13), strongly suggests a similarity of the structures, hence, the existence of a hydration spine in solution.
The same conclusion follows from the comparison with the NMR data obtained by Behling and Kearns (17). A slight optimization of our models gave an adequate description of the mutual positions of all the protons except adenines H2 of adjacent nucleotides. The obtained models fit the NMR data clearly better than the classic B form (Table 1).

Behling and Kearns noted (17) that AH2-H1' interactions are sensitive to the minor groove width. According to their data the AH2-TH1' distance is less than 0.45 nm and is smaller than AH2-AH1'. The energetically optimal models of poly(dA):poly(dT) with the spine of hydration and the X-ray model satisfy these conditions due to a narrow minor groove, while the B form does not (Fig. 1 and Table 1). Drew and Travers (23) suggested that DNA A/T runs without a TpA step in solution have a narrower minor groove than the B form. This allowed them to explain the observed pattern of DNA digestion by various nucleases. Our results support their concept and give the value of about 0.9-0.95 nm for the minor groove width. Our calculations also show that the models of poly(dA):poly(dT) with the spine of hydration and a groove width of about 1.1 nm (intermediate between 0.95 nm and 1.2 nm for the B form) are less energetically favourable and demonstrate a worse fit to the NMR data.

The only requirement following from the NMR experiments (17) which is not fulfilled by our models is for the AH2-AH2 distance to be close to 0.32 nm. This requirement would be fulfilled if AH2 protons were close to the helix axis, and this would lead to a sharp energy increase and to a much worse R-value for the X-ray model. The poly(dA):poly(dT) structure with such a position of AH2 protons is far from the optimum even without restraints imposed by the existence of the spine of hydration (see RESULTS). It should be also noted that in all X-ray models of poly(dA):poly(dT) the AH2-AH2

distance considerably exceeds 0.32 nm (2,4,18) and, therefore, does not fit the NMR data (17). We have also calculated this distance from coordinates of atoms of the six variants of the CGCGAATTCGCG dodecamer (the Brookhaven Protein Data Bank) where the structure of A/T runs is similar to poly(dA): poly(dT) in fibers (3,4). The minimal AH2-AH2 distance was 0.37 nm and most distances were longer than 0.39 nm.

It can be concluded that the poly(dA):poly(dT) structure in which AH2 protons are close to the helix axis is hardly probable from the stereochemical point of view. To solve this contradiction, it seems worth-while to revise the interpretation of the NMR data for AH2 protons (17,24); see also the Note to Table 1.

The positions of other protons are well described by the model represented in Fig. 1A. Although the NMR requirements alone do not provide the unique solution to the structure, the similarity of the discussed experimental and theoretical models of the structure strongly suggests that the model in Fig. 1A (or its slightly modified versions) adequately describes the poly(dA):poly(dT) double helix in a condensed state and in solution.

ACKNOWLEDGEMENTS

We thank Drs. I.Ya. Skuratovskii, V.I. Poltev, I.Ya. Gukowsky and R.A. Abagyan for critical comments of the work. We are very grateful to Dr. V.L. Florentiev for helpful discussions of the NMR data.

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