1. Zoom in on the middle of the dodecamer, and find the N3 position of T7 on the A chain (in the command window it should say "Atom: N3 140 Group: T 7 Chain:A"). Then find the N1 atom of A6 on the B chain. Now measure the distance between the N3 of T7 and the N1 of A6. What kind of weak interaction does this distance correspond to?

\[ 2.8 \text{ Å}, \quad \text{H-Bond} \]

b. Find the phosphorus atoms belonging to T7 and T8, and measure their interatomic distance. This value is near the maximum possible P-P distance for adjacent nucleotides in an RNA or DNA chain.

Chain A: 6.3 Å
Chain B: 6.7 Å

2. In an x-ray fiber diffraction experiment, your diffraction pattern gives a "helical cross" with a strong meridional reflection on the 5th layer line corresponding to a Bragg angle of 30°, using Cu Ka radiation (1.5 Å wavelength). Predict the structure of your molecule.

\[ n \lambda = 2d \sin \theta \]
\[ n = 1 \]
\[ \lambda = 1.5 \text{ Å} \]
\[ 2 \sin 30° = 0.5 \]
\[ d = \frac{(1)(1.5 \text{ Å})}{2(0.5)} = 1.5 \text{ Å} \]

Structural elements:
1. Molecule is a helix
2. Within a repeat (not necessarily a full turn)
   - Every 5x1.5 Å = 7.5 Å
3. And spacings of some sort every 1.5 Å perpendicular to the helical axis

3. What were the two independent lines of reasoning that indicated to Watson and Crick that there are two chains in the DNA double helix?
   1. 24 nucleotides per unit cell, 12 periphery per unit cell
   2. A dyad (2-fold symmetry) axis perpendicular to helical axis implies two antiparallel chains

4. List and compare the (i) interatomic distances and (ii) bond energies for: (a) covalent bonds (b) electrostatic interactions, (c) hydrogen bonds and (d) van der Waals interactions.
   a) i. Atom-specific, N1-2 Å
      ii. \( \Delta q \leq 80 \text{ kcal/mol} \)
   b) i. N2.5-3.5 Å
      ii. \( \Delta q \leq 185 \text{ kcal/mol} \)
   c) i. \( \approx 2.5-3.0 \text{ Å} \) in general
      ii. \( \Delta H_{\text{vac}} \leq 5 \text{ kcal/mol} \)
      \( \Delta H_{R} \leq 1 \text{ kcal/mol} \)
   d) i. N3-4 Å, depends on van der Waals
      ii. \( \Delta q \leq 1-2 \text{ kcal/mol} \)

5. Pauling noted a correlation between bond energies and bond distances. From your answer to question #5, what do you conclude?

They are inversely proportional: the greater the bond distance, the weaker the bond.
7. In what ways do the properties of water influence the strength of: (a) electrostatic interactions; (b) hydrogen bonding; and (c) hydrophobic interactions. Explain in physical and chemical terms.

<table>
<thead>
<tr>
<th>Electrostatic</th>
<th>in H₂O</th>
<th>Why</th>
</tr>
</thead>
<tbody>
<tr>
<td>weaker</td>
<td>high dielectric constant ( \varepsilon = 81 )</td>
<td></td>
</tr>
</tbody>
</table>

| H-bond | weaker | competition |

| Hydrophobic | stronger | non-interference w/ H₂O structure |

8. Alkaline pH (e.g., pH 11-12) is used to denature DNA (i.e., cause strand separation). Explain how this works, based on your knowledge of pK's and weak interactions.

- High pH favors "wrong" base tautomers and new negative charges.

9. Binding of a protein to DNA has a Gibbs free energy of \(-15\) kcal/mol at 37°C. Calculate the Kd (dissociation constant) for the binding reaction.

\[
K_d = \text{concentration at which the protein is half bound to DNA} = \frac{[\text{DNA+protein}]}{[\text{DNA}][\text{protein}]} \\
\Delta G = -RT \ln K \\
K_d = e^{-\frac{\Delta G}{RT}} = e^{-\frac{\Delta G}{RT}} \approx 2.66 \times 10^{-11} \text{ M}
\]

10. Association of two DNA oligonucleotide strands into a double helix has a Kd (dissociation constant) of \(10^{-9}\) at 37°C. Calculate the Gibbs free energy for the association reaction.

\[
\Delta G = -RT \ln K \\
\Delta G = -(1.9872 \times 10^{-3} \text{ Kcal/mol} \cdot K)(310 \text{ K}) \ln 10^{-9} \\
\Delta G = 12.76 \text{ Kcal/mol}, \text{ for association reaction} \quad \Delta G = -12.76 \text{ Kcal/mol}
\]