

Nucleic Acids

The Other Biomolecule

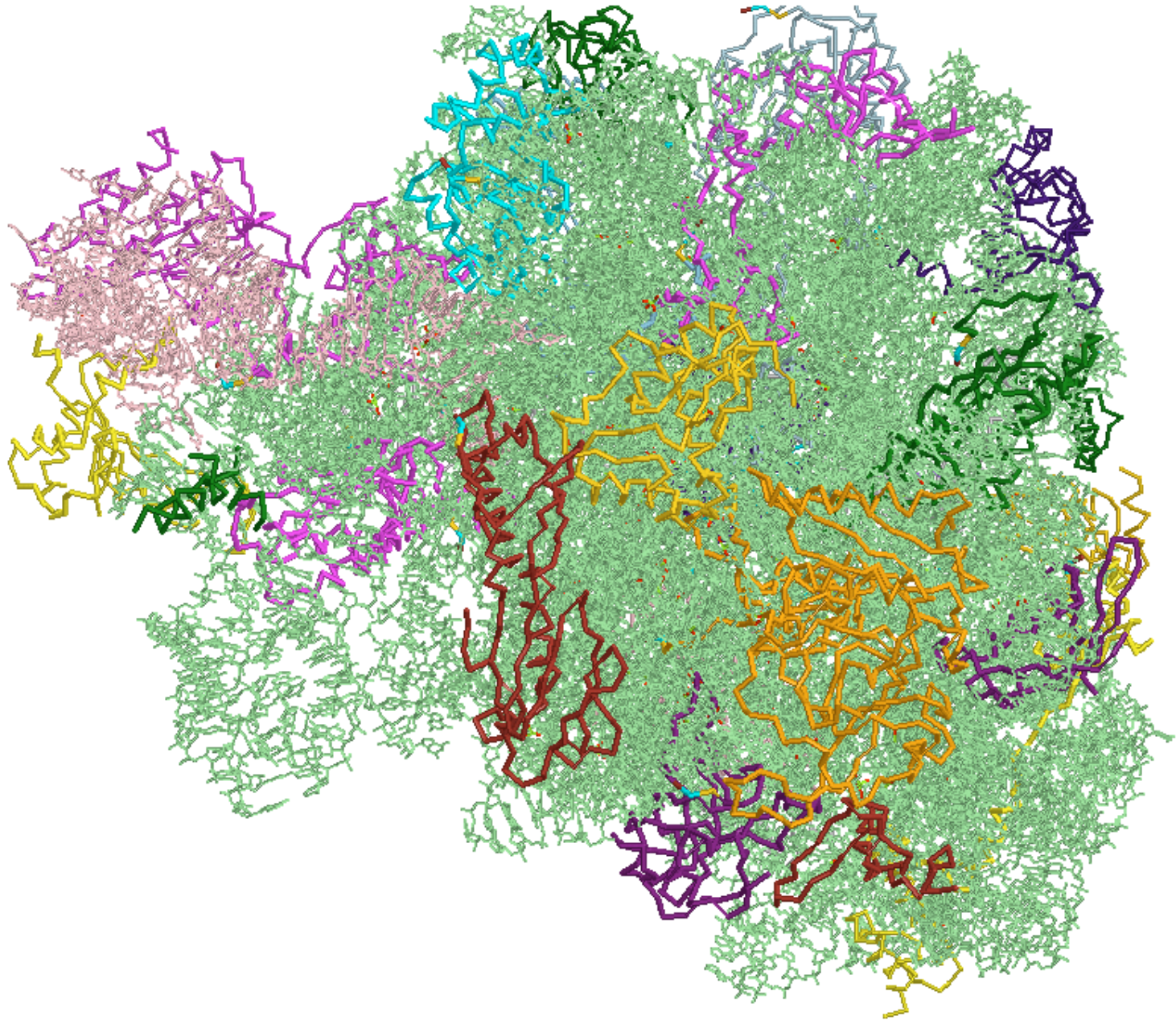
Nucleic Acids

The Other Biomolecule

details are different
principles are the same

Ribosome

An RNA machine with protein cofactors



What stabilizes protein structures?

What stabilizes protein structures?

What *directs* protein structures?

The DNA Duplex

The DNA Duplex

What stabilizes the duplex?

The DNA Duplex

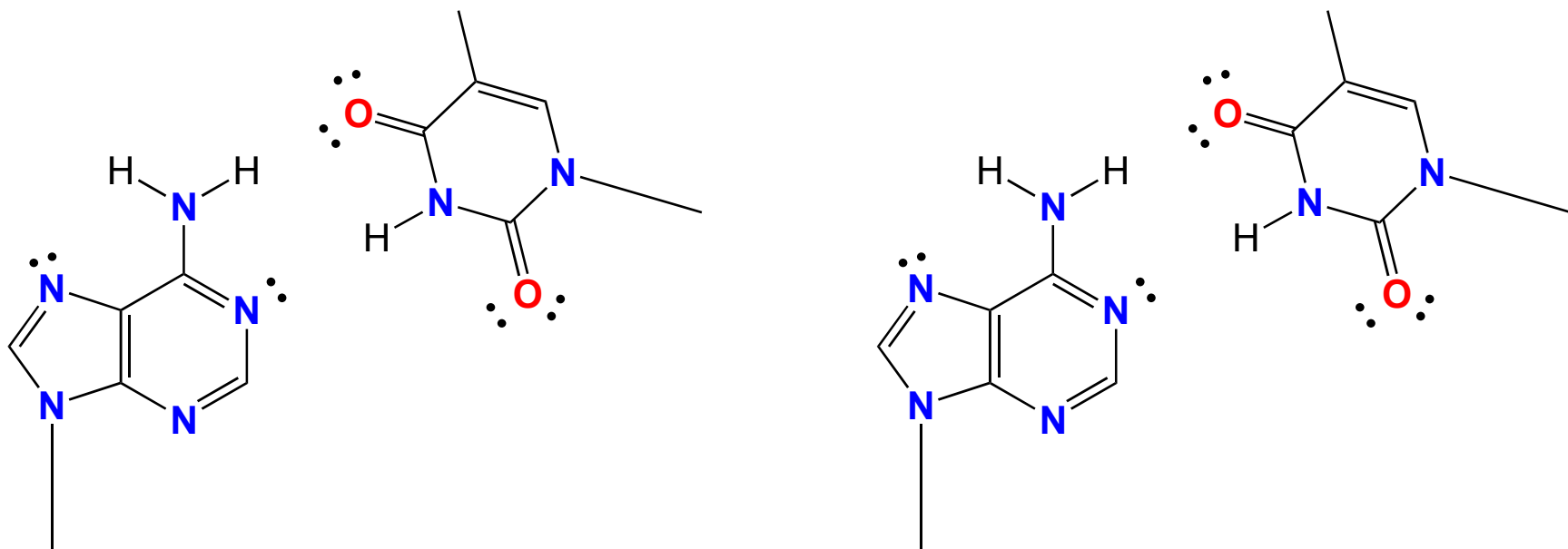
What stabilizes the duplex?

What *directs* duplex structure?

Which is most stable?

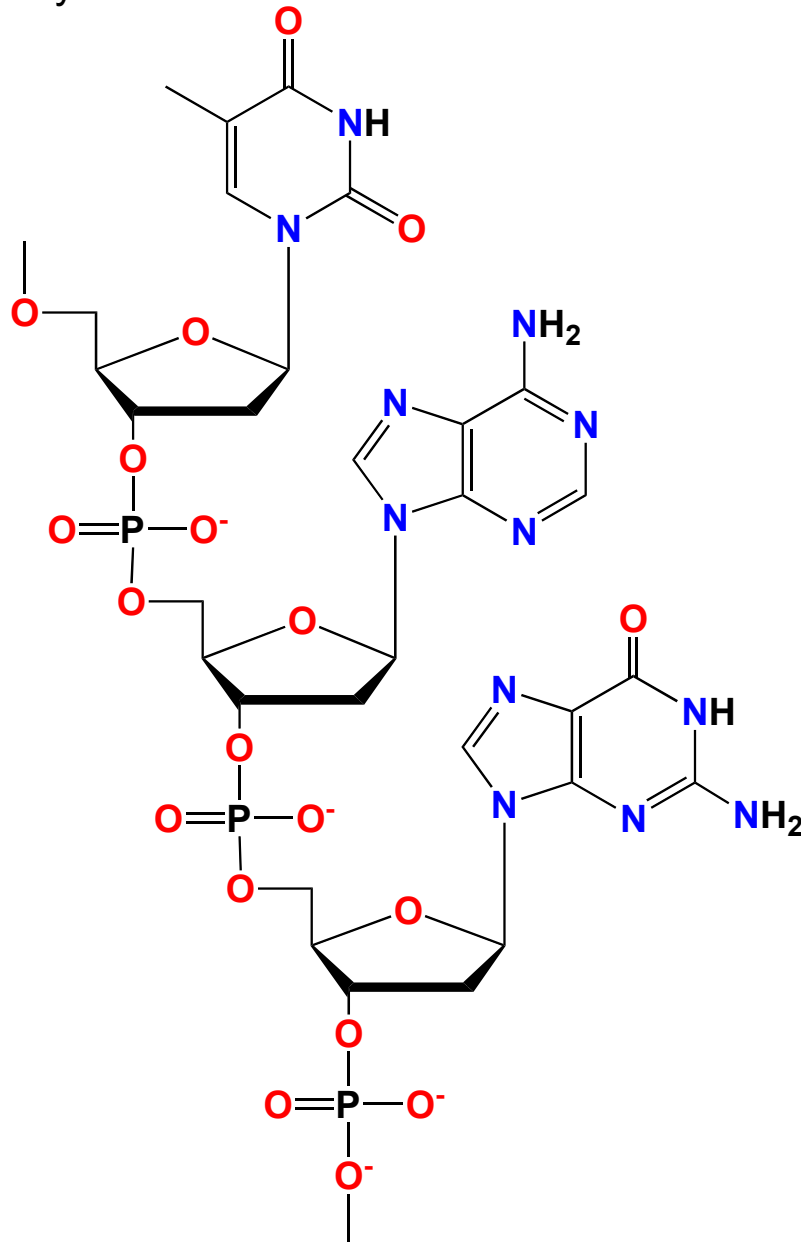
5' -ACCGCCGACGT-3'
3' -TGGCGGCTGCA-5'

5' -ACCGCCGACGT-3'
3' -AGGCGGCTGCC-5'



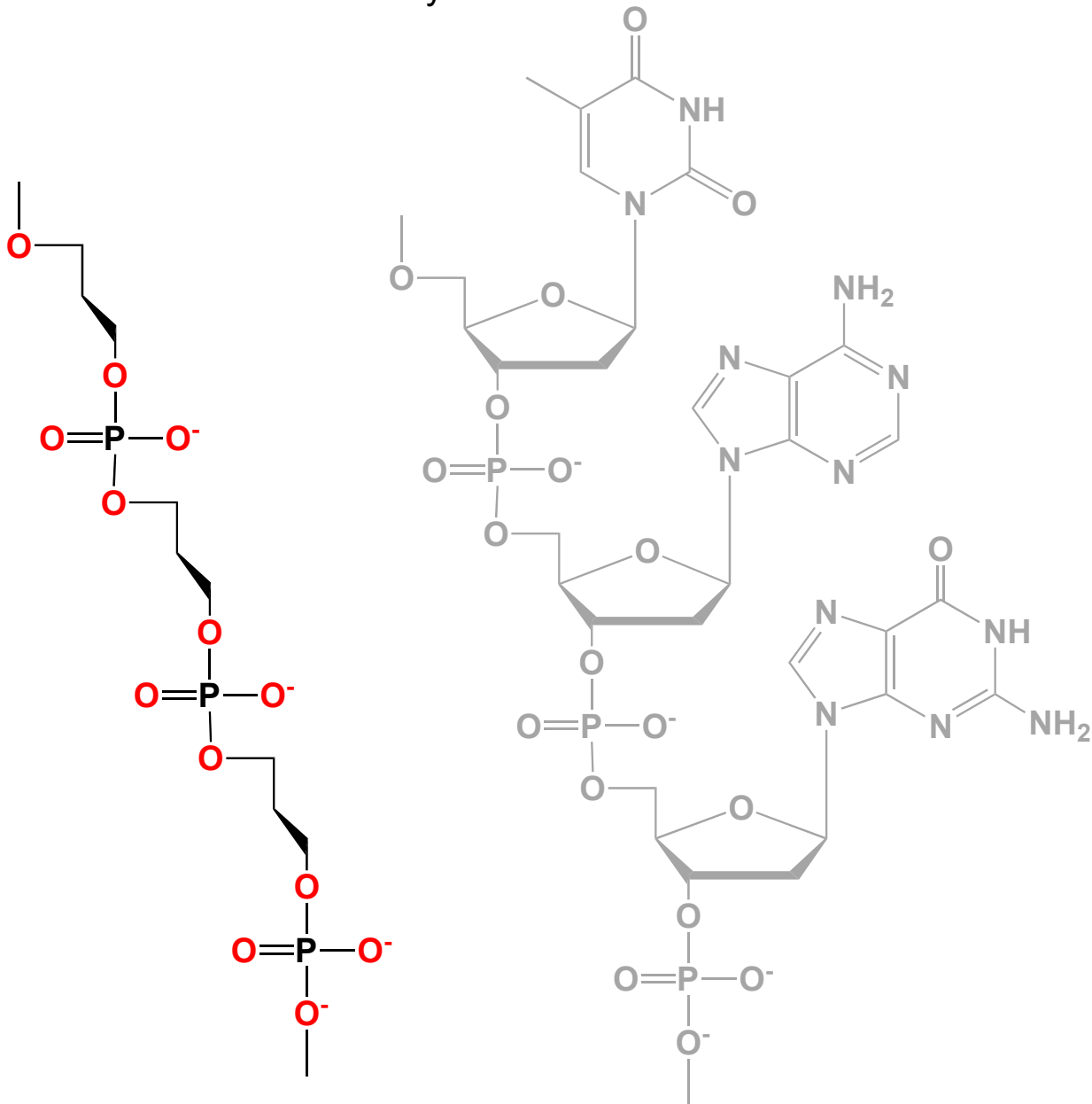
DNA

A look at the Chemistry



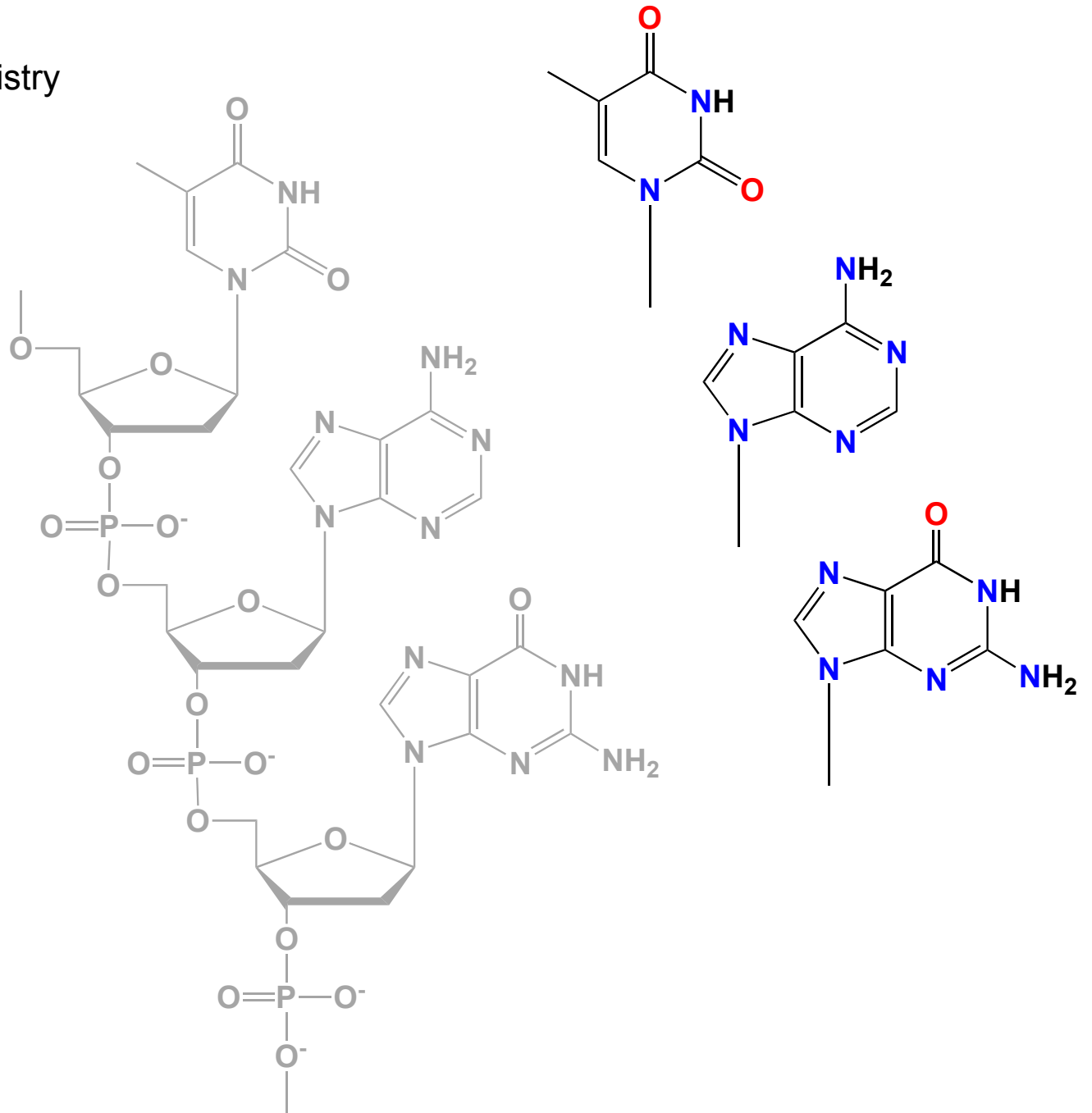
DNA

A look at the Chemistry



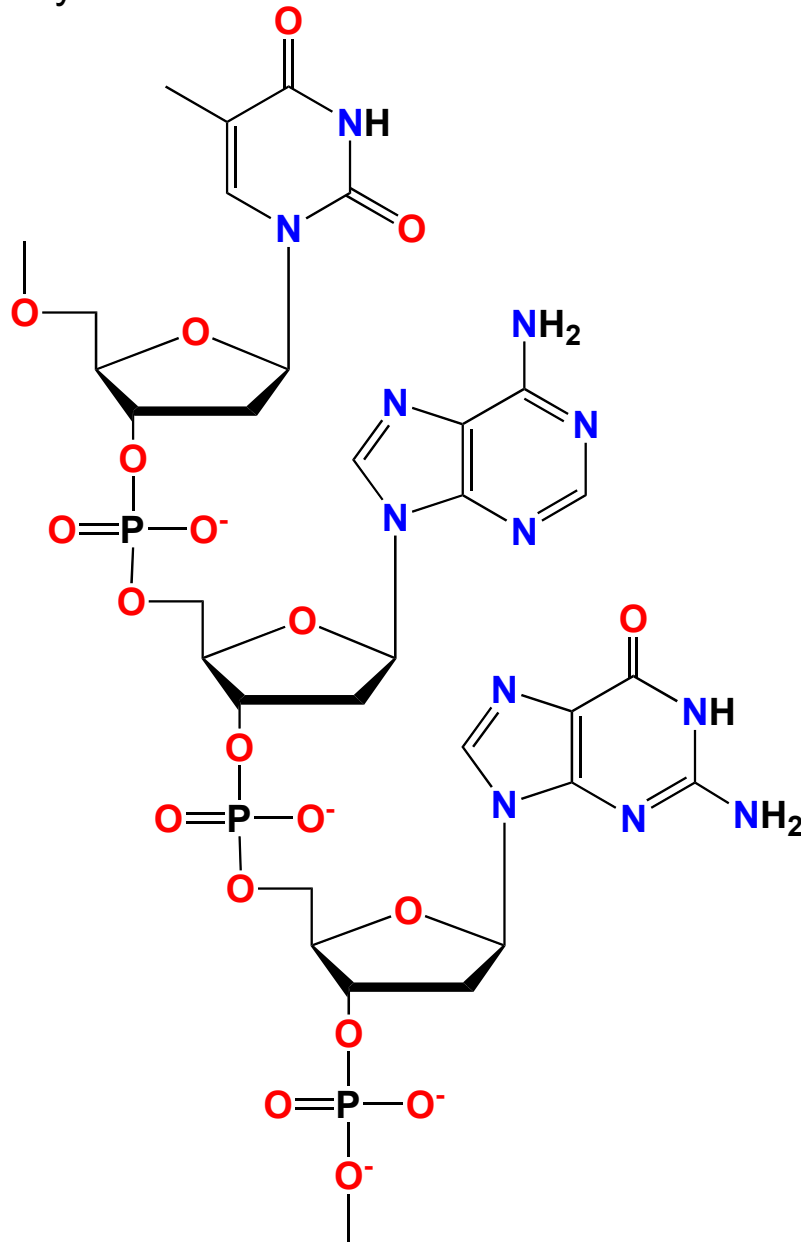
DNA

A look at the Chemistry



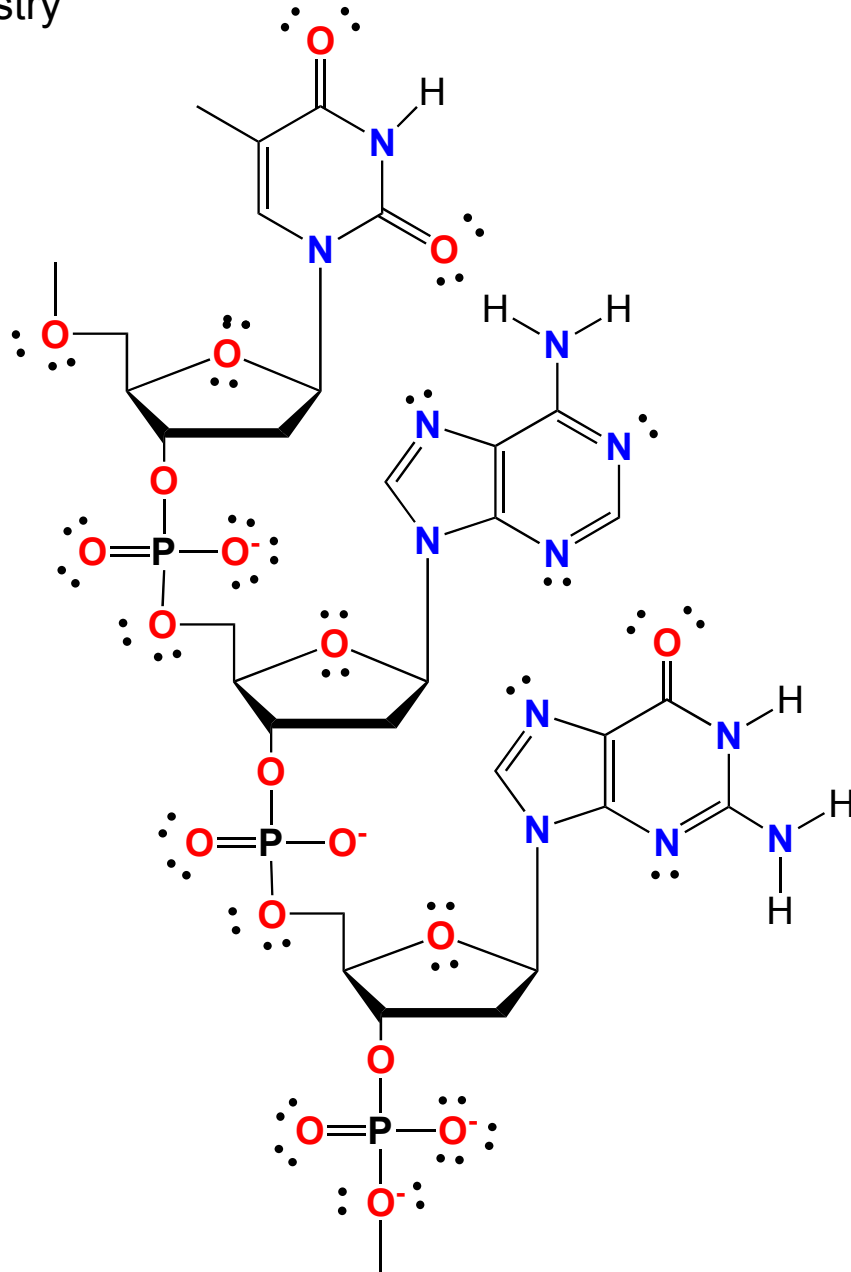
DNA

A look at the Chemistry



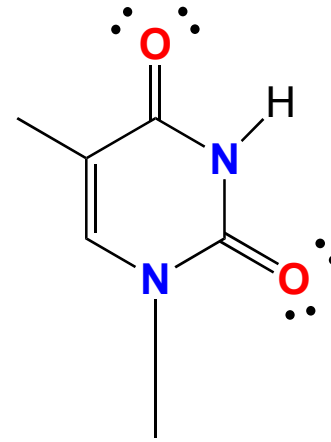
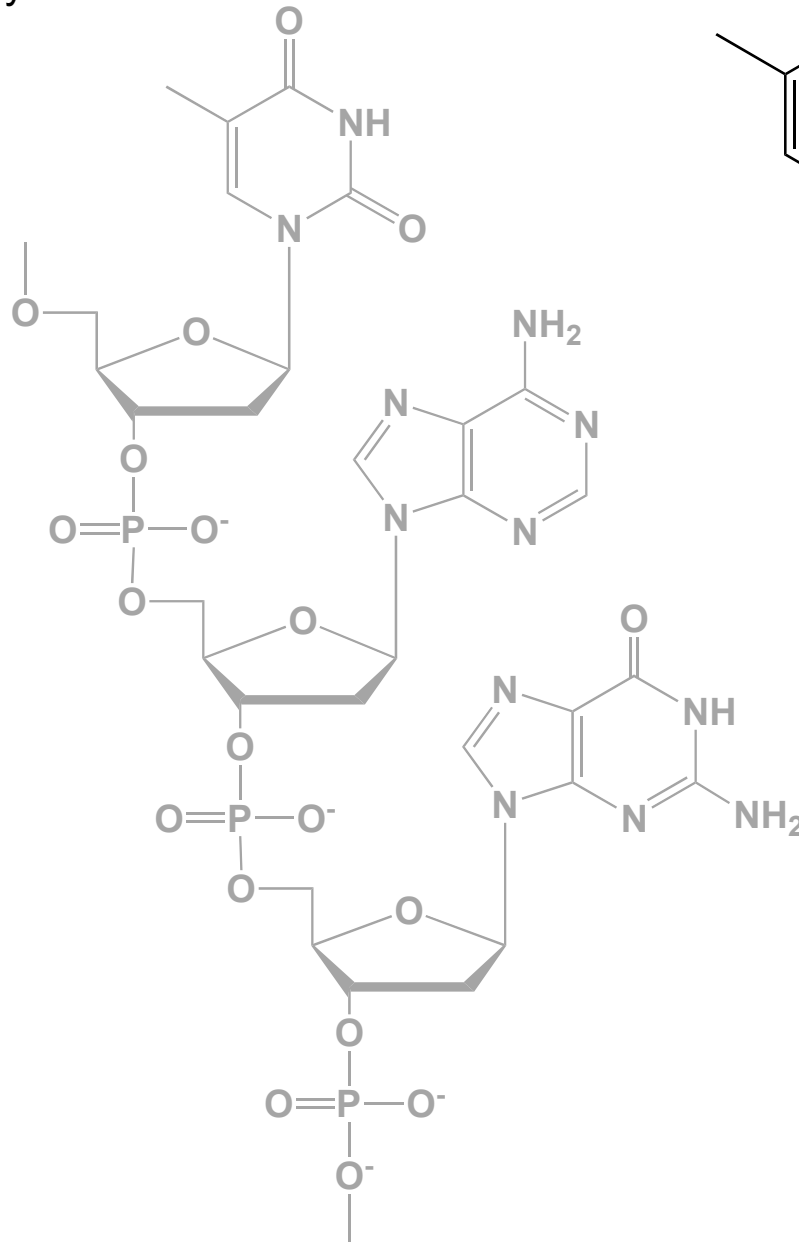
DNA

A look at the Chemistry



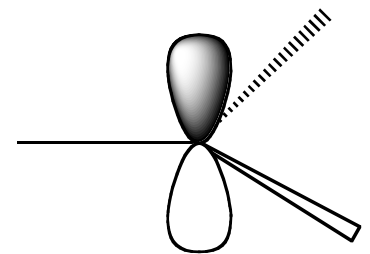
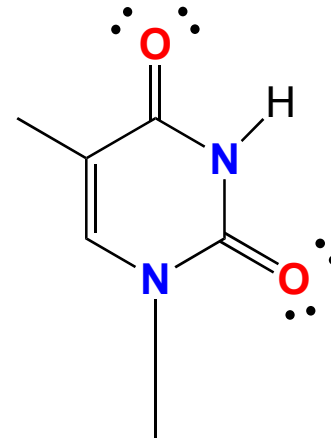
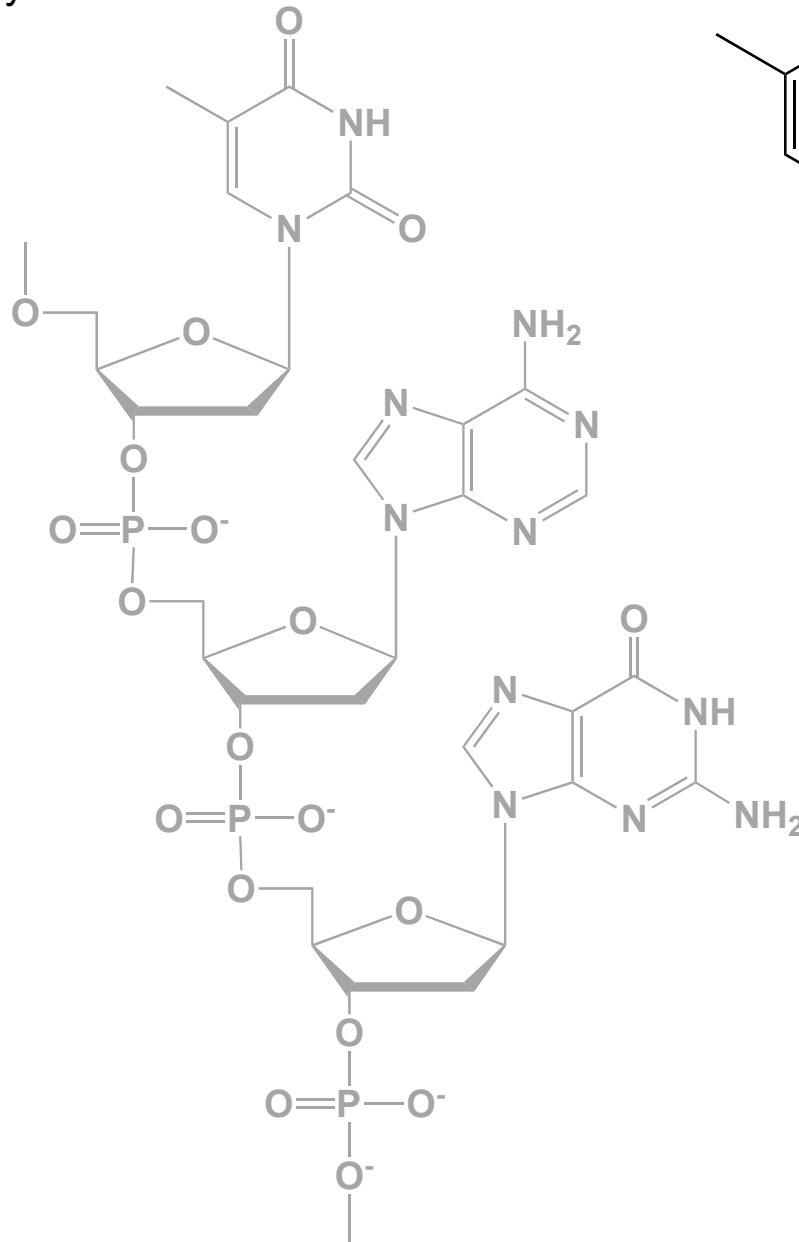
DNA

A look at the Chemistry



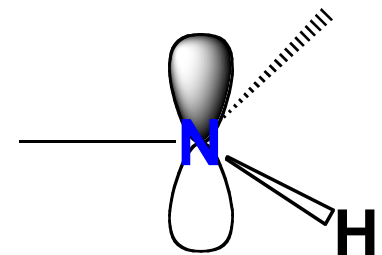
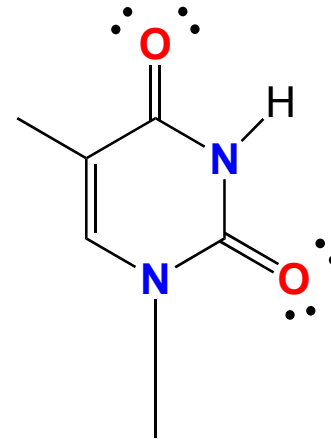
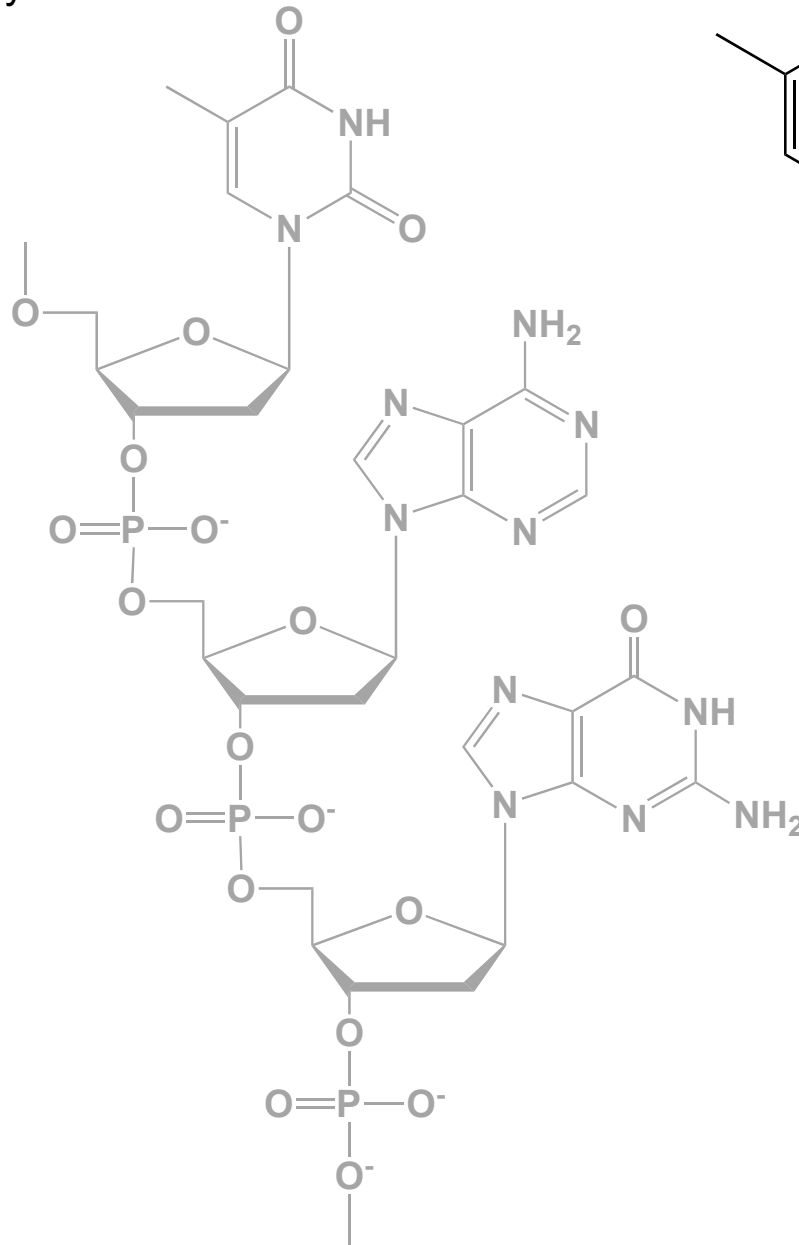
DNA

A look at the Chemistry



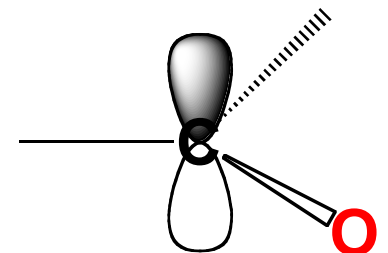
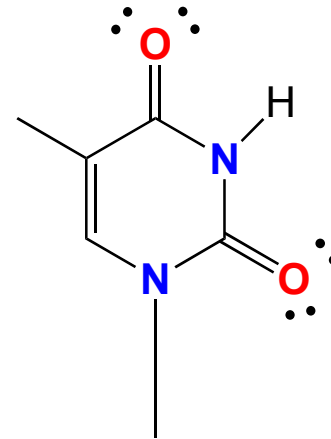
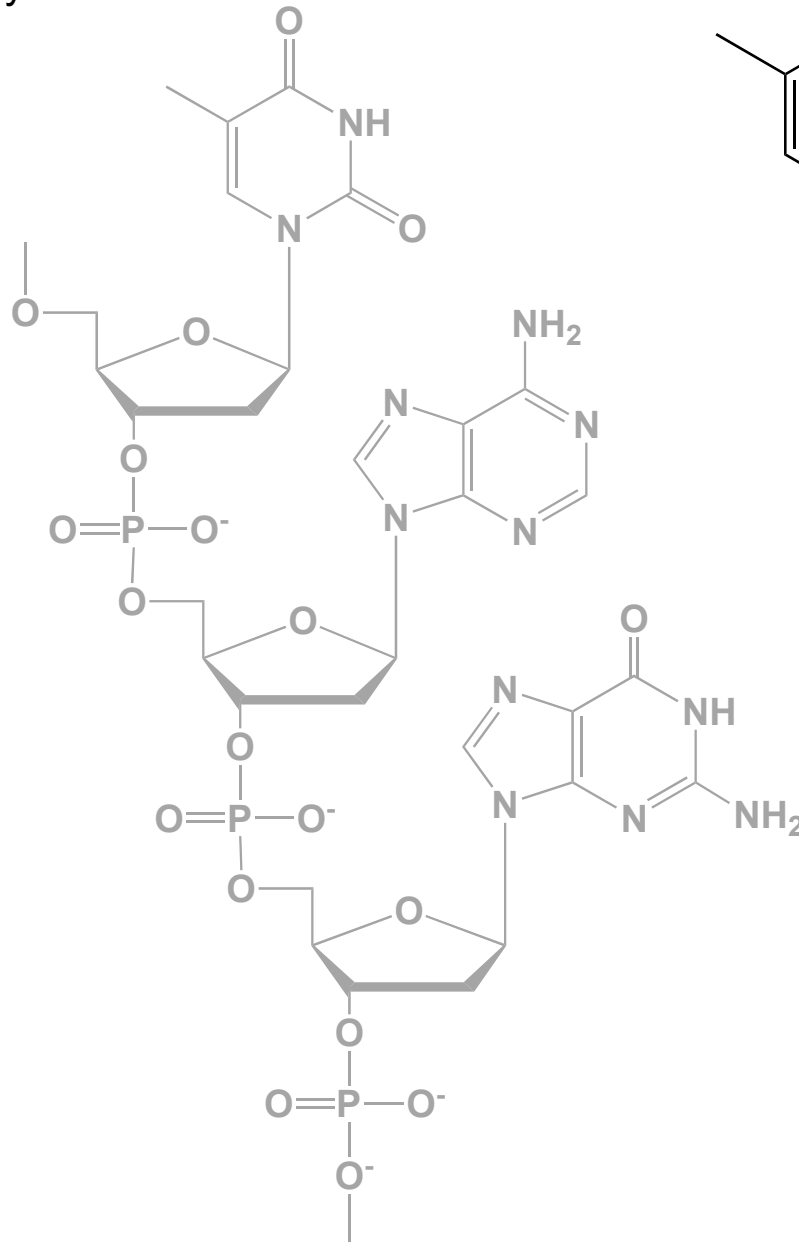
DNA

A look at the Chemistry



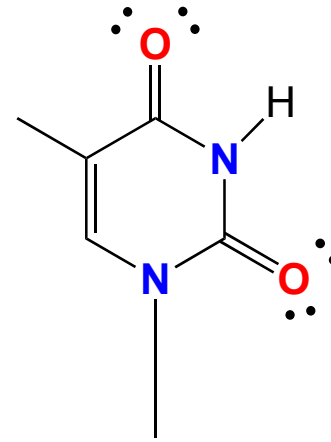
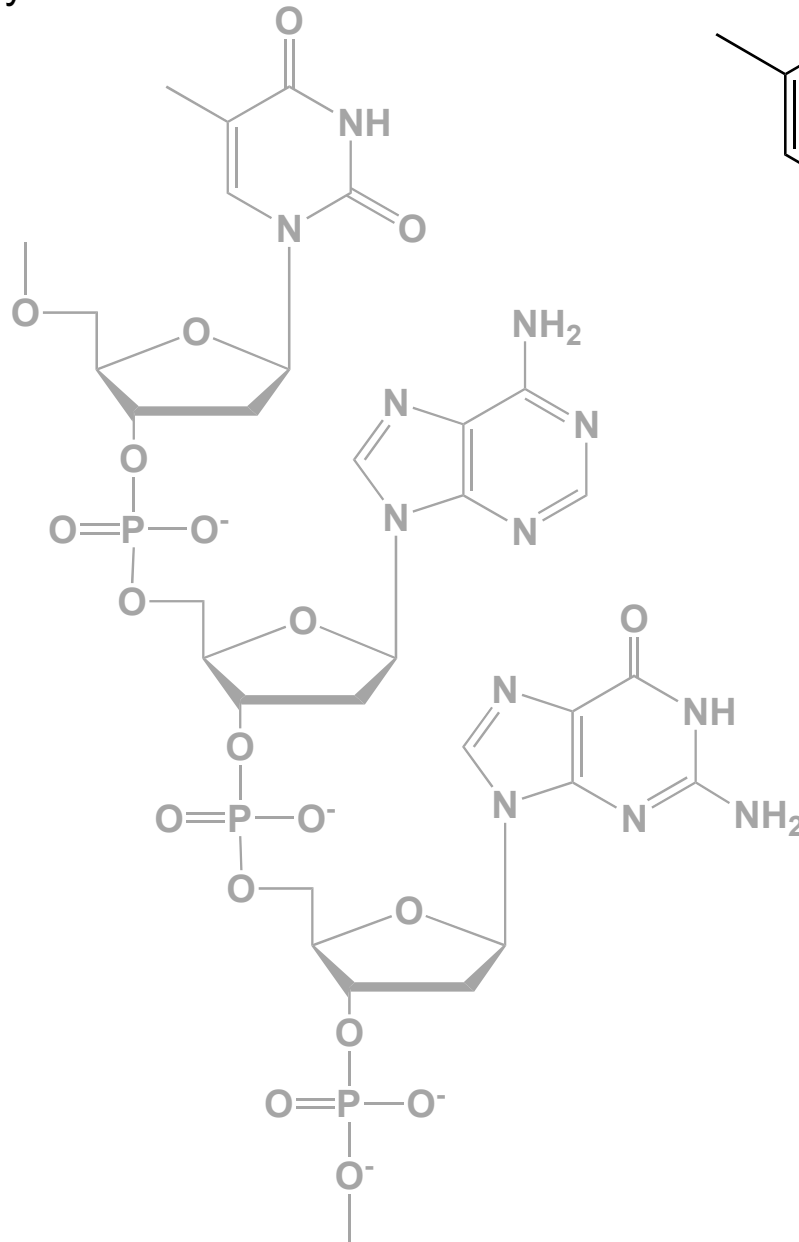
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A look at the Chemistry



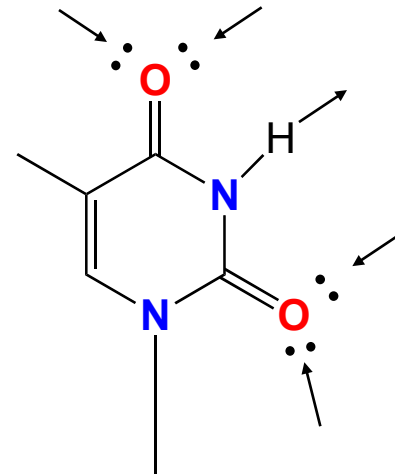
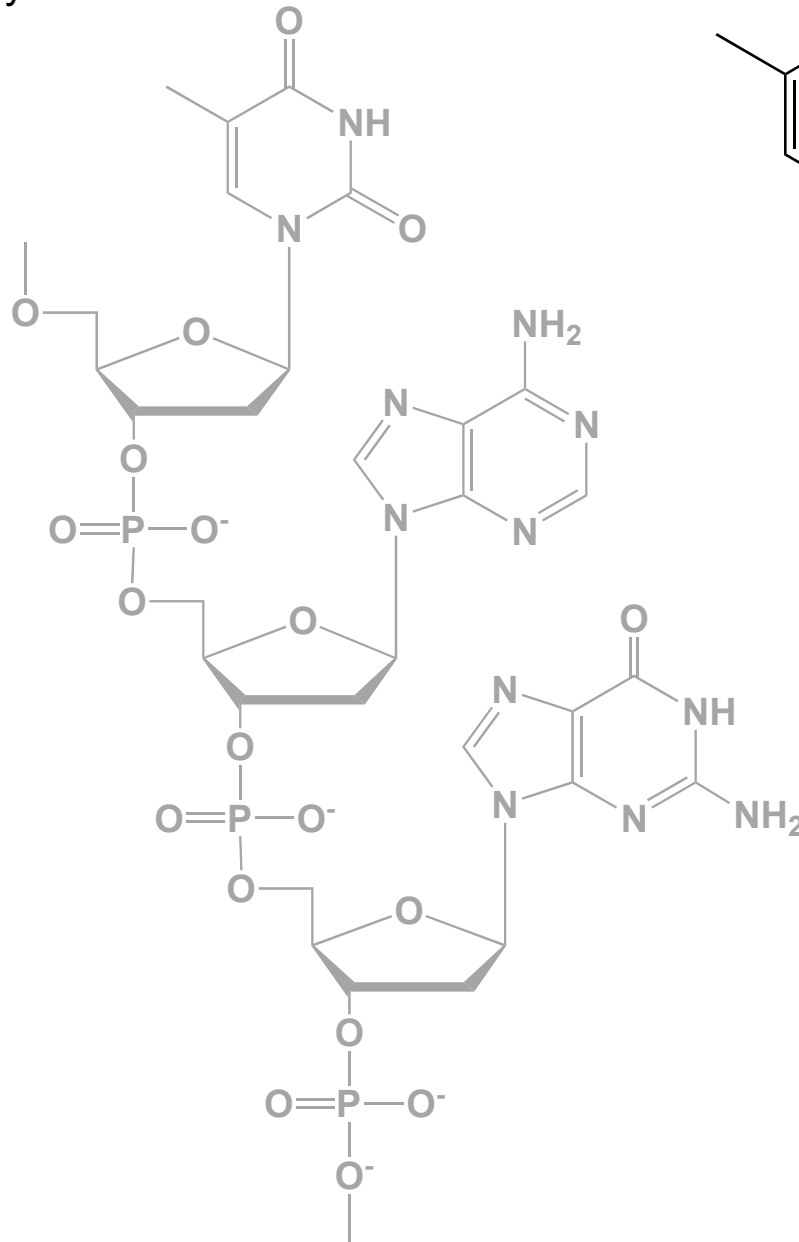
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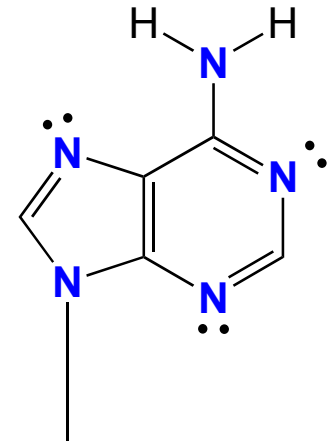
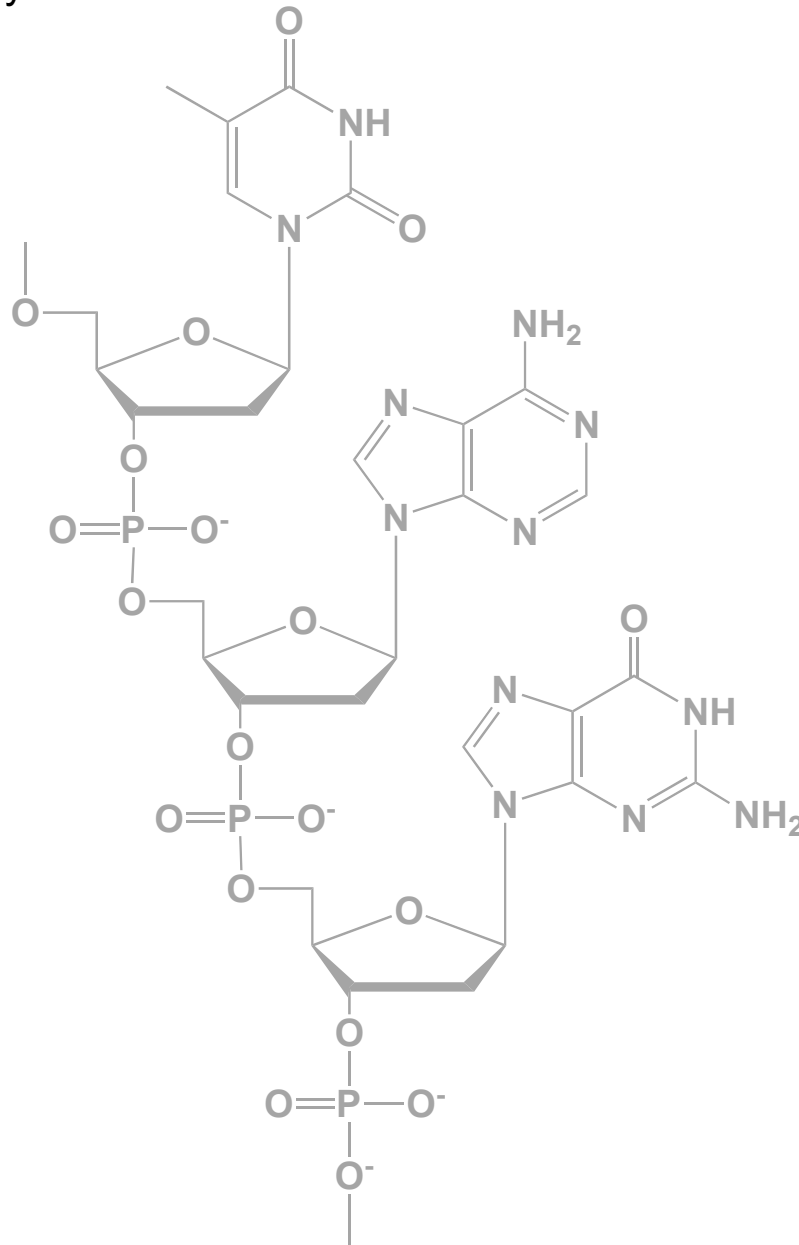
DNA

A look at the Chemistry



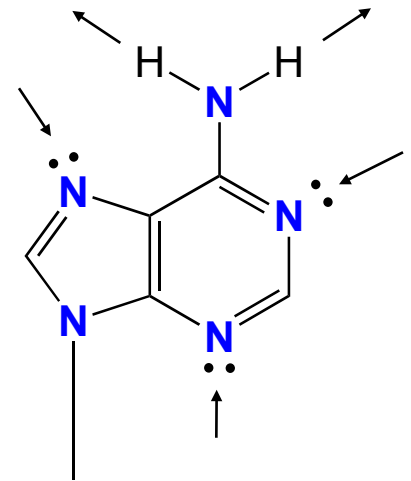
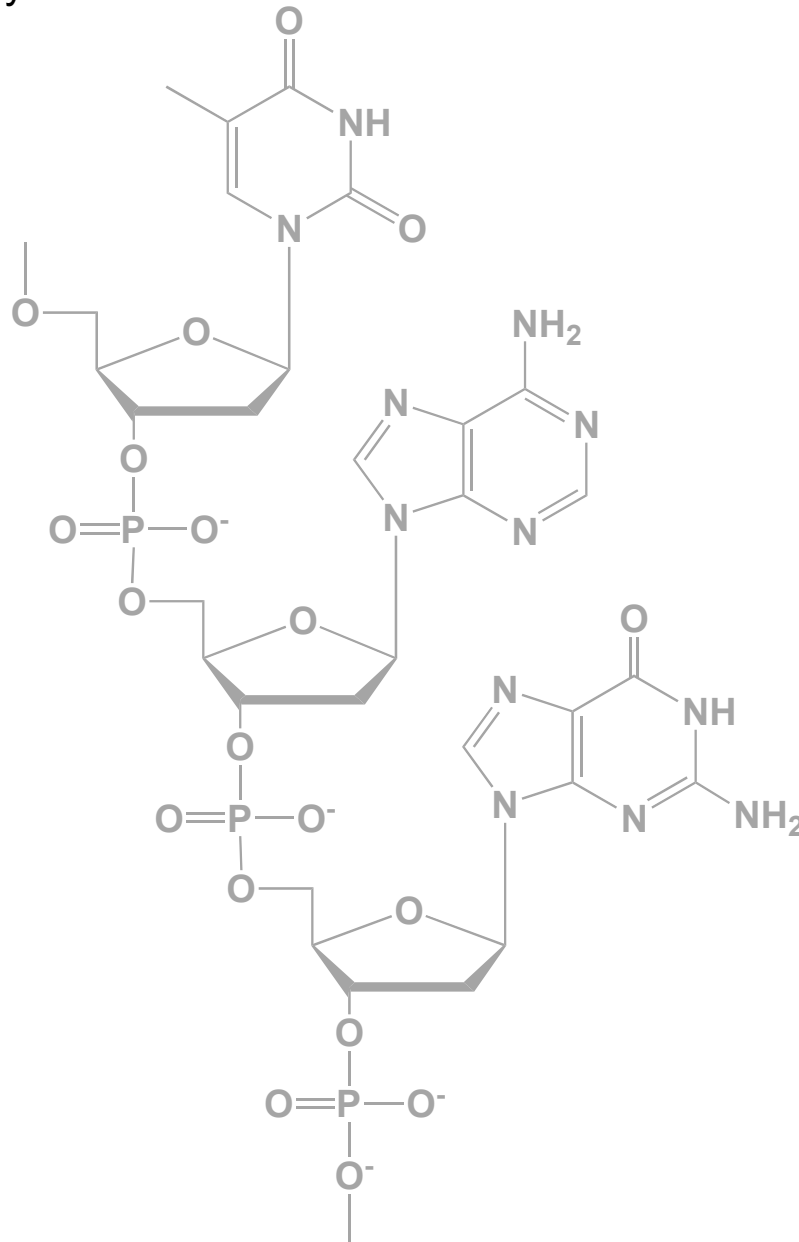
DNA

A look at the Chemistry



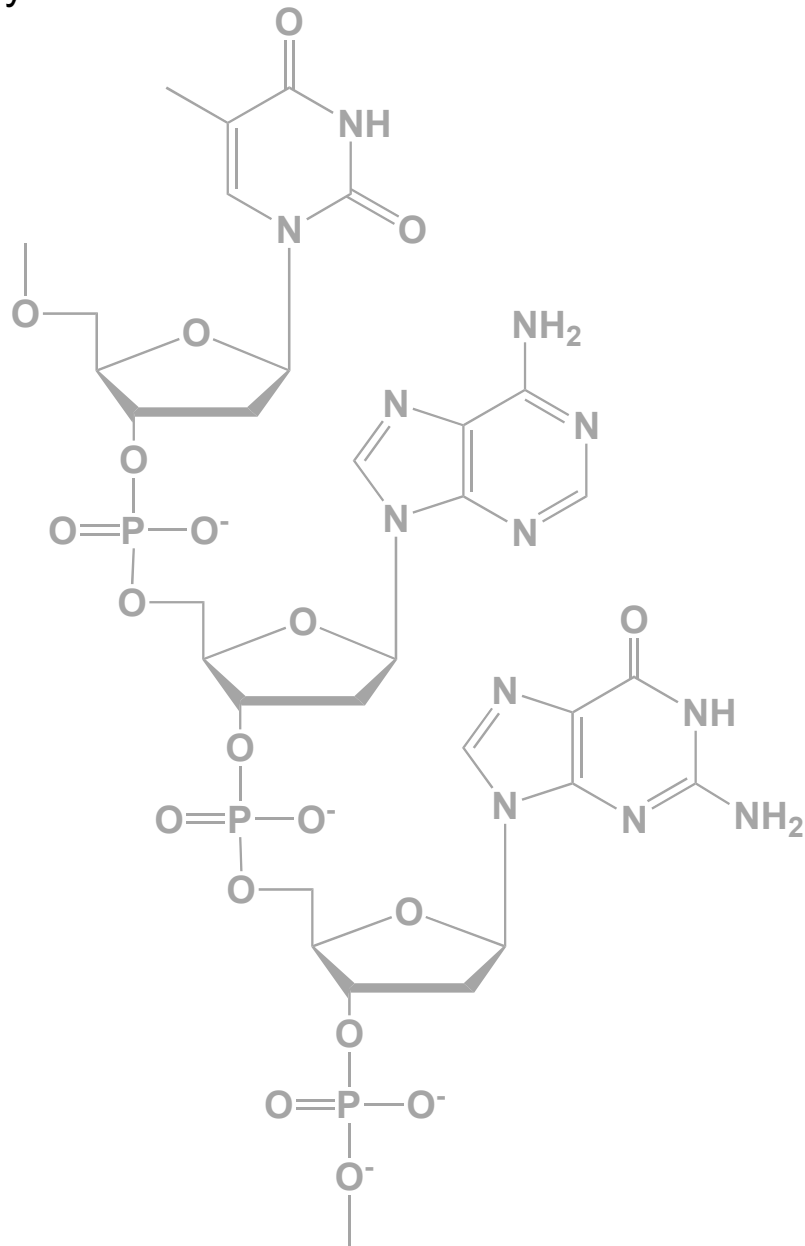
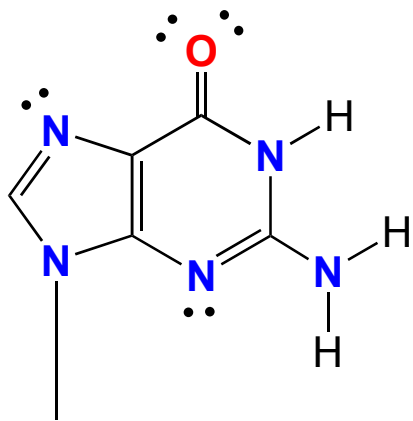
DNA

A look at the Chemistry



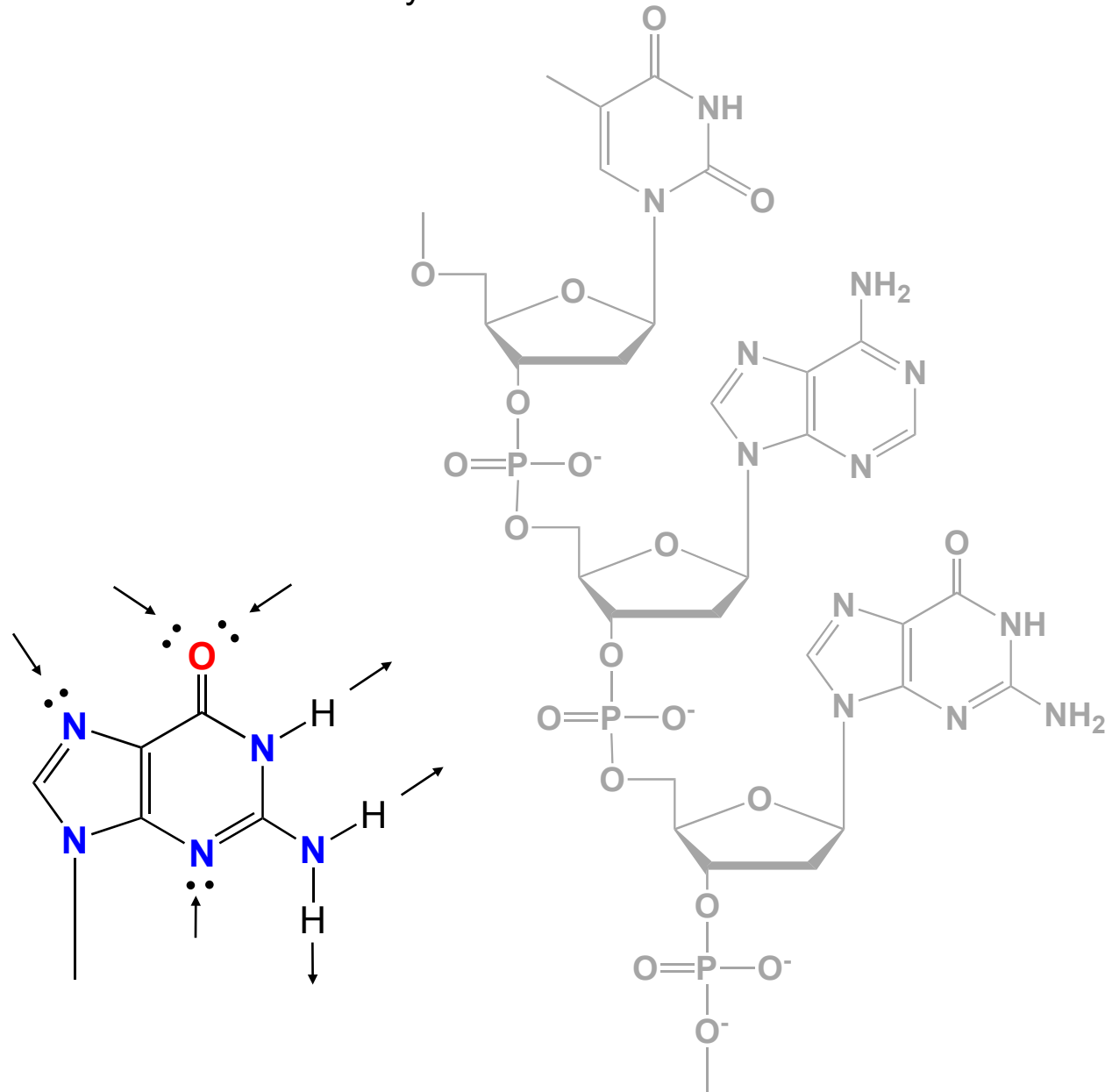
DNA

A look at the Chemistry

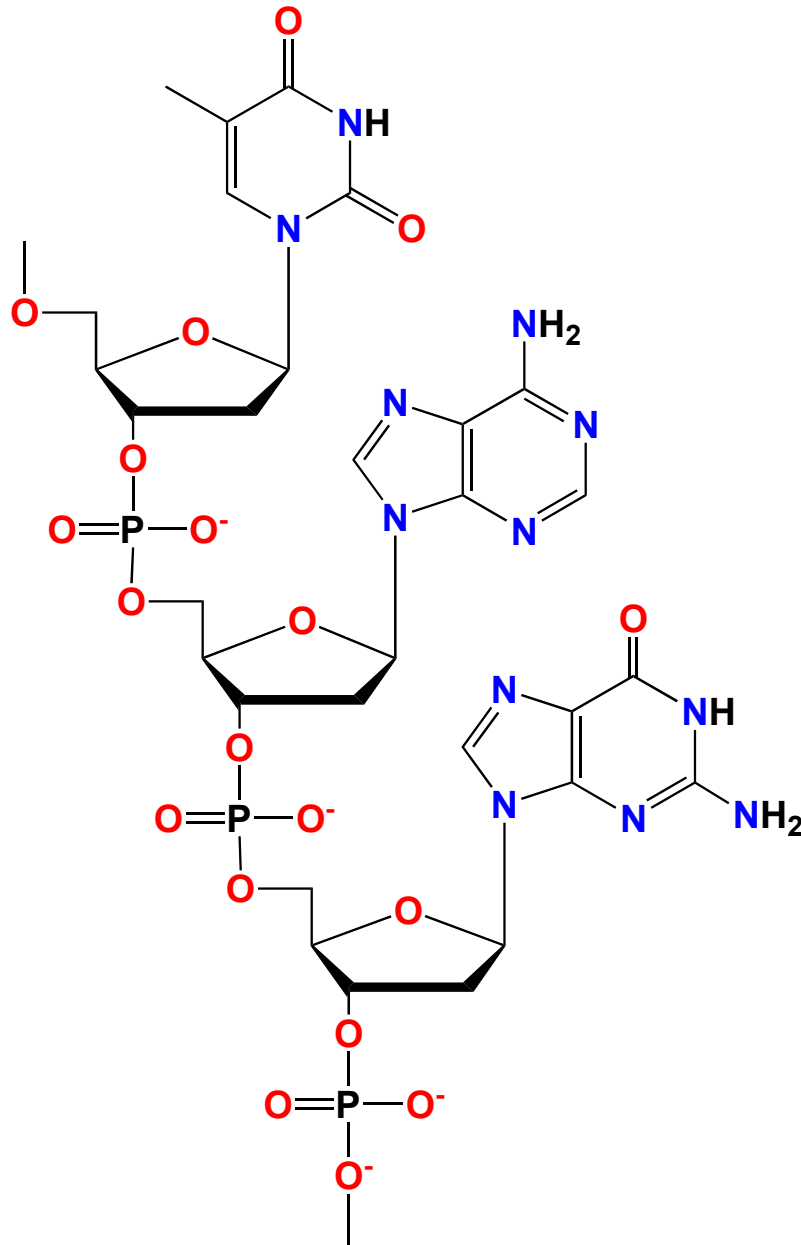


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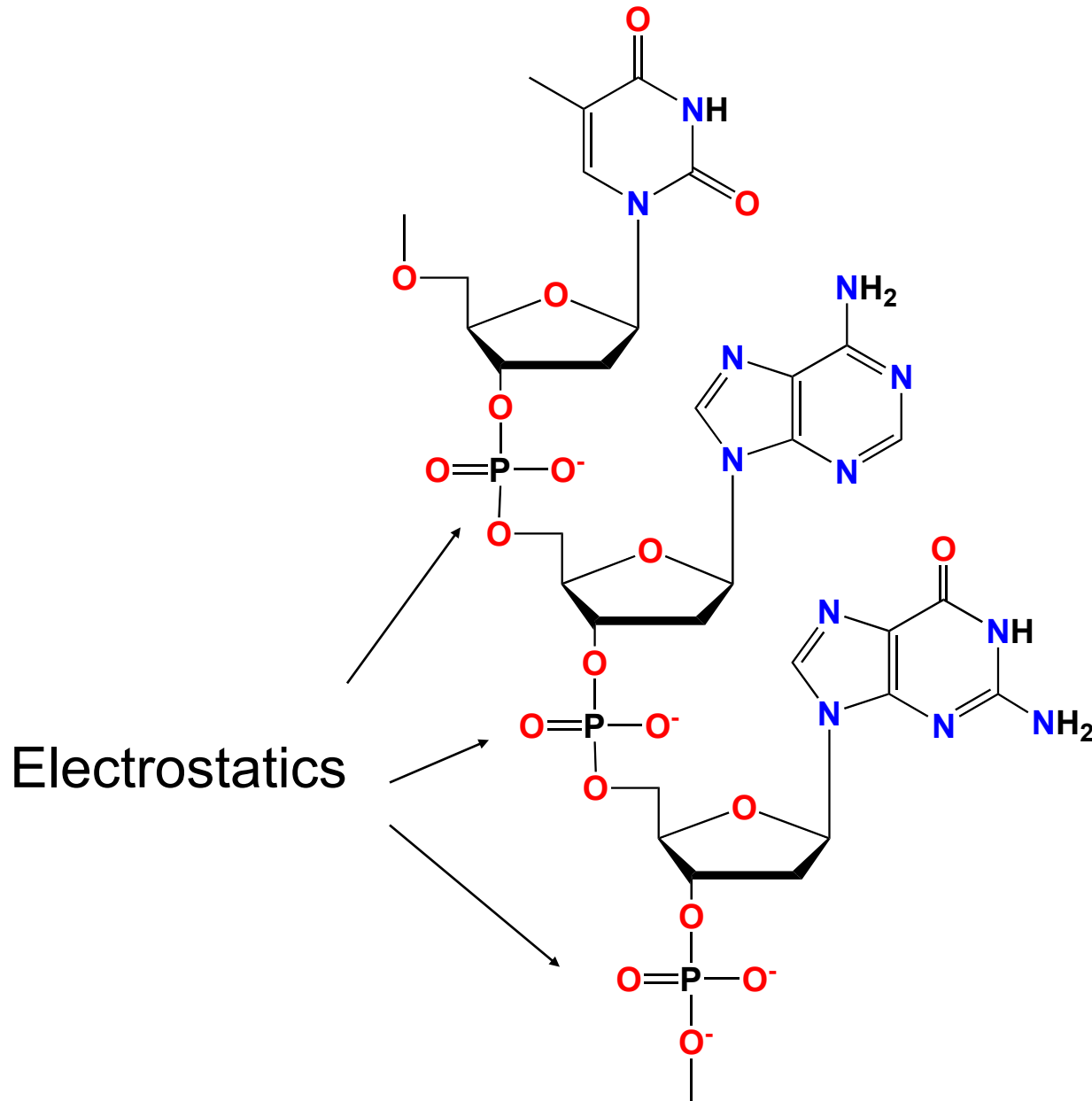
A look at the Chemistry



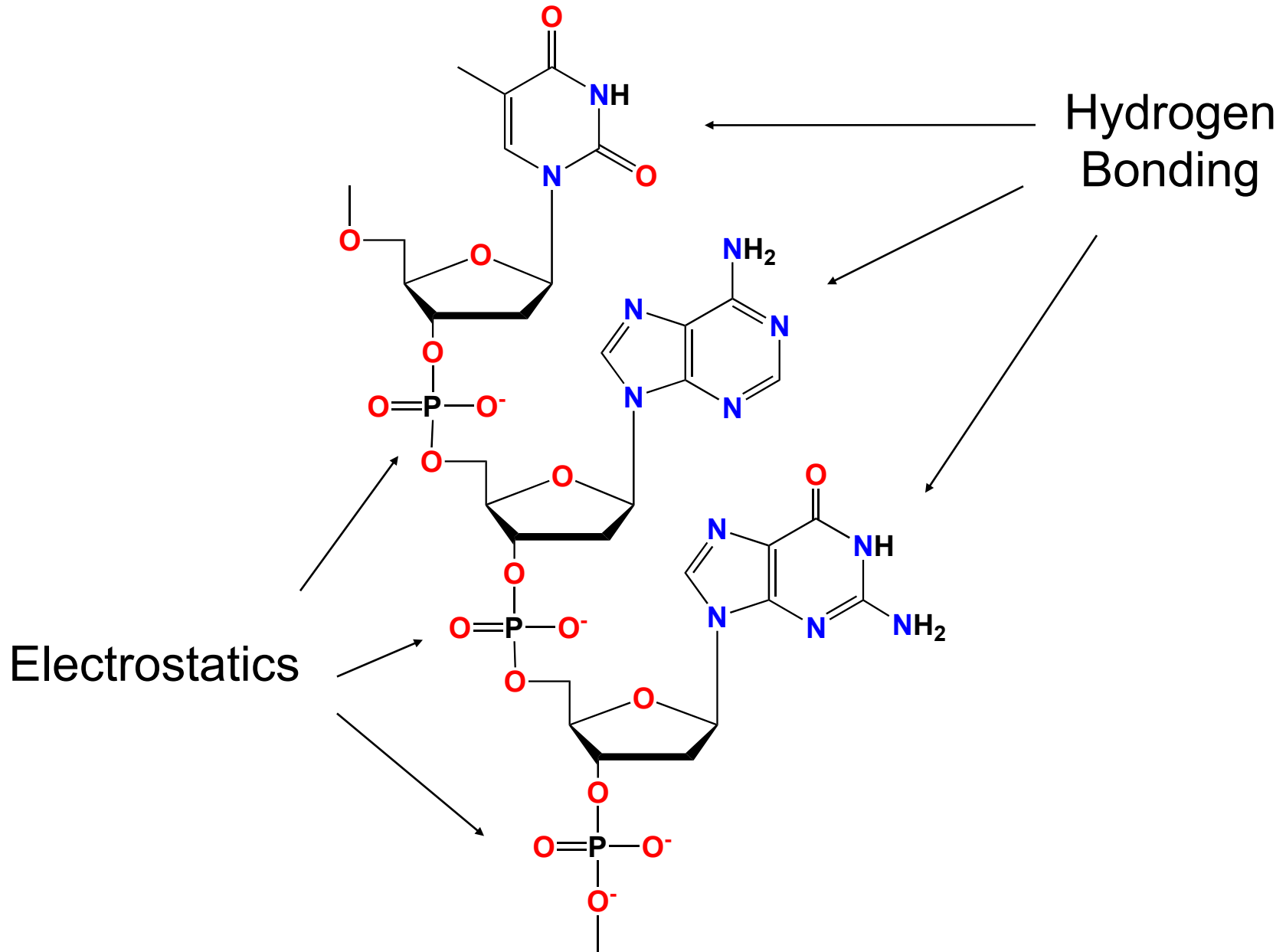
What forces are important?



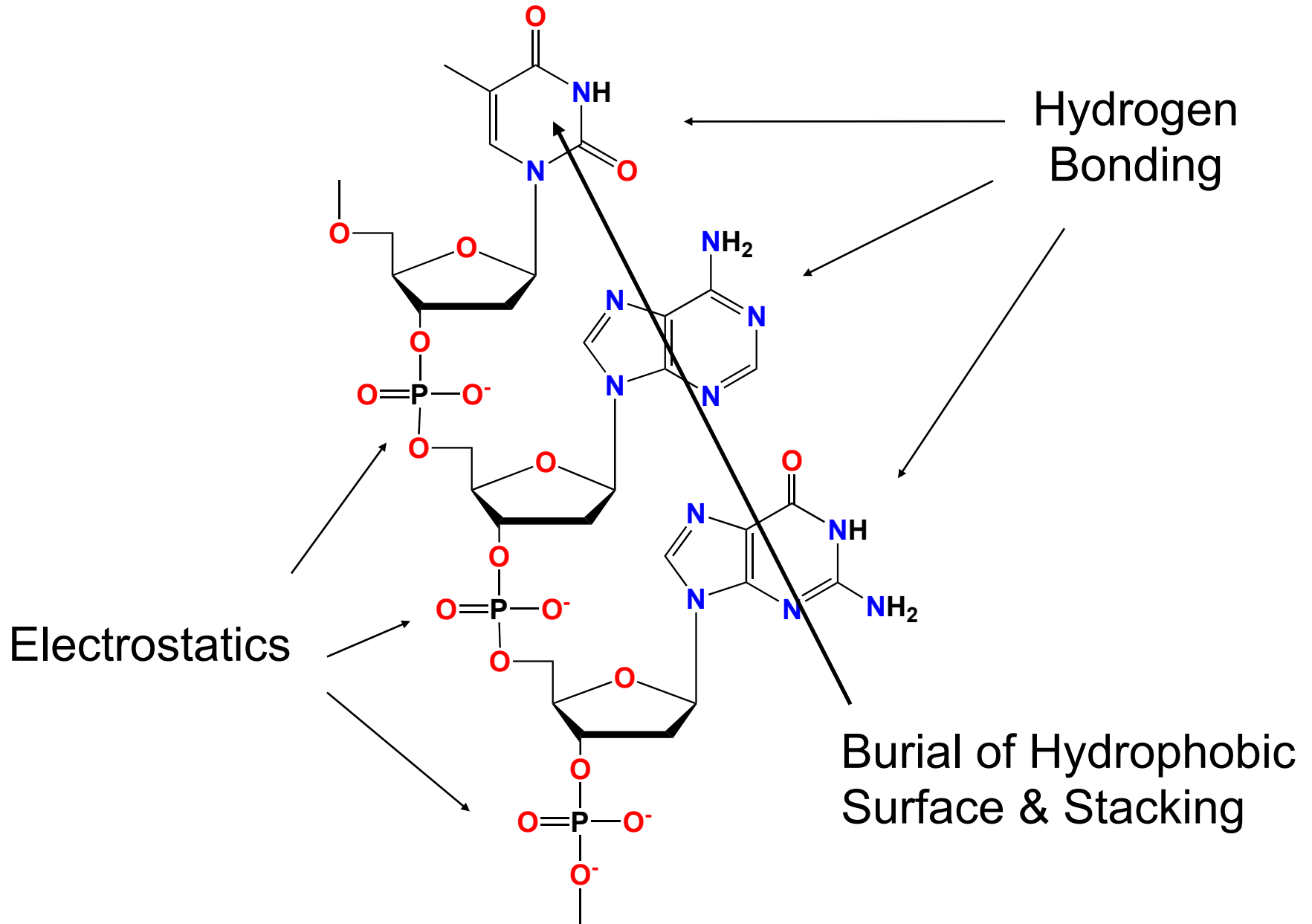
What forces are important?



What forces are important?



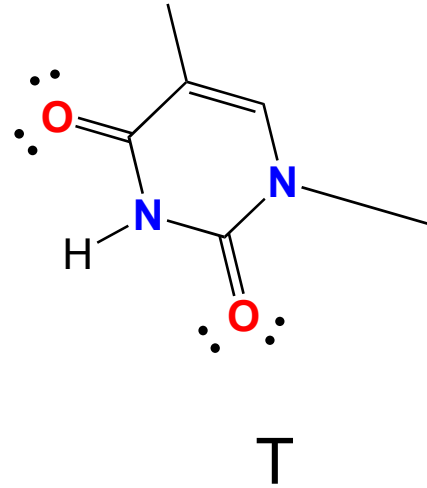
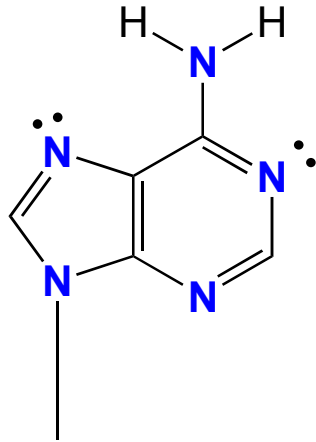
What forces are important?



Base Pairing

(Donors matched to Acceptors)

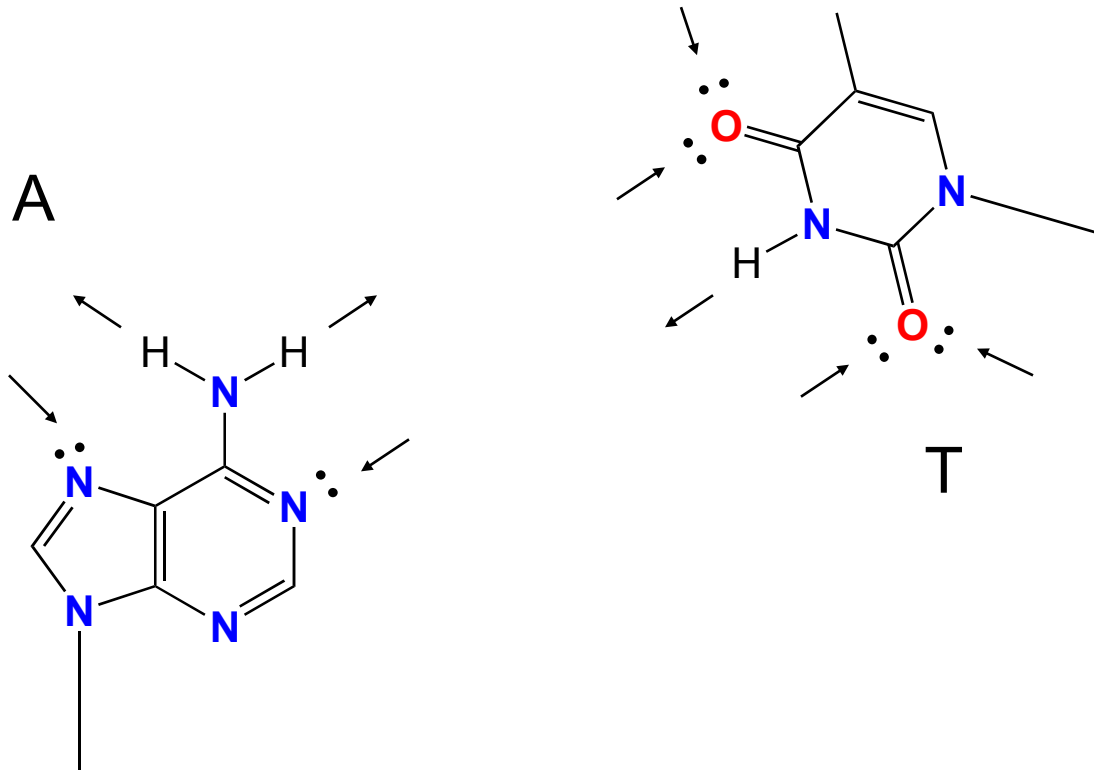
A



T

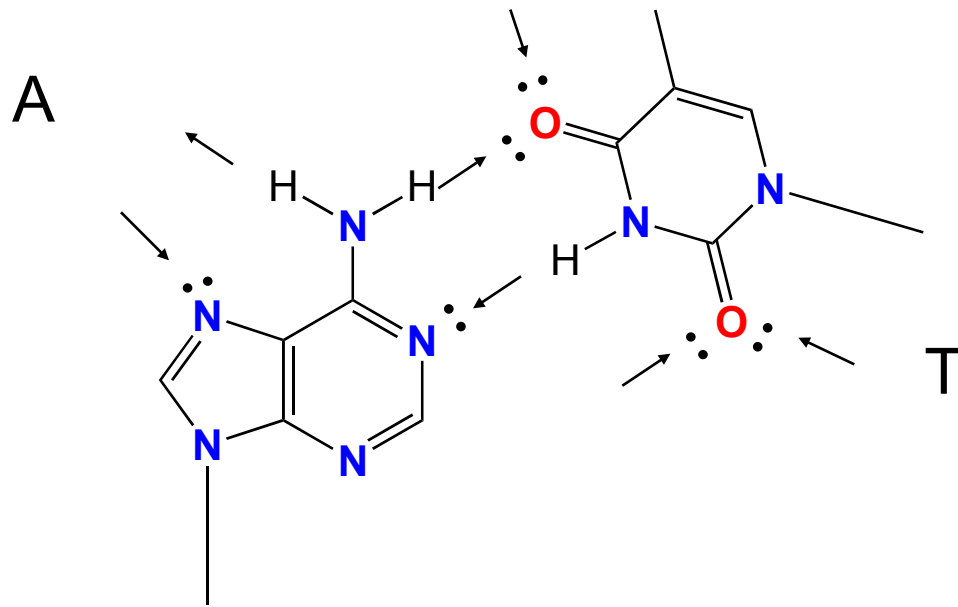
Base Pairing

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Base Pairing

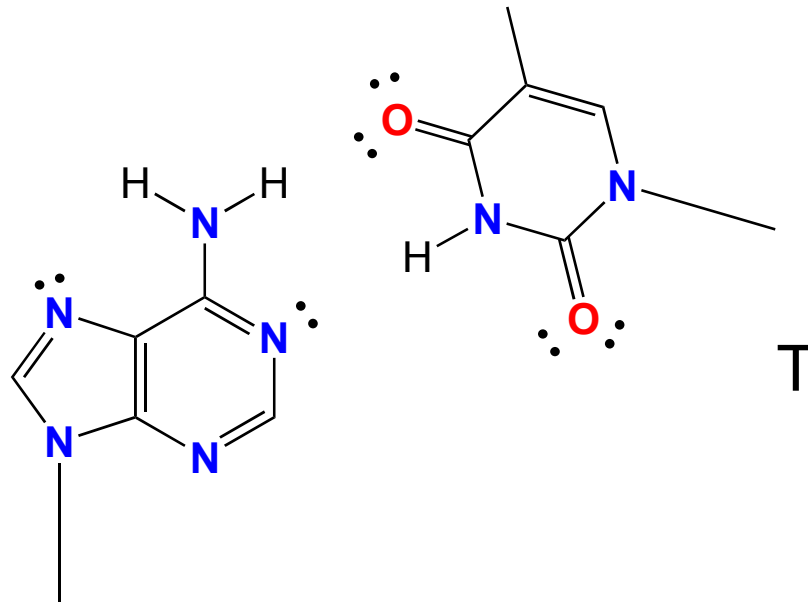
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Base Pairing

(Donors matched to Acceptors)

A



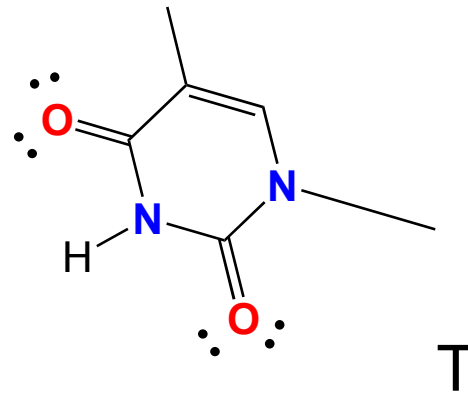
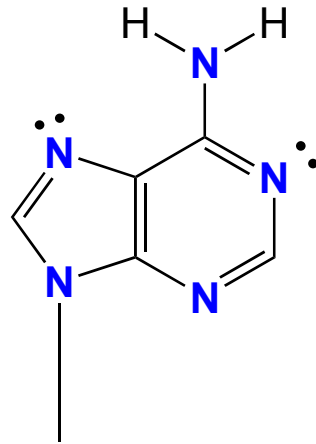
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Base Pairing

(Donors matched to Acceptors)

Major Groove

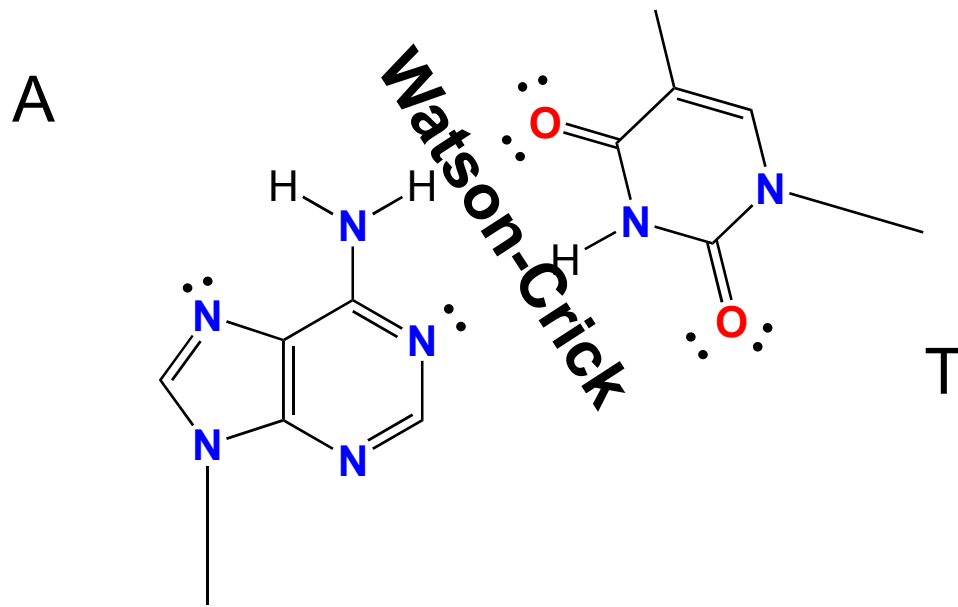
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Minor Groove

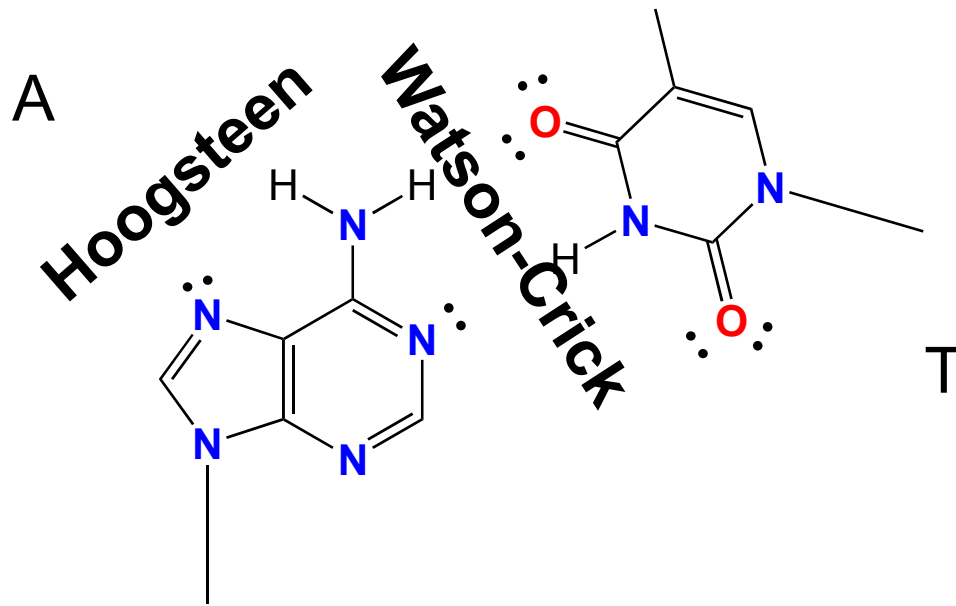
Base Pairing

(Donors matched to Acceptors)



Base Pairing

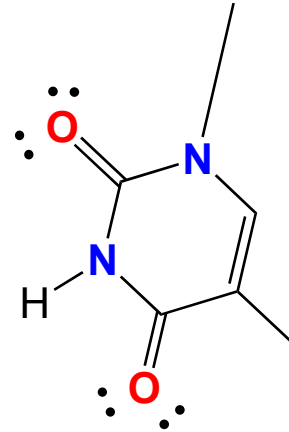
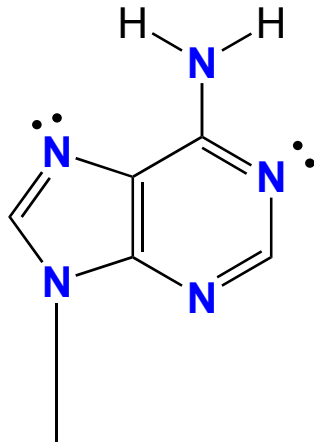
(Donors matched to Acceptors)



Base Pairing

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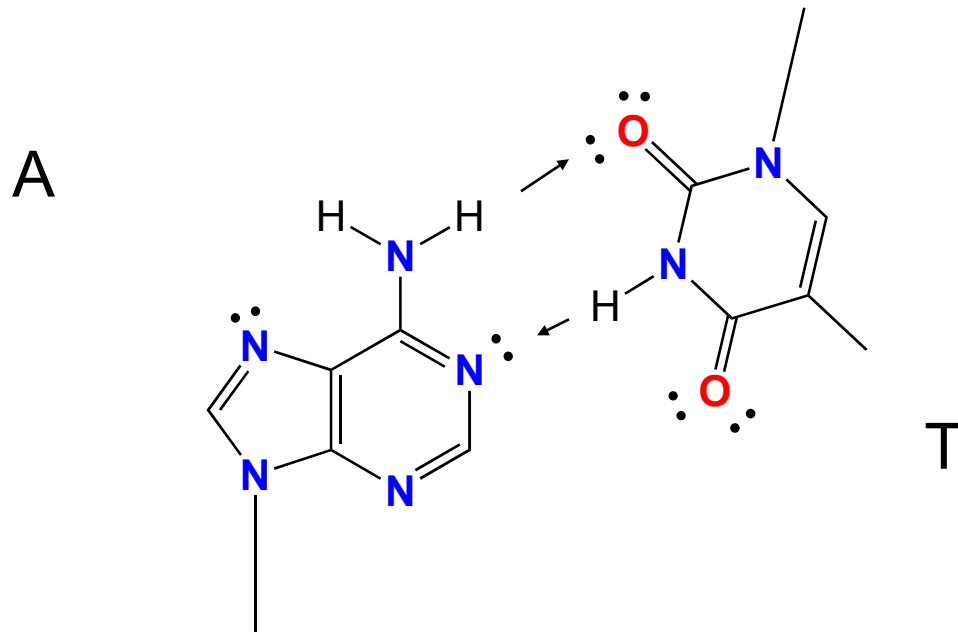
A



T

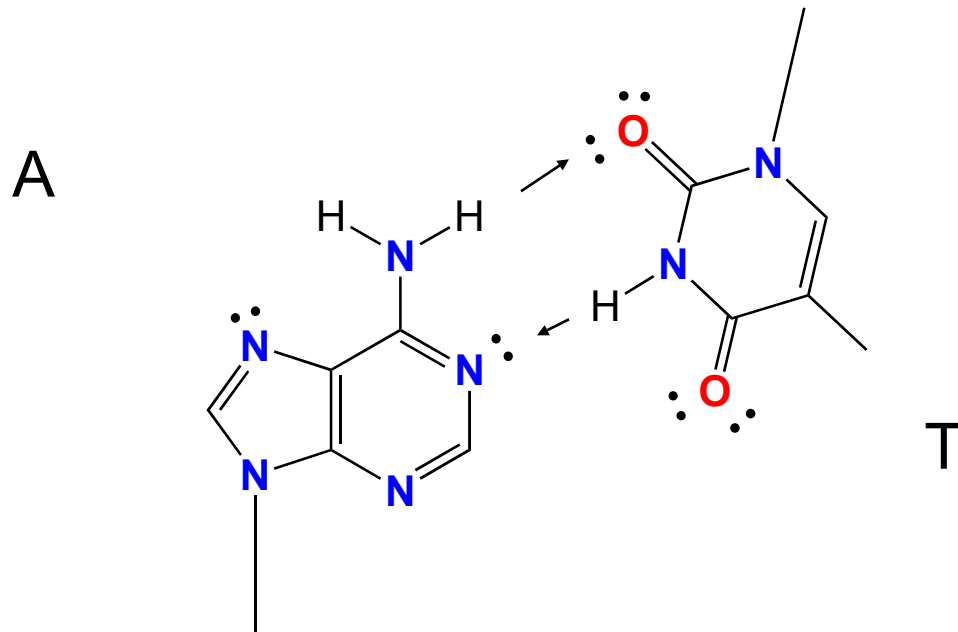
Base Pairing

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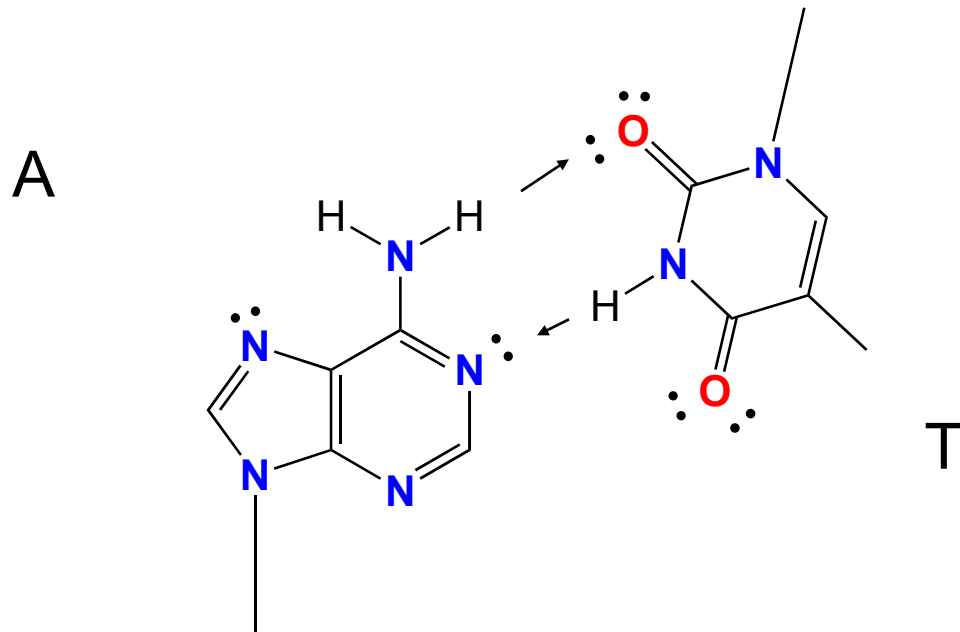
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Good base pairing

Base Pairing

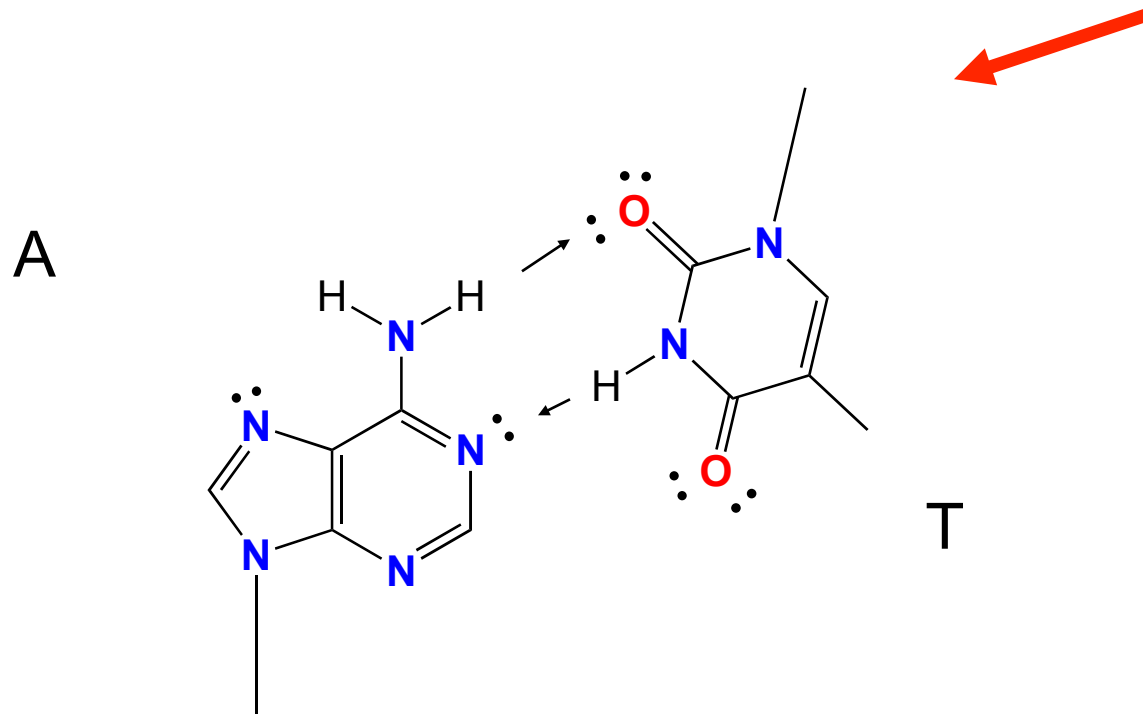
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Good base pairing
Watson-Crick facing

Base Pairing

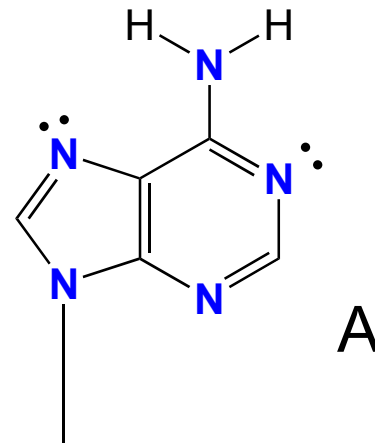
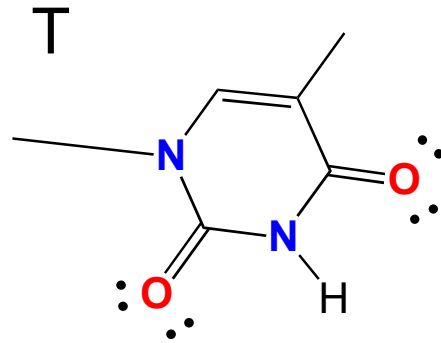
(Donors matched to Acceptors)



Good base pairing
Watson-Crick facing
but *Anti-Watson-Crick* orientation

Base Pairing

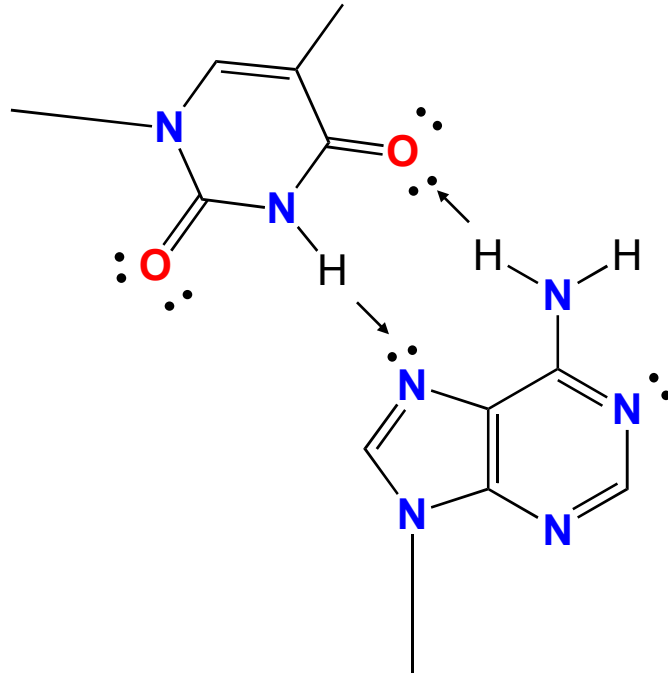
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Base Pairing

(Donors matched to Acceptors)

T

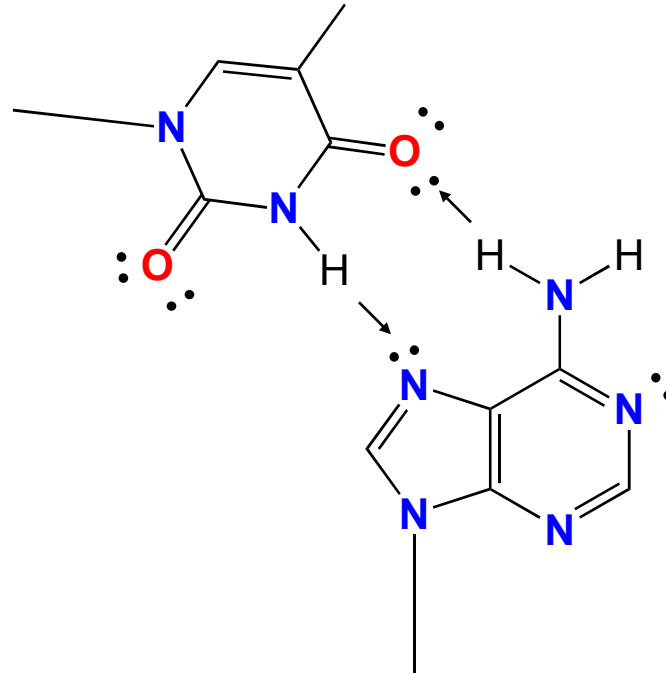


A

Base Pairing

(Donors matched to Acceptors)

T



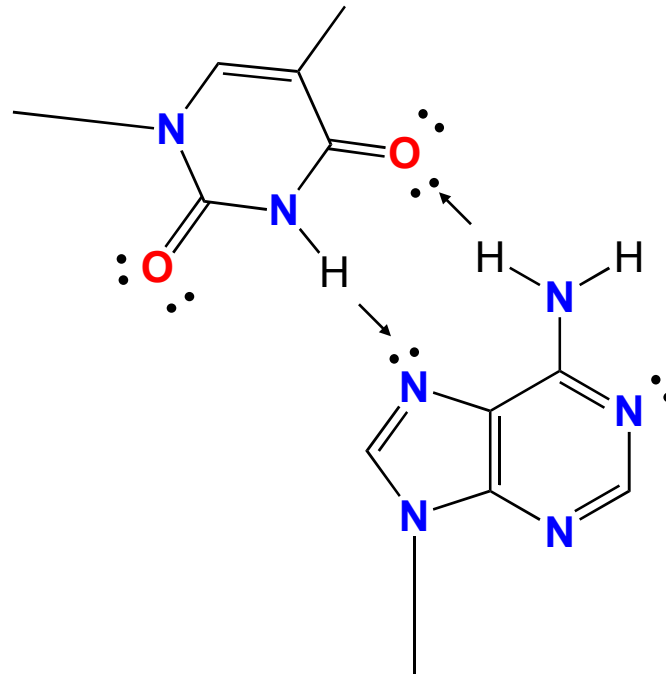
A

Good base pairing

Base Pairing

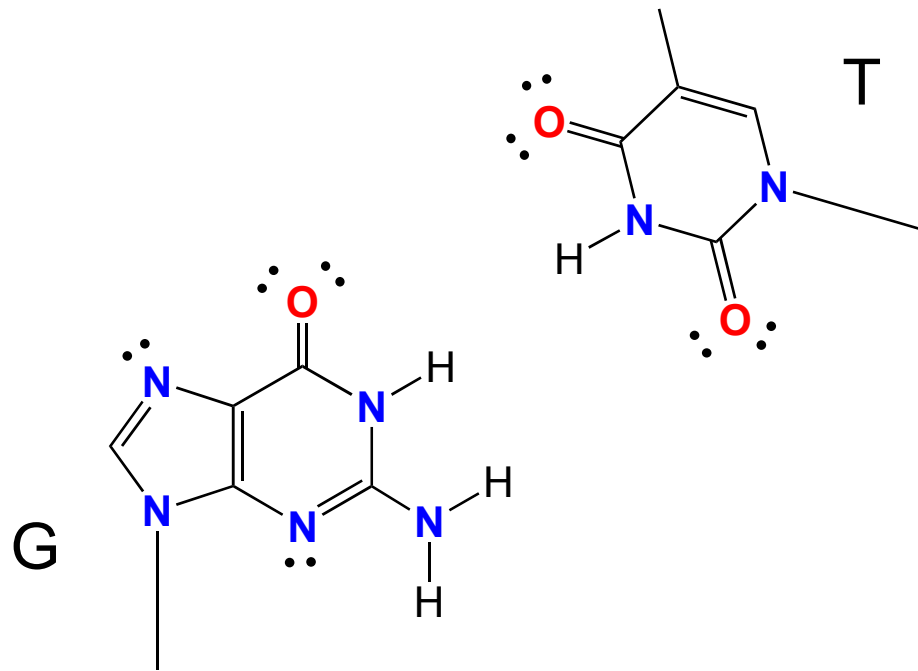
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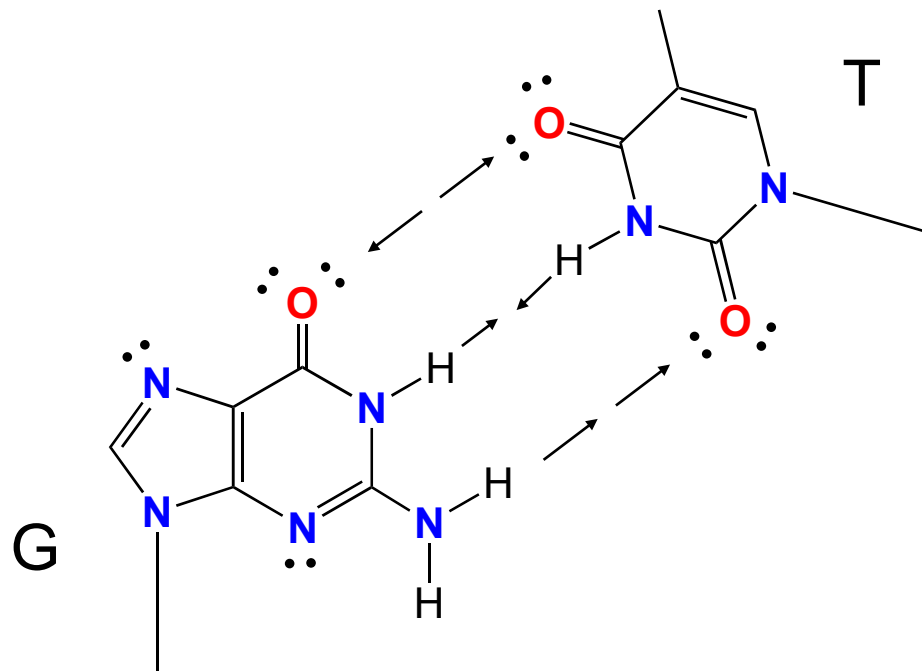
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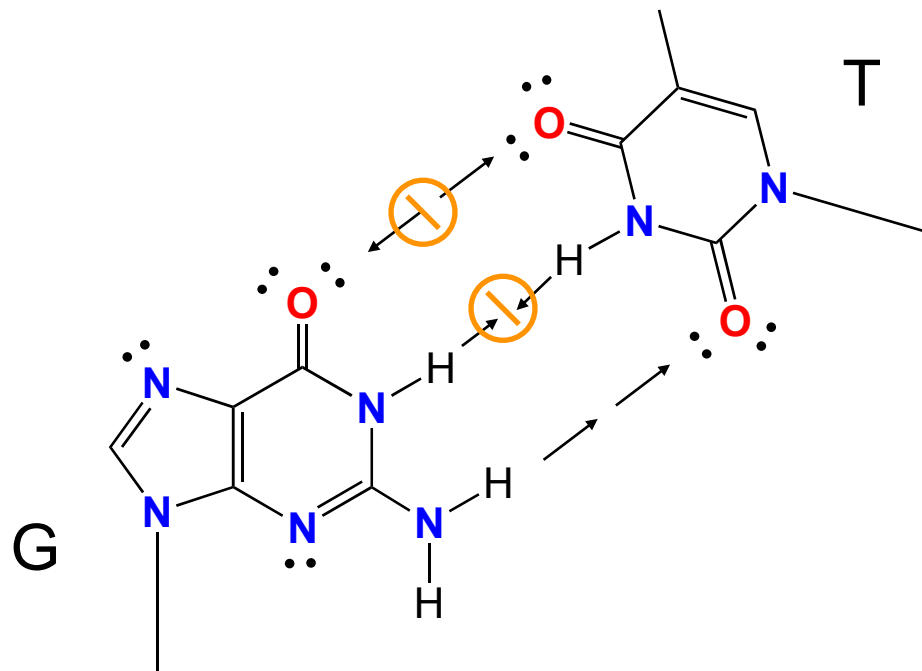


A

Good base pairing
WC-Hoogsteen facing

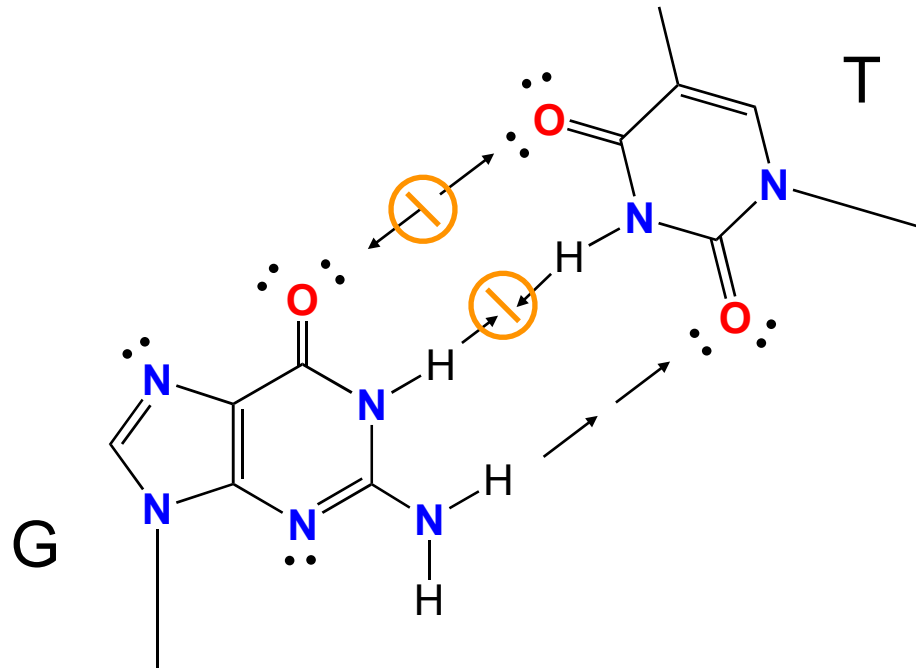


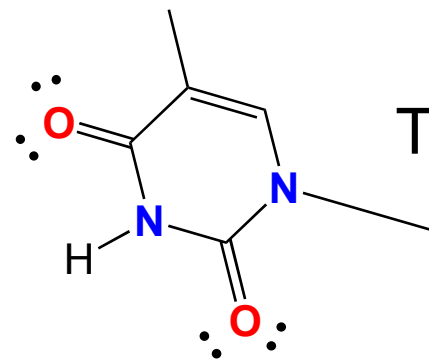
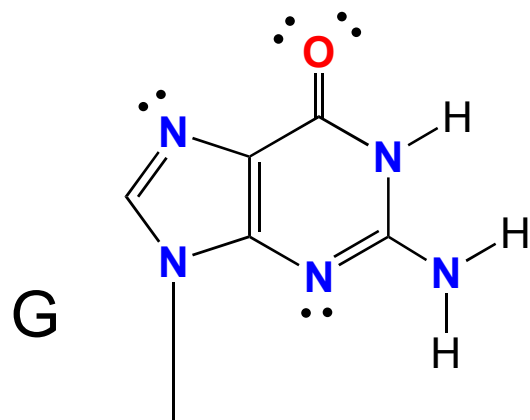


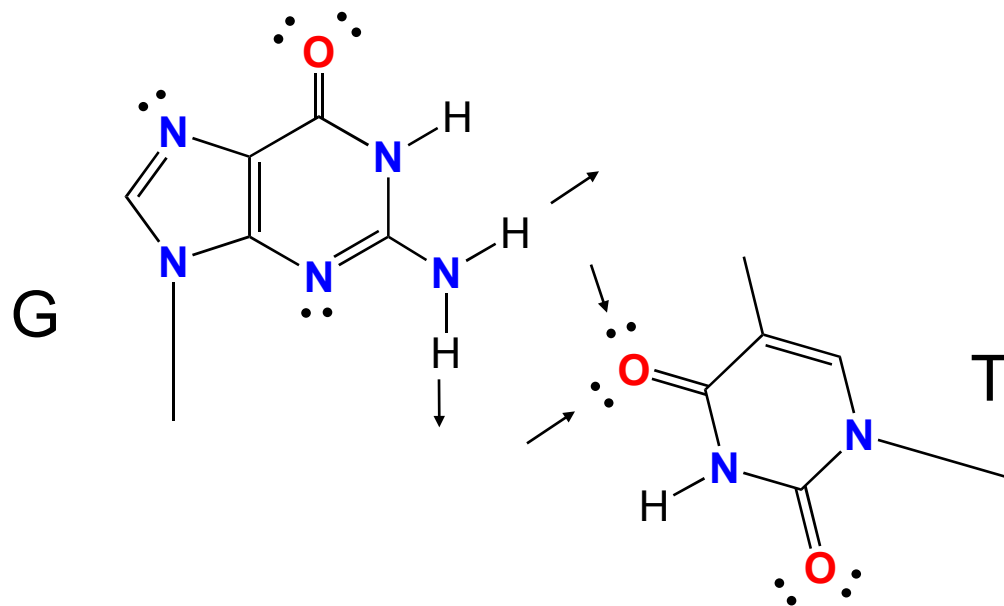


Bad Base Pairing

(Donors *not* matched to Acceptors)

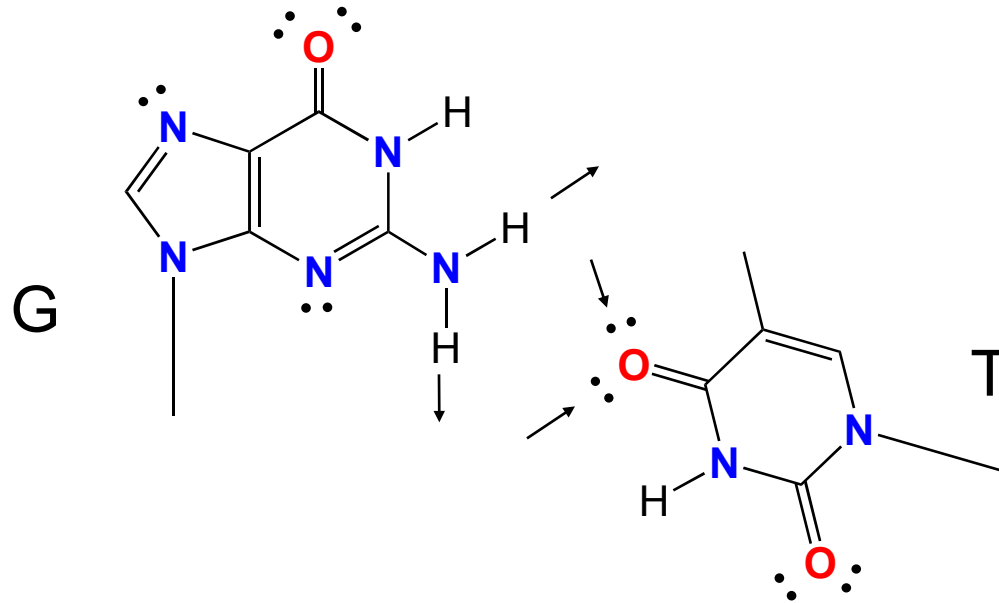




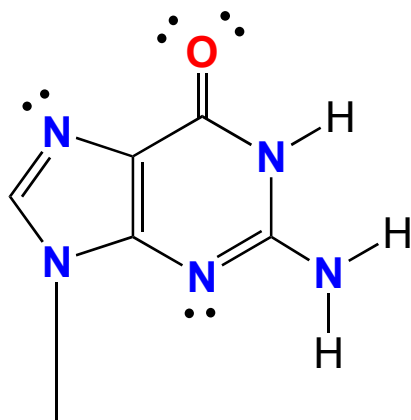


Bad Base Pairing

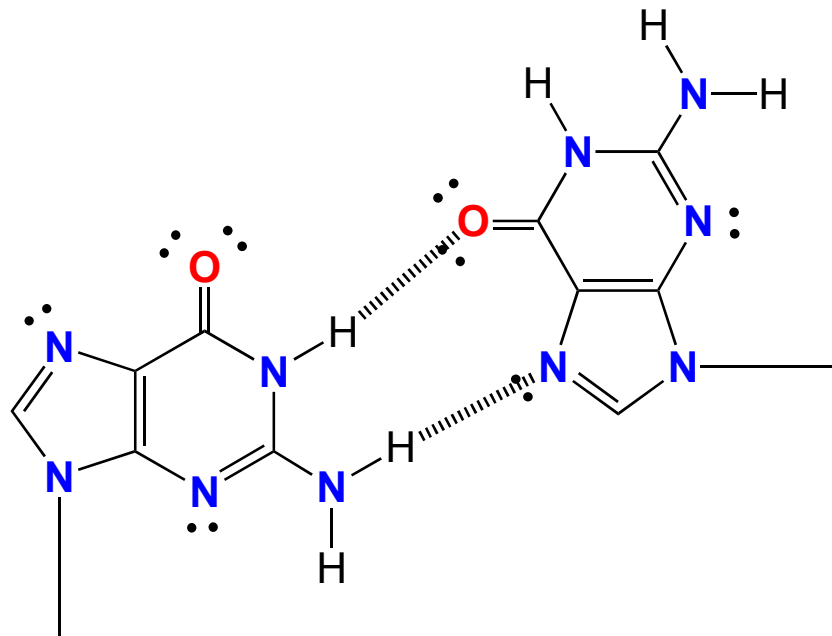
(Donors to Acceptors with *terrible angles*)



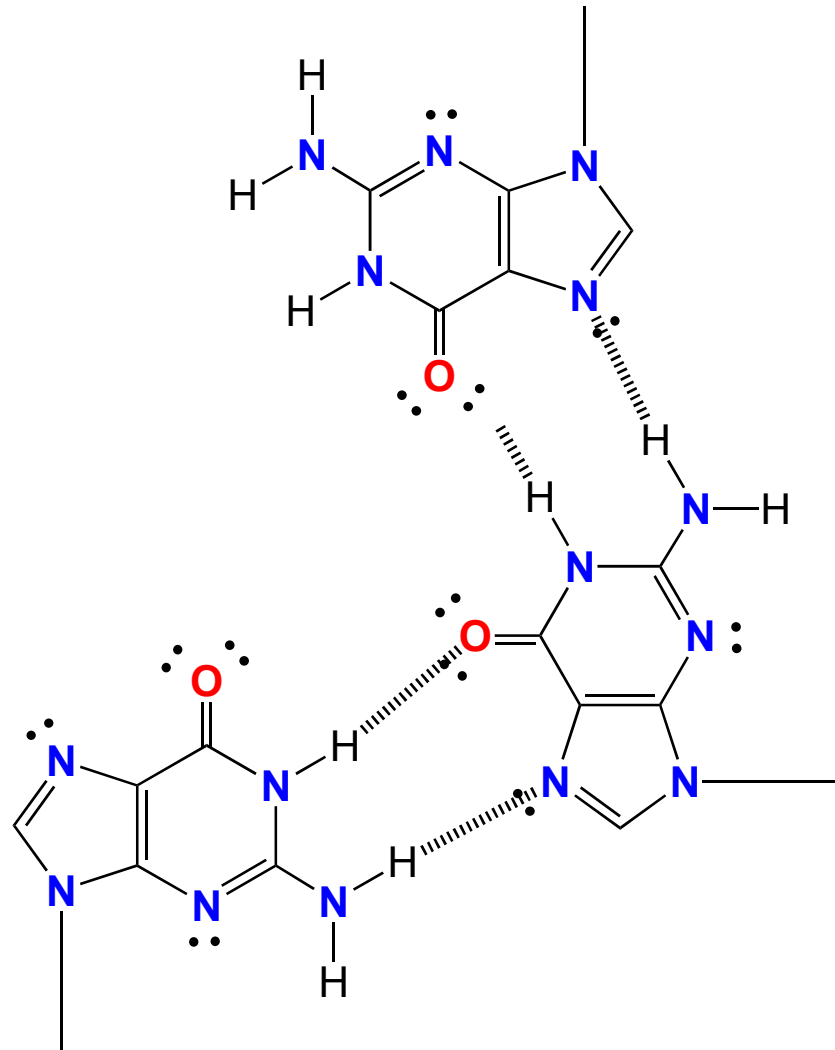
Wild (but good) Base Pairing



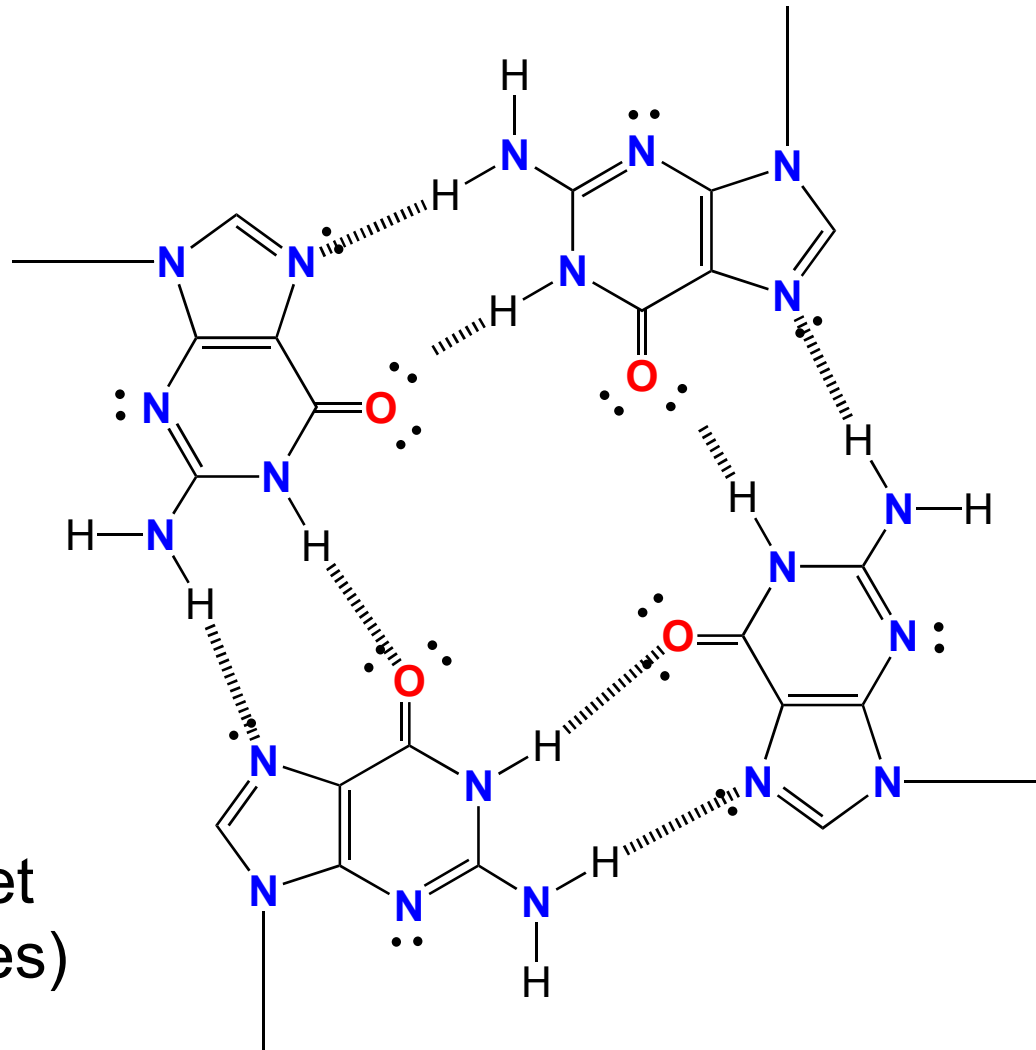
Wild (but good) Base Pairing



Wild (but good) Base Pairing

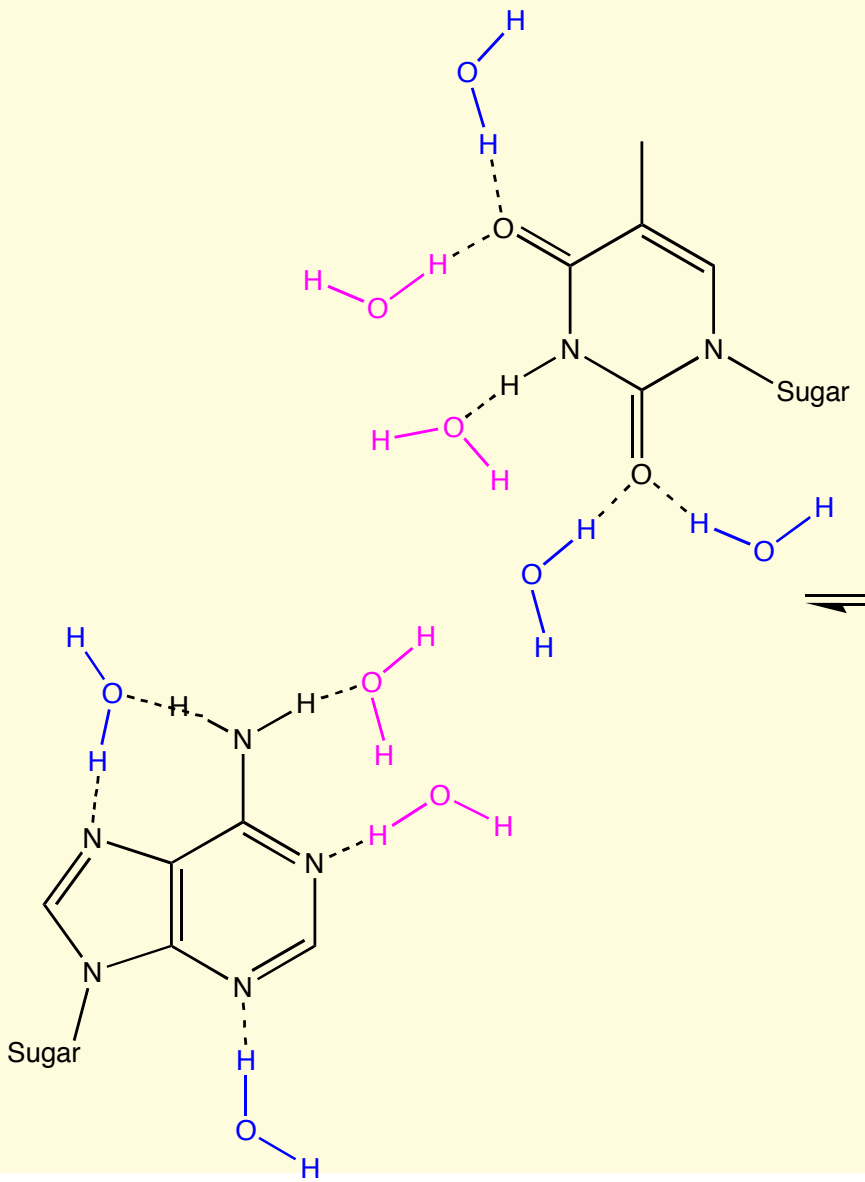


Wild (but good) Base Pairing



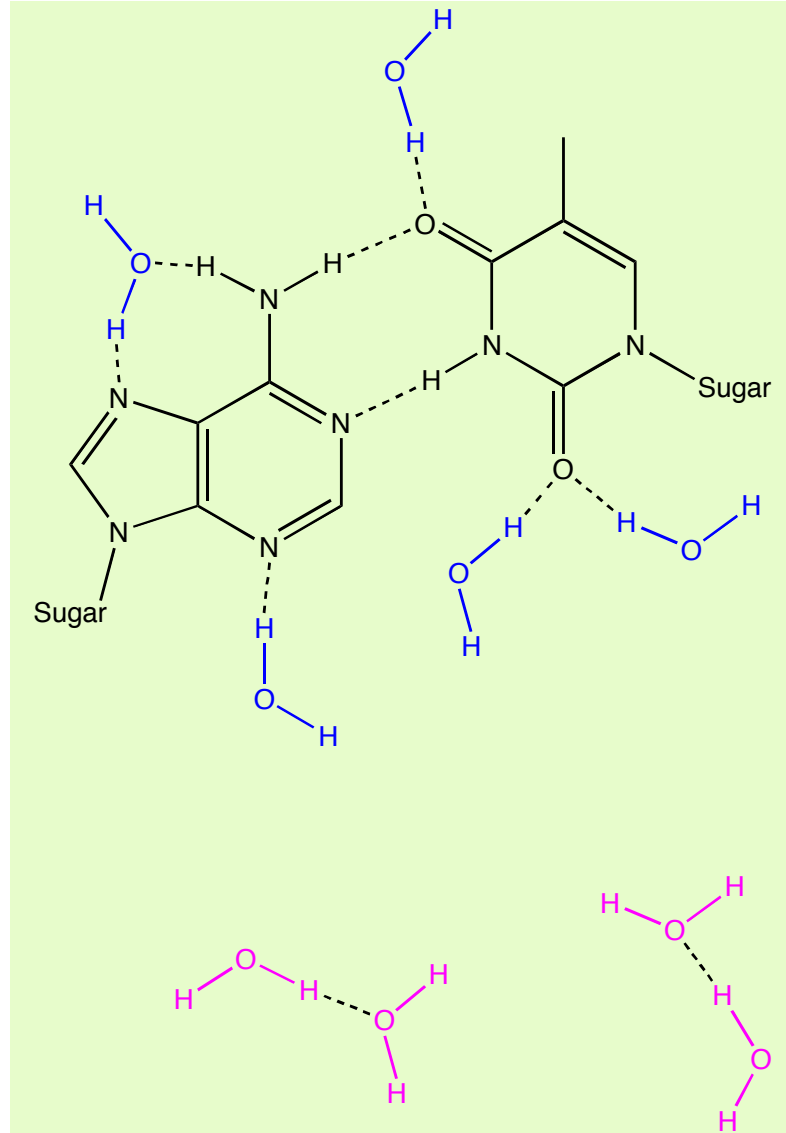
G-quartet
(Telomeres)

AT Base Pair



Ten H-Bonds

Ten H-Bonds



How important are H-bonds in DNA?

J. Am. Chem. Soc., Vol. 117, No. 7, 1995 1867

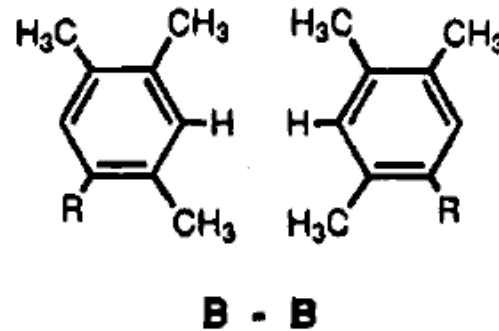
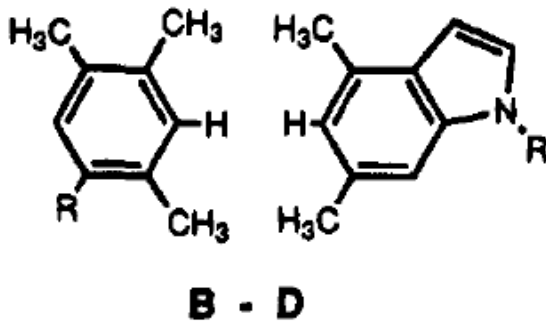
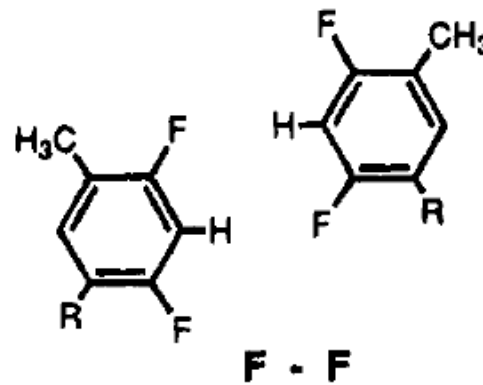
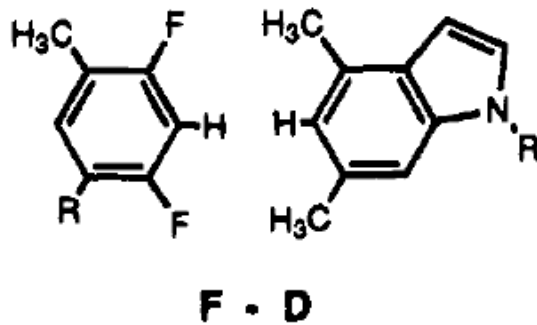
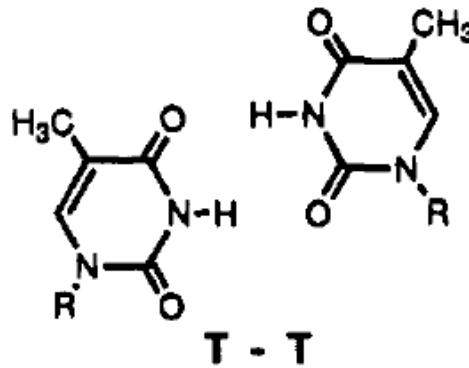
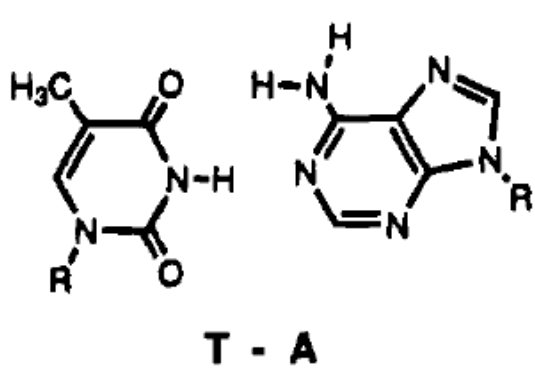


Table 1. Free Energies and Melting Temperatures for Dodecamer Duplexes Containing a Variable T-X, F-X, B-X, or D-X Base Pair (X = A, T, C, G)

duplex	T_m (°C) ^a	$-\Delta G_{25}^{\circ}$ (kcal)
5'-CTTTTC[T]TTCTT 3'-GAAAAG[A]AAGAA	39.4	12.3
5'-CTTTTC[T]TTCTT 3'-GAAAAG[C]AAGAA	26.4	8.7
5'-CTTTTC[T]TTCTT 3'-GAAAAG[G]AAGAA	30.7	9.3
5'-CTTTTC[T]TTCTT 3'-GAAAAG[T]AAGAA	27.1	8.9
5'-CTTTTC[F]TTCTT 3'-GAAAAG[A]AAGAA	21.4	7.4
5'-CTTTTC[F]TTCTT 3'-GAAAAG[C]AAGAA	25.0	8.2
5'-CTTTTC[F]TTCTT 3'-GAAAAG[G]AAGAA	23.0	8.0
5'-CTTTTC[F]TTCTT 3'-GAAAAG[T]AAGAA	20.2	7.3
5'-CTTTTC[B]TTCTT 3'-GAAAAG[A]AAGAA	21.0	7.5
5'-CTTTTC[B]TTCTT 3'-GAAAAG[C]AAGAA	22.9	7.8
5'-CTTTTC[B]TTCTT 3'-GAAAAG[G]AAGAA	20.1	7.6
5'-CTTTTC[B]TTCTT 3'-GAAAAG[T]AAGAA	20.3	6.7
5'-CTTTTC[D]TTCTT 3'-GAAAAG[A]AAGAA	20.8	7.4
5'-CTTTTC[D]TTCTT 3'-GAAAAG[C]AAGAA	22.2	7.6
5'-CTTTTC[D]TTCTT 3'-GAAAAG[G]AAGAA	19.7	7.4
5'-CTTTTC[D]TTCTT 3'-GAAAAG[T]AAGAA	17.6	6.9

^a Conditions: 100 mM NaCl, 10 mM MgCl₂, 10 mM Na · PIPES, pH 7.0, 1.6 μM each strand.

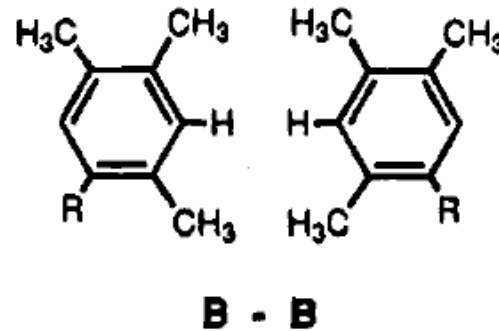
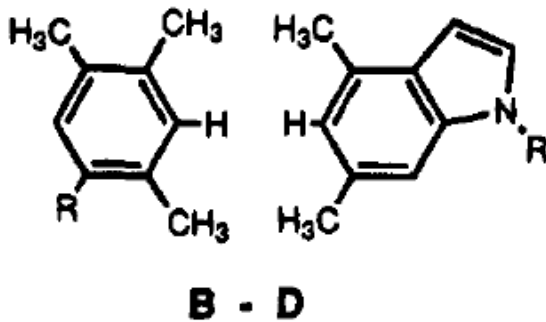
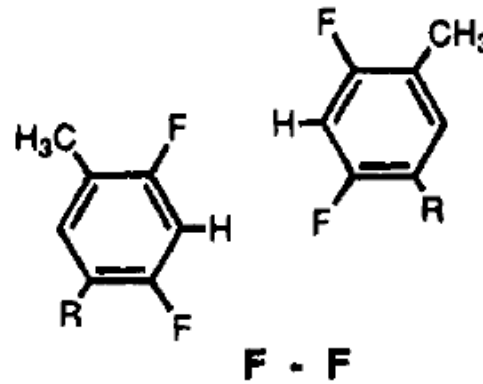
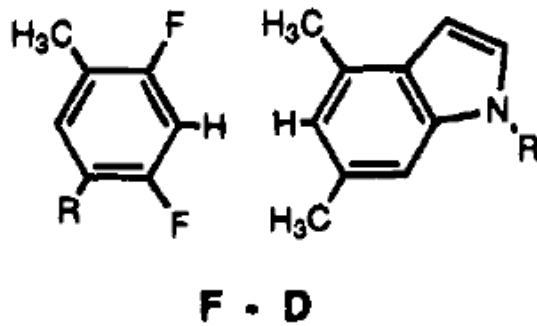
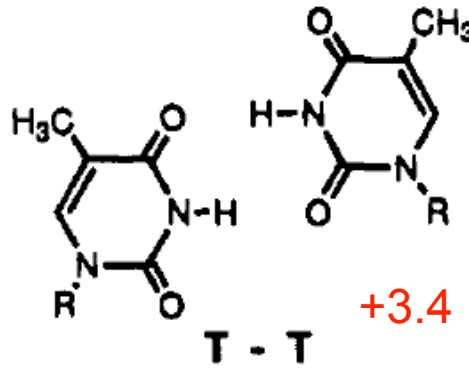
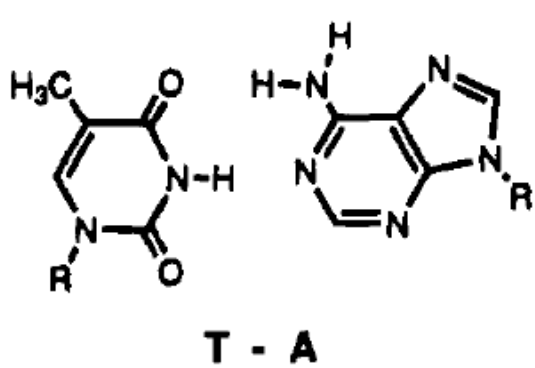
How important are H-bonds in DNA?

J. Am. Chem. Soc., Vol. 117, No. 7, 1995 1867

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5'-CTTTTC T TTCTT 3'-GAAAAG A AAGAA	39.4	12.3
5'-CTTTTC F TTCTT 3'-GAAAAG C AAGAA	26.4	8.7
5'-CTTTTC D TTCTT 3'-GAAAAG T AAGAA	30.7	9.3
5'-CTTTTC B TTCTT 3'-GAAAAG T AAGAA	27.1	8.9
5'-CTTTTC F TTCTT 3'-GAAAAG A AAGAA	21.4	7.4
5'-CTTTTC F TTCTT 3'-GAAAAG C AAGAA	25.0	8.2
5'-CTTTTC F TTCTT 3'-GAAAAG G AAGAA	23.0	8.0
5'-CTTTTC F TTCTT 3'-GAAAAG T AAGAA	20.2	7.3
5'-CTTTTC B TTCTT 3'-GAAAAG A AAGAA	21.0	7.5
5'-CTTTTC B TTCTT 3'-GAAAAG C AAGAA	22.9	7.8
5'-CTTTTC B TTCTT 3'-GAAAAG G AAGAA	20.1	7.6
5'-CTTTTC B TTCTT 3'-GAAAAG T AAGAA	20.3	6.7
5'-CTTTTC D TTCTT 3'-GAAAAG A AAGAA	20.8	7.4
5'-CTTTTC D TTCTT 3'-GAAAAG C AAGAA	22.2	7.6
5'-CTTTTC D TTCTT 3'-GAAAAG G AAGAA	19.7	7.4
5'-CTTTTC D TTCTT 3'-GAAAAG T AAGAA	17.6	6.9

^a Conditions: 100 mM NaCl, 10 mM MgCl₂, 10 mM Na · PIPES, pH 7.0, 1.6 μM each strand.



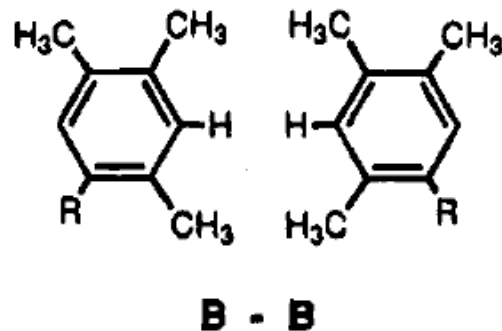
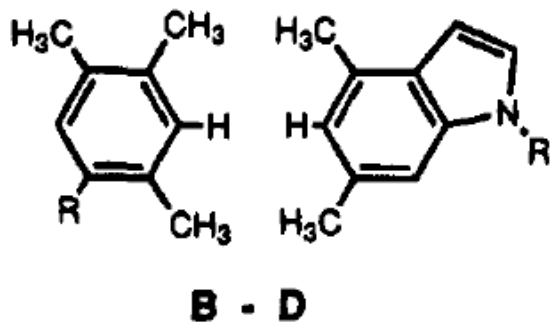
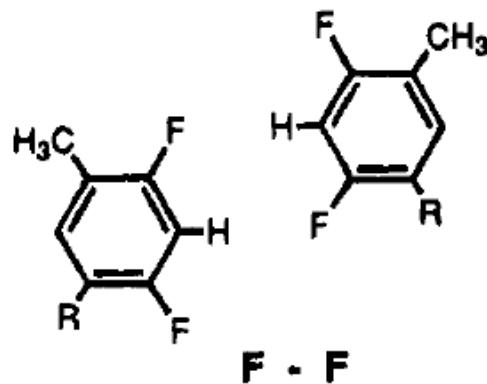
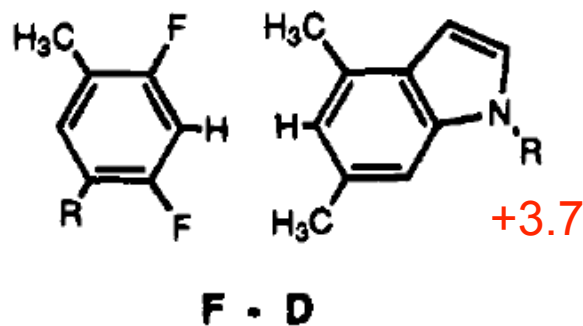
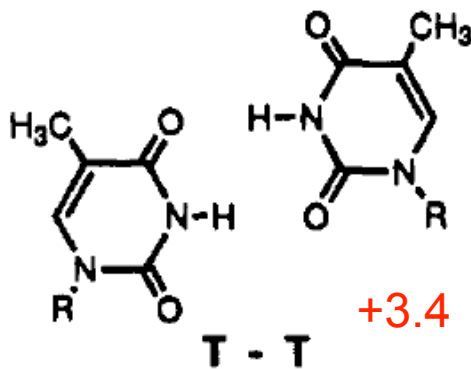
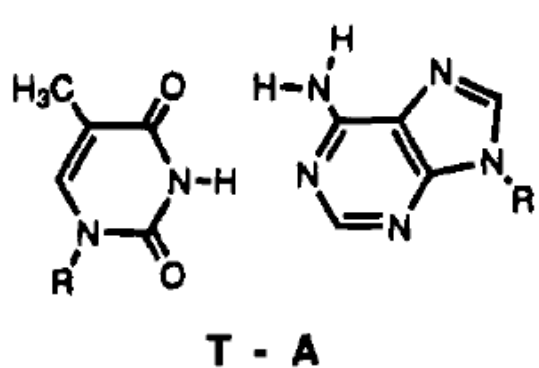
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5'-CTTTTC[B]TTCTT 3'-GAAAAG[T]AAGAA	20.3	6.7
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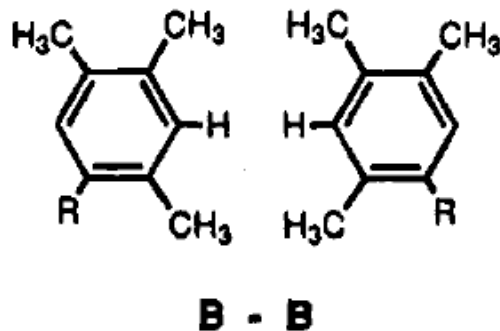
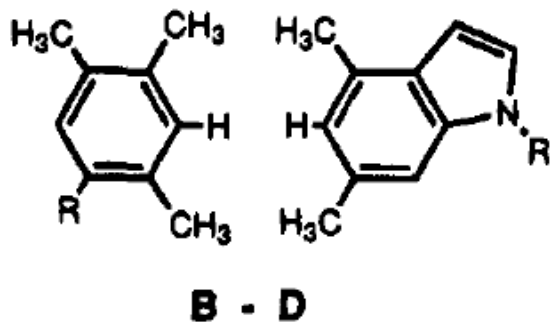
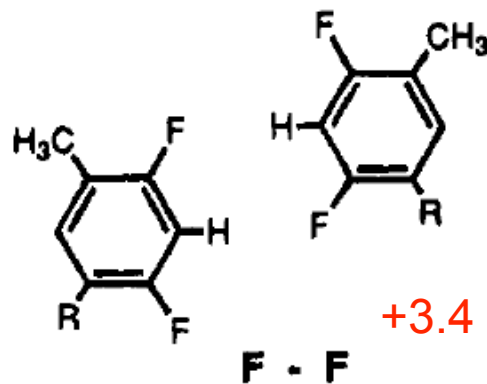
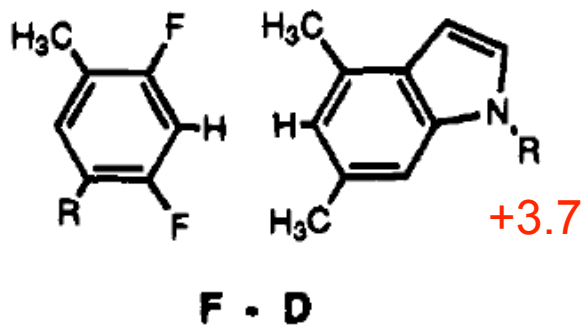
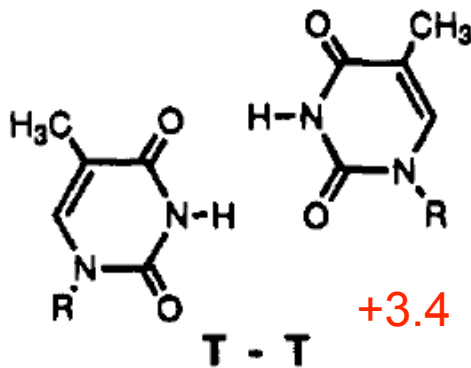
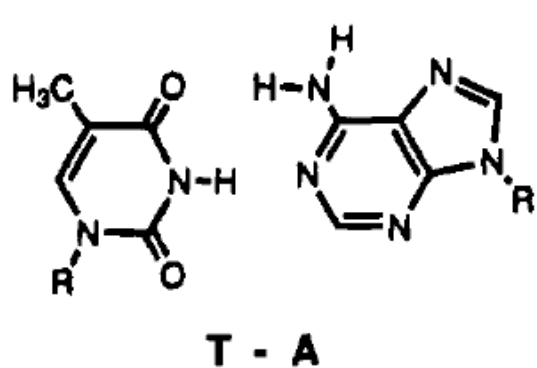


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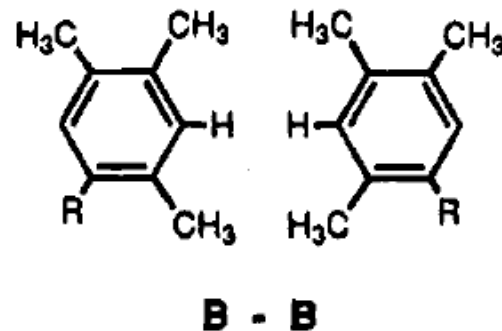
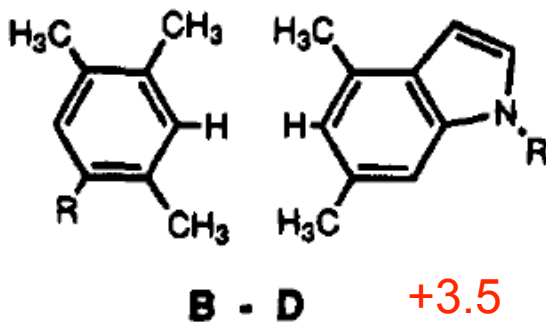
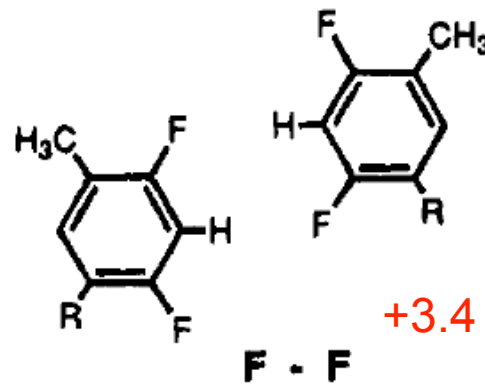
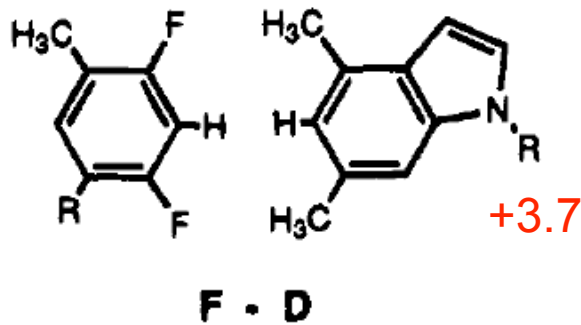
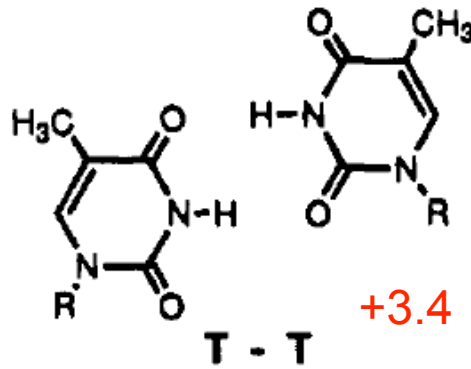
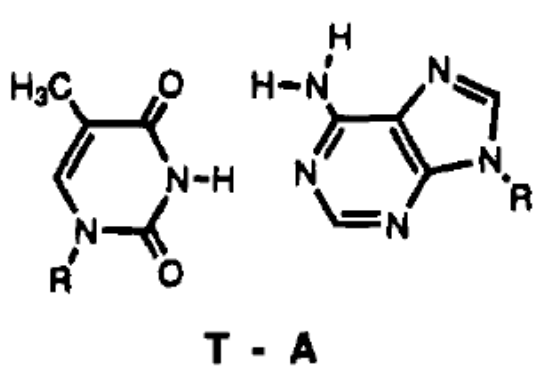
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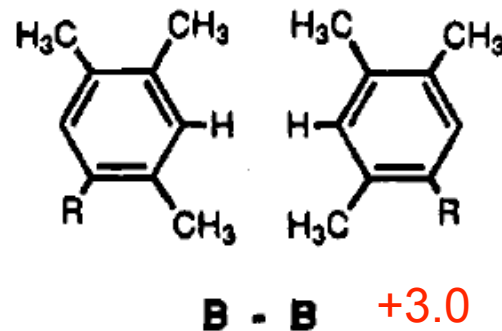
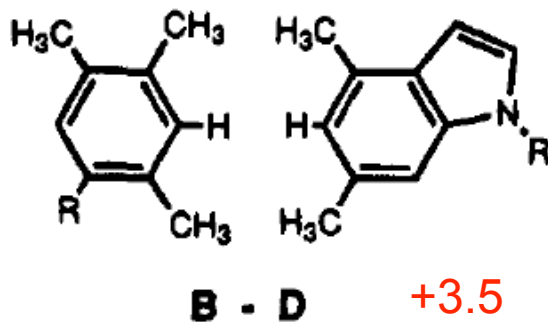
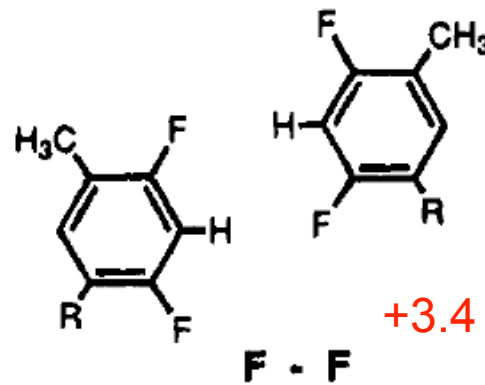
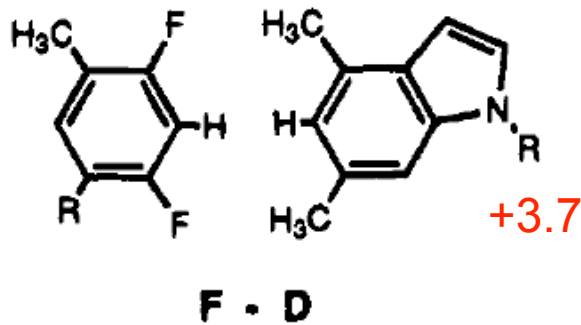
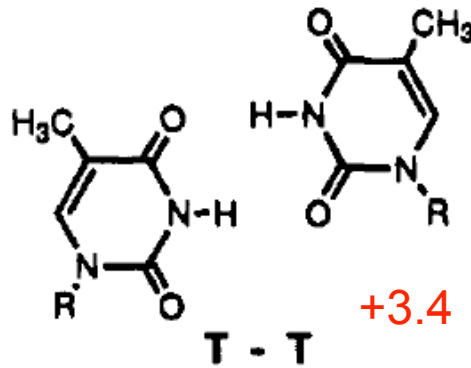
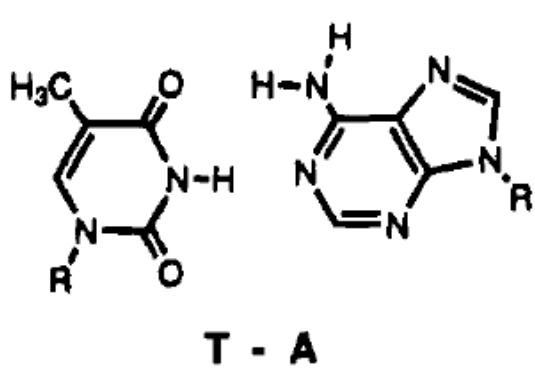
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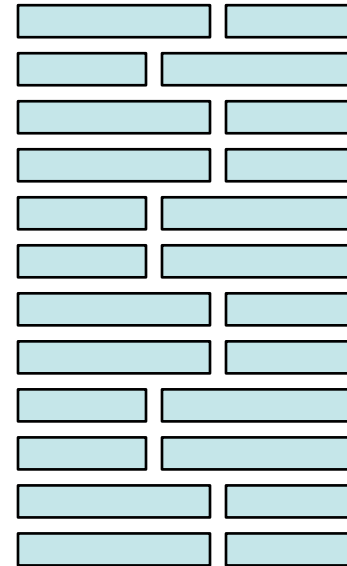
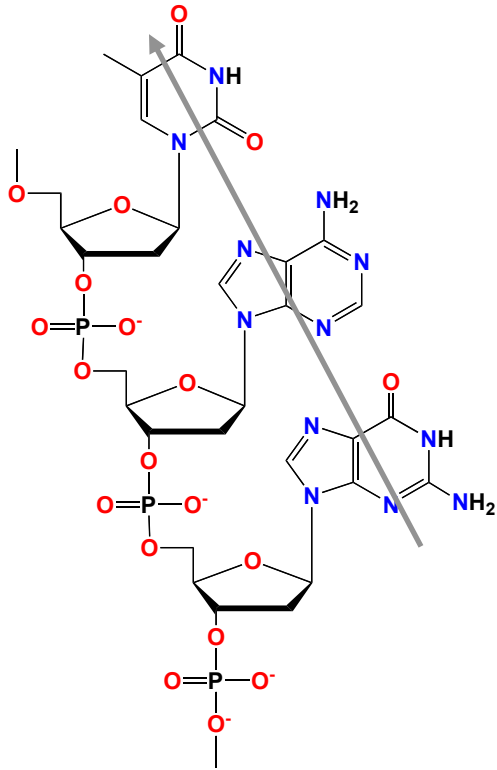
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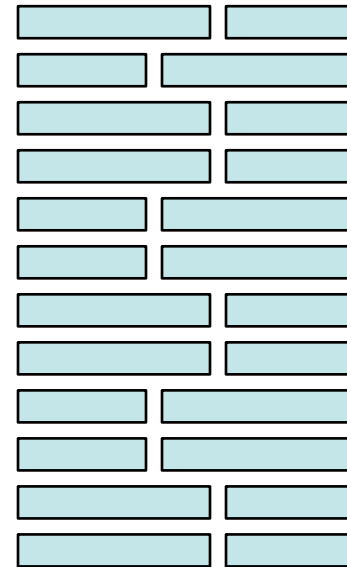
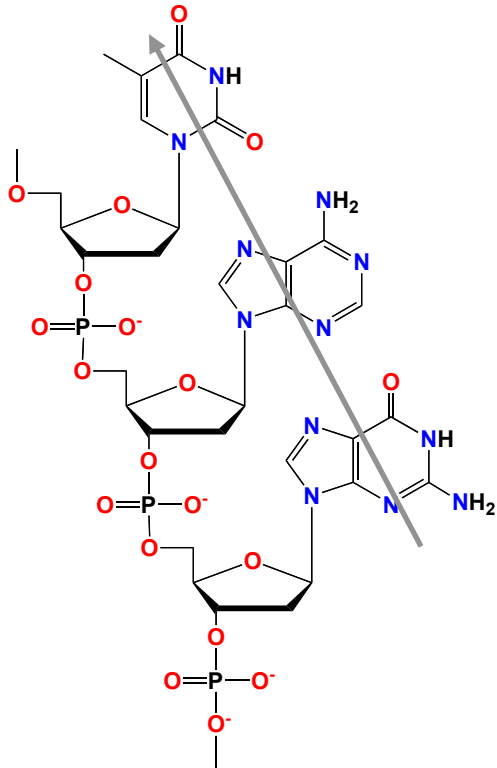
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Burial of hydrophobic surface drives helix formation (hydrophobic core / stacking interactions)

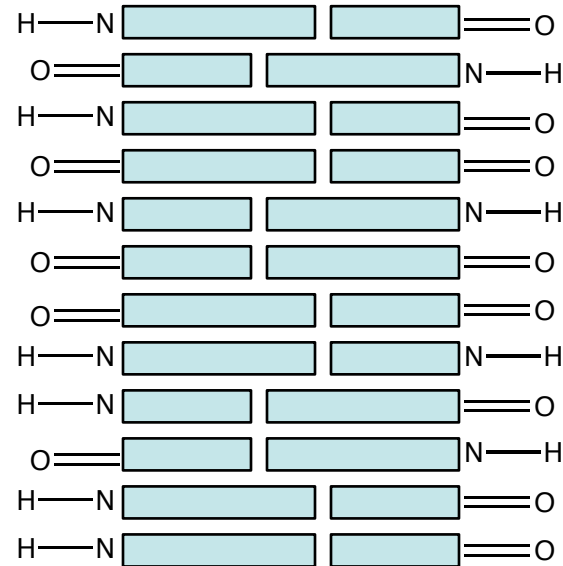
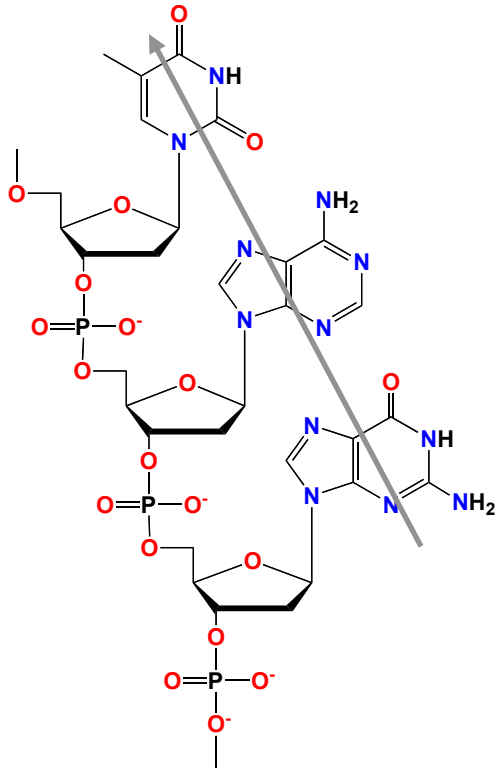


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Flat faces are nonpolar

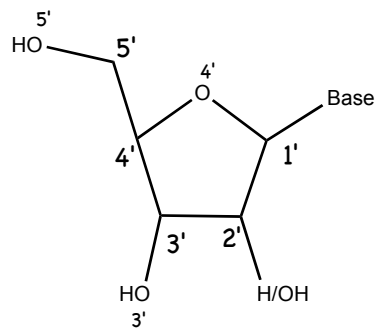
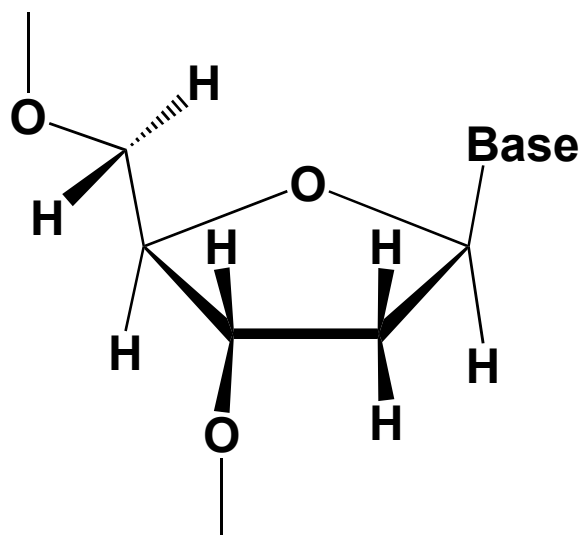
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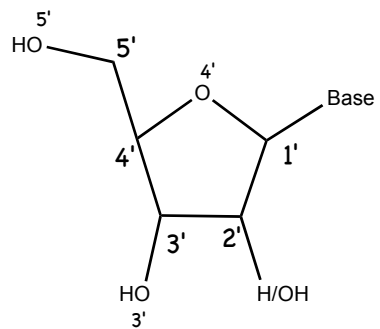
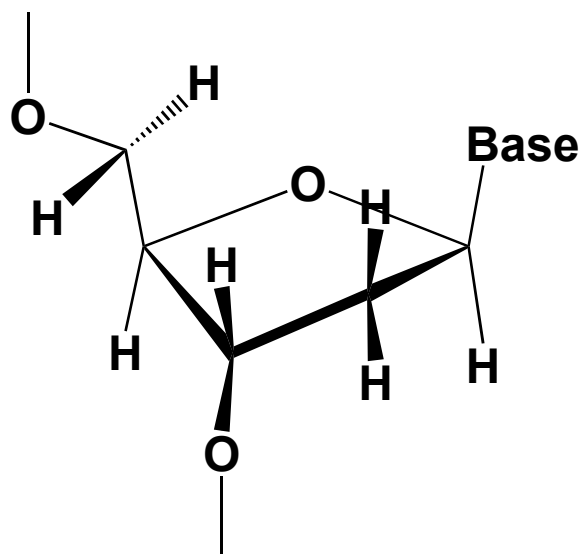
Flat faces are nonpolar
Edges are very polar (can H-bond)

Other chemical constraints

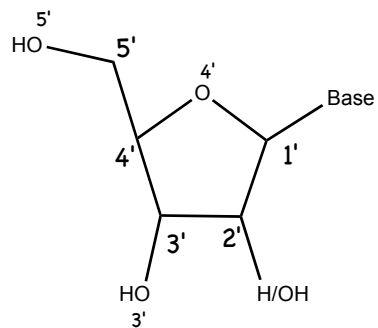
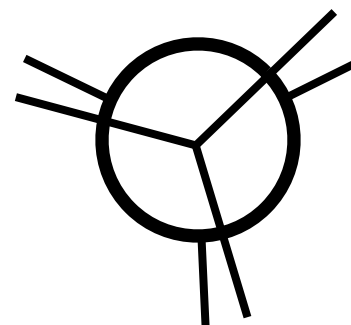
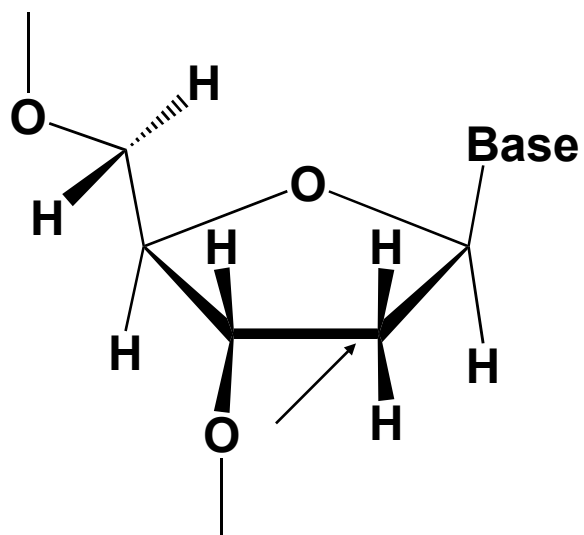
Furanose Sugar Ring



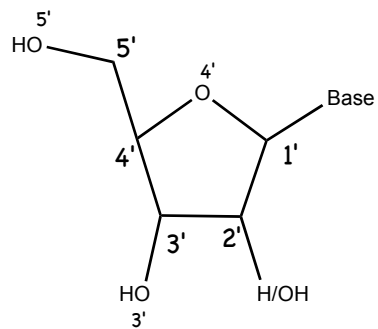
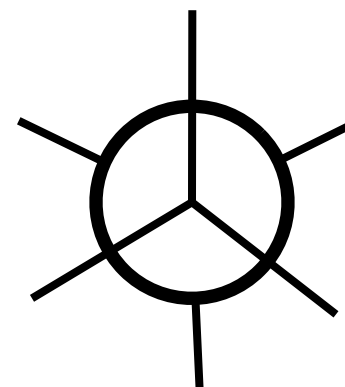
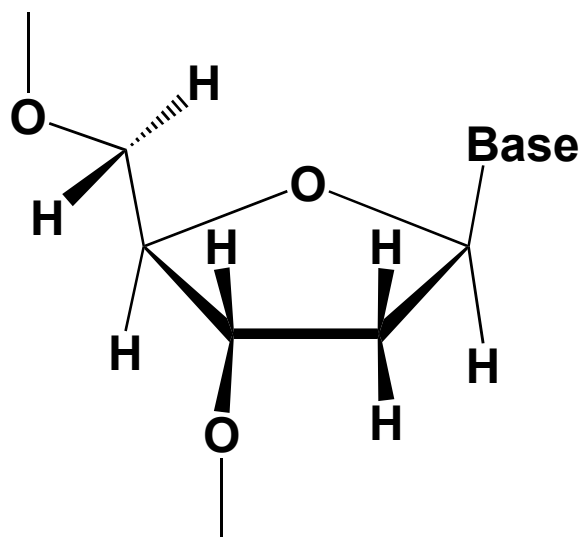
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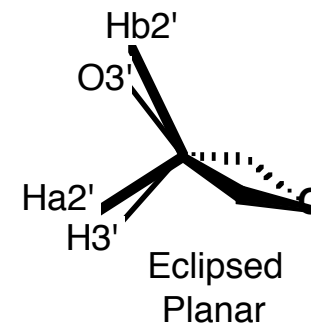
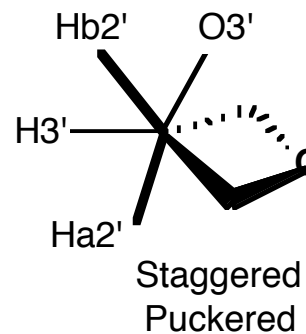
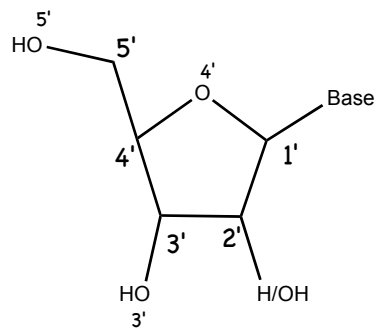
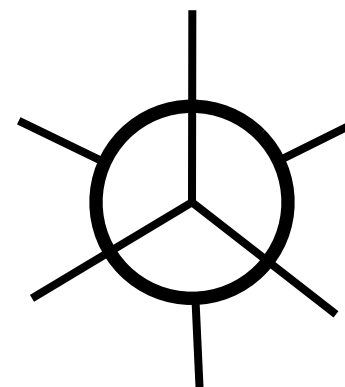
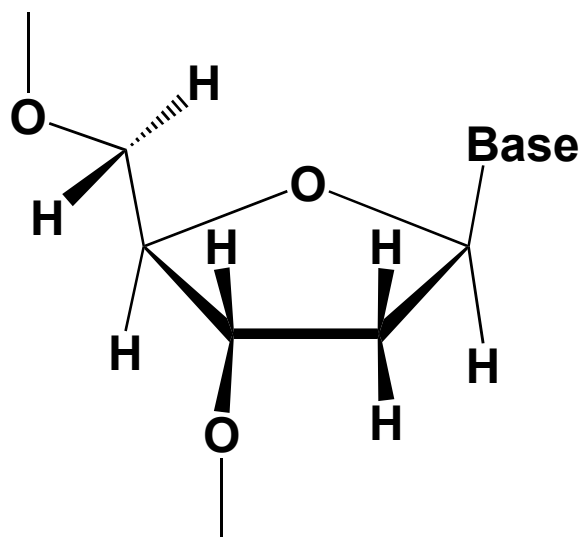
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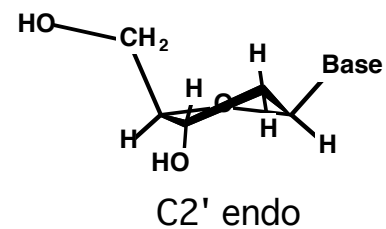
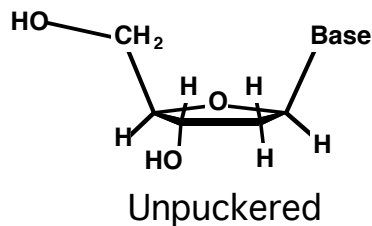
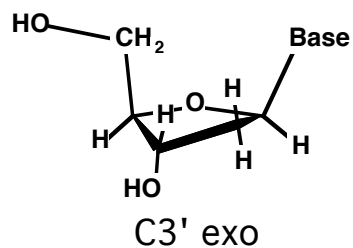
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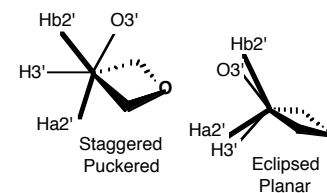
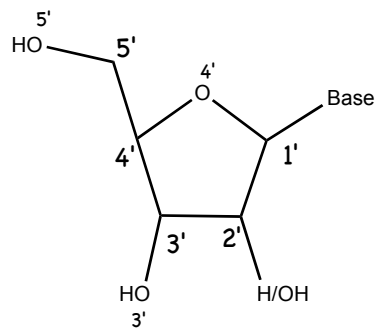
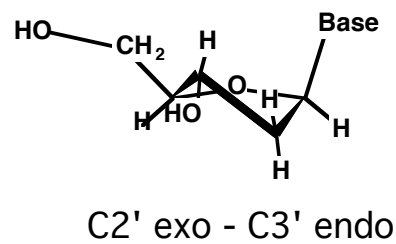
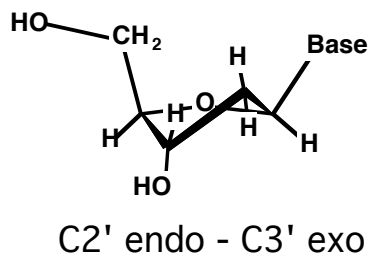
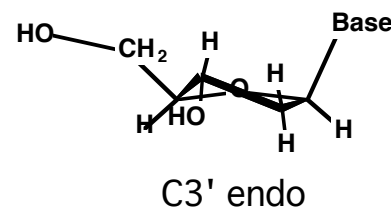
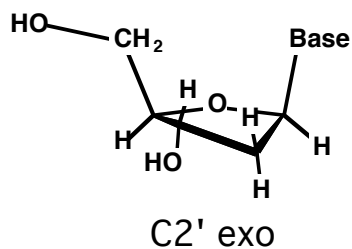
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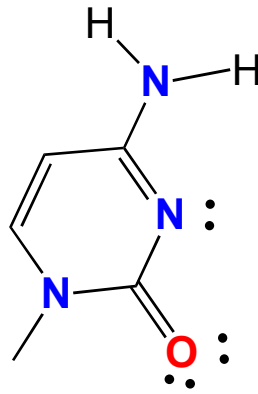


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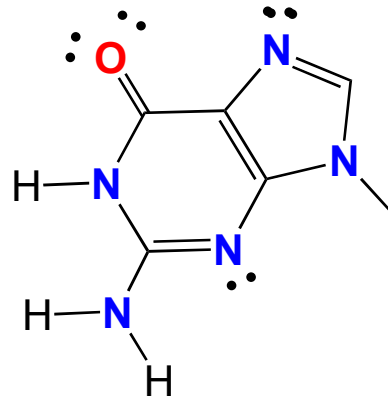


Why is Watson-Crick so good?

C

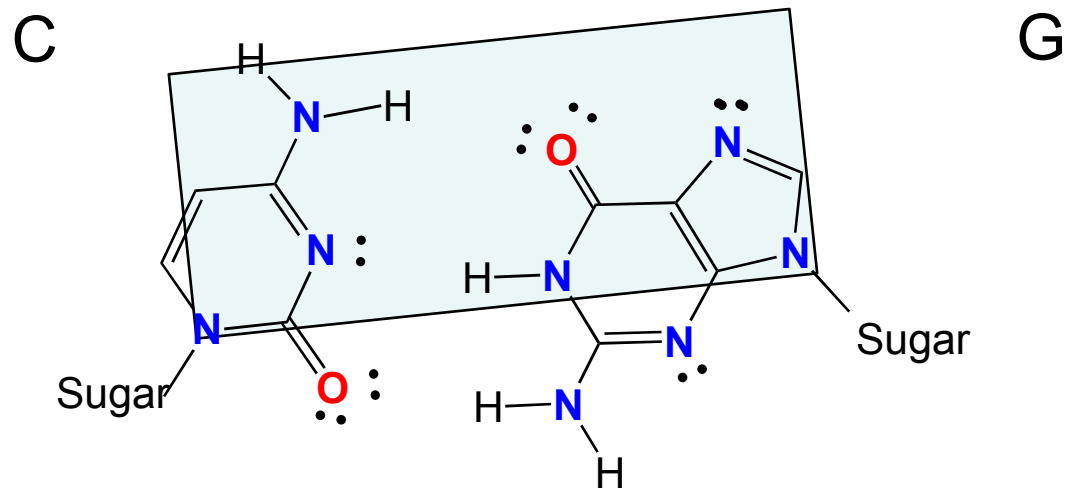


G



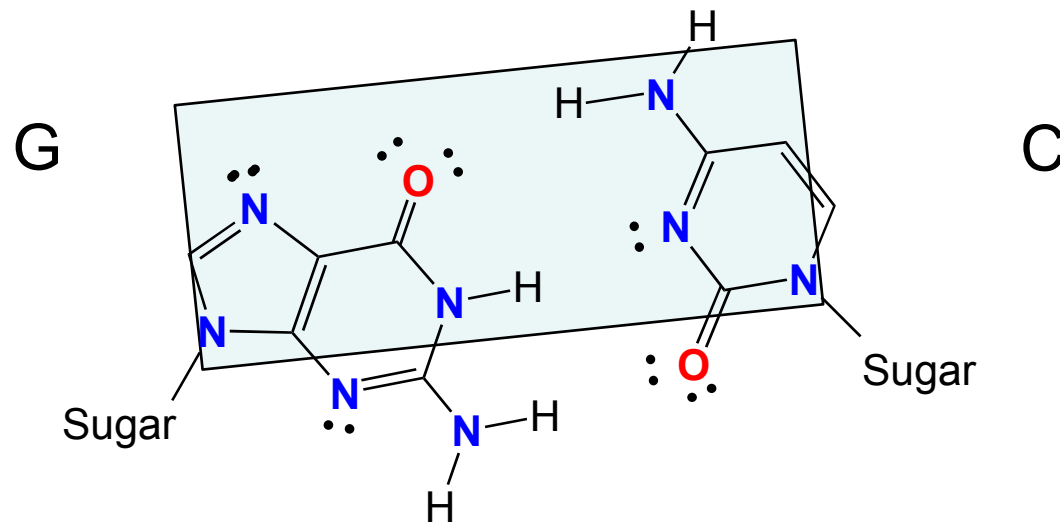
All four WC base pairs
are
isosteric

Why is Watson-Crick so good?



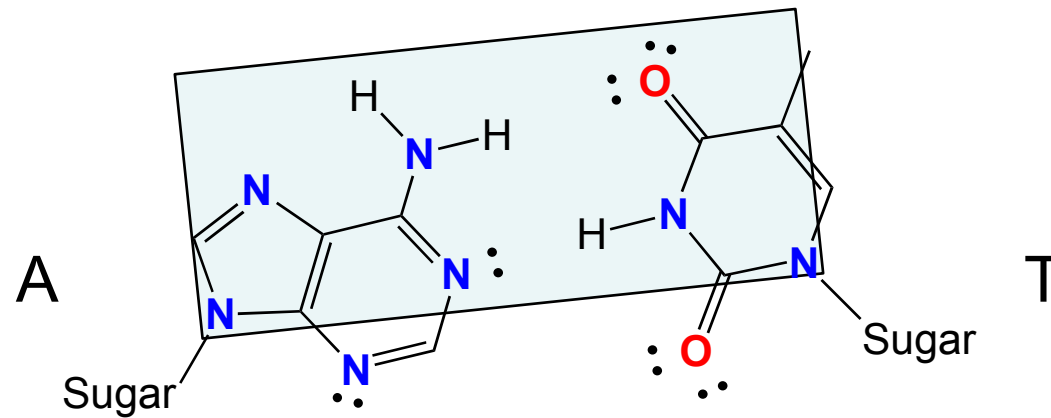
All four WC base pairs
are
isosteric

Why is Watson-Crick so good?



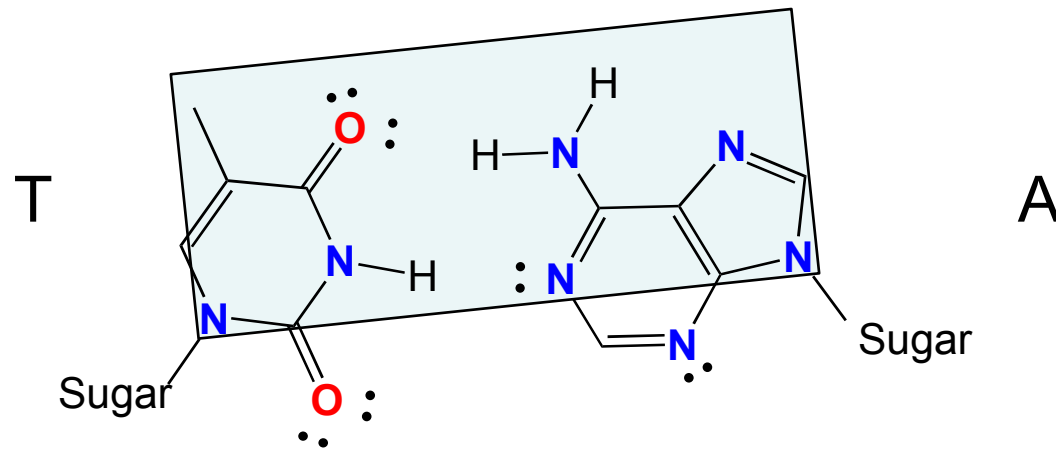
All four WC base pairs
are
isosteric

Why is Watson-Crick so good?



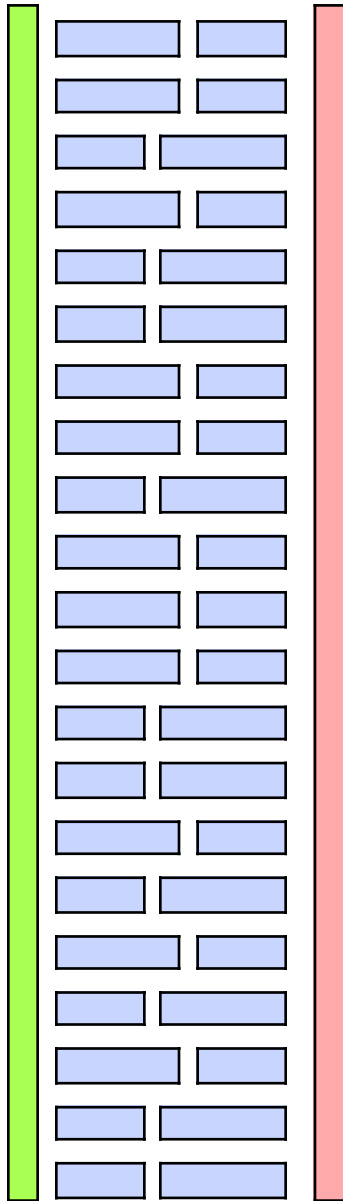
All four WC base pairs
are
isosteric

Why is Watson-Crick so good?

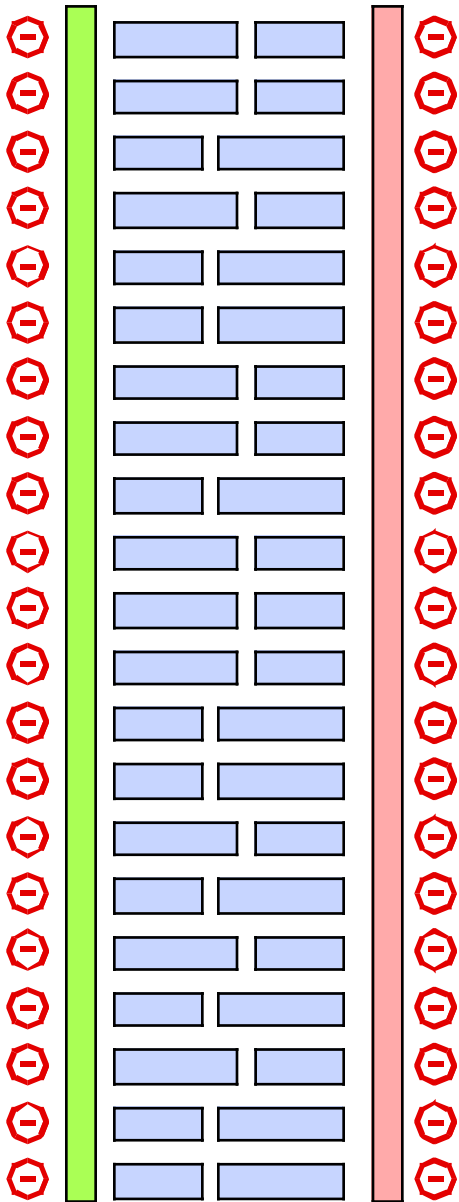


All four WC base pairs
are
isosteric

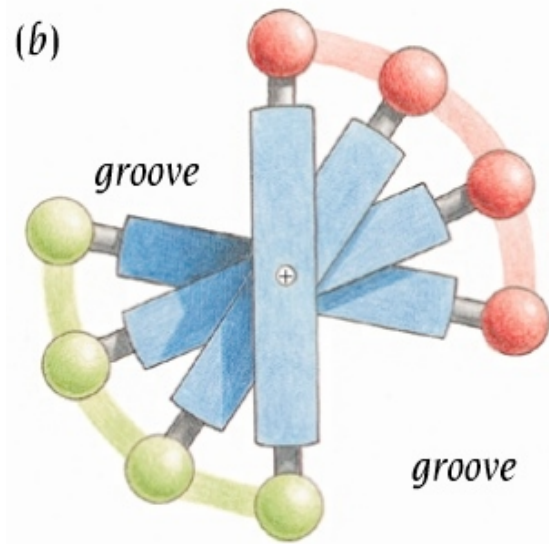
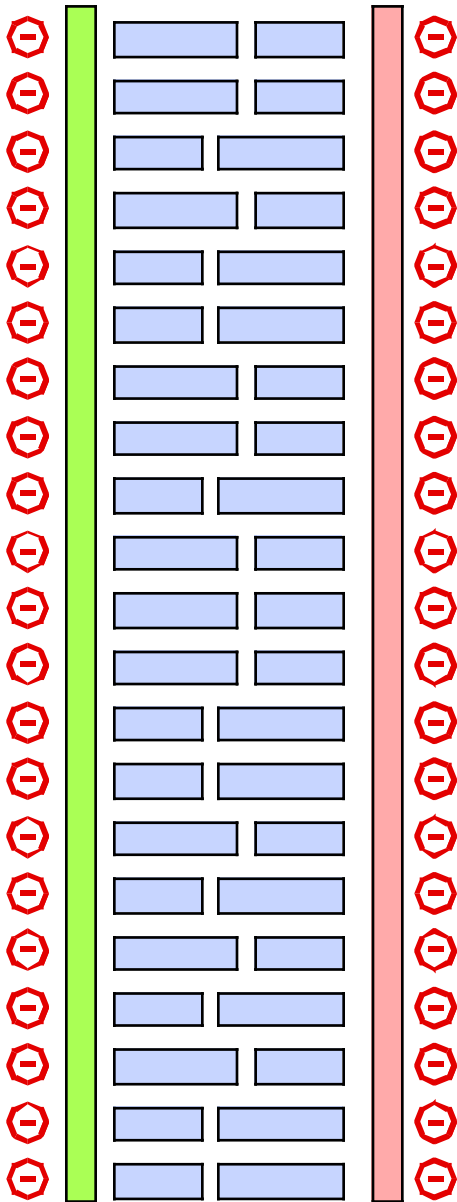
Why *a helix*?



Why *a helix*?

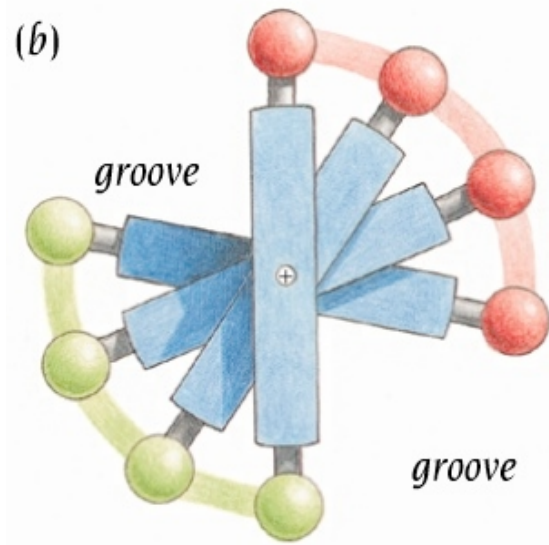
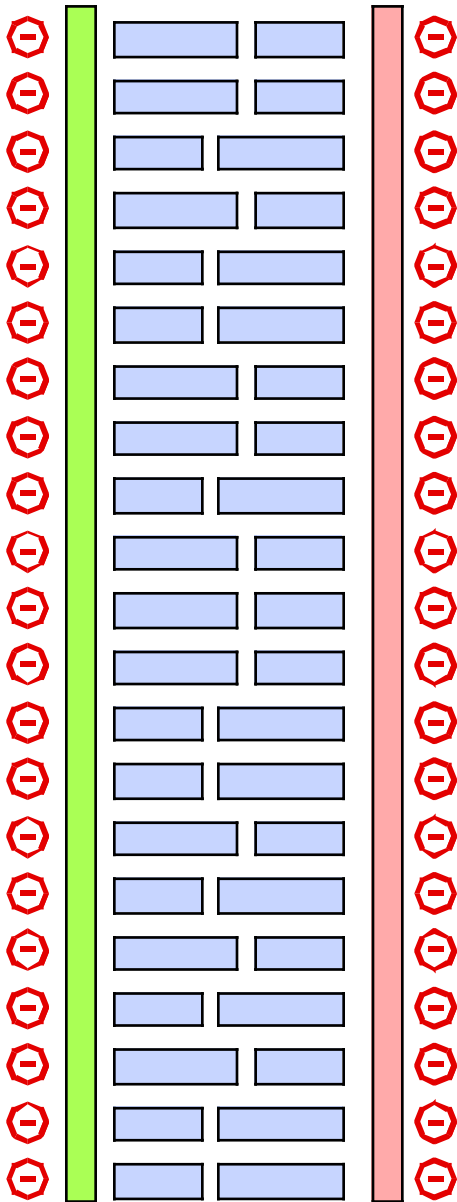


Why a *helix*?

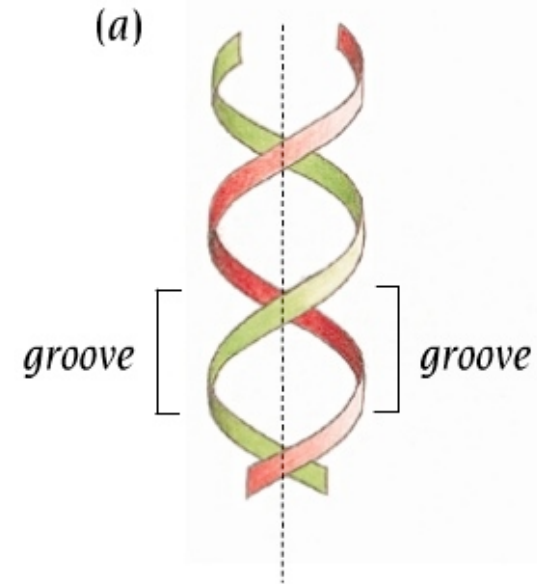


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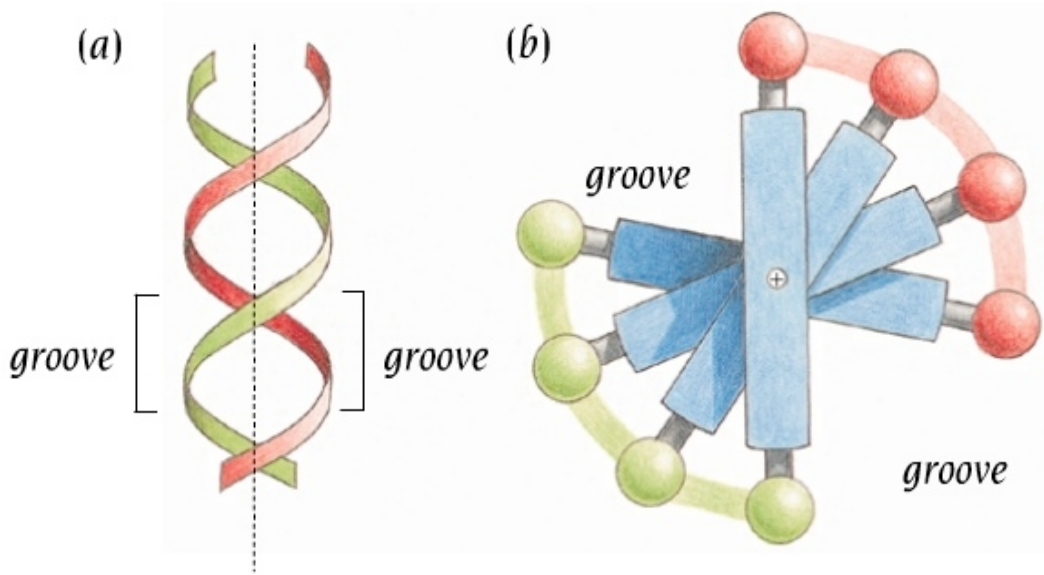
Why a *helix*?



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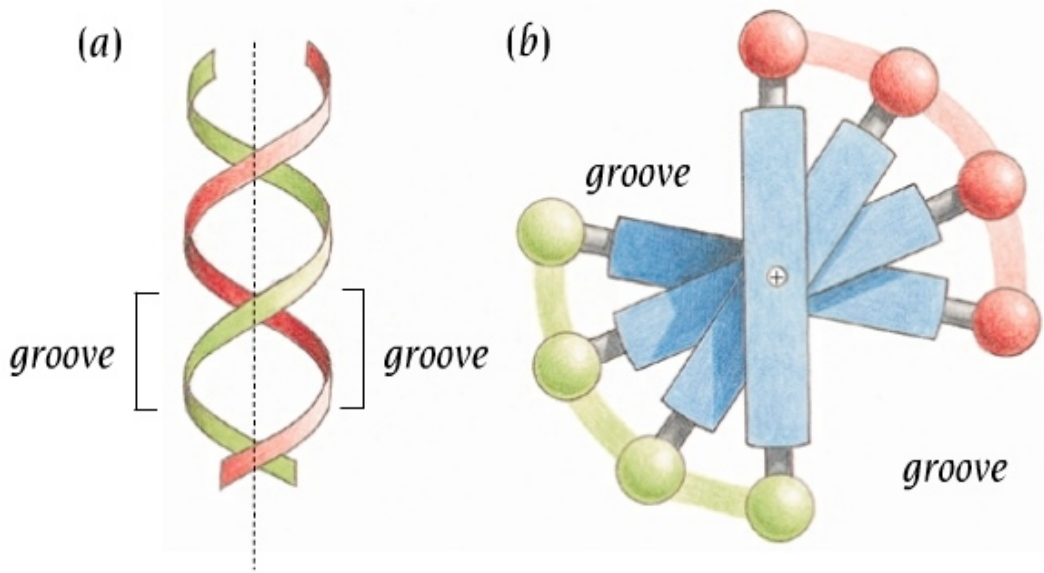


Why *major* and *minor* grooves?

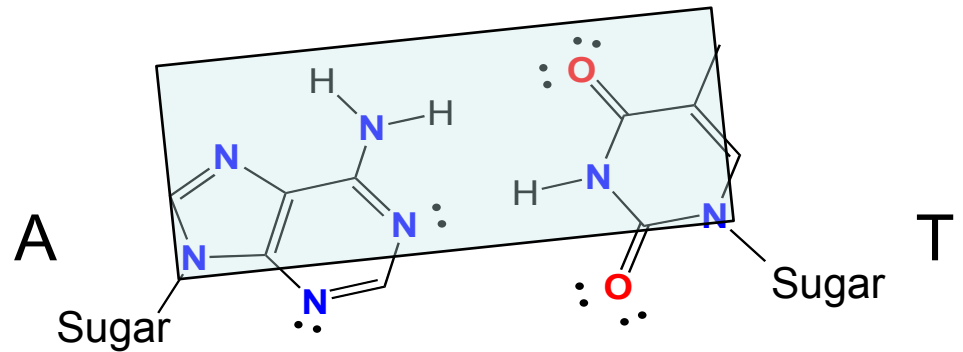


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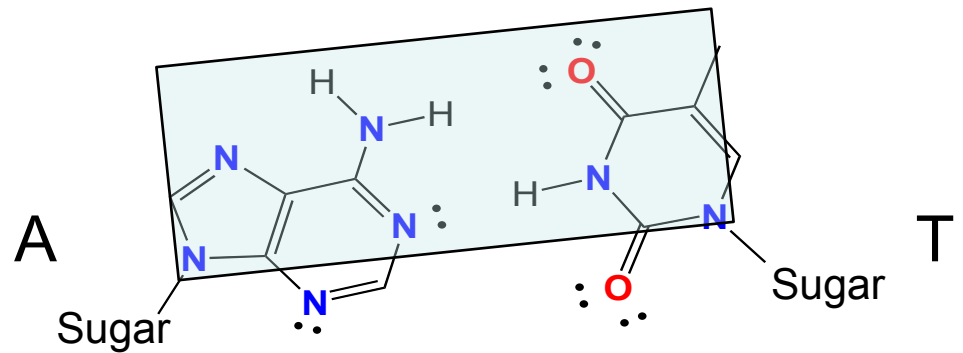
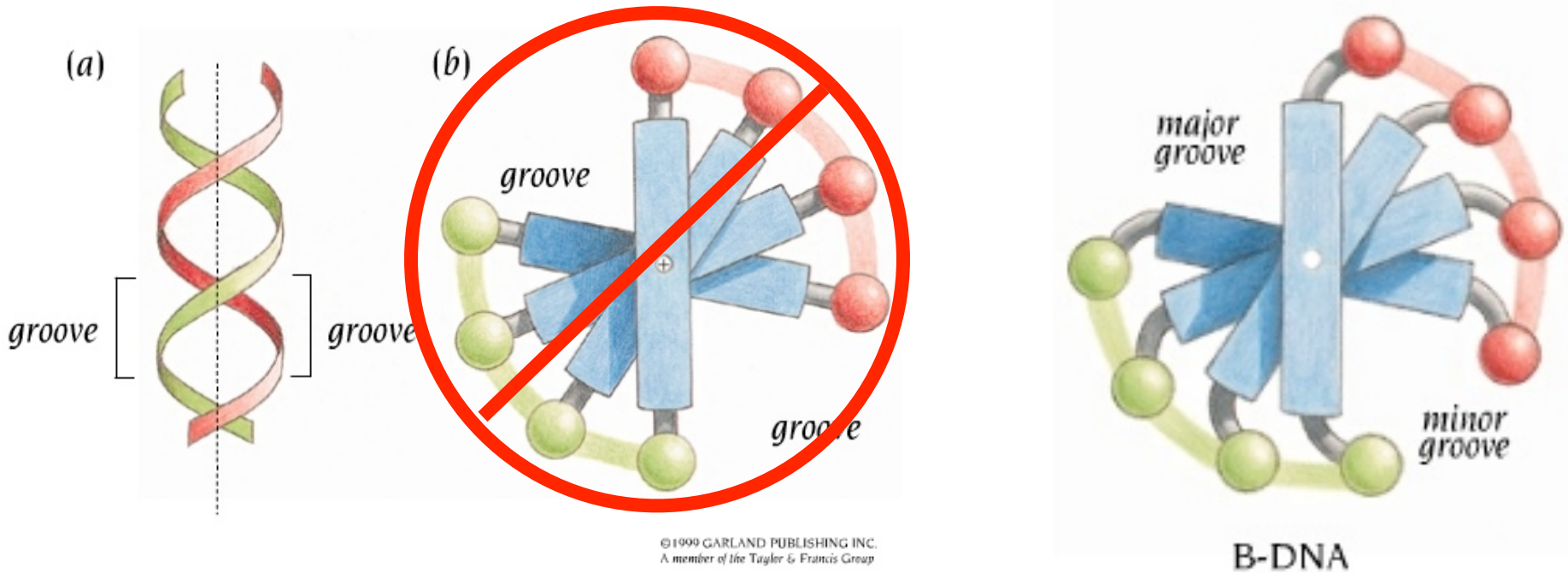
Why *major* and *minor* grooves?



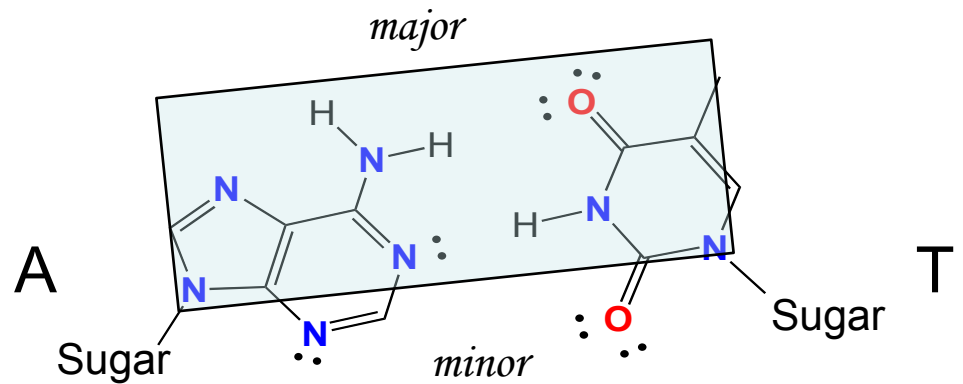
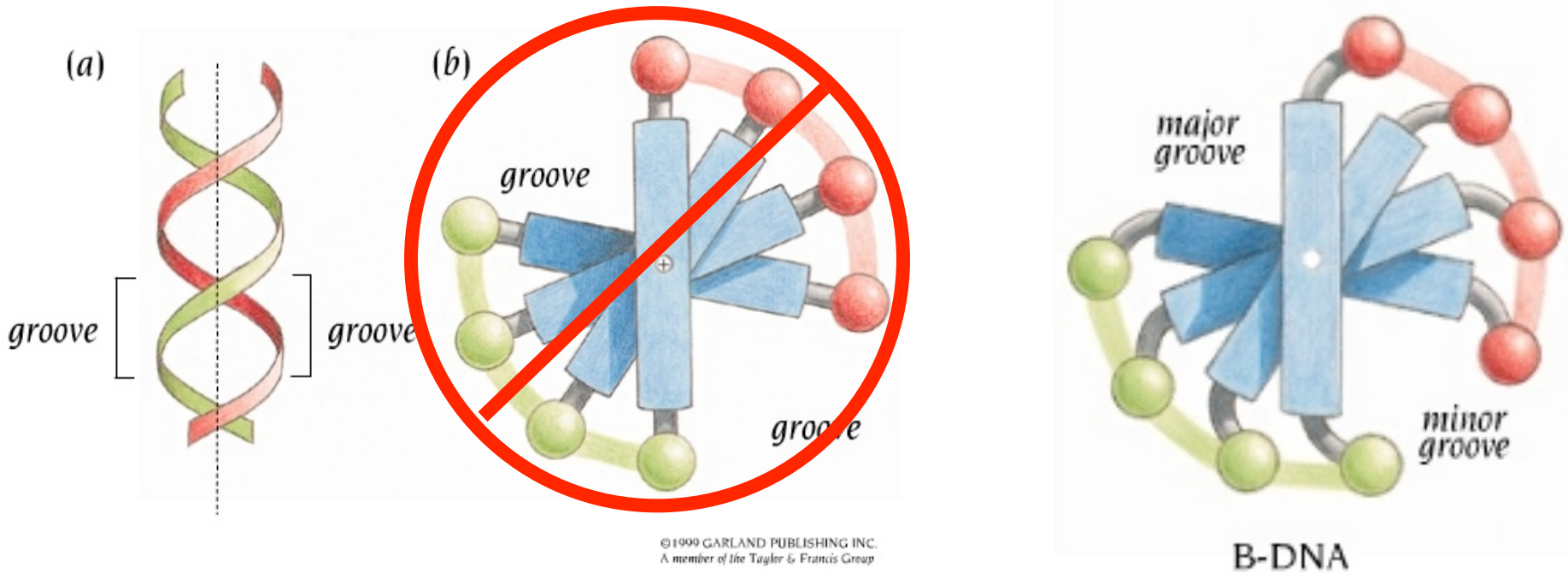
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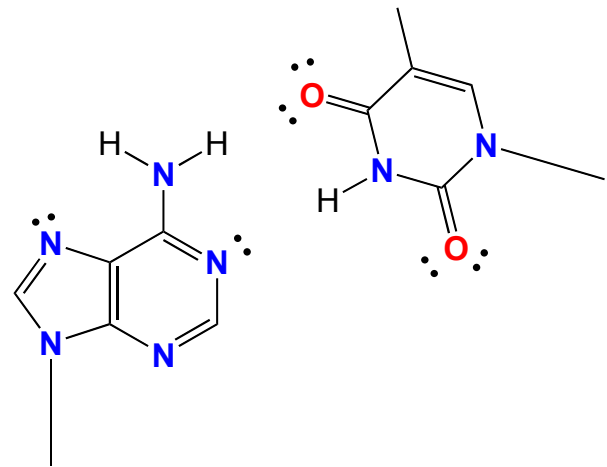
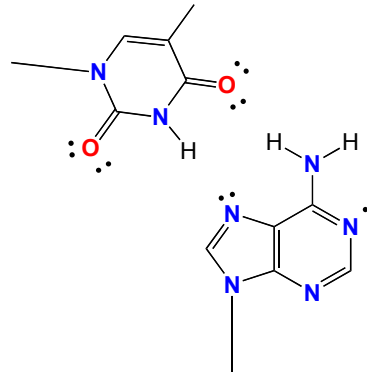
Why *major* and *minor* grooves?



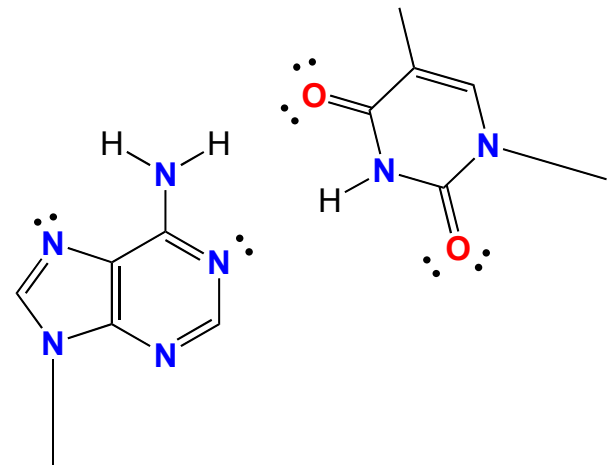
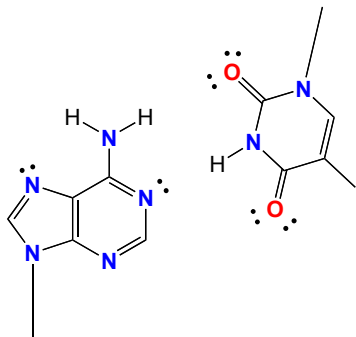
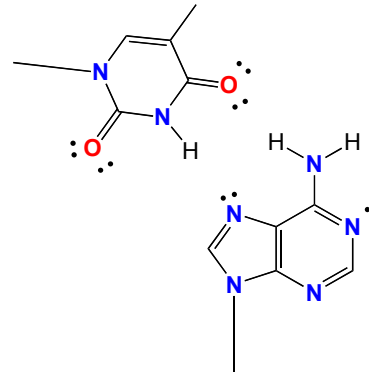
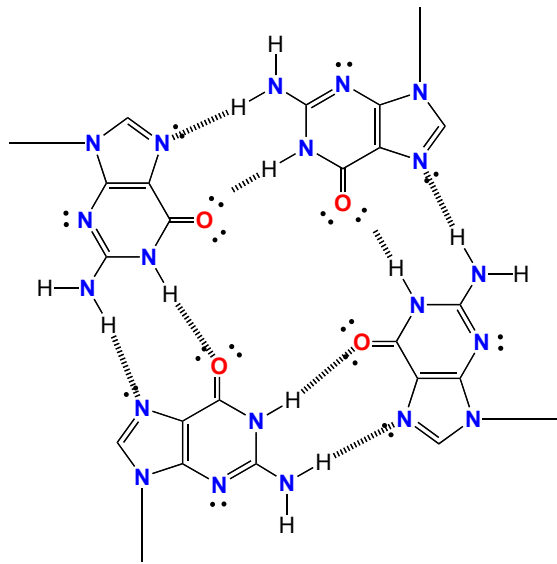
Why *major* and *minor* grooves?



Nucleic Acid - Nucleic Acid Recognition

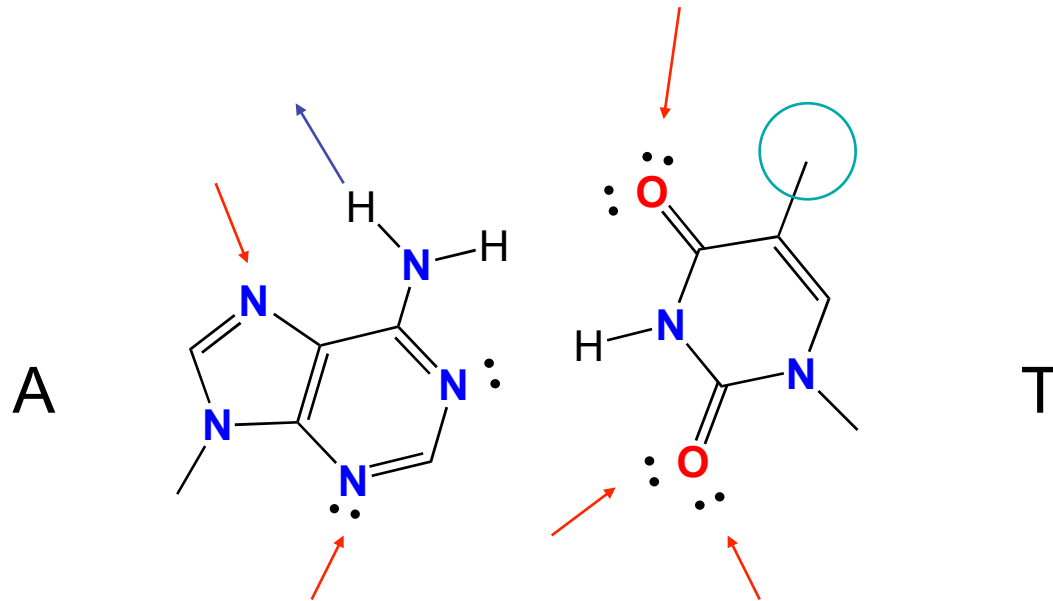


Nucleic Acid - Nucleic Acid Recognition



Why is the major groove so good?

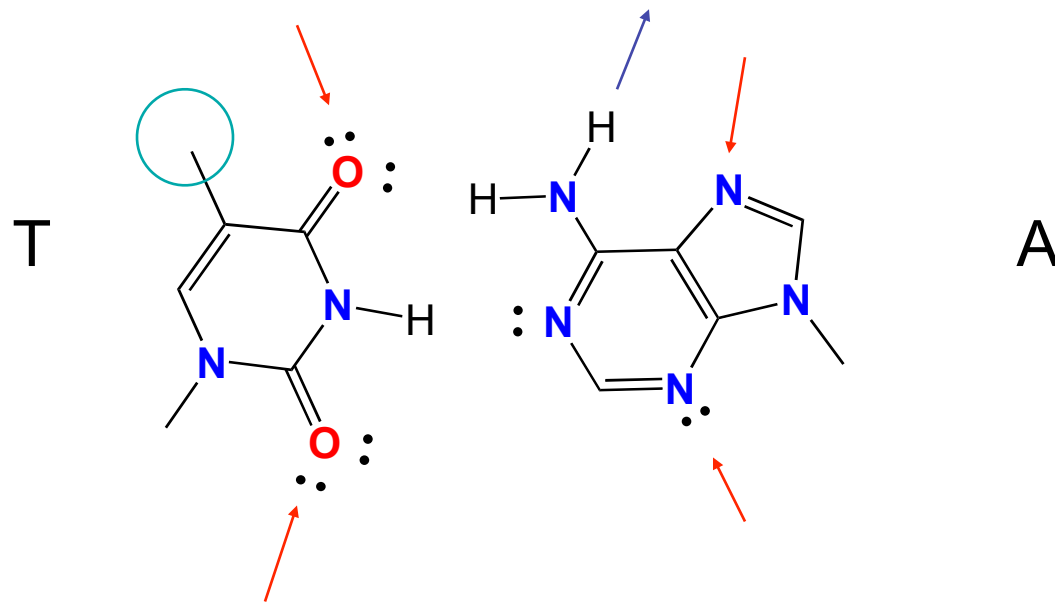
Major Groove



Minor Groove

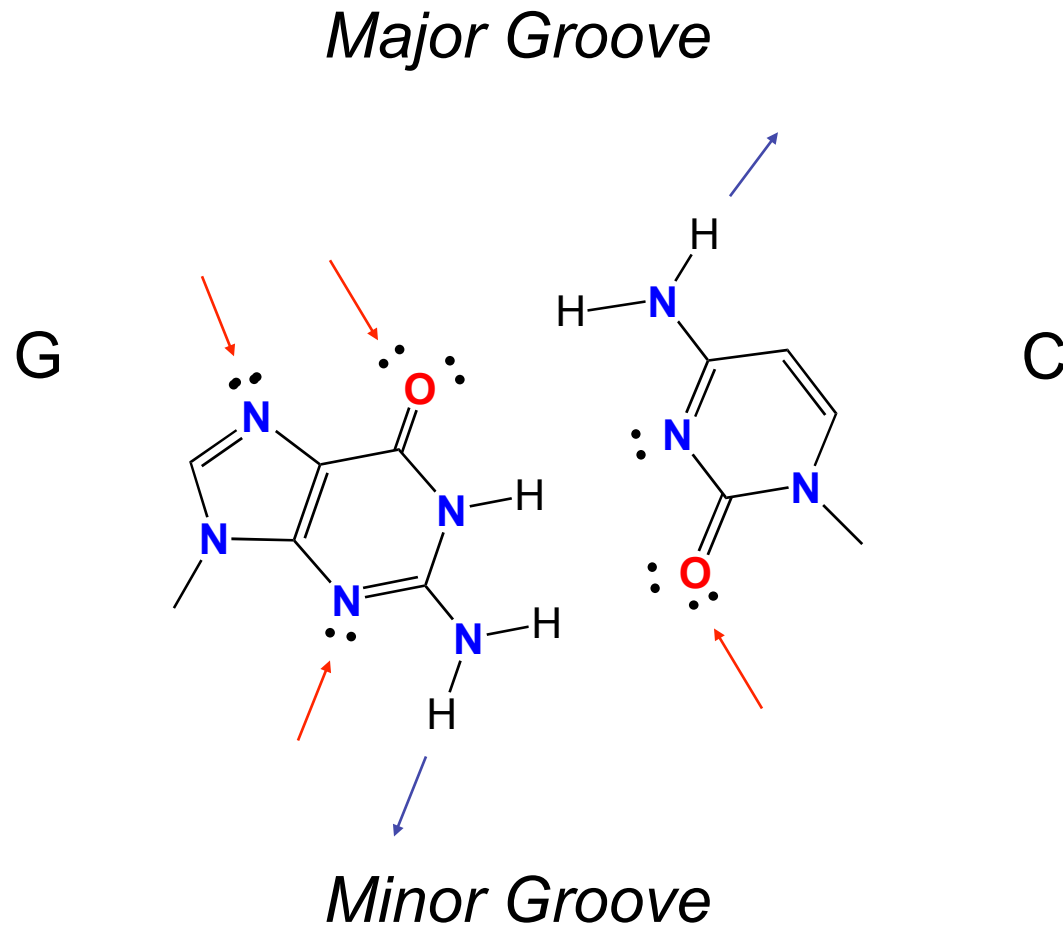
Why is the major groove so good?

Major Groove



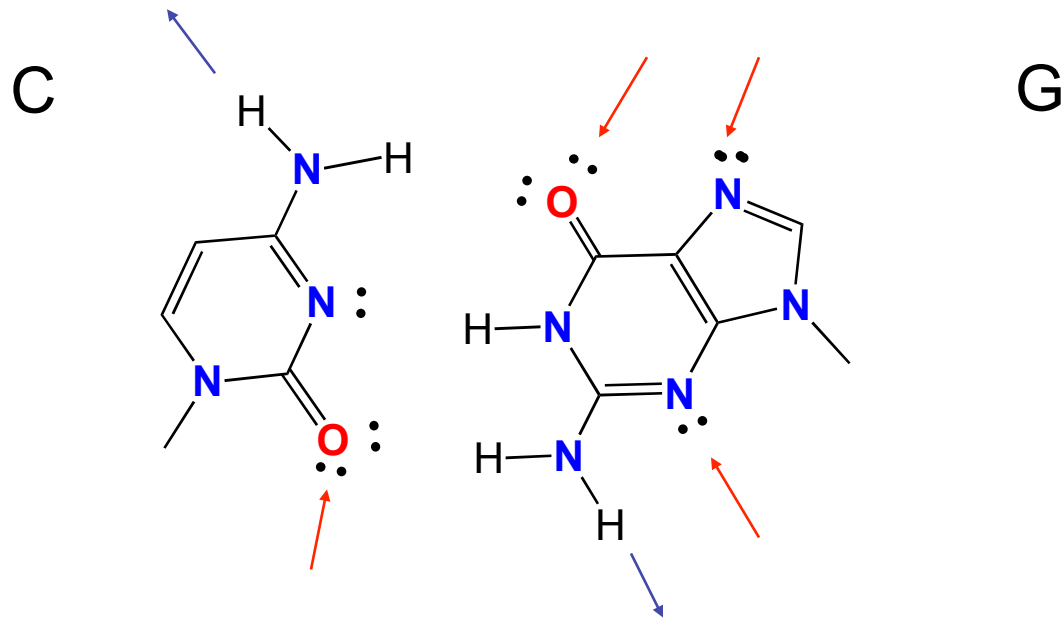
Minor Groove

Why is the major groove so good?



Why is the major groove so good?

Major Groove



Minor Groove

Bases that polymerases like

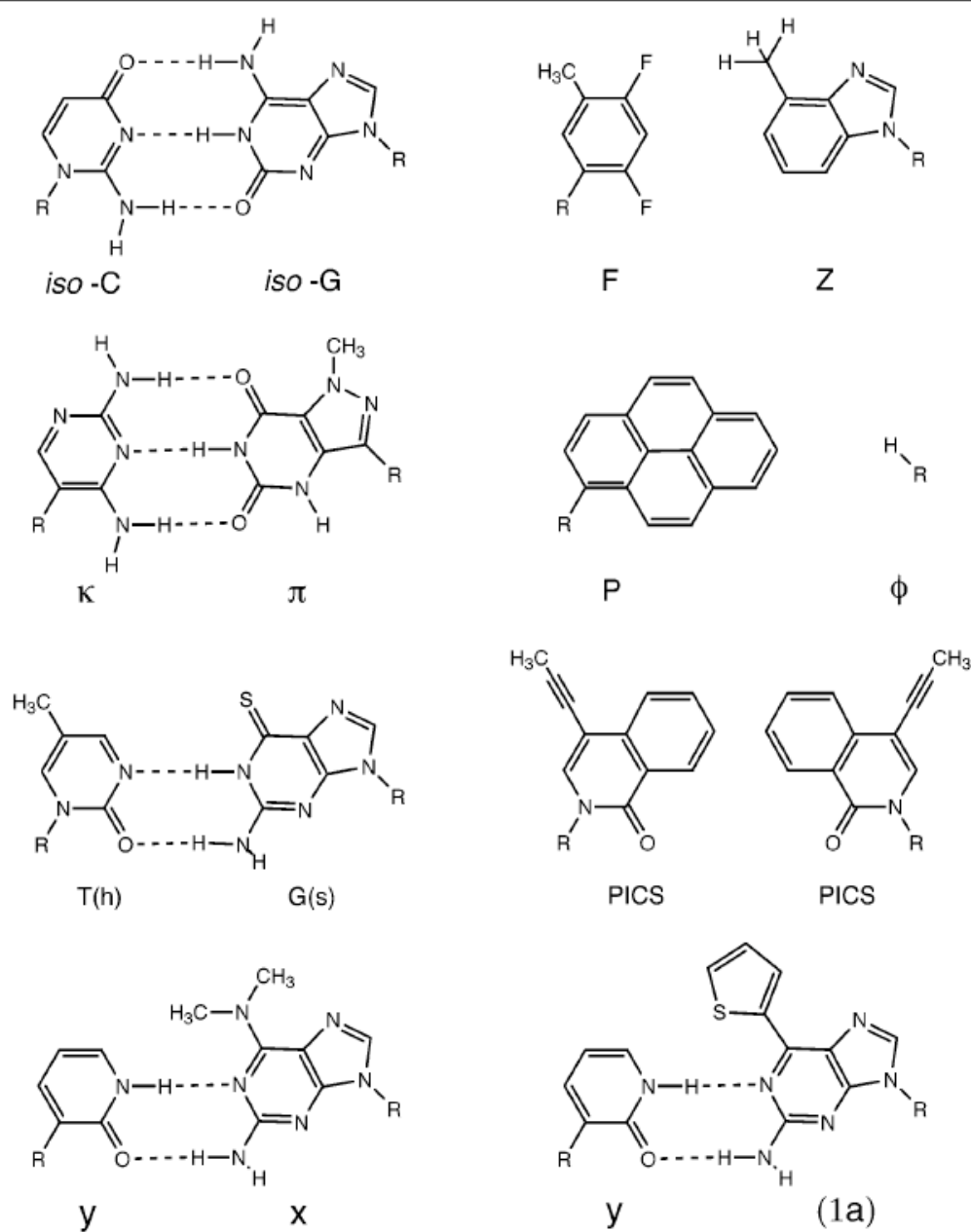
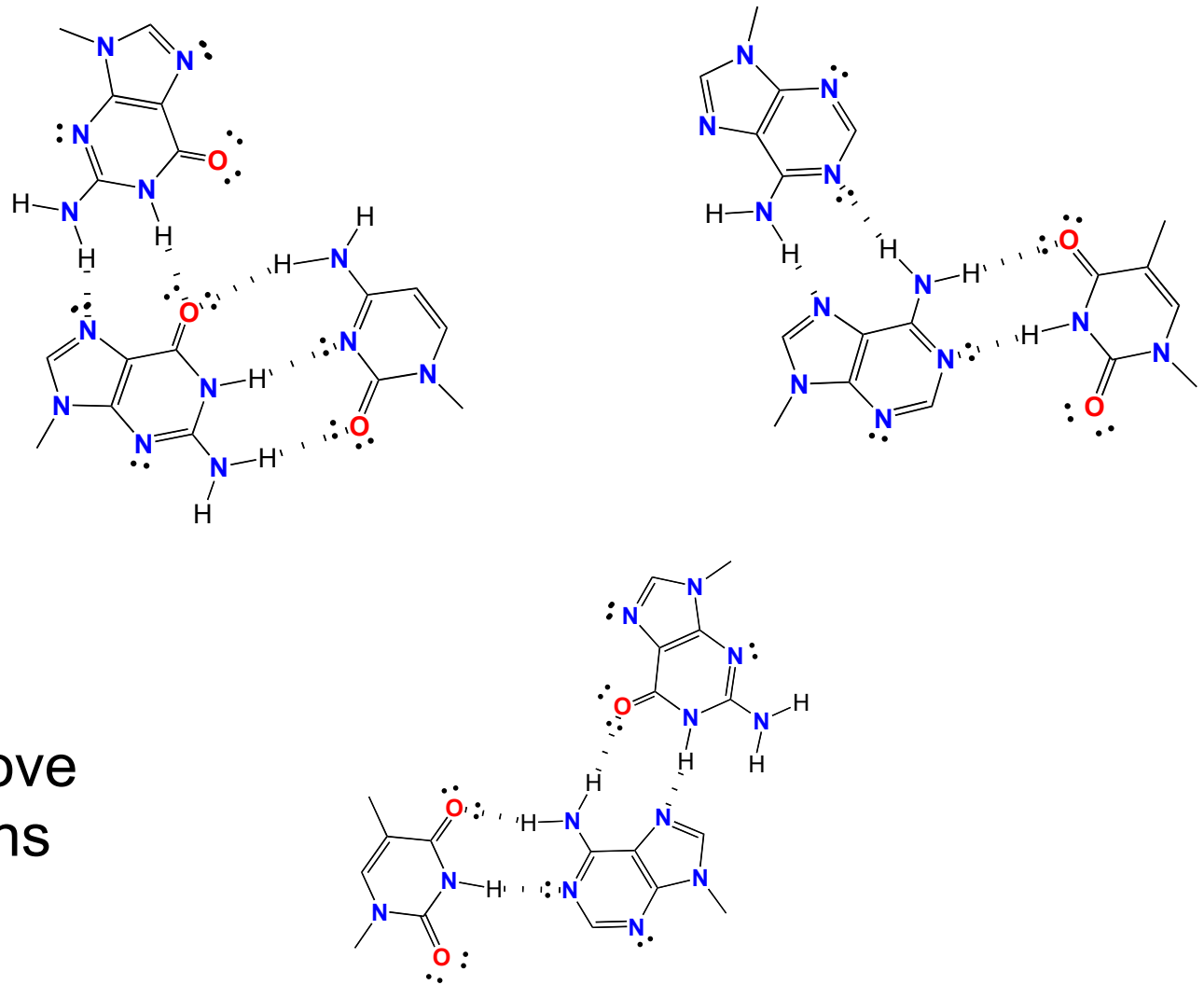


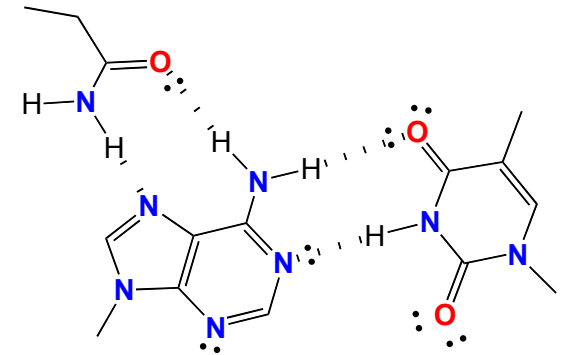
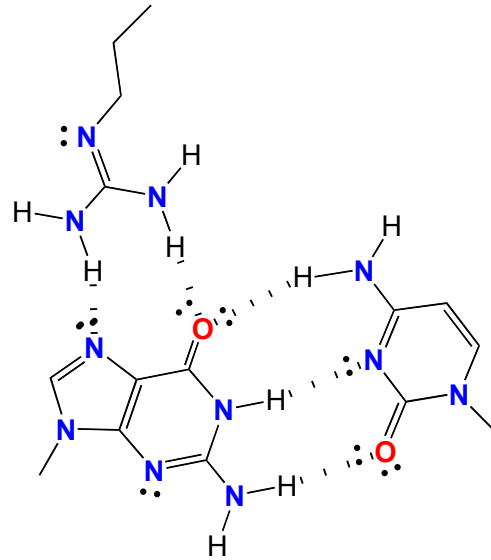
FIGURE 7. Examples of DNA base replacements designed to form stable pairs and/or to be replicated selectively by DNA polymerase enzymes.^{17,23,24,49,54,55}

Nucleic Acid “Triples / Platforms”

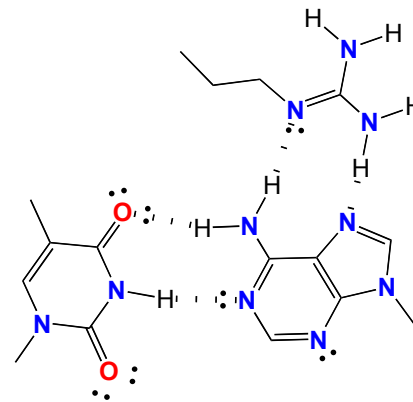


Major Groove
Interactions

Protein - Nucleic Acid Interactions



Major Groove Interactions

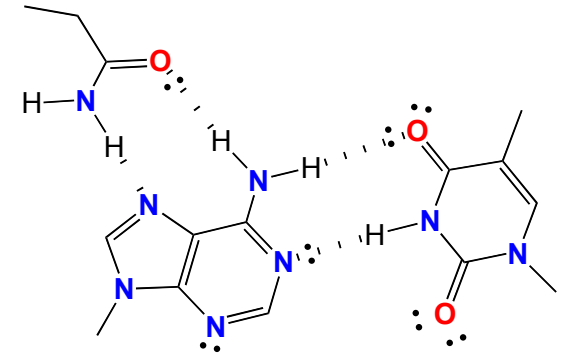
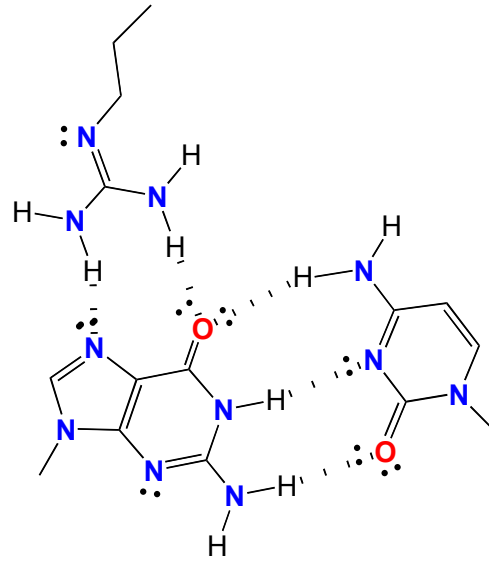


Protein - Nucleic Acid Interactions

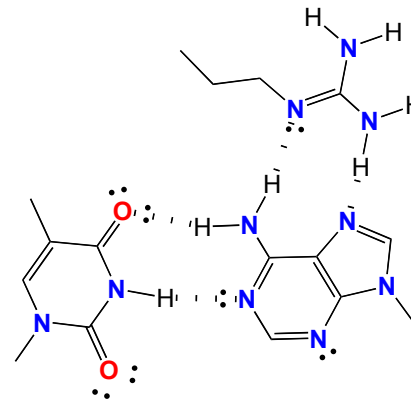
Gln

Asn

Arg



Major Groove Interactions



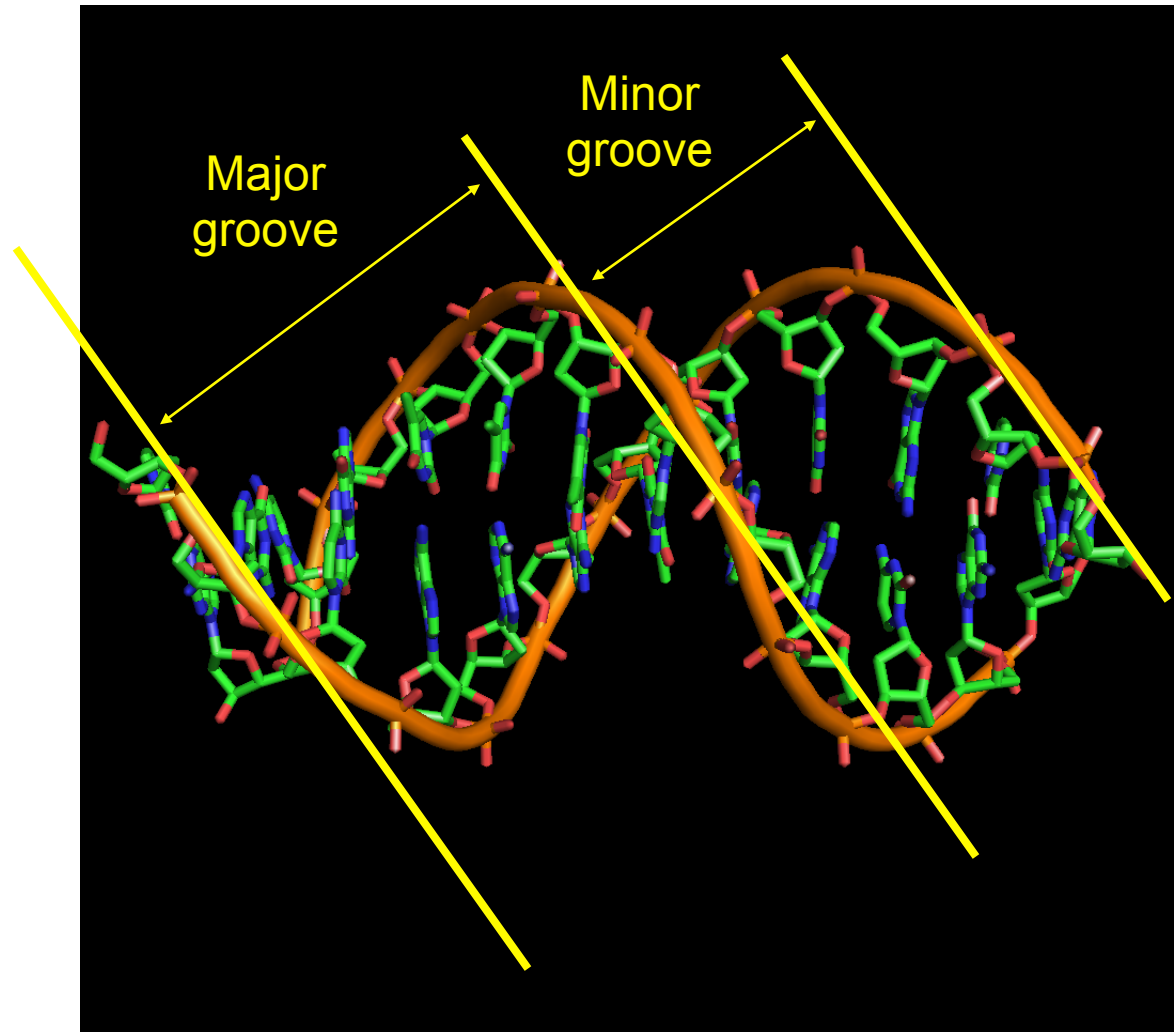
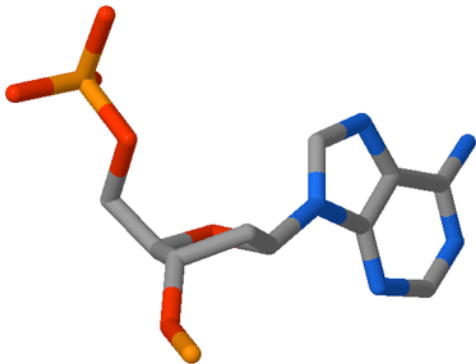
B-form DNA

B-form

Residues per turn = 10
Twist per base pair = 36°
Rise per pair = 3.4\AA
c2'-endo

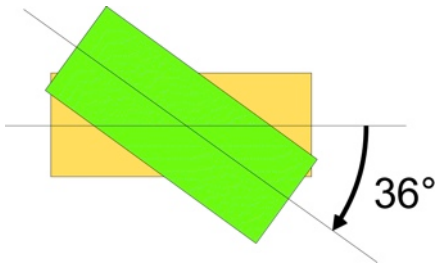
Minor groove width = 5.7\AA
Major groove width = 11.7\AA

Minor groove depth = 7.5\AA
Major groove depth = 8.8\AA



B-form DNA

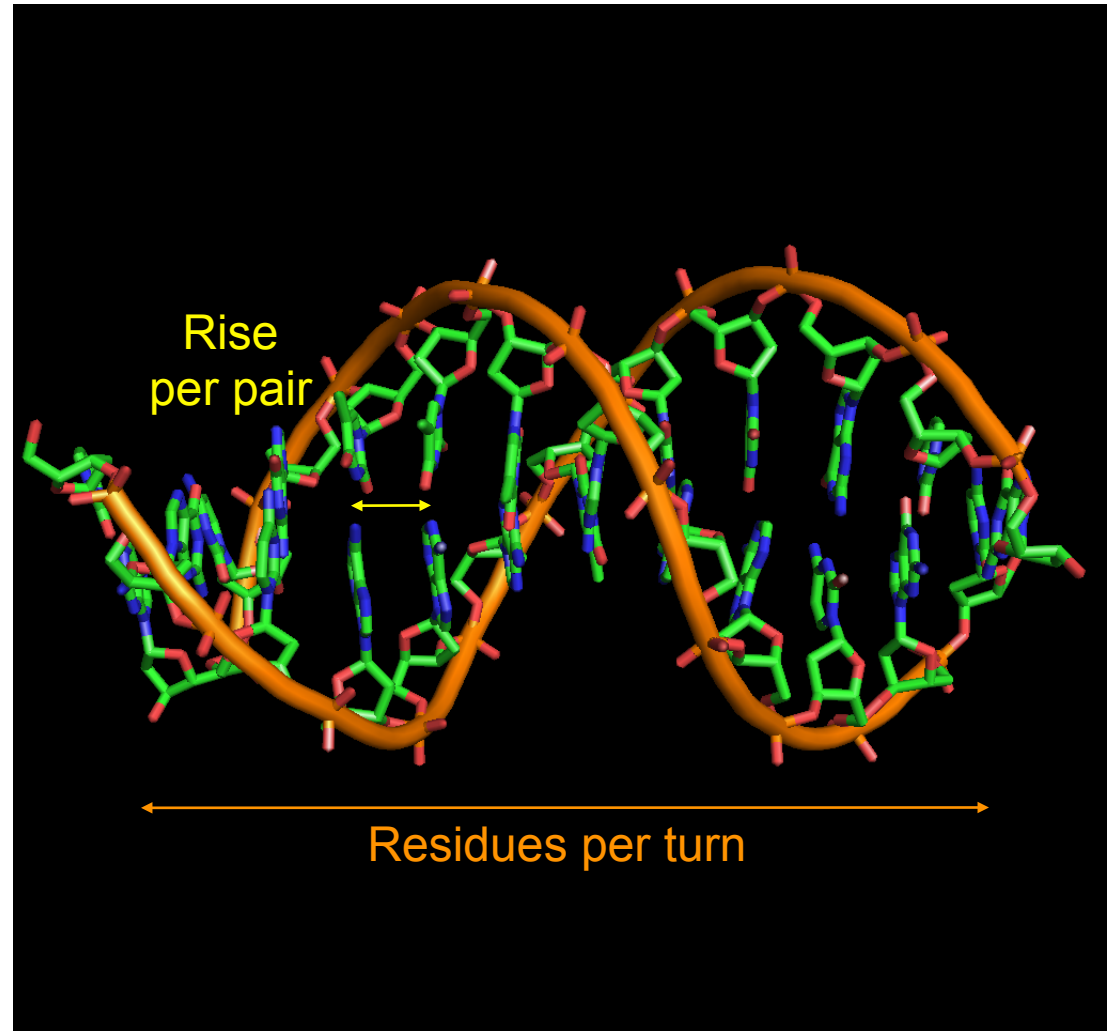
Residues per turn = 10
Twist per base pair = 36°



Rise per pair = 3.4\AA
c2'-endo

Minor groove width = 5.7\AA
Major groove width = 11.7\AA

Minor groove depth = 7.5\AA
Major groove depth = 8.8\AA

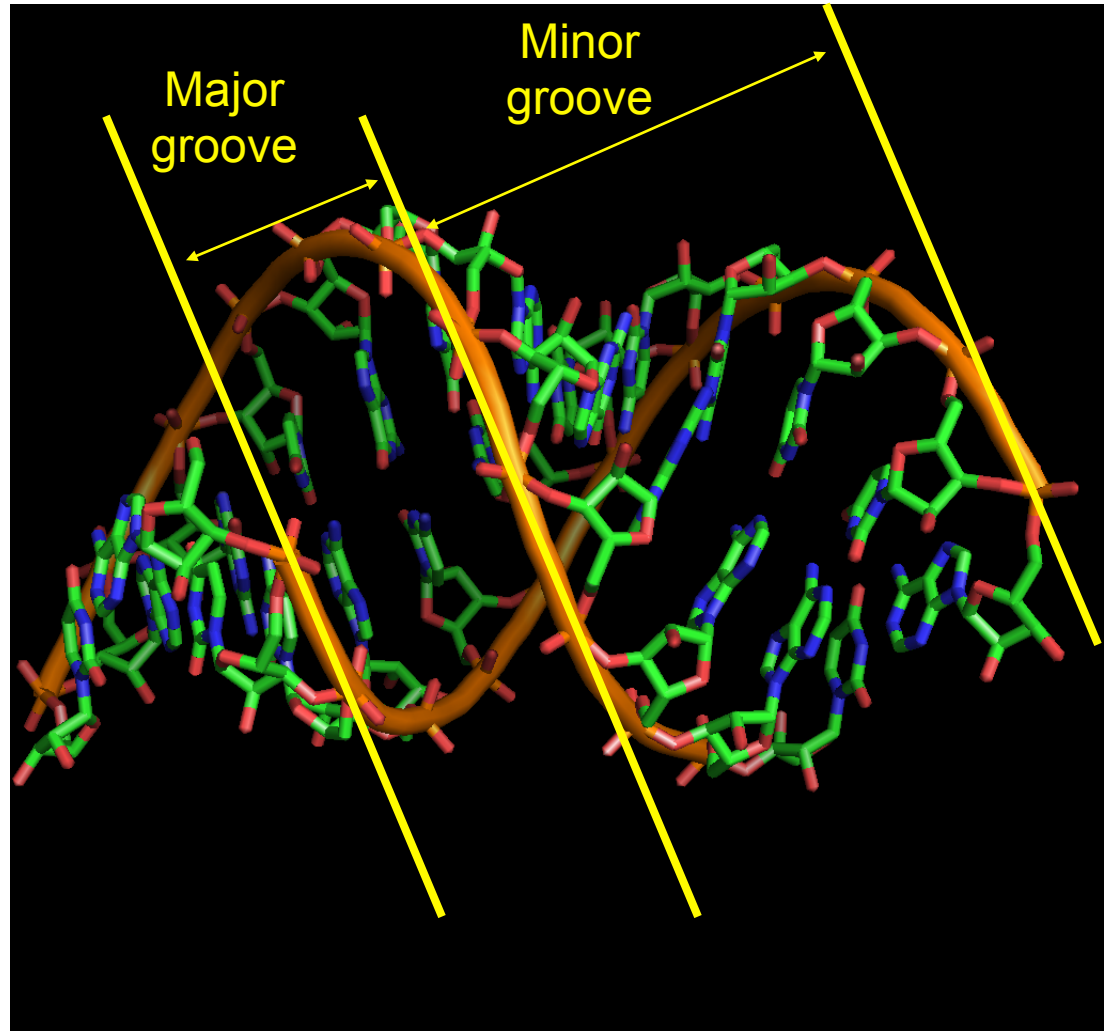
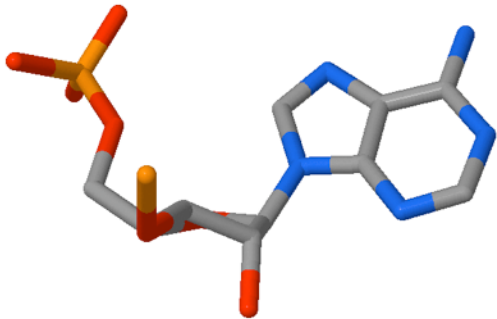


A-form RNA

Residues per turn = 11
Twist per base pair = 33°
Rise per pair = 2.9\AA
c3'-endo

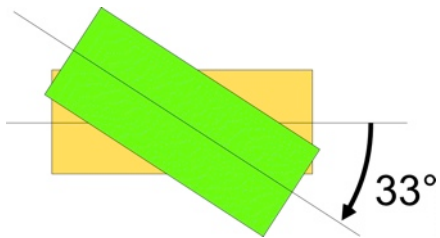
Minor groove width = 11\AA
Major groove width = 2.7\AA

Minor groove depth = 2.8\AA
Major groove depth = 13.5\AA



A-form RNA

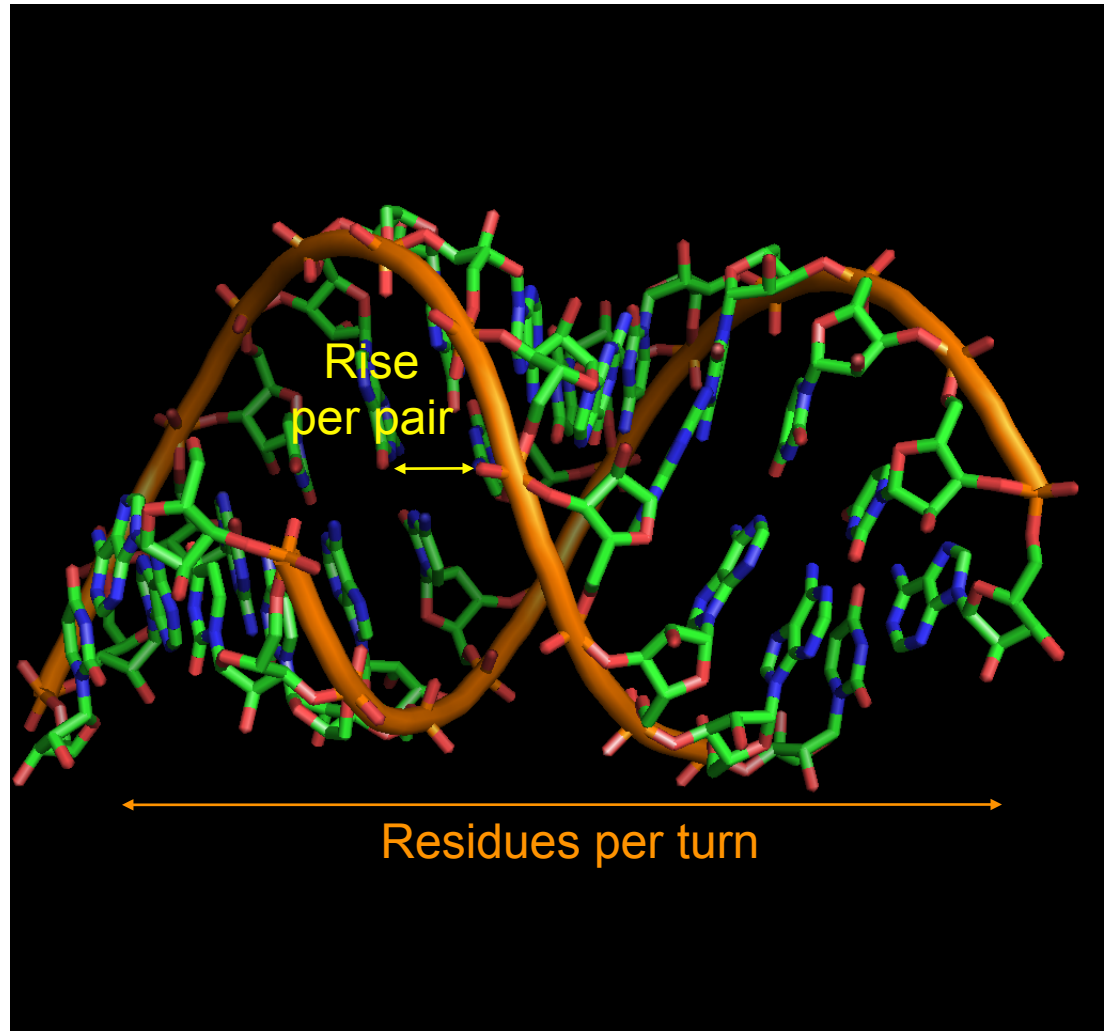
Residues per turn = 11
Twist per base pair = 33°



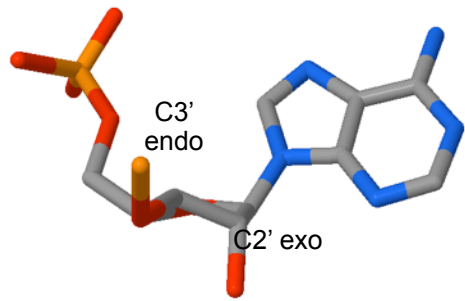
Rise per pair = 2.9\AA
c3'-endo

Minor groove width = 11\AA
Major groove width = 2.7\AA

Minor groove depth = 2.8\AA
Major groove depth = 13.5\AA



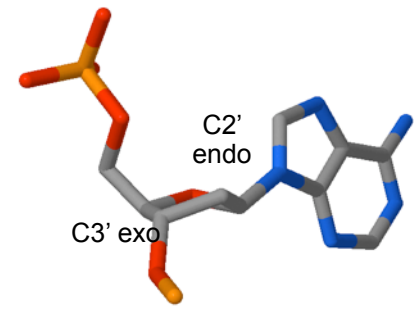
Compare



A-form (RNA)

Minor groove width = 11\AA
Major groove width = 2.7\AA

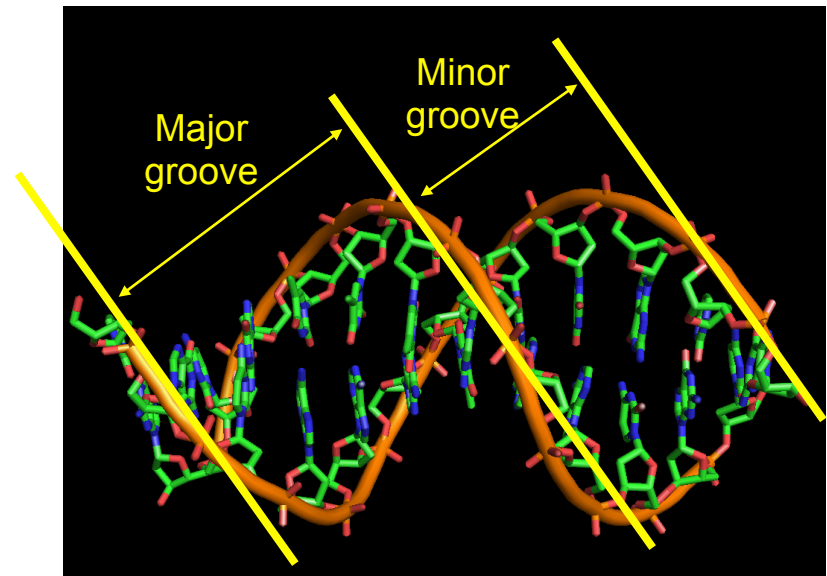
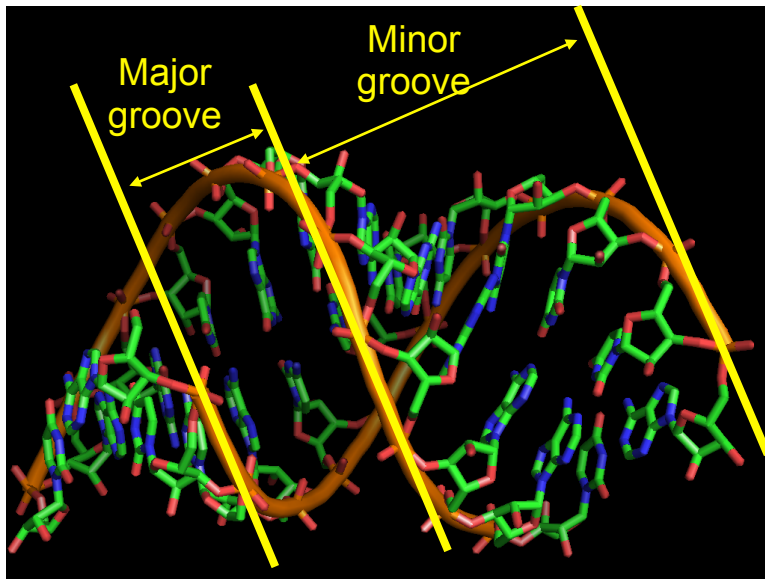
Minor groove depth = 2.8\AA
Major groove depth = 13.5\AA



B-form (DNA)

Minor groove width = 5.7\AA
Major groove width = 11.7\AA

Minor groove depth = 7.5\AA
Major groove depth = 8.8\AA



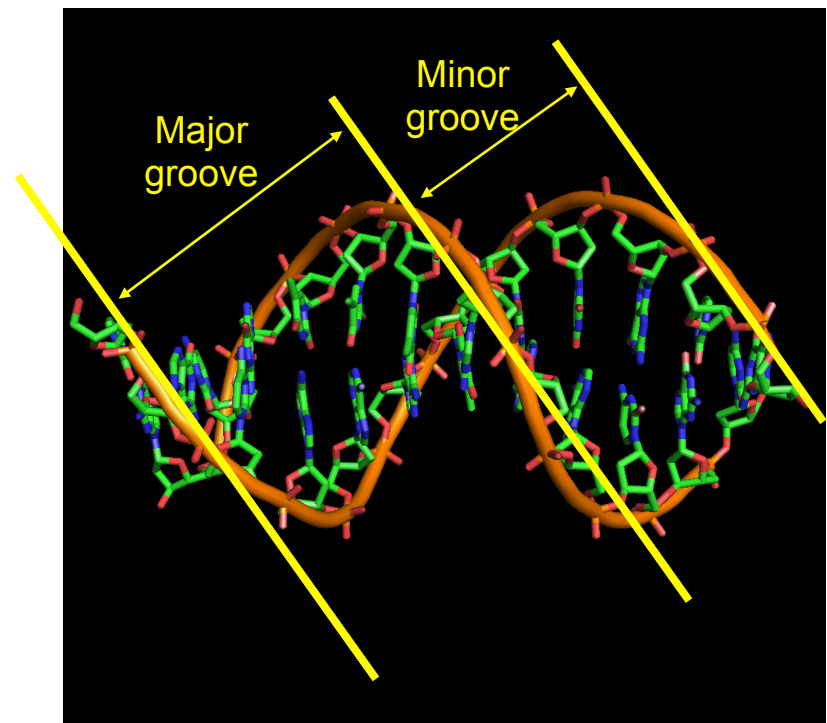
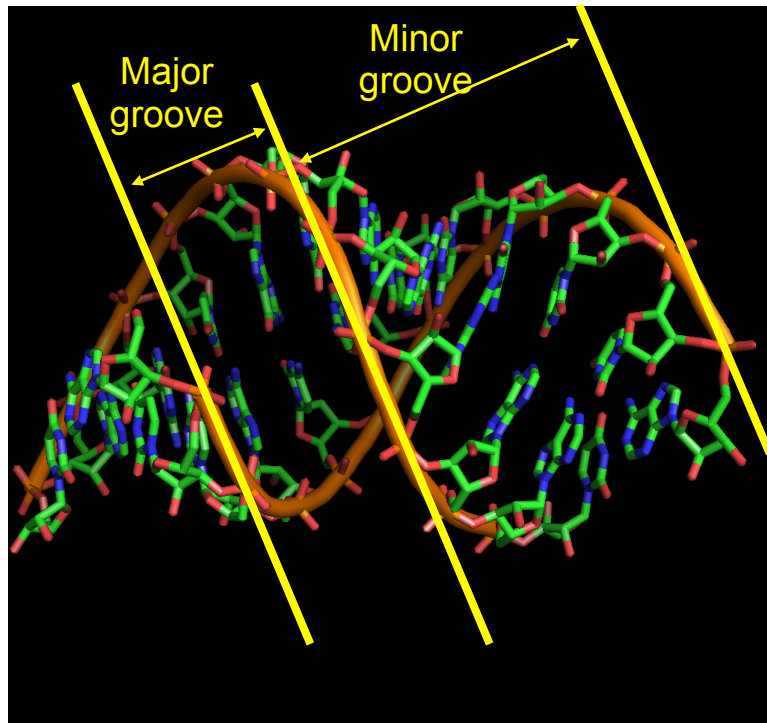
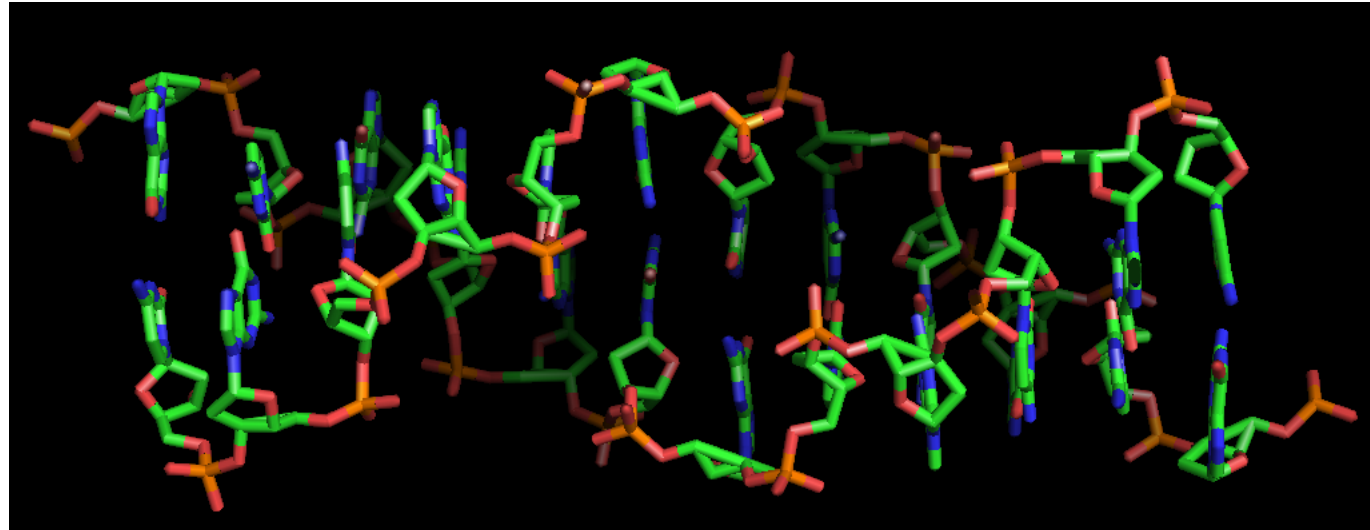
Z-DNA

Residues per turn = 12
Twist per base pair = $-9 / -51^\circ$

Rise per pair = 3.7\AA
c3'-endo(syn) / c2'-endo

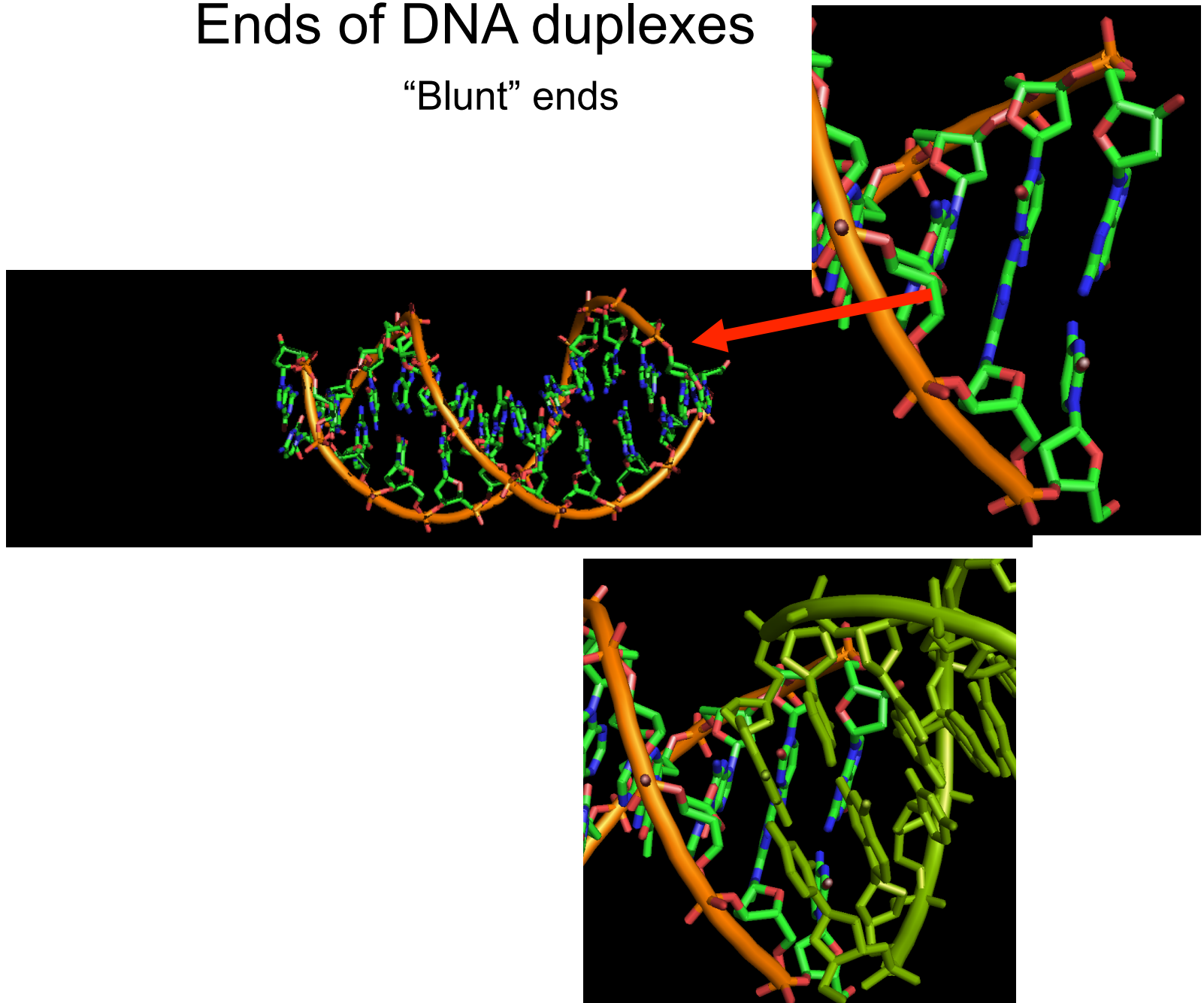
Minor groove width = 2.0\AA
Major groove width = 8.8\AA

Minor groove depth = 13.8\AA
Major groove depth = 3.7\AA



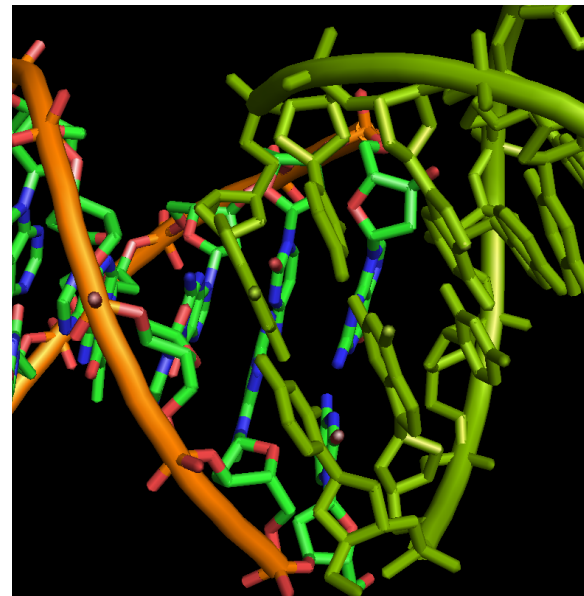
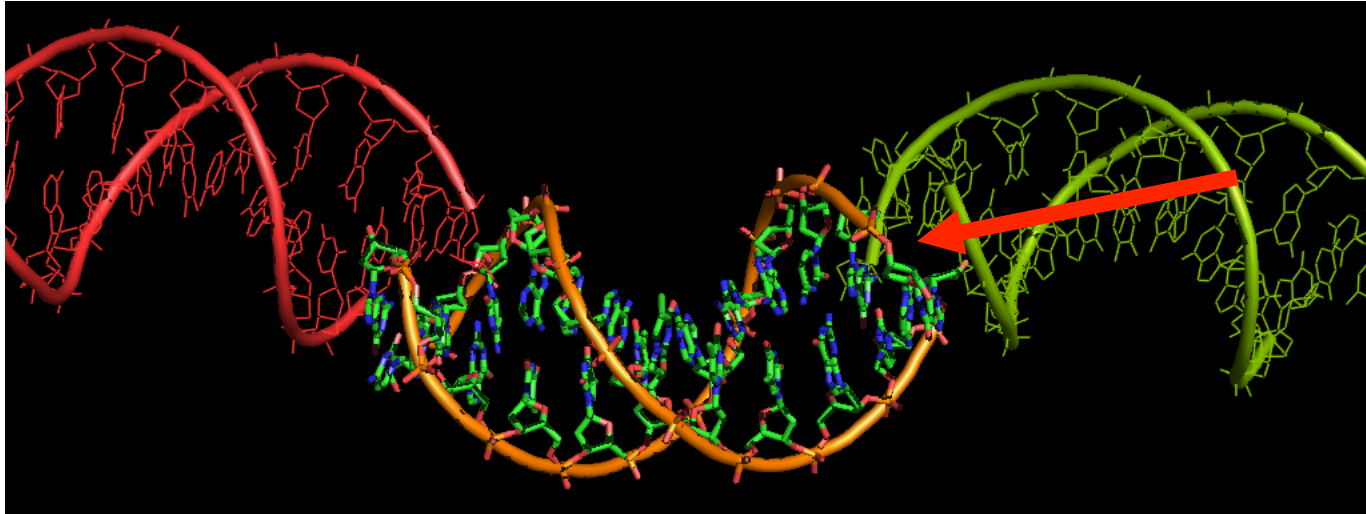
Ends of DNA duplexes

“Blunt” ends

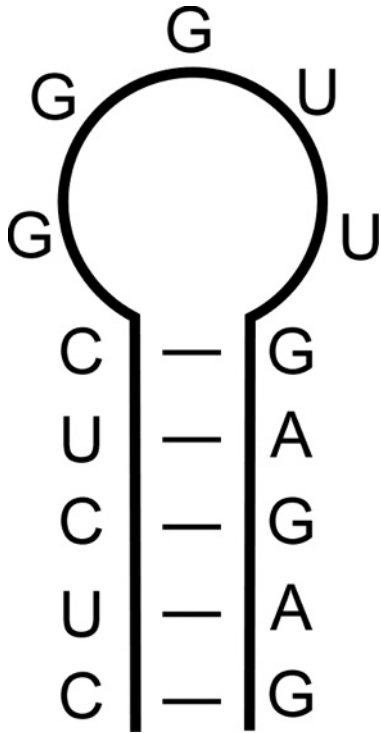


Ends of DNA duplexes

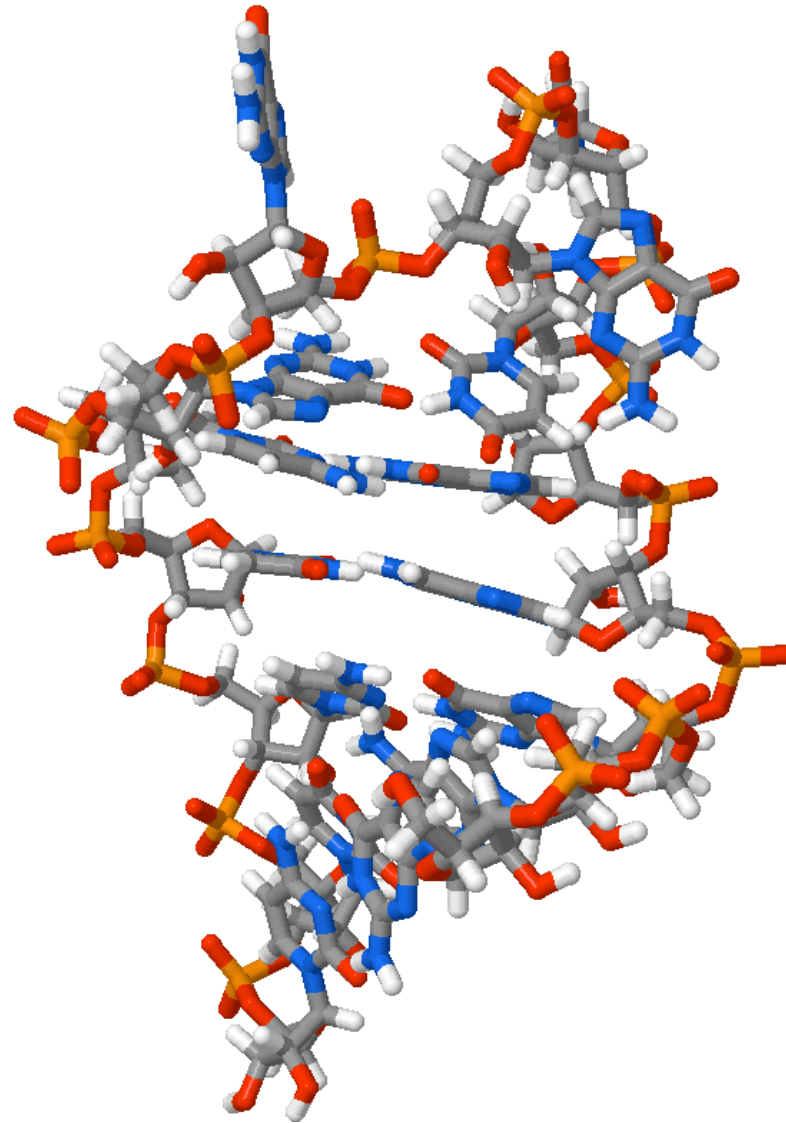
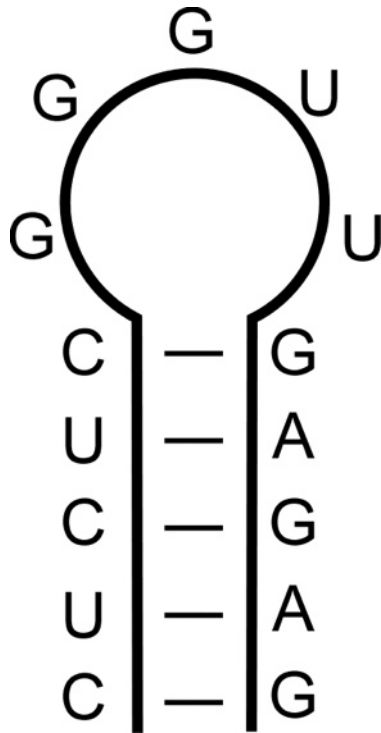
“Blunt” ends



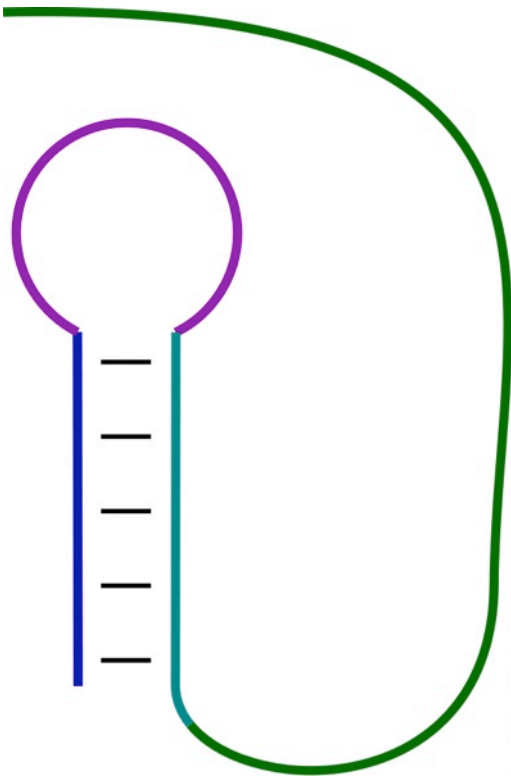
Simple Structure - Hairpin



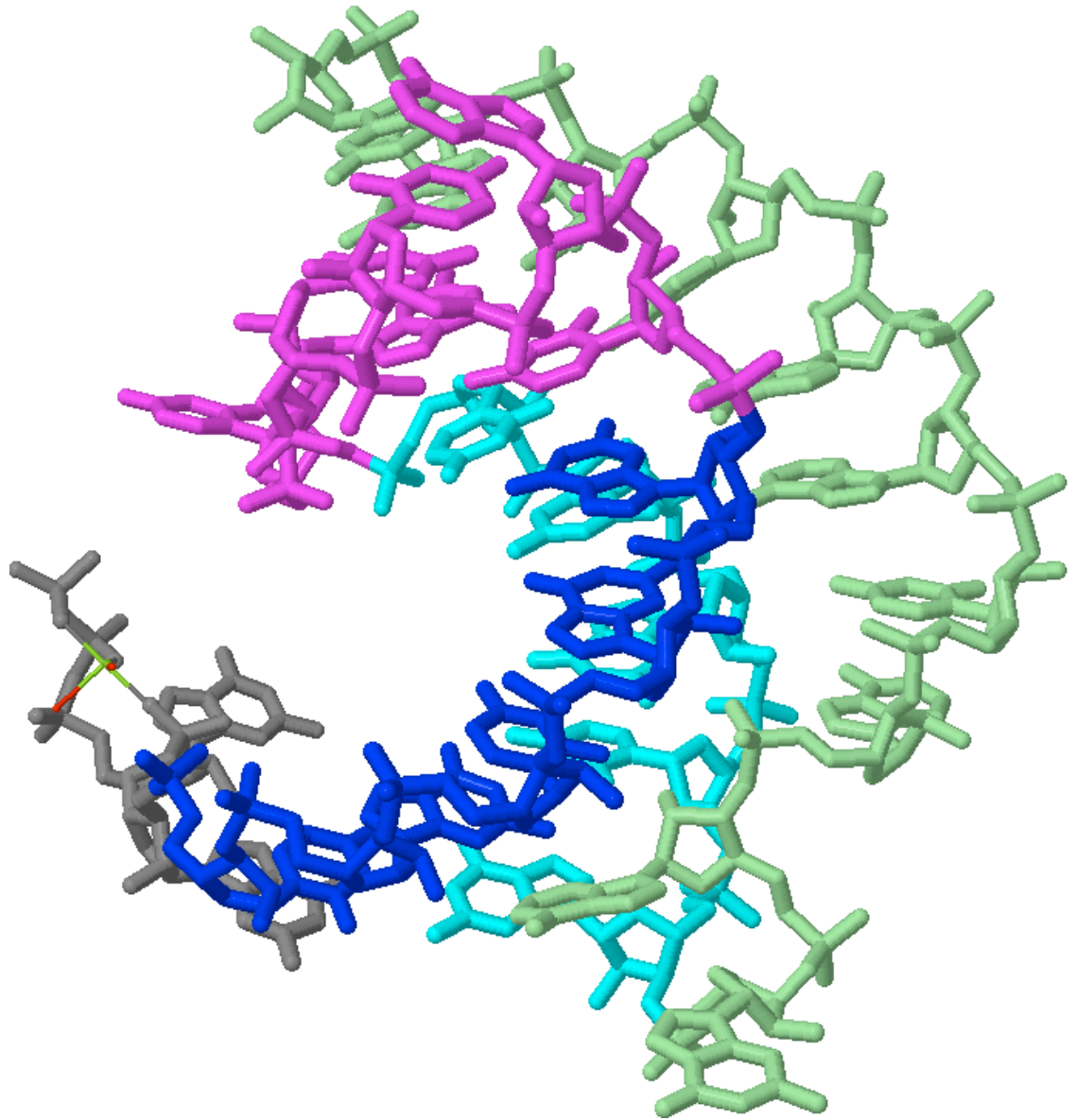
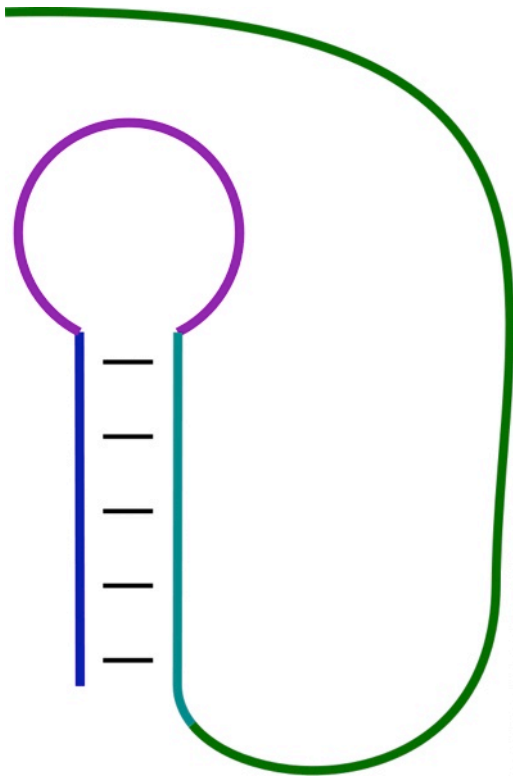
Simple Structure - Hairpin



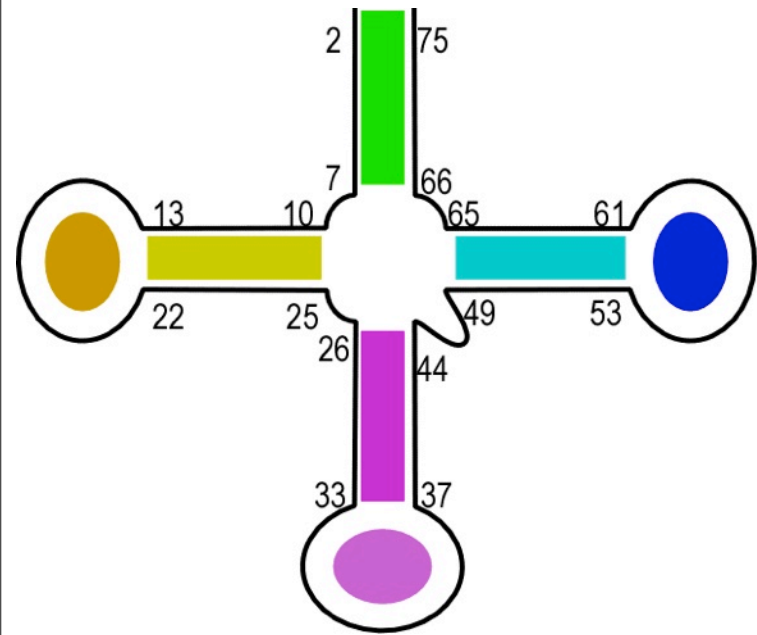
Classic Structure - Pseudoknot



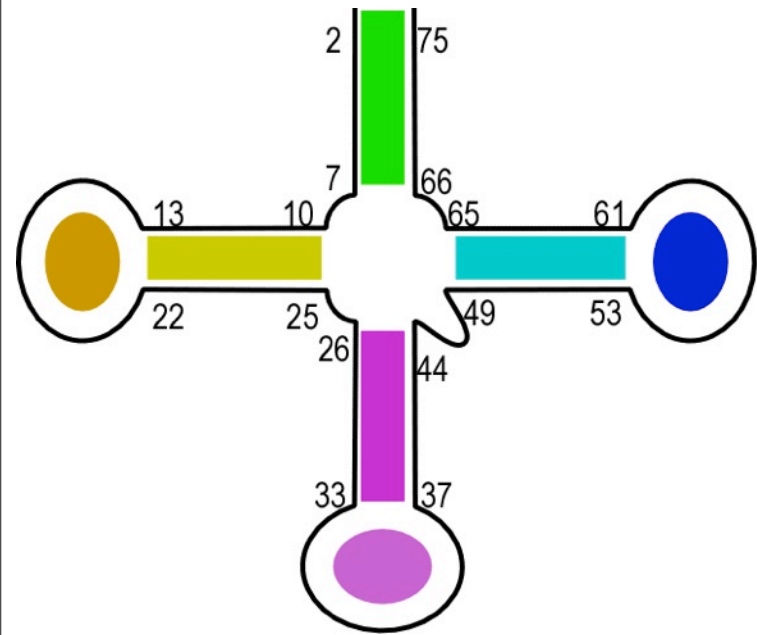
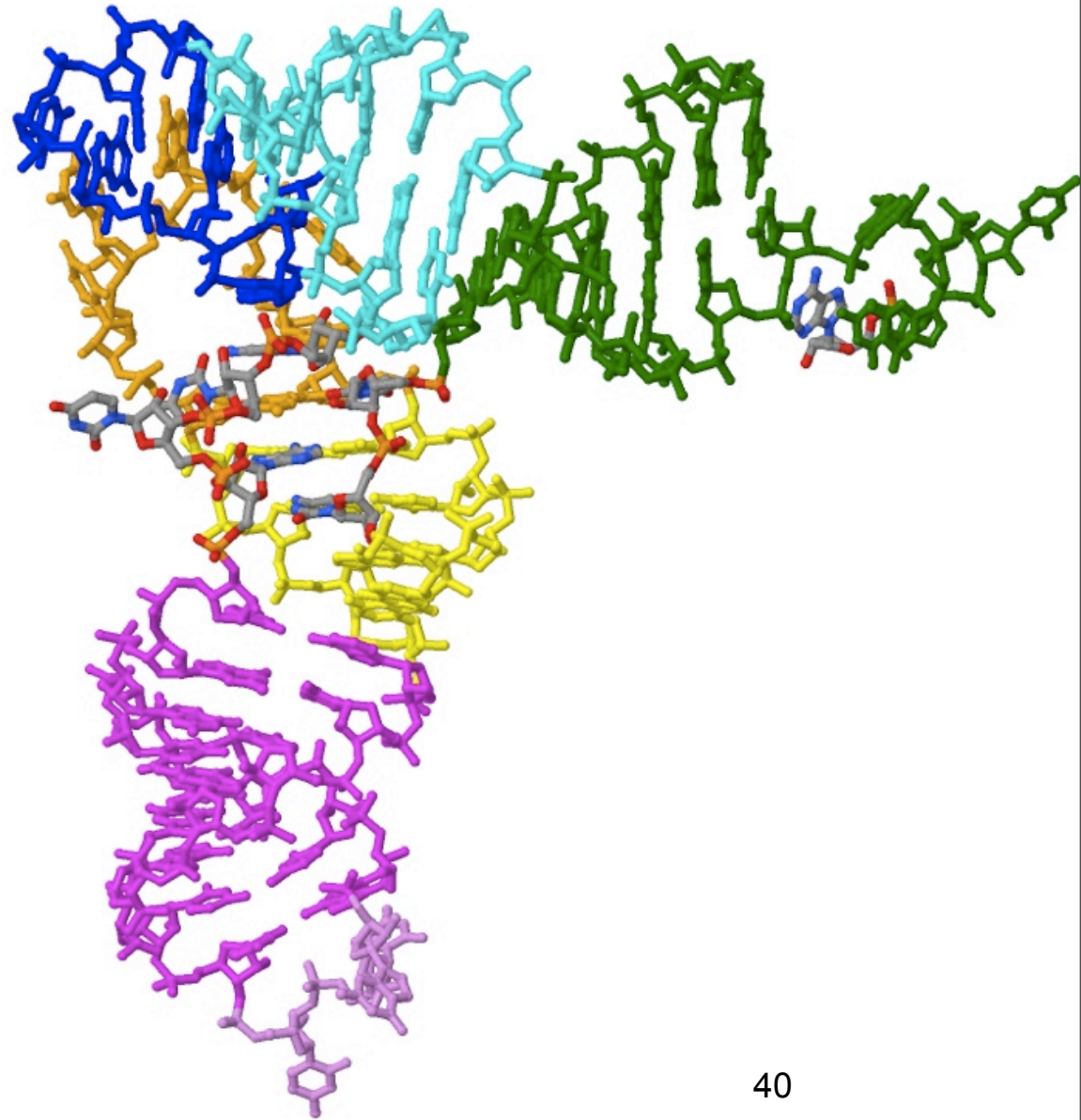
Classic Structure - Pseudoknot



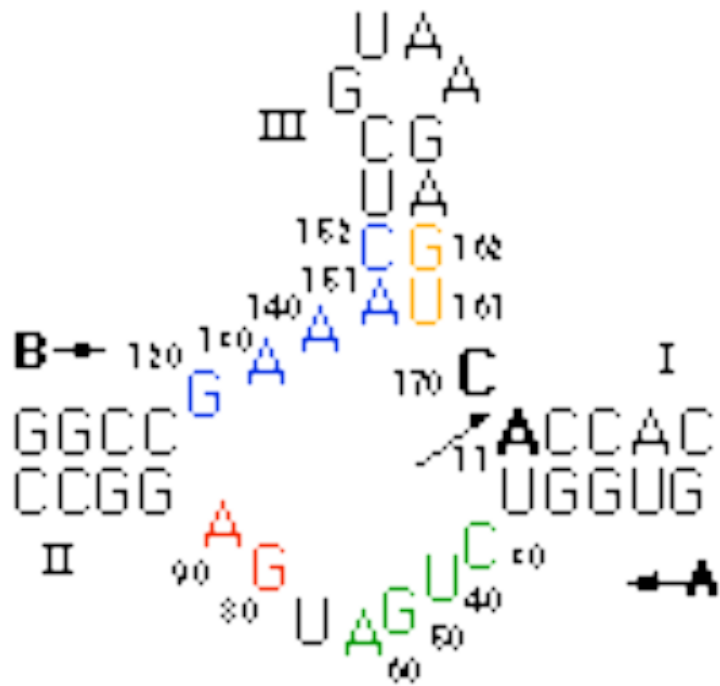
tRNA



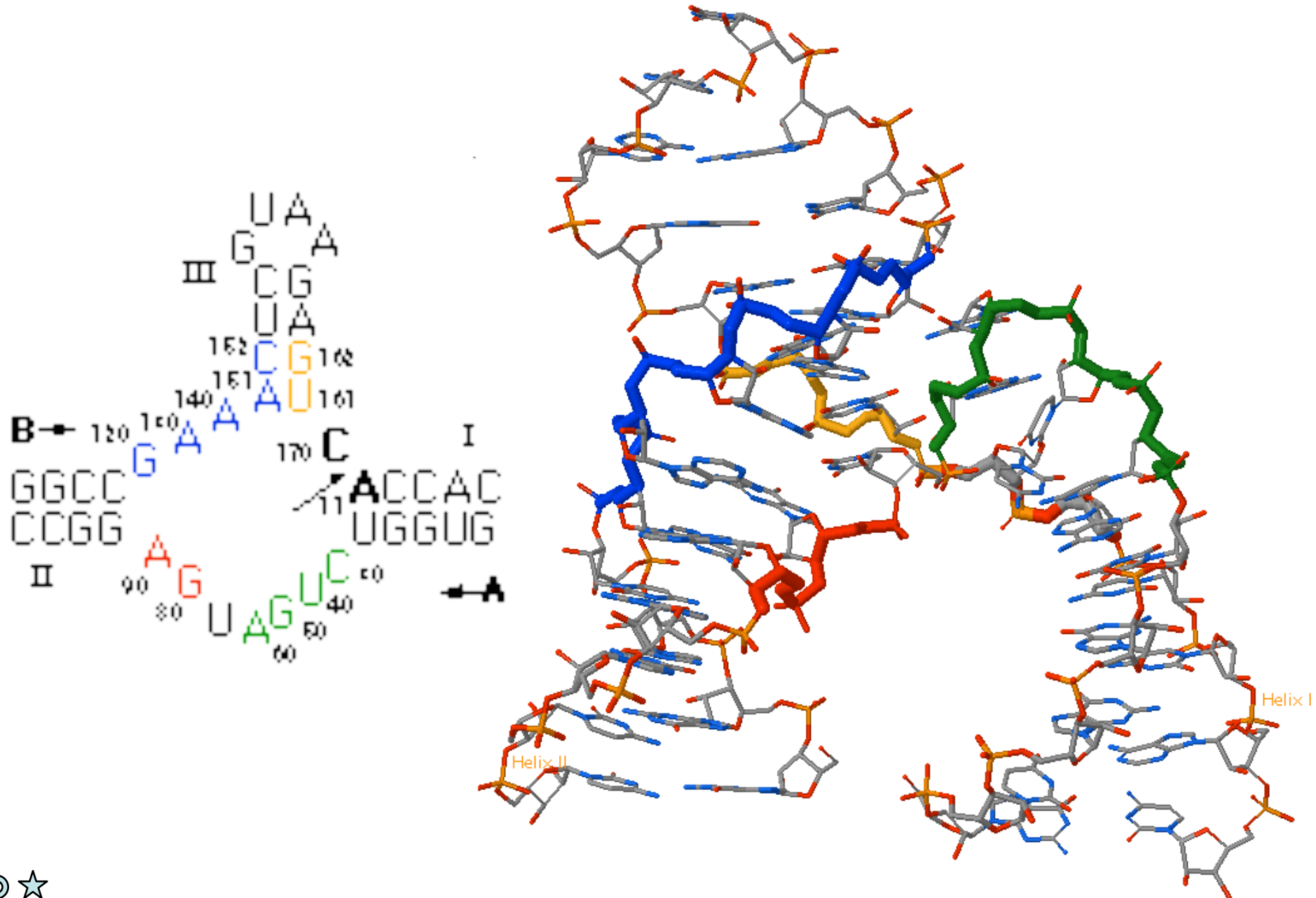
tRNA



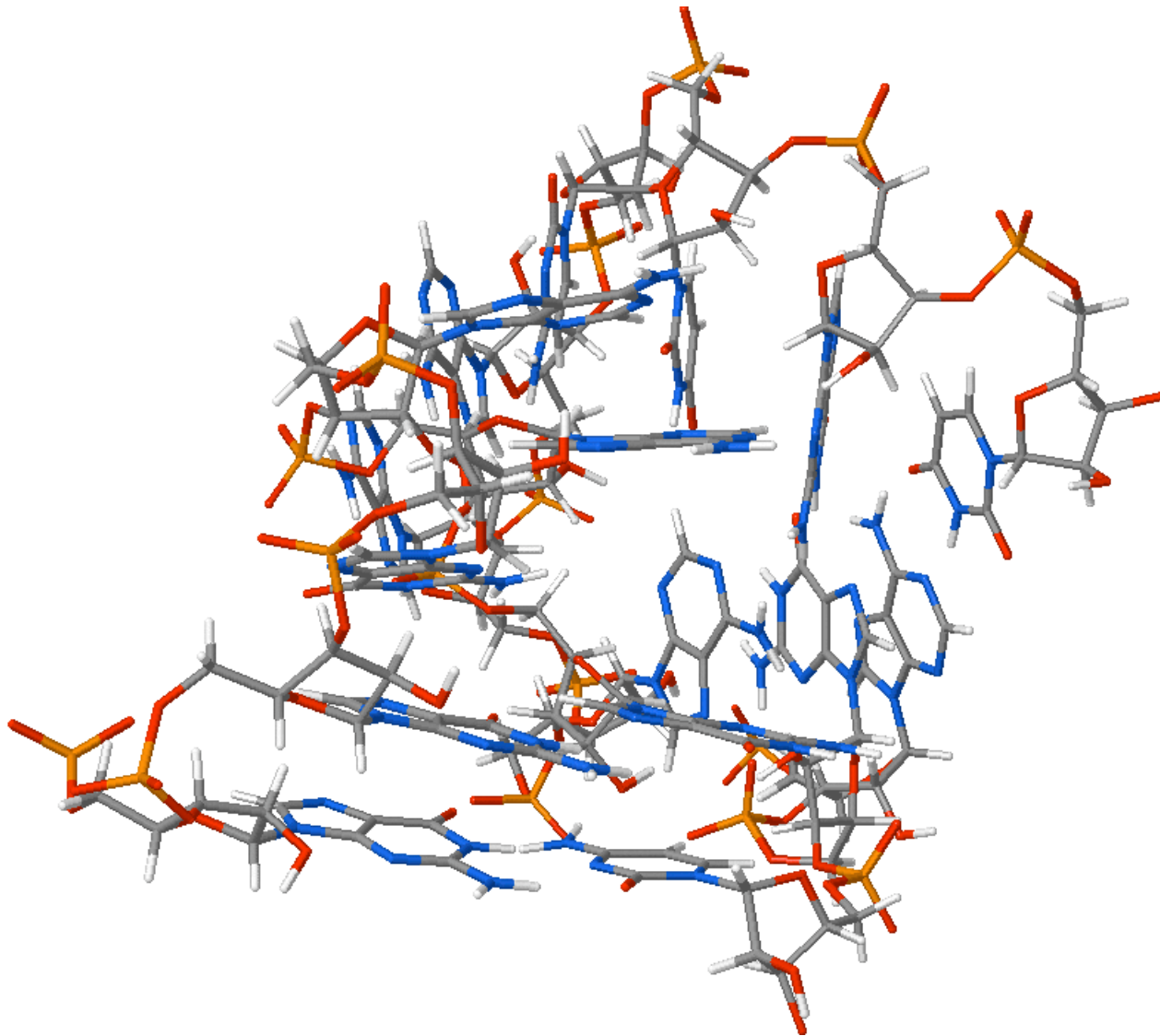
Hammerhead Ribozyme



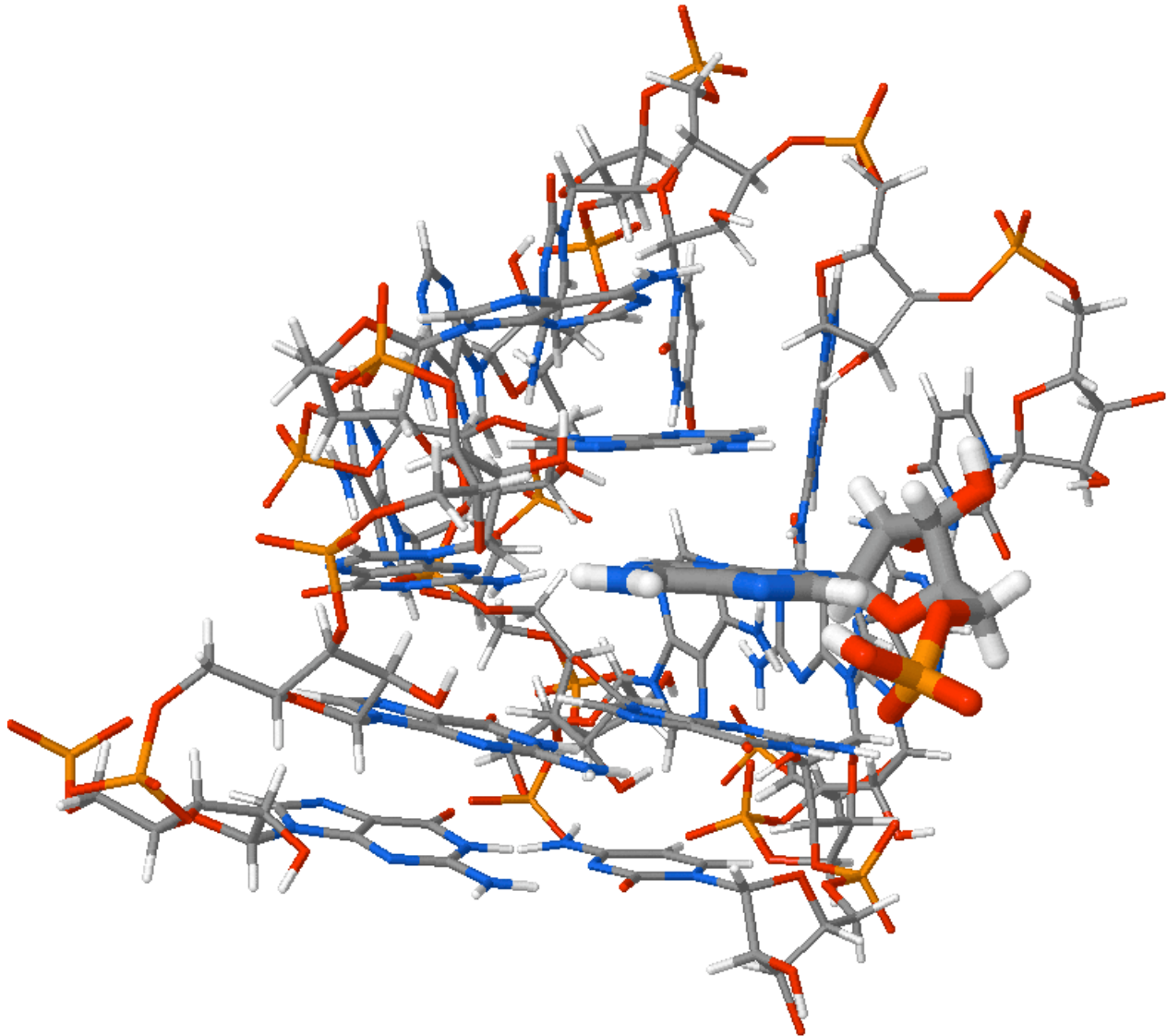
Hammerhead Ribozyme



AMP Aptamer

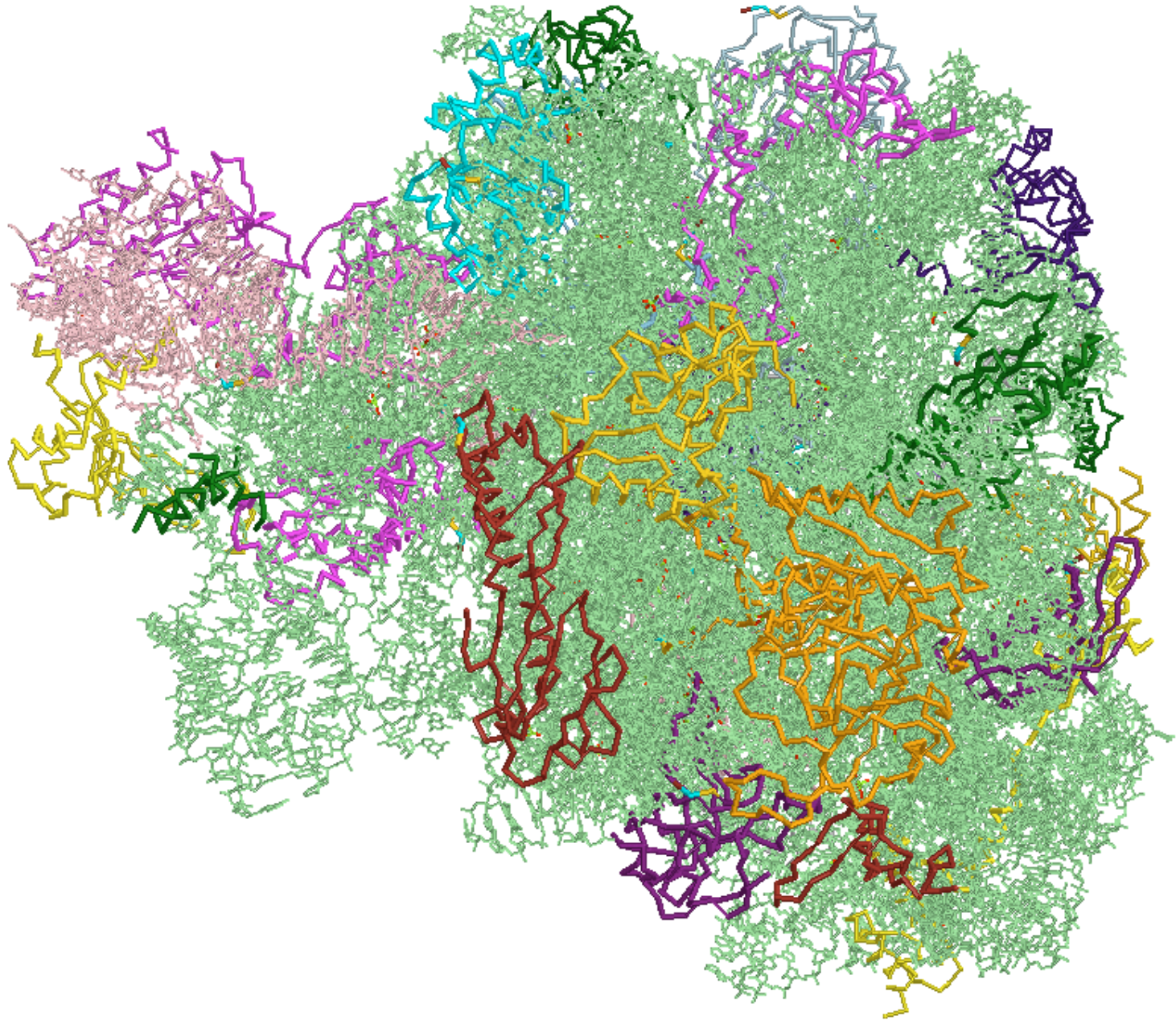


AMP Aptamer



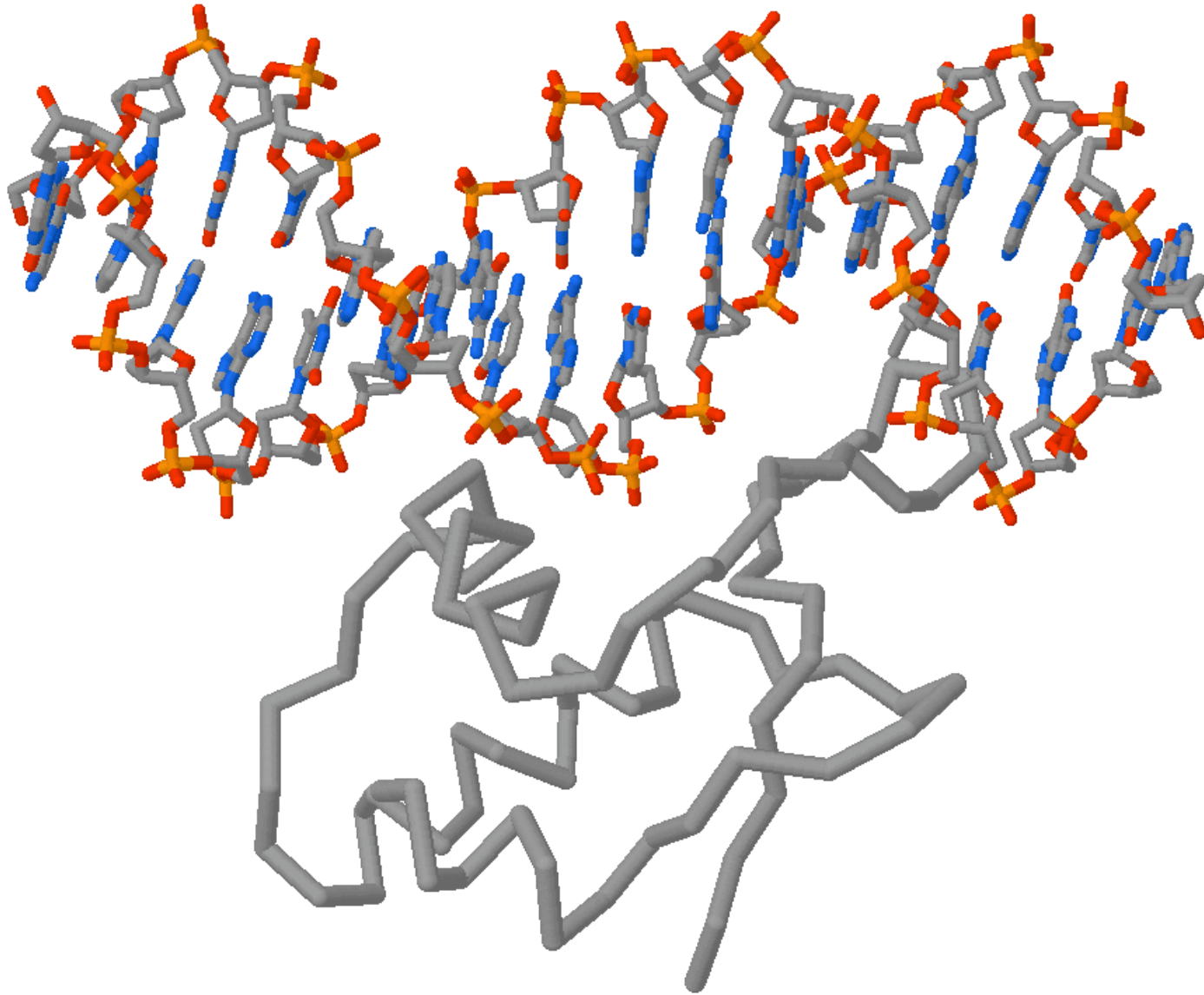
Ribosome

An RNA machine with protein cofactors



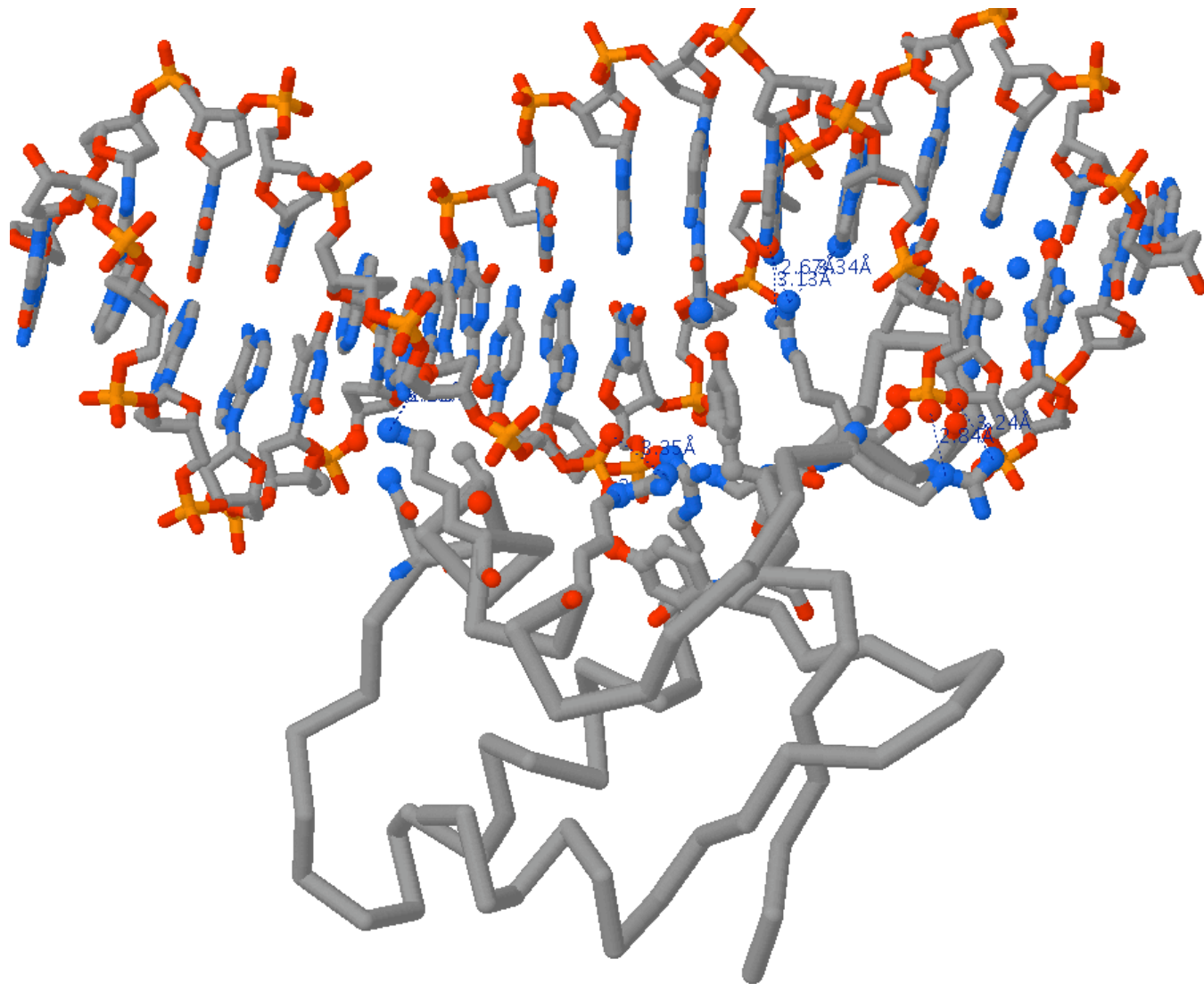
Winged Helix DNA Binding Domain

Classic helix-turn-helix



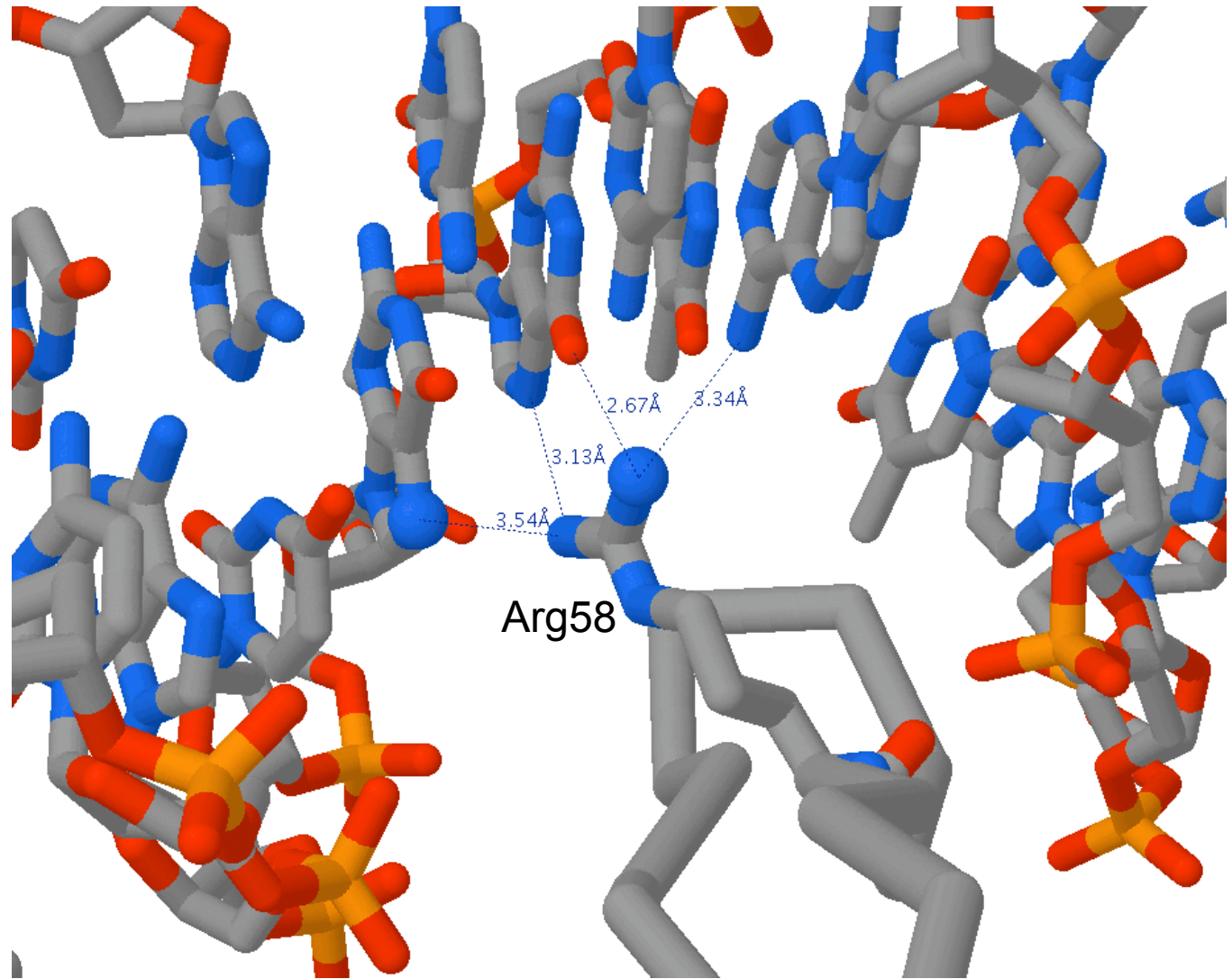
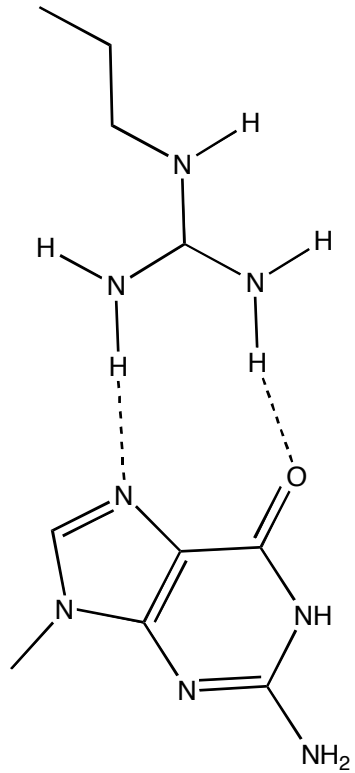
Winged Helix DNA Binding Domain

Classic helix-turn-helix



Winged Helix DNA Binding Domain

Classic helix-turn-helix



Hrfx1 bound to its X-box binding site