Assignment-13

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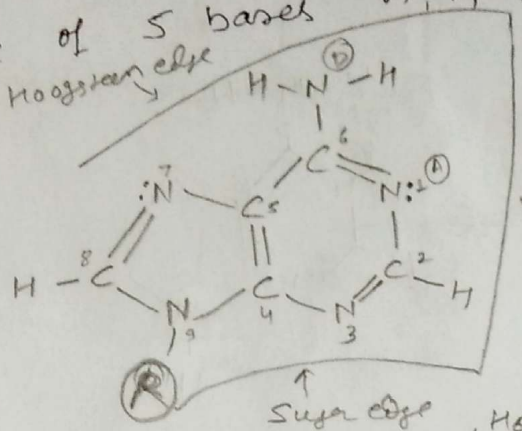
(1) Lewis structure of 5 bases A, T, U, G, C

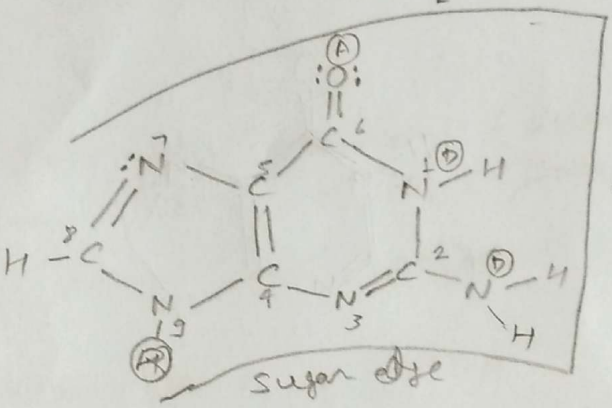
Purines :—

Adenine – (A)



Ⓓ – H bond donor
Ⓐ – H bond acceptor

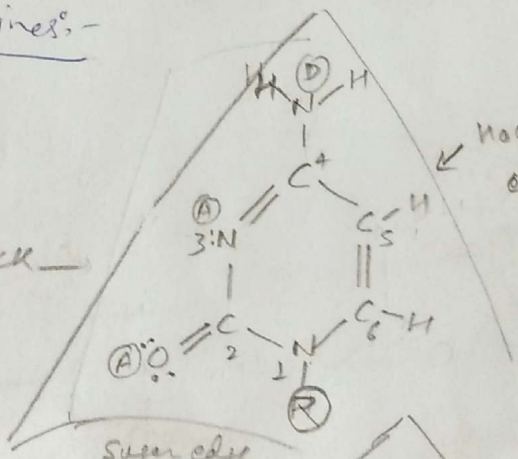
Guanine – (G)



Pyrimidines :–

Cytosine – (C)

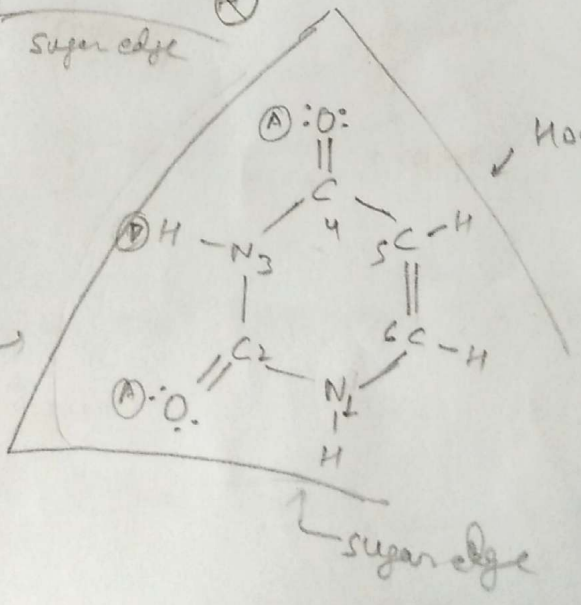
watson-Crick edge



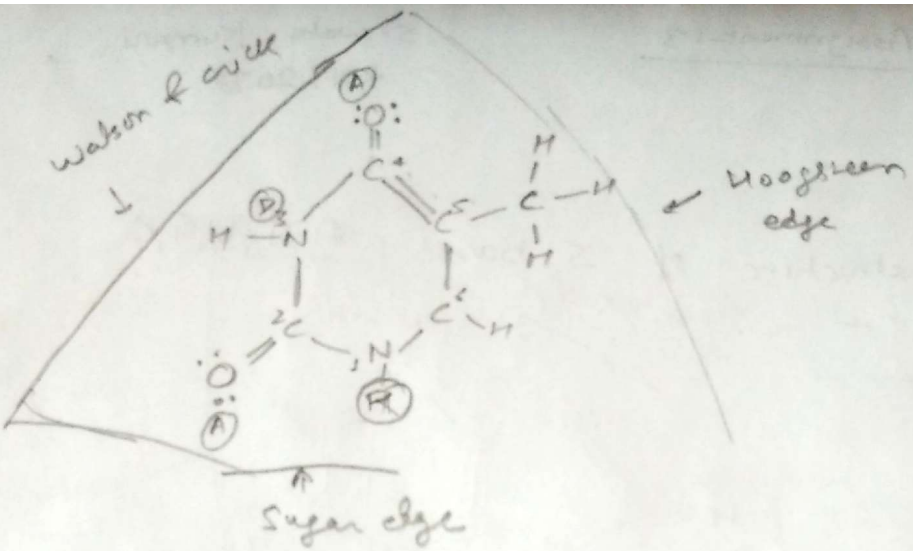
Uracil – (U)

[only in RNA]

watson & Crick edge

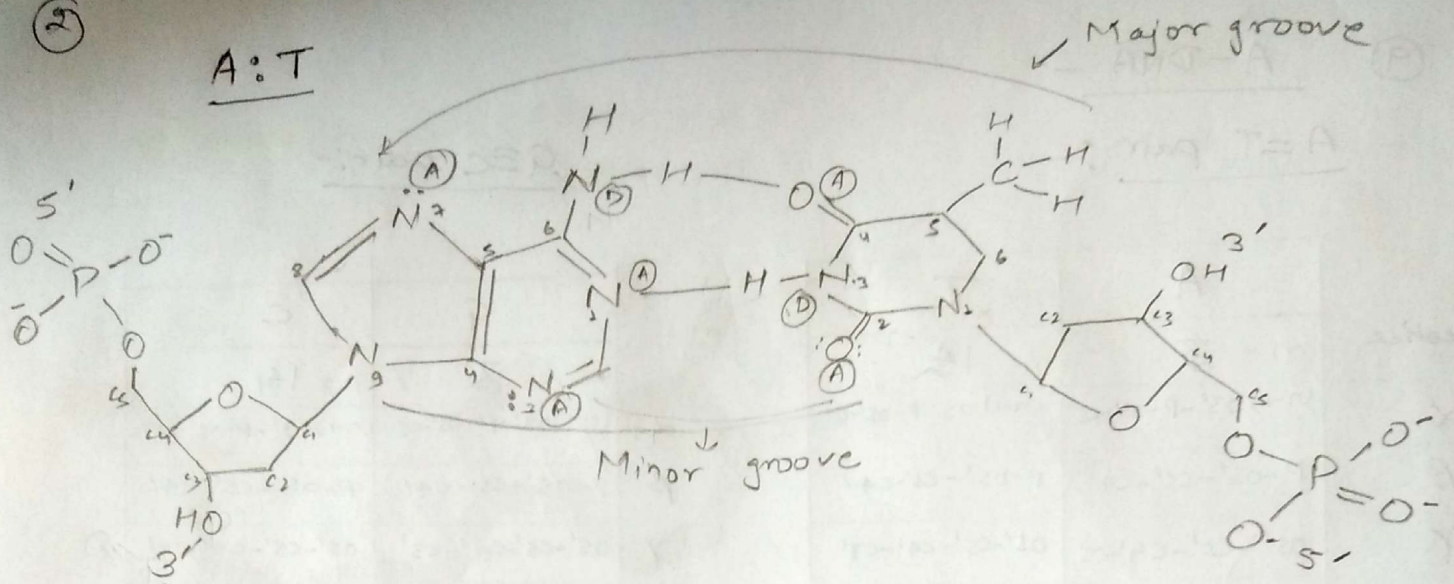


Thymine (T) — [in DNA only]



(2)

A : T



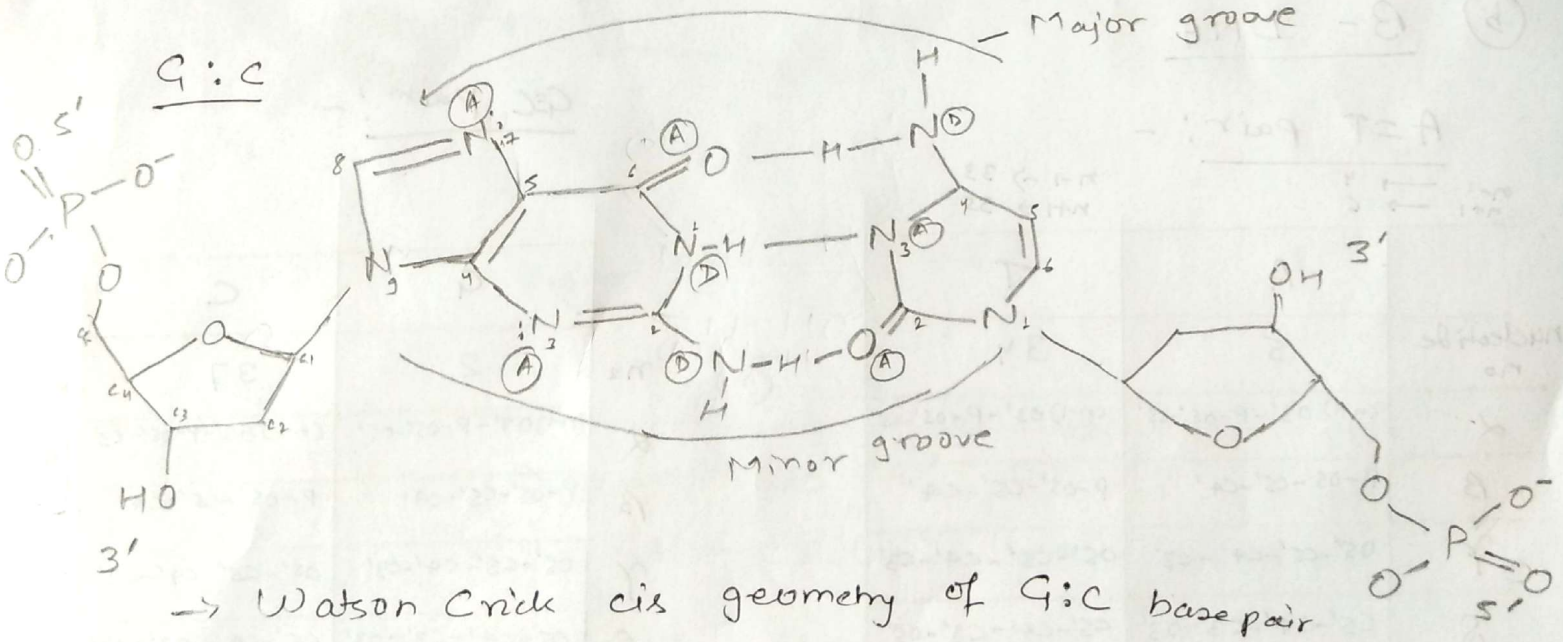
→ Watson Crick cis geometry (orientation of glycosidic bond same side) of A : T base pair

→ Hbond donor and acceptor in Major & Minor groove :-

Major groove - ADA

Minor groove - AA AA

G : C



→ Watson Crick cis geometry of G : C base pair

→ H-bond donor & Acceptor in Minor & Major groove

Major groove - AAD

Minor groove - ADA

4.

(a) A-DNA -

A=T pair :-

	A	T
nucleotide no	n = 5	n = 12
α	(n-1) O3'-P-O5'-C5'	(n-1) O3'-P-O5'-C5'
β	P-O5'-C5'-C4'	P-O5'-C5'-C4'
γ	O5'-C5'-C4'-C3'	O5'-C5'-C4'-C3'
δ	C5'-C4'-C3'-O3'	C5'-C4'-C3'-O3'
ε	C4'-C3'-O3'-P	C4'-C3'-O3'-P
ξ	C3'-O3'-P-O5' (n+1)	C3'-O3'-P-O5' (n+1)
χ	O4'-C1'-N9-C4	O4'-C1'-N1-C2
Sugar packer	C3' endo	C3' endo

n-1 = 4
n+1 = 6

n-1 = 11
n+1 = 13

G≡C pair:-

	G	C
	n = 3	n = 16
α	(n-1)O3'-P-O5'-C5'	(n-1)O3'-P-O5'-C5'
β	P-O5'-C5'-C4'	P-O5'-C5'-C4'
γ	O5'-C5'-C4'-C3'	O5'-C5'-C4'-C3'
δ	C5'-C4'-C3'-O3'	C5'-C4'-C3'-O3'
ε	C4'-C3'-O3'-P	C4'-C3'-O3'-P
ξ	C3'-O3'-P-O5'	C3'-O3'-P-O5'
χ	O4'-C1'-N9-C4	O4'-C1'-N1-C2
Sugar packer	C3' endo	C3' endo

n-1 = 2	13
n+1 = 4	15

(b) B-DNA

A=T pair :-

n-1 → 4
n+1 → 6

n-1 → 33
n+1 → 35

	A	T
nucleotide no	5	34
α	(n-1) O3'-P-O5'-C5' (4th, 5th)	(n-1)O3'-P-O5'-C5' (33)
β	P-O5'-C5'-C4' (5)	P-O5'-C5'-C4'
γ	O5'-C5'-C4'-C3'	O5'-C5'-C4'-C3'
δ	C5'-C4'-C3'-O3'	C5'-C4'-C3'-O3'
ε	C4'-C3'-O3'-P	C4'-C3'-O3'-P
ξ	C3'-O3'-P-O5' (n+1) (34)	C3'-O3-P-O5' (n+1) (35)
χ	O4'-C1'-N9-C4 (52)	O4'-C1'-N1-C2 (53rd)
Sugar packer	C2' endo	C2' endo

G≡C pair :-

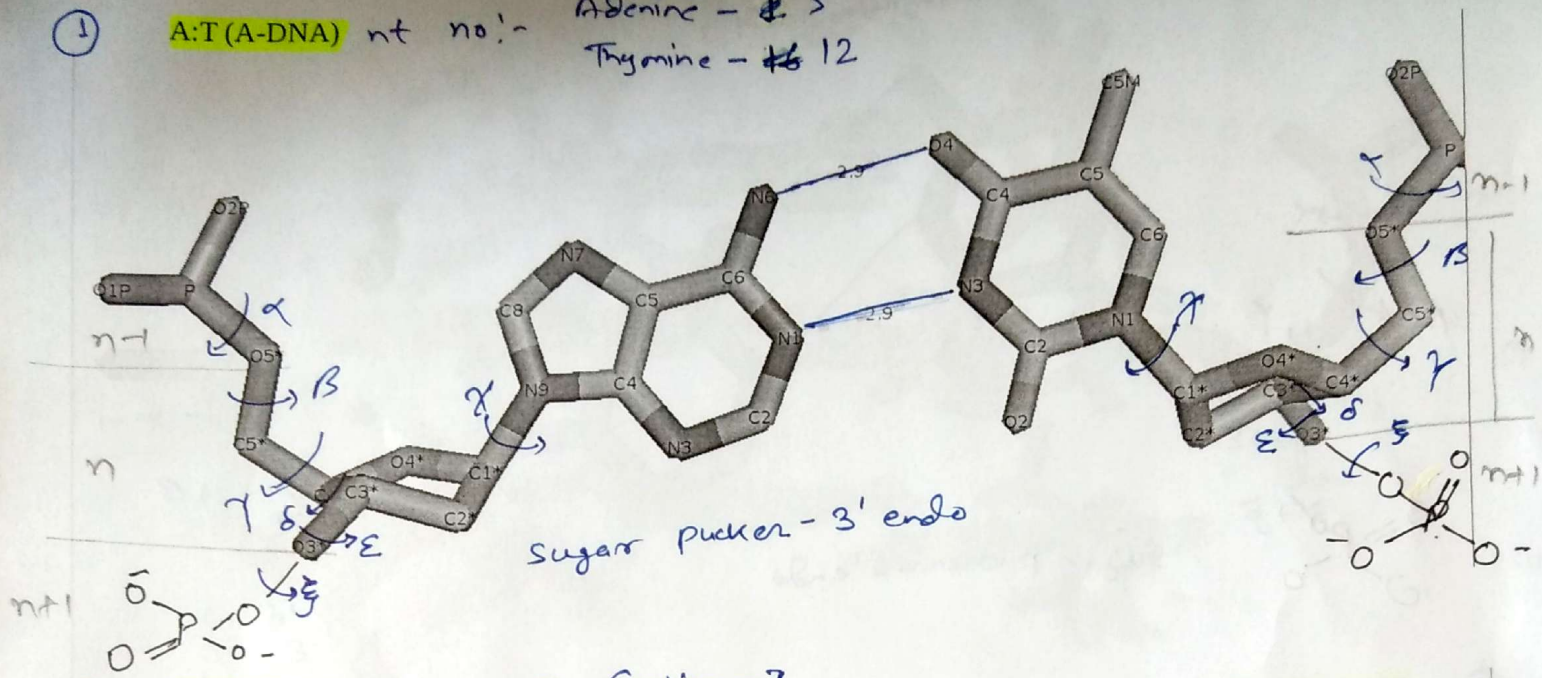
	G	C
n =	2	37
α	(n-1)O3'-P-O5'-C5'	(n-1)O3'-P-O5'-C5'
β	P-O5'-C5'-C4'	P-O5'-C5'-C4'
γ	O5'-C5'-C4'-C3'	O5'-C5'-C4'-C3'
δ	C5'-C4'-C3'-O3'	C5'-C4'-C3'-O3'
ε	C4'-C3'-O3'-P	C4'-C3'-O3'-P
ξ	C3'-O3'-P-O5' (n+1)	C3'-O3-P-O5' (n+1)
χ	O4'-C1'-N9-C4	O4'-C1'-N1-C2
Sugar packer	C2' endo	C2' endo

n+1 = for G
n-1 = for G

for n-1
n+1

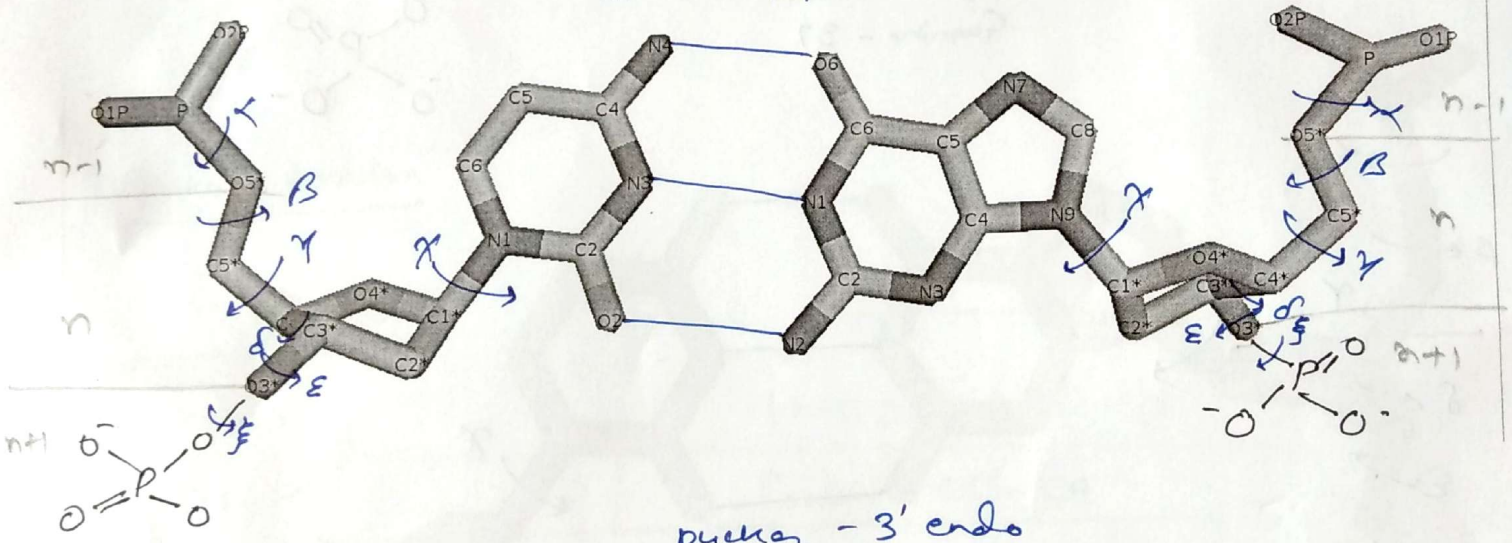
A-DNA

① A:T (A-DNA) nt no:- Adenine – 5
Thymine – 12



Sugar pucker – 3' endo

② C:G (A-DNA) nt no – Cytosine – 3
Guanine – 14



Sugar pucker – 3' endo

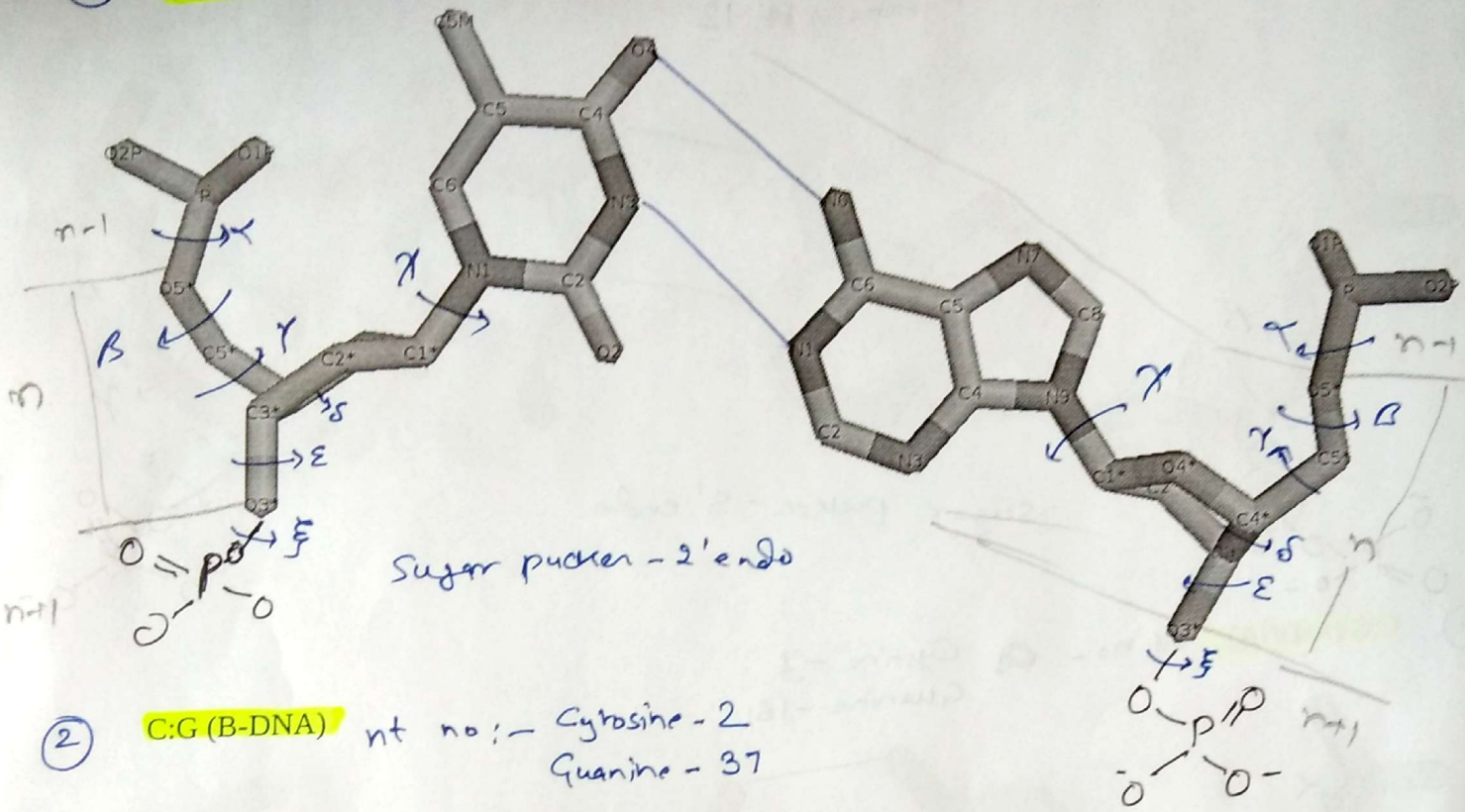
Backbone torsion angle → P – O5' (α), O5' – C5' (β), C5' – C4' (γ), C4' – C3' (δ), C3' – O3' (ε)

O3' – P (ξ)

Glycosidic angle (χ) → O4' – C1' – N1' – C2 (Thymine & Cytosine)
O4' – C1' – N9' – C4 (Adenine & Guanine)

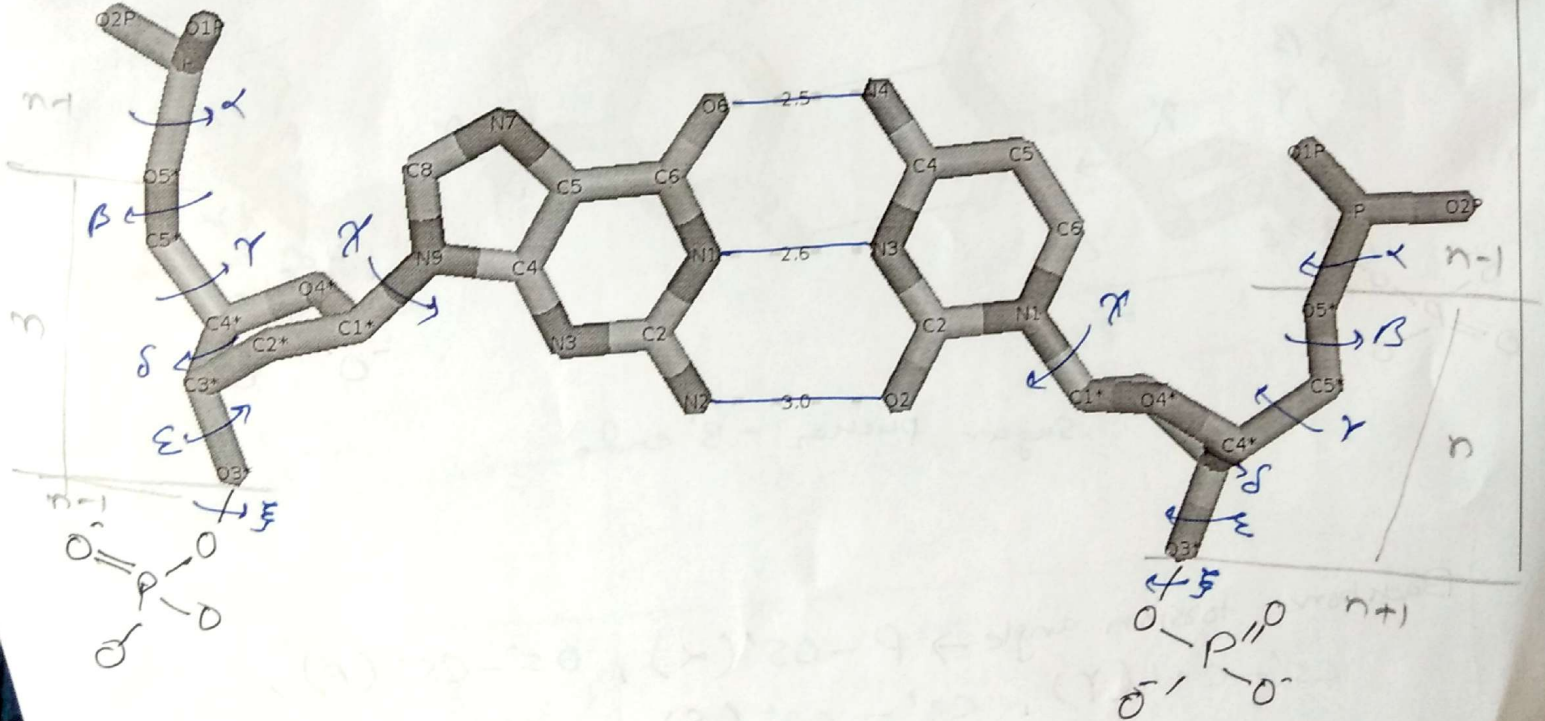
B-DNA

① A:T (B-DNA) nt no:- Adenine - 5
Thymine - 34



Sugar pucker - 2'endo

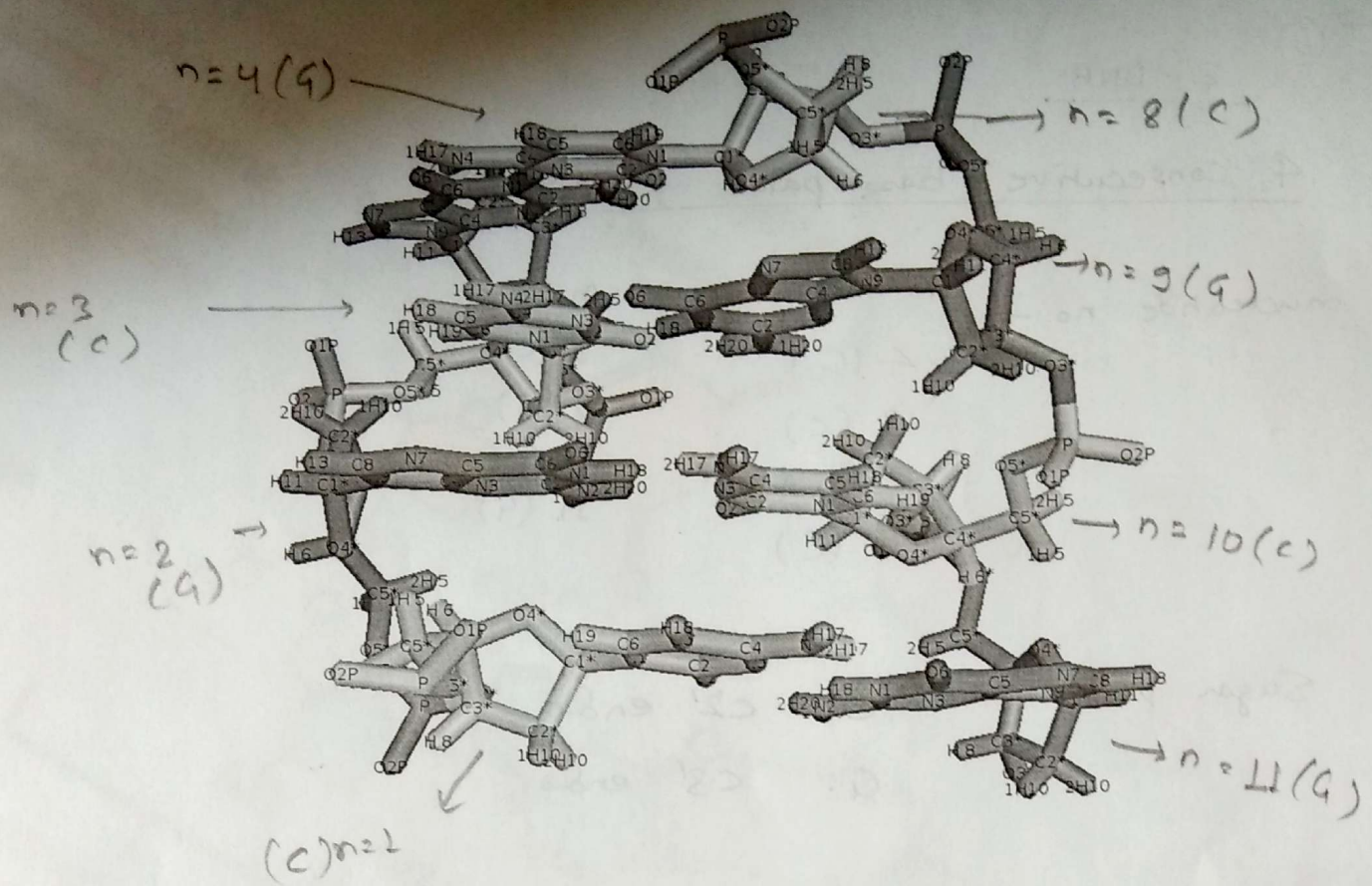
② C:G (B-DNA) nt no:- Cytosine - 2
Guanine - 37



Sugar pucker - 2'endo

Backbone torsion → P-O5'(α), O5'—C5'(β), C5'-C4'(γ)
C4'—C3'(δ), C3'-O3'(ε), O3'-P(ξ)
Glycosidic angle (χ) → O4'-C1'-N1-C2 (Thy, Cyt), O4'-C1'-N9-C4 (A,G)

4(b) Z-DNA



Backone torsion

Torsion angle	atom involved
α	(n-1) O3′ – P – O5′ – C5′
β	P – O5′ – C5′ – C4′
γ	O5′ – C5′ – C4′ – C3′
δ	C5′ – C4′ – C3′ – O3′
ε	C4′ – C3′ – O3′ – P
ζ	C3′ – O3′ – P – O5′ (nH)
χ	O4′ – C1′ – N9 – C4 (for guanine) O4′ – C1′ – N1 – C2 (for cytosine)

4 (b)

2-DNA

4 consecutive base pair parameters

nucleotide no –

n	n
4 (G)	8 (C)
3 (C)	9 (G)
2 (G)	10 (C)
1 (C)	11 (G)

Sugar pucker – C: C2' endo

G: C3' endo