

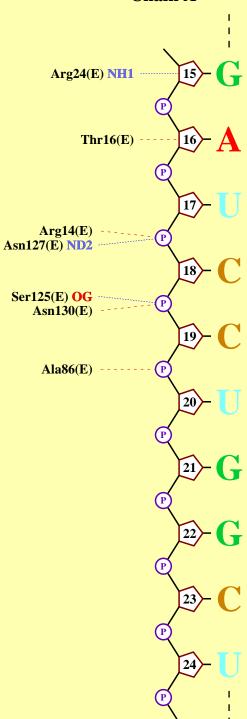
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



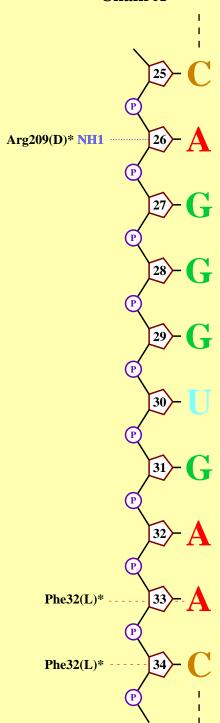
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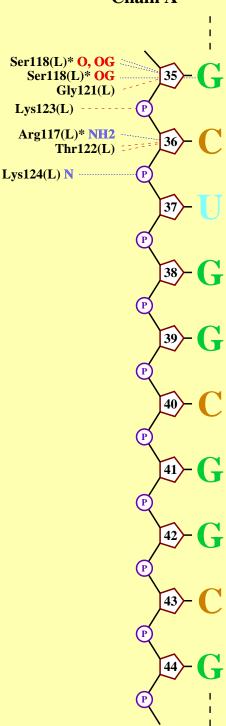
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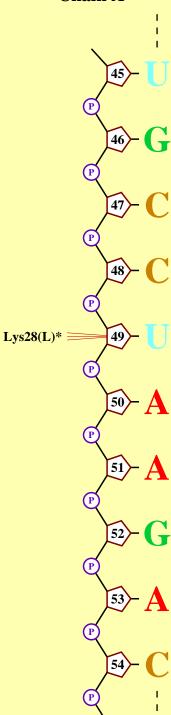
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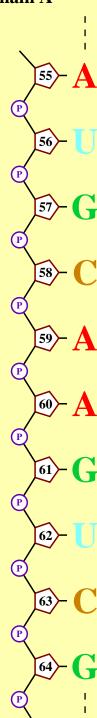
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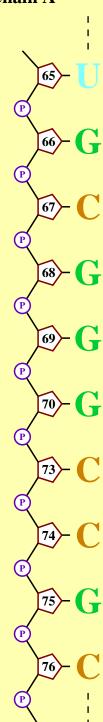
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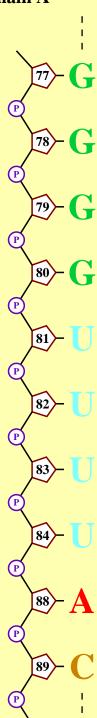
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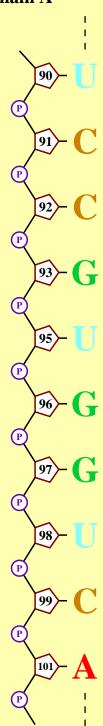
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Chain A Gln18(T) NE2 104 Lys14(T) NZ Arg22(T) 106 Arg15(T) NH2, NE 107 108 109 Arg25(P)* O 110

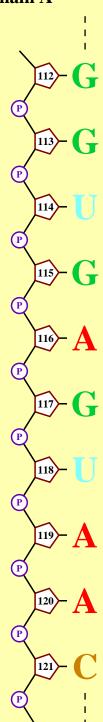
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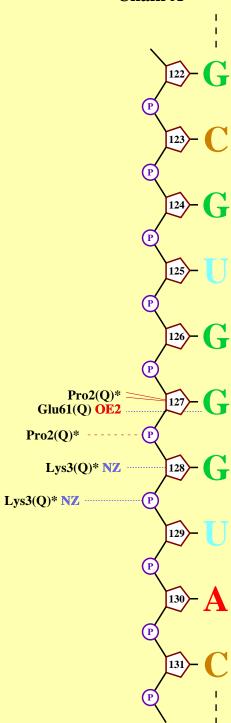
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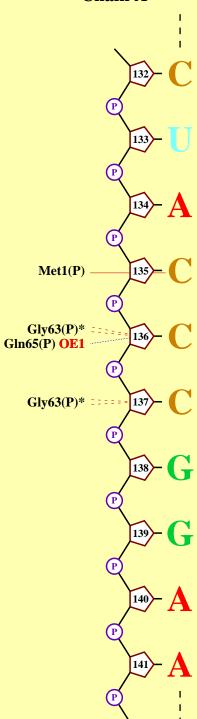
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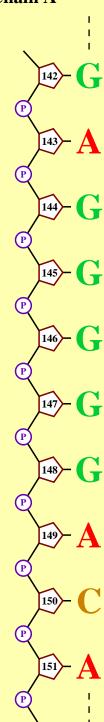
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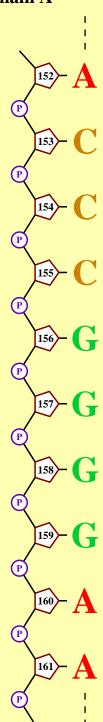
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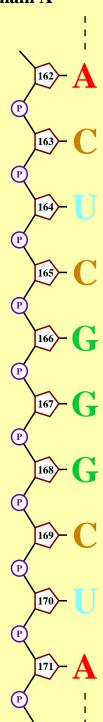
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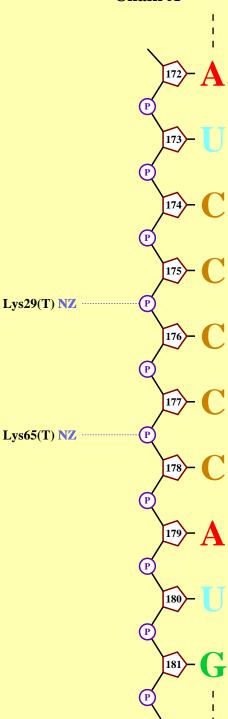
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Chain A 184 185 Lys81(T) NZ Met85(T)* ==== 186 Ser82(T) ===== (P Arg89(T)* NH1 Ser105(T)* N 187 Arg86(T) Arg89(T)* NH1 Ser105(T)* OG 188 189 190 Met85(T)* Gly101(T) O Gly102(T) O Gly103(T) O 191

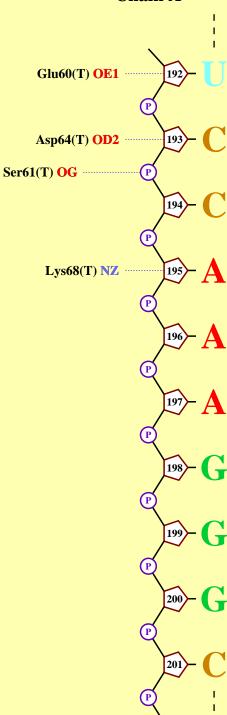
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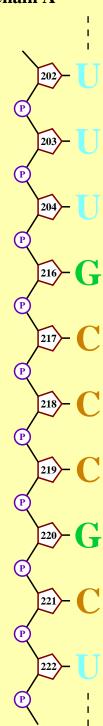
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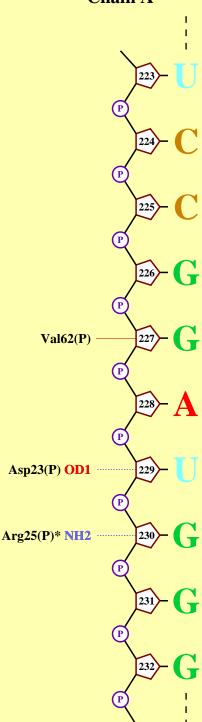
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Chain A Arg70(Q) Lys40(Q)* NZTyr42(Q) Lys40(Q)*NZ

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Chain A Ser99(Q) = Lys100(Q)

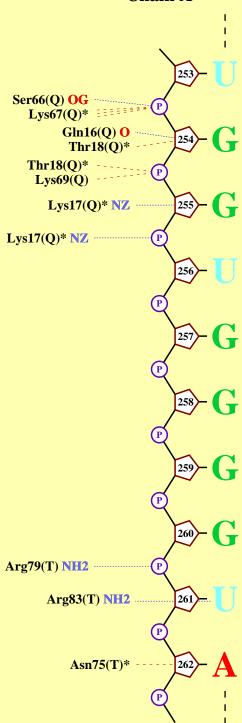
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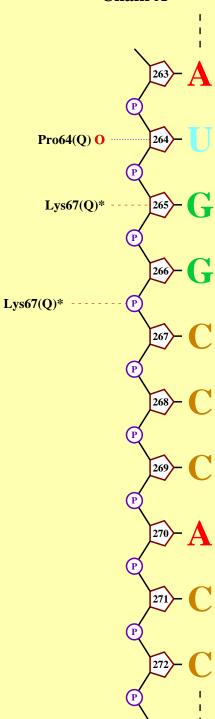
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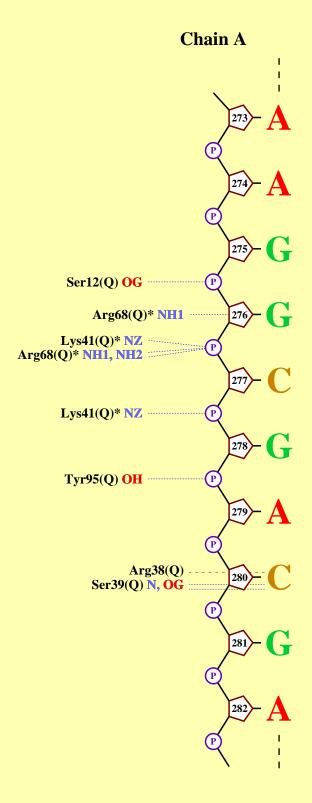
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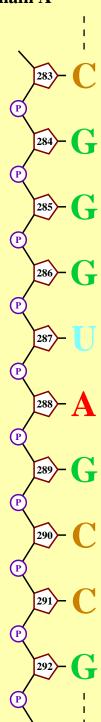
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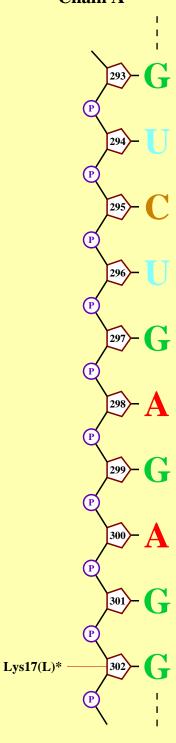
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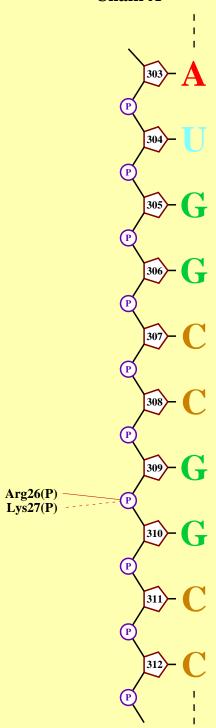
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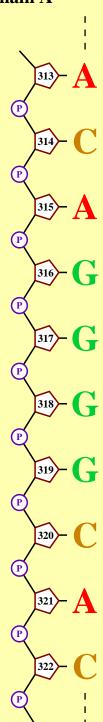
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Chain A Ser70(T)* Ser70(T)* Leu10(T)

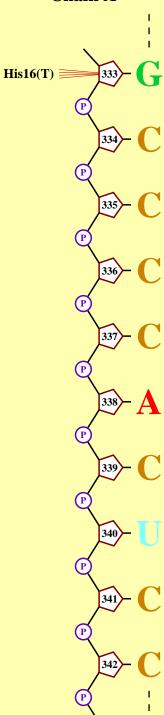
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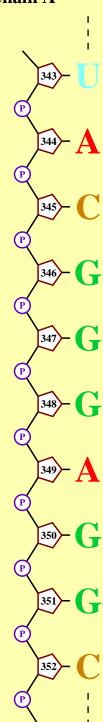
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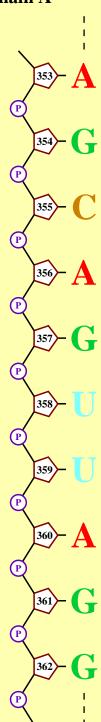
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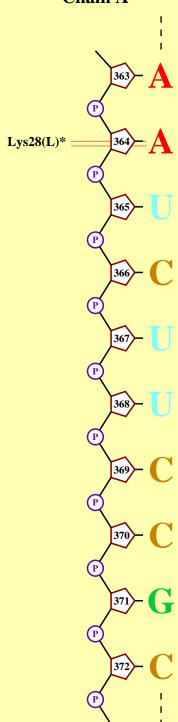
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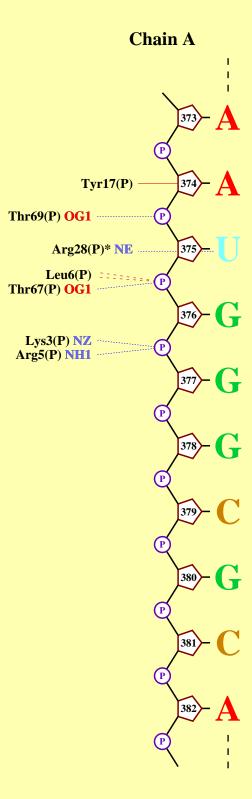
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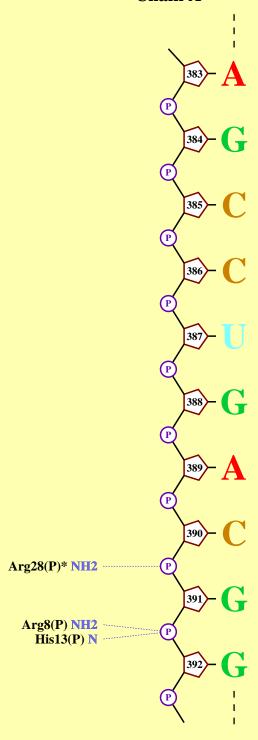
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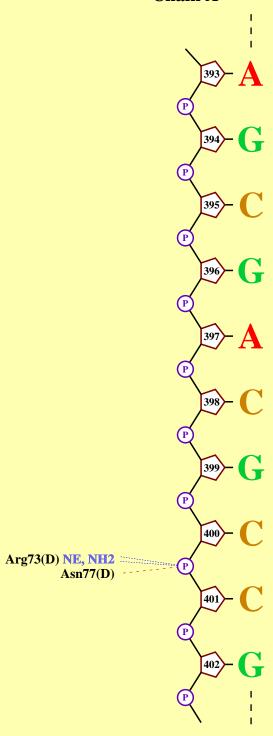
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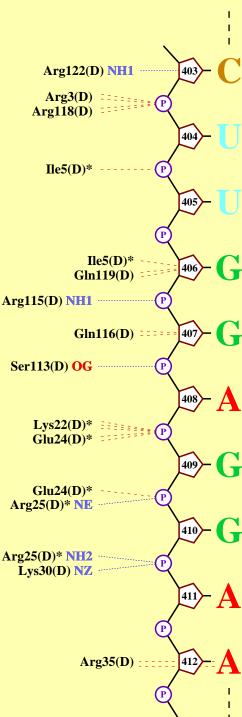
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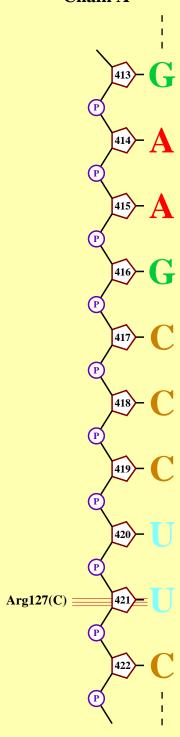
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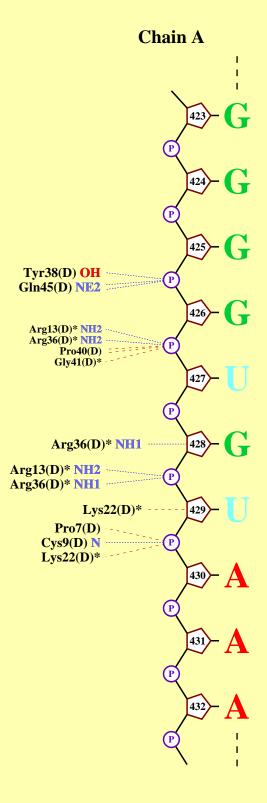
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Chain A **Glu156(D) Leu155(D)** His123(D)* His125(D) NE2 His123(D)*

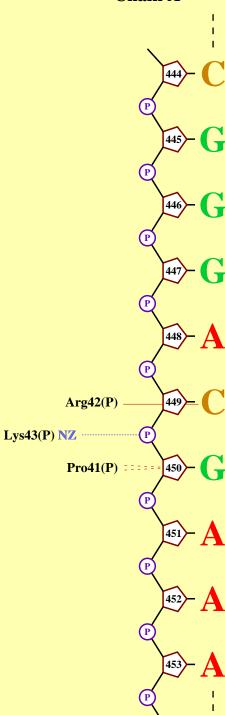
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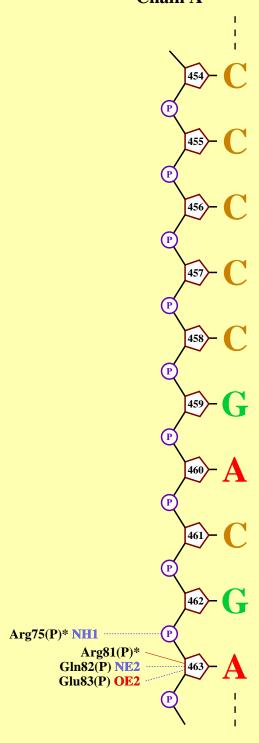
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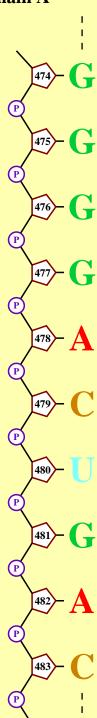
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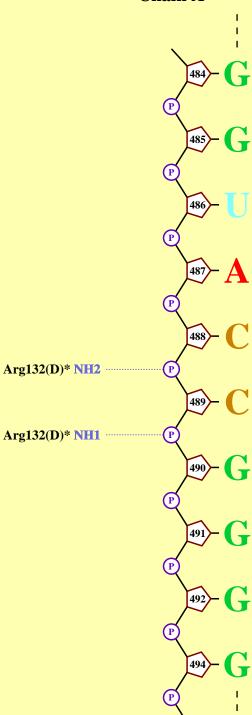
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Chain A 498 500 Arg117(L)* NH2 501 Ser118(L)* N 502 Ser116(L) OG Lys119(L) 503

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Chain A Arg209(D)* NH2 508 Ser52(D) OG 510 His43(D)*

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Chain A Ser50(L) OG Ala51(L) Leu52(L) N Glu73(L) OE1 Lys54(L)Tyr69(L) OH Gly72(L) N Asn49(L)* Asp92(L) OD2

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Chain A Asn49(L)* Asn49(L)* :::: Asn49(L)* **Glu161(C)** Gly159(C) O

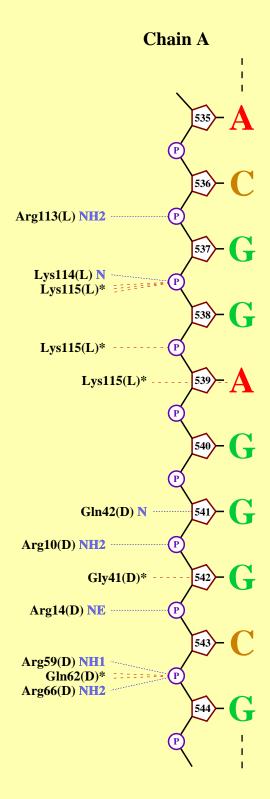
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Chain A **Glu72(D)** 550 Pro31(L) 0 Arg86(L)* Arg86(L)* **Gly87(L)** Ser22(L)

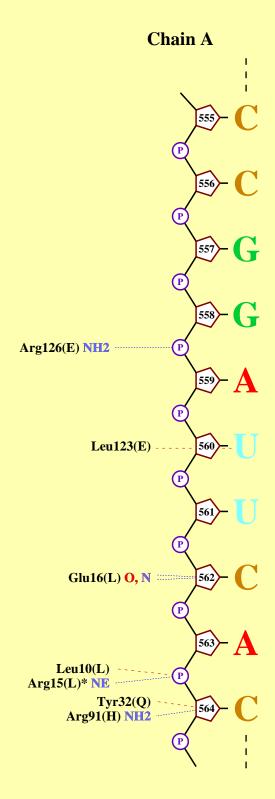
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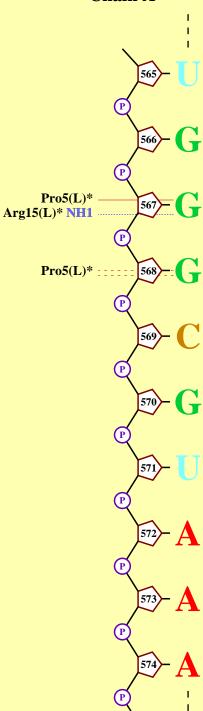
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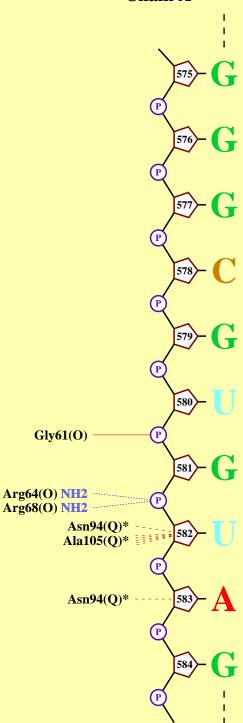
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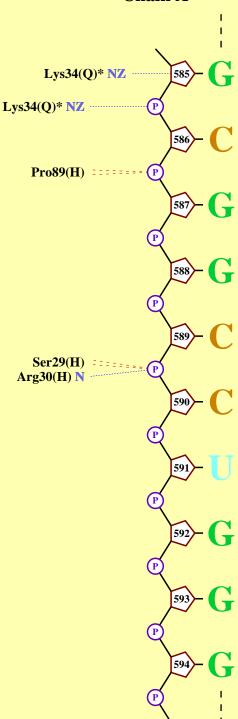
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Chain A 595 P 596 C Tyr94(H)*

Tyr94(H)* P

Val95(H)

Gly130(H)

Val97(H) N

P

600

601 — P 602 — A P 603 — I

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Chain A Arg18(P) NH2 610

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Chain A **Arg141(D) NH1** 617 Val133(D) Asp134(D) N, OD1 Leu135(D) 620

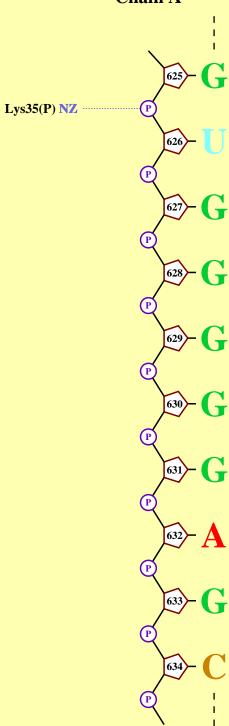
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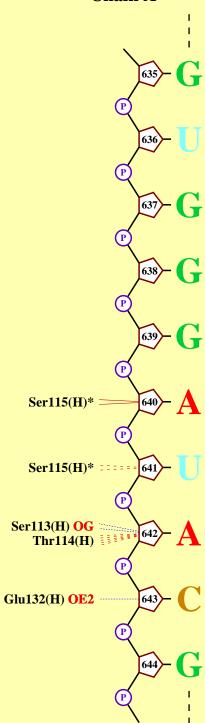
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Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



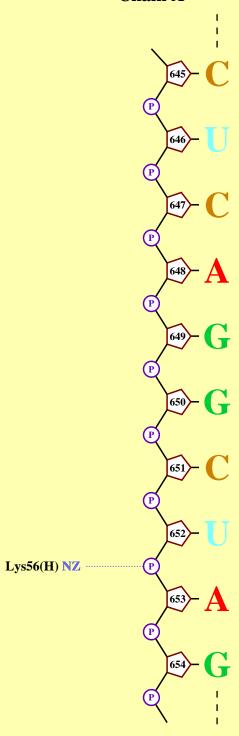
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



Key

- Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

--- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number

Chain A Gln28(O)* ≡ Thr22(O) **OG1** Gln28(O)* Lys8(O)* NZ 658 Lys8(O)* NZ **Ile12(O)** Lys5(O) NZ 660 Arg64(R)* NH1

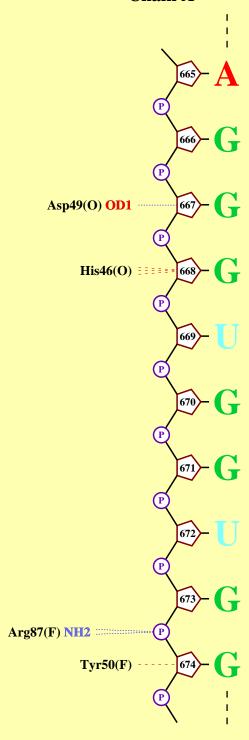
Key

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- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



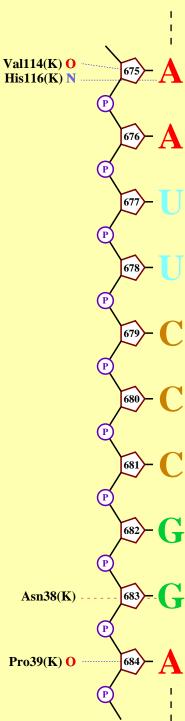
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

--- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



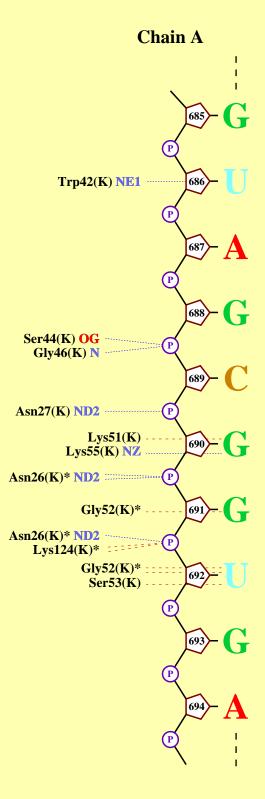
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



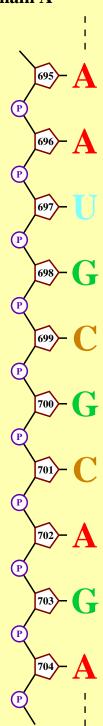
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



Key

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- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

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88 Water molecule and number

Chain A **Ile29(K)** Thr31(K) OG1 Arg85(K)* NH1 707 Gly37(K) **O** Tyr20(K) 708 709 Lys54(F)* 710 Lys54(F)*

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Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number

Chain A Asn117(K) ND2 Lys49(R)* Phe81(R) O Lys49(R)* Ile50(R) O, N Arg74(R) NH1 Gln63(R)*Lys71(R) Gln63(R)*

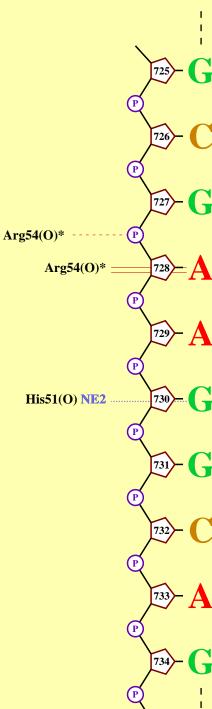
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



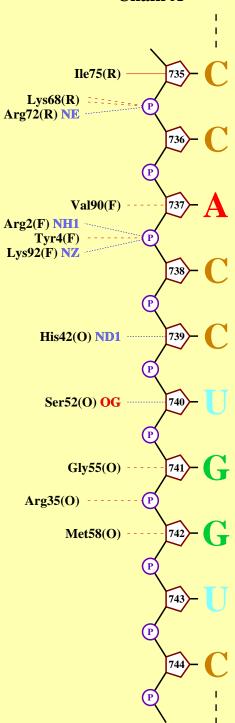
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



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 - * Residue/water on plot more than once

Hydrogen bond to DNA

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88 Water molecule and number

Chain A Asp21(O) OD1 Gly23(O) O 750 **Phe18(O)** Tyr69(O) OH Met1(H) ::::

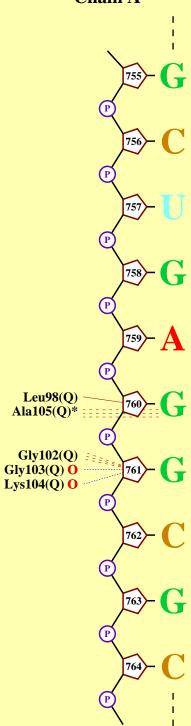
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



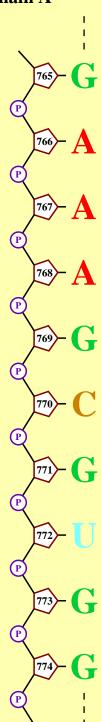
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Hydrogen bond to DNA

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88 Water molecule and number



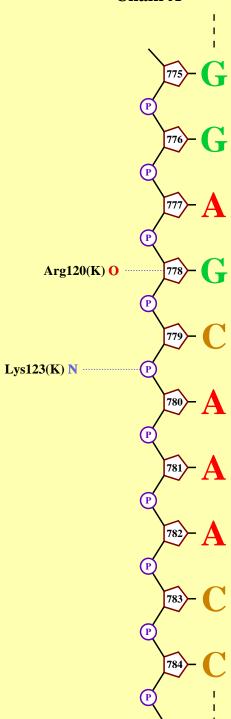
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- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

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88 W Water molecule and number



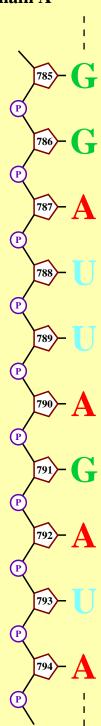
Key

- 3 Backbone sugar and base-number
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Hydrogen bond to DNA

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88 Water molecule and number



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Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



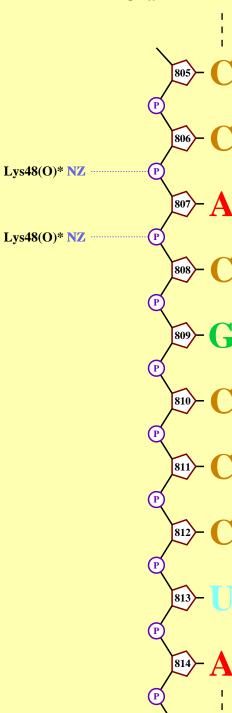
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88 Water molecule and number



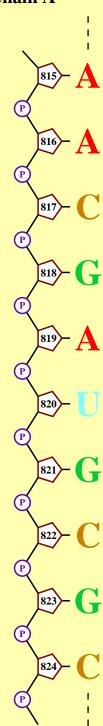
Key

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Hydrogen bond to DNA

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88 Water molecule and number



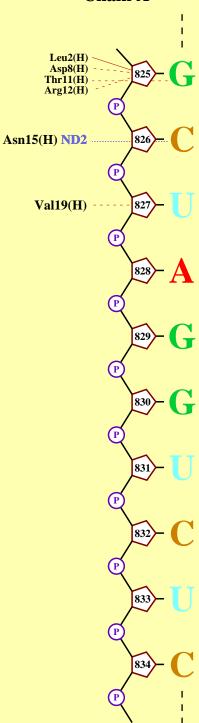
Key

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88 W Water molecule and number



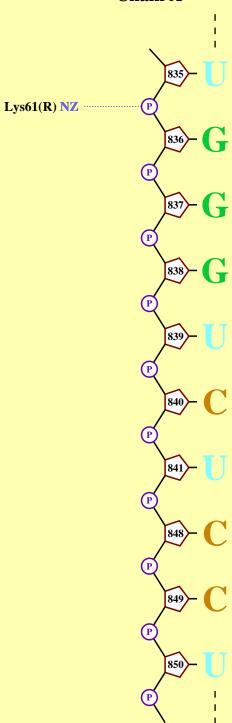
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Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



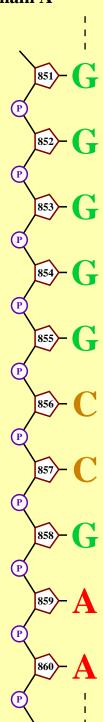
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88 Water molecule and number



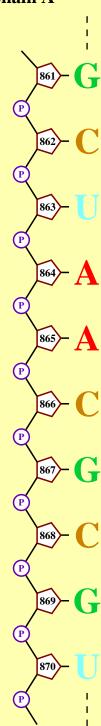
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Hydrogen bond to DNA

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88 W Water molecule and number



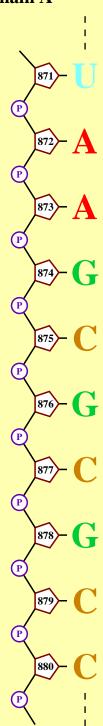
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- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

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88 W Water molecule and number



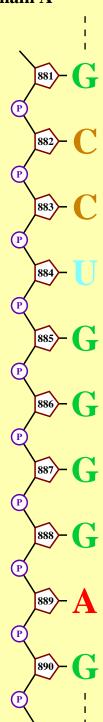
Key

- 3 Backbone sugar and base-number
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88 W Water molecule and number



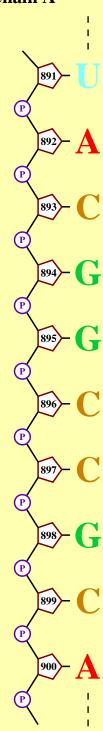
Key

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88 Water molecule and number



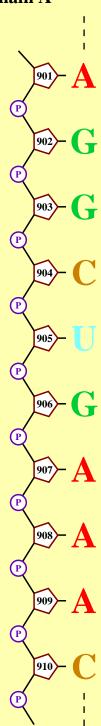
Key

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Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



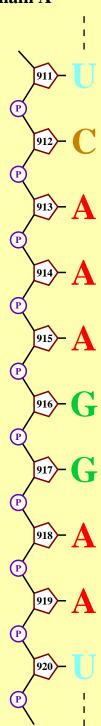
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Hydrogen bond to DNA

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88 W Water molecule and number



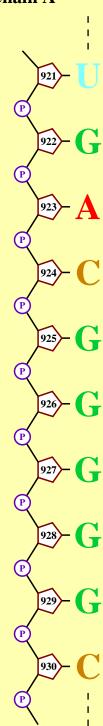
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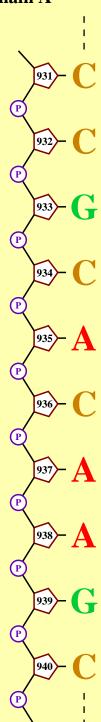
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Hydrogen bond to DNA

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88 W Water molecule and number



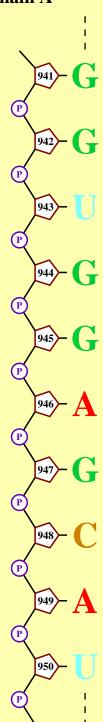
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88 W Water molecule and number



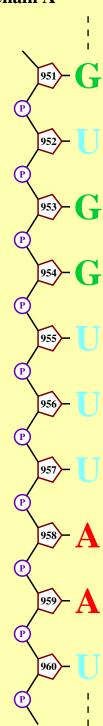
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 - * Residue/water on plot more than once

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88 W Water molecule and number



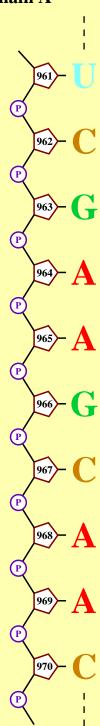
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Hydrogen bond to DNA

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88 Water molecule and number



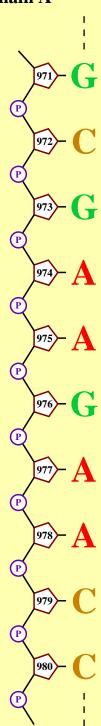
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- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

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88 W Water molecule and number



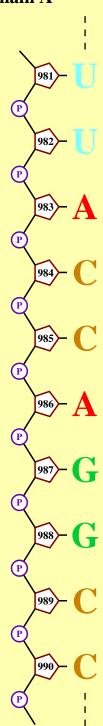
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88 W Water molecule and number



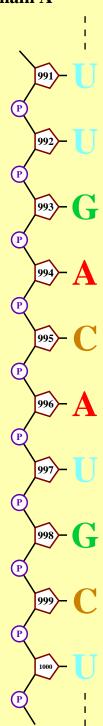
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Hydrogen bond to DNA

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88 Water molecule and number



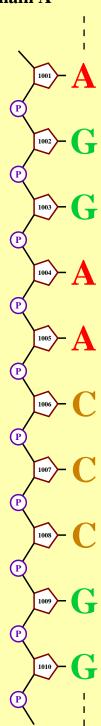
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Hydrogen bond to DNA

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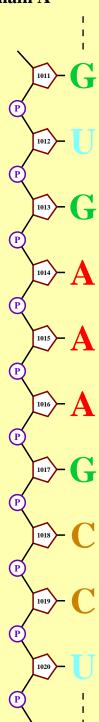
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88 Water molecule and number



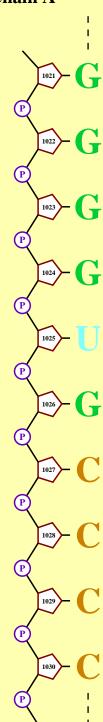
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- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

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88 Water molecule and number



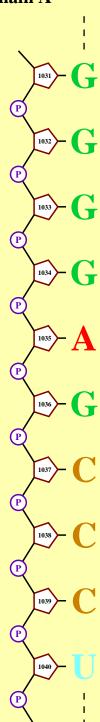
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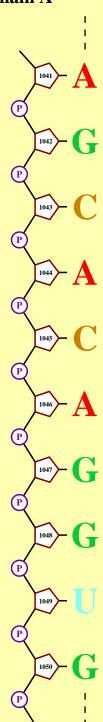
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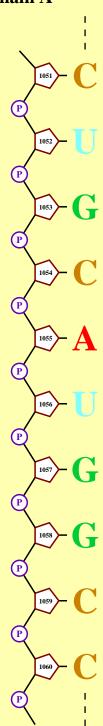
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- P Phosphate group
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Hydrogen bond to DNA

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88 W Water molecule and number



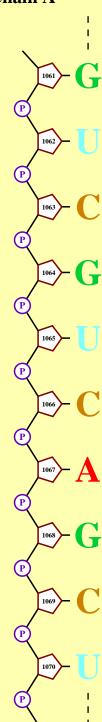
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- P Phosphate group
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88 Water molecule and number



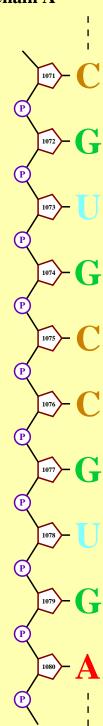
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88 W Water molecule and number



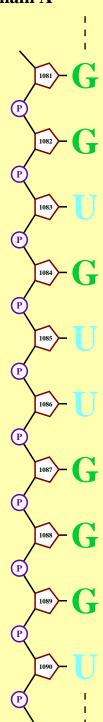
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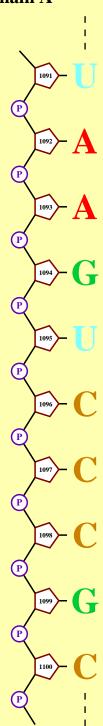
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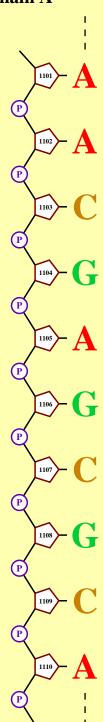
Key

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88 W Water molecule and number



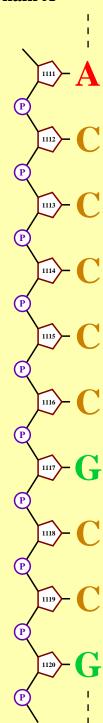
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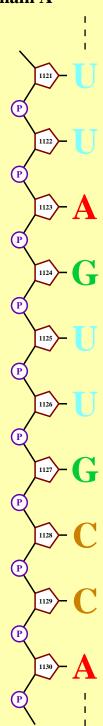
Key

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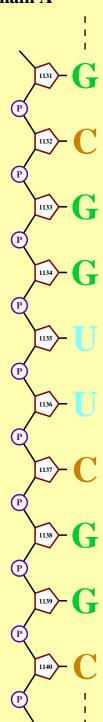
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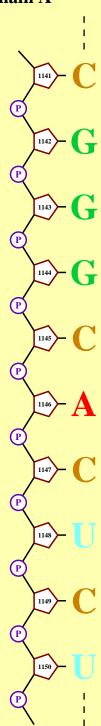
Key

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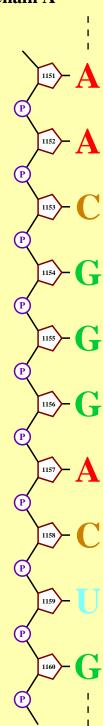
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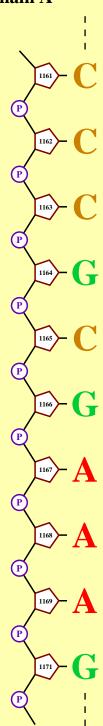
Key

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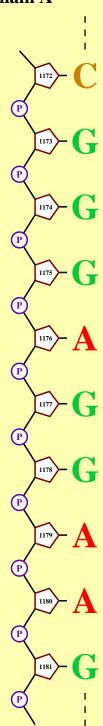
Key

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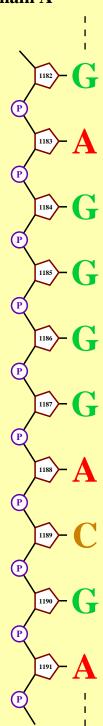
Key

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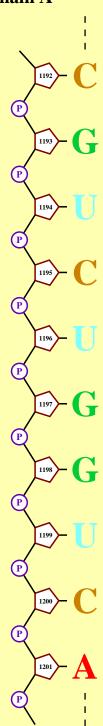
Key

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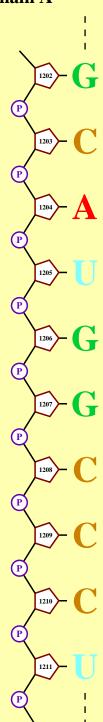
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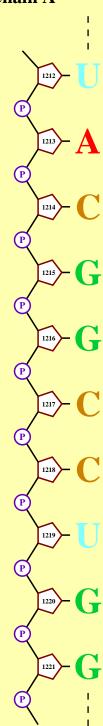
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-- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



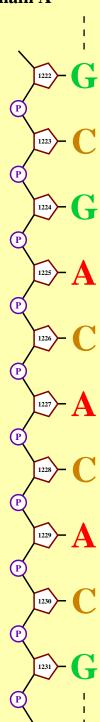
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



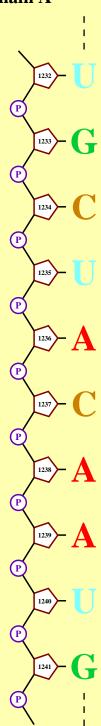
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



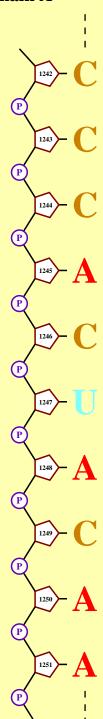
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



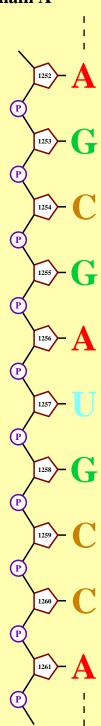
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



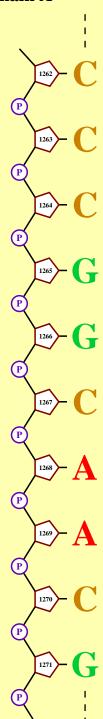
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



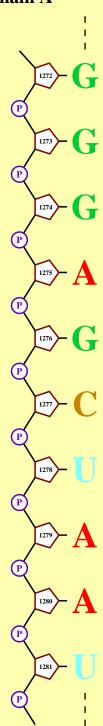
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



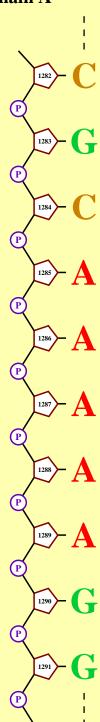
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



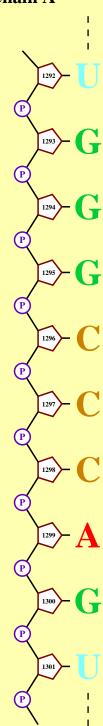
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



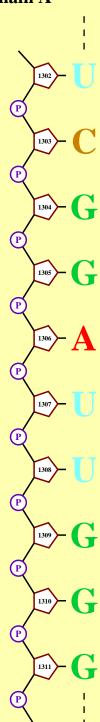
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



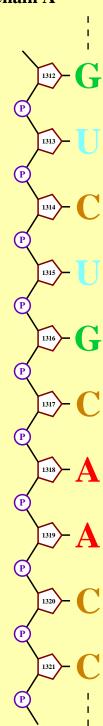
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



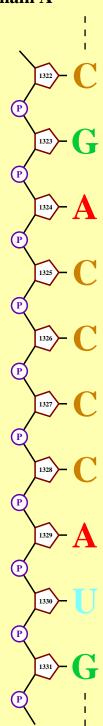
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



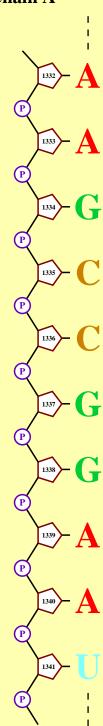
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



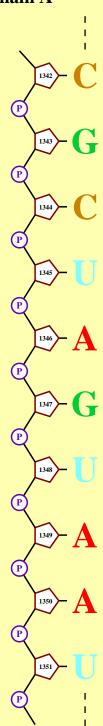
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



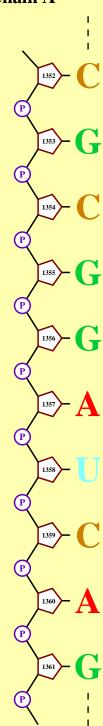
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



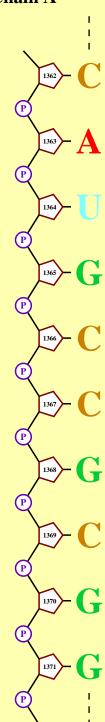
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



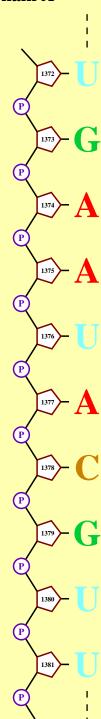
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



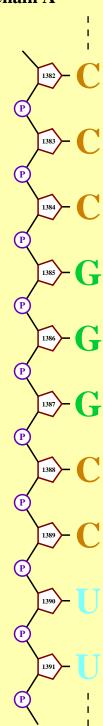
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



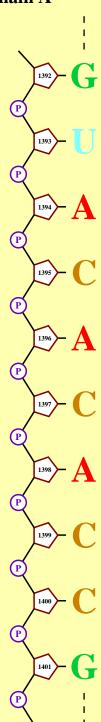
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



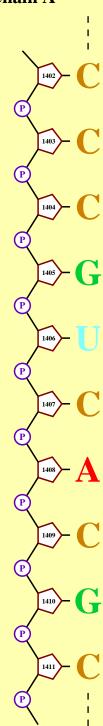
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



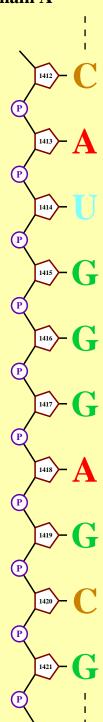
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number



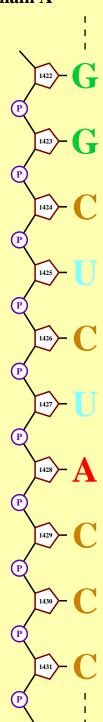
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



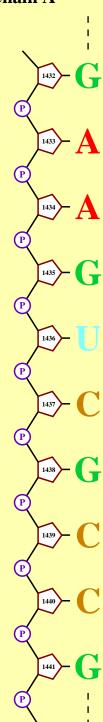
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



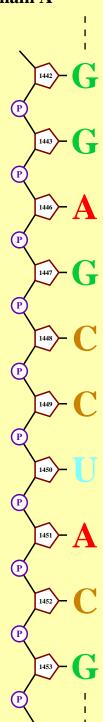
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



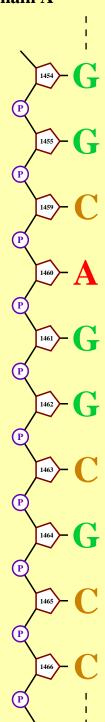
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



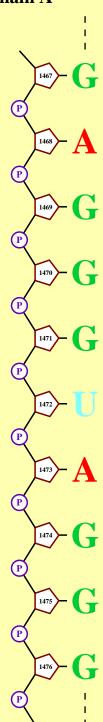
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- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



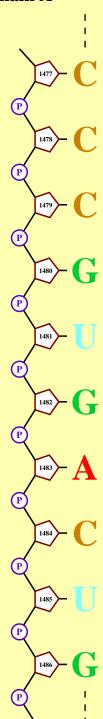
Key

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- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



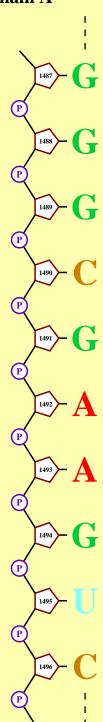
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

-- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



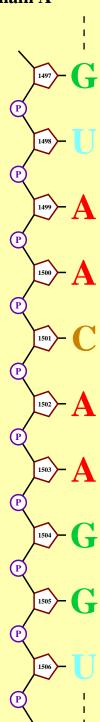
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



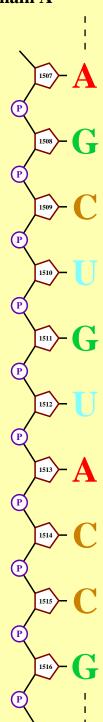
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



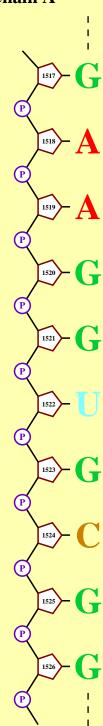
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



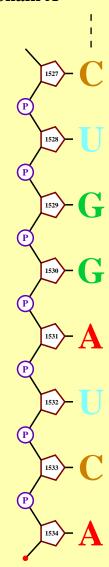
Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

- Nonbonded contact to DNA (< 3.35A)

88 W Water molecule and number



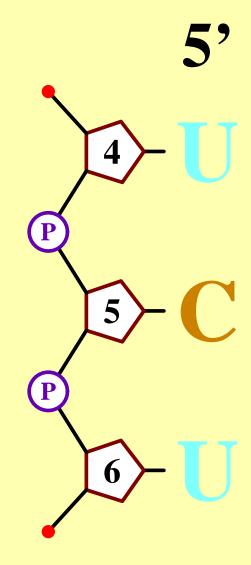
Key

- 3 Backbone sugar and base-number
- Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA
Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number

Chain X



Key

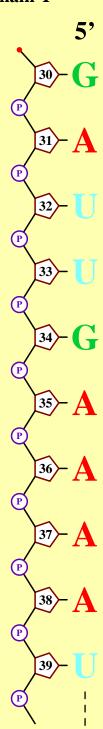
- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number

Chain Y



Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

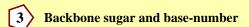
- Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number

Chain Y



Key

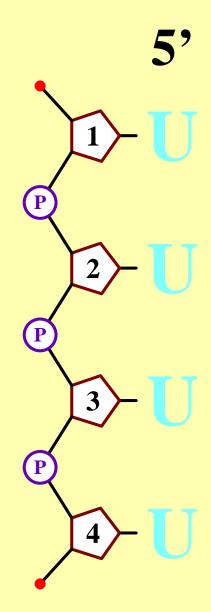


P Phosphate group

* Residue/water on plot more than once

Hydrogen bond to DNA
Nonbonded contact to DNA (< 3.35A)
Water molecule and number

Chain Z



Key

- 3 Backbone sugar and base-number
- P Phosphate group
 - * Residue/water on plot more than once

Hydrogen bond to DNA

Nonbonded contact to DNA (< 3.35A)

88 Water molecule and number