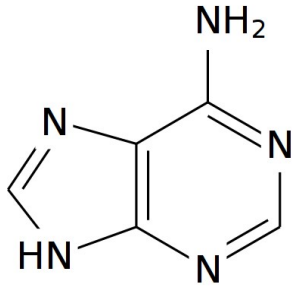
Bioinformatics III

Analysis and prediction of 3D macromolecule structures

Lecture 7 – geometry of nucleic acids

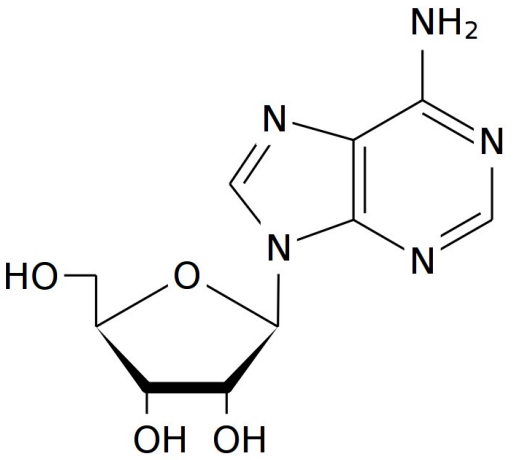
Saulius Gražulis
2022

Chemical structure of nucleotides

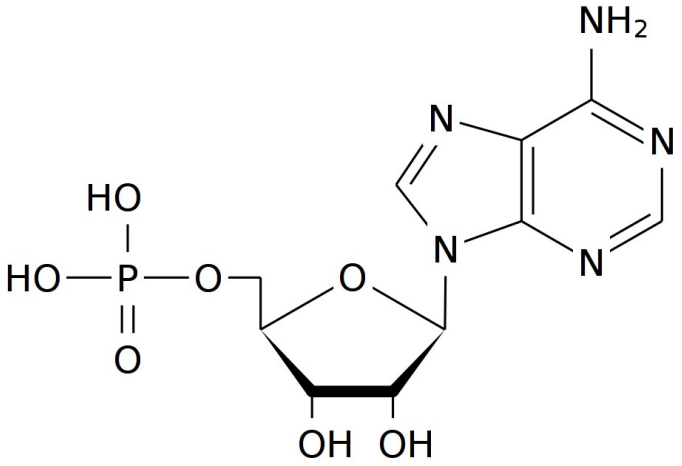


Bases

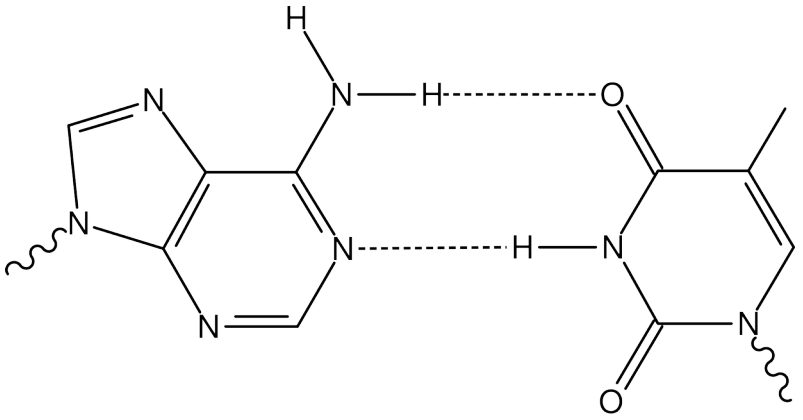
Nucleosides (glycosides)



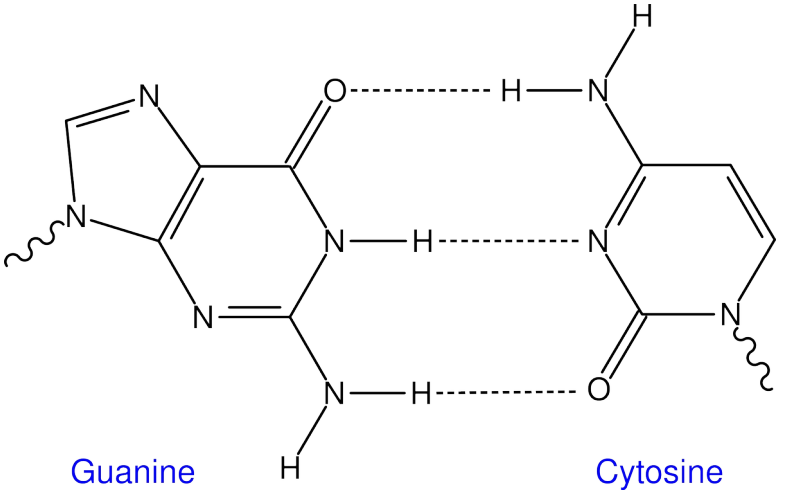
Nucleotides (phosphates of glycosides)



Watson-Crick pairs

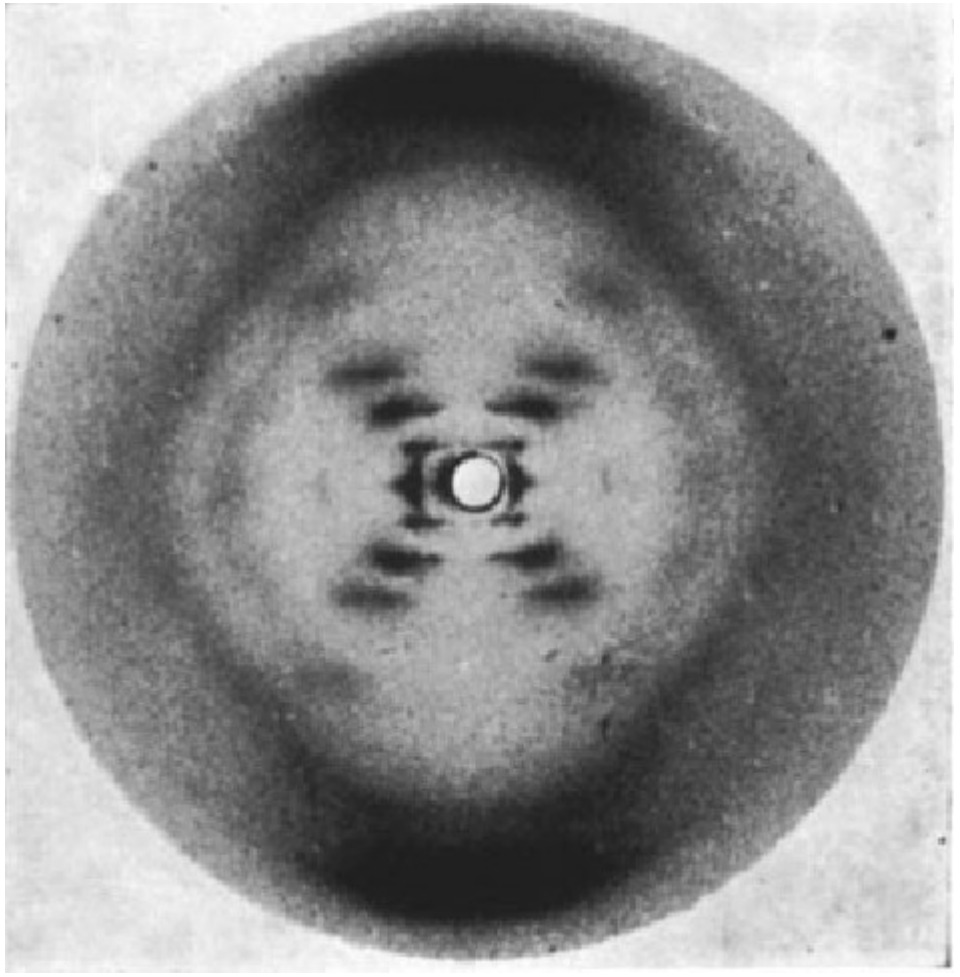


Adenine Thymine

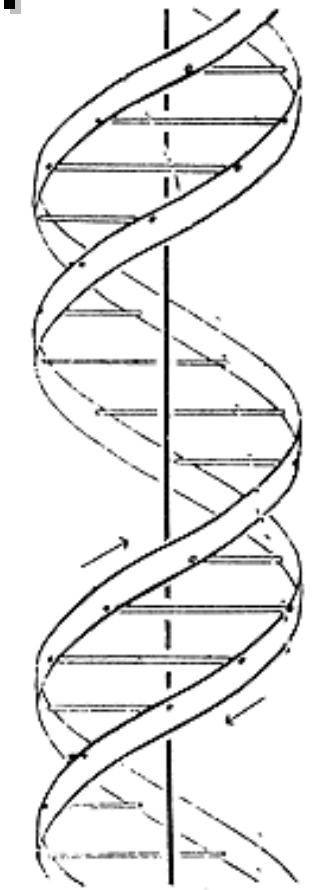


Guanine Cytosine

X-ray analysis and the Watson-Crick model



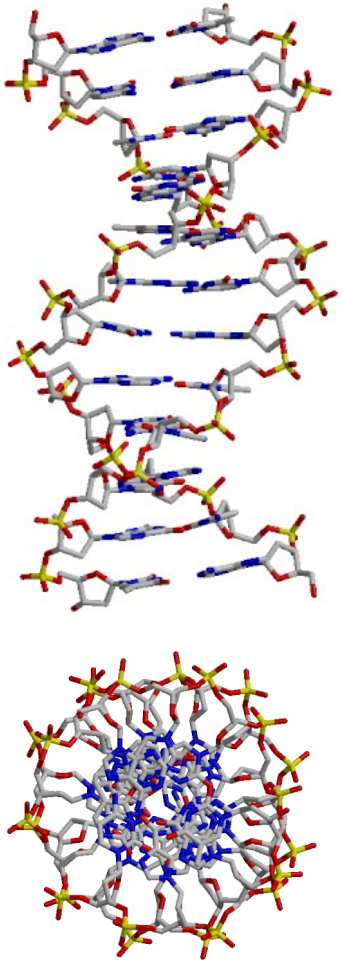
Franklin, R. E. & Gosling, R. G. (1953) Nature **171**, 740



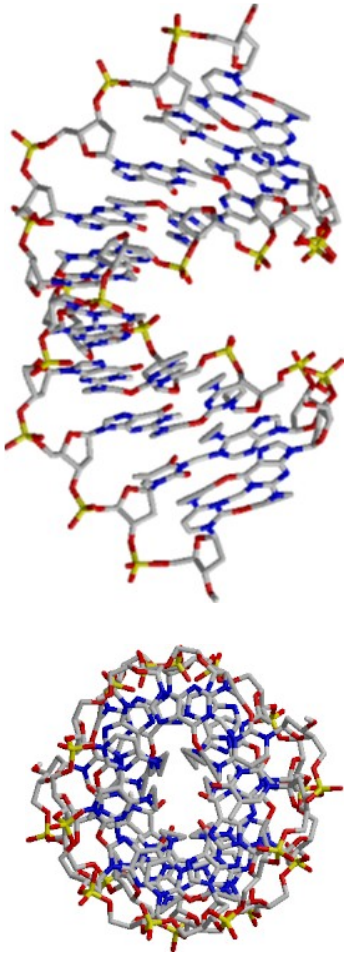
This figure is purely diagrammatic. The two ribbons symbolize the two phosphate—sugar chains, and the horizontal rods the pairs of bases holding the chains together. The vertical line marks the fibre axis

Watson & Crick,(1953) Nature **171**, 737

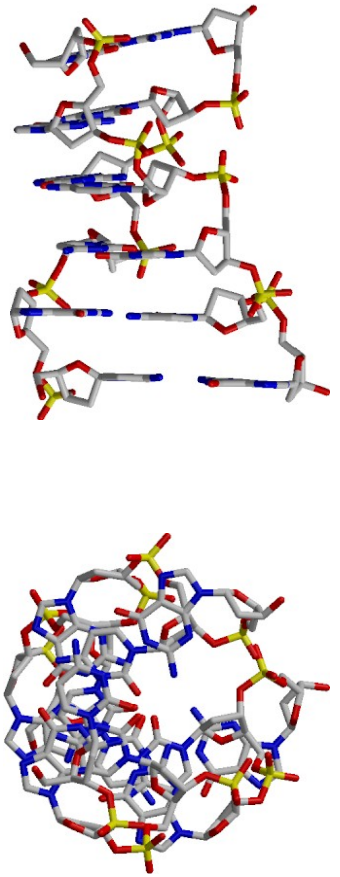
Double helix



B form (DNR)



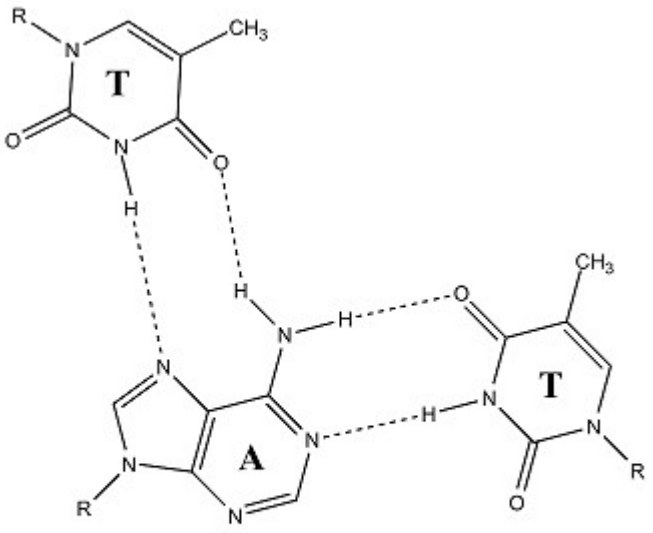
A form (DNR)



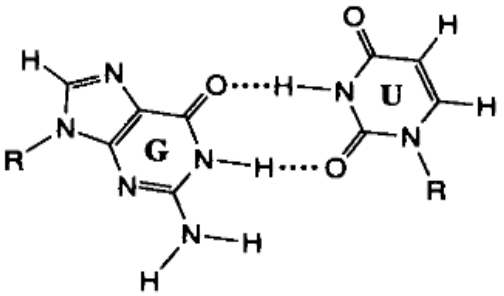
Z form (DNR)

„Non-standard“ pairs, triplexes, quadruplexes

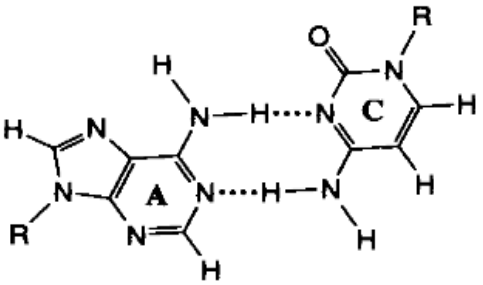
Hoogsteen base pairs



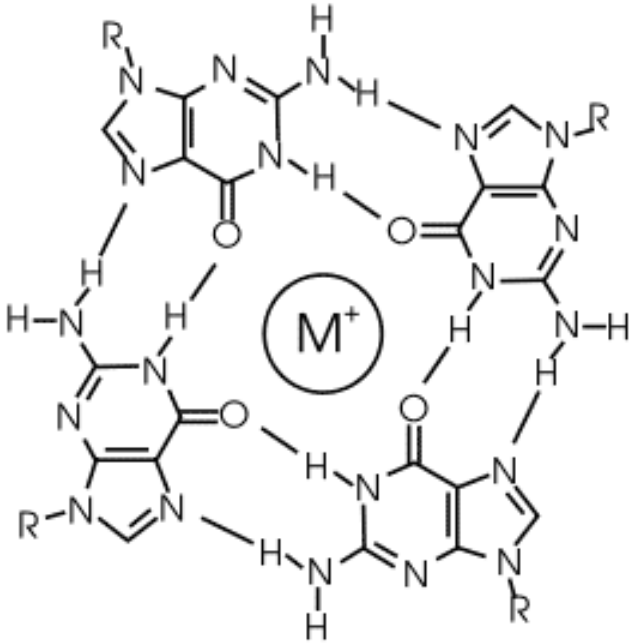
TA*T

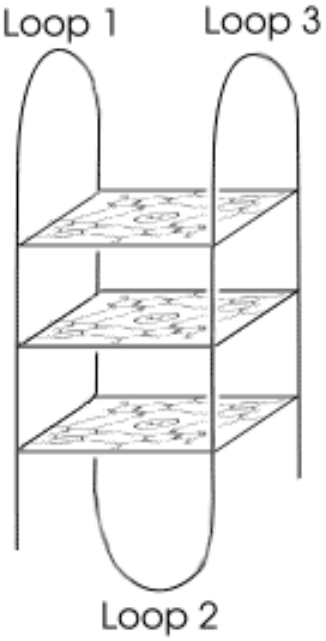


G·U Wobble

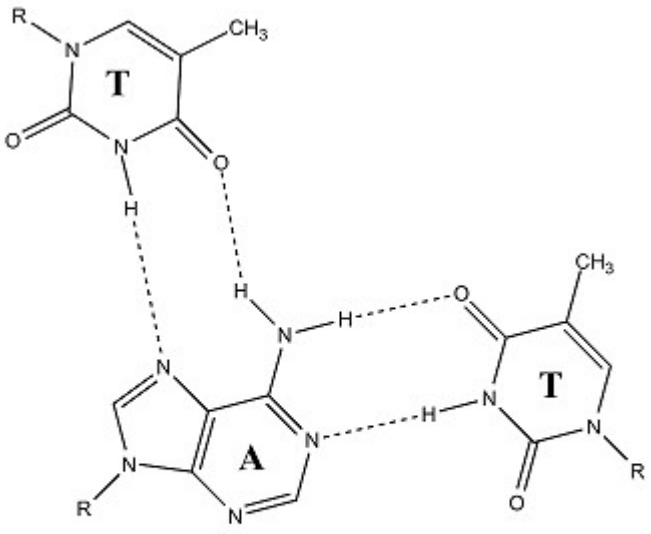


A·C Reverse wobble





Hoogsteen base pairs – experimental observation



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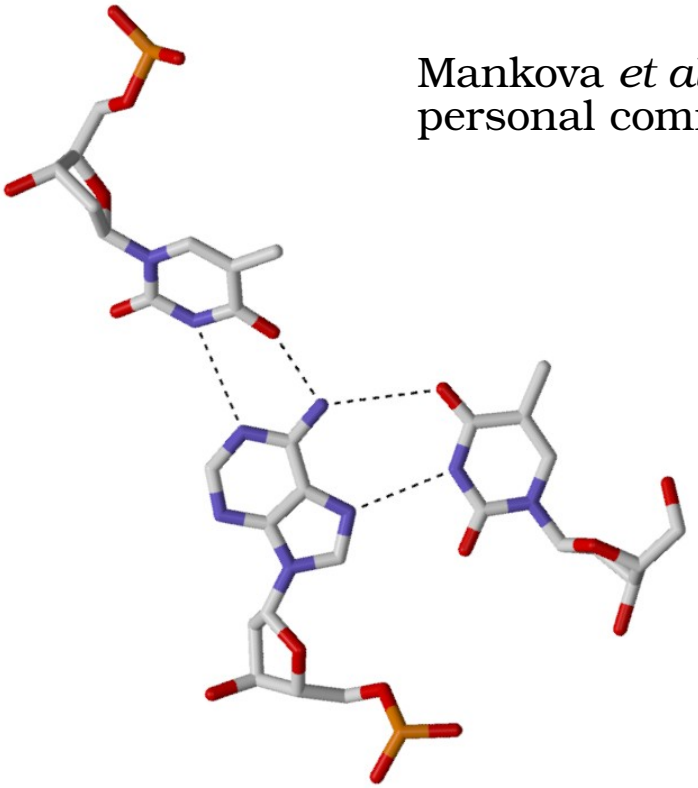
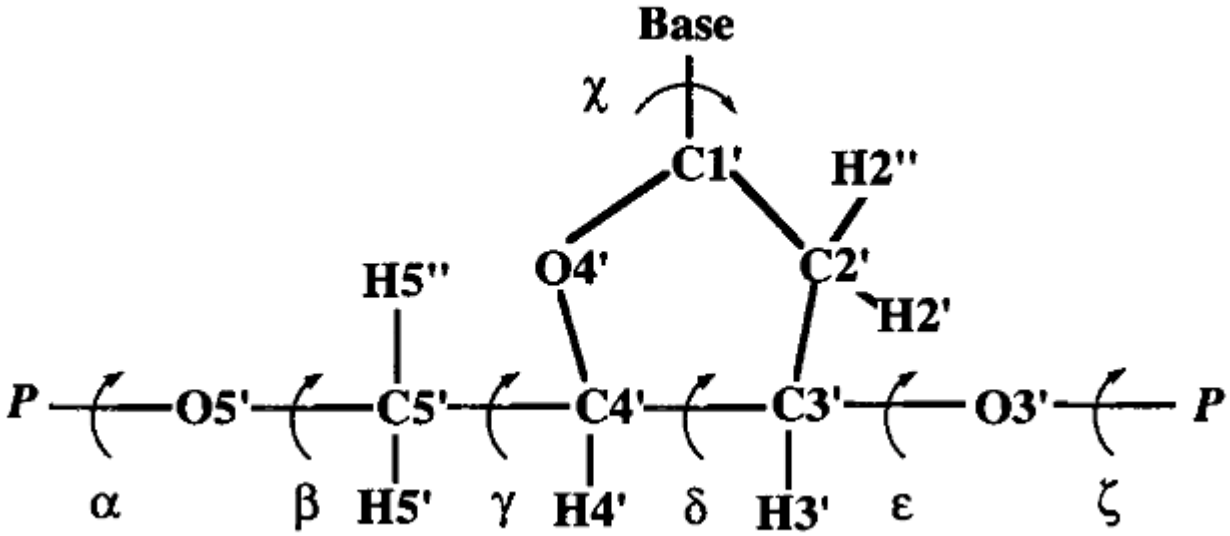


Mankova *et al.*, personal comm.

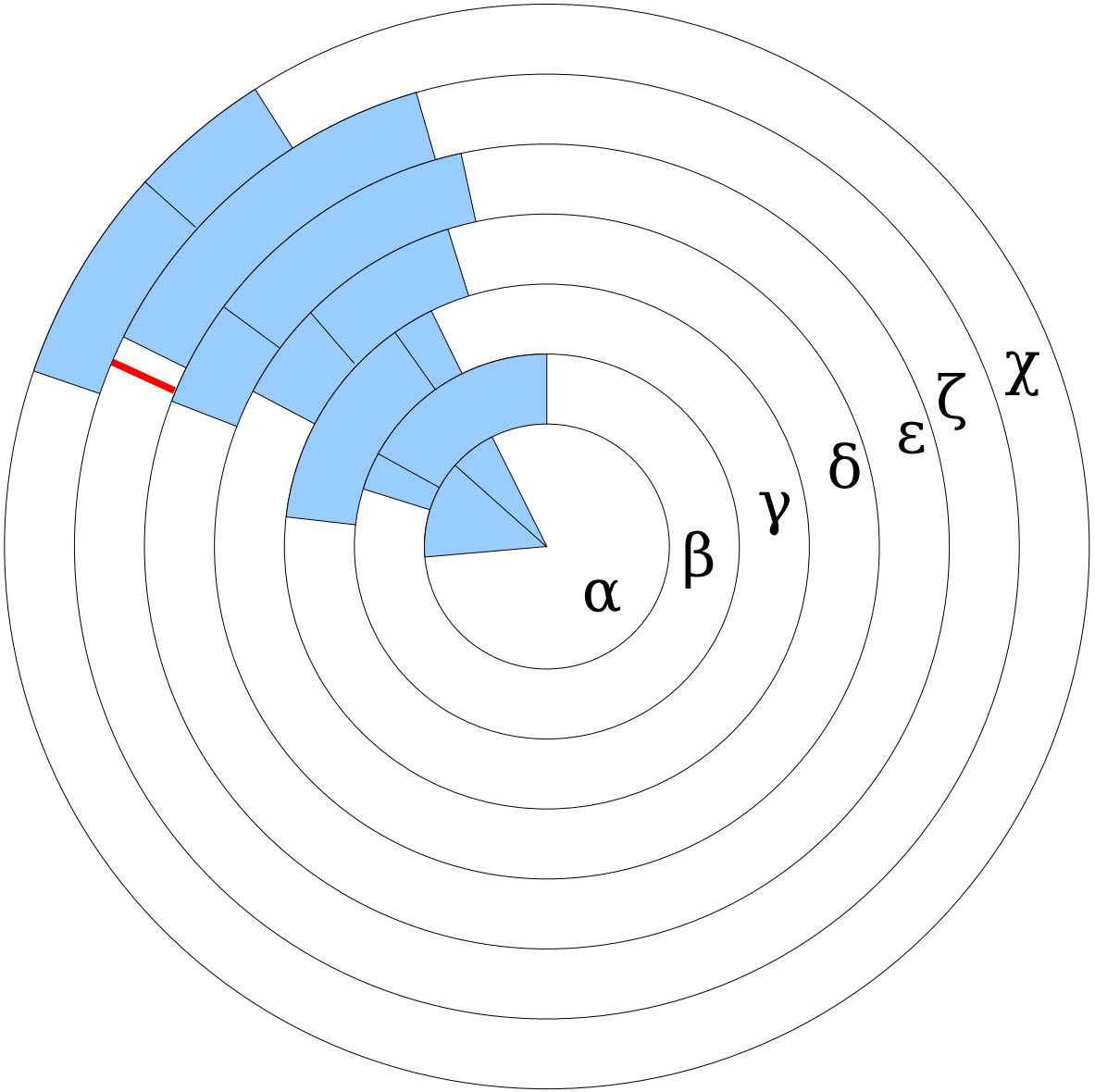
Wikipedia:
http://en.wikipedia.org/wiki/Hoogsteen_base_pair
http://upload.wikimedia.org/wikipedia/commons/0/06/Hoogsteen.png

Backbone angles of NAs

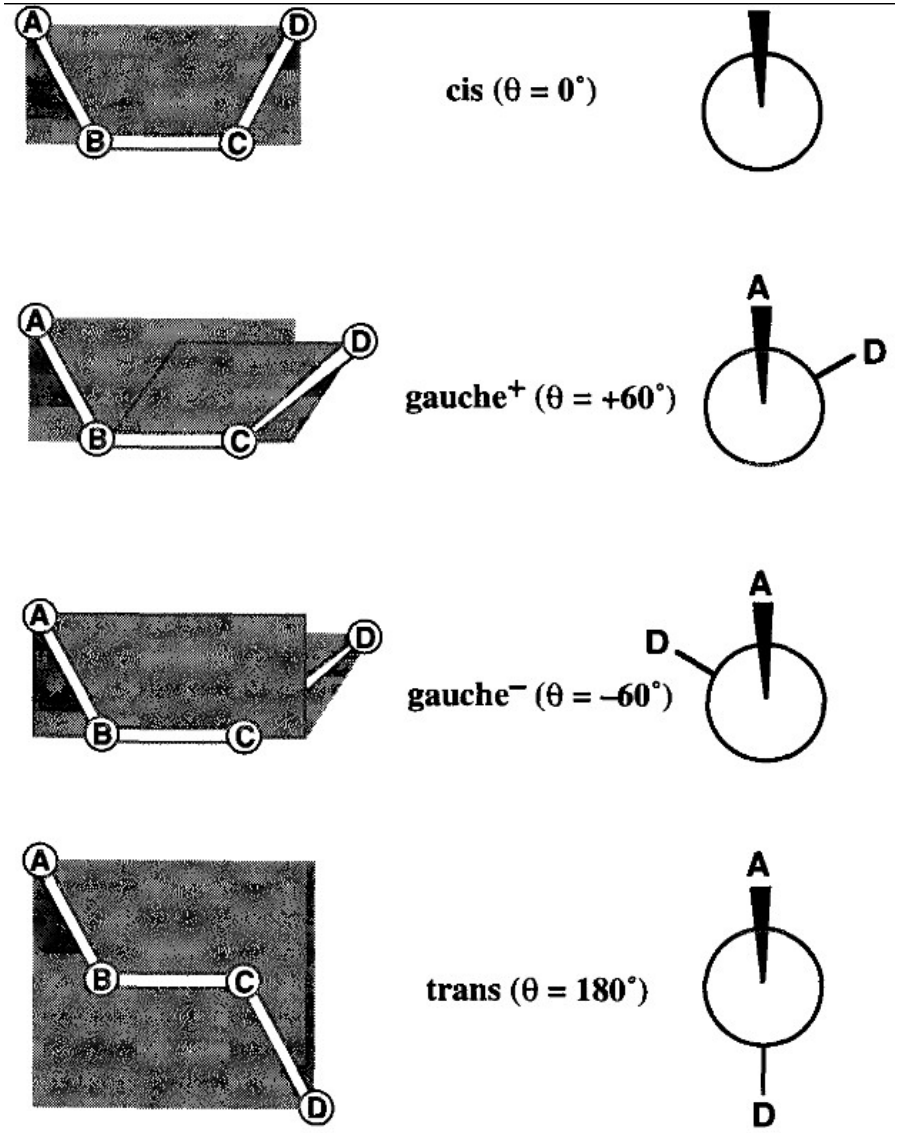


Bloomfield, Crothers, Tinoco
Nucleic Acids – structure, properties & functions
University Science Books, California, 2000, p. 17

Bond angle diagrams



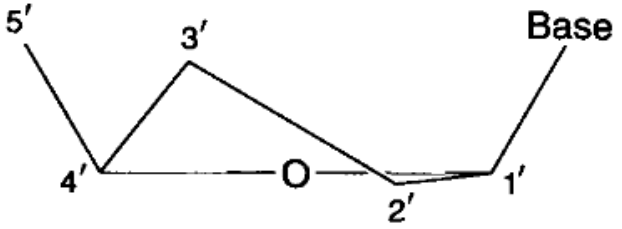
Bond angle values



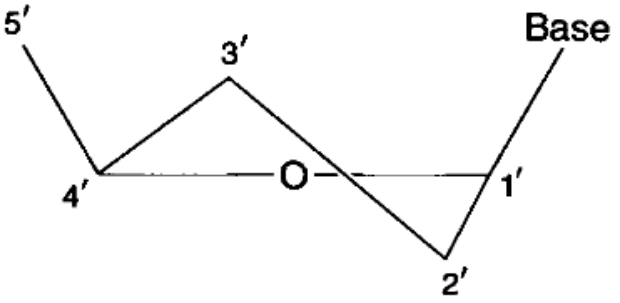
Bloomfield *et al.* 2000, p. 18

Sugar ring conformation

North (N) conformers–
A-form double strands

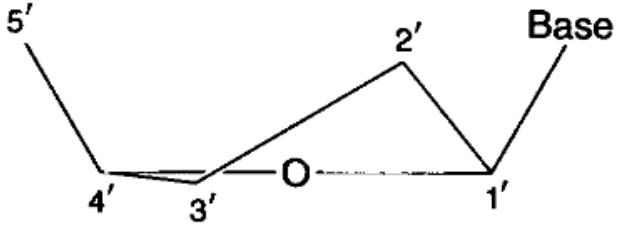


3′-*endo*
Phase angle, $P = 18°$
Envelope

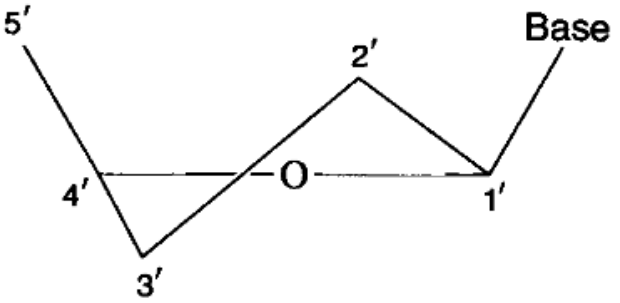


3′-*endo*, 2′-*exo*
Phase angle, $0° < P < 18°$
Twist

South (S) conformers–
B-form double strands



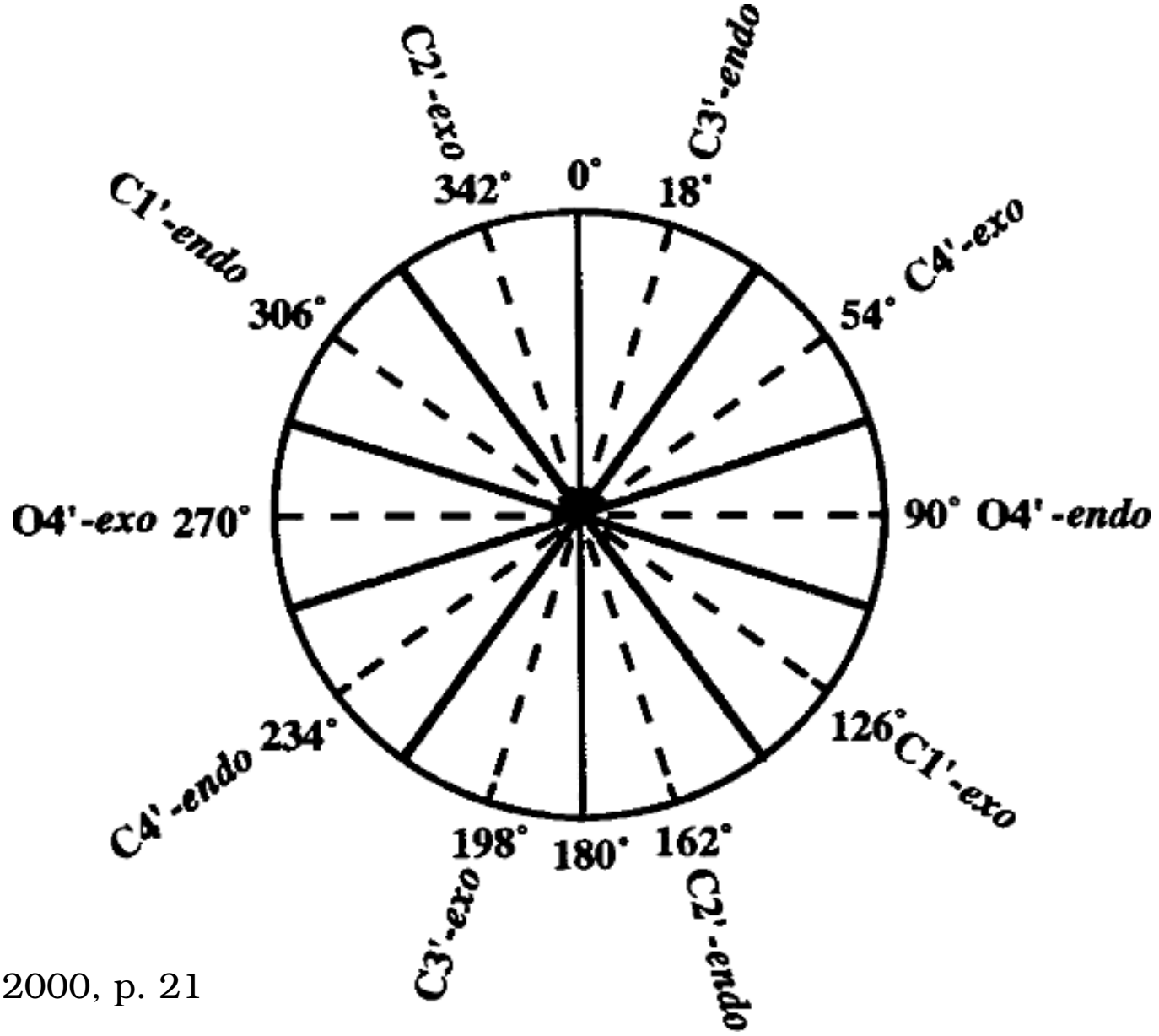
2′-*endo*
Phase angle, $P = 162°$
Envelope



2′-*endo*, 3′-*exo*
Phase angle, $162° < P < 180°$
Twist

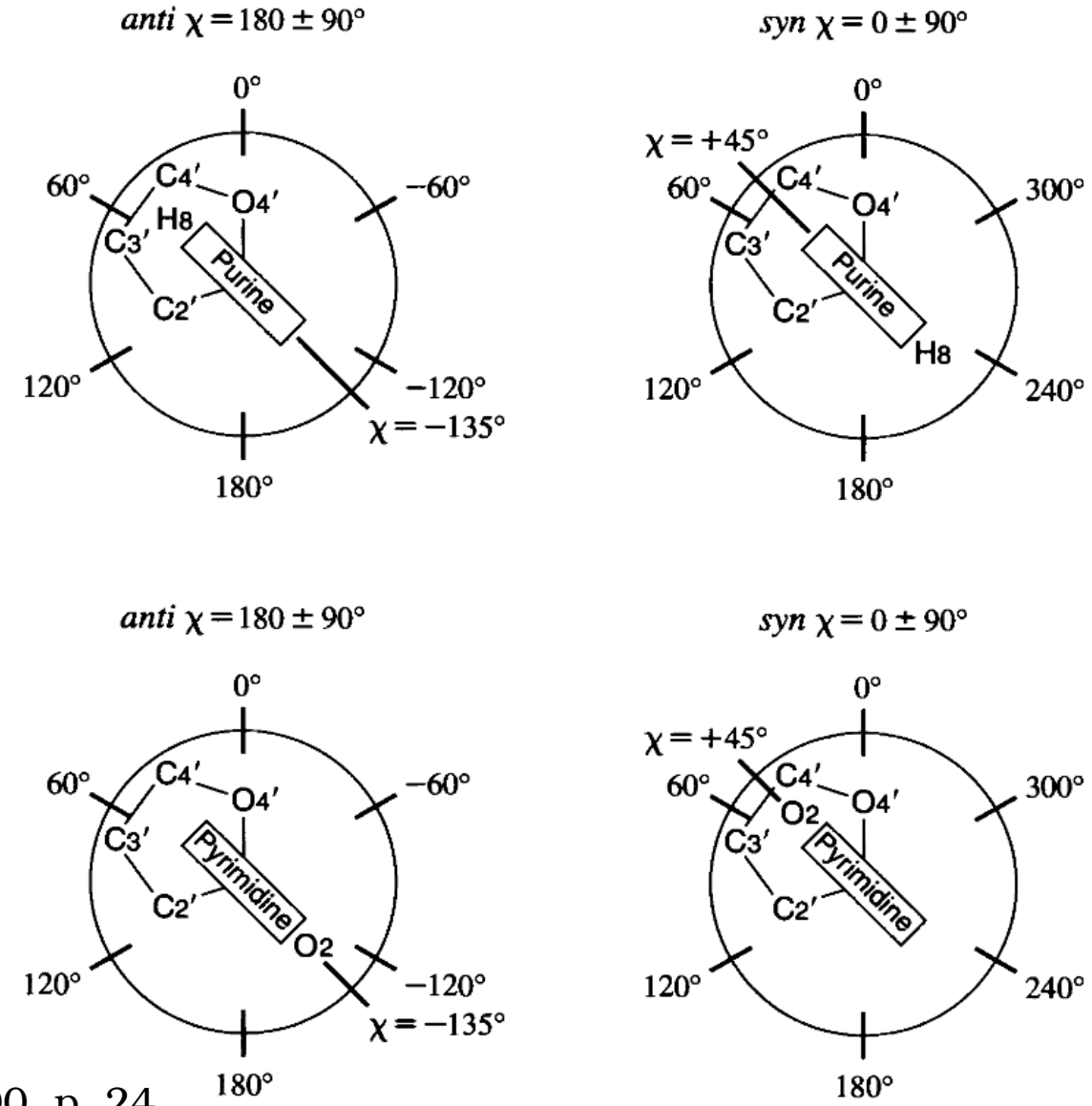
Bloomfield *et al.* 2000, p. 19

Pseudorotation angles



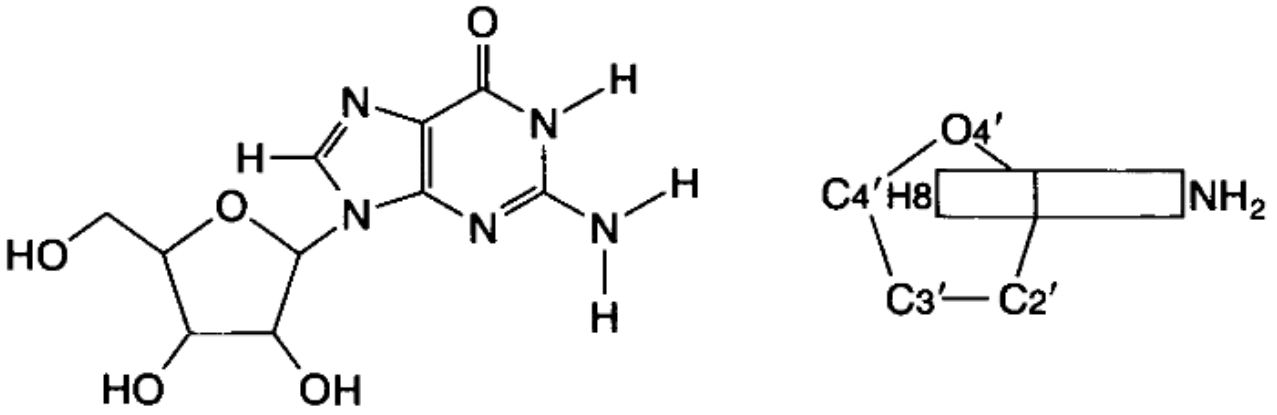
Bloomfield *et al.* 2000, p. 21

Syn and *anti* configurations

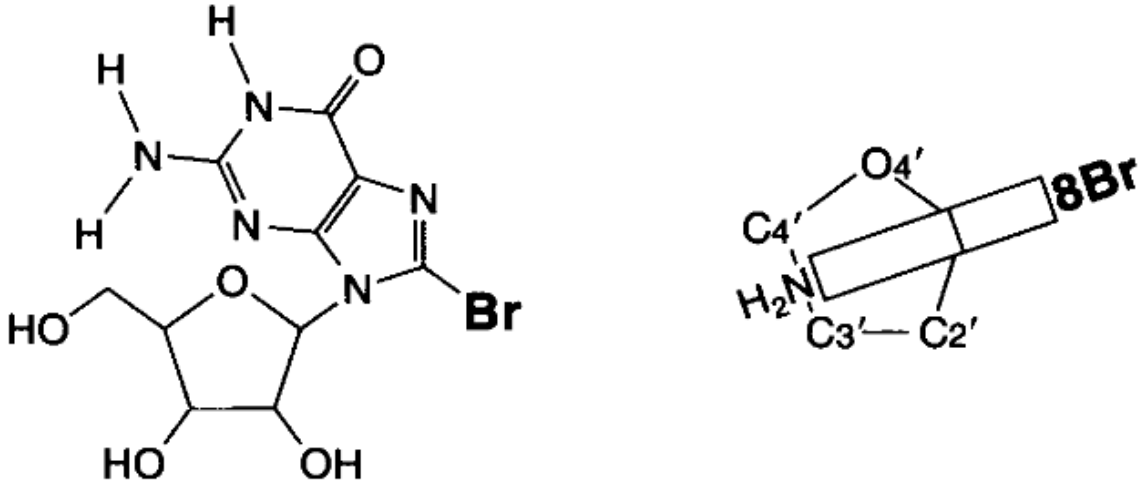


Bloomfield *et al.* 2000, p. 24

Influence of a large (Br) substituent



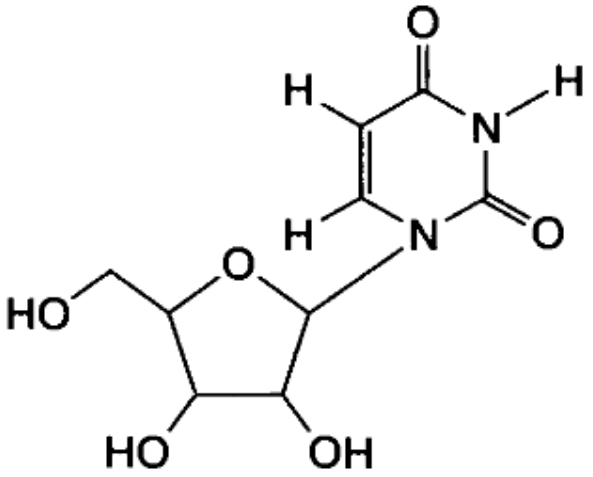
anti Guanosine

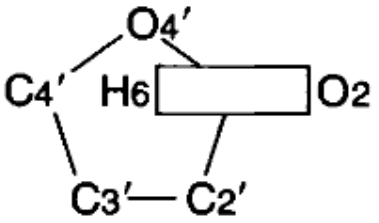


syn 8-Bromoguanosine

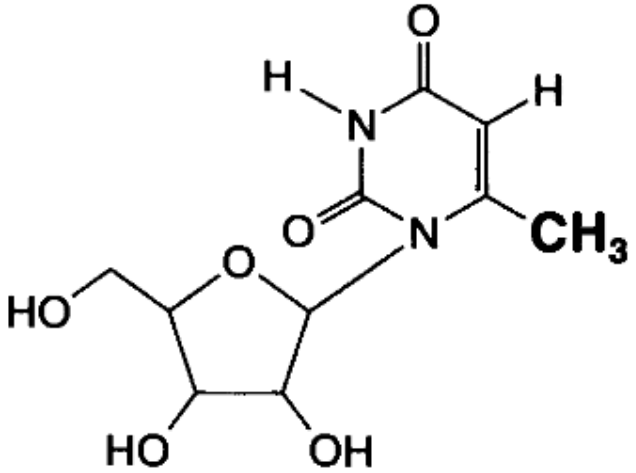
Bloomfield *et al.* 2000, p. 23

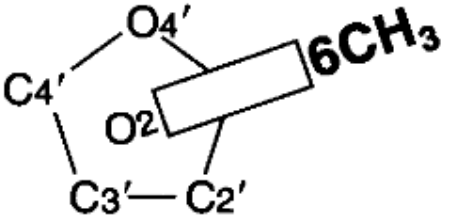
Syn/Anti variants





anti Uridine



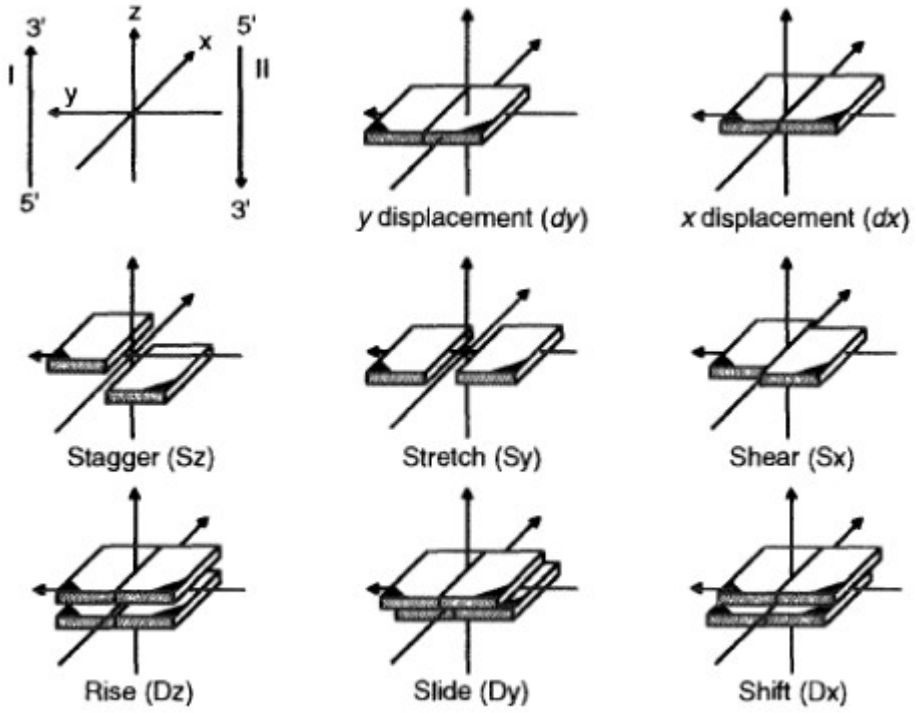


syn 6-Methyluridine

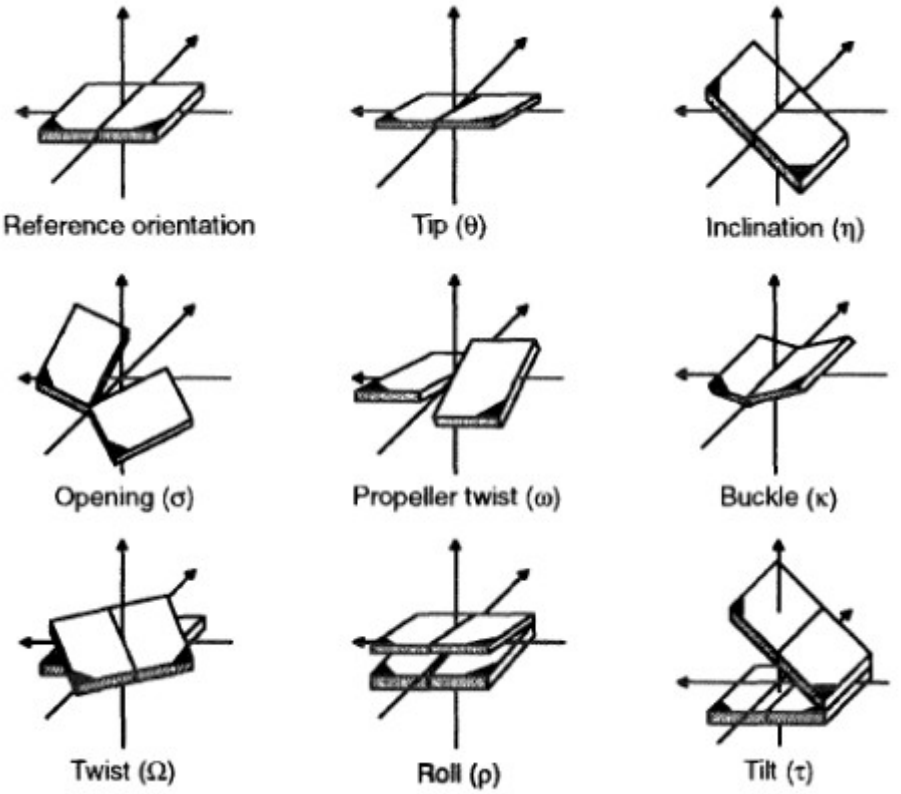
Bloomfield *et al.* 2000, p. 23

Base pair relative position

Translation

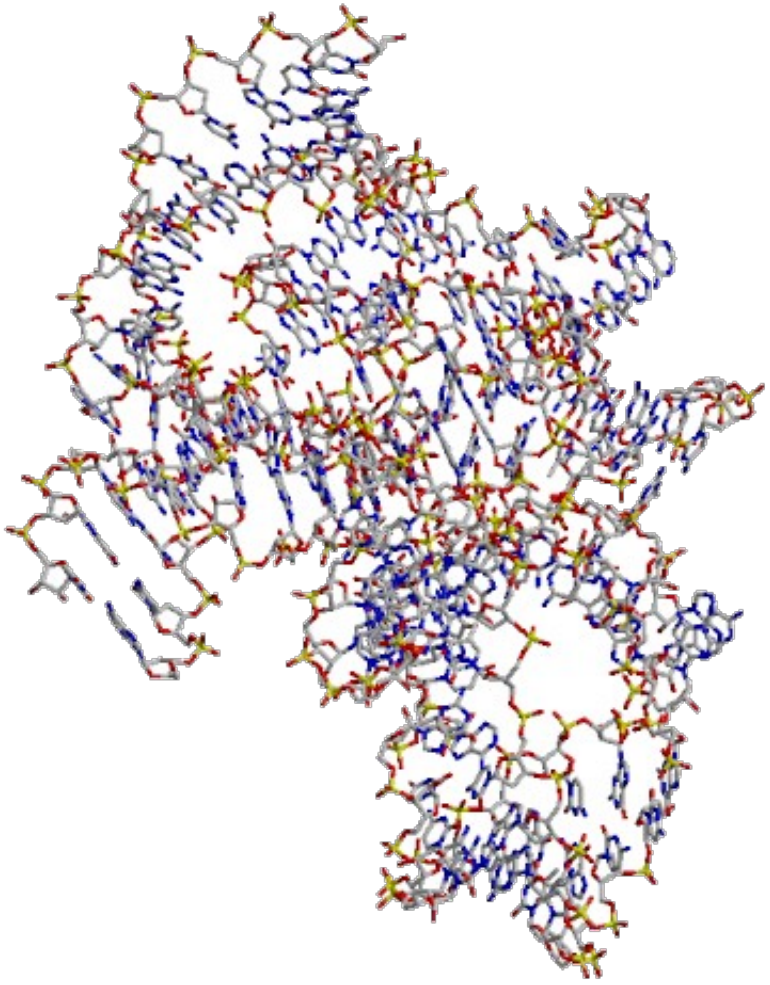


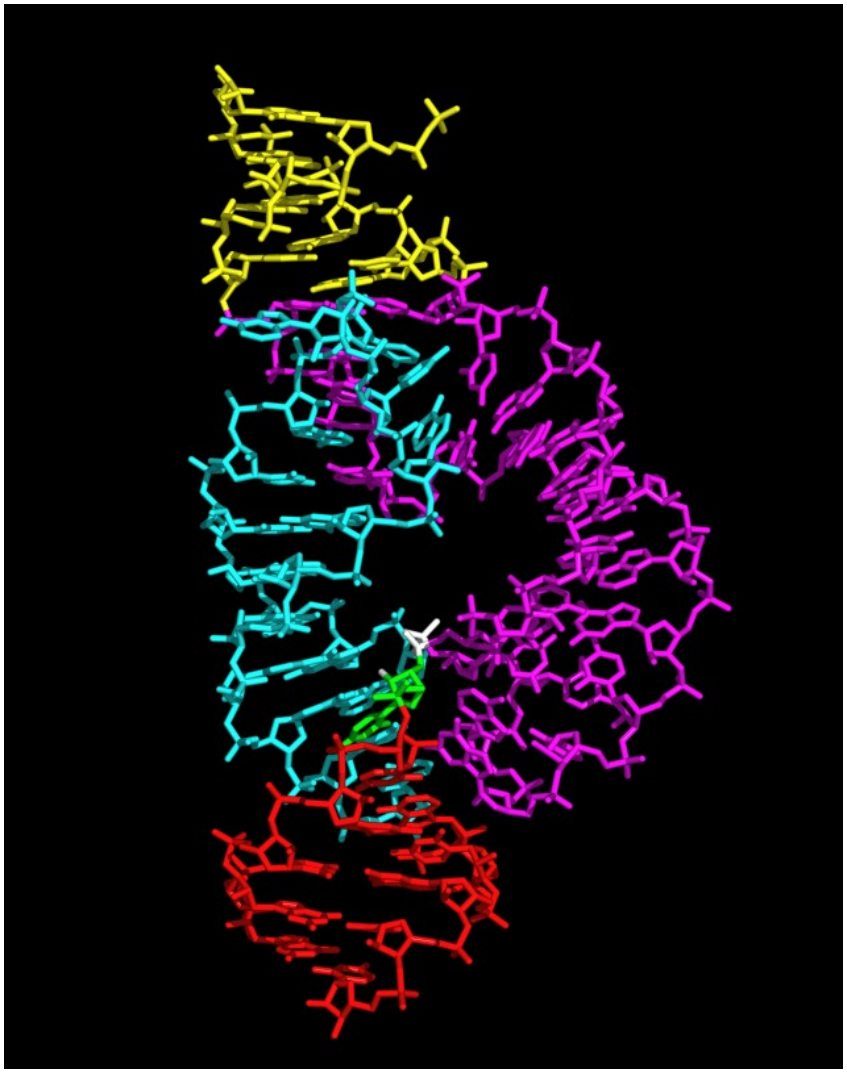
Rotattion



Bloomfield *et al.* 2000, p. 94

RNA secondary structure

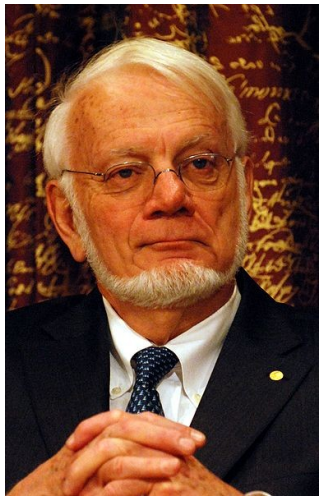




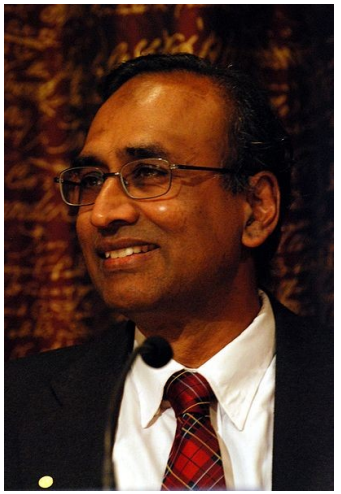
Hammerhead rybosime

Ribosome

Ada Yonath

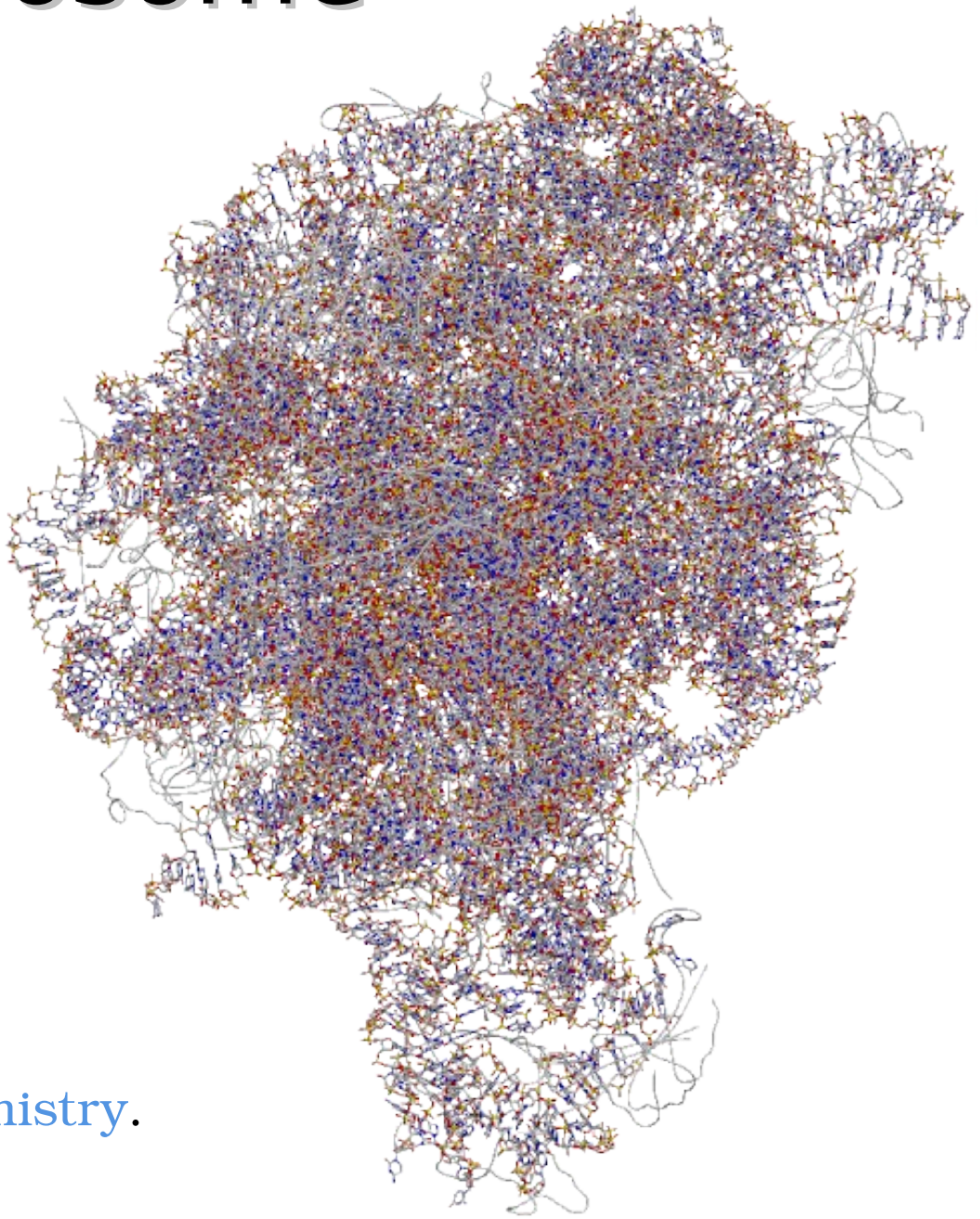


Thomas A. Steitz



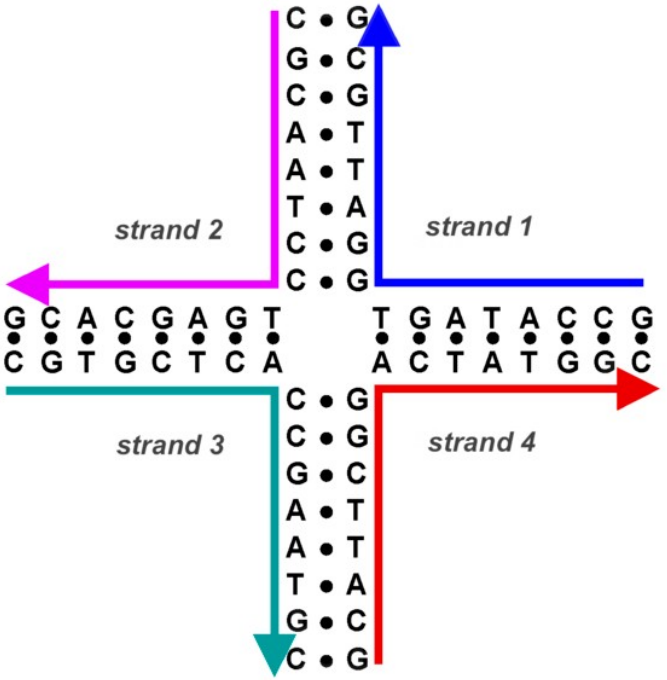
Venkatraman Ramakrishnan

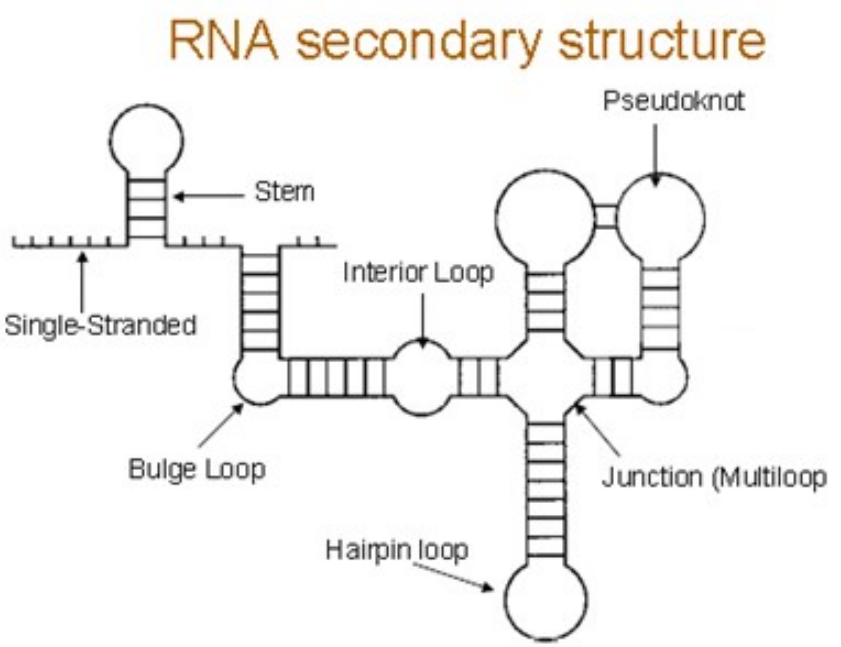
The Nobel Prize in Chemistry.
2009



sources: Wikipedia, The Protein Data Bank (PDB)

RNA secondary structure prediction





http://en.wikipedia.org/wiki/RNA_structure

http://en.wikipedia.org/wiki/List_of_RNA_structure_prediction_software