

The geometry of DNA: a structural revision

Mark E. Curtis

Thule House, 18 Tobson, Bernera, Isle of Lewis, HS2 9NA, UK.

Email: mark@curtisdna.com

I would like to suggest a modification to the structure for the salt of deoxyribose nucleic acid (D.N.A.) that was proposed by Francis Crick and James Watson in April 1953.

In 1995 I began an investigation into the structure of DNA with the intention of producing a series of drawings and paintings of the double helix. My interest stemmed from certain features of my work as an artist, specifically my inquiries into the nature and depiction of space. In the manner of renaissance perspectival artists such as Uccello, I embarked on scale drawings of the helical structure using the standard textbook dimensions that derive from x-ray diffraction data. In the course of this work, discrepancies emerged, and it became clear to me that the Crick and Watson structure does not conform to geometric principles. Indeed my attempts to translate their theory from two into three dimensions ran into considerable topological problems.

Since the article in nature was published, their proposal would appear to have been fully vindicated by almost all-available empirical evidence. However, I have since discovered that a growing minority do recognise flaws in Crick and Watson's conclusions, specifically in terms of its topology and thereby the ability of the structure to replicate itself. Although some research has even gone so far as to question the very existence of the double helical structure itself, my proposal retains the double helix as its fundamental basis.

Without compromising the essence of their structure, I propose a resolution of the geometrical inconsistencies by means of a simple change in the position of alignment between the purines and pyrimidines. This realignment is founded entirely upon geometric principles and further investigation revealed a series of mathematical equations that describe a three-dimensional geometric helix that conforms to the known ratios of DNA. In this paper, I will demonstrate the mathematical basis for this re-reading of DNA and moreover the simplicity and purity it engenders, when applied to the molecular structure of the bases.

The Double Helix

The structure of the salt of deoxyribose nucleic acid is undoubtedly a double helix, with ten bases to each turn. Moreover, the approximate dimensions of a complete turn of DNA's helix are well known: the diameter of the helix is 20\AA (angstroms), the base height is 3.4\AA and thus the helix extension is 34\AA . These data enabled a simplified and systematic perspective projection of the structure, see **fig1** below.

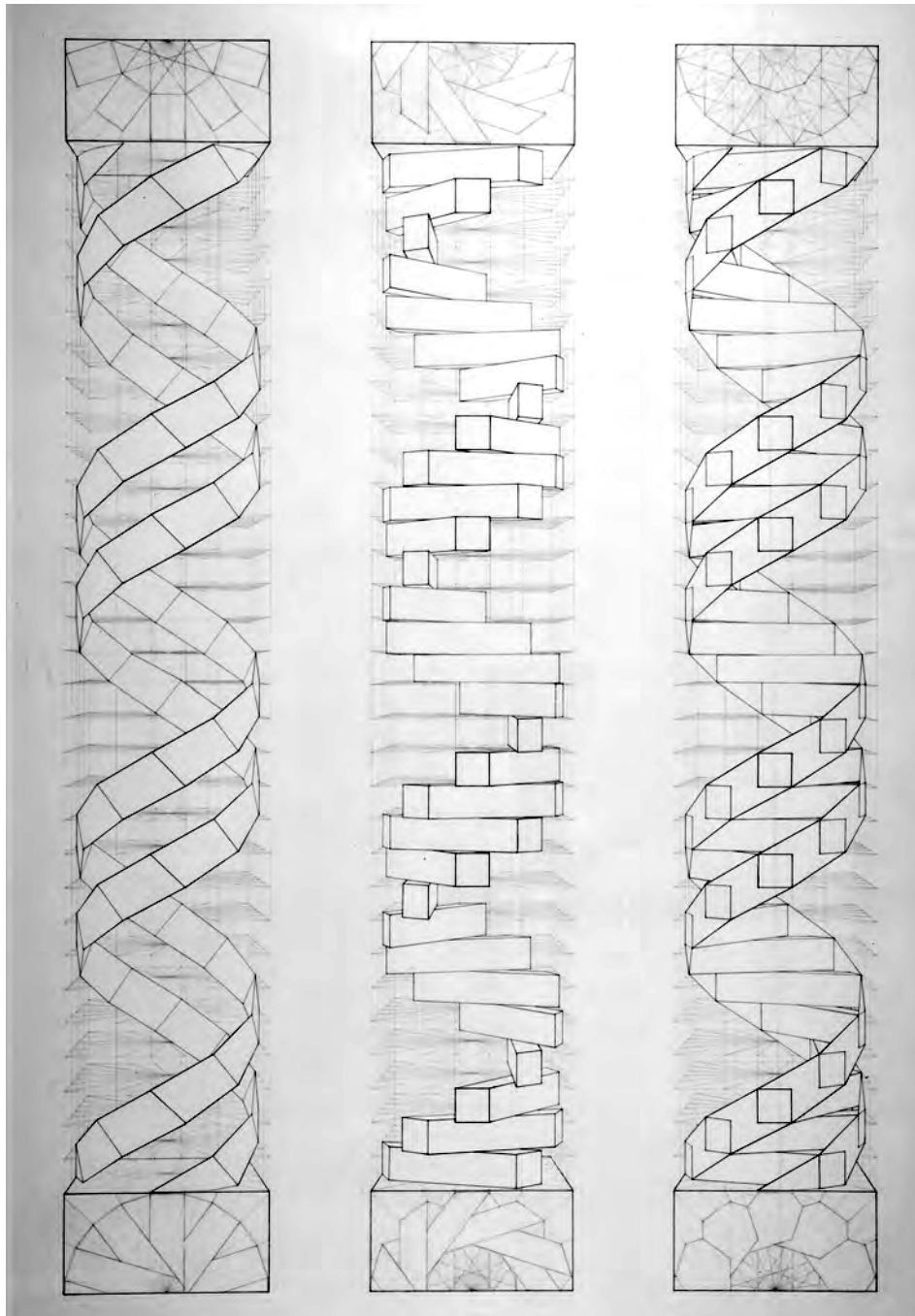


fig 1

The Mathematics

Although, theoretically, it is possible to construct a helix from almost any series of polygons, there happens to be only one polygonal formation that would fulfil all the necessary criteria: ten regular pentagons orientated about a decagon, see **fig 2** below.

When translated into three-dimensional space, these pentagons would become prisms with all lengths equal (**ii**).

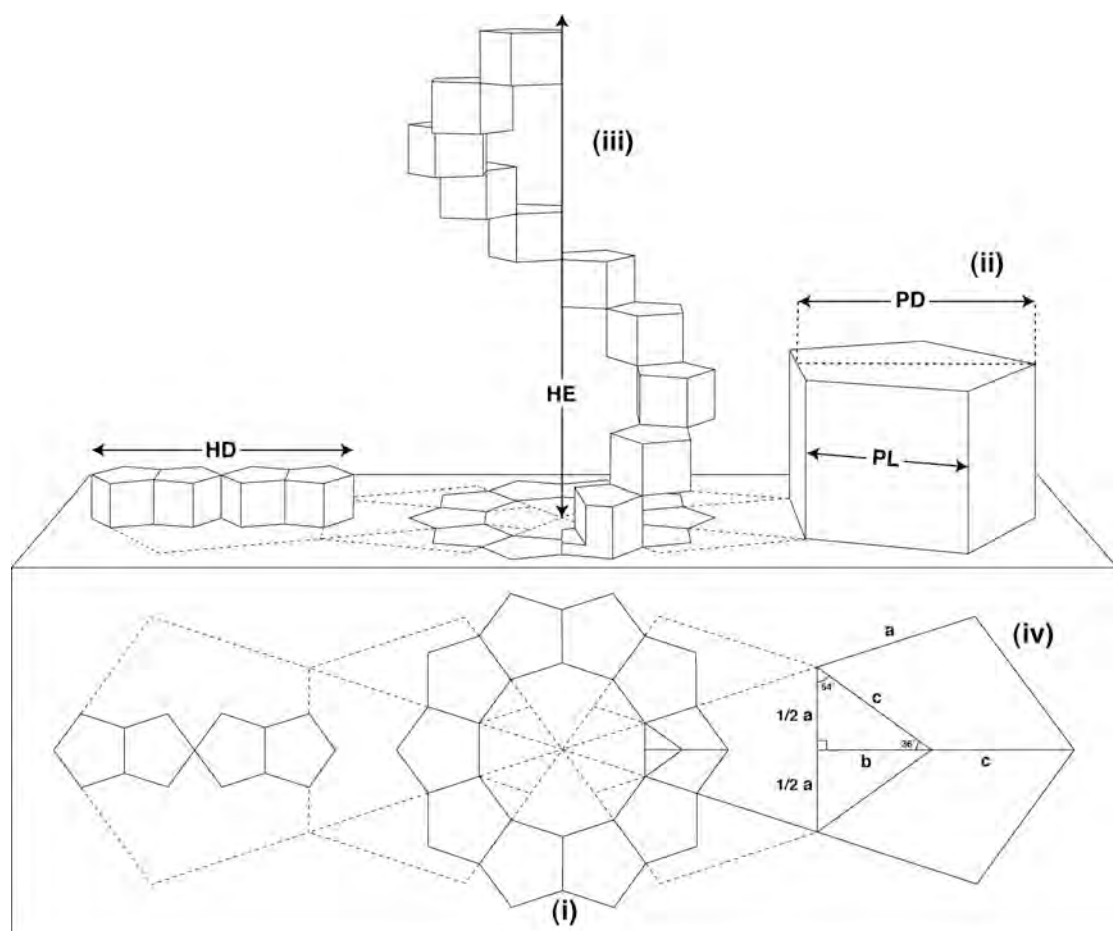


fig 2

A complete turn of the helix is formed by progressive rotation and extension of the ten regular prismatic pentagons (**iii**).

It follows, therefore, that the diameter of the helix (**HD**) and the height of the helix extension (**HE**) have a direct and constant proportional ratio to the pentagon length (**PL**) and pentagon diameter (**PD**).

In order to establish the precise nature of this ratio we must devise some trigonometrical equations.

The values of **a b c (iv)** are ascertained as follows:

$$1/2a = c \times \sin 36^\circ$$

$$b = c \times \cos 36^\circ$$

$$c = 1/2a \div \sin 36^\circ \text{ or } b \div \cos 36^\circ$$

The values of PL and PD may be determined as follows:

$$PL = 2 \times 1/2a = a$$

$$PD = b + c$$

It follows, therefore, that:

$$HD = 4 \times (b + c)$$

$$HE = 10 \times a$$

The above equations enable us to establish the mathematical constant ratios correct to ten decimal places:

$$PL = 1$$

$$PD = 1.5388417686$$

$$HD = 6.1553670744$$

$$HE = 10$$

From these ratios, it is possible to come by a set of interrelated equations that would determine any of the measurements of a helix constructed from regular prismatic pentagons:

$$PL = PD \div 1.5388417686 \text{ or } HD \div 6.1553670744 \text{ or } HE \div 10$$

$$PD = PL \times 1.5388417686 \text{ or } HD \div 4$$

$$HD = PL \times 6.1553670744 \text{ or } PD \times 4$$

$$HE = PL \times 10$$

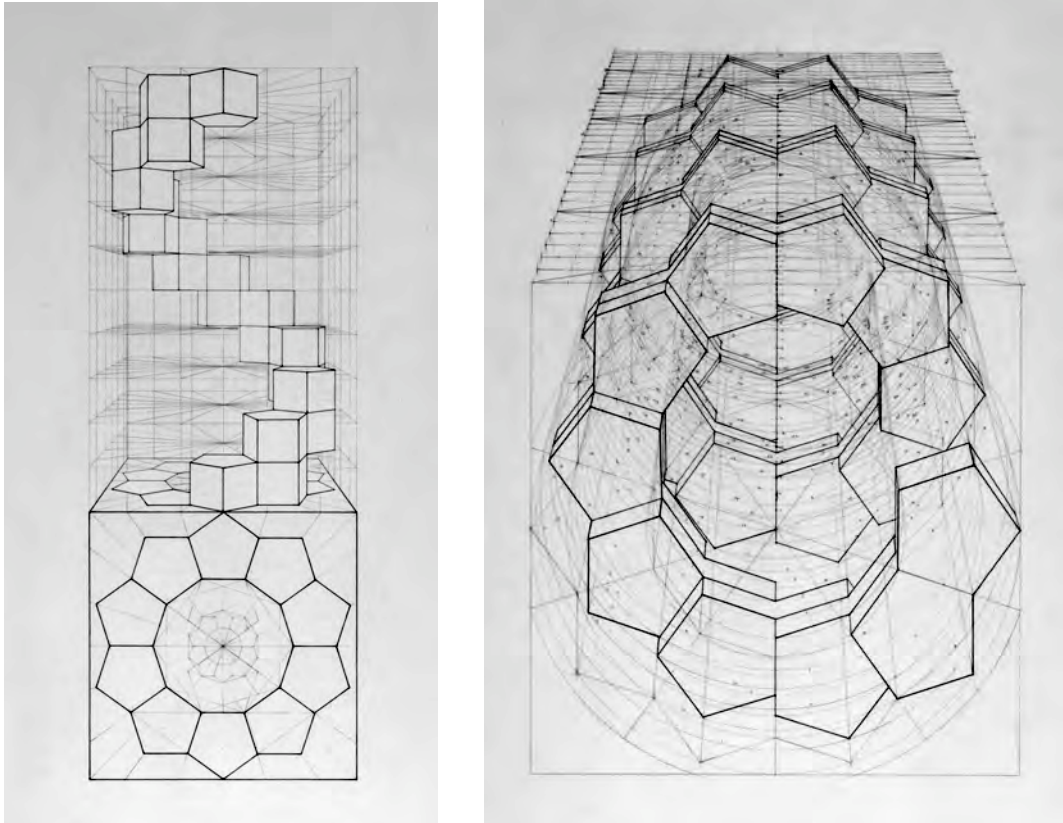
We now find ourselves in a position to apply any one of the known dimensions of DNA to the above equations. For example, if the PL – i.e. the base height – is known to be approximately 3.4 Å:

$$PD = 3.4 (PL) \times 1.5388417686 = 5.23206201324 \text{ \AA}$$

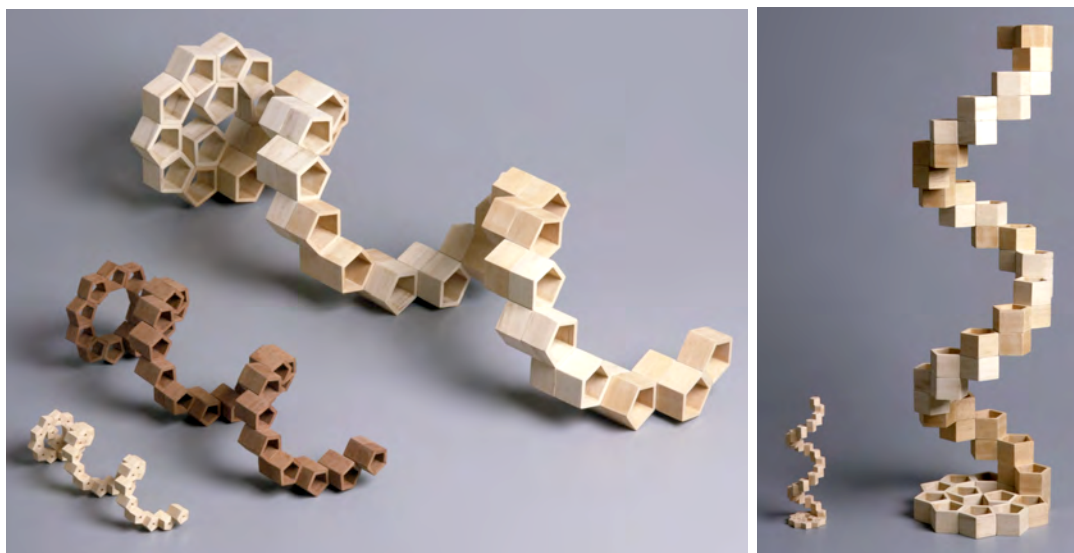
$$HD = 3.4 (PL) \times 6.1553670744 = 20.928248053 \text{ \AA}$$

$$HE = 3.4 (PL) \times 10 = 34 \text{ \AA}$$

These figures would appear to cohere with the known dimensions of DNA, as revealed by the x-ray diffraction data and we now find ourselves in a position to construct an exact dimensional composite of the DNA double helix.



In **fig 2** I used single prismatic pentagons to illustrate the 3-dimensional helix. However, to ensure stability in the structure as it would exist in reality, it is necessary to place adjacent pentagons on each plane and then stack accordingly, thereby creating the double helix.



The application of geometry to the DNA molecular structure

The pairing of purines and pyrimidines in the Crick and Watson proposal locates the molecular pentagons that make up a part of the purines on the outside of the paired bases (**fig 4**). However, it has been demonstrated that a more fluent geometry would require adjacent pentagons at the heart of the base pairing. It is therefore necessary to re-orientate the established molecular pairing, so that the pentagons of adenine (A) and guanine (G) form hydrogen bonds to the hexagonal structures of both thymine (T) and cytosine (C) (**fig 5**). This spatial arrangement of the hydrogen bonds enables the necessary adjacent second pentagon to become viable. Moreover, it also accords with our understanding of molecular bonding and maintains the specificity of G with C and A with T.

Fig 4 Crick and Watson pairings

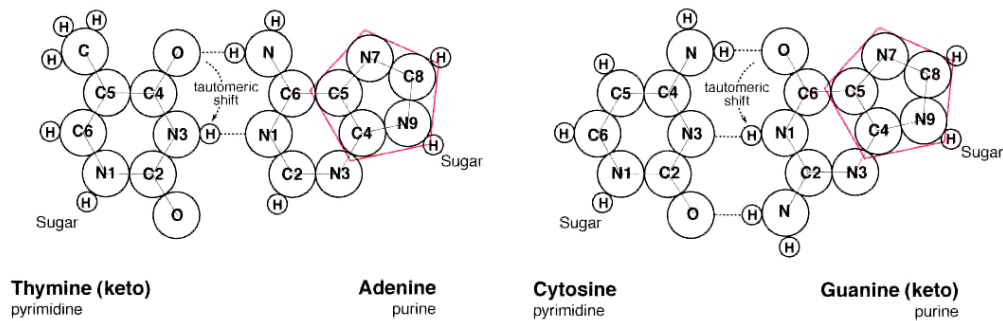
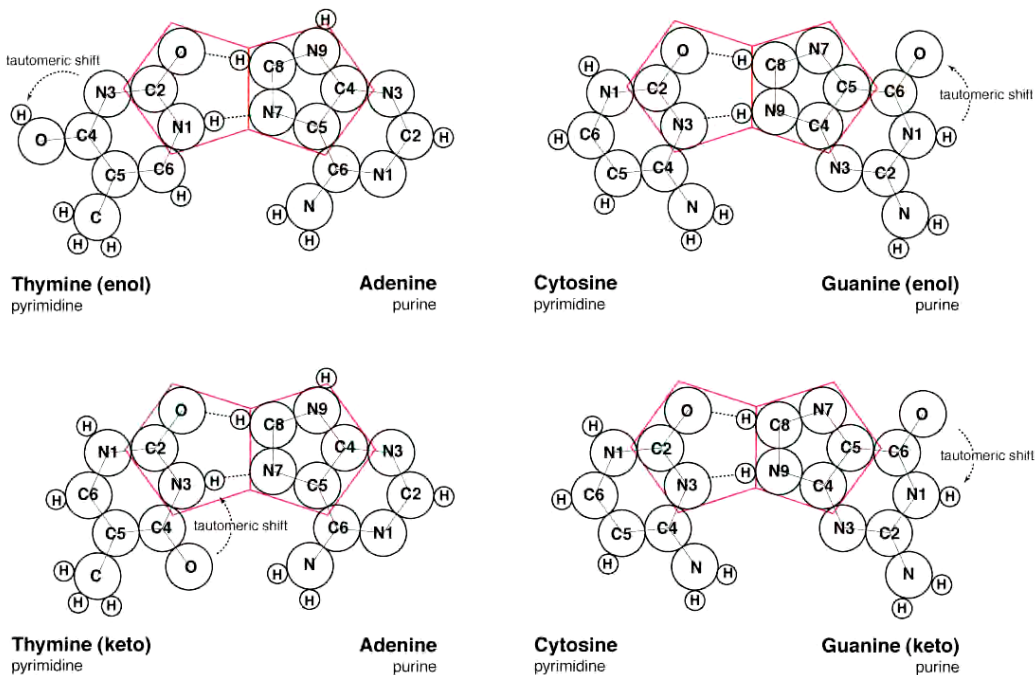
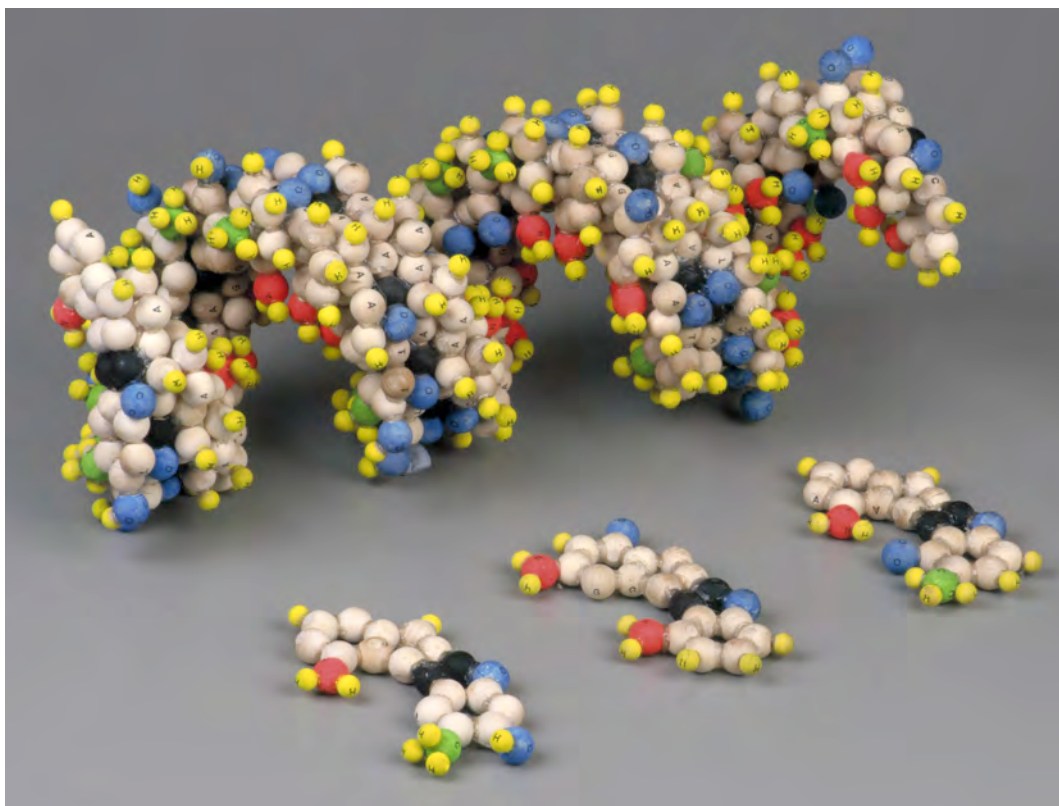


Fig 5 Proposed pentagonal pairings



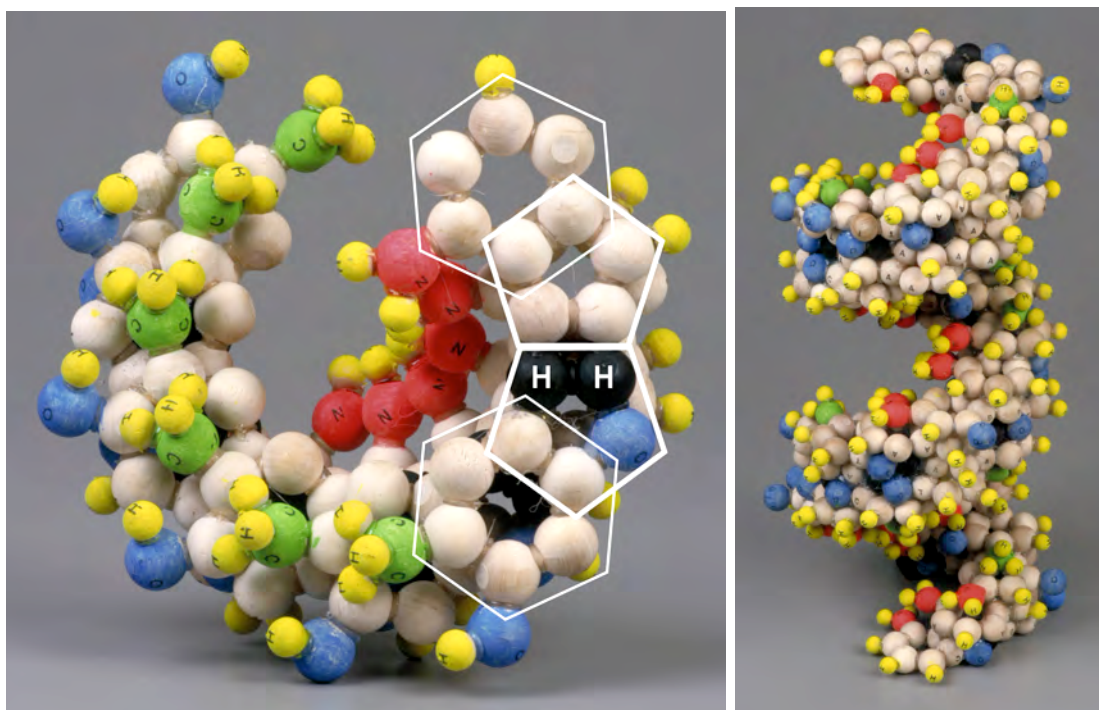
At this point, it would seem appropriate to refer to the different formations that the molecules of guanine and thymine can take, namely the enol and keto states. Guanine and thymine may exist in either enol or keto configurations and are believed to pass through tautomeric shifts from one to the other – in other words, an indiscernible and spontaneous leap by the hydrogen atom from a specific oxygen atom to a specific nitrogen atom or vice-versa. The Crick and Watson proposal requires the keto formation, whereas this alternate proposal would appear to be viable in either of the formations.

In addition, it should be noted that presently the sugar-phosphate chains are depicted attached to N(1) of the pyrimidines and N(9) of the purines by covalent (glycosidic) bonds. However, both prior to 1953 and even today, when the molecules are represented in isolation, hydrogen atoms are illustrated attached to these nitrogen atoms. For the purposes of this proposal, the four hydrogens are retained and one of them – guanine N(9) – now plays a practical role in the pairing of guanine with cytosine.



This alternative geometrical formulation reveals each base pairing to be an almost mirror image of the other, allowing a structure which, when fully assembled, exhibits both uniformity and stability. Most importantly perhaps, the alignment of the ‘spurs’ – that is to say, the NH₂’s (G, C & A) or CH₃ (T) – on each base pair is consistent. If either base pair were

inverted, these spurs would naturally project in the opposite direction without upsetting the main generative architecture of the helix. This ensures that the spurs attached to cytosine and adenine construct a constant sequence specific 'secondary helix' within the space generated by the primary helix, and that the spurs attached to guanine and thymine provide a sequence specific 'capping' of the cavities generated by the conformation of the primary helix. This sets in motion a simple and seemingly clockwork mechanism that may be utilised in the coding for amino acids and subsequent protein structures.

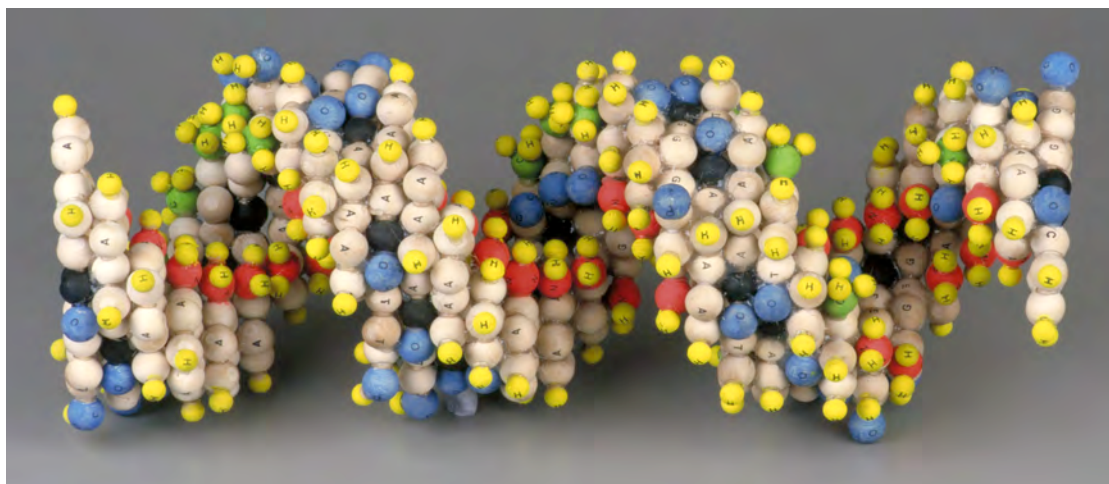
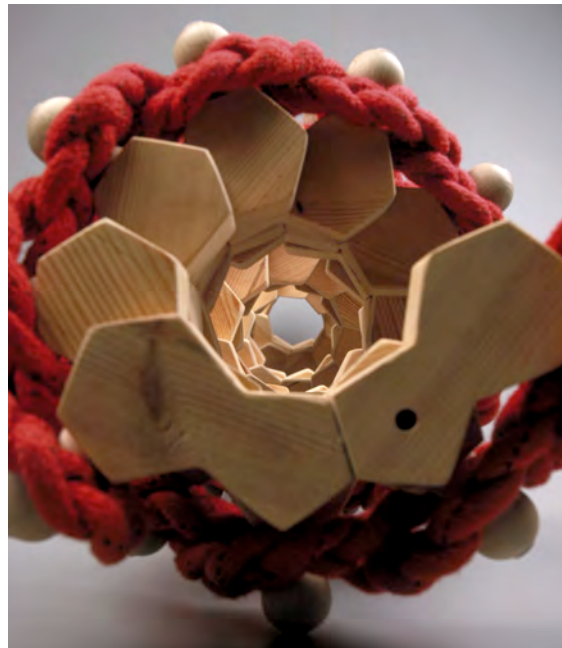


With respect to the sugar-phosphate chains, it has already been stated that at present, covalent bonds are used to attach them to the bases. The nature of the C/W proposal is such that it both requires and also relies in entirety on the sugar phosphate chains to corral the bases into the helix.

While it would be possible to incorporate covalent bonds into this proposal, I must say that, to my mind, the nature of this revised structure does suggest a strong possibility that the sugar phosphate chains may be secured by means of multiple hydrogen bonds. The sheer quantities of accessible hydrogen and oxygen on both the revised structure and also on the sugar-phosphate chains would perhaps tie in with such a suggestion. The first point of separation will inevitably continue to be the hydrogen bonds that hold base to base because they have considerably less resistance than the multiplicity of bonds that would hold the base-pair's to the sugar-phosphate chains.

Conclusions

This proposed structure for DNA is wholly founded upon mathematical principles. Although the geometrical modification to the base pairings is relatively minor, the resulting double helix manifests a clarity altogether distinct from that offered by Crick and Watson and it would appear to shed light upon a number of areas of continuing uncertainty.



The implications of these findings are inevitably far-reaching and would potentially affect many areas of research. However, these lie beyond my own capacity to evaluate and I will restrict myself to reiterating the principal features of this proposal:

- Geometric equations predict the dimensions of DNA's structure. Not only does the pentagonal geometry predict the helical dimensions but it would also demonstrate 'principle causation'.
- The pentagonal geometry provides the dynamics required to build a consistent, stable and uniform helical structure and also establishes *why* there should be consistently ten bases contained within a single turn of the helix. Incidentally, when converted to the molecular dimension I would certainly predict degrees of variation, certainly between 9.5 and 10.5 bases per turn, but perhaps even more.
- Both the hollow centre and side-by-side structural formation ensure instant access at any point within the helix. This would permit the DNA (even circular) to open and close during its replication functions without entangling itself.
- The modification to the base pairing would appear to be able to exist in either the enol or keto formations.
- While the sugar-phosphate backbones will undoubtedly prove integral to the stability of the helical structure, it is the geometry of the base-pair molecules themselves that is ultimately responsible for the formation of the helix.

I have now set down a reinterpretation of DNA's structure as I see it. It should be remembered that, by necessity, I publish this paper in my capacity as an artist and in the knowledge that nothing I have set down has yet been subjected to scientific scrutiny. It should be read as such, allowing the visual material to complement the text and vice-versa. This, after all, was the trigger for my initial interest. Aware of the further implications, I offer it in the hope that it may stimulate wider research and debate.

Mark E. Curtis

Addendum

Since my first offering of this proposal in 1997 it has met, perhaps not altogether surprisingly, with a decidedly cool response. However, that said, I remain no less convinced that there is a case to answer and that more specific scientific research needs to be undertaken - I therefore continue to maintain what I have done so already with confidence, and would like to offer the following quote from Plato as some justification for my apparent dogmatism.

“We must in my opinion begin by distinguishing between that which always is and never becomes from that which is always becoming but never is. The one is apprehensible by intelligence with the aid of reasoning, being eternally the same, the other is the object of opinion and irrational sensation, coming to be and ceasing to be, but never fully real. In addition, everything that becomes or changes must do so owing to some cause; for nothing can come to be without a cause. Whenever, therefore, the maker of anything keeps his eye on the eternally unchanging and uses it as his pattern for the form and function of his product the result must be good; whenever he looks to something that has come to be and uses a model that has come to be, the result is not good.”

Plato - Timaeus. (28)

Unfortunately, I have neither the access nor indeed the understanding to take these ideas any further and feel it both wise and prudent to leave any potential future areas of research to those people with a more specialist knowledge. In response to those whose minds appear fixed within the present paradigm and who would use its ‘issue’ to pick holes in some of the detail of this alternate proposal I can but quote Thomas Kuhn:

“...the choice between competing paradigms regularly raises questions that cannot be resolved by the criteria of normal science. To the extent, as significant as it is incomplete, that two scientific schools disagree about what is a problem and what a solution, they will inevitably talk through each other when debating the relative merits of their respective paradigms. In the partially circular arguments that regularly result, each paradigm will be shown to satisfy more or less the criteria that it dictates for itself and to fall short of a few of those dictated by its opponent... The normal scientific tradition that emerges from a scientific revolution is not only incompatible but often actually incommensurable with that which has gone before... Because it has that character, the choice is not and cannot be determined merely by the evaluative procedures characteristic of normal science, for these depend in part upon a particular paradigm, and that paradigm is at issue.”

Thomas Kuhn - The Structure of Scientific Revolutions. Ch IX & XII

Finally, I should like to mention that over these last 10 years I have both unearthed and also been pointed towards numerous papers, articles and books that I believe to be well worth revisiting in the light of this geometry. In particular I would draw attention to the following:

Papers

- Crick, F. H. C. & Watson, J. D. (1953) *Nature*, vol **171**, 737-738.
Gamow, G. (1954) *Nature*, vol **173**, 318.
Furberg, S. (1949) *Nature*, vol **164**, 22.
Pauling, L. & Corey, R. B. (1953) *Proc. Natl. Acad. Sci*, **39**, 84-96
Hoogsteen, K. (1959) *Acta. Cryst*, vol **12**, 822.
Hoogsteen, K. (1963) *Acta. Cryst*, vol **16**, 907-916.
Root-Bernstein, R. (1996) *Art Journal*, **Sp**, 47-55.
Bansal, M. (2003) *Current Science*, vol **85**, 1556-1563.

Books

- Levene, P. A. & Bass, L. W. (1931) 'Nucleic Acids'.
Todd, A. (1956) 'Nucleic Acids'.
Thompson, D'arcy (1961) 'On Growth and Form' abridged edition.
Watson, J. D. (1968) 'The Double Helix'.
Olby, R. (1974) 'The Path to the Double Helix'.
Freeland Judson, H. (1979) 'The Eighth Day of Creation'.
Crick, F. H. C. (1989) 'What Mad Pursuit'.
Maddox, B. (2002) 'Rosalind Franklin: The Dark Lady of DNA'.