is no *obvious* formula for its construction ; and what is obvious, of course, varies between observers. Perhaps it should therefore be a matter of some surprise that present probability theory applied to science in fact works as well as it does ; and if we could discover how it is that it does work so well, we might be able to see how it is that it does not appear to work quite well enough.

I wish to express my gratitude to the Perrott Electors of Trinity College, Cambridge, under whom the new description of this psychical research problem was originally made, and to Prof. A. C. Hardy, of Oxford, who generously provided a grant for the research to continue in his Department. I should also like to thank Sir Ronald Fisher, by whose writings and conversation I have been greatly helped.

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EVIDENCE FOR 2-CHAIN HELIX IN CRYSTALLINE STRUCTURE OF SODIUM DEOXYRIBONUCLEATE

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WATSON AND CRICK[1] have proposed a structure for sodium deoxyribonucleate consisting of two co-axial helical chains related by a diad axis. We have shown[2] that the main features of their structure are consistent with certain important features of our X-ray diagrams of structure B (the high-humidity less-ordered form of the salt). A subsequent closer investigation of density and water content in relation to the prominent equatorial spacing, and also of equatorial intensities calculated from a projection of the proposed structure (kindly provided by Watson and Crick), makes it clear that in detail the structure is not consistent with the observed equatorial reflexions. Both density and intensity considerations lead us to favour a more compact helical structure in which the phosphorus atoms lie on a helix of radius about 8·5 A. rather than 10 A. This value also lies within the range of spread of the more diffuse layer-line peaks.

We are more concerned here, however, with evidence which confirms in principle the type of structure suggested by Watson and Crick, than with criticism on points of detail.

If a 2-chain helical molecule exists in structure B, then such a molecule, in modified form, must also exist in structure A (the crystalline form obtained at 75 per cent relative humidity), since the change $A \rightleftharpoons B$ is readily reversible. The purpose of this communication is to point to evidence for a 2-chain helical molecule in structure A.

For structure A we have measured the positions and intensities of reflexions and have calculated the cylindrically averaged Patterson function[3]. The work

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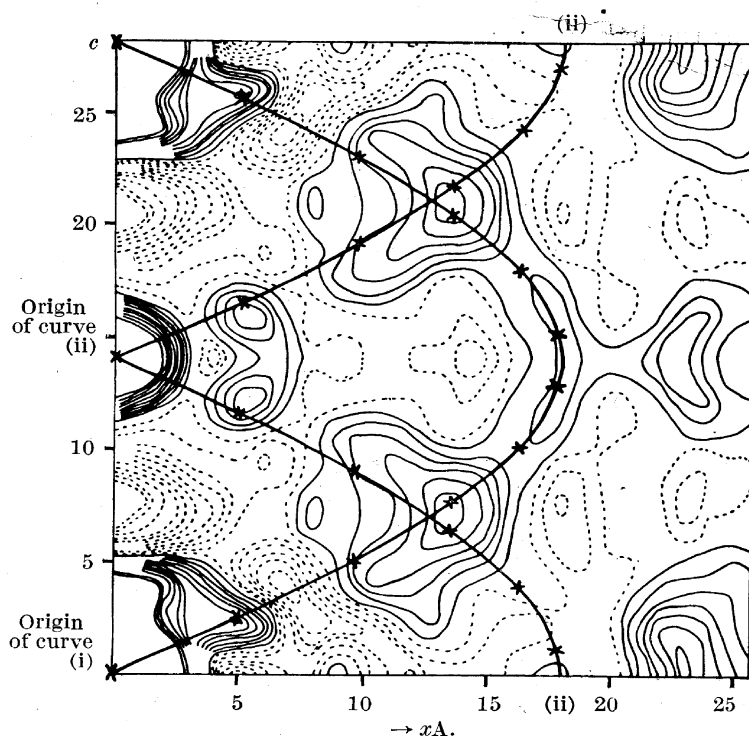
Fig. 1.　Cylindrical Patterson function of crystalline sodium deoxyribonucleate.　×, theoretical peak for *intra*-helical P – P vector

is described in detail elsewhere[4]. The Patterson function is reproduced in Fig. 1. The theoretical curve for the Patterson function of a smooth helix of radius 9·0 A. is also shown (curve (i)). The very strong peak at height $c = \frac{1}{2}$ on the fibre axis suggests that the phosphate groups of the two chains are separated by approximately $\frac{1}{2}c$. We therefore added to Fig. 1 curve (ii), which completes the theoretical Patterson function for two smooth co-axial helices separated by $\frac{1}{2}c$ (c is the pitch of the helix). Curves (i) and (ii) together clearly pass through a large proportion of the important Patterson peaks. Moreover, if we take into account the fact that the real structure contains, not smooth helices, but phosphate groups equally spaced along such helices, the agreement is even better.

The only near-meridional reflexion in the X-ray diagram of structure A is a rather weak one on the eleventh layer-line. This suggests that there are eleven nucleotides per turn of the helix. (This is sufficiently near to the number ten, found for structure B[1,2,5], for the reversible transformation $A \rightleftharpoons B$ to be plausible.) Further, we may suppose that the well-resolved peak at 5·7 A. from the pseudo-origin peak at $c = \frac{1}{2}$ represents a P – P vector, and this distance is exactly that between neighbouring phosphorus atoms if eleven are equally spaced along one turn of a helix of radius 9 A. In Fig. 1 we have marked with a cross the theoretical positions of intra-molecular Patterson peaks to be expected for this arrangement, assuming that the phosphorus atoms on one helix lie vertically above those on the other. The agreement with the observed Patterson peaks is seen to be remarkably good.

In Fig. 2 we have marked on the Patterson function the positions of all inter-molecular P – P vectors obtained when, in the unit cell described below, there is one molecule (that is, two chains) associated with each lattice point. The circles in Fig. 2 have each only 1/11 of the weight of the crosses in Fig. 1, and 1/22 and 1/44 of the weight of the pseudo-lattice points (relating phosphate residues only) shown by crosses

near the half-cell height in Fig. 2. The lattice points relating the whole structure are denoted by larger crosses near to the origin level in c. In addition to this weighting, for correlation with the cylindrically averaged Patterson function, the weight of each calculated peak should be considered as inversely proportional to x, since in averaging it must be spread over a circle of radius x. When these factors are taken into account, it will be seen that agreement between calculated and observed Patterson peaks is still good.

Space group, density and the unit cell. Using the cylindrical Patterson function, we have been able to identify the lattice vectors (indicated in Fig. 2) and hence to index all 66 observed reflexions. The unit cell is face-centred monoclinic having $a = 22 \cdot 0$ A.; $b = 39 \cdot 8$ A.; $c = 28 \cdot 1$ A.; $\beta = 96\frac{1}{2}°$. If the unit cell is truly monoclinic, the space-group can only be $C2$, since the molecule contains asymmetric carbon atoms. Again, since the structure of the phosphate sugar backbone chain is non-centric, the symmetry axis cannot pass through such a chain, but must relate the chains one to another in pairs. There must, therefore, be an even number of chains associated with each lattice point.

In order to calculate the number of nucleotides in the unit cell, it is necessary to know both the density and the water content. Unfortunately, these quantities can only be measured on a polycrystalline mass, and there must remain some uncertainty as to the true density and water content of the crystallites. Our measurements[5] gave a density of $1 \cdot 47$ gm./c.c. at 75 per cent relative humidity and a water content of about 40 per cent of the dry weight (or about $8H_2O$ per nucleotide). We have confirmed that the specimens used for these measurements were in the form of structure A and not structure B. These results correspond to twenty-three nucleotides per lattice point, which is in reasonable agreement with the suggestion that the primitive unit cell contains eleven nucleotides on each of two chains.

The three-dimensional Patterson function. After establishing the unit cell and indexing the reflexions, the complete three-dimensional Patterson function
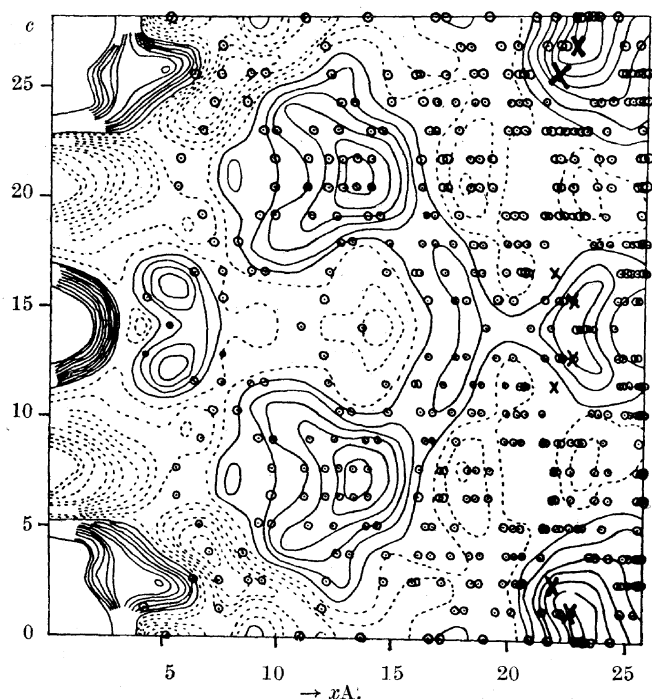

Fig. 2. Cylindrical Patterson function of crystalline sodium deoxyribonucleate. ⊙, theoretical peak for *inter*-helical P – P vector
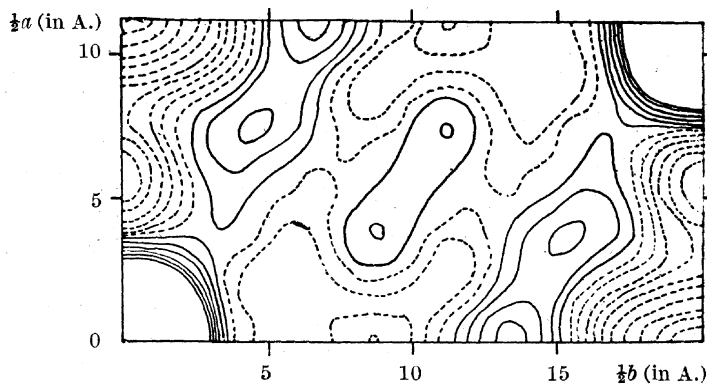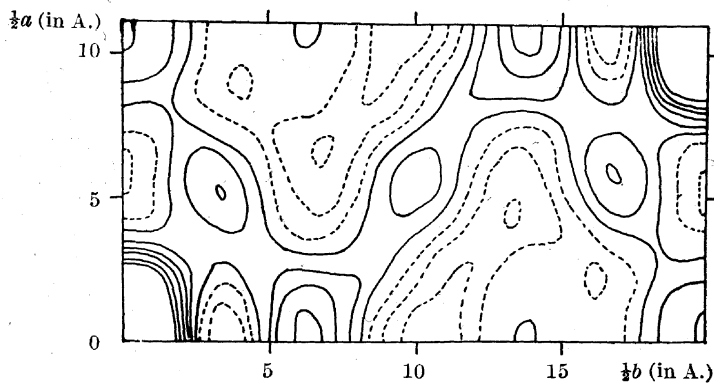

Fig. 3 (i)

Fig. 3 (ii)

Three-dimensional Patterson function of crystalline sodium deoxyribonucleate. Sections in $a - b$ plane at (i) $c = 0$, (ii) $c = \frac{1}{4}$

was calculated. This will be published and discussed in detail elsewhere. The $a - b$ sections at heights $c = 0$ and $c = \frac{1}{2}$ are shown in Fig. 3. The very strong peak at $a = b = 0$, $c = \frac{1}{4}$ suggests a pseudo-halving of the unit cell. On the other hand, all features of the zero section other than the origin peak are almost entirely reversed in the section $c = \frac{1}{2}$. This at once suggests that only a part of the structure repeats at $c = \frac{1}{2}$. This is exactly what would occur for two co-axial chains related by a diad axis, as suggested by Watson and Crick. The phosphate groups repeat at $c = \frac{1}{2}$, as indicated in Fig. 1; but, since the two chains run in opposite directions, this will not be true of the rest of the molecule.

Relationship between structure A and structure B. In conclusion, we suggest that the unit in structure A is, as in structure B, two co-axial helical chains running in opposite directions. In the change from B to A the number of residues per turn increases from ten to eleven and the pitch of the helix decreases from 34 A. to 28 A. In structure A the phosphate groups lie on a helix of radius 9 A., with a separation of approximately $\frac{1}{2}c$ between the phosphate groups of the two co-axial chains.

The vertical component of the inter-base distance is thus decreased from $3 \cdot 4$ A. in structure B to $2 \cdot 55$ A. in structure A. This indicates that in structure A the planes of the bases cannot be perpendicular to the fibre axis. The positions of the strong reflexions on the sixth, seventh and eighth layer-lines suggest that the angle of tilt is about $25°$.

We are grateful to Prof. J. T. Randall for his interest and encouragement. One of us (R. E. F.) acknowledges the award of a Turner and Newall Fellowship.   [June 25.

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