STRUCTURE OF POLYGLYCINE II

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VERY recently Bamford and his colleagues[1] have described their work on a second form of polyglycine, which they call polyglycine II. The purpose of this communication is to suggest a structure for this substance.

Bamford *et al.*[1] have shown clearly that polyglycine can give two types of X-ray diagram according to the method of precipitation. Polyglycine I gives strong reflexions at 4·4 A. and 3·45 A., and is thus some kind of β-structure; that is, the polypeptide chains are almost but not quite fully extended, and hydrogen bonds are formed between neighbouring chains (in approximately the same plane) to form sheets of parallel or anti-parallel chains. Polyglycine II, on the other hand, gives a very strong reflexion at 4·15 A., and a moderately strong one at 3·1 A. Only a powder diagram has so far been obtained. Bamford *et al.*[1] have shown that the X-ray picture cannot be easily explained in terms of any well-known configuration of the polypeptide chain.

The structure we propose is simple. All the polypeptide chains are parallel and each one has a threefold screw axis. The chains are packed in a hexagonal array, each chain being hydrogen-bonded to each of its six neighbours. These hydrogen bonds lie roughly perpendicular to the screw axis, and, as implied above, run in several directions and not merely in one direction as in a β-structure. This can be seen in Fig. 1, which is a projection of the structure looking down the screw axis.

Another view of the structure is shown in Fig. 2. This is a projection along the x-axis and perpendicular to the screw axis (the z-axis), which runs vertically. The easiest way to visualize the structure is to look at one of the residues at the bottom of the figure. This shows that the planar peptide group is inclined at about 35° to the fibre axis, and has its plane perpendicular to that of the paper. There is thus an infinite sequence of hydrogen bonds running from one cell to the next, perpendicular to the paper and joining residues of adjacent chains. It follows that the atoms of these residues all lie on an inclined lathe. There is another set of such lathes at a level 3·1 A. higher in the structure, but due to the 120° rotation of the screw axis these lathes run at an angle to the paper. At 3·1 A. higher again there is a third set of lathes, again at an angle to the paper. Above that the structure is repeated.

The formal crystallographic description of the structure is: $a = 4{\cdot}8$ A., $c = 9{\cdot}3$ A., space group PS_1, one residue per asymmetric unit. The calculated density is 1·54 gm./c.c.; observed density[1], 1·43 gm./c.c. (It is often found for this type of material that the calculated density is 5–10 per cent higher than the observed.) The co-ordinates of the atoms

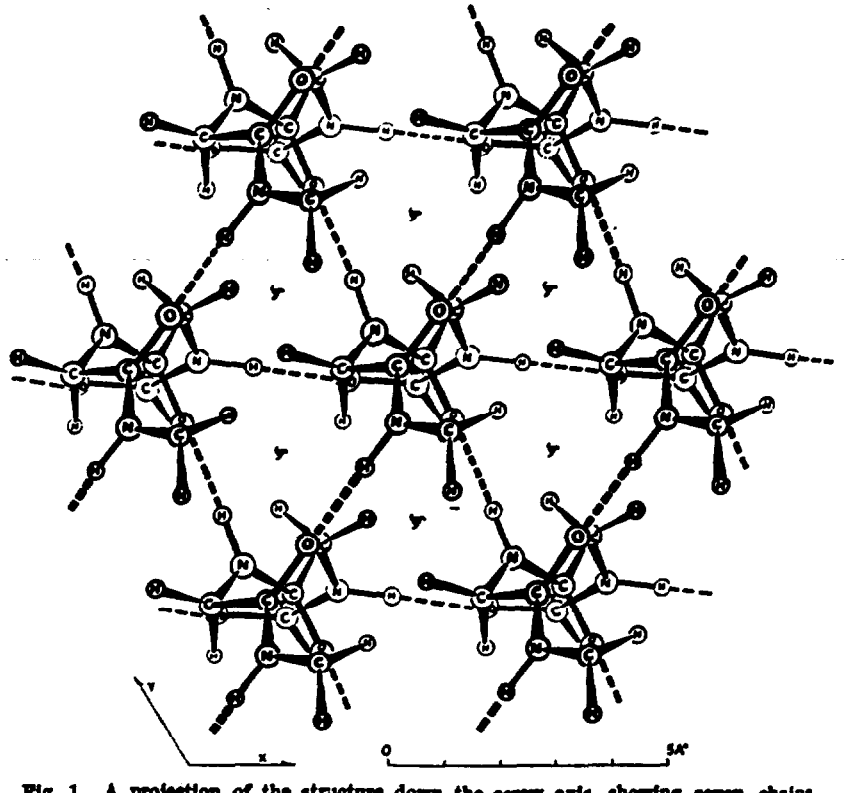

Fig. 1. A projection of the structure down the screw axis, showing seven chains. Hydrogen bonds, drawn as dashed lines, run in a number of directions linking neighbouring chains together

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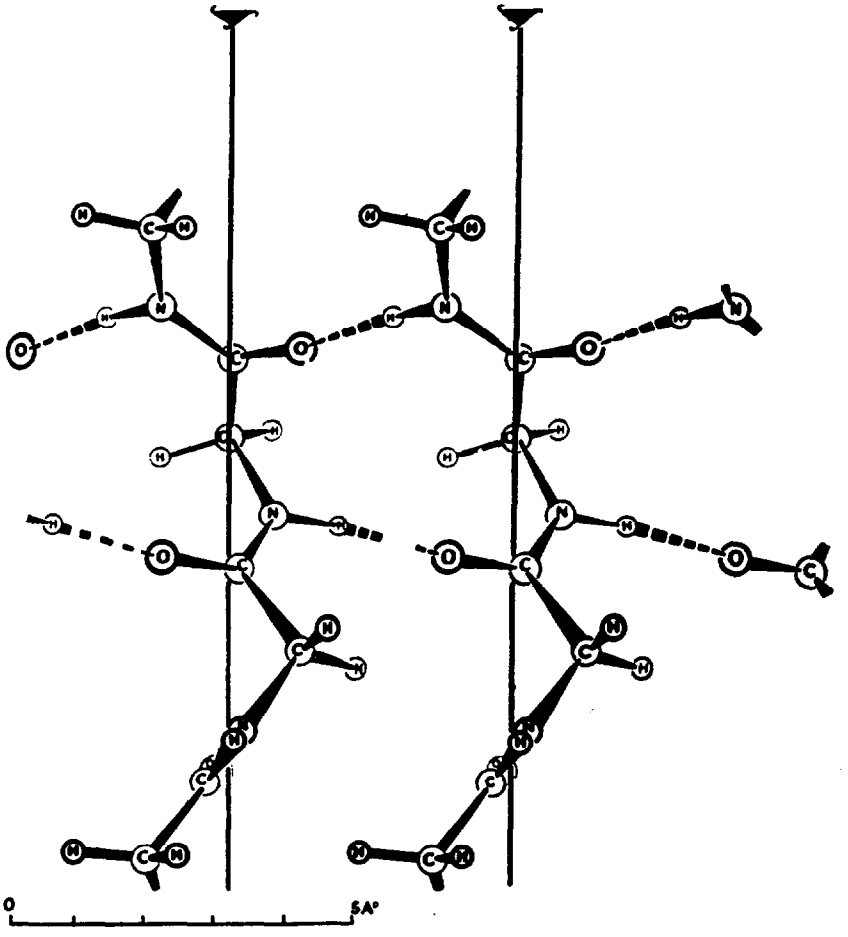

Fig. 2. A projection of the structure with the screw axis vertical. One *x*-axis points towards the reader; the chain on the right has been drawn as nearer to the reader than the chain on the left (see Fig. 1). Note the planar peptide groups edge-on at the bottom of the figure. The hydrogen bonds from these groups are almost perpendicular to the paper

of one asymmetric unit (excepting hydrogen atoms) are given in Table 1, to the nearest 0·05 A.

In building the structure we have adopted the standard Pauling–Corey[2] bond-distances and angles. The hydrogen bond-distance (nitrogen to oxygen) is 2·76 A., which is a little short, but quite acceptable[2]. The hydrogen bond is almost straight, as can be seen from the figures. All the van der Waals distances are acceptable, and in fact space-filling models show that the chains pack together in a comfortable manner.

Since there is no asymmetric carbon atom in polyglycine, the mirror image structure (space group $P3_1$) is equally possible.

We have calculated the spacings and intensities expected from this structure for all reflexions out to 1·8 A. Dr. C. H. Bamford and his colleagues have kindly shown us the original of the powder photograph (their Fig. 1). Their X-ray data are in good qualitative agreement with our calculations. The very strong 4·15 A. reflexion is 10$\bar{1}$0. A glance at Fig. 1 shows that this will be intense. The 3·1-A. reflexion has a small contribution from 0003, but is mostly due to 10$\bar{1}$2, spacing 3·09 A. The strength of this reflexion is mainly produced by the inclined planes of the peptide groups which make up the lathes described above.

We thus feel confident that polyglycine II has the structure we have described, or a closely similar structure. It should be realized, however, that there is a family of possible structures of this general type. All these would have in common polypeptide backbones with three-fold screw axes and a repeat of about 9·3 A. There are only two possible ways of achieving this backbone: the one we have described, and an analogous one in which the nitrogen atom is close to the fibre axis. Such chains can have either right-handed screws, or left-handed, and can be combined in various ways, either parallel or anti-parallel. So far as we can see, the structure we have described is the simplest member of the family. Stimulated by a suggestion by Dr. A. Elliott, we have found that it is possible to remove a chain from the structure and then replace it running in the opposite direction. All the hydrogen bonds can be remade and at first glance the modified structure looks very similar to the original, so that its X-ray diffraction pattern will also be similar. Only a very detailed study of the experimental results will enable one to say whether the simple structure is strictly correct, or only a first approximation.

Whatever the outcome of such studies, we feel that the present qualitative agreement with the experimental evidence makes it almost certain that the structure of polyglycine II is of this general type. This enables us to conclude that only polyglycine can form such a lattice—there is no room for side-chains in the lattice unless some of the hydrogen bonds are broken.

We see no special reason why a single polyglycine chain should take up this precise configuration; this is presumably dictated by the interaction between neighbouring chains, which imposes the exact three-fold screw axis. We note with interest that polyproline, the structure of which has recently been reported by Cowan and McGavin[4], and which is unable to form hydrogen bonds, takes up a similar backbone configuration.

As yet it has not been possible to obtain[1] a fibre diagram of polyglycine II. This is probably because any process used to produce orientation will tend to stretch the structure, and it will then pass over to the more extended β-form of polyglycine I.

We should like to thank Dr. Bamford and his colleagues both for showing us their X-ray photographs and for helpful discussion. [Sept. 20

Table 1. Atomic co-ordinates, in a hexagonal frame, in angstrom units

	C_α	O	C	N
x	− 0·05	− 1·25	− 0·1	+ 1·1
y	− 1·3	− 0·15	− 0·3	+ 0·3
z	0·0	+ 1·3	+ 1·15	+ 1·95

[1] Bamford, C. H., Brown, L., Cant, E. M., Elliott, A., Hanby, W. E., and Malcolm, B. R., *Nature*, 176, 396 (1955).
[2] Corey, R. B., and Pauling, L., *Proc. Roy. Soc.*, B, 141, 10 (1953).
[3] Donohue, J., *J. Phys. Chem.*, 56, 502 (1952).
[4] Cowan, P. M., and McGavin, S., Comm. to 3rd Int. Cong. Biochem., 2.64 (1955); *Nature*, 176, 501 (1955).