

the precise ψ position since $\psi = 15^\circ$ was near this large crystallographic peak and hence it represented only a small plateau on the fall-off from this peak. To illustrate this plateau, Fig. 1(a) shows the difference between the fall-off along $\varphi = 21^\circ$ (the final φ value) and an arbitrary direction ($\varphi = 10^\circ$). From this Figure, the ψ value of the local twofold axis was determined to be 17° . Fig. 1(b) shows the φ dependence of the rotation function. There is a narrow peak at 21° and a broad unexplained peak between 25° and 50° . Fig. 1(c) shows the κ dependence of the rotation function. The magnitude of the rotation function for the null rotation ($\kappa = 180^\circ$) is 81. The average background of the function was 67.9 with a standard deviation of 6.8.

It should be emphasized that these calculations were made before any phases were known and were based only on the native X-ray intensities to 7.9 Å resolution. However, knowledge of the spatial relationship between the two subunits has been helpful in interpreting a 3.0 Å resolution electron-density map of s-MDH (Hill, Tsernoglou, Webb & Banaszak, 1972).

After this map was interpreted, a three-dimensional least-squares fit of the α -carbon positions in the two subunits to a twofold symmetry axis (molecular dyad) indicated that the 'best' directions for the rotation function angles are $\kappa = 180^\circ$, $\psi = 17^\circ$, $\varphi = 21^\circ$. The orientation of the molecular dyad obtained from the molecular model is marked by ar-

rows in Fig. 1(a), (b) and (c) to permit comparison with the results from the rotation function. Although the results in φ were made ambiguous by the broad peak, the values for κ and ψ are certainly consistent with these results.

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Crystallographic data for carbobenzoxy-L-alanyl- β -alanine. By A. DEL PRA, *Institute of Organic Chemistry, 35100 Padova, Italy*

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Crystals of carbobenzoxy-L-alanyl- β -alanine have been examined by X-ray methods. They crystallize in the orthorhombic system, space group $P2_12_12_1$, with $a = 17.02$, $b = 15.60$, $c = 5.91$ Å and $Z = 4$.

Carbobenzoxy-L-alanyl- β -alanine, $C_6H_5-CH_2-O-CO-NH-CH(CH_3)-CO-NH-(CH_2)_2-COOH$, is the monomer used for obtaining the sequential polypeptide poly-L-alanyl- β -alanine, which is a good model for the study, both in the solid state and in solution, of the conformational properties of co-polyamides.

The compound was prepared by basic hydrolysis of carbobenzoxy-L-alanyl- β -alanine ethyl ester (Scatturin and co-workers, 1973, in preparation). Single crystals were grown from ethanol solution as colourless prisms, with rectangular cross section, elongated along [001]. The crystal symmetry and unit-cell dimensions were determined from Weissenberg and precession photographs of zero and upper layers. The unit cell chosen proved to be reduced (Buerger, 1957).

The crystal density was measured by flotation in KBr solution. The physical and crystallographic data are reported in Table 1.

No further work is contemplated.

I thank Dr A. Scatturin for the samples of carbobenzoxy-L-alanyl- β -alanine.

Table 1. *Crystallographic data*

M.W.	294
m.p.	132°C
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a	17.02 ± 2 Å
b	15.60 ± 2
c	5.91 ± 1
V	1569.2 Å ³
D_x	1.24 g cm ⁻³
D_m	1.23
Z	4
$F(000)$	624
μ (Mo $K\alpha$)	8.06 cm ⁻¹
μ (Mo $K\alpha$)	1.02

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