Diagrams and tables relating to the structure of B-Poly-L-alanine referenced as 'Dr Dover'

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Publication/Creation

July 1968

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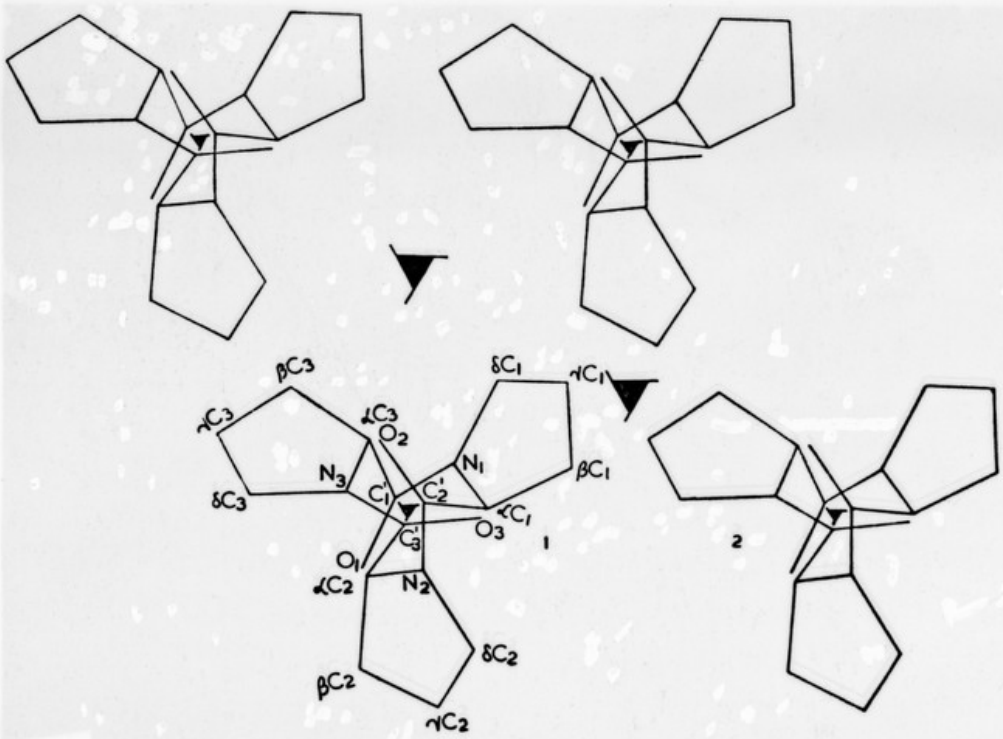

Fig. 2. Projection of the molecular chain on the a, b plane. The position indicated is $\psi = 0°$ from which the chain is rotated through intervals of 5°.

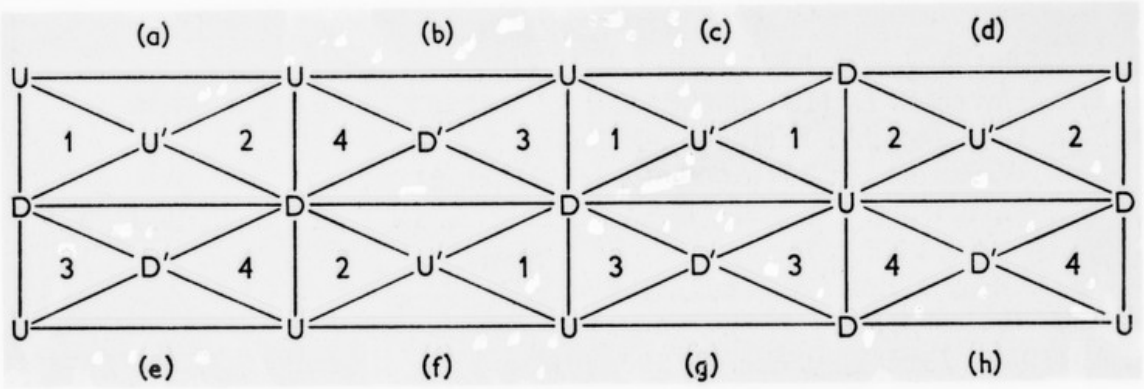

FIG. 3. The eight possible unit cells in the statistical structure of β-poly-L-alanine. U and D are up-pointing and down-pointing chains, respectively. U′ and D′ are similar chains translated ΔZ along the z-axis. Triangles of molecules within which the same intermolecular interactions occur are labelled with the same number.

they were not imposed as a feature of the model, their occurrence is striking testimony to the credibility of the refined model); C . . . C distances of 3·2 Å between

varies as ΔZ varies. If ΔZ were 0·25 Å less, and ω correspondingly changed,

TABLE 2

Values of initial and final parameters in the refinement

	τ_{23}	τ_{34}	τ_{45}	θ_1	θ_2	θ_3
Initial value	−141·0°	−180·0°	−105·0°	15·0°	65·0°	35·0°
Refined value	−134·7°	−181·5°	−101·2°	25·2°	60·0°	49·6°
	u	v	w	ΔZ	K	B
Initial value	−0·25 Å	0·53 Å	1·72 Å	0·00 Å	18·0	3·00 Å^2
Refined value	−0·14 Å	0·79 Å	1·34 Å	0·65 Å	18·7	6·51 Å^2
	R	Φ				
Initial value	0·360	$9{\cdot}5\times10^5$				
Refined value	0·136	$1{\cdot}3\times10^5$				

TABLE 3

Atomic co-ordinates of one peptide unit

TABLE 1

	$\theta_x°$	$\theta_y°$	$\theta_z°$	$\tau_{23}°$	$\tau_{34}°$	$\tau_{45}°$	$\phi_2°$	$\phi_3°$	$\phi_4°$	t(Å)	$\psi°$	K	B(Å^2)
AW	−77·0	36·2	−142·1	50·5	179·0	174·4	109·5	114·0	123·0	4·15	172·7	1·410	2·00
ADW	−79·5	38·1	−142·1	47·5	179·8	177·4	109·7	115·4	120·9	4·17	175·1	1·415	2·23

Initial (AW) and final (ADW) parameters in this refinement (symbols are defined in the text and in Fig. 1 except t, ψ, K, B which are respectively the relative translation and orientation of the antiparallel chains at each molecular site in the statistical crystal structure, and the scale factor and thermal vibration parameter).

(It is of interest that the chain angle at αC, $\phi 2$, has a value very near the theoretical tetrahedral one of 109°28′ This contrasts with the high values (about 112°) found in aliphatical hydrocarbons.)

(b)

FIG. 1. Diagram of poly-L-alanine chain showing (a) conformational parameters and atom numbering system; (b) the stereochemistry of the refined model.

TABLE 2

Cylindrical polar co-ordinates for an alanyl residue in α-poly-L-alanine

	R(Å)	ϕ (degrees)	Z(Å)
αC	2·288	0	0
H (on αC)	3·013	13·54	−0·485
βC	3·294	−17·63	0·808
O	1·906	78·33	−0·761
C′	1·664	72·41	0·441
N	1·548	27·35	0·906
H (on N)	1·539	18·57	1·878

Initial value	−0·26 Å	0·53 Å	1·72 Å	0·90 Å	18·7	3·80 Å²
Refined value	−0·14 Å	0·79 Å	1·34 Å	0·65 Å	18·7	6·51 Å²

	R	Φ
Initial value	0·360	$9{\cdot}5\times10^5$
Refined value	0·136	$1{\cdot}3\times10^5$

TABLE 3

Atomic co-ordinates of one peptide unit

Atom	X (Å)	Y (Å)	Z (Å)
C′	−0·49	−0·13	3·56
O	−1·70	0·13	3·53
N	0·33	0·13	2·56
H (on N)	1·30	−0·10	2·58
αC	−0·14	0·79	1·34
H (on αC)	−1·21	0·70	1·27
βC	0·24	2·28	1·37

The co-ordinates in Å of the second peptide group in the chain are $-X, -Y, Z + 6{\cdot}89/2$. The co-ordinates of the next (antiparallel) chain in the pleated sheet are

$$X + 4{\cdot}73,\ -Y,\ -Z - 2{\cdot}67 + 6{\cdot}89.$$

5. Discussion

(a) *Stereochemistry*

In the statistical crystal the chains in any locality exhibit polarity and eight different unit cells are possible. These are shown in Fig. 3. Only four different kinds of molecular interactions occur between the smallest triangles of molecules, and

were measured photometrically using a Joyce–Loebl recording microdensitometer. Ideal

tudes are given in Table 1, together with estimates of the 6 below threshold $(h + k)$-even reflexions which occur in the region where diffracted intensity was recorded.

TABLE 1

Observed and calculated structure amplitudes for β-poly-L-alanine

h k	$l = 0$		$l = 1$		$l = 2$		$l = 3$	
	F_{obs}	F_{calc}	F_{obs}	F_{calc}	F_{obs}	F_{calc}	F_{obs}	F_{cal}
0 2	113	119	54	47	59	59	—	—
1 1	79	71	61	60	22	22	27	26
1 3	(6)	(15)	24	27	10	8	18	20
0 4	109	106	(9)	(11)	26	29		
2 0	52	49	35	22	21	16		
2 2	(8)	(5)	26	29	(9)	(2)		
1 5	11	13	18	29	(10)	(4)		
2 4	21	31	21	26	29	28		
0 6								
3 1	29	22	15	11				

Round brackets imply below threshold; —, not recorded.

3. The Structure Model and its Parameters

The model we have adopted has protein chains arranged antiparallel and capable of being joined by intramolecular hydrogen bonds (see Fig. 1). There are two peptide units related by a 2-fold screw axis per c-axis repeat. The *anti-parallel* arrangement is the only likely one when this distance is 6·9 Å: reasonably linear

Fig. 3.4 SCHEMATIC REPRESENTATION OF A DNA–DAUNOMYCIN DIFFRACTION PATTERN.

D. DOVER.