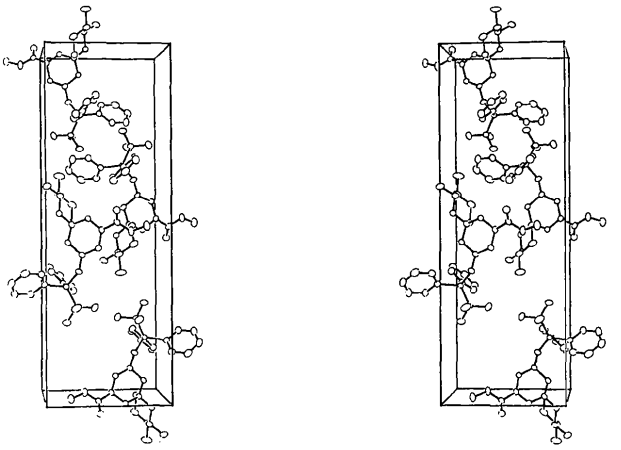

Fig. 2. Stereoscopic view of the unit cell of a milbemycin β_3 intermediate. The *a* axis points from right to left, the *c* axis points downwards, and the *b* axis points into the plane of the paper.

Related literature. This compound, which was prepared from (*S*)-citronellene by Attwood *et al.* (1985), is a key intermediate in the total synthesis of the spiroketal macrocyclic lactone milbemycin β_3. Takiguchi, Mishima, Okuda, Terao, Aoki & Fukuda (1980) have reported the structure of this natural product, and Williams, Barner, Nishitani & Phillips (1982) have established its absolute stereochemistry by synthesis.

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N,N'-Bis(*p*-chlorobenzylidene)-1,3-propanediamine

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Abstract. $C_{17}H_{16}Cl_2N_2$, $M_r = 319{\cdot}23$, monoclinic, $P2_1$, $a = 7{\cdot}371$ (3), $b = 30{\cdot}406$ (19), $c = 7{\cdot}268$ (4) Å, $\beta = 96{\cdot}23$ (4)°, $V = 1619$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}31$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å, $\mu = 3{\cdot}97$ cm^{-1}, $F(000) = 664$, $T = 291$ K, $R = 0{\cdot}067$ for 1205 observed reflections. The two independent molecules in the asymmetric unit are similar and have a *trans* configuration around the imine bonds. In each molecule, the two Cl—C_6H_5—C=N—C moieties are planar (maximum deviation from mean planes <0·05 Å) and perpendicular to each other (in both molecules the angle between the mean planes is 86°).

Experimental. Parallelepipedal crystal, 0·25 × 0·2 × 0·4 mm. Lattice parameters refined using 15 reflections in range $5 < 2\theta < 15°$. Syntex $P2_1$, graphite-monochromatized Mo $K\alpha$ radiation. 2436 $hk\pm l$ independent reflections with $\sin\theta/\lambda < 0{\cdot}561$ Å^{-1}; $0 \le h \le 8$, $0 \le k \le 33$, $-7 \le l \le 7$, 1205 with $I \ge 2{\cdot}5\sigma(I)$. Standard reflection (131) checked every 50 reflections: no significant deviation. Structure solved by *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Least-squares refinement with *SHELX*76 (Sheldrick, 1976), *F* magnitudes; isotropic then anisotropic temperature factors gave $R = 0{\cdot}067$, $wR = 0{\cdot}062$ including H atoms at calculated positions. $w = 1/(\sigma^2 + 0{\cdot}00039F^2)$. Final max. shift to e.s.d. = 0·38. $S = 1{\cdot}85$. Max. and min. heights in final difference Fourier synthesis = 0·28 and −0·32 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). The atomic parameters are given in Table 1,* mean values of selected bond lengths and angles in Table 2. Fig. 1 is a view of one of the two independent molecules (*A*), showing the numbering of the atoms; Fig. 2 shows the packing in the unit cell (program *PLUTO*; Motherwell & Clegg, 1978).

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and a full list of bond lengths and angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42637 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/86/030383-02$01.50

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* ($Å^2$)

$$B_{eq} = \tfrac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	Molecule *A*				Molecule *B*			
	x	*y*	*z*	B_{eq}	*x*	*y*	*z*	B_{eq}
Cl(1)	11601 (8)	6231	18 (8)	6·96	12474 (7)	−2803 (2)	−3988 (7)	6·35
Cl(2)	2144 (7)	2109 (2)	7921 (7)	6·15	4541 (7)	1371 (3)	5060 (7)	6·46
C(0)	10447 (26)	4268 (7)	9039 (29)	6·32	3531 (29)	−838 (8)	−3063 (29)	6·17
C(1)	8925 (30)	4603 (8)	8212 (34)	6·61	4289 (35)	−1158 (8)	−1601 (32)	5·75
N(2)	9568 (21)	4804 (7)	6591 (23)	5·19	5938 (26)	−1353 (6)	−2124 (23)	5·65
C(3)	9544 (27)	5213 (9)	6443 (29)	5·26	6017 (29)	−1763 (8)	−2093 (23)	4·19
C(4)	10038 (23)	5467 (8)	4918 (31)	3·87	7579 (35)	−2001 (8)	−2620 (25)	5·25
C(5)	10545 (26)	5253 (7)	3351 (32)	5·16	7499 (29)	−2462 (8)	−2514 (24)	5·21
C(6)	11042 (30)	5478 (8)	1848 (33)	5·80	9069 (35)	−2711 (7)	−2946 (22)	5·69
C(7)	11063 (23)	5943 (8)	1937 (31)	5·13	10608 (28)	−2499 (6)	−3519 (23)	4·13
C(8)	10527 (26)	6159 (8)	3485 (32)	5·86	10665 (25)	−2045 (8)	−3556 (25)	5·24
C(9)	10171 (27)	5908 (7)	4938 (33)	5·22	9209 (26)	−1801 (7)	−3109 (24)	4·32
C(1′)	10607 (27)	3869 (7)	7909 (28)	5·02	4788 (26)	−438 (7)	−3291 (26)	5·29
N(2′)	8843 (23)	3620 (7)	7598 (23)	5·68	4936 (22)	−179 (6)	−1580 (22)	5·22
C(3′)	8824 (36)	3219 (8)	8298 (30)	5·70	4374 (29)	205 (8)	−1505 (31)	5·12
C(4′)	7134 (34)	2960 (8)	8108 (28)	5·05	4366 (22)	487 (7)	58 (28)	3·53
C(5′)	5519 (29)	3118 (7)	7321 (26)	4·17	3641 (26)	915 (7)	−22 (29)	4·68
C(6′)	4027 (28)	2865 (7)	7240 (26)	5·00	3639 (26)	1187 (8)	1382 (29)	4·71
C(7′)	4121 (25)	2437 (7)	7976 (23)	3·86	4435 (24)	1045 (7)	3052 (32)	4·31
C(8′)	5810 (26)	2287 (7)	8743 (22)	3·36	5241 (27)	641 (8)	3417 (30)	4·84
C(9′)	7256 (27)	2530 (7)	8785 (24)	4·35	5231 (28)	354 (7)	1814 (35)	6·07

Table 2. *Mean values of bond lengths* (Å) *and angles* (°)

C(7)–Cl(1)	1·72 (1)	C(1′)–C(0)–C(1)	114 (1)
C(7′)–Cl(2)	1·76 (1)	N(2)–C(1)–C(0)	108 (1)
C(1)–C(0)	1·54 (2)	C(3)–N(2)–C(1)	118 (1)
C(1′)–C(0)	1·51 (2)	C(4)–C(3)–N(2)	125 (2)
N(2)–C(1)	1·44 (2)	N(2′)–C(1′)–C(0)	111 (1)
C(3)–N(2)	1·25 (2)	C(3′)–N(2′)–C(1′)	120 (1)
C(4)–C(3)	1·44 (2)	C(4′)–C(3′)–N(2′)	125 (2)
N(2′)–C(1′)	1·48 (2)	C(6)–C(7)–Cl(1)	119 (1)
C(3′)–N(2′)	1·28 (2)	C(8)–C(7)–Cl(1)	121 (1)
C(4′)–C(3′)	1·44 (2)	C(6′)–C(7′)–Cl(2)	122 (1)
		C(8′)–C(7′)–Cl(2)	117 (1)

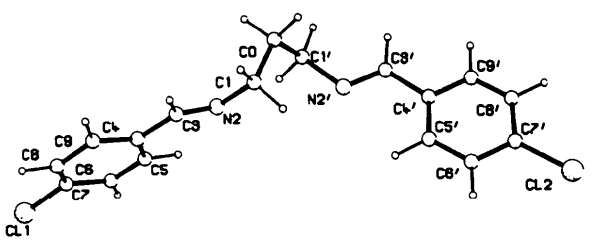

Fig. 1. View of molecule *A* and atom numbering.

Fig. 2. Packing of the unit cell.

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