cycle $(\Delta/\sigma)_{max} = 0.033$. Final difference synthesis $(\Delta\rho)_{max} = 0.26$, $(\Delta\rho)_{min} = -0.25$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1* gives the atom parameters. Fig. 1 shows the molecular structure and the atomic numbering scheme drawn by *ORTEP*II (Johnson, 1976).

Related literature. The compound was synthesized according to Altman, Gorecki, Wilchek, Votano & Rich (1983). Votano, Altman, Wilchek, Gorecki & Rich (1984) have described the effect of this compound on erythrocytes containing deoxyhemoglobin S.

We thank Professor G. A. Petsko for his useful discussion. One of us (SKB) was supported by a Natural Sciences and Engineering Research Council of Canada postdoctoral fellowship.

* Lists of structure-factor amplitudes, anisotropic thermal parameters, bond lengths and bond angles, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43676 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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The Structure of an Antisickling Agent, L-Phenylalanine Benzyl Ester Monochloride

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Abstract. L-Phenylalanine benzyl ester monochloride, $C_{16}H_{18}NO_2^+.Cl^-$, $M_r = 291.8$, orthorhombic, $P2_12_12_1$, $a = 5.221$ (1), $b = 8.674$ (1), $c = 33.880$ (3) Å, $V = 1534.7$ (1) Å^3, $Z = 4$, $D_x = 1.262$ g cm^{-3} λ(Cu $K\alpha$) $= 1.5418$ Å, $\mu = 20.8$ cm^{-1}, $F(000) = 616$, $T = 283$ K, $R = 0.052$ for 1247 unique observed reflections. The molecule adopts a compact and amphipathic conformation. Peptide torsion angles: L-Phe: $\psi_{T'} = 37.5$ (4), Cα(L-Phe)–C(L-Phe)–O(benzyl)–C(benzyl) $= -176.5$ (5), $\chi^1 = -171.4$ (6), $\chi^{2,1} = 65.9$ (8)°; benzyl: C(L-Phe)–O(benzyl)–C(benzyl)–C(1)(benzyl) $= -153.2$ (7), O(benzyl)–C(benzyl)–C(1)(benzyl)–C(2)(benzyl) $= -47.5$ (8)°. Intramolecular edge-to-face interaction between phenyl rings: phenyl(L-Phe)–phenyl(benzyl) centroid separation = 5.07 (1) Å and dihedral angle = 79.7 (8)°. Intermolecular hydrogen bonds: N(L-Phe)–H···O(L-Phe′) = 2.839 (6), N(L-Phe)–H···Cl = 3.252 (4) and N(L-Phe)–H···Cl′ = 3.080 (4) Å. Intermolecular edge-to-face interaction between phenyl rings: phenyl(L-Phe)–phenyl(benzyl′) $d = 5.00$ (1) Å and dihedral angle = 79.7 (8)°.

Experimental. Rectangular crystal by evaporation from aqueous solution at neutral pH, 0.1 × 0.2 × 0.6 mm, Nicolet *P*3 diffractometer, Ni-filtered radiation, ω-scan method, $(\sin\theta)/\lambda < 0.58$ Å^{-1}, lattice parameters from the 2θ values of 15 reflections with $40.40 < 2\theta < 49.54°$, no absorption correction, $h = 0$ to 10, $k = 0$ to 10, $l = 0$ to 40, reflections 0,0,16, 020 and 400 as intensity standards, intensity variation < 2%. 1550 unique reflections measured, 303 excluded during refinement [$F < 2\sigma(F)$], chloride counterion position from Patterson function, other non-H atoms from Fourier syntheses based on phases defined by chloride counterion; least-squares refinement using *SHELX*76 (Sheldrick, 1976), *F* magnitudes, unit weights; isotropic and then anisotropic temperature factors gave $R = 0.052$ and $S = 0.86$ with H atoms at positions

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Table 1. *Atomic coordinates and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

$U_{eq} = \frac{1}{3}(U_{11}+U_{22}+U_{33})$.

	x	y	z	U_{eq}(Å^2)
Cl	0·1026 (3)	0·08943 (17)	0·22891 (4)	0·064
C(*F*1)	0·3025 (11)	0·5730 (6)	0·18898 (14)	0·052
O(*F*1)	0·4372 (9)	0·4764 (5)	0·20322 (11)	0·077
N(*F*1)	0·3801 (8)	0·7572 (5)	0·24128 (10)	0·050
C*A*(*F*1)	0·3205 (10)	0·7447 (6)	0·19843 (13)	0·045
C*B*(*F*1)	0·5285 (10)	0·8228 (7)	0·17436 (15)	0·057
C*G*(*F*1)	0·4606 (11)	0·8350 (7)	0·13148 (15)	0·056
C*D*1(*F*1)	0·2567 (12)	0·9277 (8)	0·11964 (17)	0·073
C*E*1(*F*1)	0·1942 (15)	0·9390 (10)	0·0800 (2)	0·095
C*Z*(*F*1)	0·3277 (18)	0·8547 (10)	0·0523 (2)	0·098
C*E*2(*F*1)	0·5305 (18)	0·7649 (10)	0·0634 (2)	0·101
C*D*2(*F*1)	0·5960 (14)	0·7541 (8)	0·10338 (18)	0·077
O(*B*2)	0·1209 (9)	0·5458 (4)	0·16247 (10)	0·063
C(*B*2)	0·0792 (18)	0·3818 (6)	0·15331 (18)	0·096
C1(*B*2)	−0·0244 (12)	0·3710 (7)	0·11260 (17)	0·063
C2(*B*2)	0·0825 (14)	0·4492 (8)	0·08153 (17)	0·081
C3(*B*2)	−0·0038 (15)	0·4315 (10)	0·0434 (2)	0·096
C4(*B*2)	−0·2071 (17)	0·3372 (10)	0·0365 (2)	0·101
C5(*B*2)	−0·3203 (16)	0·2576 (10)	0·0664 (3)	0·105
C6(*B*2)	−0·2342 (14)	0·2739 (8)	0·1055 (2)	0·086

calculated or located by difference synthesis. 183 parameters varied: x,y,z,U_{ij} for non-H atoms. A single U for all backbone H atoms, and a single U for all phenyl-ring H atoms. x,y,z for three amino terminal H atoms located by difference synthesis. In final cycle $(\Delta/\sigma)_{max} = 0{\cdot}107$. Final difference synthesis $(\Delta\rho)_{max} = 0{\cdot}21$, $(\Delta\rho)_{min} = -0{\cdot}27$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1* gives the atom parameters. Fig. 1 shows the molecular structure and the atom-numbering scheme drawn by *ORTEP*II (Johnson, 1976).

Related literature. The compound was synthesized according to Gorecki, Acquaye, Wilchek, Votano & Rich (1980). Related structures were reported by Burley & Wang (1987*a*,*b*) and Fujii, Burley & Wang (1987). A mechanism of antisickling action was proposed by Burley, Wang, Votano & Rich (1986). The intra- and intermolecular edge-to-face interactions between phenyl rings are enthalpically favorable (Burley & Petsko, 1986).

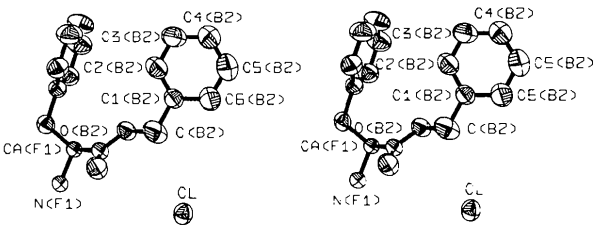

Fig. 1. Stereodrawing of the molecular structure showing the numbering scheme. The thermal ellipsoids are drawn at the 50% level.

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