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1-Benzoyl-6-ethyl-5-(phenylsulfonyl)perhydropyrrolo[3,4-*b*]pyrrole

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.127
Data-to-parameter ratio = 31.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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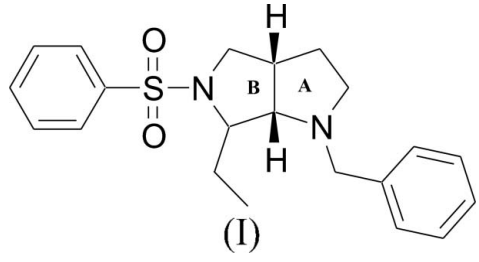
In the title compound, $C_{21}H_{26}N_2O_2S$, one of the pyrrolidine rings adopts a twist conformation, while the other is in an envelope conformation. Weak C—H···O interactions stabilize the crystal structure.

Comment

Pyrrole derivatives have *in vitro* activity against mycobacteria and candidae (Biava *et al.*, 2005). Some of these derivatives are used as platelet-activating factor (PAF) antagonists (Le Naour *et al.*, 1994). These derivatives inhibit cytokine-dependent induction of human immunodeficiency virus (HIV) expression in chronically infected promonocytic cells (Weissman *et al.*, 1993). Pyrroles possess anti-inflammatory (Fernandes *et al.*, 2004), antiviral (Borthwick *et al.*, 2003), antifungal and antimicrobial activities (Amal Raj *et al.*, 2003). In view of this importance, an X-ray crystallographic analysis of the title compound, (I), was carried out and the results are presented here.



(I)

Bond lengths and angles in (I) (Fig. 1) are comparable with those observed in a similar structure, 1-(3-nitrophenyl)-5-tosylperhydropyrrolo[3,4-*b*]pyrrole (Gayathri *et al.*, 2006). The sums of the bond angles around N1 (331.4°) and N2 (350.9°) indicate that N1 is sp^3-hybridized and N2 is sp^2-hybridized. The N1/C2–C4/C7 pyrrolidine ring adopts a twist conformation, with an asymmetry parameter (Nardelli, 1983) ΔC_2(C3) of 3.1 (2)°, and puckering parameters (Cremer & Pople, 1975) q_2 and φ of 0.412 (2) Å and 163.3 (3)°, respectively. The other pyrrolidine ring (N2/C4–C7) is in an envelope conformation, with ΔC_s(C4), q_2 and φ values of 3.8 (2)°, 0.356 (2) Å and 248.3 (2)°, respectively. The deviation of atom C4 from the mean plane defined by atoms N2, C5, C6 and C7 is 0.520 (1) Å. The dihedral angle between the C9–C14 and C15–C20 phenyl rings is 66.84 (9)°.

A weak C—H···O interaction is observed in the molecular structure. In the crystal structure, the molecules are linked into a three-dimensional framework by C—H···O intermolecular interactions (Table 1).

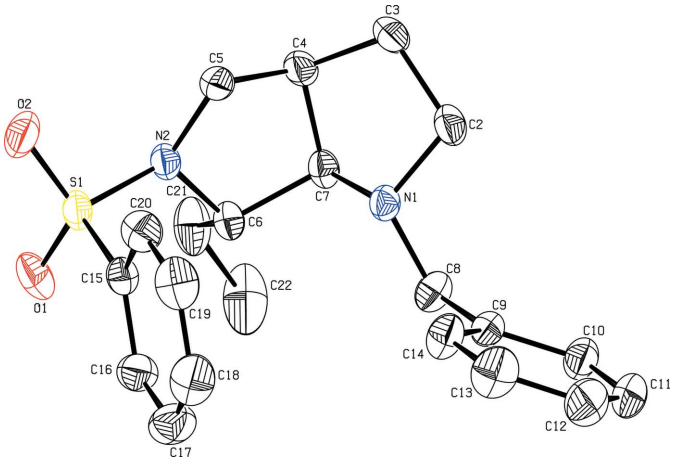


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted.

Experimental

A mixture of 2-(*N*-allyl-*N*-tosylamino)butanal (1 mmol) and *N*-benzylglycine (1 mmol) in toluene (20 ml) was refluxed until the disappearance of the starting materials, as evidenced by thin-layer chromatography. The solvent was evaporated under vacuum and the residue was then column-chromotographed with a hexane–ethyl acetate mixture (8:2 *v*/*v*) to obtain the title compound, which was ecrystallized from ethyl acetate.

Crystal data

$C_{21}H_{26}N_2O_2S$
M_r = 370.50
Orthorhombic, $P2_12_12_1$
a = 8.1022 (2) Å
b = 9.9925 (2) Å
c = 24.8288 (5) Å
V = 2010.17 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa-APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*: Sheldrick, 1996)
T_{min} = 0.803, T_{max} = 0.883
(expected range = 0.878–0.965)
39402 measured reflections
7377 independent reflections
5770 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.127
S = 1.05
7377 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Absolute structure: Flack (1983), with 3223 Friedel pairs
Flack parameter: 0.52 (6)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5B···O1^{i}	0.97	2.48	3.190 (2)	130
C11—H11···O2^{ii}	0.93	2.57	3.472 (2)	164
C21—H21A···O1	0.97	2.53	3.160 (3)	123

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, -y+1, z-\frac{1}{2}$.

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C). The value of the Flack parameter indicates inversion twinning.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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