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cis-1-(4-Bromophenyl)-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) = 0.004 Å
R factor = 0.035
wR factor = 0.088
Data-to-parameter ratio = 18.8

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

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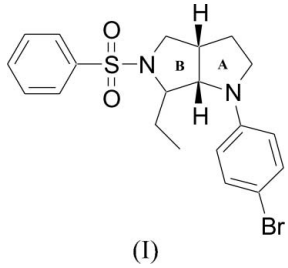
In the title compound, $C_{20}H_{23}BrN_2O_2S$, both pyrrolidine rings adopt twist conformations. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds and π–π interactions.

Comment

Pyrrolopyrrole compounds exhibit anti-inflammatory and analgesic activities (Rooks *et al.*, 1982; Muchowski *et al.*, 1989). Inhibitors of human cytomegalovirus (HCMV) protease have been designed based on the 5-oxo-hexahydropyrrolo[3,2-*b*]pyrrole ring system (Borthwick *et al.*, 2000). It has been shown that *N*-substituted pyrrole derivatives inhibit human immunodeficiency virus type-1 (HIV-I) (Jiang *et al.*, 2004). These derivatives also possess antileukemic activity (Anderson & Mach, 1987) and some of them are used as platelet activating factor (PAF) antagonists (Weissman *et al.*, 1993; Le Naour *et al.*, 1994). In view of this biological importance, the crystal structure of the title compound, (I), has been determined and the results are presented here.



(I)

Bond lengths and angles in (I) (Fig. 1) agree with those observed in a similar structure, *cis*-1-(4-bromophenyl)-6-ethyl-5-tosylperhydropyrrolo[3,4-*b*]pyrrole (Chinnakali *et al.*, 2007). The sums of the bond angles around atoms N1 (357.3°) and N2 (352.1°) indicate sp^2-hybridization. Atom S1 has a distorted tetrahedral geometry, with angles O1—S1—O2 [120.06 (14)°] and N2—S1—O2 [106.52 (13)°] deviating significantly from the ideal value, as a result of the Thorpe–Ingold effect (Bassindale, 1984).

Both pyrrolidine rings A (N1/C2–C4/C7) and B (N2/C4–C7) adopt twist conformations. The puckering parameters (Cremer & Pople, 1975) and the asymmetry parameters (Nardelli, 1983) are q_2 = 0.320 (3) Å and φ = 87.2 (5)° and ΔC_2(N1) = 3.1 (3)° for ring A, and q_2 = 0.281 (3) Å, φ = 302.4 (5)° and ΔC_2(C5) = 1.7 (3)° for ring B. The two aromatic rings are almost parallel to one another with a dihedral angle of 4.9 (2)°.

In the crystal structure, C—H···O intermolecular hydrogen bonds link the molecules into a three-dimensional framework

(Table 1). In addition, a π–π interaction involving the C8–C13 ring of the molecule at (x, y, z) and the C14–C19 ring of the molecule at $(-1+x, y, z)$ is observed, with a centroid–centroid distance of 3.632 (2) Å.

Experimental

A mixture of 2-(*N*-allyl-*N*-tosylamino)butanal (1 mmol) and 2-(*p*-bromo)phenylthiazolidine-4-carboxylic acid (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-chromatographed with a hexane–ethyl acetate mixture (8:2) to obtain the title compound.

Crystal data

$C_{20}H_{23}BrN_2O_2S$
M_r = 435.37
Orthorhombic, $Pna2_1$
a = 7.9894 (2) Å
b = 18.8355 (5) Å
c = 12.9451 (4) Å
V = 1948.03 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.23 mm^{-1}
T = 293 (2) K
0.25 × 0.17 × 0.15 mm

Data collection

Bruker Kappa APEX2 area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.640, T_{max} = 0.715
16756 measured reflections
4421 independent reflections
3229 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.088
S = 1.02
4421 reflections
235 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), 2097 Friedel pairs
Flack parameter: 0.003 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1^{i}	0.93	2.53	3.433 (4)	164
C20—H20A···O2^{ii}	0.97	2.57	3.453 (4)	151

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

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).

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).

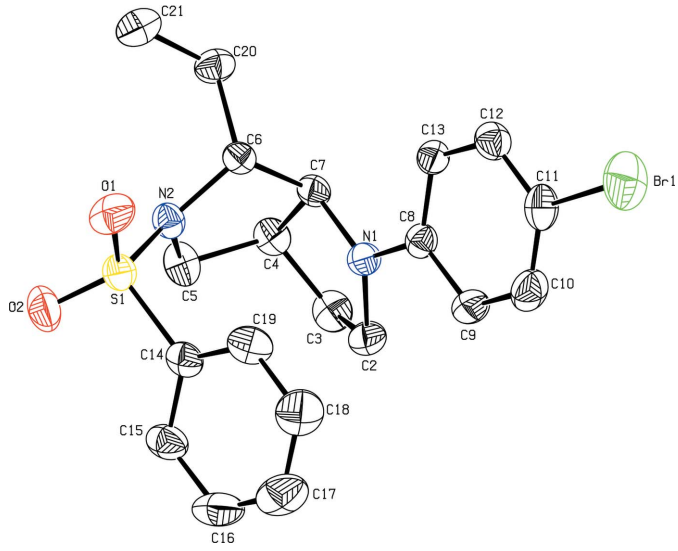


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted.

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