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(3a*R*,6*S*,6a*R*)-6-Benzyl-1-(4-bromophenyl)-5-tosyl-*cis*-perhydropyrrolo[3,4-*b*]pyrrole

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The title compound, $C_{26}H_{27}BrN_2O_2S$, has two fused pyrrolidine rings, each in a twist conformation.

Key indicators

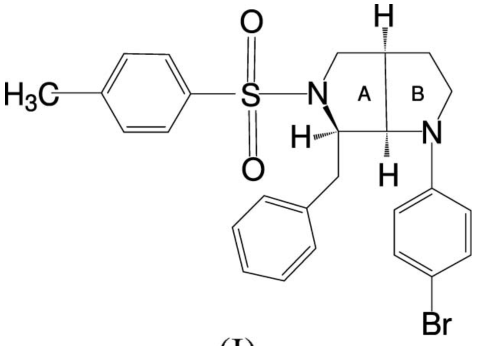
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.048
wR factor = 0.153
Data-to-parameter ratio = 19.0

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

Comment

In recent years, polyhydroxylated piperidine, pyrrolidine, indolizidine and pyrrolizidine alkaloids have attracted much attention, owing to their ability to act as selective glycosidase inhibitors. Such inhibition may be useful for the treatment of diabetes, cancer, malaria and some viral infections including AIDS (Kilonda *et al.*, 1995). Pyrrolidine compounds are capable of exhibiting antimicrobial and antifungal activity (Amal Raj *et al.*, 2003).

The title compound, (I), has two fused pyrrolidine rings, each in a twist conformation. The puckering parameters (Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Nardelli, 1983) for the pyrrolidine ring A (N1/C1–C4) are $q2$ = 0.286 (4) Å, φ = −85.4 (8)°, ΔC_2(N1) = 3.4 (5), and for the pyrrolidine ring B (N2/C3/C2/C5/C6) are $q2$ = 0.345 (4) Å, φ = 84.0 (6)°, ΔC_2(N2) = 5.2 (6). The geometric parameter are in the normal ranges (Allen *et al.*, 1987). The sums of the bond angles around atoms N1 and N2 of the pyrrolidine rings (349.1 and 356.1°, respectively) indicate that N1 and N2 have almost trigonal planar coordination. The dihedral angle between the bromophenyl and phenyl rings is 79.1 (1)°.



(I)

Experimental

A mixture of (*S*)-2-(*N*-allyl-*N*-tosylamino)-3-phenylpropanal (1 mmol) and *N*-(*p*-bromophenyl)glycine (1 mmol) in 20 ml of toluene was refluxed under Dean–Stark conditions, until the disappearance of the starting materials, as evidenced by thin-layer chromatography. The solvent was then evaporated in vacuum and the residue was column chromatographed using a hexane–ethyl acetate

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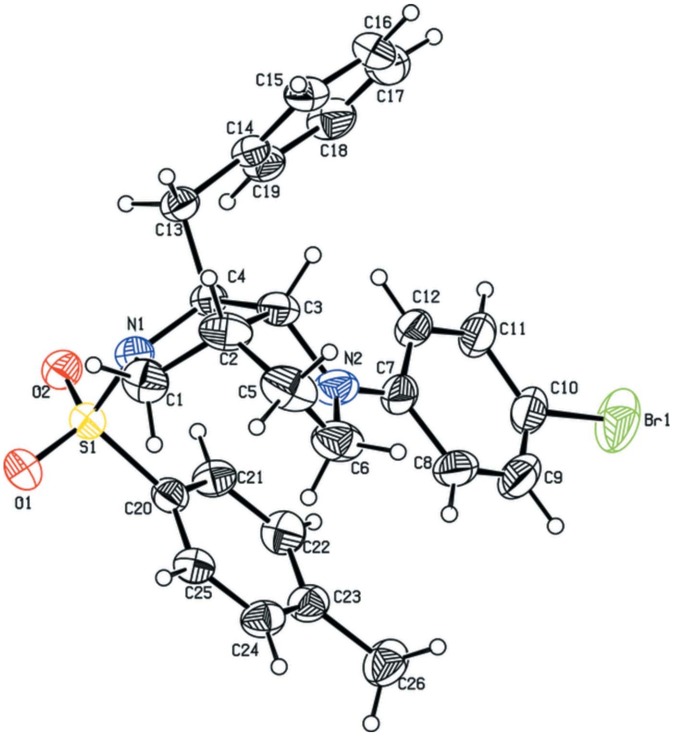

Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

mixture (8:2) to obtain the title compound. The title compound was crystallized from an ethyl acetate solution by slow evaporation.

Crystal data

$C_{26}H_{27}BrN_2O_2S$
$M_r = 511.47$
Orthorhombic, $P2_12_12_1$
$a = 20.9376\ (11)$ Å
$b = 10.5821\ (6)$ Å
$c = 11.0154\ (6)$ Å
$V = 2440.6\ (2)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.80$ mm^{-1}
$T = 293\ (2)$ K
0.24 × 0.23 × 0.21 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
20524 measured reflections
5499 independent reflections
3825 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.153$
$S = 1.07$
5499 reflections
289 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.80$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.67$ e Å^{-3}
Absolute structure: Flack (1983), 2297 Friedel pairs
Flack parameter: 0.031 (13)

Table 1
Selected bond angles (°).

C7—N2—C6	122.0 (4)	C4—N1—C1	111.9 (3)
C7—N2—C3	123.7 (3)	C4—N1—S1	118.7 (2)
C6—N2—C3	111.3 (4)	C1—N1—S1	119.5 (2)

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with aromatic C—H distances of 0.93 Å, methyl C—H distances of 0.96 Å and methylene C—H distances of 0.97 Å, and with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$ for methyl H and $1.2U_{\rm eq}({\rm C})$ for other H.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

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