Acta Crystallographica Section E
**Structure Reports
Online**

ISSN 1600-5368

3-(4-Bromophenyl)-6-(*p*-tosyl)perhydrothiazolidino[3,4-*a*]pyrrolo[4,5-*c*]pyrrole

Venugopal Kavitha,[a] Dasara Raju Gayathri,[b] Devadasan Velmurugan,[b]* Krishnan Ravikumar[c] and Mahalingam Poornachandran[d]

[a]Bioinformatics Research Institute, Ashok Nagar, Chennai 600 083, India, [b]Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, [c]Laboratory of X-ray Crystallography, Indian Institute of Chemical Technology, Hyderabad 500 007, India, and [d]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India

Correspondence e-mail: d_velu@yahoo.com

Received 10 April 2006
Accepted 26 April 2006

Key indicators

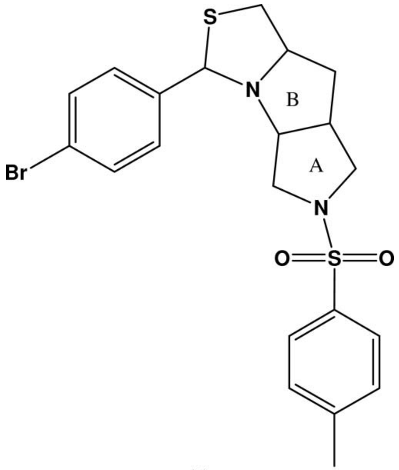
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.126
Data-to-parameter ratio = 19.5

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

In the title compound, $C_{21}H_{23}BrN_2O_2S_2$, the two pyrrolidine rings adopt envelope conformations and the thiazolidine ring adopts a twisted conformation with a pseudo-twofold axis passing through the S atom and the C—N ring-fusion bond. The crystal packing is stabilized by a C—H···π interaction between inversion-related molecules.

Comment

Pyrrole occurs widely in nature and is a structural part of porphyrin heme, chlorophyll and vitamin B12. It has been shown that *N*-substituted pyrrole derivatives inhibit human immunodeficiency virus type-I (HIV-I) (Jiang *et al.*, 2004). Thiazolidine and its derivatives have diverse biological importance, such as local anesthetic, antiseizure, antitubercular, antibacterial, anti-amebic, antidiabetic, anti-inflammatory (Chaurasia, 1971; Zimenkovsky *et al.*, 1999), anti-oxidant (Rachinskii, 1964) and flavor-enhancing properties, and the presence of N—C—S in the ring enhances the antifungal activity (Eswaramoorthy *et al.*, 1991).



(I)

In the title compound, (I), the S1—C8 bond length is long compared with S1—C7, while the N2—C8 bond is short compared with N2—C6 and N2—C3 (Table 1). These long and short bonds may be due to the bromophenyl substitution at C8. The sums of the bond angles around N1 (343.4°) and N2 (333.3°) indicate sp^3-hybridization. Atom Br1 deviates by 0.185 (1) Å from the mean plane of the benzene ring C9–C14. The two fused pyrrolidine rings (N1/C1–C4, *A*, and C2/C3/N2/C5/C6, *B*) adopt envelope conformations; atom N1 in ring *A* lies 0.609 (2) Å above the C1–C4 mean plane and atom C6 in ring *B* lies 0.562 (3) Å below the N2/C3/C2/C5 mean plane.

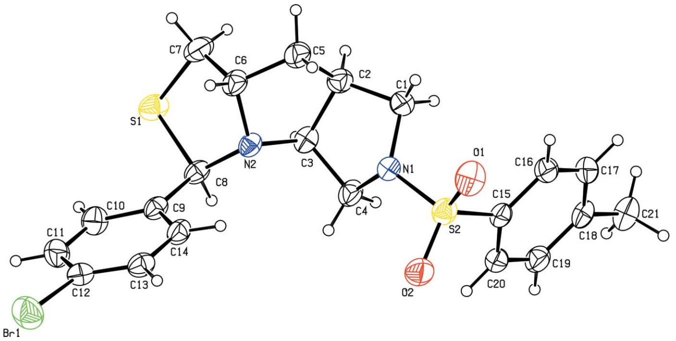


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

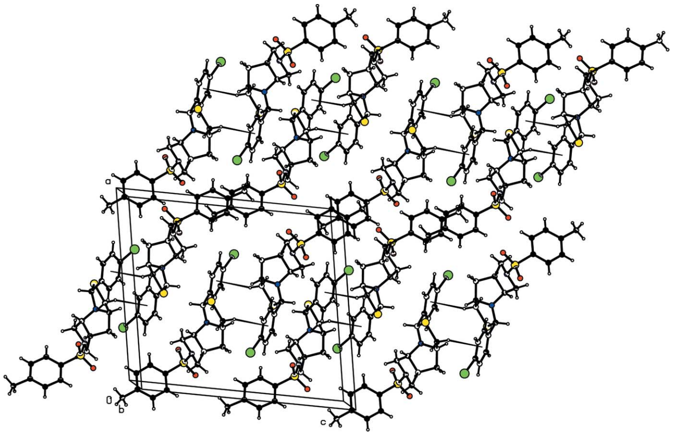


Figure 2
The molecular packing of (I), viewed down the *b* axis, showing C—H$\cdots\pi$ interactions as dashed lines.

The thiazolidine ring adopts a twisted conformation with a pseudo-twofold axis passing through atom S1 and the C6—N2 bond. The puckering parameters (Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Nardelli, 1983) are q_2 = 0.409 (2) Å, φ = −179.5 (4)° and $\Delta_s(N_1)$ = 0.003 (1) for ring *A*, q_2 = 0.366 (3) Å, φ = −75 (1)° and $\Delta_s(C_6)$ = 0.016 (3) for ring *B*, and q_2 = 0.368 (3) Å, φ = 19.9 (4)° and $\Delta_s(S_1)$ = 0.006 (1) for the thiazolidine ring.

In the crystal packing, the molecules are linked into centrosymmetric dimers by a pair of C—H$\cdots\pi$ interactions (Fig. 2 and Table 2). Atom C7 at (x, y, z) acts as a donor, through atom H7*B*, to the benzene ring C9–C14 at ($1 - x$, $2 - y$, $1 - z$) with the H7*B*$\cdots$*Cg*1 distance of 2.73 Å (*Cg*1 is the centroid of the C9—C14 ring).

Experimental

A solution of *N*-allyl-*N*-(2-oxo-ethyl)-4-methylbenzene-sulfonamide (1 mmol) and 2-(*p*-bromophenyl)thiazolidine-4-carboxylic acid (1.2 mmol) in toluene (20 ml) was refluxed under Dean–Stark conditions for 2 h. After completion of the reaction the mixture was chromatographed over silica gel using a hexane and ethyl acetate (9:1) mixture to yield the title compound. Single crystals were grown by slow evaporation of an ethyl acetate solution.

Crystal data

$C_{21}H_{23}BrN_2O_2S_2$
M_r = 479.44
Monoclinic, $P2_1/c$
a = 15.3215 (8) Å
b = 8.0676 (4) Å
c = 17.1663 (9) Å
β = 100.119 (1)°
V = 2088.88 (19) Å^3
Z = 4
D_x = 1.525 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.19 mm^{-1}
T = 293 (2) K
Block, colorless
0.23 × 0.22 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
23302 measured reflections
4943 independent reflections
3520 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.030
$\theta_{\rm max}$ = 28.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.126
S = 0.96
4943 reflections
254 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0658P)^2 + 1.1265P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.001
$\Delta\rho_{\rm max}$ = 0.89 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.53 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.480 (3)	C8—S1	1.869 (2)
C3—N2	1.469 (3)	C12—Br1	1.893 (3)
C4—N1	1.473 (3)	C15—S2	1.763 (3)
C6—N2	1.463 (3)	N1—S2	1.627 (2)
C7—S1	1.795 (3)	O1—S2	1.423 (2)
C8—N2	1.441 (3)	O2—S2	1.428 (2)
C4—N1—C1	105.6 (2)	O1—S2—O2	120.3 (1)
C4—N1—S2	118.9 (2)	O1—S2—N1	106.7 (1)
C1—N1—S2	118.9 (2)	O2—S2—N1	106.6 (1)
C8—N2—C6	109.9 (2)	O1—S2—C15	108.0 (1)
C8—N2—C3	115.8 (2)	O2—S2—C15	108.4 (1)
C6—N2—C3	107.6 (2)	N1—S2—C15	106.0 (1)
C7—S1—C8	92.6 (1)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots$*A*	*D*—H	H$\cdots$*A*	*D*$\cdots$*A*	*D*—H$\cdots$*A*
C7—H7*B*$\cdots$*Cg*1$^{\rm i}$	0.97	2.73	3.632 (4)	156

Symmetry code: (i) $-x+1, -y+2, -z+1$.

All H atoms were positioned geometrically and allowed to ride on their parent C atoms, with C—H distances in the range 0.93–0.98 Å and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

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).

Financial support from the University Grants Commission (UGC-SAP) and Department of Science and Technology

Acta Cryst. (2006). E**62**, o2146–o2148 Kavitha *et al.* • $C_{21}H_{23}BrN_2O_2S_2$ **o2147**

(DST-FIST), Government of India, is acknowledged for providing facilities to the department. DRG and DV thank the University Grants Commission (UGC), India, for funding.

References

Bruker (2001). *SMART* (Version. 5.625) and *SAINT* (Version 6.28a). Bruker AXS Inc., Madison, Wisconsin, USA.

Chaurasia, M. R. (1971). *Indian J. Pharm.* **33**, 17–19.

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Eswaramoorthy, S., Ponnuswamy, M. N., Raju, K. S. & Czerwinski, E. W. (1991). *Acta Cryst.* C**47**, 171–173.

Jiang, S., Lu, H., Liu, S., Zhao, Q., He, Y. & Debnath, A. K. (2004). *Antimicrob. Agents Chemother.* **48**, 4349–4359.

Nardelli, M. (1983). *Acta Cryst.* C**39**, 1141–1142.

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.

Rachinskii, F. Yu. (1964). *Akad. Nauk SSSR*, **4**, 256–264.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Zimenkovsky, B., Lesyk, R., Vladzimirska, O., Nektegayev, I., Golota, S. & Chorniy, I. (1999). *J. Pharm. Pharmacol.* **51**, 264.

o2148 Kavitha *et al.* • $C_{21}H_{23}BrN_2O_2S_2$ *Acta Cryst.* (2006). E**62**, o2146–o2148