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2-(4-Chlorophenyl)-5-(phenylsulfonyl)perhydro-1,3-thiazolo[3,4-*a*]pyrrolo[4,5-*c*]pyrrole

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.030
wR factor = 0.080
Data-to-parameter ratio = 23.0

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

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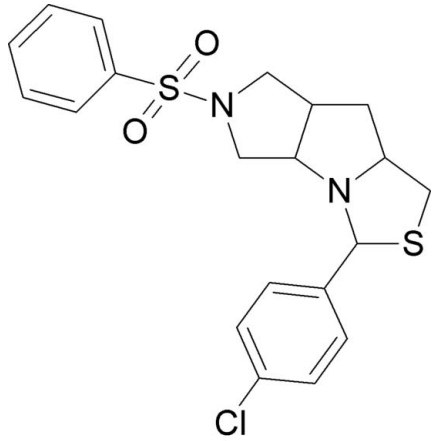
The thiazolidine ring and the two pyrrolidine rings in the title compound, $C_{20}H_{21}ClN_2O_2S_2$, adopt twisted conformations. In the crystal structure, the molecules translated by a unit cell along the *a* axis are linked by intermolecular C—H···O hydrogen bonds into a chain and inversion-related molecules in adjacent chains are interconnected *via* C—H···π interactions to form a double-stranded chain.

Comment

Some pyrrolo[1,2-*c*]thiazole derivatives are used as platelet-activating factor (PAF) antagonists (Weissman *et al.*, 1993; Le Naour *et al.*, 1994). They also inhibit cytokine-dependent induction of human immunodeficiency virus (HIV) expression in chronically infected promonocytic cells (Weissman *et al.*, 1993). 5-Oxo-hexahydropyrrolo[3,2-*b*]pyrroles have been found to act as inhibitors of human cytomegalovirus protease (Borthwick *et al.*, 2000). Since the title compound, (I), also contains a pyrrolopyrrole and a pyrrolothiazole unit it may also exhibit some biological activity.



(I)

The molecular structure of (I) is illustrated in Fig. 1. Bond lengths and angles in (I) agree with those observed in a similar structure, 2-(4-bromophenyl)-5-(phenylsulfonyl)perhydrothiazolo[3,4-*a*]pyrrolo [4,5-*c*]pyrrole, (II) (Kumar *et al.*, 2006). The configuration around atom N1 is nearly planar, whereas atom N2 exhibits a pyramidal geometry. The thiazolidine ring and the two pyrrolidine rings (N1/C1–C4 and N2/C3/C2/C5/C6) adopt twisted conformations. The Cremer & Pople (1975) puckering parameters q_2 and φ are, respectively: 0.397 (1) Å and 124.9 (2) ° for the thiazolidine ring, 0.363 (1) Å and 60.7 (2)° for the pyrrolidine ring (N1/C1–C4), and 0.419 (1) Å and 198.1 (2)° for the pyrrolidine ring (N2/C3/C2/C5/C6).

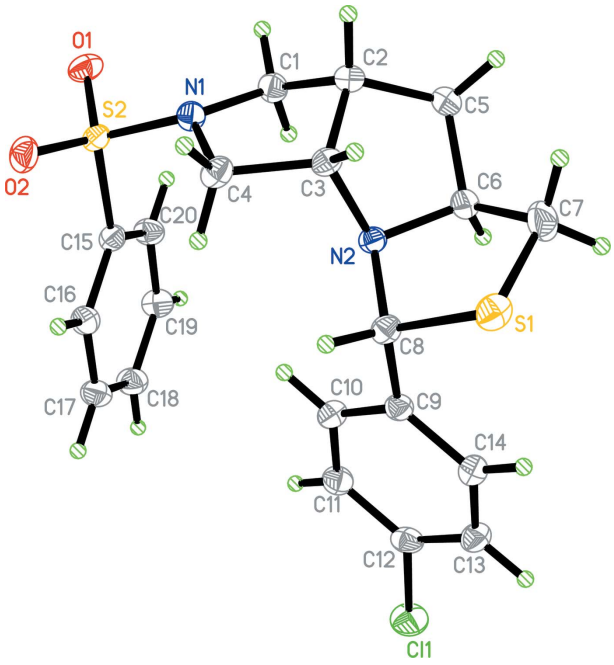


Figure 1
The structure of (I), showing 60% probability displacement ellipsoids and the atomic numbering scheme.

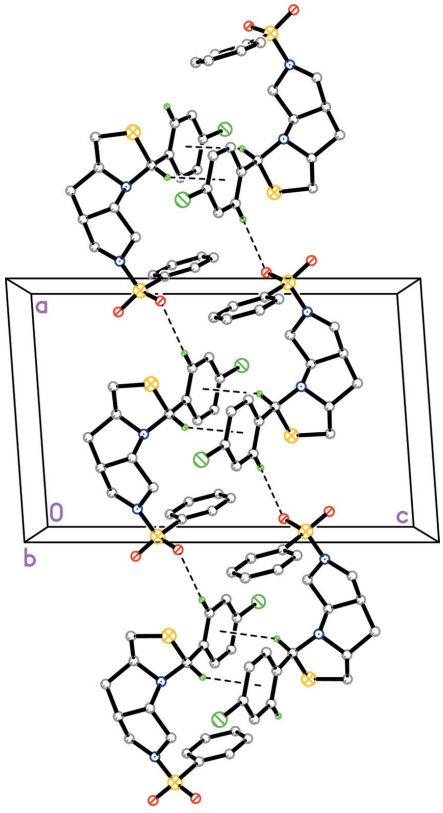


Figure 2
A view of a hydrogen-bonded (dashed lines) double-stranded chain in (I). Only the H atoms involved in hydrogen bonding are shown.

The crystal packing of (I) reveals that molecules translated by a unit cell along the *a* axis are linked by intermolecular C—H···O hydrogen bonds (Table 1) into chains. Inversion-related molecules in adjacent chains are interconnected *via* C—H···π interactions, involving the C9–C14 benzene rings (centroid *Cg*1), to form double-stranded chains along the *a* axis (Fig. 2).

A superimposed fit of the non-H atoms of (I) and the corresponding atoms in (II) (Kumar *et al.*, 2006) gives an r.m.s. deviation of 0.038 Å. This indicates that the conformation of (I) is not significantly altered by replacing the Br atom in (II) by a Cl atom. The pattern of intermolecular C—H···π hydrogen bonding is identical in the crystal structures of (I) and (II).

Experimental

A solution of *N*-allyl-*N*-(2-oxoethyl)benzenesulfonamide (1 mmol) and 2-(*p*-chlorophenyl)thiazolidine-4-carboxylic acid (1.2 mmol) in dry toluene (30 ml) was refluxed for 4 h. After completion of the reaction, the solvent was evaporated off vacuum and the residue was chromatographed (SiO_2) using a hexane–ethyl acetate (9:1) mixture, to yield the title compound. Compound (I) was recrystallized from ethyl acetate.

Crystal data

$C_{20}H_{21}ClN_2O_2S_2$
M_r = 420.96
Monoclinic, $P2_1/c$
a = 10.4869 (2) Å
b = 11.2536 (2) Å
c = 16.4220 (2) Å
β = 94.052 (1)°
V = 1933.20 (6) Å^3
Z = 4
D_x = 1.446 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 100 (2) K
Block, colourless
0.56 × 0.33 × 0.32 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.795, T_{max} = 0.874
25474 measured reflections
5600 independent reflections
5046 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 30.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
S = 1.03
5600 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 0.9249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

*Cg*1 is the centroid of the ring C9–C14.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···S1	1.00	2.83	3.2274 (11)	104
C14—H14···S1	0.95	2.66	3.1103 (13)	110
C14—H14···O2^{i}	0.95	2.51	3.3863 (14)	153
C16—H16···O2	0.95	2.57	2.9246 (15)	102
C8—H8···*Cg*1^{ii}	1.00	2.61	3.4999 (12)	148

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z+1$.

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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References

Borthwick, A. D., Angier, S. J., Crame, A. J., Exall, A. M., Haley, T. M., Hart, G. J., Mason, A. M., Pennell, A. M. K. & Weingarten, G. G. (2000). *J. Med. Chem.* **43**, 4452–4464.
Bruker (2005). *APEX2* (Version 1.27), *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Kumar, R. P., Gayathri, D., Velmurugan, D., Ravikumar, K. & Poornachandran, M. (2006). *Acta Cryst.* E**62**, o2429–o2431.
Le Naour, R., Clayette, P., Henin, Y., Mabondzo, A., Raoul, H., Bousseau, A. & Dormont, D. (1994). *J. Gen. Virol.* **75**, 1379–1388.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Weissman, D., Poli, G., Bousseau, A. & Fauci, A. S. (1993). *Proc. Natl Acad. Sci. USA*, **90**, 2537–2541.