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6-Ethyl-1-(4-fluorophenyl)-5-(phenylsulfonyl)-perhydro-*cis*-pyrrolo[3,4-*b*]pyrrole

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In the title compound, $C_{20}H_{23}FN_2O_2S$, one of the pyrrolidine rings adopts an envelope conformation, while the other is in a twist conformation. The molecules are linked into *C*(6) chains by C—H···O hydrogen bonds.

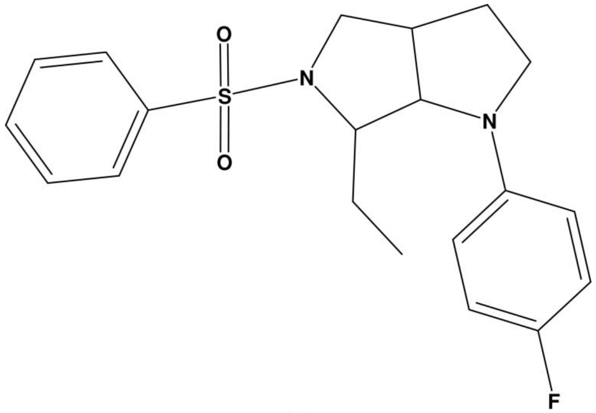
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.057
wR factor = 0.150
Data-to-parameter ratio = 18.7

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

Comment

The pyrrolidine ring occurs in many families of biologically important compounds. Many pyrrolidine derivatives with varying properties have been synthesized as a result of the ease of substitution and modifications at several positions (Baldwin *et al.*, 1994). Pyrrolidine derivatives have been found to exhibit antimicrobial, antifungal (Amal Raj *et al.*, 2003), anti-inflammatory (Fernandes *et al.*, 2004) and antiviral (Borthwick *et al.*, 2003) activities. We report here the crystal structure of the title compound, (I).



(I)

The bond lengths in (I) (Fig. 1) show normal values (Allen *et al.*, 1987). The sums of the bond angles (Table 1) around atoms N1 (351.8°) and N2 (357.8°) indicate that they are sp^2-hybridized. Atom F1 deviates from the plane of the C15–C20 benzene ring by 0.026 (3) Å.

The N1/C7–C10 pyrrolidine ring adopts an envelope conformation, with atom C9 deviating by 0.452 (3) Å from the mean plane of other ring atoms. The other pyrrolidine ring (C8/C9/N2/C14/C13) adopts a twist conformation with a pseudo-twofold axis passing through atom N2 and the C8—C13 bond. The puckering parameters (Cremer & Pople, 1975) and the smallest displacement asymmetry parameters (Nardelli, 1983) are q_2 = 0.284 (3) Å and φ = 295.5 (6)° and Δ_S(C9) = 5.3 (3)° for the N1/C7–C10 pyrrolidine ring, and q_2 = 0.325 (3) Å, φ = 91.1 (5)° and Δ_2(N2) = 1.3 (3)° for the other pyrrolidine ring. The dihedral angle between the C1–C6 and C15–C20 rings is 11.0 (2)°.

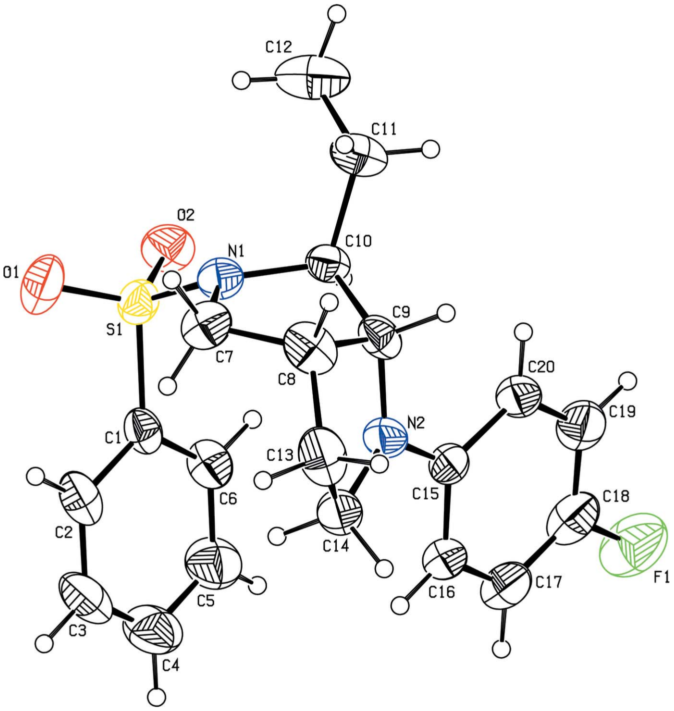


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

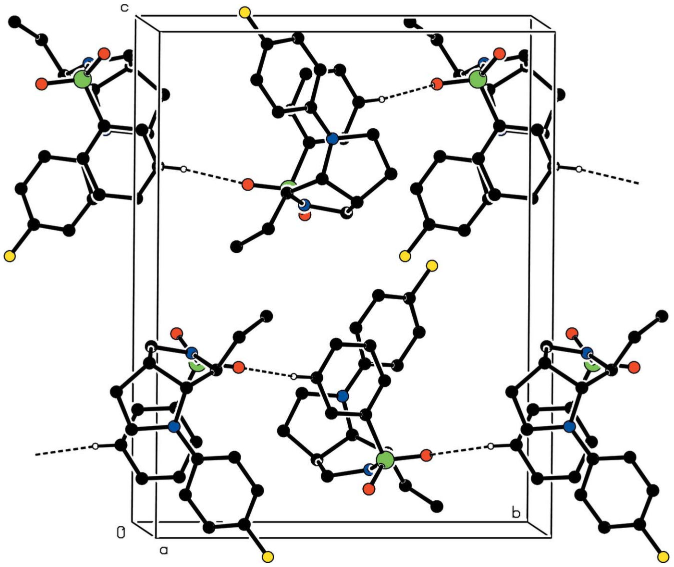


Figure 2
The molecular packing of (I), viewed approximately down the *a* axis. For clarity, H atoms not involved in the hydrogen bonds (dashed lines) have been omitted.

The C3—H3···O2($2 - x$, $-\frac{1}{2} + y$, $\frac{1}{2} - z$) hydrogen bond (Table 2) links the molecules into a *C*(6) chain running along the *b* axis.

Experimental

A solution of 2-(*N*-allyl-*N*-benzenesulfonylamino)butanal (1 mmol) and *p*-fluorophenylglycine (1.2 mmol) in dry toluene (20 ml) was refluxed until completion of the reaction as evidenced by thin-layer chromatography. The solvent was evaporated under vacuum and the residue was column chromatographed (silica gel, 100–200 mesh) using a hexane–ethyl acetate (9:1) mixture, yielding the title compound which was recrystallized by slow evaporation of an ethyl acetate solution.

Crystal data

$C_{20}H_{23}FN_2O_2S$
M_r = 374.46
Orthorhombic, $P2_12_12_1$
a = 7.8671 (4) Å
b = 13.6413 (7) Å
c = 17.4200 (9) Å
V = 1869.47 (17) Å^3
Z = 4
Mo *Kα* radiation
μ = 0.20 mm^{-1}
T = 293 (2) K
0.23 × 0.22 × 0.21 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: none
16247 measured reflections
4395 independent reflections
3627 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.150
S = 1.05
4395 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.38 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983); 1847 Friedel pairs
Flack parameter: 0.41 (9)

Table 1
Selected geometric parameters (Å, °).

C1—S1	1.770 (3)	C15—N2	1.379 (4)
C7—N1	1.481 (3)	C18—F1	1.383 (4)
C9—N2	1.450 (4)	N1—S1	1.617 (2)
C10—N1	1.481 (3)	O1—S1	1.434 (2)
C14—N2	1.469 (3)	O2—S1	1.422 (2)
C7—N1—C10	110.9 (2)	O2—S1—O1	120.2 (2)
C7—N1—S1	117.8 (2)	O2—S1—N1	106.9 (1)
C10—N1—S1	123.1 (2)	O1—S1—N1	106.4 (1)
C15—N2—C9	123.2 (2)	O2—S1—C1	107.4 (1)
C15—N2—C14	122.1 (2)	O1—S1—C1	106.6 (1)
C9—N2—C14	112.5 (2)	N1—S1—C1	108.9 (1)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2$^{\rm i}$	0.93	2.59	3.504 (4)	168

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

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93–0.98 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(methyl C) or 1.2$U_{\rm eq}$(C). The value of the Flack parameter indicates inversion twinning.

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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