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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å  
Disorder in main residue  
 $R$  factor = 0.053  
 $wR$  factor = 0.152  
Data-to-parameter ratio = 11.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 1-(4-Bromo-2-fluorophenyl)-3-trifluoromethyl-1H-pyrazol-5-yl benzenesulfonate

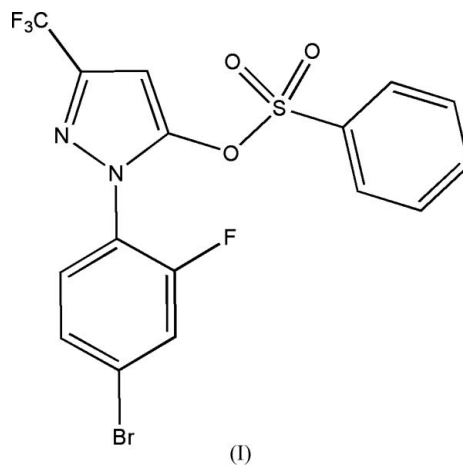
The molecular structure of the title compound,  $\text{C}_{16}\text{H}_9\text{BrF}_4\text{N}_2\text{O}_3\text{S}$ , is stabilized by an intramolecular  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bond. In the crystal structure, supramolecular layers are formed parallel to the  $bc$  plane by an intermolecular  $\text{C}-\text{H} \cdots \text{F}$  hydrogen bond. The  $\text{CF}_3$  group was found to be disordered.

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## Comment

3-(Trifluoromethyl)pyrazole derivatives have active fungicidal properties (Hwang *et al.*, 1994; Liu & Li, 2004), as well as insecticidal activities (Kim *et al.*, 1989). In a search for new compounds with improved properties, the title compound, (I), was obtained *via* benzenesulfonation of 1-(4-bromo-2-fluorophenyl)-3-trifluoromethyl-1H-pyrazol-5-one. The crystal structures of some related compounds have been reported previously (Li, Duan *et al.*, 2005; Li, Li *et al.*, 2005).The molecular structure of (I) is illustrated in Fig. 1 and shows that the rings are all planar. The dihedral angles between the pyrazole and the benzene rings at N1 and S1 are  $60.1$  (3)° and  $50.9$  (3)°, respectively.The molecular structure of (I) is stabilized by an intramolecular  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bond (Table 1). In the crystal structure (Fig. 2), supramolecular layers are formed parallel to the  $bc$  plane by an intermolecular  $\text{C16}-\text{H16} \cdots \text{F1}$  hydrogen bond. There are no significant interactions between these layers.

## Experimental

Benzenesulfonyl chloride (0.35 g, 2.0 mmol) in benzene (6 ml) was added dropwise to a suspension of 1-(4-bromo-2-fluorophenyl)-3-trifluoromethyl-1H-pyrazol-5-one (0.65 g, 2.0 mmol) [prepared according to the literature method of Liu &amp; Li (2004)], anhydrous

sodium carbonate (0.21 g, 2.0 mmol), a catalytic amount of tetrabutylammonium chloride in benzene (10 ml) and water (1 ml), over approximately 30 min at 283 K. The resulting mixture was stirred at room temperature for an additional 1 h. The benzene layer was collected and evaporated under reduced pressure. The crude product was recrystallized from ethyl acetate/petroleum ether (1:1 v/v) to give (I) as a colorless solid (0.80 g, yield: 86%; m.p. 342–343 K). Suitable single crystals were grown from a solution in ethyl acetate/*n*-hexane (1:1 v/v).

#### Crystal data

$C_{16}H_9BrF_4N_2O_3S$

$M_r = 465.22$

Monoclinic,  $P2_1/c$

$a = 19.740$  (4) Å

$b = 9.5361$  (18) Å

$c = 9.7230$  (18) Å

$\beta = 101.699$  (3)°

$V = 1792.3$  (6) Å<sup>3</sup>

$Z = 4$

$D_x = 1.724$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

Cell parameters from 1907

reflections

$\theta = 2.4$ – $22.6$ °

$\mu = 2.47$  mm<sup>-1</sup>

$T = 293$  (2) K

Block, colorless

$0.30 \times 0.24 \times 0.20$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.525$ ,  $T_{\max} = 0.638$

8850 measured reflections

3161 independent reflections

1656 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.058$

$\theta_{\text{max}} = 25.0$ °

$h = -23 \rightarrow 23$

$k = -11 \rightarrow 11$

$l = -11 \rightarrow 8$

#### Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.053$

$wR(F^2) = 0.152$

$S = 1.01$

3161 reflections

272 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 2.3366P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.84$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.71$  e Å<sup>-3</sup>

**Table 1**

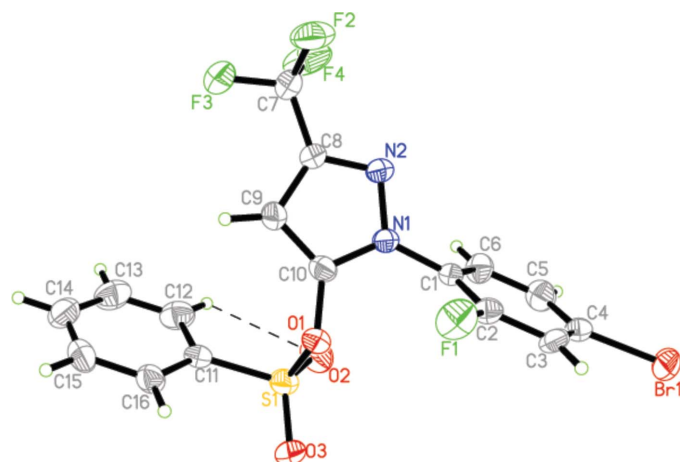
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12 $\cdots$ O2	0.93	2.56	2.927 (10)	104
C16—H16 $\cdots$ F1 <sup>1</sup>	0.93	2.52	3.428 (7)	166

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

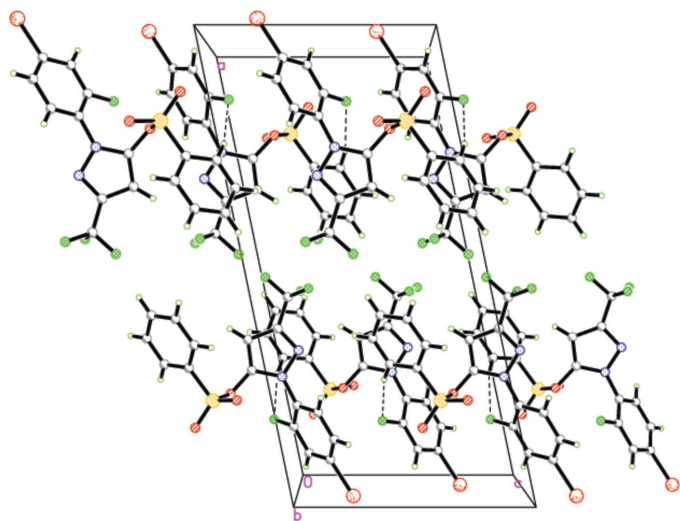
H atoms were positioned geometrically ( $C-H = 0.93$  Å) and constrained to ride on their parent atoms, with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ . The  $CF_3$  group was found to be disordered and two distinct conformations were observed. The site occupancies refined to 0.623 (2) and 0.377 (2).

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.



**Figure 1**

The molecular structure of compound (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. The dashed line indicates an intramolecular hydrogen bond. Only the major component of the disordered  $CF_3$  group is shown.



**Figure 2**

A crystal packing diagram for compound (I).  $C-H\cdots F$  hydrogen bonds are indicated by dashed lines. Only the major component of the disordered  $CF_3$  group is shown.

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