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4-(5-Phenyl-3-trifluoromethyl-1*H*-pyrazol-1-yl)benzenesulfonamide

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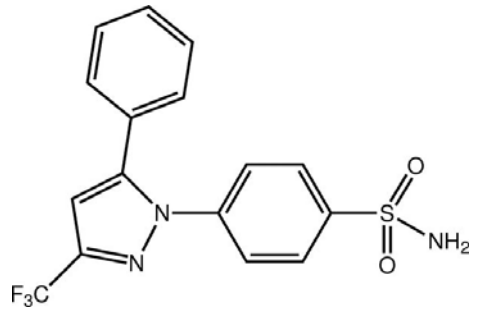
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.113; data-to-parameter ratio = 15.2.

Significant twists between the aromatic rings are evident in the structure of the title compound, $C_{16}H_{12}F_3N_3O_2S$. With reference to the pyrazole plane, the N- and C-bound benzene rings form dihedral angles of 57.12 (11) and 29.75 (11)°, respectively. The dihedral angle between the benzene rings is 52.82 (11)°. The presence of N—H···O(sulfonamide) and N—H···N(pyrazole) hydrogen bonds lead to supramolecular tubes along the *b*-axis direction. These are connected into layers *via* C—H···O interactions involving a bifurcated O atom (not involved in the N—H···O hydrogen bonding). Layers stack along the *a*-axis direction.

Related literature

For background to the biological applications of related species, see: Faidallah *et al.* (2007); Al-Saadi *et al.* (2008). For the crystal structure of a related species, see: Dev *et al.* (1999).



Experimental

Crystal data

$C_{16}H_{12}F_3N_3O_2S$
M_r = 367.35
Monoclinic, $P2_1/c$
a = 16.2430 (7) Å
b = 4.9461 (2) Å
c = 21.2383 (8) Å
β = 111.231 (5)°
V = 1590.47 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 100 K
0.40 × 0.10 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.735, T_{max} = 1.000
7901 measured reflections
3560 independent reflections
2876 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 1.06
3560 reflections
234 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1···O1^{i}	0.84 (3)	2.14 (3)	2.911 (2)	153 (2)
N3—H2···N2^{ii}	0.87 (2)	2.21 (3)	3.049 (3)	164 (2)
C9—H9···O2^{iii}	0.95	2.49	3.376 (3)	155
C16—H16···O2^{iv}	0.95	2.55	3.137 (2)	120

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5083).

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