4-(5-Phenyl-3-trifluoromethyl-1H-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_{3}N_{3}O_{2}S. 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_{3}N_{3}O_{2}S

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 Kα 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

Refinement

R[F^2 > 2σ(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

Δρ_{max} = 0.34 e Å^{-3}

Δρ_{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–H1i –O1v 0.84 (3) 2.14 (3) 2.91 (2) 153 (2)
N3–H2v –O2iv 0.87 (2) 2.21 (3) 3.04 (3) 164 (2)
C9–H9 –O2iv 0.95 2.49 3.37 (3) 155
C16–H16 –O2iv 0.95 2.55 3.13 (2) 120

Symmetry codes: (i) x, y − 1, z; (ii) −x + 1, −y + 1, −z + 1; (iii) −x + 1, y + 1/2, −z + 1/2

Data collection: CrysAlis PRO (Agilent, 2010); cell refinement: 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).

References


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