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4-(3-Methyl-5-phenyl-1*H*-pyrazol-1-yl)-benzenesulfonamide

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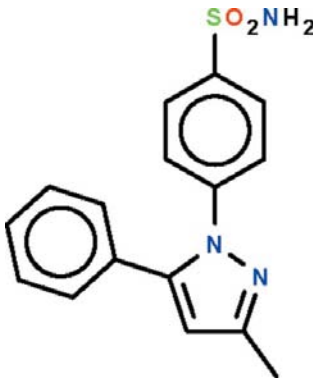
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 15.1.

With respect to the planar five-membered ring of the title compound, $C_{16}H_{15}N_3O_2S$, the phenyl ring is aligned at 47.0 (1)° and the phenylene ring at 37.6 (1)°. The amino group has the N atom in a pyramidal geometry; the group is a hydrogen-bond donor to the sulfonyl O atom of one molecule and to the pyrazole N atom of another molecule, resulting in the formation of a layer parallel to the *bc* plane.

Related literature

For the synthesis, see: Gosselin *et al.* (2006); Organ & Mayer (2003).



Experimental

Crystal data

$C_{16}H_{15}N_3O_2S$
M_r = 313.37
Monoclinic, $C2/c$
a = 28.2545 (8) Å
b = 11.9135 (4) Å
c = 9.3739 (3) Å
β = 91.016 (3)°
V = 3154.85 (17) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 1.91 mm^{-1}
T = 100 K
0.30 × 0.03 × 0.03 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.598, T_{max} = 0.945
6579 measured reflections
3137 independent reflections
2689 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.03
3137 reflections
208 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N3^{i}	0.92 (2)	1.98 (2)	2.878 (2)	164 (2)
N1—H2···O1^{ii}	0.86 (2)	2.07 (2)	2.930 (2)	177 (2)

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

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: *X-SEED* (Barbour, 2001); 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: BT5609).

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