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4-(3,5-Dimethyl-1*H*-pyrazol-1-yl)-benzenesulfonamide

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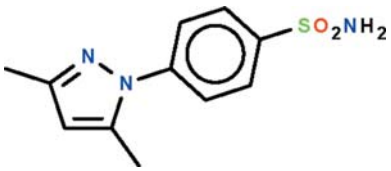
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 14.1.

The two aromatic rings of the title compound, $C_{11}H_{13}N_3O_2S$, are inclined at an angle of 47.81 (4)°. The N atom of the amino unit is pyramidally coordinated; one H atom interacts with the sulfamyl O atom of an adjacent molecule, forming a centrosymmetric hydrogen-bonded dimer. The dimers are linked by N—H···N hydrogen bonds, generating a three-dimensional network.

Related literature

For the synthesis and medicinal properties of the title compound, see: Grueneberg *et al.* (2002); Wright *et al.* (1964).



Experimental

Crystal data

$C_{11}H_{13}N_3O_2S$
M_r = 251.30
Monoclinic, $P2_1/n$
a = 7.9649 (1) Å
b = 11.7827 (2) Å
c = 12.2720 (2) Å
β = 91.720 (1)°
V = 1151.18 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.47 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.02 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.525, T_{max} = 0.952
8510 measured reflections
2312 independent reflections
2215 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
S = 1.07
2312 reflections
164 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 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}	0.87 (1)	2.13 (1)	2.966 (2)	160 (2)
N3—H1···N2^{ii}	0.87 (1)	2.94 (2)	3.501 (2)	124 (2)

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

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: *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: BT5610).

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