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4-(5-Oxo-3-phenyl-4,5-dihydro-1*H*-pyrazol-1-yl)benzenesulfonamide

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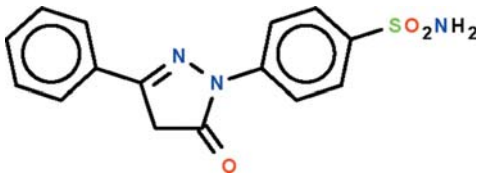
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.121; data-to-parameter ratio = 13.2.

With respect to the aliphatic planar five-membered ring (r.m.s. deviation = 0.011 Å) of the title compound, $C_{15}H_{13}N_3O_2S$, the phenyl ring is aligned at 6.9 (1)° and the phenylene ring at 2.4 (1)°, so that the three rings are nearly coplanar. 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 ketonic O atom of another molecule, resulting in the formation of a layer parallel to the *bc* plane.

Related literature

For the synthesis, see: Casoni (1956); Itano (1955).



Experimental

Crystal data

$C_{15}H_{13}N_3O_3S$
M_r = 315.34
Monoclinic, $P2_1/c$
a = 13.6794 (4) Å
b = 13.4304 (4) Å
c = 7.3678 (2) Å
β = 91.055 (3)°
V = 1353.38 (7) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.29 mm^{-1}
T = 100 K
0.30 × 0.05 × 0.05 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.546, T_{max} = 0.894
10404 measured reflections
2731 independent reflections
2444 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.121
S = 1.06
2731 reflections
207 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.73 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
N3—H1···O3^{i}	0.88 (1)	2.12 (1)	2.975 (2)	164 (2)
N3—H2···O2^{ii}	0.87 (1)	2.12 (1)	2.978 (2)	168 (2)

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

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: BT5611).

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