

4-(3-Methyl-4,5-dihydro-1H-benzo[g]-indazol-1-yl)benzenesulfonamide

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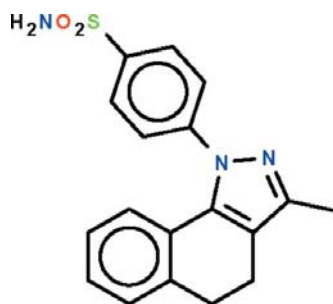
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.068; wR factor = 0.184; data-to-parameter ratio = 14.4.

In the title compound, $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_2\text{S}$, the aromatic ring bearing the sulfamide unit is aligned at $61.65(1)^\circ$ with respect to the pyrrole ring; its amino group forms $\text{N}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds to neighboring molecules, generating sheets in the ac plane.

Related literature

For the crystal structure of a pyrrole synthesized using 2-acetyltetralone as a reactant, see: Portilla *et al.* (2007).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_2\text{S}$
 $M_r = 339.41$
Monoclinic, $P2_1/n$
 $a = 4.8838(1)$ Å
 $b = 27.3894(4)$ Å
 $c = 12.2399(2)$ Å
 $\beta = 94.738(1)^\circ$

$V = 1631.67(5)$ Å³
 $Z = 4$
Cu $K\alpha$ radiation
 $\mu = 1.89$ mm⁻¹
 $T = 100$ K
 $0.30 \times 0.25 \times 0.20$ mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
 $T_{\min} = 0.600$, $T_{\max} = 0.703$

11808 measured reflections
3255 independent reflections
3166 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$
 $wR(F^2) = 0.184$
 $S = 1.11$
3255 reflections
226 parameters
14 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.70$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.65$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1}\cdots\text{N3}^{\text{i}}$	0.88 (1)	2.05 (1)	2.925 (4)	173 (5)
$\text{N1}-\text{H2}\cdots\text{O2}^{\text{ii}}$	0.88 (1)	1.95 (2)	2.806 (4)	165 (4)

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

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: *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5614).

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