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# 4-(3,7-Dimethyl-4-oxo-4,5-dihydroisoxazolo[4,5-*d*]pyridazin-5-yl)benzenesulfonamide

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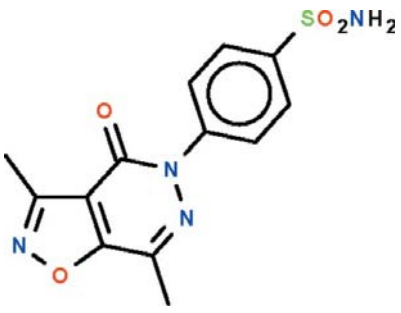
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.033; $wR$ factor = 0.096; data-to-parameter ratio = 9.1.

The nine-membered fused-ring system of the title pyridazine derivative, $C_{13}H_{12}N_4O_4S$, is approximately planar (r.m.s. deviation 0.027 Å), and the benzene ring of the phenylsulfamide substituent is aligned at 43.5 (1)° to the fused-ring system. The amine group of the sulfonamide substituent forms an N—H···O hydrogen bond to the ketonic O atom of two neigboring molecules to generate a chain running along the *c* axis.

## Related literature

For a related structure, see: Abdel-Aziz *et al.* (2010). For the biological activity of the class of pyridazines, see: Faid-Allah *et al.* (2011); Makki & Faid-Allah (1996).




## Experimental

### Crystal data

$C_{13}H_{12}N_4O_4S$
$M_r$ = 320.33
Orthorhombic, *Fdd*2
$a$ = 18.0113 (4) Å
$b$ = 35.5302 (11) Å
$c$ = 8.2900 (2) Å
$V$ = 5305.1 (2) Å$^3$
$Z$ = 16
Cu $K\alpha$ radiation
$\mu$ = 2.43 mm$^{-1}$
$T$ = 100 K
0.30 × 0.20 × 0.05 mm

### Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.529, $T_{max}$ = 0.888
7699 measured reflections
1886 independent reflections
1870 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.096
$S$ = 1.08
1886 reflections
207 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$
Absolute structure: Flack (1983), 441 Friedel pairs
Flack parameter: 0.026 (18)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N4—H1···O2$^{i}$ | 0.95 (3) | 2.09 (4) | 3.012 (3) | 163 (3) |
| N4—H2···O2$^{ii}$ | 0.85 (5) | 2.11 (5) | 2.933 (3) | 162 (4) |

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

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: XU5287).

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