

4-(5,3'-Dimethyl-5'-oxo-2-phenyl-2',5'-dihydro-2H-[3,4]bipyrazol-1'-yl)-benzenesulfonamide monohydrate

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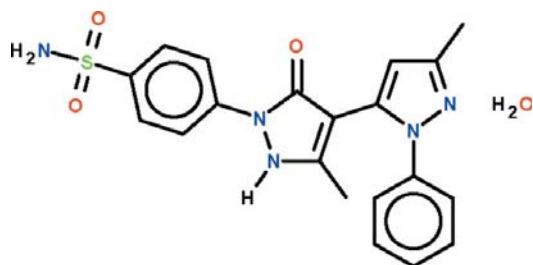
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Key indicators: single-crystal X-ray study; *T* = 100 K; mean $\sigma(\text{C}-\text{C})$ = 0.003 Å; *R* factor = 0.048; *wR* factor = 0.130; data-to-parameter ratio = 15.2.

In the title compound, C₂₀H₁₉N₅O₃S·H₂O, the pyrazole ring is connected to a pyrazolone ring, and the two five-membered rings are aligned at 45.0 (1)°. The pyrazole ring is connected to a phenyl ring and the two are twisted by 42.7 (1)°. Finally, the pyrazolone ring is connected to a benzene ring and the two are twisted by 19.5 (1)°. The N—H and —NH₂ portions and the solvent water molecules are engaged in N—H···N, N—H···O and O—H···O hydrogen-bonding interactions to generate a three-dimensional network.

Related literature

For related pyrazole–benzenesulfonamides, see: Al-Youbi *et al.* (2011); Asiri *et al.* (2011).



Experimental

Crystal data

C₂₀H₁₉N₅O₃S·H₂O

M_r = 427.48

Monoclinic, *P*2₁/*c*

a = 11.1570 (5) Å

b = 12.3305 (5) Å

c = 14.9228 (5) Å

β = 107.142 (4)°

V = 1961.75 (14) Å³

Z = 4

Mo *K*α radiation

μ = 0.21 mm⁻¹

T = 100 K

0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2010)

*T*_{min} = 0.941, *T*_{max} = 0.960

9403 measured reflections

4382 independent reflections

3259 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.039

Refinement

R[*F*² > 2σ(*F*²)] = 0.048

wR(*F*²) = 0.130

S = 1.01

4382 reflections

288 parameters

5 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}}$ = 0.51 e Å⁻³

$\Delta\rho_{\text{min}}$ = -0.54 e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ··· <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> — <i>H</i> ··· <i>A</i>
N3—H3···N2 ⁱ	0.88 (1)	2.05 (1)	2.927 (3)	175 (2)
N5—H51···O1 ⁱ	0.88 (1)	2.05 (1)	2.913 (3)	165 (2)
N5—H52···O1W ⁱⁱ	0.88 (1)	2.09 (1)	2.932 (3)	161 (2)
O1W—H11···O1	0.84 (1)	1.94 (1)	2.769 (2)	169 (3)
O1W—H12···O2 ⁱⁱⁱ	0.84 (1)	2.38 (2)	3.158 (2)	154 (3)

Symmetry codes: (i) *x*, -*y* + $\frac{3}{2}$, *z* + $\frac{1}{2}$; (ii) -*x* + 1, -*y* + 1, -*z* + 1; (iii) *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: XU5305).

References

- Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, Oxfordshire, England.
Al-Youbi, A. O., Asiri, A. M., Faidallah, H. M., Alamry, K. A. & Ng, S. W. (2011). *Acta Cryst.* **E67**, o2428.
Asiri, A. M., Faidallah, H. M., Al-Youbi, A. O. & Ng, S. W. (2011). *Acta Cryst.* **E67**, o2427.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.