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

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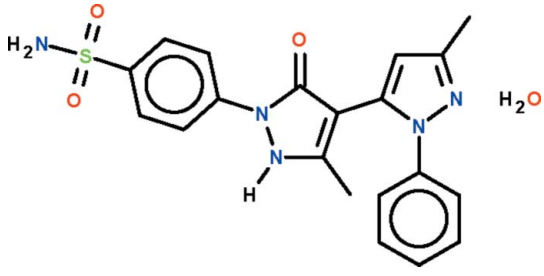
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.130; data-to-parameter ratio = 15.2.

In the title compound, $C_{20}H_{19}N_5O_3S\cdot H_2O$, 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 –NH_2 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

$C_{20}H_{19}N_5O_3S\cdot H_2O$ M_r = 427.48
Monoclinic, $P2_1/c$
a = 11.1570 (5) Å
b = 12.3305 (5) Å
c = 14.9228 (5) Å
β = 107.142 (4)°
V = 1961.75 (14) Å^3
Z = 4
Mo $K\alpha$ 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 $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 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
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
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).

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