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(2*Z*)-1-(5-Hydroxy-3-methyl-1-phenyl-1*H*-pyrazol-4-yl)-3-(4-methoxyanilino)-but-2-en-1-one

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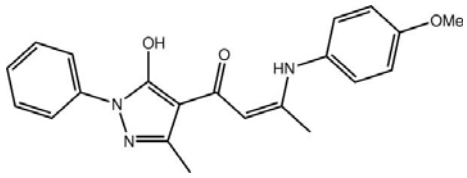
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.104; data-to-parameter ratio = 15.4.

The central residue in the title compound, $C_{21}H_{21}N_3O_3$, is close to planar (r.m.s. deviation = 0.0753 Å for all non-H atoms from OH to NH inclusive): the hydroxy, amino and carbonyl groups all lie to the same side of the molecule (the conformation about the ethene bond is *Z*), facilitating the formation of intramolecular O—H···O and N—H···O hydrogen bonds that close *S*(6) rings. However, overall the molecule is twisted as the terminal aromatic rings are not coplanar with the central plane [dihedral angles = 20.55 (5) and 80.90 (4)° for the N-bound phenyl ring and the methoxybenzene ring, respectively]. The dihedral angle between the rings is 82.14 (7)°. Supramolecular layers in the *ac* plane mediated by C—H···π interactions are found in the crystal.

Related literature

For background to the synthesis, see: Gelin *et al.* (1983); Bendaas *et al.* (1999). For the structure of the 4-chloro derivative, see: Asiri *et al.* (2011).



Experimental

Crystal data

$C_{21}H_{21}N_3O_3$
M_r = 363.41
Monoclinic, $P2_1/n$
a = 9.5717 (3) Å
b = 16.9516 (6) Å
c = 11.3143 (4) Å
β = 104.946 (4)°
V = 1773.70 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.837, T_{max} = 1.000
8486 measured reflections
3939 independent reflections
3145 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.104
S = 1.05
3939 reflections
255 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the N1,N2,C1–C3 and C15–C20 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.86 (1)	1.68 (1)	2.4963 (15)	156 (2)
N3—H3···O2	0.89 (1)	1.92 (1)	2.6447 (16)	138 (2)
C14—H14b···*Cg*1^{i}	0.98	2.88	3.5542 (18)	127
C21—H21c···*Cg*2^{ii}	0.98	2.76	3.5195 (17)	134

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

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: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); 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: HB6355).

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