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(*E*)-4-[4-(Benzyloxy)-3-methoxybenzylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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Key indicators

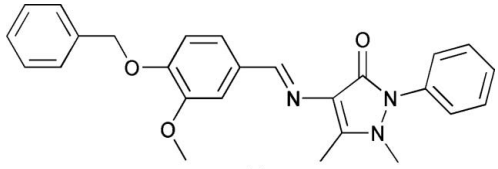
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.131
Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{26}H_{25}N_3O_3$, was prepared by the reaction of 4-(benzyloxy)-3-methoxybenzaldehyde and 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one. The central benzene ring makes dihedral angles of 28.58 (7), 67.98 (6) and 86.16 (7)° with the pyrazole ring and the two terminal phenyl rings, respectively. The N atoms of the pyrazole ring have pyramidal environments.

Comment

The metal complexes of Schiff bases exhibit various biological activities (Kahwa *et al.*, 1986). A large number of such compounds have been synthesized to develop protein and enzyme mimics (Santos *et al.*, 2001). In continuation of our search for new Schiff bases functioning as ligands, we present the molecular and crystal structure of the title compound, (I).



(I)

In (I) (Fig. 1), the bond lengths and angles (Table 1) are within normal ranges. The central benzene ring (C8–C13) makes dihedral angles of 67.98 (6) and 86.16 (7)° with the two terminal phenyl rings (C21–C26 and C2–C7, respectively). In the pyrazole ring, atoms N2 and N3 have pyramidal environments, proved by the sum of bond angles being less than 360°, namely 352.6 and 347.2° for N2 and N3, respectively. The crystal packing (Fig. 2) is stabilized by van der Waals forces.

Experimental

An anhydrous ethanol solution of 4-(benzyloxy)-3-methoxybenzaldehyde (2.42 g, 10 mmol) was added to an anhydrous ethanol

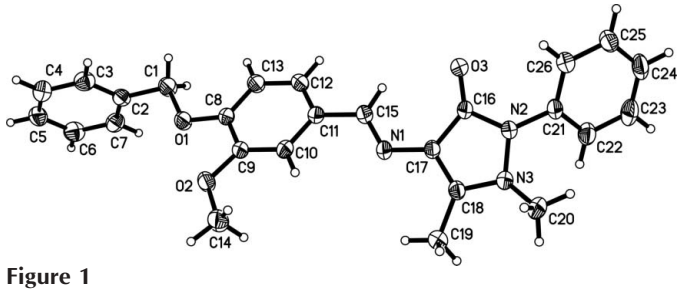


Figure 1
View of (I), with displacement ellipsoids drawn at the 30% probability level.

solution of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol). The mixture was stirred at 350 K for 5 h under nitrogen, whereupon a yellow precipitate appeared. The product was isolated, recrystallized from ethanol, and then dried *in vacuo* to give the pure compound in 89% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{26}H_{25}N_3O_3$	$Z = 2$
$M_r = 427.49$	$D_x = 1.274$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.432$ (2) Å	Cell parameters from 2027 reflections
$b = 9.550$ (2) Å	$\theta = 2.6$–$25.5°$
$c = 12.711$ (3) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 83.986$ (4)°	$T = 294$ (2) K
$\beta = 84.986$ (3)°	Block, yellow
$\gamma = 78.772$ (4)°	0.20 × 0.16 × 0.08 mm
$V = 1114.2$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3902 independent reflections
φ and ω scans	2666 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.028$
$T_{min} = 0.975$, $T_{max} = 0.993$	$\theta_{max} = 25.0°$
5706 measured reflections	$h = -11 \rightarrow 11$
	$k = -4 \rightarrow 11$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0707P)^2 + 0.1077P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.131$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.14$ e Å^{-3}
3902 reflections	Extinction correction: *SHELXL97*
293 parameters	Extinction coefficient: 0.027 (4)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.368 (2)	N1—C17	1.396 (2)
O1—C1	1.427 (2)	N2—C16	1.401 (2)
O2—C9	1.370 (2)	N2—N3	1.402 (2)
O2—C14	1.405 (2)	N2—C21	1.428 (2)
O3—C16	1.235 (2)	N3—C18	1.362 (2)
N1—C15	1.277 (2)	N3—C20	1.462 (2)
C8—O1—C1	116.99 (14)	N3—N2—C21	119.32 (14)
C9—O2—C14	118.39 (15)	C18—N3—N2	106.79 (14)
C15—N1—C17	121.43 (16)	C18—N3—C20	122.75 (16)
C16—N2—N3	109.49 (14)	N2—N3—C20	117.57 (15)
C16—N2—C21	123.78 (16)	O1—C1—C2	108.56 (15)

H atoms were included in calculated positions and refined using a riding-model approximation, with constrained C—H bond lengths and isotropic displacement parameters [C—H = 0.93 Å for aromatic CH, 0.97 Å for CH_2 and 0.96 Å for CH_3, and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(C methyl)].

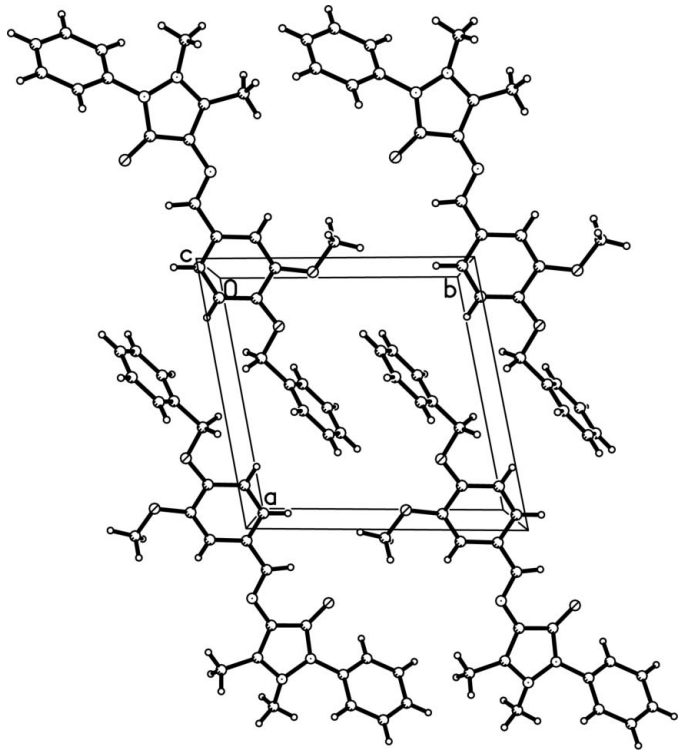


Figure 2
The crystal packing, viewed down the *c* axis.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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