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

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In the title compound, $C_{26}H_{24}ClN_3O_3$, the vanillin group makes dihedral angles of 8.09 (9), 74.91 (8) and 44.66 (9)° with the pyrazolone ring, the terminal chlorobenzene ring and the terminal phenyl ring, respectively. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds.

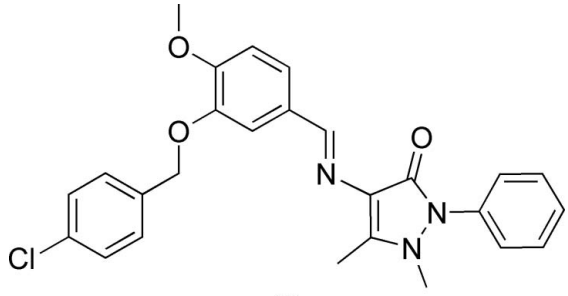
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.126
Data-to-parameter ratio = 13.4

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

Comment

Schiff bases have received a good deal of attention in the development of coordination chemistry because of their significant biological activity (Kahwa *et al.*, 1986). Consequently, significant effort has been devoted to the synthesis of Schiff base derivatives to develop protein and enzyme mimics (Santos *et al.*, 2001). Among the large number of these compounds, 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures (*E*)-(4)-(3-ethoxy-4-hydroxybenzylideneamino)-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Han & Zhen, 2005) and (*E*)-4-(3-ethoxy-4-(2-phenoxyethoxy)benzylideneamino)-2,3-dimethyl-1-phenyl-1,2-dihydropyrazol-5-one (Zhang *et al.*, 2006) have been reported. We report here the synthesis and structure of the title compound, (I) (Fig. 1).



(I)

The bond lengths and angles in (I) are within normal ranges. The pyrazolone ring (C16/C17/C20/N1/N2/N3/O3) is almost planar, with an r.m.s. deviation for fitted atoms of 0.0307 Å. It makes a dihedral angle of 44.54 (9)° with the attached phenyl ring (C21–C26). The vanillin group (C8–C13/C15/O1/O2) is nearly planar, with an r.m.s. deviation for the fitted atoms of 0.0167 Å, and makes dihedral angles of 8.09 (9), 74.91 (8) and 44.66 (9)° with the the pyrazolone ring (C16/C17/C20/N1/N2/N3/O3), the terminal chlorobenzene ring (C1–C6) and the terminal phenyl ring (C21–C26), respectively.

The crystal packing in (I) is stabilized by weak non-classical intermolecular C—H···O hydrogen bonds (Table 1) that form an infinite network (Fig. 2).

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Experimental

An anhydrous ethanol solution (20 ml) of 3-(4-chlorobenzyloxy)-4-methoxybenzaldehyde (2.77 g, 10 mmol) was added to an anhydrous ethanol solution (20 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) and the mixture was stirred at 350 K for 3 h under nitrogen, giving a yellow precipitate. The product was then isolated and recrystallized from ethanol, and then dried *in vacuo* to give the pure compound in 79% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{26}H_{24}ClN_3O_3$
M_r = 461.93
Triclinic, $P\overline{1}$
a = 9.801 (7) Å
b = 10.017 (7) Å
c = 13.394 (10) Å
α = 72.699 (12)°
β = 87.461 (12)°
γ = 67.245 (12)°
V = 1154.0 (14) Å^3
Z = 2
D_x = 1.329 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 294 (2) K
Block, yellow
0.40 × 0.34 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.914, T_{max} = 0.961
5895 measured reflections
4039 independent reflections
2485 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 1.01
4039 reflections
301 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.2246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C24—H24···O2^{i}	0.93	2.51	3.338 (4)	148
C12—H12···O3^{ii}	0.93	2.47	3.370 (4)	163

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

H atoms were included in calculated positions (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

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*.

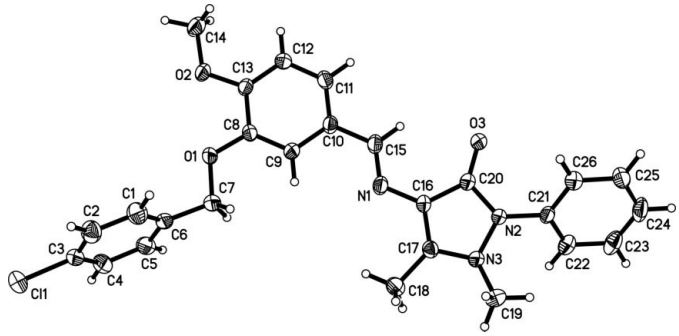

Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

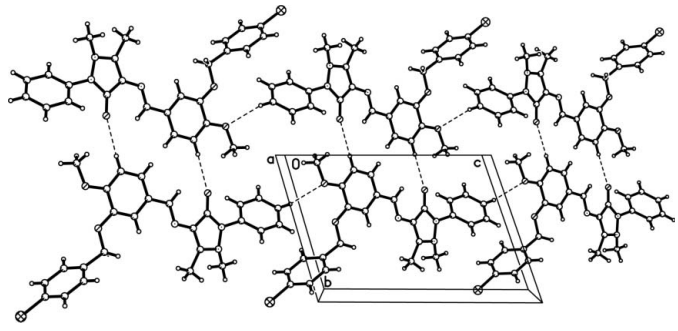

Figure 2
Packing diagram for (I), with C—H···O hydrogen bonds drawn as dashed lines.

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