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

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The title compound, $C_{27}H_{26}ClN_3O_3$, was prepared by reacting 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one and 4-(4-chlorobenzyloxy)-3-ethoxybenzaldehyde. The central ethylvanillin group makes dihedral angles of 63.00 (11), 31.83 (7) and 74.47 (8)° with the chlorobenzene ring, the pyrazolone ring and the terminal phenyl ring, respectively. Packing is stabilized by intermolecular C—H···O hydrogen bonds that form centrosymmetric dimers.

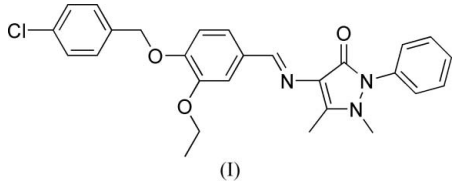
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.055
wR factor = 0.165
Data-to-parameter ratio = 13.9

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

Comment

Schiff base ligands have received a good deal of attention in the development of coordination chemistry for more than 100 years (Kahwa *et al.*, 1986). Among the large number of compounds, 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one forms a variety of Schiff bases with aldehydes (Han & Zhen, 2005; Shi, 2005). In the present study we report the synthesis and molecular structure of such a compound, (I).



(I)

In the title molecule (Fig. 1), bond lengths and angles are within normal ranges. The central ethylvanillin group (C8–C13/C16/O1/O2) is planar, with an r.m.s. deviation for fitted atoms of 0.0224 Å, and it makes dihedral angles of 63.00 (11), 31.83 (7) and 74.47 (8)° with the benzene ring (C1–C6), the pyrazolone ring (C17/C18/N2/N3/C21/N1/O3) and the terminal phenyl ring (C22–C27), respectively. The pyrazolone ring is also almost planar, with an r.m.s. deviation for fitted atoms of 0.0370 Å. It makes a dihedral angle of 48.41 (9)° with the terminal phenyl ring. The crystal packing is stabilized by weak non-classical intermolecular C—H···O=C hydrogen bonds (Table 1) that form centrosymmetric dimers (Fig. 2).

Experimental

An anhydrous (99.5%) ethanol solution of 4-(4-chlorobenzyloxy)-3-ethoxybenzaldehyde (2.91 g, 10 mmol) was added to an anhydrous ethanol solution of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) and the mixture stirred at 350 K for 3 h under nitrogen, whereupon a yellow precipitate appeared. The product was then isolated and recrystallized from ethanol, and dried *in vacuo* to give pure (I) in 82% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{27}H_{26}ClN_3O_3$
M_r = 475.96
Triclinic, $P\overline{1}$
a = 10.019 (2) Å
b = 10.355 (2) Å
c = 12.824 (3) Å
α = 77.080 (4)°
β = 83.710 (4)°
γ = 71.133 (4)°
V = 1226.1 (4) Å^3
Z = 2
D_x = 1.289 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 294 (2) K
Block, yellow
0.34 × 0.30 × 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} = 0.928, T_{max} = 0.963
6294 measured reflections
4299 independent reflections
2253 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.165
S = 1.05
4299 reflections
310 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0704P)^2 + 0.1725P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C26—H26···O3^{i}	0.93	2.60	3.395 (4)	144

Symmetry code: (i) $-x, -y-1, -z+1$.

All H atoms were included in calculated positions and refined using a riding-model. Constrained C—H bond lengths and isotropic U_{iso}(H) parameters: 0.93 Å and 1.2U_{eq}(C) for aromatic, 0.97 Å and 1.2U_{eq}(C) for methylene, and 0.96 Å and 1.5U_{eq}(C) for methyl H atoms.

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

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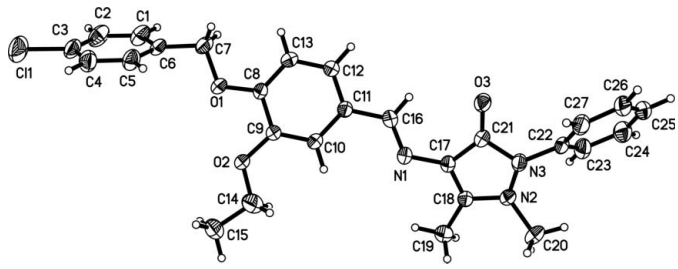

Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

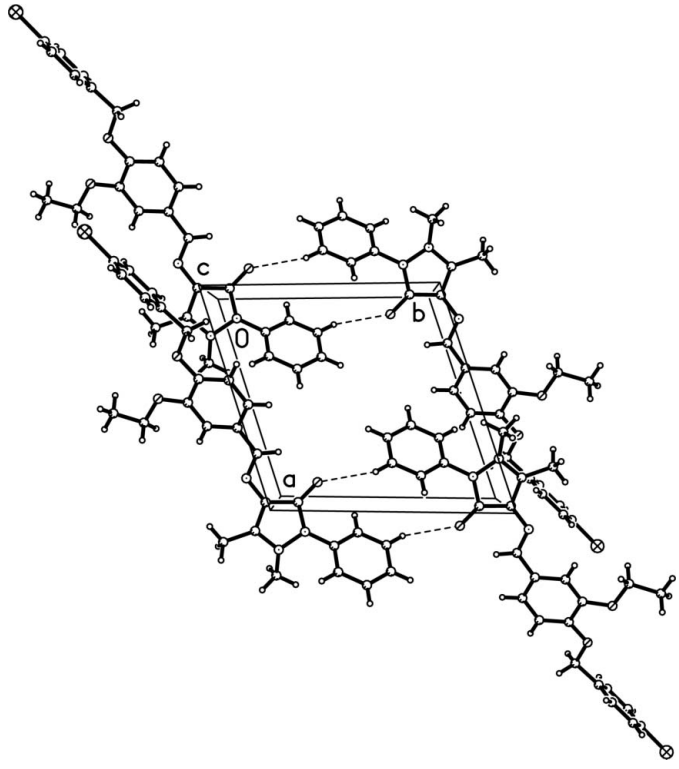

Figure 2
A view, down the *c* axis, of the packing arrangement in the crystal structure of (I). Intermolecular hydrogen bonds are represented by dashed lines.

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