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(*E*)-1,5-Dimethyl-4-[3-(2-phenoxyethoxy)-benzylideneamino]-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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In the title compound, $C_{26}H_{25}N_3O_3$, the central benzene ring makes dihedral angles of 13.93 (7), 54.45 (6) and 80.83 (5)°, respectively, with the pyrazolone ring, the attached phenyl ring and the other terminal phenyl ring. The crystal structure is stabilized by a couple of weak non-classical intermolecular C—H···O interactions, forming an infinite network.

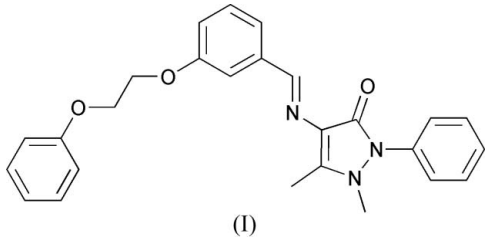
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.138
Data-to-parameter ratio = 15.9

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

Comment

There has been steady growth of interest in the structure and reactivity of Schiff bases due to their potential biological activities such as antibacterial and antitumor (Klayman *et al.*, 1979). Among the large number of compounds, 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one forms a variety of Schiff bases with aldehydes, and the syntheses and crystal structures of some of them, such as (*E*)-1,5-dimethyl-4-{2-[2-(2-nitrophenoxy)-ethoxy]benzylideneamino}-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Diao & Chen, 2006) (*E*)-4-[3-(4-chlorobenzyloxy)-4-methoxybenzylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Duan *et al.*, 2006), have been reported. We report here the synthesis and structure of the title compound, (I).



(I)

In the title molecule (Fig. 1), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The pyrazolone ring (C16–C18/N1–N3/O3) is nearly planar, with an r.m.s. deviation for fitted atoms of 0.0394 Å. It makes a dihedral angle of 54.99 (6)° with the attached phenyl ring (C21–C26). The central benzene ring (C9–C15/O2) is essentially planar, with

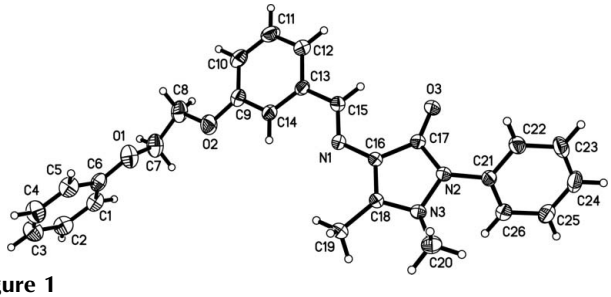


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

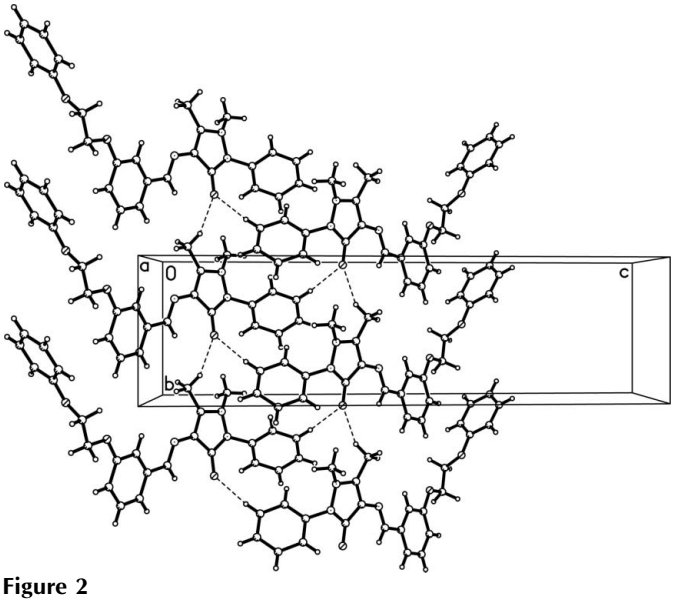


Figure 2
Intermolecular hydrogen-bonding interactions (dashed lines) in (I).

an r.m.s. deviation for fitted atoms of 0.0084 Å. It makes dihedral angles of 13.93 (7), 80.83 (5) and 54.45 (6)°, respectively, with the the pyrazolone ring (C16–C18/N1–N3/O3) and the terminal (C1–C6 and C21–C26) phenyl rings.

The crystal structure is stabilized by a couple of weak non-classical intermolecular C—H···O interactions (Table 1), forming an infinite network (Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 3-(2-phenoxyethoxy)benzaldehyde (2.42 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a yellow precipitate. The product was isolated, recrystallized from acetonitrile, and then dried in a vacuum to give the pure compound in 85% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{26}H_{25}N_3O_3$
M_r = 427.49
Monoclinic, $P2_1/c$
a = 11.3949 (18) Å
b = 7.4456 (12) Å
c = 26.791 (4) Å
β = 95.392 (3)°
V = 2262.9 (6) Å^3
Z = 4
D_x = 1.255 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
Block, yellow
0.30 × 0.24 × 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} = 0.958, T_{max} = 0.984
12330 measured reflections
4635 independent reflections
2621 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.138
S = 0.99
4635 reflections
291 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0654P)^2 + 0.2074P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19A···O3^{i}	0.96	2.31	3.137 (2)	144
C25—H25···O3^{ii}	0.93	2.45	3.368 (3)	169

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

H atoms were included in calculated positions and refined using a riding-model approximation: C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2; C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene; C—H = 0.96 Å and U_{iso}(H) = 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*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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