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4-[(*E*)-4-(2-{4-[(*E*)-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yl)iminomethyl]phenoxy}-ethoxy)benzylideneamino]-1,5-dimethyl-1-phenyl-1*H*-dihydropyrazol-3(2*H*)-one

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In the title compound, $C_{38}H_{36}N_6O_4$, a crystallographic center of symmetry is located at the mid-point of the central C—C bond. The 4-hydroxybenzaldehyde residue makes dihedral angles of 8.09 (9) and 68.93 (7)°, respectively, with the pyrazolone ring and the terminal phenyl ring. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds that link molecules into one-dimensional extended chains.

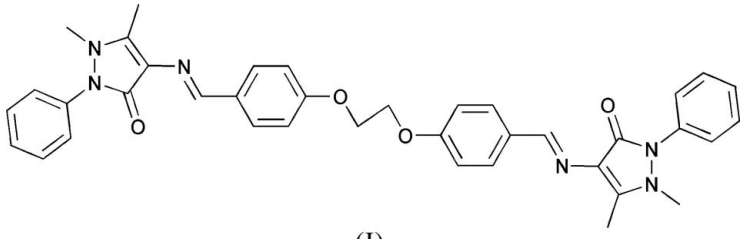
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.131
Data-to-parameter ratio = 15.4

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 owing to their potential biological activities, such as antibacterial and antitumor (Klayman *et al.*, 1979). Consequently, many Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics, such as models to mimic hydrolase in the hydrolysis of *p*-nitrophenyl picolinate (Li *et al.*, 2005). Among the large number of such compounds, 4-amino-1,5-dimethyl-2-phenyl-pyrazol-3-one forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures of some of them, such as (*E*)-1,5-dimethyl-4-{2-[2-(2-nitrophenoxy)-ethoxy]benzyl-ideneamino}-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Diao & Chen, 2006) and (*E*)-4-[3-ethoxy-4-(2-phenoxyethoxy)benzylidene-amino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Zhang *et al.*, 2006), have been reported. We report here the synthesis and structure of the title compound, (I).



(I)

In (I) (Fig. 1), a crystallographic center of symmetry is located at the mid-point of the central C1—C1^{i} bond [symmetry code: (i) $-x+2, -y, -z$]. The bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The pyrazolone ring (C9–C11/N1–N3/O2) is almost planar, with an r.m.s. deviation for fitted atoms of 0.0475 Å. It makes a dihedral angle of 60.87 (7)° with its attached phenyl ring (C14–C19). The 4-hydroxybenzaldehyde residue (C2–C8/O1) is essentially planar, with an r.m.s. deviation for the fitted atoms of 0.0127 Å. This plane makes dihedral angles of 8.09 (9) and 68.93 (7)°, respectively, with the pyrazolone ring (C9–C11/N1–N3/O2) and the terminal (C14–C19) phenyl ring.

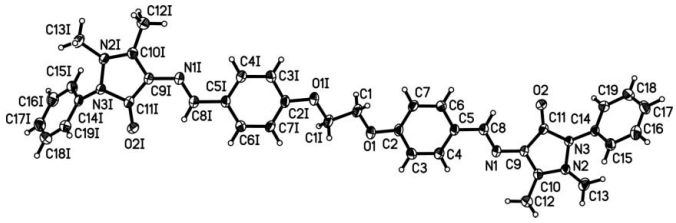


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level [symmetry code: (I) $-x+2, -y, -z$].

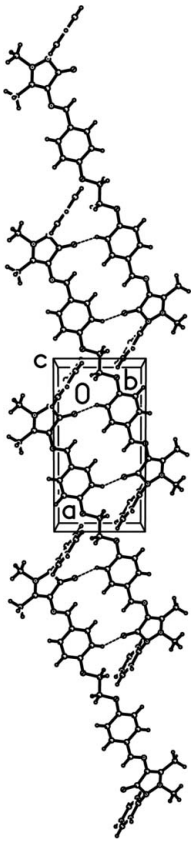


Figure 2
Packing diagram for (I), with hydrogen bonds drawn as dashed lines.

The crystal packing is stabilized by weak non-classical intermolecular C—H···O hydrogen bonds (Table 1). These C—H···O hydrogen bonds link molecules into one-dimensional extended chains (Fig. 2).

Experimental

An anhydrous ethanol solution (100 ml) of 4-[2-(4-formyl-phenoxy)ethoxy]benzaldehyde (2.70 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 was 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 82% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an *N*,*N*-dimethylformamide solution.

Crystal data

$C_{38}H_{36}N_6O_4$
$M_r = 640.73$
Monoclinic, $P2_1/c$
$a = 13.199$ (5) Å
$b = 6.802$ (3) Å
$c = 18.841$ (7) Å
$\beta = 102.315$ (7)°
$V = 1652.6$ (11) Å^3
$Z = 2$
$D_x = 1.288$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 294$ (2) K
Block, yellow
0.38 × 0.26 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.951$, $T_{max} = 0.983$
9053 measured reflections
3383 independent reflections
1892 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 26.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.131$
$S = 1.00$
3383 reflections
219 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.1695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O2^{ii}	0.93	2.50	3.332 (3)	150

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

H atoms were included in calculated positions and refined using the riding model approximation: C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H; C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene CH_2; C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl CH_3.

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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