Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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Received 16 November 2006
Accepted 17 November 2006

In the title compound, $C_{25}H_{21}Cl_2N_3O_2$, the central benzene ring makes dihedral angles of 65.61 (10), 12.95 (15) and 39.49 (14)°, respectively, with the dichlorobenzene ring, the pyrazolone ring and the terminal phenyl ring. Intermolecular C—H···O interactions help to consolidate the crystal packing.

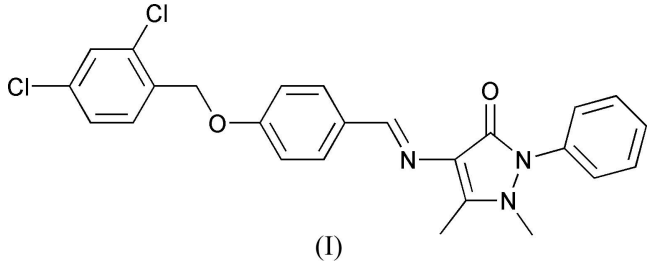
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.048
wR factor = 0.128
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

We are currently studying the reactions of Schiff bases with aldehydes (Han & Zhen, 2005). As part of this work, we report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).



(I)

The bond lengths and angles in (I) are within their normal ranges (Allen *et al.*, 1987). The pyrazolone ring (atoms C15–C17/N1–N3/O2) is close to being planar, with an r.m.s. deviation for the fitted atoms of 0.043 Å. It makes a dihedral angle of 49.67 (12)° with the attached phenyl ring (C20–C25). The central benzene ring makes dihedral angles of 65.61 (10), 12.95 (15) and 39.49 (14)° with the dichlorobenzene ring (C1–C6), the pyrazolone ring (C15–C17/N1—N3/O2) and the phenyl ring (C20–C25), respectively.

The crystal packing in (I) is stabilized by weak C—H···O interactions (Table 1). The shorter of these [C21—H21···O1^{i}; symmetry code: (i) $2-x, 1-y, 1-z$] results in inversion-related dimers. Two further, very weak, intermolecular C—H···O bonds complete the structure (Fig. 2).

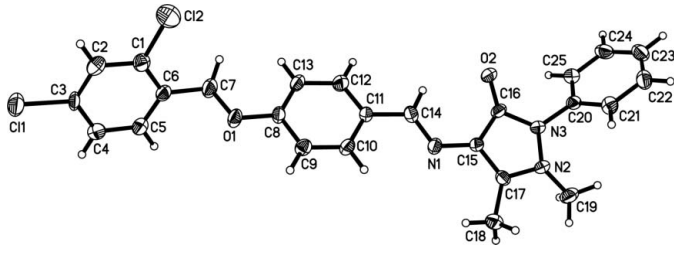


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

Experimental

An anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) was added to an anhydrous ethanol solution (100 ml) of 4-(2,4-dichlorobenzyloxy)benzaldehyde (2.81 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 82% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{25}H_{21}Cl_2N_3O_2$
M_r = 466.35
Monoclinic, $P2_1/c$
a = 16.560 (4) Å
b = 6.9670 (19) Å
c = 19.771 (5) Å
β = 100.601 (5)°
V = 2242.1 (10) Å^3
Z = 4
D_x = 1.382 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 294 (2) K
Block, yellow
0.28 × 0.24 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.897, T_{max} = 0.938
10220 measured reflections
3885 independent reflections
1552 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.128
S = 0.99
3885 reflections
291 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 0.2963P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C21—H21···O1^{i}	0.93	2.47	3.323 (5)	152
C18—H18C···O2^{ii}	0.96	2.57	3.526 (5)	174
C4—H4···O2^{iii}	0.93	2.60	3.233 (5)	126

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, y-1, z$; (iii) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$.

The 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).

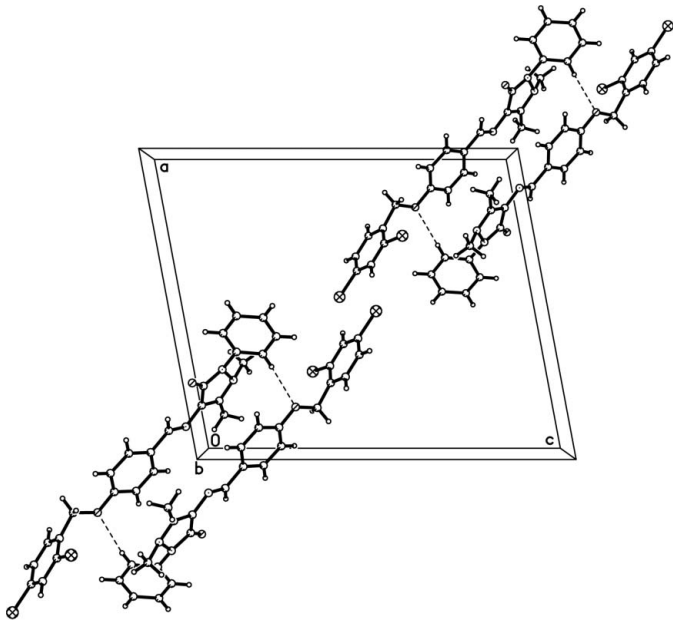


Figure 2
A partial packing diagram for (I), with the dimer-forming C—H···O interactions shown as dashed lines.

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*.

The project was supported by the Foundation of the Education Department of Hebei Province (grant No. 606022).

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