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1-Acetyl-3-(4-chlorophenyl)-5-(4-fluoro-3-phenoxyphenyl)-1H-pyrazole

In the title compound, $C_{23}H_{18}ClFN_2O_2$, the dihedral angles between the pyrazole ring and the attached chlorophenyl ring, the planar acetyl group and the fluorobenzene ring of the phenoxyphenyl unit are 3.3 (1), 5.2 (2) and 74.9 (1)°, respectively. The crystal structure is stabilized by intermolecular C—H⋯O hydrogen bonds and a short Cl⋯F contact.

Comment

Some pyrazoles are known to possess considerable anti-microbial, antiviral, antitumour, anti-inflammatory, anti-histaminic and phytotoxic activities (Mahajan *et al.*, 1991; Janus *et al.*, 1999; Katayama & Oshiyama, 1997; Badawey & El-Ashmawey, 1998; Mishra *et al.*, 1998; Bernard *et al.*, 1985). As part of our ongoing interest in such compounds (Gloe *et al.*, 2000), we report here the structure of the title compound, (I) (Fig. 1, Table 1).


(I)
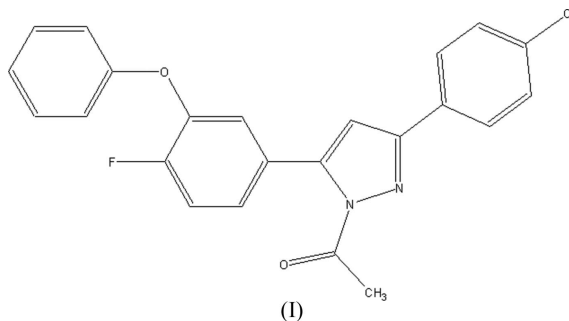
The pyrazole ring of (I) is essentially planar, with a maximum deviation from the ring plane of 0.185 (2) Å for atom C13. The chlorophenyl substituent subtends an angle of 3.3 (1)° to this plane, while the fluorobenzene ring of the phenoxyphenyl unit is inclined at an angle of 74.9 (1)°. There is some evidence for delocalization in the pyrazole ring: while the C13—N1 bond distance corresponds to a single bond, the N1—N2 bond is short and compares well with similar values reported in the literature (Hökelek, Kilic & Hayvali, 2002; Hökelek, Kilic, Isikalan *et al.*, 2002).
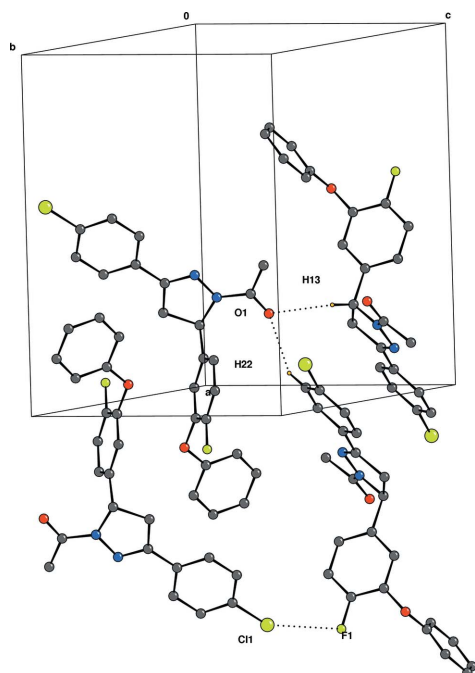
In the crystal structure, C—H⋯O intermolecular inter-actions form molecular chains along the crystallographic screw axis and in the *c*-glide plane (Fig. 2, Table 2). Furthermore, a short Cl1⋯F1 contact [3.231 (2) Å; symmetry code $(-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2})$] provides additional stability (Fig. 2).

Experimental

Single crystals of compound (I) (Mohan, 2006) were grown by slow evaporation of a solution in acetone at 275–277 K.
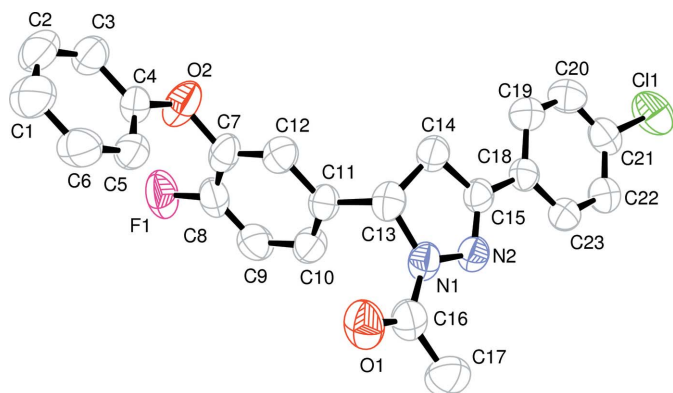
Figure 1
A view of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted.

Figure 2
The C—H···O interactions and the Cl···F short contact in the crystal structure (dotted lines). Other H atoms have been omitted for clarity.

Crystal data

$C_{23}H_{18}ClFN_2O_2$	$Z = 4$
$M_r = 408.84$	$D_x = 1.338$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 14.577\ (10)$ Å	$\mu = 0.22$ mm^{-1}
$b = 9.342\ (6)$ Å	$T = 290\ (2)$ K
$c = 14.994\ (10)$ Å	Block, colourless
$\beta = 96.237\ (11)°$	$0.41 \times 0.28 \times 0.28$ mm
$V = 2030\ (2)$ Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	15482 measured reflections
	4216 independent reflections
φ and ω scans	3210 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.020$
$T_{min} = 0.894$, $T_{max} = 0.941$	$\theta_{max} = 27.3°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.046$	$+ 0.4522P]$
$wR(F^2) = 0.128$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
4216 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
334 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

F1—C8	1.356 (2)	N2—N1	1.384 (2)
O2—C4	1.377 (2)	N1—C16	1.360 (3)
O1—C16	1.215 (2)	N1—C13	1.466 (2)
C4—O2—C7	118.97 (14)	N1—C16—C17	116.77 (18)
O1—C16—N1	119.7 (2)		
C19—C18—C15—C14	−3.8 (3)	C13—N1—C16—C17	175.10 (18)
C10—C11—C13—C14	96.6 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···O1^i	0.96 (2)	2.55 (2)	3.385 (3)	146 (2)
C22—H22···O1^{ii}	0.90 (2)	2.50 (2)	3.309 (3)	150 (2)

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

The H atoms on the methyl atom C17 were positioned geometrically and allowed to ride on the parent atom, with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$. The remaining H atoms were located in a difference Fourier map and refined isotropically. The refined C—H bond lengths are in the range 0.87 (3)–0.97 (2) Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1999) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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