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3-Ethoxycarbonyl-1-phenyl-1*H*-pyrazol-5-yl 4-chlorobenzoate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.046
wR factor = 0.131
Data-to-parameter ratio = 15.2

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

In the title compound, $C_{19}H_{15}ClN_2O_4$, the molecules are held together by π–π stacking interactions. The ethyl group was found to be disordered.

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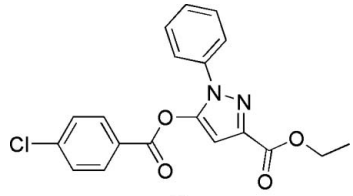
Comment

3-Substituted pyrazole derivatives have active biological properties (Vasilev *et al.*, 1981; Kim *et al.*, 1989; Hwang & Kim, 1994; Liu & Li, 2004). Recently, various new pyrazole derivatives have been prepared and their crystal structures reported by our group (Li, Li *et al.*, 2005; Li, Duan *et al.*, 2005; Guo *et al.*, 2005; Duan *et al.*, 2005). As a continuation of our project, the title compound, (I), was obtained *via* 4-chlorobenzoylation of commercially available ethyl 5-oxo-1-phenyl-2,5-dihydro-1*H*-pyrazole-3-carboxylate.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The dihedral angle between the pyrazole and phenyl rings is 31.19 (15)°, that between the pyrazole and chlorophenyl rings is 74.32 (15)°.

In the crystal structure (Fig. 2), π–π stacking interactions are observed. There is a weak π–π interaction between the phenyl ring at (x, y, z) and that at $(-x, \frac{1}{2}+y, \frac{1}{2}-z)$, with a centroid–centroid separation of 5.543 (2) Å. There is a strong

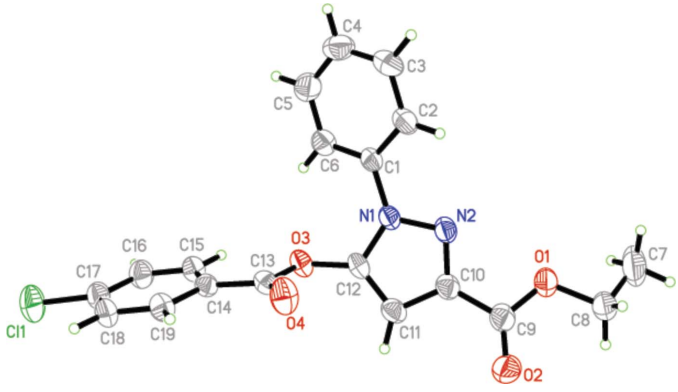


Figure 1
The molecular structure of (I), with the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. Only the major component of the disordered ethyl group is shown.

π–π interaction between the chlorophenyl ring at (x, y, z) and that at ($1-x$, $1-y$, $1-z$), with centroid–centroid and interplanar separations of 3.918 (18) and 3.491 Å, respectively.

Experimental

The title compound was obtained, according to the method of Li, Li *et al.* (2005) as colorless blocks (yield 84.0%, m.p. 394.5–395.7 K). Single crystals suitable for X-ray diffraction were grown from a solution of ethyl acetate/*n*-hexane (1:1 *v*/*v*).

Crystal data

$C_{19}H_{15}ClN_2O_4$
M_r = 370.78
Monoclinic, $P2_1/c$
a = 13.426 (3) Å
b = 5.9078 (11) Å
c = 23.142 (4) Å
β = 100.051 (3)°
V = 1807.4 (6) Å^3
Z = 4
D_x = 1.363 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1480 reflections
θ = 2.6–20.3°
μ = 0.24 mm^{-1}
T = 294 (2) K
Block, colorless
0.20 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.954, T_{max} = 0.977
9758 measured reflections
3700 independent reflections
1603 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 26.4°
$h = -16 \rightarrow 16$
$k = -7 \rightarrow 3$
$l = -28 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.131
S = 0.97
3700 reflections
243 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0025 (8)

H atoms were positioned geometrically and constrained to ride on their parent atoms [C—H = 0.93 Å for Csp^2—H and 0.97 Å for CH_2 groups, with U_{iso}(H) = 1.2U_{eq}(C), and C—H = 0.96 Å for methyl groups, with U_{iso}(H) = 1.5U_{eq}(C)]. The ethyl group was found to be disordered over two sites. The site-occupancy factors refined to 0.538 (18) and 0.462 (18).

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

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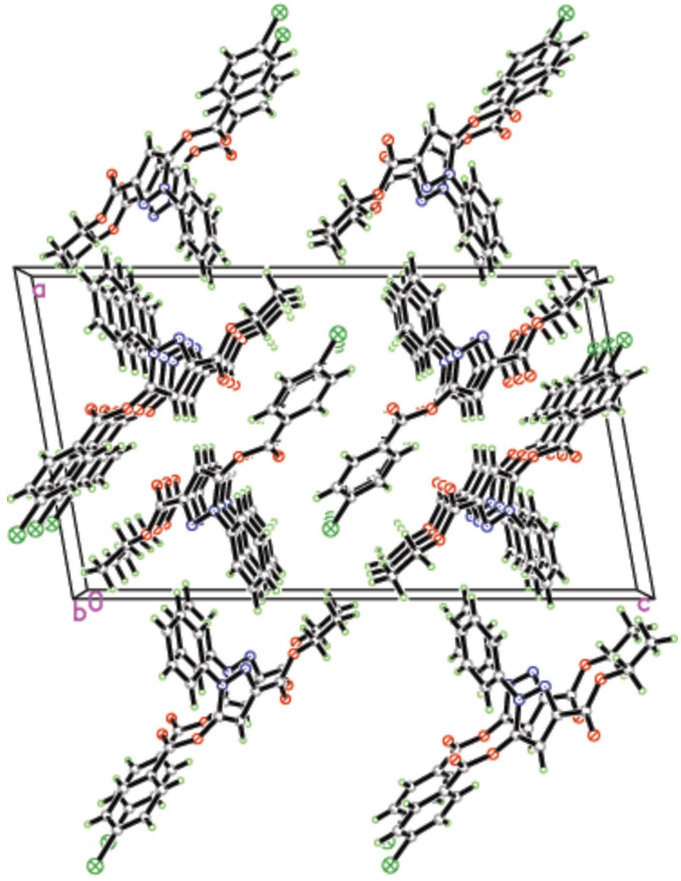

Figure 2
A packing diagram for (I). The molecules are held together by π–π stacking interactions. Only the major component of the disordered ethyl group is shown.

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