Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 1-(4-*tert*-butylbenzyl)-3-(4-chlorophenyl)-1*H*-pyrazole-5-carboxylate

Yong Xia,[a] Wen-Liang Dong,[a] Xiao-Ling Ding[b] and Bao-Xiang Zhao[a]*

[a]School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China, and [b]College of Advanced Professional Technology, Qingdao University, Qingdao 266061, People's Republic of China
Correspondence e-mail: sduzhao@hotmail.com

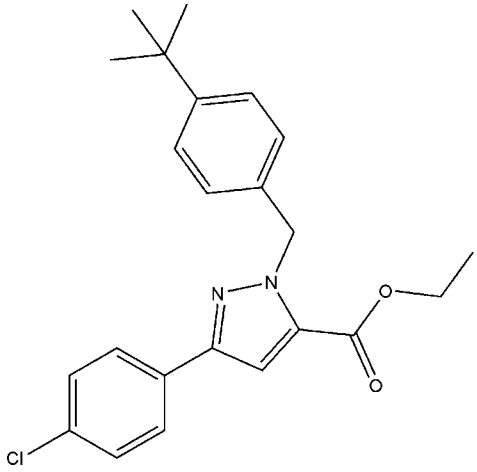
Received 16 May 2007; accepted 12 June 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.198; data-to-parameter ratio = 18.8.

In the title structure, $C_{23}H_{25}ClN_2O_2$, there are weak intramolecular C—H···N and C—H···O hydrogen bonds. There is a C=O···*Cg* interaction (*Cg* is the centroid of the pyrazole ring) and the distance between the centroids of the ring and the C=O bond is 3.017 (3) Å. The angle between the pyrazole ring and the chlorophenyl ring is 12.85 (13)°. The crystal packing is stabilized mainly by van der Waals forces.

Related literature

For related literature, see: Finn *et al.* (2003); Menozzi *et al.* (1997); Pevarello *et al.* (2004); Regan *et al.* (2002); Wustrow *et al.* (1998); Xia *et al.* (2007).



Experimental

Crystal data

$C_{23}H_{25}ClN_2O_2$
M_r = 396.90
Triclinic, $P\overline{1}$
a = 7.9351 (1) Å
b = 11.9430 (2) Å
c = 12.6558 (2) Å
α = 70.432 (1)°
β = 79.340 (1)°
γ = 71.023 (1)°
V = 1064.78 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 293 (2) K
0.44 × 0.35 × 0.32 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.841, T_{max} = 0.939
15955 measured reflections
4824 independent reflections
3237 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.198
S = 1.07
4824 reflections
257 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···N1	0.93	2.56	2.865 (3)	100
C13—H13*A*···O2	0.97	2.37	2.925 (3)	116

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This study was supported by the Foundation of the Ministry of Education (grant No. 104112) and the Natural Science Foundation of Shandong Province (grant No. Y2005B12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2052).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2* software suite. Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Finn, J., Mattia, K., Morytko, M., Ram, S., Yang, Y., Wu, X., Mak, E., Gallant, P. & Keith, D. (2003). *Bioorg. Med. Chem. Lett.* **13**, 2231–2234.
Menozzi, G., Mosti, L., Fossa, P., Mattioli, F. & Ghia, M. J. (1997). *J. Heterocycl. Chem.* **34**, 963–968.
Pevarello, P. *et al.* (2004). *J. Med. Chem.* **47**, 3367–3380.
Regan, J., Breitfelder, S., Cirillo, P., Gilmore, T., Graham, A. G., Hickey, E., Klaus, B., Madwed, J., Moriak, M., Moss, N., Pargellis, C., Pav, S., Proto, A., Swinamer, A., Tong, L. & Torcellini, C. (2002). *J. Med. Chem.* **45**, 2994–3008.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Wustrow, D. J., Capiris, T., Rubin, R., Knobelsdorf, J. A., Akunne, H., Davis, M. D., MacKenzie, R., Pugsley, T. A., Zoski, K. T., Heffner, T. G. & Wise, L. D. (1998). *Bioorg. Med. Chem. Lett.* **8**, 2067–2070.
Xia, Y., Ding, X.-L., Ge, Y.-Q., Liu, L.-D. & Zhao, B.-X. (2007). *Acta Cryst.* E**63**, o394–o395.

 doi:10.1107/S1600536807028814

supplementary materials

Acta Cryst. (2007). E**63**, o3257 [**doi:10.1107/S1600536807028814**]

Ethyl 1-(4-*tert*-butylbenzyl)-3-(4-chlorophenyl)-1*H*-pyrazole-5-carboxylate

Y. Xia, W.-L. Dong, X.-L. Ding and B.-X. Zhao

Comment

Pyrazole nucleus has pronounced pharmacological applications in antibacterial (Finn *et al.*, 2003), anti-anxiety (Wustrow *et al.*, 1998) antipyretic, analgesic and anti-inflammatory drugs (Menozzi *et al.*, 1997). Due to the easy preparation and rich biological activity the pyrazole framework represents an interesting template for combinatorial as well as for medicinal chemistry (Regan *et al.*, 2002; Pevarello *et al.*, 2004).

Experimental

The title compound has been synthesized according to Xia *et al.* (2007): A mixture of ethyl 3-(4-chlorophenyl)-1*H*-pyrazole-5-carboxylate (0.01 mol), 1-*tert*-butyl-4-(chloromethyl)benzene (0.01 mol) and potassium carbonate (0.01 mol) in acetonitrile (20 ml) was heated to reflux for 5 h. The solvent was removed under reduced pressure and the residue was extracted with ethyl acetate (30 ml). The organic phase was washed with brine and dried over anhydrous magnesium sulfate. After evaporation of the solvent under reduced pressure, a solid was obtained with a yield equal to 75%. The solid was dissolved in ethyl acetate/petroleum ether (1:2 *v*/*v*). The crystals of the title compound were obtained by evaporation of the solution at room temperature over a period of one week.

Refinement

All the H atoms except H11B and H23A were discernible in the difference Fourier map. Nevertheless, the found H atoms as well as H11B and H23A were placed into calculated positions and refined using a riding model with C—H = 0.97 Å (for CH_2 groups) and 0.96 Å (for CH_3 groups); $U_{iso}(H) = 1.2U_{eq}(CH_2)$ or $U_{iso}(H) = 1.5U_{eq}(CH_3)$.

Figures

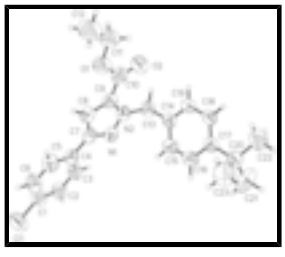


Fig. 1. The structure of the title molecule showing displacement ellipsoids drawn at the 50% probability level. The H atoms are depicted as spheres of arbitrary radii.

Ethyl 1-(4-*tert*-butylbenzyl)-3-(4-chlorophenyl)-1*H*-pyrazole-5- carboxylate

Crystal data

$C_{23}H_{25}ClN_2O_2$ $Z = 2$

M_r = 396.90	F_{000} = 420
Triclinic, $P\bar{1}$	D_x = 1.238 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.93510 (10) Å	Cell parameters from 4831 reflections
b = 11.9430 (2) Å	θ = 2.7–24.0º
c = 12.6558 (2) Å	μ = 0.20 mm^{-1}
α = 70.4320 (10)º	T = 293 (2) K
β = 79.3400 (10)º	Block, colourless
γ = 71.0230 (10)º	0.44 × 0.35 × 0.32 mm
V = 1064.78 (3) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	4824 independent reflections
Radiation source: fine-focus sealed tube	3237 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 293(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (APEX2; Bruker, 2005)	h = −10→10
T_{min} = 0.841, T_{max} = 0.939	k = −14→15
15955 measured reflections	l = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.059	H-atom parameters constrained
$wR(F^2)$ = 0.198	$w = 1/[\sigma^2(F_o^2) + (0.098P)^2 + 0.2242P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
4824 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
257 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
96 constraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8400 (3)	0.1190 (3)	−0.2742 (2)	0.0733 (6)
C2	0.9389 (4)	0.0694 (2)	−0.1824 (2)	0.0757 (6)
H2	1.0090	−0.0127	−0.1645	0.091*
C3	0.9325 (3)	0.1431 (2)	−0.1173 (2)	0.0693 (6)
H3	1.0011	0.1101	−0.0560	0.083*
C4	0.8268 (3)	0.26521 (19)	−0.14063 (17)	0.0581 (5)
C5	0.7294 (3)	0.3124 (2)	−0.2340 (2)	0.0731 (6)
H5	0.6578	0.3941	−0.2520	0.088*
C6	0.7373 (3)	0.2398 (3)	−0.3006 (2)	0.0818 (7)
H6	0.6726	0.2731	−0.3637	0.098*
C7	0.8169 (3)	0.34127 (18)	−0.06786 (17)	0.0570 (5)
C8	0.7448 (3)	0.46923 (19)	−0.08634 (18)	0.0615 (5)
H8	0.6916	0.5274	−0.1497	0.074*
C9	0.7694 (3)	0.4904 (2)	0.00879 (18)	0.0613 (5)
C10	0.7236 (3)	0.6070 (2)	0.0386 (2)	0.0695 (6)
C11	0.6048 (5)	0.8229 (3)	−0.0261 (3)	0.1026 (10)
H11A	0.5388	0.8196	0.0469	0.123*
H11B	0.7125	0.8451	−0.0270	0.123*
C12	0.4977 (6)	0.9139 (3)	−0.1125 (4)	0.1328 (14)
H12A	0.5684	0.9241	−0.1835	0.199*
H12B	0.4550	0.9915	−0.0954	0.199*
H12C	0.3978	0.8873	−0.1165	0.199*
C13	0.8939 (3)	0.3461 (2)	0.19562 (19)	0.0672 (6)
H13A	0.9302	0.4120	0.2050	0.081*
H13B	0.9930	0.2710	0.2119	0.081*
C14	0.7343 (3)	0.32618 (18)	0.27736 (17)	0.0570 (5)
C15	0.6616 (4)	0.2337 (2)	0.2844 (2)	0.0899 (9)
H15	0.7122	0.1827	0.2384	0.108*
C16	0.5160 (4)	0.2151 (2)	0.3581 (2)	0.0894 (9)
H16	0.4705	0.1517	0.3603	0.107*
C17	0.4343 (3)	0.28730 (17)	0.42923 (16)	0.0550 (5)
C18	0.5076 (3)	0.37929 (19)	0.42172 (18)	0.0625 (5)
H18	0.4575	0.4300	0.4681	0.075*
C19	0.6542 (3)	0.3991 (2)	0.34712 (19)	0.0649 (5)
H19	0.6991	0.4630	0.3442	0.078*
C20	0.2712 (3)	0.2639 (2)	0.50910 (19)	0.0656 (5)
C21	0.3156 (5)	0.1280 (3)	0.5793 (3)	0.1250 (13)
H21A	0.3416	0.0766	0.5306	0.188*
H21B	0.2153	0.1137	0.6319	0.188*
H21C	0.4179	0.1081	0.6196	0.188*
C22	0.2155 (5)	0.3413 (4)	0.5903 (3)	0.1224 (13)
H22A	0.3128	0.3224	0.6344	0.184*

H22B	0.1139	0.3227	0.6391	0.184*
H22C	0.1846	0.4277	0.5486	0.184*
C23	0.1175 (4)	0.2919 (4)	0.4406 (3)	0.1135 (11)
H23A	0.0880	0.3775	0.3967	0.170*
H23B	0.0155	0.2754	0.4902	0.170*
H23C	0.1515	0.2405	0.3915	0.170*
Cl1	0.85235 (12)	0.02856 (9)	−0.35989 (7)	0.1085 (3)
N1	0.8817 (2)	0.28689 (16)	0.03336 (14)	0.0599 (4)
N2	0.8527 (2)	0.37855 (16)	0.07868 (14)	0.0608 (4)
O1	0.6522 (3)	0.70272 (15)	−0.04525 (16)	0.0877 (5)
O2	0.7491 (3)	0.61609 (18)	0.12555 (17)	0.0940 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0674 (14)	0.0919 (16)	0.0694 (14)	−0.0270 (12)	0.0013 (11)	−0.0345 (13)
C2	0.0834 (16)	0.0710 (14)	0.0694 (15)	−0.0120 (11)	−0.0080 (12)	−0.0254 (11)
C3	0.0754 (14)	0.0671 (12)	0.0588 (12)	−0.0090 (10)	−0.0143 (10)	−0.0166 (10)
C4	0.0538 (11)	0.0643 (11)	0.0507 (11)	−0.0168 (9)	−0.0002 (8)	−0.0125 (9)
C5	0.0651 (13)	0.0763 (14)	0.0687 (14)	−0.0062 (11)	−0.0145 (11)	−0.0185 (11)
C6	0.0742 (15)	0.1045 (19)	0.0702 (15)	−0.0202 (14)	−0.0202 (12)	−0.0279 (14)
C7	0.0513 (10)	0.0613 (11)	0.0526 (11)	−0.0147 (8)	0.0003 (8)	−0.0131 (9)
C8	0.0615 (12)	0.0595 (11)	0.0563 (12)	−0.0159 (9)	−0.0030 (9)	−0.0103 (9)
C9	0.0567 (11)	0.0627 (11)	0.0608 (12)	−0.0207 (9)	0.0039 (9)	−0.0147 (9)
C10	0.0684 (14)	0.0683 (13)	0.0700 (15)	−0.0245 (10)	0.0044 (11)	−0.0187 (11)
C11	0.128 (3)	0.0693 (16)	0.114 (2)	−0.0187 (16)	−0.021 (2)	−0.0345 (16)
C12	0.190 (4)	0.0763 (19)	0.129 (3)	−0.015 (2)	−0.047 (3)	−0.031 (2)
C13	0.0619 (13)	0.0826 (14)	0.0589 (12)	−0.0215 (10)	−0.0065 (10)	−0.0215 (11)
C14	0.0607 (11)	0.0599 (11)	0.0504 (10)	−0.0151 (9)	−0.0077 (8)	−0.0167 (8)
C15	0.110 (2)	0.0854 (16)	0.0934 (19)	−0.0455 (15)	0.0363 (16)	−0.0576 (15)
C16	0.109 (2)	0.0850 (16)	0.0991 (19)	−0.0534 (15)	0.0329 (16)	−0.0563 (15)
C17	0.0585 (11)	0.0550 (10)	0.0524 (11)	−0.0129 (8)	−0.0085 (8)	−0.0182 (8)
C18	0.0717 (13)	0.0629 (11)	0.0592 (12)	−0.0157 (10)	−0.0041 (10)	−0.0300 (10)
C19	0.0761 (14)	0.0671 (12)	0.0645 (13)	−0.0285 (10)	−0.0059 (10)	−0.0281 (10)
C20	0.0584 (12)	0.0759 (13)	0.0676 (13)	−0.0196 (10)	−0.0026 (10)	−0.0285 (11)
C21	0.102 (2)	0.116 (2)	0.112 (3)	−0.0306 (19)	0.0248 (19)	0.005 (2)
C22	0.108 (2)	0.179 (4)	0.122 (3)	−0.072 (2)	0.043 (2)	−0.095 (3)
C23	0.0793 (19)	0.162 (3)	0.105 (2)	−0.0364 (19)	−0.0122 (17)	−0.042 (2)
Cl1	0.1159 (6)	0.1348 (7)	0.1051 (6)	−0.0420 (5)	−0.0072 (5)	−0.0687 (5)
N1	0.0590 (10)	0.0627 (10)	0.0534 (10)	−0.0146 (7)	−0.0020 (7)	−0.0155 (8)
N2	0.0589 (10)	0.0675 (10)	0.0535 (10)	−0.0187 (8)	−0.0008 (7)	−0.0160 (8)
O1	0.1104 (14)	0.0619 (9)	0.0899 (13)	−0.0174 (9)	−0.0180 (10)	−0.0233 (9)
O2	0.1237 (16)	0.0853 (12)	0.0800 (12)	−0.0315 (11)	−0.0052 (11)	−0.0333 (10)

Geometric parameters (Å, °)

C1—C6	1.367 (4)	C13—C14	1.509 (3)
C1—C2	1.376 (4)	C13—H13A	0.9700
C1—Cl1	1.741 (3)	C13—H13B	0.9700

C2—C3	1.377 (3)	C14—C19	1.375 (3)
C2—H2	0.9300	C14—C15	1.375 (3)
C3—C4	1.388 (3)	C15—C16	1.372 (4)
C3—H3	0.9300	C15—H15	0.9300
C4—C5	1.386 (3)	C16—C17	1.384 (3)
C4—C7	1.472 (3)	C16—H16	0.9300
C5—C6	1.378 (4)	C17—C18	1.371 (3)
C5—H5	0.9300	C17—C20	1.529 (3)
C6—H6	0.9300	C18—C19	1.386 (3)
C7—N1	1.340 (3)	C18—H18	0.9300
C7—C8	1.400 (3)	C19—H19	0.9300
C8—C9	1.369 (3)	C20—C23	1.510 (4)
C8—H8	0.9300	C20—C22	1.519 (4)
C9—N2	1.361 (3)	C20—C21	1.525 (4)
C9—C10	1.479 (3)	C21—H21A	0.9600
C10—O2	1.200 (3)	C21—H21B	0.9600
C10—O1	1.320 (3)	C21—H21C	0.9600
C11—C12	1.430 (5)	C22—H22A	0.9600
C11—O1	1.452 (3)	C22—H22B	0.9600
C11—H11A	0.9700	C22—H22C	0.9600
C11—H11B	0.9700	C23—H23A	0.9600
C12—H12A	0.9600	C23—H23B	0.9600
C12—H12B	0.9600	C23—H23C	0.9600
C12—H12C	0.9600	N1—N2	1.337 (2)
C13—N2	1.470 (3)		
C6—C1—C2	120.5 (2)	C19—C14—C15	116.9 (2)
C6—C1—Cl1	120.0 (2)	C19—C14—C13	122.20 (19)
C2—C1—Cl1	119.5 (2)	C15—C14—C13	120.86 (19)
C1—C2—C3	119.0 (2)	C16—C15—C14	121.4 (2)
C1—C2—H2	120.5	C16—C15—H15	119.3
C3—C2—H2	120.5	C14—C15—H15	119.3
C2—C3—C4	121.9 (2)	C15—C16—C17	122.4 (2)
C2—C3—H3	119.1	C15—C16—H16	118.8
C4—C3—H3	119.1	C17—C16—H16	118.8
C5—C4—C3	117.6 (2)	C18—C17—C16	115.9 (2)
C5—C4—C7	121.28 (19)	C18—C17—C20	123.57 (18)
C3—C4—C7	121.12 (19)	C16—C17—C20	120.53 (19)
C6—C5—C4	120.8 (2)	C17—C18—C19	122.06 (18)
C6—C5—H5	119.6	C17—C18—H18	119.0
C4—C5—H5	119.6	C19—C18—H18	119.0
C1—C6—C5	120.2 (2)	C14—C19—C18	121.34 (19)
C1—C6—H6	119.9	C14—C19—H19	119.3
C5—C6—H6	119.9	C18—C19—H19	119.3
N1—C7—C8	110.64 (19)	C23—C20—C22	109.6 (2)
N1—C7—C4	119.66 (18)	C23—C20—C21	108.9 (3)
C8—C7—C4	129.70 (19)	C22—C20—C21	107.4 (3)
C9—C8—C7	105.23 (19)	C23—C20—C17	109.0 (2)
C9—C8—H8	127.4	C22—C20—C17	112.5 (2)
C7—C8—H8	127.4	C21—C20—C17	109.21 (19)

N2—C9—C8	106.89 (19)	C20—C21—H21A	109.5
N2—C9—C10	122.4 (2)	C20—C21—H21B	109.5
C8—C9—C10	130.7 (2)	H21A—C21—H21B	109.5
O2—C10—O1	123.6 (2)	C20—C21—H21C	109.5
O2—C10—C9	125.8 (2)	H21A—C21—H21C	109.5
O1—C10—C9	110.6 (2)	H21B—C21—H21C	109.5
C12—C11—O1	109.3 (3)	C20—C22—H22A	109.5
C12—C11—H11A	109.8	C20—C22—H22B	109.5
O1—C11—H11A	109.8	H22A—C22—H22B	109.5
C12—C11—H11B	109.8	C20—C22—H22C	109.5
O1—C11—H11B	109.8	H22A—C22—H22C	109.5
H11A—C11—H11B	108.3	H22B—C22—H22C	109.5
C11—C12—H12A	109.5	C20—C23—H23A	109.5
C11—C12—H12B	109.5	C20—C23—H23B	109.5
H12A—C12—H12B	109.5	H23A—C23—H23B	109.5
C11—C12—H12C	109.5	C20—C23—H23C	109.5
H12A—C12—H12C	109.5	H23A—C23—H23C	109.5
H12B—C12—H12C	109.5	H23B—C23—H23C	109.5
N2—C13—C14	111.33 (17)	N2—N1—C7	105.59 (16)
N2—C13—H13A	109.4	N1—N2—C9	111.65 (17)
C14—C13—H13A	109.4	N1—N2—C13	118.38 (17)
N2—C13—H13B	109.4	C9—N2—C13	129.60 (19)
C14—C13—H13B	109.4	C10—O1—C11	115.5 (2)
H13A—C13—H13B	108.0		
C6—C1—C2—C3	0.2 (4)	C15—C16—C17—C18	0.1 (4)
Cl1—C1—C2—C3	177.90 (19)	C15—C16—C17—C20	179.4 (3)
C1—C2—C3—C4	1.2 (4)	C16—C17—C18—C19	0.2 (3)
C2—C3—C4—C5	−1.4 (4)	C20—C17—C18—C19	−179.0 (2)
C2—C3—C4—C7	177.9 (2)	C15—C14—C19—C18	0.5 (3)
C3—C4—C5—C6	0.3 (4)	C13—C14—C19—C18	−180.0 (2)
C7—C4—C5—C6	−178.9 (2)	C17—C18—C19—C14	−0.6 (3)
C2—C1—C6—C5	−1.2 (4)	C18—C17—C20—C23	113.9 (3)
Cl1—C1—C6—C5	−178.9 (2)	C16—C17—C20—C23	−65.4 (3)
C4—C5—C6—C1	1.0 (4)	C18—C17—C20—C22	−8.0 (3)
C5—C4—C7—N1	166.2 (2)	C16—C17—C20—C22	172.7 (3)
C3—C4—C7—N1	−13.0 (3)	C18—C17—C20—C21	−127.2 (3)
C5—C4—C7—C8	−12.9 (3)	C16—C17—C20—C21	53.5 (3)
C3—C4—C7—C8	167.9 (2)	C8—C7—N1—N2	−0.4 (2)
N1—C7—C8—C9	0.2 (2)	C4—C7—N1—N2	−179.63 (17)
C4—C7—C8—C9	179.34 (19)	C7—N1—N2—C9	0.4 (2)
C7—C8—C9—N2	0.1 (2)	C7—N1—N2—C13	174.07 (17)
C7—C8—C9—C10	179.0 (2)	C8—C9—N2—N1	−0.3 (2)
N2—C9—C10—O2	−2.0 (4)	C10—C9—N2—N1	−179.39 (18)
C8—C9—C10—O2	179.1 (2)	C8—C9—N2—C13	−173.1 (2)
N2—C9—C10—O1	176.88 (19)	C10—C9—N2—C13	7.9 (3)
C8—C9—C10—O1	−1.9 (3)	C14—C13—N2—N1	−89.9 (2)
N2—C13—C14—C19	−117.6 (2)	C14—C13—N2—C9	82.4 (3)
N2—C13—C14—C15	61.9 (3)	O2—C10—O1—C11	0.1 (4)
C19—C14—C15—C16	−0.2 (4)	C9—C10—O1—C11	−178.9 (2)

C13—C14—C15—C16	−179.7 (3)	C12—C11—O1—C10	−168.5 (3)
C14—C15—C16—C17	−0.1 (5)		

Hydrogen-bond geometry (Å, °)

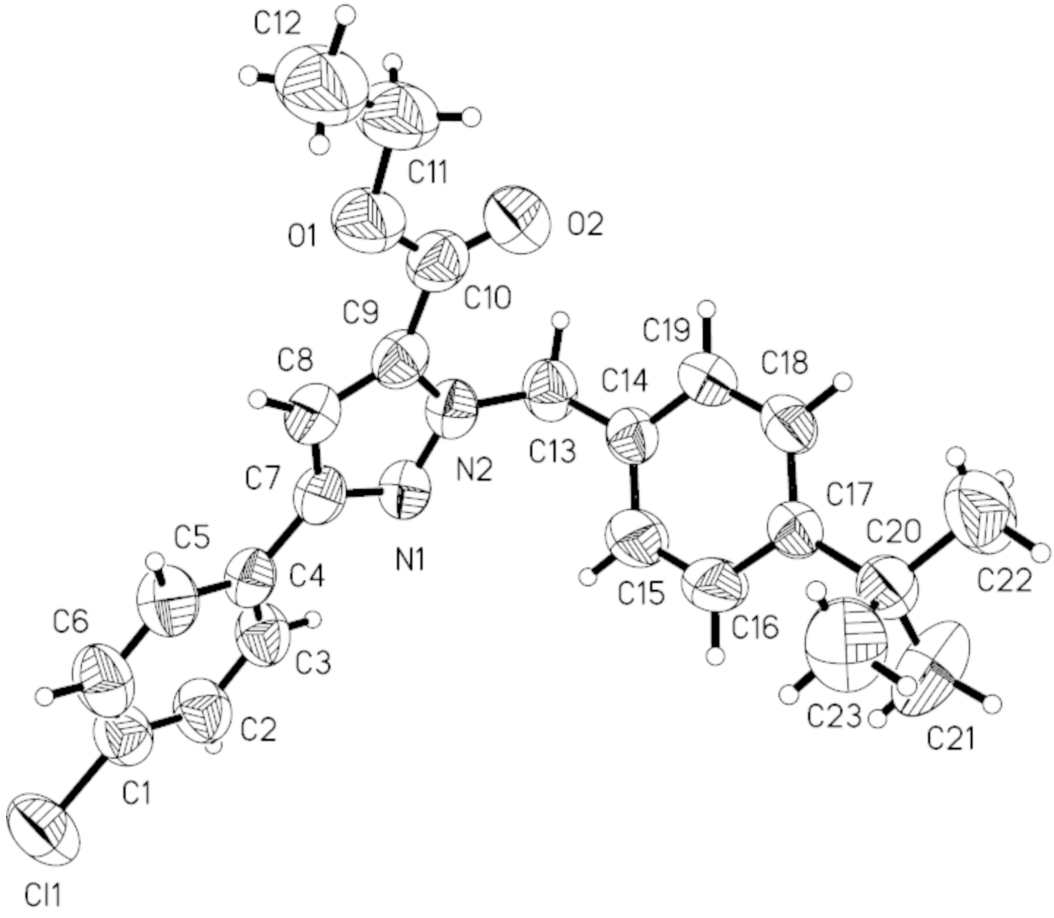
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···N1	0.93	2.56	2.865 (3)	100
C13—H13A···O2	0.97	2.37	2.925 (3)	116

Y—X···π-ring interactions calculated by PLATON [Spek (2003). J. Appl. Cryst. 36, 7–13]. Cg^i is the centroid of the pyrazole ring N1/N2/C9/C8/C7

Y-*X*···*Cg*	Y-*X*	*X*···*Cg*	Y···*Cg*	D-H···*Cg*
C10-O2···$Cg1^i$	1.200 (3)	3.503 (3)	3.623 (3)	85.95 (17)

Symmetry code: (i) 2 − *x*, 1 − *y*, −*z*.

Fig. 1


C12
C11
O1
O2
C10
C9
C8
C19
C18
C14
C13
N2
C7
C17
C5
C20
C4
N1
C22
C15
C6
C16
C3
C23
C2
C21
C1
Cl1