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1-(4-*tert*-Butylbenzyl)-3-(4-chlorophenyl)-1*H*-pyrazole-5-carboxylic acid

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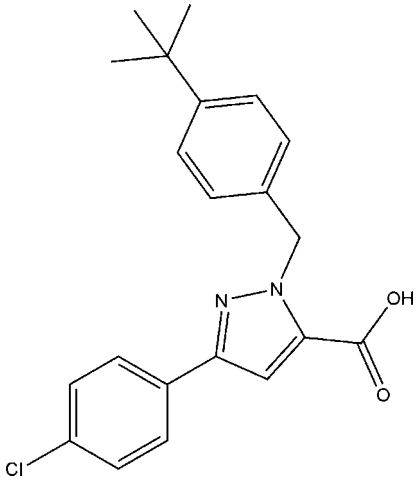
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.182; data-to-parameter ratio = 18.4.

In the title compound, $C_{21}H_{21}ClN_2O_2$, the pyrazole and chlorobenzene rings are coplanar and make a dihedral angle of 79.7 (2)° with the *tert*-butylbenzene ring. The crystal structure displays intermolecular O—H···O hydrogen bonding.

Related literature

For related literature, see: Jia *et al.* (2004); Cottineau *et al.* (2002); Finn *et al.* (2003); Wei *et al.* (2006); Xia *et al.* (2007).



Experimental

Crystal data

$C_{21}H_{21}ClN_2O_2$
M_r = 368.85
Triclinic, $P\overline{1}$
a = 6.6835 (1) Å
b = 12.3218 (3) Å
c = 12.6783 (3) Å
α = 105.714 (2)°
β = 102.714 (1)°
γ = 96.003 (2)°
V = 965.32 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 (2) K
0.48 × 0.24 × 0.09 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.905, T_{max} = 0.980
15167 measured reflections
4403 independent reflections
2700 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.182
S = 0.92
4403 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1^{i}	0.82	1.81	2.624 (2)	177

Symmetry code: (i) $-x+3, -y+1, -z+1$.

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2063).

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supplementary materials

Acta Cryst. (2007). E**63**, o3125 [**doi:10.1107/S1600536807027006**]

1-(4-*tert*-Butylbenzyl)-3-(4-chlorophenyl)-1*H*-pyrazole-5-carboxylic acid

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

Comment

The pyrazole framework plays an essential role in biologically active compounds. Many pyrazole derivatives are known to exhibit a wide range of biological properties such as anticoagulant (Jia *et al.*, 2004), antipyretic, antibacterial, hypoglycaemic, antihyperglycaemic, analgesic, anti-inflammatory, sedative–hypnotic (Cottineau *et al.*, 2002; Finn *et al.*, 2003), and antitumour (Wei *et al.*, 2006) activities.

In the title compound, $C_{21}H_{21}ClN_2O_2$ (I), shown in Fig. 1, the pyrazole (C7—C9/N1/N2) and benzene (C1—C6) rings are coplanar within 0.01° and subtend a dihedral angle of 79.7 (2)° with the *tert*-butylbenzyl ring (C12—C17). The crystal structure displays a strong intermolecular O2—H2A···O1 interaction which leads to formation of hydrogen bonded dimeric units (Table 1 and Fig. 2).

Experimental

A mixture of ethyl 1-(4-*tert*-butylbenzyl)-3-(4-chlorophenyl)-1*H*-pyrazole-5-carboxylate (0.01 mol) that was synthesized according to a literature procedure (Xia *et al.*, 2007) and potassium hydroxide (0.02 mol) in ethanol (40 ml) was heated to reflux for 3 h. The solvent was removed under reduced pressure and the residue was dissolved in water and acidified with hydrochloric acid (10%). The precipitate was filtered and dried to give a white solid (yield 95%). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid in acetone at room temperature for 3 d.

Refinement

All H atoms were placed at geometrically calculated positions and allowed to ride with C—H = 0.97Å (for CH_2 groups) and 0.96Å (for CH_3 groups), and O—H = 0.82 Å; their isotropic displacement parameters were set to 1.2 times (CH_2 groups) or 1.5 times (CH_3 and O—H groups) the equivalent displacement parameter of their parent atoms.

Figures

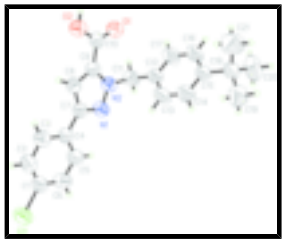

Fig. 1. **Fig 1** The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level for non-H atoms.

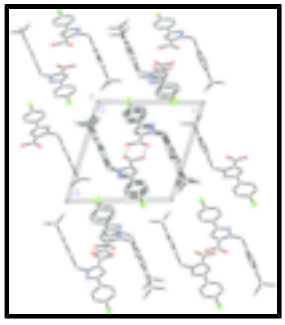

Fig. 2. **Fig 2** Packing view of (I), shown down the *a* axis. Hydrogen bonds leading to dimeric units are drawn as dashed lines.

1-(4-*tert*-Butylbenzyl)-3-(4-chlorophenyl)-1*H*-pyrazole-5-carboxylic acid

Crystal data

$C_{21}H_{21}ClN_2O_2$	$Z = 2$
$M_r = 368.85$	$F_{000} = 388$
Triclinic, $P\overline{1}$	$D_x = 1.269$ Mg m^{-3}
$a = 6.68350$ (10) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 12.3218$ (3) Å	Cell parameters from 3163 reflections
$c = 12.6783$ (3) Å	$\theta = 2.8$–23.6º
$\alpha = 105.714$ (2)º	$\mu = 0.22$ mm^{-1}
$\beta = 102.7140$ (10)º	$T = 293$ (2) K
$\gamma = 96.003$ (2)º	Plate, colourless
$V = 965.32$ (4) Å^3	0.48 × 0.24 × 0.09 mm

Data collection

Bruker APEX II CCD area-detector diffractometer	4403 independent reflections
Radiation source: fine-focus sealed tube	2700 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 293$(2) K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -8 \rightarrow 8$
$T_{min} = 0.905$, $T_{max} = 0.980$	$k = -15 \rightarrow 15$
15167 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.050$	H-atom parameters constrained
$wR(F^2) = 0.182$	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.244P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 0.92	$(\Delta/\sigma)_{max} < 0.001$
4403 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
239 parameters	$\Delta\rho_{min} = -0.17$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 calculating *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	0.1226 (4)	0.07086 (19)	0.3376 (2)	0.0712 (6)
C2	0.2138 (4)	0.1251 (2)	0.2756 (2)	0.0882 (8)
H2	0.1396	0.1232	0.2037	0.106*
C3	0.4169 (4)	0.1832 (2)	0.3194 (2)	0.0844 (7)
H3	0.4781	0.2203	0.2764	0.101*
C4	0.5299 (3)	0.18702 (17)	0.42565 (18)	0.0614 (5)
C5	0.4330 (4)	0.1310 (2)	0.4865 (2)	0.0762 (6)
H5	0.5053	0.1331	0.5588	0.091*
C6	0.2311 (4)	0.0718 (2)	0.4422 (2)	0.0829 (7)
H6	0.1697	0.0329	0.4836	0.099*
C7	0.7457 (3)	0.24819 (16)	0.47313 (18)	0.0604 (5)
C8	0.8730 (3)	0.30918 (17)	0.42691 (18)	0.0627 (5)
H8	0.8383	0.3212	0.3563	0.075*
C9	1.0592 (3)	0.34740 (16)	0.50741 (18)	0.0603 (5)
C10	1.2526 (4)	0.41398 (17)	0.50558 (19)	0.0635 (5)
C11	1.1879 (4)	0.32868 (19)	0.7064 (2)	0.0723 (6)
H11A	1.3256	0.3220	0.6951	0.087*
H11B	1.1483	0.2699	0.7392	0.087*
C12	1.1974 (3)	0.44418 (19)	0.78821 (18)	0.0649 (5)
C13	1.0193 (4)	0.4834 (2)	0.8071 (2)	0.0868 (8)
H13	0.8903	0.4379	0.7676	0.104*
C14	1.0277 (4)	0.5887 (2)	0.8832 (2)	0.0891 (8)
H14	0.9038	0.6122	0.8937	0.107*
C15	1.2125 (3)	0.65996 (19)	0.94393 (18)	0.0669 (6)
C16	1.3897 (4)	0.6194 (3)	0.9236 (3)	0.1062 (11)
H16	1.5190	0.6646	0.9627	0.127*
C17	1.3814 (4)	0.5149 (3)	0.8477 (3)	0.1017 (10)

H17	1.5051	0.4916	0.8364	0.122*
C18	1.2253 (4)	0.7780 (2)	1.0281 (2)	0.0778 (6)
C19	1.0071 (5)	0.8031 (3)	1.0371 (3)	0.1174 (11)
H19A	0.9430	0.7489	1.0670	0.176*
H19B	0.9226	0.7969	0.9632	0.176*
H19C	1.0201	0.8792	1.0867	0.176*
C20	1.3529 (7)	0.7854 (3)	1.1457 (3)	0.1262 (13)
H20A	1.2867	0.7292	1.1725	0.189*
H20B	1.3622	0.8604	1.1966	0.189*
H20C	1.4902	0.7713	1.1422	0.189*
C21	1.3251 (7)	0.8704 (3)	0.9879 (4)	0.1315 (13)
H21A	1.3187	0.9444	1.0358	0.197*
H21B	1.2517	0.8617	0.9111	0.197*
H21C	1.4680	0.8635	0.9913	0.197*
Cl1	−0.13478 (10)	−0.00033 (6)	0.28340 (6)	0.0938 (3)
N1	0.8497 (3)	0.24867 (15)	0.57708 (16)	0.0668 (5)
N2	1.0407 (3)	0.30882 (14)	0.59649 (15)	0.0643 (5)
O1	1.4087 (3)	0.44336 (14)	0.58439 (14)	0.0768 (4)
O2	1.2374 (3)	0.43813 (15)	0.41032 (14)	0.0803 (5)
H2A	1.3497	0.4729	0.4113	0.120*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0608 (13)	0.0616 (12)	0.0773 (14)	0.0088 (10)	0.0171 (11)	−0.0002 (10)
C2	0.0760 (16)	0.1025 (19)	0.0709 (15)	−0.0056 (14)	0.0053 (13)	0.0204 (14)
C3	0.0798 (16)	0.0944 (17)	0.0725 (15)	−0.0052 (13)	0.0172 (13)	0.0241 (13)
C4	0.0611 (12)	0.0511 (10)	0.0671 (12)	0.0102 (9)	0.0197 (10)	0.0072 (9)
C5	0.0665 (14)	0.0834 (15)	0.0759 (14)	0.0050 (12)	0.0143 (12)	0.0262 (12)
C6	0.0690 (15)	0.0851 (16)	0.0945 (18)	0.0018 (12)	0.0243 (14)	0.0289 (14)
C7	0.0623 (12)	0.0483 (10)	0.0639 (12)	0.0077 (9)	0.0169 (10)	0.0062 (8)
C8	0.0688 (13)	0.0545 (11)	0.0613 (11)	0.0077 (9)	0.0187 (10)	0.0112 (9)
C9	0.0655 (12)	0.0469 (10)	0.0656 (12)	0.0084 (9)	0.0211 (10)	0.0096 (9)
C10	0.0679 (13)	0.0520 (10)	0.0676 (13)	0.0081 (9)	0.0220 (11)	0.0106 (9)
C11	0.0684 (14)	0.0708 (13)	0.0747 (14)	0.0067 (11)	0.0081 (11)	0.0274 (11)
C12	0.0578 (12)	0.0715 (13)	0.0630 (12)	0.0026 (10)	0.0092 (10)	0.0247 (10)
C13	0.0565 (13)	0.0803 (16)	0.1011 (19)	−0.0058 (11)	0.0084 (13)	0.0070 (14)
C14	0.0572 (14)	0.0888 (17)	0.1026 (19)	0.0058 (12)	0.0121 (13)	0.0083 (14)
C15	0.0597 (12)	0.0746 (13)	0.0606 (12)	−0.0040 (10)	0.0091 (10)	0.0219 (10)
C16	0.0536 (14)	0.114 (2)	0.108 (2)	−0.0141 (14)	0.0096 (14)	−0.0162 (18)
C17	0.0515 (13)	0.111 (2)	0.111 (2)	0.0024 (13)	0.0132 (14)	−0.0079 (17)
C18	0.0788 (16)	0.0740 (14)	0.0697 (14)	−0.0030 (12)	0.0123 (12)	0.0157 (11)
C19	0.109 (2)	0.111 (2)	0.113 (2)	0.0151 (19)	0.035 (2)	−0.0011 (19)
C20	0.160 (3)	0.107 (2)	0.0766 (18)	0.007 (2)	−0.008 (2)	0.0073 (17)
C21	0.158 (3)	0.089 (2)	0.157 (3)	0.001 (2)	0.065 (3)	0.043 (2)
Cl1	0.0648 (4)	0.0897 (5)	0.1040 (5)	−0.0023 (3)	0.0161 (3)	0.0024 (4)
N1	0.0624 (11)	0.0606 (10)	0.0721 (11)	0.0007 (8)	0.0161 (9)	0.0165 (8)
N2	0.0618 (11)	0.0580 (9)	0.0677 (11)	0.0046 (8)	0.0137 (9)	0.0153 (8)

O1	0.0684 (10)	0.0830 (11)	0.0738 (10)	−0.0029 (8)	0.0172 (8)	0.0226 (8)
O2	0.0777 (11)	0.0827 (11)	0.0757 (10)	−0.0071 (9)	0.0174 (8)	0.0262 (8)

Geometric parameters (Å, °)

C1—C2	1.359 (4)	C12—C13	1.375 (3)
C1—C6	1.360 (4)	C13—C14	1.379 (4)
C1—Cl1	1.743 (2)	C13—H13	0.9300
C2—C3	1.383 (4)	C14—C15	1.370 (3)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.378 (3)	C15—C16	1.381 (4)
C3—H3	0.9300	C15—C18	1.534 (3)
C4—C5	1.380 (3)	C16—C17	1.371 (4)
C4—C7	1.468 (3)	C16—H16	0.9300
C5—C6	1.381 (3)	C17—H17	0.9300
C5—H5	0.9300	C18—C21	1.519 (4)
C6—H6	0.9300	C18—C20	1.519 (4)
C7—N1	1.346 (3)	C18—C19	1.544 (4)
C7—C8	1.399 (3)	C19—H19A	0.9600
C8—C9	1.368 (3)	C19—H19B	0.9600
C8—H8	0.9300	C19—H19C	0.9600
C9—N2	1.363 (3)	C20—H20A	0.9600
C9—C10	1.465 (3)	C20—H20B	0.9600
C10—O1	1.218 (3)	C20—H20C	0.9600
C10—O2	1.306 (3)	C21—H21A	0.9600
C11—N2	1.460 (3)	C21—H21B	0.9600
C11—C12	1.503 (3)	C21—H21C	0.9600
C11—H11A	0.9700	N1—N2	1.343 (2)
C11—H11B	0.9700	O2—H2A	0.8200
C12—C17	1.361 (3)		
C2—C1—C6	120.3 (2)	C15—C14—C13	122.2 (2)
C2—C1—Cl1	120.1 (2)	C15—C14—H14	118.9
C6—C1—Cl1	119.6 (2)	C13—C14—H14	118.9
C1—C2—C3	120.1 (3)	C14—C15—C16	115.6 (2)
C1—C2—H2	119.9	C14—C15—C18	123.1 (2)
C3—C2—H2	119.9	C16—C15—C18	121.4 (2)
C4—C3—C2	120.9 (2)	C17—C16—C15	122.3 (2)
C4—C3—H3	119.5	C17—C16—H16	118.9
C2—C3—H3	119.5	C15—C16—H16	118.9
C3—C4—C5	117.6 (2)	C12—C17—C16	121.8 (2)
C3—C4—C7	121.5 (2)	C12—C17—H17	119.1
C5—C4—C7	120.8 (2)	C16—C17—H17	119.1
C4—C5—C6	121.4 (2)	C21—C18—C20	109.4 (3)
C4—C5—H5	119.3	C21—C18—C15	109.6 (2)
C6—C5—H5	119.3	C20—C18—C15	110.7 (2)
C1—C6—C5	119.6 (2)	C21—C18—C19	107.3 (3)
C1—C6—H6	120.2	C20—C18—C19	108.1 (3)
C5—C6—H6	120.2	C15—C18—C19	111.6 (2)
N1—C7—C8	110.39 (19)	C18—C19—H19A	109.5

N1—C7—C4	119.21 (19)	C18—C19—H19B	109.5
C8—C7—C4	130.4 (2)	H19A—C19—H19B	109.5
C9—C8—C7	105.5 (2)	C18—C19—H19C	109.5
C9—C8—H8	127.2	H19A—C19—H19C	109.5
C7—C8—H8	127.2	H19B—C19—H19C	109.5
N2—C9—C8	107.10 (19)	C18—C20—H20A	109.5
N2—C9—C10	122.7 (2)	C18—C20—H20B	109.5
C8—C9—C10	130.2 (2)	H20A—C20—H20B	109.5
O1—C10—O2	124.3 (2)	C18—C20—H20C	109.5
O1—C10—C9	123.5 (2)	H20A—C20—H20C	109.5
O2—C10—C9	112.2 (2)	H20B—C20—H20C	109.5
N2—C11—C12	113.02 (18)	C18—C21—H21A	109.5
N2—C11—H11A	109.0	C18—C21—H21B	109.5
C12—C11—H11A	109.0	H21A—C21—H21B	109.5
N2—C11—H11B	109.0	C18—C21—H21C	109.5
C12—C11—H11B	109.0	H21A—C21—H21C	109.5
H11A—C11—H11B	107.8	H21B—C21—H21C	109.5
C17—C12—C13	116.6 (2)	N2—N1—C7	105.68 (17)
C17—C12—C11	122.0 (2)	N1—N2—C9	111.31 (18)
C13—C12—C11	121.4 (2)	N1—N2—C11	118.34 (18)
C12—C13—C14	121.4 (2)	C9—N2—C11	130.25 (19)
C12—C13—H13	119.3	C10—O2—H2A	109.5
C14—C13—H13	119.3		
C6—C1—C2—C3	−1.0 (4)	C11—C12—C13—C14	179.1 (3)
Cl1—C1—C2—C3	178.9 (2)	C12—C13—C14—C15	0.1 (5)
C1—C2—C3—C4	0.1 (4)	C13—C14—C15—C16	0.2 (4)
C2—C3—C4—C5	−0.1 (4)	C13—C14—C15—C18	179.3 (2)
C2—C3—C4—C7	179.9 (2)	C14—C15—C16—C17	0.0 (5)
C3—C4—C5—C6	0.9 (4)	C18—C15—C16—C17	−179.1 (3)
C7—C4—C5—C6	−179.1 (2)	C13—C12—C17—C16	0.8 (5)
C2—C1—C6—C5	1.8 (4)	C11—C12—C17—C16	−178.9 (3)
Cl1—C1—C6—C5	−178.16 (19)	C15—C16—C17—C12	−0.5 (5)
C4—C5—C6—C1	−1.7 (4)	C14—C15—C18—C21	−117.2 (3)
C3—C4—C7—N1	−179.6 (2)	C16—C15—C18—C21	61.9 (4)
C5—C4—C7—N1	0.4 (3)	C14—C15—C18—C20	122.0 (3)
C3—C4—C7—C8	−0.5 (3)	C16—C15—C18—C20	−58.9 (4)
C5—C4—C7—C8	179.5 (2)	C14—C15—C18—C19	1.6 (4)
N1—C7—C8—C9	−0.2 (2)	C16—C15—C18—C19	−179.3 (3)
C4—C7—C8—C9	−179.43 (19)	C8—C7—N1—N2	−0.2 (2)
C7—C8—C9—N2	0.6 (2)	C4—C7—N1—N2	179.10 (16)
C7—C8—C9—C10	178.73 (19)	C7—N1—N2—C9	0.6 (2)
N2—C9—C10—O1	−2.6 (3)	C7—N1—N2—C11	177.22 (17)
C8—C9—C10—O1	179.5 (2)	C8—C9—N2—N1	−0.7 (2)
N2—C9—C10—O2	177.59 (18)	C10—C9—N2—N1	−179.06 (17)
C8—C9—C10—O2	−0.3 (3)	C8—C9—N2—C11	−176.87 (19)
N2—C11—C12—C17	−131.2 (3)	C10—C9—N2—C11	4.8 (3)
N2—C11—C12—C13	49.1 (3)	C12—C11—N2—N1	−97.8 (2)
C17—C12—C13—C14	−0.6 (4)	C12—C11—N2—C9	78.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1^{i}	0.82	1.81	2.624 (2)	177

Symmetry codes: (i) −*x*+3, −*y*+1, −*z*+1.

Fig. 1

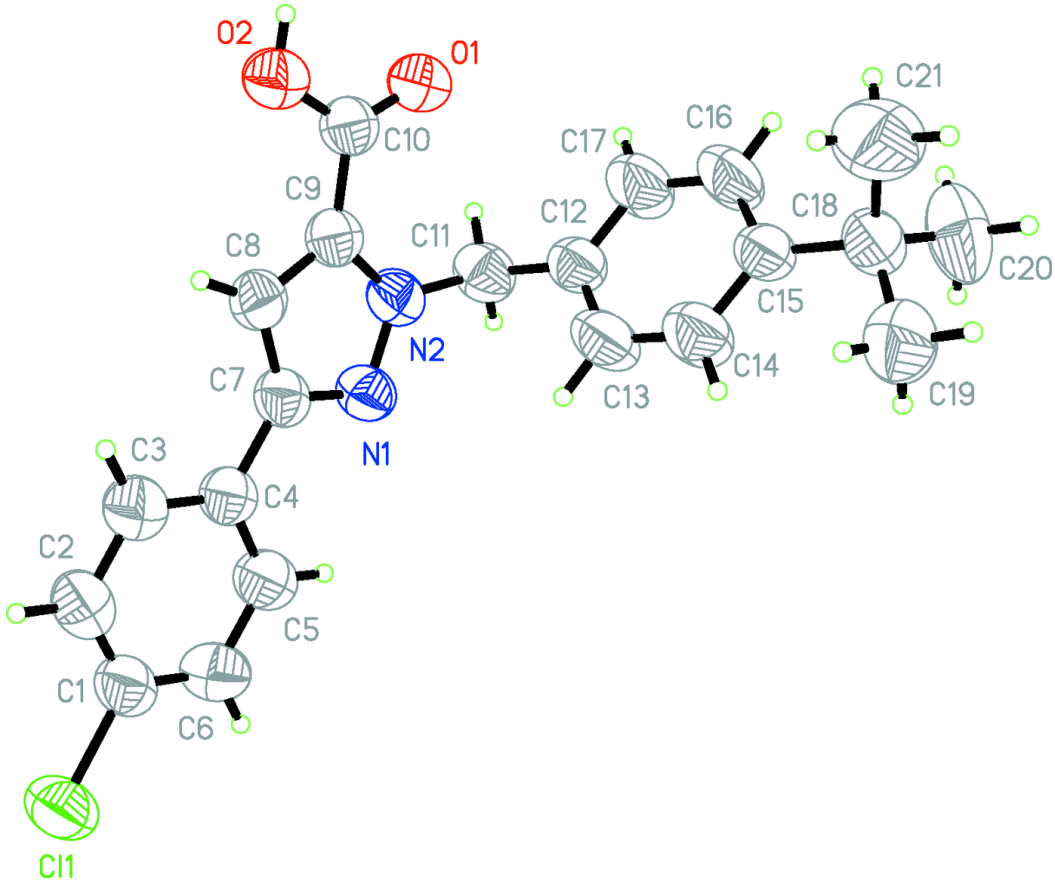
O2
O1
C10
C9
C8
C11
C12
C17
C16
C21
C18
C20
C15
N2
C7
C14
C13
C19
N1
C3
C4
C2
C5
C1
C6
Cl1

Fig. 2