Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-Benzyl-*N*-(4-chlorophenyl)acrylamide

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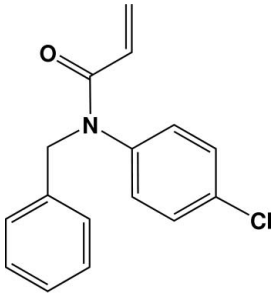
Received 17 November 2007; accepted 29 November 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.064; wR factor = 0.158; data-to-parameter ratio = 18.3.

In the molecular structure of the title compound, $C_{16}H_{14}ClNO$, the acrylamide unit is essentially planar and makes dihedral angles of 80.06 (12) and 68.91 (13)°, respectively, with the benzene and phenyl rings. The dihedral angle between the two rings is 49.79 (11)°. In the crystal structure, molecules are connected *via* weak C—H···O and C—H···π interactions, forming a molecular tape running along the *b* axis.

Related literature

For related literature, see: Fairlamb (2004); Hu *et al.* (2003); Park & Hoffmann (1990); Otero & Cantero (1995); Riggi *et al.* (1992).



Experimental

Crystal data

$C_{16}H_{14}ClNO$
M_r = 271.73
Monoclinic, $P2_1/n$
a = 9.215 (4) Å
b = 9.210 (4) Å
c = 17.090 (8) Å
β = 102.842 (6)°
V = 1414.2 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 291 (2) K
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.93, T_{max} = 0.94
11395 measured reflections
3172 independent reflections
1666 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.158
S = 1.06
3172 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

*Cg*1 is the mid-point of atoms C15 and C16.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.53	3.405 (4)	157
C6—H6···*Cg*1^{ii}	0.93	3.02	3.75 (2)	136

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $-x, -y+1, -z+1$. *Cg*1 is the mid-point of atoms C15 and C16.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Science Foundation of Anhui Province (project No. 2004kj164zd), the Education Department of Anhui Province Program (grant Nos. 2006K J006TD and TD200707) and the National Science Foundation of China (project No. 20572001) for financial support of this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2254).

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supporting information

Acta Cryst. (2008). E**64**, o206 [https://doi.org/10.1107/S160053680706432X]

N-Benzyl-*N*-(4-chlorophenyl)acrylamide

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S1. Comment

Many active molecules in nature contain highly functionalized heterocyclic rings (Fairlamb, 2004). In recent research, we report a novel palladium catalyzed Heck intermolecular reactions of aryl halides with the nitron-containing olefins (Hu *et al.*, 2003). We found that polyene amide was prepared by two steps (Riggi *et al.*, 1992). The substrate of *N*-benzyl-*N*-(4-chlorophenyl)acrylamide is used to obtain this pyrrole skeleton (Park & Hoffmann, 1990; Otero & Cantero, 1995).

In this paper, we report the crystal structure of the title compound, $C_{16}H_{14}ClNO$ (Fig. 1). The crystal data show that all bond lengths and angles in the title compound have normal values. The bond length of C15=C16 is 1.288 (4) Å, belonging to typical C_{sp2}—C_{sp2} double bonds. The molecule contains two six-membered rings, A (C1—C6) and B (C8—C13). Rings A and B are not coplanar, the dihedral angle between ring A and ring B being 49.79 (11)°. In the structure there are a weak intermolecular C—H···O interaction [C2—H2···O1^{i}, symmetry code: (i) -*x*, -*y*, 1 - *z*] and a C—H···π interaction [C6—H6···*Cg*1^{ii}, *Cg*1 is the centroid of atoms C15 and C16; symmetry code: (ii) -*x*,1 - *y*,1 - *z*]. These weak intermolecular interactions extended the title compound molecules into a one-dimensional chain structure (Fig. 2) along the *b* axis.

S2. Experimental

The solution of 4-chlorobenzenamine (12.75 g, 0.1 mol) and triethylamine (14 ml, 0.1 mol) in CCl_4 (20 ml) was placed in a three-necked flask equipped with reflux condenser, dropping funnel and mechanical stirrer. The 1-chloromethylbenzene (13.91 g, 0.11 mol) in CCl_4 (20 ml) was added at a rate such as to produce gentle reflux at room temperature. The crude product was recrystallized from C_2H_5OH; yield (21.54 g, 90%). *N*-benzyl-4-chlorobenzenamine (10.89 g, 0.05 mol) was stirred at ice-water in the presence of 2-propenoyl chloride (4.9 ml, 0.06 mol) and triethylamine (8.4 ml, 0.06 mol) in CCl4 (20 ml). The mixture was washed with water and the organic layer was dried by $MgSO_4$. The crude product was purified by flash column chromatography on silica gel (light petroleum/EtOAc, 8:1) to obtain the product (8.23 g, 61%). Colorless crystals of the *N*-benzyl-3-(4-chlorophenyl)-3-phenyl-propanamide suitable for X-ray diffraction were obtained from an ethyl acetate solution over one week.

S3. Refinement

H atoms were placed in calculated positions with C—H distances 0.93–0.97 Å and treated as riding, with U_{iso}(H) = 1.2U_{eq}(C).

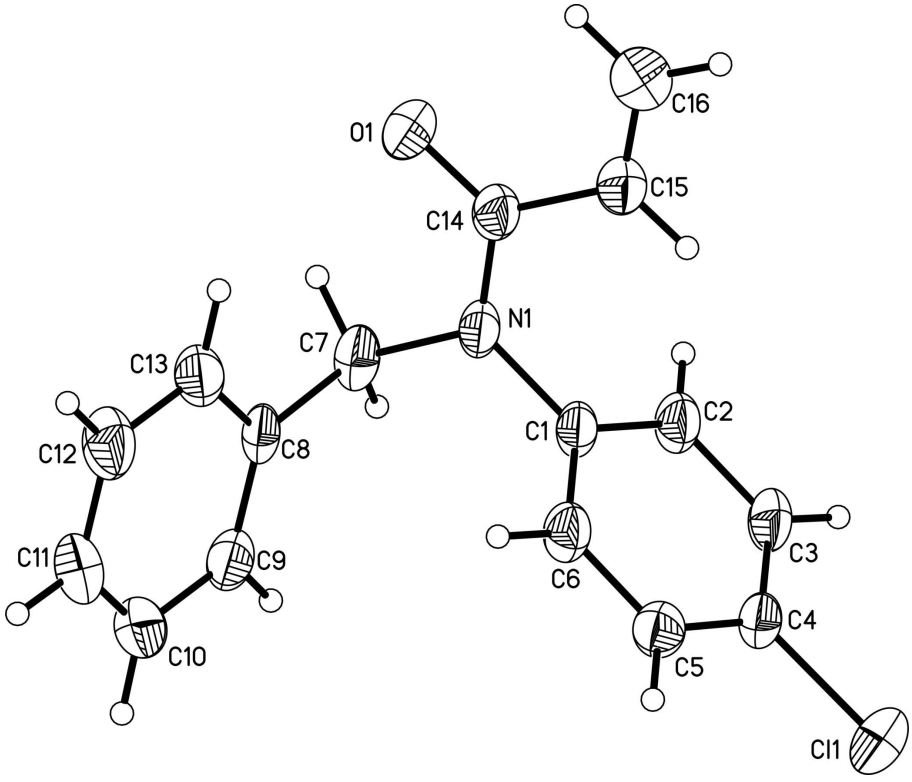

Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids with numbering scheme.

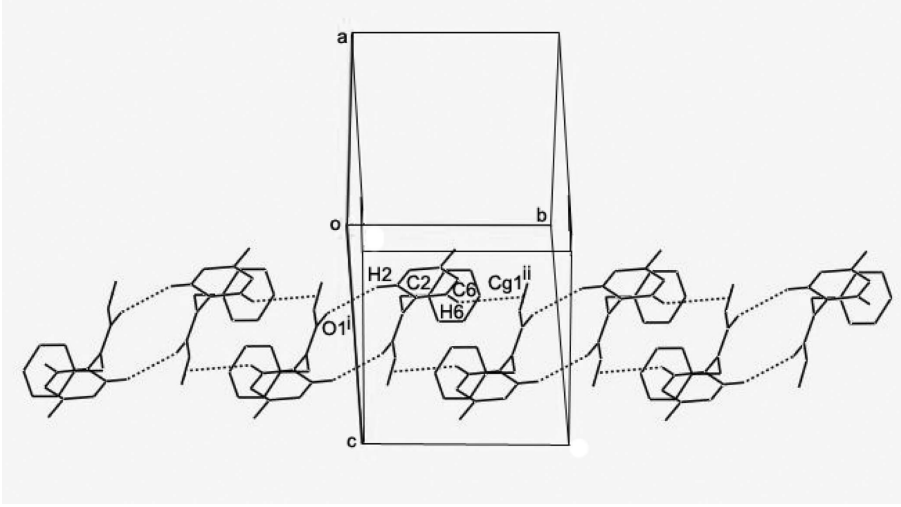

Figure 2

View of the chain packing of (I) approximately down the *a* axis. H atoms have been omitted except H2 and H6 for clarity [symmetry codes: (i) -*x*, -*y*, 1 - *z*; (ii) -*x*, 1 - *y*, 1 - *z*].

N-Benzyl-*N*-(4-chlorophenyl)acrylamide

Crystal data

$C_{16}H_{14}ClNO$
$M_r = 271.73$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.215$ (4) Å
$b = 9.210$ (4) Å
$c = 17.090$ (8) Å
$\beta = 102.842$ (6)°
$V = 1414.2$ (12) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.276$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3741 reflections
$\theta = 2.1$–25.4°
$\mu = 0.26$ mm^{-1}
$T = 291$ K
Block, colourless
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.93$, $T_{max} = 0.94$
11395 measured reflections
3172 independent reflections
1666 reflections with $I > 2\sigma(I)$
$R_{int} = 0.057$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -20 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.158$
$S = 1.06$
3172 reflections
173 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.55P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.008 (2)

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.
Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
9.0764 (0.0047) *x* - 0.6878 (0.0111) *y* - 1.1393 (0.0196) *z* = 0.3034 (0.0082)
* -0.0078 (0.0020) C1 * 0.0033 (0.0020) C2 * 0.0052 (0.0021) C3 * -0.0091 (0.0020) C4 * 0.0045 (0.0020) C5 * 0.0039 (0.0020) C6
Rms deviation of fitted atoms = 0.0060
4.7161 (0.0105) *x* - 5.4299 (0.0094) *y* + 8.4686 (0.0192) *z* = 4.7812 (0.0131)
Angle to previous plane (with approximate e.s.d.) = 49.79 (0.11)
* 0.0026 (0.0019) C8 * 0.0023 (0.0020) C9 * -0.0059 (0.0022) C10 * 0.0046 (0.0023) C11 * 0.0004 (0.0023) C12 * -0.0040 (0.0021) C13
Rms deviation of fitted atoms = 0.0037

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1090 (3)	0.2996 (3)	0.42821 (14)	0.0487 (7)
C2	0.0953 (3)	0.2145 (3)	0.36048 (15)	0.0586 (8)
H2	0.0888	0.1141	0.3641	0.070*
C3	0.0913 (3)	0.2801 (3)	0.28706 (15)	0.0623 (8)
H3	0.0824	0.2240	0.2410	0.075*
C4	0.1004 (3)	0.4277 (3)	0.28296 (15)	0.0561 (7)
C5	0.1168 (3)	0.5138 (3)	0.35022 (16)	0.0586 (7)
H5	0.1250	0.6141	0.3466	0.070*
C6	0.1209 (3)	0.4476 (3)	0.42326 (16)	0.0565 (7)
H6	0.1318	0.5039	0.4694	0.068*
C7	0.2646 (3)	0.2115 (3)	0.55720 (15)	0.0607 (8)
H7A	0.3338	0.1858	0.5242	0.073*
H7B	0.2612	0.1311	0.5934	0.073*
C8	0.3224 (3)	0.3442 (3)	0.60604 (15)	0.0524 (7)
C9	0.4397 (3)	0.4235 (3)	0.59152 (16)	0.0606 (8)
H9	0.4840	0.3961	0.5499	0.073*
C10	0.4933 (4)	0.5435 (4)	0.63763 (19)	0.0716 (9)
H10	0.5720	0.5966	0.6264	0.086*
C11	0.4310 (4)	0.5840 (4)	0.69955 (19)	0.0747 (9)
H11	0.4680	0.6637	0.7312	0.090*
C12	0.3137 (4)	0.5065 (4)	0.71468 (19)	0.0776 (10)
H12	0.2704	0.5342	0.7566	0.093*
C13	0.2590 (3)	0.3874 (3)	0.66831 (16)	0.0641 (8)
H13	0.1788	0.3360	0.6791	0.077*
C14	−0.0055 (3)	0.1827 (3)	0.52919 (16)	0.0569 (7)
C15	−0.1547 (4)	0.2031 (3)	0.47419 (17)	0.0622 (8)
H15	−0.1607	0.2433	0.4237	0.075*
C16	−0.2751 (4)	0.1660 (4)	0.4955 (2)	0.0807 (10)
H16A	−0.2702	0.1258	0.5459	0.097*
H16B	−0.3669	0.1796	0.4604	0.097*
Cl1	0.09117 (12)	0.51004 (11)	0.18992 (5)	0.0938 (4)
N1	0.1152 (3)	0.2311 (2)	0.50484 (12)	0.0537 (6)
O1	0.0044 (3)	0.1269 (2)	0.59589 (12)	0.0769 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0522 (16)	0.0546 (17)	0.0341 (13)	−0.0008 (13)	−0.0014 (12)	−0.0025 (11)
C2	0.074 (2)	0.0544 (17)	0.0410 (15)	−0.0033 (15)	−0.0019 (14)	−0.0061 (12)
C3	0.073 (2)	0.073 (2)	0.0352 (15)	−0.0065 (16)	0.0005 (14)	−0.0101 (13)

C4	0.0506 (17)	0.074 (2)	0.0385 (15)	−0.0049 (14)	−0.0020 (13)	0.0064 (13)
C5	0.0630 (19)	0.0550 (17)	0.0540 (17)	−0.0017 (14)	0.0053 (14)	0.0020 (13)
C6	0.0683 (19)	0.0553 (18)	0.0420 (15)	0.0004 (14)	0.0036 (14)	−0.0072 (13)
C7	0.0650 (19)	0.0652 (19)	0.0442 (15)	0.0101 (15)	−0.0045 (14)	0.0000 (13)
C8	0.0536 (17)	0.0630 (18)	0.0326 (13)	0.0028 (14)	−0.0074 (12)	0.0008 (12)
C9	0.0597 (19)	0.077 (2)	0.0411 (15)	0.0046 (17)	0.0035 (14)	0.0050 (14)
C10	0.060 (2)	0.081 (2)	0.066 (2)	−0.0098 (17)	−0.0038 (17)	0.0063 (17)
C11	0.069 (2)	0.085 (2)	0.060 (2)	−0.0075 (19)	−0.0065 (17)	−0.0151 (17)
C12	0.079 (2)	0.099 (3)	0.0520 (18)	−0.004 (2)	0.0088 (17)	−0.0219 (17)
C13	0.0554 (18)	0.085 (2)	0.0488 (17)	−0.0074 (16)	0.0057 (14)	−0.0068 (15)
C14	0.074 (2)	0.0511 (17)	0.0410 (15)	−0.0084 (15)	0.0031 (15)	−0.0050 (12)
C15	0.068 (2)	0.0663 (19)	0.0489 (17)	−0.0113 (16)	0.0054 (15)	−0.0012 (14)
C16	0.061 (2)	0.0653 (2)	0.053 (2)	−0.009 (2)	0.0097 (19)	−0.0015 (18)
Cl1	0.1158 (8)	0.1115 (8)	0.0498 (5)	−0.0131 (6)	0.0093 (5)	0.0202 (5)
N1	0.0605 (15)	0.0593 (15)	0.0345 (11)	−0.0032 (12)	−0.0044 (11)	−0.0001 (10)
O1	0.0958 (17)	0.0819 (15)	0.0480 (12)	−0.0129 (12)	0.0052 (11)	0.0133 (11)

Geometric parameters (Å, º)

C1—C6	1.372 (4)	C8—C13	1.382 (4)
C1—C2	1.380 (3)	C9—C10	1.383 (4)
C1—N1	1.443 (3)	C9—H9	0.9300
C2—C3	1.386 (4)	C10—C11	1.363 (4)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.365 (4)	C11—C12	1.367 (5)
C3—H3	0.9300	C11—H11	0.9300
C4—C5	1.376 (4)	C12—C13	1.381 (4)
C4—Cl1	1.747 (3)	C12—H12	0.9300
C5—C6	1.382 (4)	C13—H13	0.9300
C5—H5	0.9300	C14—O1	1.235 (3)
C6—H6	0.9300	C14—N1	1.347 (4)
C7—N1	1.476 (3)	C14—C15	1.495 (4)
C7—C8	1.509 (4)	C15—C16	1.288 (4)
C7—H7A	0.9700	C15—H15	0.9300
C7—H7B	0.9700	C16—H16A	0.9300
C8—C9	1.371 (4)	C16—H16B	0.9300
C6—C1—C2	120.4 (2)	C8—C9—C10	121.2 (3)
C6—C1—N1	120.2 (2)	C8—C9—H9	119.4
C2—C1—N1	119.4 (2)	C10—C9—H9	119.4
C1—C2—C3	119.4 (3)	C11—C10—C9	120.1 (3)
C1—C2—H2	120.3	C11—C10—H10	119.9
C3—C2—H2	120.3	C9—C10—H10	119.9
C4—C3—C2	119.4 (3)	C10—C11—C12	119.4 (3)
C4—C3—H3	120.3	C10—C11—H11	120.3
C2—C3—H3	120.3	C12—C11—H11	120.3
C3—C4—C5	121.8 (3)	C11—C12—C13	120.6 (3)
C3—C4—Cl1	119.2 (2)	C11—C12—H12	119.7

C5—C4—Cl1	119.0 (2)	C13—C12—H12	119.7
C4—C5—C6	118.4 (3)	C12—C13—C8	120.5 (3)
C4—C5—H5	120.8	C12—C13—H13	119.8
C6—C5—H5	120.8	C8—C13—H13	119.8
C1—C6—C5	120.5 (3)	O1—C14—N1	121.7 (3)
C1—C6—H6	119.8	O1—C14—C15	120.1 (3)
C5—C6—H6	119.8	N1—C14—C15	118.1 (2)
N1—C7—C8	113.8 (2)	C16—C15—C14	121.3 (3)
N1—C7—H7A	108.8	C16—C15—H15	119.4
C8—C7—H7A	108.8	C14—C15—H15	119.4
N1—C7—H7B	108.8	C15—C16—H16A	120.0
C8—C7—H7B	108.8	C15—C16—H16B	120.0
H7A—C7—H7B	107.7	H16A—C16—H16B	120.0
C9—C8—C13	118.1 (3)	C14—N1—C1	123.8 (2)
C9—C8—C7	121.8 (3)	C14—N1—C7	119.7 (2)
C13—C8—C7	120.1 (3)	C1—N1—C7	116.6 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.93	2.53	3.405 (4)	157
C6—H6···*Cg*1^{ii}	0.93	3.02	3.75 (2)	136

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