Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Chlorophenyl)pyrrolidine-1-carboxamide

Yu-Feng Li

Microscale Science Institute, Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China
Correspondence e-mail: liyufeng8111@163.com

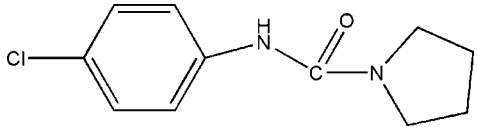
Received 19 May 2011; accepted 20 June 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.130; data-to-parameter ratio = 18.9.

In the title molecule, $C_{11}H_{13}ClN_2O$, the five-membered ring has an envelope conformation. In the crystal, molecules are linked into chains along [100] by intermolecular N—H···O hydrogen bonds.

Related literature

For the medicinal properties of pyrrolidine compounds, see: Yang *et al.* (1997). For a related structure, see: Köhn *et al.* (2004).



Experimental

Crystal data

$C_{11}H_{13}ClN_2O$
M_r = 224.68
Orthorhombic, *Pbca*
a = 9.4498 (19) Å
b = 10.856 (2) Å
c = 21.930 (4) Å
V = 2249.7 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 293 K
0.23 × 0.19 × 0.19 mm

Data collection

Bruker SMART CCD diffractometer
20387 measured reflections
2576 independent reflections
2264 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.130
S = 1.07
2576 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.86	2.21	2.9184 (15)	140

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author would like to thank the Natural Science Foundation of Shandong Province (No. Y2008B23).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5257).

References

Bruker (1997). *SMART* and *SAINT*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Köhn, U., Günther, W., Görls, H. & Anders, E. (2004). *Tetrahedron Asymmetry*, **15**, 1419–1426.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, D., Soulier, J. L., Sicsic, S., Mathe-Allainmat, M., Bremont, B., Croci, T., Cardamone, R., Aureggi, G. & Langlois, M. (1997). *J. Med. Chem.* **40**, 608–621.

supporting information

Acta Cryst. (2011). E**67**, o1792 [doi:10.1107/S1600536811024111]

N-(4-Chlorophenyl)pyrrolidine-1-carboxamide

Yu-Feng Li

S1. Comment

Pyrrolidine compounds have been shown to have medicinal properties (Yang *et al.*, 1997). The crystal structure of the title compound is presented herein. The molecular structure of the title compound is shown in Fig. 1. The five-membered ring has an envelope conformation with atom C4 forming the flap. In the crystal, the molecules are linked into chains along [100] by intermoecular N—H···O hydrogen bonds. The structure of a related compound has already been determined (Köhn *et al.*, 2004).

S2. Experimental

A mixture of pyrrolidine (0.1 mol), and (4-chlorophenyl)carbamic chloride (0.1 mol) was stirred in refluxing ethanol (20 ml) for 4 h to afford the title compound (0.079 mol, yield 79%). Colourless blocks of the title compound were obtained by recrystallization of a solution of the title compound ethanol at room temperature.

S3. Refinement

H atoms were fixed geometrically and allowed to ride on their attached atoms, with C—H distances = 0.93–0.97 Å; N—H = 0.86Å and with U_{iso}(H) = 1.2U_{eq}(C,*N*).

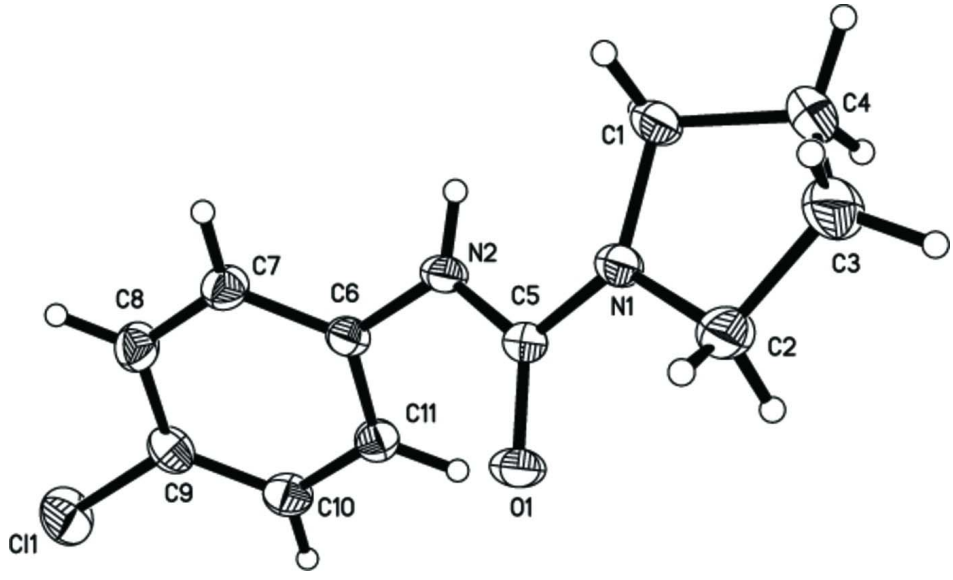


Figure 1

The molecular structure of the title compound showing 30% probability displacement ellipsoids.

N-(4-Chlorophenyl)pyrrolidine-1-carboxamide

Crystal data

$C_{11}H_{13}ClN_2O$
$M_r = 224.68$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 9.4498$ (19) Å
$b = 10.856$ (2) Å
$c = 21.930$ (4) Å
$V = 2249.7$ (8) Å^3
$Z = 8$
$F(000) = 944$
$D_x = 1.327$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2264 reflections
$\theta = 3.0$–$27.6°$
$\mu = 0.31$ mm^{-1}
$T = 293$ K
Bar, colorless
0.23 × 0.19 × 0.19 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
20387 measured reflections
2576 independent reflections
2264 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -12 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.130$
$S = 1.07$
2576 reflections
136 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
$w = 1/[\sigma^2(F_o^2) + (0.0763P)^2 + 0.5404P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
Cl1	0.10254 (6)	0.10302 (5)	0.03994 (2)	0.0685 (2)
O1	0.12968 (10)	0.43109 (12)	0.28838 (5)	0.0496 (3)
N2	0.34453 (11)	0.36694 (12)	0.25166 (5)	0.0388 (3)
H2A	0.4347	0.3673	0.2570	0.047*
C6	0.28726 (13)	0.30130 (12)	0.20175 (6)	0.0347 (3)
C10	0.12280 (16)	0.15354 (14)	0.16052 (7)	0.0434 (3)

H10A	0.0507	0.0963	0.1660	0.052*
C5	0.26031 (14)	0.43003 (13)	0.29184 (6)	0.0356 (3)
C11	0.17977 (15)	0.21521 (13)	0.20997 (6)	0.0393 (3)
H11A	0.1460	0.1990	0.2490	0.047*
N1	0.32890 (12)	0.49261 (12)	0.33577 (5)	0.0417 (3)
C9	0.17459 (17)	0.17824 (14)	0.10291 (7)	0.0445 (3)
C7	0.34090 (16)	0.32181 (14)	0.14377 (7)	0.0420 (3)
H7A	0.4150	0.3770	0.1383	0.050*
C1	0.47839 (15)	0.47967 (16)	0.35253 (7)	0.0463 (4)
H1A	0.5367	0.5390	0.3310	0.056*
H1B	0.5127	0.3973	0.3439	0.056*
C8	0.28451 (17)	0.26042 (15)	0.09408 (7)	0.0460 (4)
H8A	0.3202	0.2743	0.0552	0.055*
C2	0.24919 (18)	0.5611 (2)	0.38171 (8)	0.0584 (5)
H2B	0.1790	0.5091	0.4012	0.070*
H2C	0.2023	0.6319	0.3638	0.070*
C4	0.4771 (2)	0.5051 (2)	0.42042 (8)	0.0633 (5)
H4A	0.4543	0.4313	0.4434	0.076*
H4B	0.5677	0.5367	0.4341	0.076*
C3	0.3624 (2)	0.6009 (2)	0.42688 (10)	0.0748 (7)
H3A	0.3981	0.6822	0.4169	0.090*
H3B	0.3253	0.6021	0.4681	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0781 (4)	0.0754 (4)	0.0520 (3)	−0.0222 (2)	−0.0144 (2)	−0.0182 (2)
O1	0.0252 (5)	0.0734 (8)	0.0503 (6)	−0.0018 (5)	−0.0022 (4)	−0.0141 (5)
N2	0.0250 (5)	0.0529 (7)	0.0385 (6)	−0.0035 (4)	−0.0019 (5)	−0.0104 (5)
C6	0.0300 (6)	0.0374 (7)	0.0366 (6)	−0.0003 (5)	−0.0028 (5)	−0.0035 (5)
C10	0.0401 (7)	0.0376 (7)	0.0525 (8)	−0.0078 (6)	−0.0040 (6)	−0.0022 (6)
C5	0.0273 (6)	0.0462 (7)	0.0333 (6)	−0.0018 (5)	−0.0008 (5)	−0.0012 (5)
C11	0.0378 (7)	0.0399 (7)	0.0403 (7)	−0.0038 (5)	−0.0005 (5)	0.0017 (5)
N1	0.0278 (6)	0.0607 (8)	0.0366 (6)	0.0020 (5)	−0.0021 (5)	−0.0122 (5)
C9	0.0476 (8)	0.0423 (7)	0.0435 (7)	−0.0040 (6)	−0.0103 (6)	−0.0082 (6)
C7	0.0407 (7)	0.0434 (7)	0.0420 (7)	−0.0097 (6)	0.0024 (6)	−0.0037 (6)
C1	0.0304 (7)	0.0660 (9)	0.0427 (7)	0.0017 (6)	−0.0066 (6)	−0.0109 (7)
C8	0.0516 (8)	0.0499 (8)	0.0366 (7)	−0.0080 (6)	0.0007 (6)	−0.0041 (6)
C2	0.0386 (7)	0.0854 (12)	0.0511 (9)	0.0037 (8)	0.0039 (7)	−0.0269 (9)
C4	0.0507 (10)	0.0972 (14)	0.0419 (8)	−0.0043 (9)	−0.0111 (7)	−0.0109 (8)
C3	0.0550 (10)	0.1115 (18)	0.0580 (11)	−0.0022 (11)	−0.0013 (9)	−0.0434 (11)

Geometric parameters (Å, º)

Cl1—C9	1.7428 (15)	C7—C8	1.384 (2)
O1—C5	1.2368 (17)	C7—H7A	0.9300
N2—C5	1.3707 (18)	C1—C4	1.514 (2)
N2—C6	1.4138 (16)	C1—H1A	0.9700

N2—H2A	0.8600	C1—H1B	0.9700
C6—C7	1.387 (2)	C8—H8A	0.9300
C6—C11	1.3920 (19)	C2—C3	1.521 (3)
C10—C9	1.381 (2)	C2—H2B	0.9700
C10—C11	1.383 (2)	C2—H2C	0.9700
C10—H10A	0.9300	C4—C3	1.509 (3)
C5—N1	1.3453 (17)	C4—H4A	0.9700
C11—H11A	0.9300	C4—H4B	0.9700
N1—C2	1.4612 (19)	C3—H3A	0.9700
N1—C1	1.4664 (18)	C3—H3B	0.9700
C9—C8	1.383 (2)		

C5—N2—C6	121.82 (11)	C4—C1—H1A	111.2
C5—N2—H2A	119.1	N1—C1—H1B	111.2
C6—N2—H2A	119.1	C4—C1—H1B	111.2
C7—C6—C11	119.55 (12)	H1A—C1—H1B	109.1
C7—C6—N2	119.27 (12)	C9—C8—C7	119.31 (14)
C11—C6—N2	121.17 (12)	C9—C8—H8A	120.3
C9—C10—C11	119.02 (13)	C7—C8—H8A	120.3
C9—C10—H10A	120.5	N1—C2—C3	103.37 (14)
C11—C10—H10A	120.5	N1—C2—H2B	111.1
O1—C5—N1	121.34 (13)	C3—C2—H2B	111.1
O1—C5—N2	123.01 (12)	N1—C2—H2C	111.1
N1—C5—N2	115.65 (12)	C3—C2—H2C	111.1
C10—C11—C6	120.49 (13)	H2B—C2—H2C	109.1
C10—C11—H11A	119.8	C3—C4—C1	102.93 (15)
C6—C11—H11A	119.8	C3—C4—H4A	111.2
C5—N1—C2	120.15 (12)	C1—C4—H4A	111.2
C5—N1—C1	126.53 (12)	C3—C4—H4B	111.2
C2—N1—C1	111.87 (12)	C1—C4—H4B	111.2
C10—C9—C8	121.30 (13)	H4A—C4—H4B	109.1
C10—C9—Cl1	119.70 (12)	C4—C3—C2	104.35 (15)
C8—C9—Cl1	118.99 (12)	C4—C3—H3A	110.9
C8—C7—C6	120.25 (13)	C2—C3—H3A	110.9
C8—C7—H7A	119.9	C4—C3—H3B	110.9
C6—C7—H7A	119.9	C2—C3—H3B	110.9
N1—C1—C4	102.78 (13)	H3A—C3—H3B	108.9
N1—C1—H1A	111.2		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O1^{i}	0.86	2.21	2.9184 (15)	140

Symmetry code: (i) $x+1/2, y, -z+1/2$.