Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Chlorophenyl)-2-(naphthalen-1-yl)-acetamide

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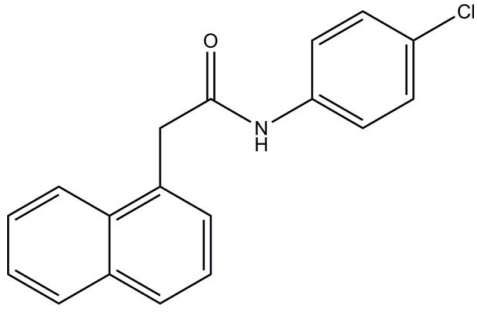
Received 8 July 2012; accepted 11 July 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.009 Å; R factor = 0.060; wR factor = 0.208; data-to-parameter ratio = 13.4.

In the title compound, $C_{18}H_{14}ClNO$, the naphthalene ring system [maximum deviation = 0.014 (9) Å] forms a dihedral angle of 74.8 (2)° with the benzene ring. In the crystal, molecules are linked *via* N—H···O hydrogen bonds into chains propagating along [010].

Related literature

For general background to and related structures of the title compound, see: Fun *et al.* (2010, 2011*a*,*b*, 2012).



Experimental

Crystal data

$C_{18}H_{14}ClNO$
M_r = 295.75
Monoclinic, $P2_1/c$
a = 19.163 (6) Å
b = 5.0458 (11) Å
c = 17.252 (4) Å
β = 116.365 (5)°
V = 1494.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 296 K
0.35 × 0.15 × 0.09 mm

Data collection

Bruker SMART APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.916, T_{max} = 0.978
9206 measured reflections
2611 independent reflections
1185 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.208
S = 1.01
2611 reflections
195 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N1···O1^{i}	0.98 (5)	1.98 (5)	2.942 (4)	166 (4)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

The authors thank Universiti Sains Malaysia (USM) for a Research University Grant (No. 1001/PFIZIK/811160). BN also thanks UGC, New Delhi, and the Government of India for the purchase of chemicals through the SAP-DRS-Phase 1 programme.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6893).

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‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5525-2009.

supporting information

Acta Cryst. (2012). E**68**, o2463 [https://doi.org/10.1107/S1600536812031613]

N-(4-Chlorophenyl)-2-(naphthalen-1-yl)acetamide

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S1. Comment

In continuation of our work on synthesis of amides (Fun *et al.*, 2010, 2011*a*,*b*, 2012), we report herein the crystal structure of the title compound.

The molecular structure is shown in Fig. 1. Bond lengths are comparable to related structures (Fun *et al.*, 2010, 2011*a*,*b*, 2012). The naphthalene ring system (C1–C10, maximum deviation of 0.014 (9) Å at atom C5) forms a dihedral angle of 74.8 (2)° with the benzene ring (C13–C18).

In the crystal structure, Fig. 2, molecules are linked *via* N1—H1N1···O1 hydrogen bonds (Table 1) into one-dimensional chains along [010].

S2. Experimental

1-Naphthalene acetic acid (0.186 g, 1 mmol), 4-chloroaniline (0.127 g, 1 mmol) and 1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide hydrochloride (1.0 g, 0.01 mol) were dissolved in dichloromethane (20 ml). The mixture was stirred in presence of triethylamine at 273 K for about 3 h. The contents were poured into 100 ml of ice-cold aqueous hydrochloric acid with stirring, which was extracted thrice with dichloromethane. Organic layer was washed with saturated $NaHCO_3$ solution and brine solution, dried and concentrated under reduced pressure to give the title compound. Colourless blocks were grown from acetone and toluene (1:1) mixture by the slow evaporation method (m.p. 449–451 K).

S3. Refinement

Atom H1N1 was located in a difference Fourier map and refined freely with N1—H1N1 = 0.98 (5) Å. The remaining H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

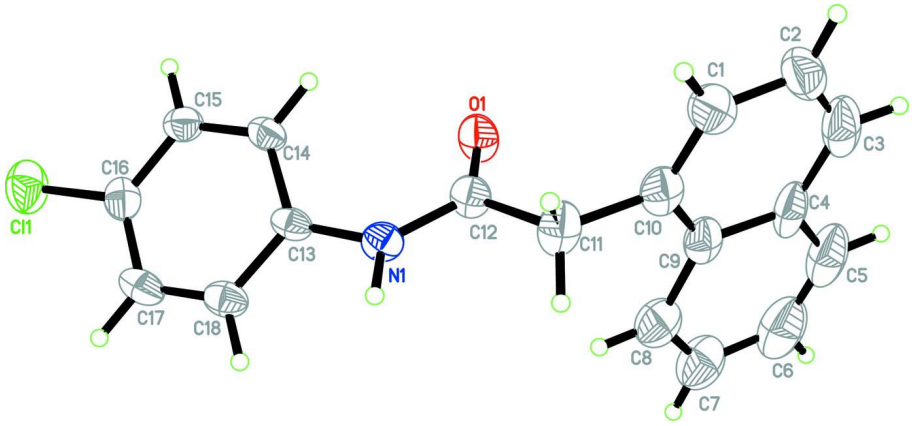

Figure 1

The molecular structure of the title compound showing 50% probability displacement ellipsoids for non-H atoms.

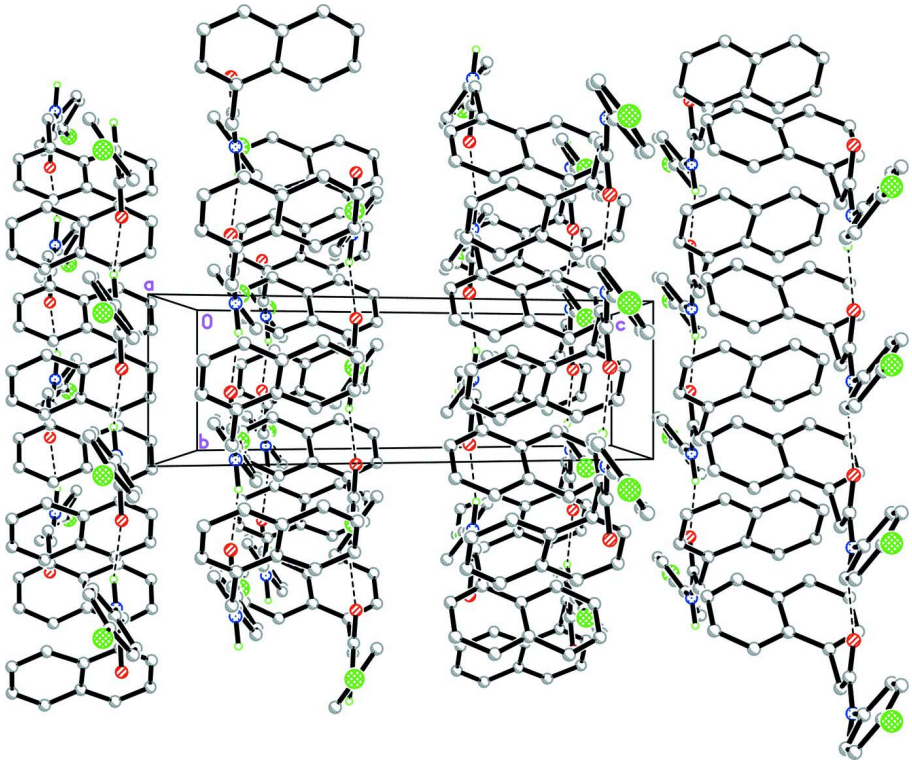

Figure 2

The crystal structure of the title compound, viewed along the *a* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

N-(4-Chlorophenyl)-2-(naphthalen-1-yl)acetamide

Crystal data

$C_{18}H_{14}ClNO$
$M_r = 295.75$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 19.163\ (6)$ Å
$b = 5.0458\ (11)$ Å
$c = 17.252\ (4)$ Å
$\beta = 116.365\ (5)°$
$V = 1494.6\ (7)$ Å^3
$Z = 4$

$F(000) = 616$
$D_x = 1.314$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1386 reflections
$\theta = 2.4$–$21.5°$
$\mu = 0.25$ mm^{-1}
$T = 296$ K
Block, colourless
0.35 × 0.14 × 0.09 mm

Data collection

Bruker SMART APEXII DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.916$, $T_{max} = 0.978$
9206 measured reflections
2611 independent reflections
1185 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -22 \rightarrow 22$
$k = -5 \rightarrow 3$
$l = -20 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.208$
$S = 1.01$
2611 reflections
195 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0913P)^2 + 0.5172P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.008 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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	0.30184 (7)	0.9142 (3)	0.11979 (9)	0.1183 (7)
O1	0.64245 (16)	0.5769 (5)	0.1247 (2)	0.0885 (10)
N1	0.6142 (2)	1.0067 (7)	0.1325 (2)	0.0681 (10)
C1	0.8073 (3)	0.5845 (12)	0.0810 (4)	0.1051 (16)
H1A	0.7783	0.6565	0.0263	0.126*
C2	0.8600 (4)	0.3825 (15)	0.0897 (6)	0.130 (2)
H2A	0.8650	0.3194	0.0418	0.156*
C3	0.9041 (4)	0.2791 (13)	0.1703 (7)	0.138 (3)
H3A	0.9402	0.1460	0.1780	0.166*
C4	0.8942 (3)	0.3771 (11)	0.2422 (5)	0.1032 (17)

C5	0.9390 (4)	0.2649 (14)	0.3251 (8)	0.147 (3)
H5A	0.9739	0.1276	0.3328	0.176*
C6	0.9296 (5)	0.363 (2)	0.3916 (7)	0.166 (3)
H6A	0.9598	0.2925	0.4463	0.199*
C8	0.8326 (3)	0.6693 (12)	0.3047 (5)	0.1102 (17)
H8A	0.7972	0.8025	0.2994	0.132*
C7	0.8779 (4)	0.5606 (17)	0.3840 (5)	0.133 (2)
H7A	0.8737	0.6209	0.4326	0.160*
C9	0.8398 (3)	0.5767 (9)	0.2290 (4)	0.0863 (14)
C10	0.7961 (3)	0.6808 (9)	0.1472 (4)	0.0880 (14)
C11	0.7373 (2)	0.9033 (9)	0.1340 (3)	0.0958 (14)
H11A	0.7606	1.0297	0.1810	0.115*
H11B	0.7266	0.9955	0.0806	0.115*
C12	0.6607 (2)	0.8082 (8)	0.1304 (3)	0.0723 (11)
C13	0.5384 (2)	0.9812 (7)	0.1258 (2)	0.0589 (10)
C14	0.4866 (2)	0.7824 (7)	0.0781 (2)	0.0666 (11)
H14A	0.5013	0.6598	0.0479	0.080*
C15	0.4140 (3)	0.7658 (8)	0.0751 (3)	0.0710 (11)
H15A	0.3801	0.6312	0.0436	0.085*
C16	0.3914 (2)	0.9466 (9)	0.1184 (3)	0.0748 (12)
C17	0.4414 (3)	1.1482 (8)	0.1643 (3)	0.0794 (13)
H17A	0.4259	1.2735	0.1931	0.095*
C18	0.5136 (3)	1.1623 (8)	0.1672 (2)	0.0717 (11)
H18B	0.5469	1.2989	0.1982	0.086*
H1N1	0.630 (3)	1.193 (10)	0.140 (3)	0.115 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0979 (10)	0.1515 (14)	0.1228 (12)	0.0188 (9)	0.0646 (9)	0.0142 (10)
O1	0.0811 (19)	0.0456 (17)	0.144 (3)	−0.0048 (15)	0.0547 (19)	−0.0001 (17)
N1	0.077 (2)	0.0456 (19)	0.080 (2)	−0.0074 (18)	0.0337 (19)	0.0019 (17)
C1	0.102 (4)	0.106 (4)	0.128 (5)	−0.025 (3)	0.069 (4)	−0.014 (4)
C2	0.111 (5)	0.121 (5)	0.196 (7)	−0.027 (4)	0.102 (5)	−0.054 (5)
C3	0.083 (4)	0.085 (4)	0.261 (10)	−0.017 (3)	0.090 (6)	−0.022 (6)
C4	0.052 (3)	0.076 (3)	0.175 (6)	−0.002 (3)	0.045 (4)	0.020 (4)
C5	0.077 (4)	0.095 (5)	0.247 (10)	−0.004 (3)	0.053 (6)	0.030 (6)
C6	0.105 (6)	0.170 (9)	0.208 (10)	−0.025 (6)	0.056 (6)	0.021 (8)
C8	0.094 (4)	0.114 (4)	0.128 (5)	−0.027 (3)	0.054 (4)	−0.001 (4)
C7	0.105 (5)	0.166 (7)	0.129 (6)	−0.022 (5)	0.052 (4)	0.011 (5)
C9	0.067 (3)	0.062 (3)	0.133 (5)	−0.015 (2)	0.048 (3)	0.001 (3)
C10	0.079 (3)	0.066 (3)	0.128 (5)	−0.019 (3)	0.054 (3)	0.003 (3)
C11	0.078 (3)	0.065 (3)	0.143 (4)	−0.006 (3)	0.049 (3)	0.020 (3)
C12	0.077 (3)	0.046 (2)	0.093 (3)	0.000 (2)	0.037 (2)	0.008 (2)
C13	0.087 (3)	0.040 (2)	0.052 (2)	0.004 (2)	0.032 (2)	0.0031 (17)
C14	0.080 (3)	0.051 (2)	0.070 (3)	0.003 (2)	0.035 (2)	−0.0098 (19)
C15	0.076 (3)	0.065 (3)	0.067 (3)	−0.005 (2)	0.026 (2)	−0.006 (2)
C16	0.077 (3)	0.092 (3)	0.064 (3)	0.016 (3)	0.039 (2)	0.015 (3)

C17	0.119 (4)	0.061 (3)	0.068 (3)	0.010 (3)	0.051 (3)	−0.003 (2)
C18	0.098 (3)	0.053 (2)	0.065 (3)	−0.002 (2)	0.038 (2)	−0.001 (2)

Geometric parameters (Å, º)

Cl1—C16	1.736 (4)	C8—C9	1.451 (7)
O1—C12	1.210 (4)	C8—H8A	0.9300
N1—C12	1.352 (5)	C7—H7A	0.9300
N1—C13	1.411 (5)	C9—C10	1.386 (6)
N1—H1N1	0.98 (5)	C10—C11	1.535 (6)
C1—C10	1.344 (7)	C11—C12	1.518 (6)
C1—C2	1.394 (8)	C11—H11A	0.9700
C1—H1A	0.9300	C11—H11B	0.9700
C2—C3	1.371 (9)	C13—C18	1.368 (5)
C2—H2A	0.9300	C13—C14	1.395 (5)
C3—C4	1.423 (9)	C14—C15	1.371 (5)
C3—H3A	0.9300	C14—H14A	0.9300
C4—C9	1.394 (7)	C15—C16	1.365 (5)
C4—C5	1.420 (10)	C15—H15A	0.9300
C5—C6	1.331 (10)	C16—C17	1.380 (6)
C5—H5A	0.9300	C17—C18	1.365 (6)
C6—C7	1.372 (10)	C17—H17A	0.9300
C6—H6A	0.9300	C18—H18B	0.9300
C8—C7	1.367 (8)		
C12—N1—C13	126.7 (3)	C1—C10—C9	118.4 (5)
C12—N1—H1N1	123 (3)	C1—C10—C11	121.6 (6)
C13—N1—H1N1	111 (3)	C9—C10—C11	120.0 (5)
C10—C1—C2	123.6 (6)	C12—C11—C10	114.0 (3)
C10—C1—H1A	118.2	C12—C11—H11A	108.7
C2—C1—H1A	118.2	C10—C11—H11A	108.7
C3—C2—C1	118.6 (7)	C12—C11—H11B	108.7
C3—C2—H2A	120.7	C10—C11—H11B	108.7
C1—C2—H2A	120.7	H11A—C11—H11B	107.6
C2—C3—C4	119.4 (7)	O1—C12—N1	123.1 (4)
C2—C3—H3A	120.3	O1—C12—C11	123.3 (4)
C4—C3—H3A	120.3	N1—C12—C11	113.7 (4)
C9—C4—C5	121.8 (7)	C18—C13—C14	117.8 (4)
C9—C4—C3	119.2 (7)	C18—C13—N1	118.7 (4)
C5—C4—C3	119.0 (7)	C14—C13—N1	123.4 (3)
C6—C5—C4	117.9 (8)	C15—C14—C13	120.7 (4)
C6—C5—H5A	121.0	C15—C14—H14A	119.7
C4—C5—H5A	121.0	C13—C14—H14A	119.7
C5—C6—C7	123.7 (10)	C16—C15—C14	120.1 (4)
C5—C6—H6A	118.2	C16—C15—H15A	119.9
C7—C6—H6A	118.2	C14—C15—H15A	119.9
C7—C8—C9	119.9 (6)	C15—C16—C17	120.0 (4)
C7—C8—H8A	120.0	C15—C16—Cl1	120.0 (4)

C9—C8—H8A	120.0	C17—C16—Cl1	119.9 (4)
C8—C7—C6	120.0 (8)	C18—C17—C16	119.5 (4)
C8—C7—H7A	120.0	C18—C17—H17A	120.2
C6—C7—H7A	120.0	C16—C17—H17A	120.2
C10—C9—C4	120.7 (6)	C17—C18—C13	121.9 (4)
C10—C9—C8	122.6 (5)	C17—C18—H18B	119.1
C4—C9—C8	116.7 (6)	C13—C18—H18B	119.1

C10—C1—C2—C3	−1.4 (8)	C8—C9—C10—C11	0.0 (6)
C1—C2—C3—C4	0.9 (9)	C1—C10—C11—C12	101.4 (5)
C2—C3—C4—C9	0.0 (8)	C9—C10—C11—C12	−79.4 (5)
C2—C3—C4—C5	178.7 (5)	C13—N1—C12—O1	−2.2 (7)
C9—C4—C5—C6	−2.3 (9)	C13—N1—C12—C11	176.7 (4)
C3—C4—C5—C6	179.0 (6)	C10—C11—C12—O1	−10.9 (7)
C4—C5—C6—C7	1.6 (12)	C10—C11—C12—N1	170.2 (4)
C9—C8—C7—C6	−0.6 (8)	C12—N1—C13—C18	149.8 (4)
C5—C6—C7—C8	−0.2 (11)	C12—N1—C13—C14	−31.2 (6)
C5—C4—C9—C10	−179.2 (4)	C18—C13—C14—C15	−1.9 (5)
C3—C4—C9—C10	−0.5 (6)	N1—C13—C14—C15	179.0 (4)
C5—C4—C9—C8	1.6 (6)	C13—C14—C15—C16	0.8 (6)
C3—C4—C9—C8	−179.7 (4)	C14—C15—C16—C17	0.7 (6)
C7—C8—C9—C10	−179.3 (4)	C14—C15—C16—Cl1	−176.3 (3)
C7—C8—C9—C4	−0.2 (7)	C15—C16—C17—C18	−1.0 (6)
C2—C1—C10—C9	0.8 (7)	Cl1—C16—C17—C18	176.0 (3)
C2—C1—C10—C11	−179.9 (4)	C16—C17—C18—C13	−0.2 (6)
C4—C9—C10—C1	0.2 (6)	C14—C13—C18—C17	1.6 (5)
C8—C9—C10—C1	179.3 (4)	N1—C13—C18—C17	−179.3 (3)
C4—C9—C10—C11	−179.1 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···O1^{i}	0.98 (5)	1.98 (5)	2.942 (4)	166 (4)

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