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Crystal structures of three *N*-(3-acetylphenyl)-quinoline-2-carboxamides

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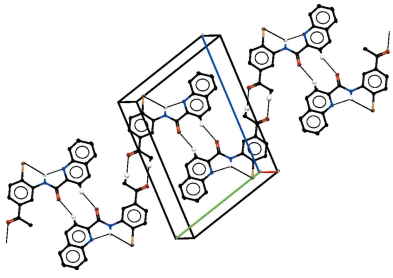
In the title compounds, *N*-(5-acetyl-2-methylphenyl)quinoline-2-carboxamide [$C_{19}H_{16}N_2O_2$, (I)], *N*-(5-acetyl-2-bromophenyl)quinoline-2-carboxamide [$C_{18}H_{13}BrN_2O_2$, (II)] and *N*-(5-acetyl-2-ethynylphenyl)quinoline-2-carboxamide [$C_{20}H_{14}N_2O_2$, (III)], the quinoline ring system is essentially planar and forms a dihedral angles of 3.68 (5) (I), 5.59 (7) (II) and 1.87 (6)° (III) with the acetyl-substituted ring. The molecular structures of (I) and (III) each feature an intramolecular N—H···N hydrogen bond, forming an *S*(5) ring, while in (II) an intramolecular bifurcated N—H···(N,Br) hydrogen bond forms two *S*(5) rings. In the crystals, weak C—H···O hydrogen bonds link molecules of (I) into *C*(7) chains long [010], molecules of (II) into chains of $R_2^2(8)$ rings along [110] and molecules of (III) into *C*(8) chains along [010]. In (I), there are no significant π–π stacking interactions under 4 Å, but in both (II) and (III), π–π interactions link the weak hydrogen-bonded chains into layers parallel to (001) [centroid–centroid disttances of 3.748 (1) Å in (II) and 3.577 (1), 3.784 (1) and 3.780 (1) Å in (III)].

1. Chemical context

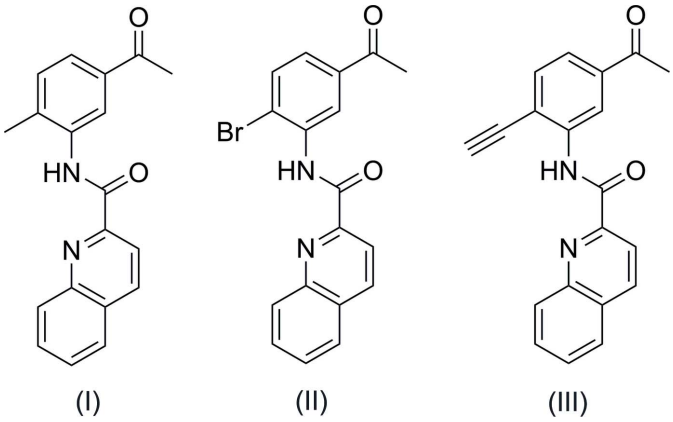
Aminoacetophenones, quinolines and carboxamides have been reported to possess many interesting pharmacological activities and they are characteristic components of a large number of biologically active compounds. The wide spectrum of biological effects of these kind of compounds includes antimicrobial (Nawar & Hosny, 2000), anticonvulsant (Pandeya *et al.*, 1998), cytotoxic (Zhao *et al.*, 2005), antimalarial (Egan *et al.*, 1994), antiproliferative (Chen *et al.*, 2006), antituberculosis/antimycobacterial (Gonec *et al.*, 2012) activities, radioligands (Matarrese *et al.*, 2001, Belloli *et al.*, 2004), calpain inhibitors (Nam *et al.*, 2008), TPSO ligand (Blair *et al.*, 2013) and pharmaceutical medicaments (Weidmann *et al.*, 2008), among others.



2. Structural commentary

The molecular structure of title compounds (I), (II) and (III) are shown in Figs. 1, 2 and 3, respectively. The quinoline ring system [C1–C9/N1 in (I), C2–C10/N1 in (II) and C12–C20/N2 in (III)] in each compound is essentially planar with maximum deviations of 0.015 (1) Å for C3 in (I), 0.017 (2) Å for C3 in (II) and 0.013 (2) Å for C17 in (III). The quinoline ring system forms dihedral angles of 3.68 (5)° (I), 5.59 (7)° (II) and 1.87 (6)° (III) with the acetyl-substituted ring [C11–C16 in (I)

and (II), C3–C8 in (III)]. In the molecular structures of (I) and (III), an intramolecular N—H···N hydrogen bond forms an *S*(5) ring while in (II) an intramolecular bifurcated N—H···(N,Br) hydrogen bond forms two *S*(5) rings (Tables 1–3).



3. Supramolecular features

In the crystals, weak C—H···O hydrogen bonds link molecules of (I) into *C*(7) chains along [010] (Fig. 4), molecules of (II) into chains of $R_2^2(8)$ rings along [110] (Fig. 5) and molecules of (III) into *C*(8) chains along [010] (Fig. 6). In (I), there are no significant π–π stacking interactions under 4 Å but in (II) π–π interactions link the weak hydrogen-bonded chains into layers parallel to (001) [centroid–centroid distance

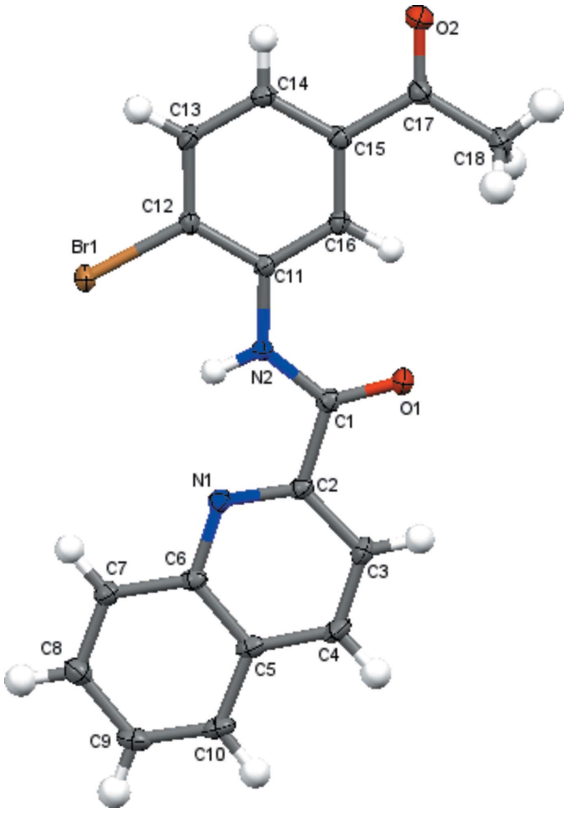


Figure 2
The molecular structure of (II), with the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

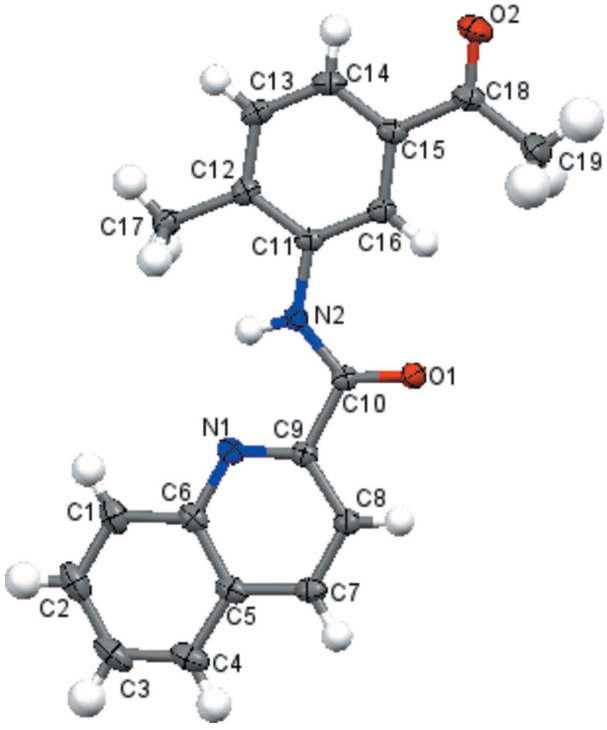


Figure 1
The molecular structure of (I), with the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

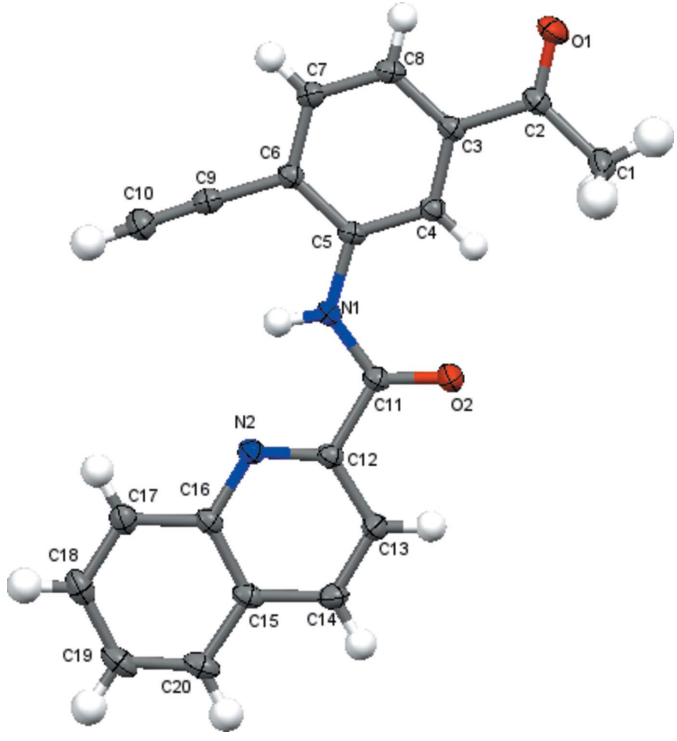


Figure 3
The molecular structure of (III), with the-atom numbering scheme and displacement ellipsoids drawn at the 50% probability level.

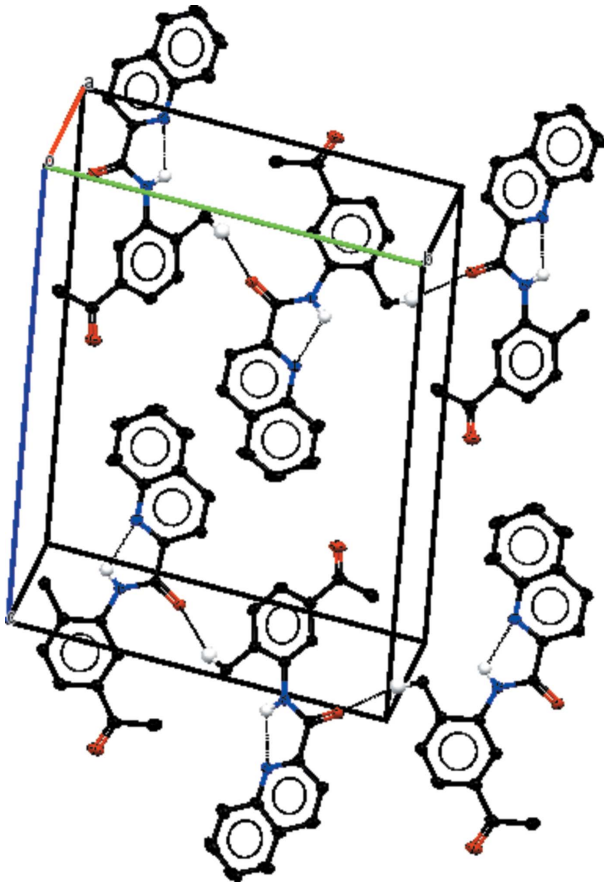


Figure 4
Part of the crystal structure of (I), with intermolecular and intramolecular hydrogen bonds shown as black dotted lines. Only H atoms involved in hydrogen bonds are shown.

*Cg*1···*Cg*2(1 + *x*, *y*, *z*) = 3.748 (1) Å; *Cg*1 and *Cg*2 are the centroids of the C5–C10 and N1/C2–C6 rings, respectively]. In (III), π–π interactions link the weak hydrogen-bonded chains into layers parallel to (001) with centroid–centroid distances

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1	0.86	2.15	2.619 (2)	114
C17—H17···O1^{i}	0.96	2.49	3.424 (2)	164

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1	0.86	2.19	2.629 (2)	112
C3—H3···O1^{i}	0.93	2.55	3.410 (2)	154
C18—H18···O2^{ii}	0.96	2.49	3.444 (2)	171
N2—H2···Br1	0.86	2.58	3.081 (1)	118

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+3, -y, -z+1$.

Table 3
Hydrogen-bond geometry (Å, °) for (III).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2	0.86	2.23	2.666 (2)	111
C10—H10···O2^{i}	0.93	2.36	3.103 (2)	136

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

*Cg*3···*Cg*4(−1 + *x*, −1 + *y*, −1 + *z*) = 3.577 (1), *Cg*4···*Cg*5(−*x* + 1, −*y* + 1, −*z* + 1) 3.784 (1) and *Cg*4···*Cg*5(−*x* + 2, −*y* + 1, −*z* + 1) = 3.780 (1) Å; *Cg*3, *Cg*4, and *Cg*5 are the centroids of the N2/C12–C16, C3–C8 and C15–C20 rings, respectively].

4. Database survey

A search of the Cambridge Structural Database (Groom *et al.* 2016; Version 1.18, April 2016) for similar compounds with an

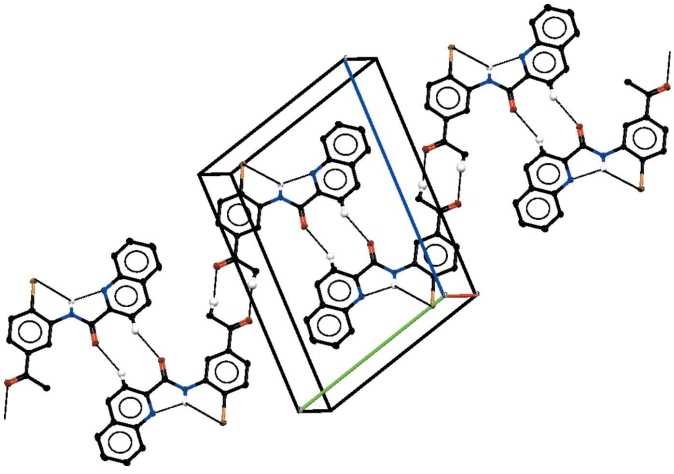


Figure 5
Part of the crystal structure of (II), with intermolecular and intramolecular hydrogen bonds shown as black dotted lines. Only H atoms involved in hydrogen bonds are shown.

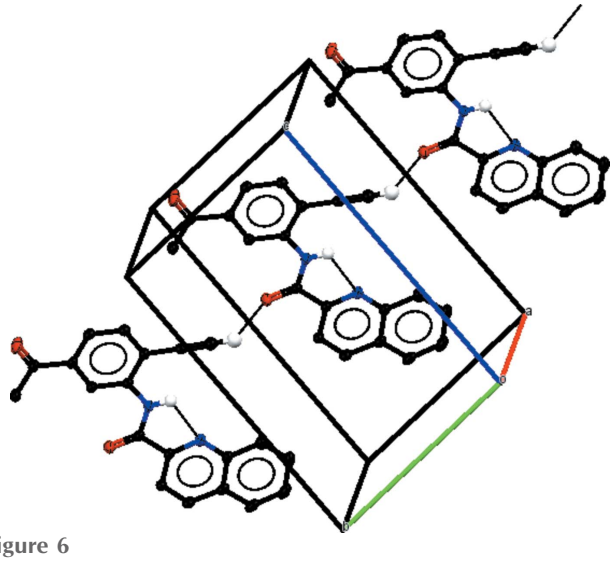


Figure 6
Part of the crystal structure of (III), with intermolecular and intramolecular hydrogen bonds shown as black dotted lines. Only H atoms involved in hydrogen bonds are shown.

Table 4
Experimental details.

	(I)	(II)	(III)
Crystal data			
Chemical formula	$C_{19}H_{16}N_2O_2$	$C_{18}H_{13}BrN_2O_2$	$C_{20}H_{14}N_2O_2$
M_r	304.34	369.21	314.33
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$	Triclinic, $P\overline{1}$
Temperature (K)	123	123	123
a, b, c (Å)	4.5787 (2), 14.7986 (7), 22.3732 (12)	4.29848 (12), 11.6353 (3), 15.5888 (4)	7.3075 (6), 8.2605 (4), 13.8196 (9)
α, β, γ (°)	90, 92.130 (5), 90	103.788 (2), 95.515 (2), 96.195 (2)	92.734 (5), 100.608 (6), 108.989 (6)
V (Å^3)	1514.93 (12)	746.76 (3)	770.11 (10)
Z	4	2	2
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.71	3.85	0.09
Crystal size (mm)	0.33 × 0.12 × 0.07	0.65 × 0.10 × 0.06	0.19 × 0.08 × 0.05
Data collection			
Diffractometer	Agilent TitanS2 GV1000	Agilent TitanS2 GV1000	Agilent SuperNova Single source at offset, Eos
Absorption correction	Analytical [*CrysAlis PRO* (Rigaku OD, 2015), based on expressions derived by Clark & Reid (1995)]	Gaussian [*CrysAlis PRO* (Rigaku OD, 2015), based on expressions derived by Clark & Reid (1995)]	Analytical [*CrysAlis PRO* (Rigaku OD, 2015), based on expressions derived by Clark & Reid (1995)]
T_{min}, T_{max}	0.869, 0.958	0.540, 0.900	0.987, 0.996
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6056, 2935, 2562	12899, 2966, 2870	20693, 5173, 3687
R_{int}	0.020	0.033	0.060
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.622	0.753
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.106, 1.04	0.024, 0.065, 1.05	0.056, 0.151, 1.04
No. of reflections	2935	2966	5173
No. of parameters	210	210	218
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.21	0.48, −0.65	0.42, −0.26

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

N-phenylquinoline-2-carboxamide skeleton resulted in twelve hits. One entry for the compound without substituents is reported (Jing & Qin, 2007). Eight are structures substituted in the 4-position of the phenyl group: one methoxy group (Qi *et al.*, 2003) and another a nitro group (Jing & Qin, 2008); one chlorine and one fluorine (Khavasi *et al.*, 2014), and two reports each for bromine (Bobal *et al.*, 2012; Khavasi *et al.*, 2014) and iodine (Qi *et al.*, 2003; Khavasi *et al.*, 2014). The rest have large organic substituents.

5. Synthesis and crystallization

Compounds (I)–(III) were prepared by refluxing a mixture of quinaldic acid, triethylamine, *p*-toluenesulfonyl chloride and the corresponding substituted aminoacetophenones (**1a**–**c**) for 24 h in DCM (Fig. 7). Acetic acid 5% was added to quench the reaction, and the organic phase was washed three times with water. After evaporation of DCM, the compounds were purified by silica column chromatography (pentane:ethyl acetate 2:1). Single crystals were obtained by slow evaporation of the respective solutions of the compounds in dichloromethane into a closed flask with petroleum ether.

***N*-(5-acetyl-2-methylphenyl)quinoline-2-carboxamide (I):** Light-yellow solid (0.700 g, yield quant, R_f PE/EA 2:1 0.52). **^{1}H NMR (400 MHz, CDCl$_3$):** δ 8.95 (*d*, ^3J = 7.7 Hz, 1H, quinol), 8.40 (*s*, 2H, ArH quinol), 8.17 (*d*, ^3J = 8.5 Hz, 1H, ArH), 7.93 (*d*, ^3J = 9.0 Hz, 1H, quinol), 7.82 (*ddd*, ^3J = 8.4, ^3J = 6.9 Hz, 1H, quinol), 7.73 (*dd*, ^3J = 7.9, 1H, ArH), 7.67 (*ddd*, ^3J = 8.1, ^3J = 6.9 Hz, 1H, quinol), 7.35 (*d*, ^3J = 7.9 Hz, 1H, quinol), 2.65 (*s*, 3H, CH_3), 2.55 (*s*, 3H, $COCH_3$). **^{13}C NMR (100 MHz,**

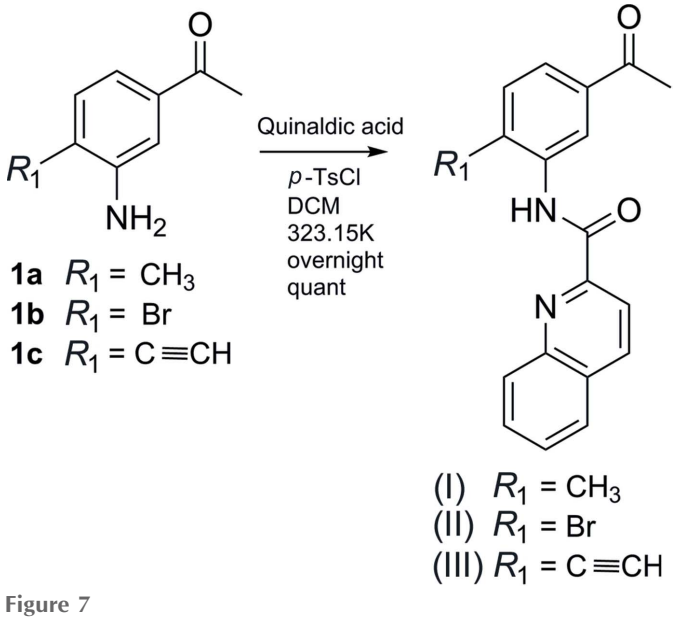


Figure 7
The reaction scheme for the synthesis of the title compounds

$CDCl_3$): δ 197.8 (C_{quat}), 162.2 (C_{quat}), 149.5 (C_{quat}), 146.2 (C_{quat}), 138.0 (C_{quat}), 136.2 (C_{quat}), 133.5 (C_{quat}), 130.7 (C_{quat}), 130.4 (+), 129.8 (+), 129.5 (+), 128.3 (+), 127.8 (+), 124.1 (+), 121.5 (+), 118.6 (+), 26.7 (+), 18.0 (+).

***N*-(5-acetyl-2-bromophenyl)quinoline-2-carboxamide (II):** Yellow solid (0.700 g, yield quant, R_f PE/EA 2:1 0.60). **^{1}H NMR (400 MHz, $CDCl_3$): δ** 9.32 (*s*, 1H), 8.40 (*d*, ^3J = 3.0 Hz, 2H), 8.23 (*d*, ^3J = 8.5 Hz, 1H), 7.94 (*d*, ^3J = 8.8 Hz, 1H), 7.83 (*t*, ^3J = 7.0 Hz, 1H), 7.69 (*m*, 3H), 2.68 (*s*, 3H, $COCH_3$). **^{13}C NMR (100 MHz, $CDCl_3$): δ** 197.3 (C_{quat}), 162.6 (C_{quat}), 149.1 (C_{quat}), 146.3 (C_{quat}), 138.2 (C_{quat}), 137.2 (C_{quat}), 136.3 (C_{quat}), 132.8 (+), 130.6 (+), 130.5 (+), 130.6 (+), 128.5 (+), 127.8 (+), 124.1 (+), 121.1 (+), 118.9 (+), 118.5 (+), 26.7 (+).

***N*-(5-acetyl-2-ethynylphenyl)quinoline-2-carboxamide (III):** Light-brown solid (0.700 g, yield quant, R_f PE/EA 2:1 0.20). **^{1}H NMR (400 MHz, $CDCl_3$): δ** 9.36 (*d*, ^3J = 1.6 Hz, 1H), 8.40 (*s*, 2H), 8.15 (*d*, ^3J = 8.5 Hz, 1H), 7.94 (*d*, ^3J = 8.2 Hz, 1H), 7.82 (*dd*, ^3J = 11.2, 4.2 Hz, 1H), 7.73 (*dd*, ^3J = 8.1, ^3J = 1.7 Hz, 1H), 7.71 (*m*, 1H), 7.63 (*d*, *J* = 8.1 Hz, 1H), 3.87 (*s*, 1H, CCH), 2.70 (*s*, 3H, CH_3). **^{13}C NMR (100 MHz, $CDCl_3$): δ** = 197.6 (C_{quat}), 162.8 (C_{quat}), 149.2 (C_{quat}), 146.3 (C_{quat}), 140.1 (C_{quat}), 138.0 (C_{quat}), 132.5 (+), 130.4 (+), 129.9 (+), 129.5 (+), 128.4 (+), 127.8 (+), 122.6 (+), 119.1 (+), 118.6 (+), 115.7 (+), 87.1 (C_{quat}), 79.0 (+), 26.8 (+).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. All non-hydrogen atoms were refined anisotropically. Hydrogen-atom positions were calculated geometrically and refined using the riding model. N–H = 0.86 Å, C—H = 0.96 Å for methyl H atoms and 0.93 Å for all other; U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(C_{methyl}).

Acknowledgements

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supporting information

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Crystal structures of three *N*-(3-acetylphenyl)quinoline-2-carboxamides

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Computing details

For all compounds, data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

(I) *N*-(5-Acetyl-2-methylphenyl)quinoline-2-carboxamide

Crystal data

$C_{19}H_{16}N_2O_2$
M_r = 304.34
Monoclinic, $P2_1/c$
a = 4.5787 (2) Å
b = 14.7986 (7) Å
c = 22.3732 (12) Å
β = 92.130 (5)°
V = 1514.93 (12) Å^3
Z = 4
$F(000)$ = 640
D_x = 1.334 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3477 reflections
θ = 6.0–74.2°
μ = 0.71 mm^{-1}
T = 123 K
Block, dark gray
0.33 × 0.12 × 0.07 mm

Data collection

Agilent TitanS2 GV1000 diffractometer
Radiation source: gradient vaccum rotating-anode X-ray tube, GV1000 (Cu) X-ray Source
Mirror monochromator
Detector resolution: 4.1818 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlis PRO (Rigaku OD, 2015), based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.869, T_{max} = 0.958
6056 measured reflections
2935 independent reflections
2562 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 74.4°, θ_{min} = 3.6°
h = −5→5
k = −18→17
l = −27→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.106
S = 1.04
2935 reflections
210 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0608P)^2 + 0.2546P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.59998 (18)	0.50983 (6)	0.24602 (4)	0.0250 (2)
O2	1.4993 (2)	0.62002 (8)	0.05885 (5)	0.0410 (3)
N2	0.7067 (2)	0.65842 (7)	0.26763 (5)	0.0217 (2)
H2	0.6628	0.7001	0.2925	0.026*
N1	0.3450 (2)	0.65936 (7)	0.35561 (5)	0.0223 (2)
C10	0.5705 (2)	0.57873 (8)	0.27553 (5)	0.0197 (2)
C9	0.3690 (2)	0.58150 (8)	0.32767 (5)	0.0200 (2)
C16	1.0023 (2)	0.62534 (8)	0.18077 (5)	0.0225 (3)
H16	0.9290	0.5668	0.1784	0.027*
C11	0.9095 (2)	0.68391 (8)	0.22502 (5)	0.0205 (3)
C12	1.0191 (2)	0.77271 (8)	0.22953 (6)	0.0223 (3)
C8	0.2199 (2)	0.50181 (8)	0.34310 (6)	0.0229 (3)
H8	0.2444	0.4485	0.3219	0.028*
C15	1.2058 (2)	0.65473 (8)	0.13999 (6)	0.0239 (3)
C6	0.1639 (2)	0.66364 (9)	0.40278 (5)	0.0242 (3)
C17	0.9276 (3)	0.83545 (8)	0.27837 (6)	0.0257 (3)
H17A	0.7217	0.8470	0.2739	0.039*
H17B	1.0329	0.8913	0.2758	0.039*
H17C	0.9700	0.8080	0.3166	0.039*
C13	1.2190 (3)	0.80052 (8)	0.18796 (6)	0.0252 (3)
H13	1.2917	0.8592	0.1899	0.030*
C14	1.3123 (3)	0.74284 (9)	0.14374 (6)	0.0268 (3)
H14	1.4464	0.7630	0.1165	0.032*
C7	0.0383 (3)	0.50538 (9)	0.39030 (6)	0.0260 (3)
H7	−0.0619	0.4539	0.4018	0.031*
C5	0.0036 (2)	0.58715 (9)	0.42139 (6)	0.0256 (3)
C18	1.3186 (3)	0.59328 (9)	0.09298 (6)	0.0284 (3)
C1	0.1359 (3)	0.74684 (10)	0.43341 (6)	0.0309 (3)
H1	0.2429	0.7969	0.4218	0.037*
C4	−0.1839 (3)	0.59647 (11)	0.47008 (6)	0.0337 (3)
H4	−0.2897	0.5469	0.4830	0.040*
C3	−0.2098 (3)	0.67783 (12)	0.49810 (6)	0.0395 (4)
H3	−0.3356	0.6835	0.5296	0.047*
C2	−0.0478 (3)	0.75369 (11)	0.47989 (7)	0.0371 (3)
H2A	−0.0665	0.8085	0.4997	0.045*
C19	1.2077 (4)	0.49817 (10)	0.08911 (8)	0.0446 (4)
H19A	1.2992	0.4673	0.0570	0.067*
H19B	0.9998	0.4988	0.0818	0.067*
H19C	1.2530	0.4674	0.1261	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0249 (4)	0.0214 (4)	0.0291 (5)	0.0003 (3)	0.0072 (3)	−0.0016 (3)
O2	0.0414 (5)	0.0441 (6)	0.0388 (6)	−0.0028 (4)	0.0208 (4)	0.0001 (5)
N2	0.0217 (5)	0.0199 (5)	0.0239 (5)	0.0002 (4)	0.0055 (4)	−0.0005 (4)
N1	0.0195 (5)	0.0248 (5)	0.0226 (5)	0.0028 (4)	0.0008 (4)	0.0000 (4)
C10	0.0152 (5)	0.0210 (5)	0.0228 (6)	0.0018 (4)	0.0002 (4)	0.0018 (4)
C9	0.0163 (5)	0.0233 (5)	0.0202 (6)	0.0018 (4)	−0.0006 (4)	0.0015 (4)
C16	0.0197 (5)	0.0229 (5)	0.0250 (6)	0.0013 (4)	0.0017 (4)	0.0028 (5)
C11	0.0159 (5)	0.0229 (5)	0.0226 (6)	0.0009 (4)	0.0008 (4)	0.0050 (4)
C12	0.0188 (5)	0.0222 (6)	0.0258 (6)	0.0021 (4)	−0.0014 (4)	0.0035 (5)
C8	0.0201 (5)	0.0246 (6)	0.0240 (6)	−0.0003 (4)	0.0007 (4)	0.0011 (5)
C15	0.0200 (5)	0.0277 (6)	0.0242 (6)	0.0030 (4)	0.0028 (4)	0.0047 (5)
C6	0.0197 (5)	0.0316 (6)	0.0210 (6)	0.0051 (5)	−0.0010 (4)	0.0006 (5)
C17	0.0275 (6)	0.0211 (5)	0.0286 (6)	−0.0011 (5)	0.0017 (5)	0.0013 (5)
C13	0.0217 (5)	0.0228 (5)	0.0312 (7)	−0.0023 (4)	0.0002 (5)	0.0072 (5)
C14	0.0216 (6)	0.0308 (6)	0.0283 (7)	0.0000 (5)	0.0050 (5)	0.0081 (5)
C7	0.0201 (5)	0.0322 (6)	0.0256 (6)	−0.0028 (5)	0.0008 (5)	0.0050 (5)
C5	0.0185 (5)	0.0377 (7)	0.0205 (6)	0.0034 (5)	−0.0002 (4)	0.0038 (5)
C18	0.0246 (6)	0.0340 (7)	0.0268 (6)	0.0034 (5)	0.0057 (5)	0.0039 (5)
C1	0.0310 (6)	0.0346 (7)	0.0270 (7)	0.0079 (5)	−0.0014 (5)	−0.0046 (5)
C4	0.0243 (6)	0.0522 (8)	0.0249 (7)	0.0045 (6)	0.0047 (5)	0.0061 (6)
C3	0.0304 (7)	0.0648 (10)	0.0236 (7)	0.0138 (7)	0.0054 (5)	−0.0011 (7)
C2	0.0360 (7)	0.0479 (8)	0.0273 (7)	0.0147 (6)	−0.0015 (5)	−0.0097 (6)
C19	0.0536 (9)	0.0348 (8)	0.0472 (9)	−0.0030 (6)	0.0261 (7)	−0.0092 (7)

Geometric parameters (Å, º)

O1—C10	1.2249 (15)	C17—H17A	0.9600
O2—C18	1.2129 (17)	C17—H17B	0.9600
N2—H2	0.8600	C17—H17C	0.9600
N2—C10	1.3490 (15)	C13—H13	0.9300
N2—C11	1.4068 (15)	C13—C14	1.3861 (19)
N1—C9	1.3175 (15)	C14—H14	0.9300
N1—C6	1.3674 (16)	C7—H7	0.9300
C10—C9	1.5142 (16)	C7—C5	1.4075 (19)
C9—C8	1.4120 (16)	C5—C4	1.4188 (18)
C16—H16	0.9300	C18—C19	1.498 (2)
C16—C11	1.3940 (17)	C1—H1	0.9300
C16—C15	1.3973 (17)	C1—C2	1.365 (2)
C11—C12	1.4090 (16)	C4—H4	0.9300
C12—C17	1.5051 (17)	C4—C3	1.365 (2)
C12—C13	1.3912 (17)	C3—H3	0.9300
C8—H8	0.9300	C3—C2	1.414 (2)
C8—C7	1.3694 (17)	C2—H2A	0.9300
C15—C14	1.3937 (18)	C19—H19A	0.9600
C15—C18	1.4970 (18)	C19—H19B	0.9600

C6—C5	1.4200 (18)	C19—H19C	0.9600
C6—C1	1.4172 (18)		

C10—N2—H2	115.0	C12—C13—H13	119.2
C10—N2—C11	130.05 (10)	C14—C13—C12	121.53 (11)
C11—N2—H2	115.0	C14—C13—H13	119.2
C9—N1—C6	118.07 (10)	C15—C14—H14	119.9
O1—C10—N2	126.59 (11)	C13—C14—C15	120.17 (11)
O1—C10—C9	121.36 (10)	C13—C14—H14	119.9
N2—C10—C9	112.04 (10)	C8—C7—H7	120.1
N1—C9—C10	116.96 (10)	C8—C7—C5	119.81 (11)
N1—C9—C8	124.38 (11)	C5—C7—H7	120.1
C8—C9—C10	118.66 (10)	C7—C5—C6	118.13 (11)
C11—C16—H16	120.1	C7—C5—C4	123.06 (12)
C11—C16—C15	119.89 (11)	C4—C5—C6	118.81 (12)
C15—C16—H16	120.1	O2—C18—C15	120.37 (13)
N2—C11—C12	116.35 (10)	O2—C18—C19	120.53 (13)
C16—C11—N2	122.74 (11)	C15—C18—C19	119.10 (11)
C16—C11—C12	120.91 (11)	C6—C1—H1	119.9
C11—C12—C17	121.28 (11)	C2—C1—C6	120.15 (14)
C13—C12—C11	118.00 (11)	C2—C1—H1	119.9
C13—C12—C17	120.71 (11)	C5—C4—H4	119.9
C9—C8—H8	121.0	C3—C4—C5	120.25 (14)
C7—C8—C9	118.00 (11)	C3—C4—H4	119.9
C7—C8—H8	121.0	C4—C3—H3	119.6
C16—C15—C18	121.71 (11)	C4—C3—C2	120.85 (13)
C14—C15—C16	119.50 (12)	C2—C3—H3	119.6
C14—C15—C18	118.77 (11)	C1—C2—C3	120.34 (14)
N1—C6—C5	121.61 (11)	C1—C2—H2A	119.8
N1—C6—C1	118.80 (12)	C3—C2—H2A	119.8
C1—C6—C5	119.59 (12)	C18—C19—H19A	109.5
C12—C17—H17A	109.5	C18—C19—H19B	109.5
C12—C17—H17B	109.5	C18—C19—H19C	109.5
C12—C17—H17C	109.5	H19A—C19—H19B	109.5
H17A—C17—H17B	109.5	H19A—C19—H19C	109.5
H17A—C17—H17C	109.5	H19B—C19—H19C	109.5
H17B—C17—H17C	109.5		

O1—C10—C9—N1	−178.04 (10)	C11—C16—C15—C14	−0.49 (18)
O1—C10—C9—C8	1.81 (16)	C11—C16—C15—C18	178.04 (11)
N2—C10—C9—N1	2.76 (14)	C11—C12—C13—C14	−0.89 (17)
N2—C10—C9—C8	−177.40 (10)	C12—C13—C14—C15	0.12 (19)
N2—C11—C12—C17	1.36 (16)	C8—C7—C5—C6	−0.83 (17)
N2—C11—C12—C13	−179.66 (10)	C8—C7—C5—C4	178.99 (11)
N1—C9—C8—C7	−0.09 (18)	C15—C16—C11—N2	−179.62 (10)
N1—C6—C5—C7	0.80 (17)	C15—C16—C11—C12	−0.31 (17)
N1—C6—C5—C4	−179.03 (11)	C6—N1—C9—C10	179.88 (9)
N1—C6—C1—C2	178.65 (12)	C6—N1—C9—C8	0.04 (17)

C10—N2—C11—C16	0.95 (19)	C6—C5—C4—C3	0.34 (18)
C10—N2—C11—C12	−178.39 (11)	C6—C1—C2—C3	0.4 (2)
C10—C9—C8—C7	−179.93 (10)	C17—C12—C13—C14	178.09 (11)
C9—N1—C6—C5	−0.41 (16)	C14—C15—C18—O2	−0.05 (19)
C9—N1—C6—C1	179.89 (11)	C14—C15—C18—C19	179.31 (13)
C9—C8—C7—C5	0.49 (17)	C7—C5—C4—C3	−179.48 (12)
C16—C11—C12—C17	−177.99 (11)	C5—C6—C1—C2	−1.07 (19)
C16—C11—C12—C13	0.99 (17)	C5—C4—C3—C2	−1.0 (2)
C16—C15—C14—C13	0.59 (18)	C18—C15—C14—C13	−177.99 (11)
C16—C15—C18—O2	−178.60 (12)	C1—C6—C5—C7	−179.50 (11)
C16—C15—C18—C19	0.76 (19)	C1—C6—C5—C4	0.67 (17)
C11—N2—C10—O1	0.6 (2)	C4—C3—C2—C1	0.6 (2)
C11—N2—C10—C9	179.74 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1	0.86	2.15	2.619 (2)	114
C17—H17···O1^{i}	0.96	2.49	3.424 (2)	164

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

(II) *N*-(5-Acetyl-2-bromophenyl)quinoline-2-carboxamide

Crystal data

$C_{18}H_{13}BrN_2O_2$
M_r = 369.21
Triclinic, $P\overline{1}$
a = 4.29848 (12) Å
b = 11.6353 (3) Å
c = 15.5888 (4) Å
α = 103.788 (2)°
β = 95.515 (2)°
γ = 96.195 (2)°
V = 746.76 (3) Å^3
Z = 2
$F(000)$ = 372
D_x = 1.642 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 10806 reflections
θ = 3.9–73.8°
μ = 3.85 mm^{-1}
T = 123 K
Plank, clear colourless
0.65 × 0.10 × 0.06 mm

Data collection

Agilent TitanS2 GV1000 diffractometer
Radiation source: gradient vaccum rotating-anode X-ray tube, GV1000 (Cu) X-ray Source
Mirror monochromator
Detector resolution: 4.1818 pixels mm^{-1}
ω scans
Absorption correction: gaussian [CrysAlis PRO (Rigaku OD, 2015), based on expressions derived by Clark & Reid (1995)]
T_{min} = 0.540, T_{max} = 0.900
12899 measured reflections
2966 independent reflections
2870 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 73.7°, θ_{min} = 2.9°
h = −5→5
k = −13→14
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.065
S = 1.05
2966 reflections
210 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 0.3702P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.65$ e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0018 (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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.61589 (4)	0.18439 (2)	0.04683 (2)	0.02135 (9)
O1	0.5793 (3)	0.36128 (11)	0.39598 (8)	0.0221 (3)
O2	1.3517 (3)	−0.04850 (12)	0.36241 (9)	0.0289 (3)
N2	0.5689 (3)	0.29917 (12)	0.24400 (9)	0.0152 (3)
H2	0.4949	0.3149	0.1955	0.018*
N1	0.2021 (3)	0.45877 (12)	0.22055 (9)	0.0155 (3)
C11	0.7457 (4)	0.20417 (15)	0.23433 (11)	0.0144 (3)
C1	0.4988 (4)	0.37012 (15)	0.32082 (11)	0.0161 (3)
C6	0.0260 (4)	0.54368 (15)	0.20390 (11)	0.0159 (3)
C15	1.0588 (4)	0.07376 (15)	0.29489 (11)	0.0161 (3)
C12	0.7872 (4)	0.13977 (15)	0.14896 (11)	0.0161 (3)
C2	0.3045 (4)	0.46475 (15)	0.30427 (11)	0.0156 (3)
C16	0.8882 (4)	0.16983 (15)	0.30694 (11)	0.0158 (3)
H16	0.8683	0.2121	0.3644	0.019*
C13	0.9537 (4)	0.04208 (16)	0.13641 (11)	0.0185 (3)
H13	0.9742	−0.0006	0.0791	0.022*
C3	0.2451 (4)	0.55339 (16)	0.37799 (11)	0.0202 (4)
H3	0.3202	0.5528	0.4358	0.024*
C14	1.0880 (4)	0.00874 (16)	0.20912 (11)	0.0183 (3)
H14	1.1978	−0.0569	0.2010	0.022*
C18	1.2121 (4)	0.11879 (17)	0.46469 (11)	0.0219 (4)
H18A	0.9983	0.1174	0.4778	0.033*
H18B	1.2985	0.1991	0.4666	0.033*
H18C	1.3353	0.0903	0.5080	0.033*
C17	1.2189 (4)	0.03975 (16)	0.37334 (11)	0.0187 (3)
C7	−0.0919 (4)	0.53725 (16)	0.11481 (11)	0.0190 (3)
H7	−0.0509	0.4752	0.0692	0.023*
C8	−0.2654 (4)	0.62145 (17)	0.09514 (12)	0.0231 (4)
H8	−0.3398	0.6169	0.0362	0.028*
C9	−0.3322 (4)	0.71549 (17)	0.16407 (13)	0.0241 (4)
H9	−0.4509	0.7723	0.1501	0.029*
C4	0.0744 (4)	0.63973 (16)	0.36164 (12)	0.0221 (4)
H4	0.0344	0.7000	0.4087	0.026*

C10	−0.2242 (4)	0.72361 (16)	0.25081 (13)	0.0220 (4)
H10	−0.2703	0.7858	0.2955	0.026*
C5	−0.0422 (4)	0.63791 (15)	0.27334 (12)	0.0179 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03126 (13)	0.02289 (13)	0.01153 (11)	0.00980 (8)	0.00226 (7)	0.00496 (8)
O1	0.0320 (7)	0.0228 (7)	0.0123 (6)	0.0102 (5)	0.0028 (5)	0.0033 (5)
O2	0.0414 (8)	0.0268 (7)	0.0214 (6)	0.0190 (6)	0.0013 (6)	0.0062 (5)
N2	0.0197 (7)	0.0159 (7)	0.0116 (6)	0.0069 (5)	0.0031 (5)	0.0042 (5)
N1	0.0181 (6)	0.0141 (7)	0.0149 (6)	0.0026 (5)	0.0049 (5)	0.0034 (5)
C11	0.0159 (7)	0.0133 (8)	0.0145 (7)	0.0019 (6)	0.0036 (6)	0.0039 (6)
C1	0.0172 (7)	0.0155 (8)	0.0155 (8)	0.0016 (6)	0.0039 (6)	0.0032 (6)
C6	0.0162 (7)	0.0138 (8)	0.0189 (8)	0.0031 (6)	0.0063 (6)	0.0046 (6)
C15	0.0171 (7)	0.0164 (8)	0.0155 (8)	0.0019 (6)	0.0027 (6)	0.0053 (6)
C12	0.0194 (8)	0.0181 (8)	0.0113 (7)	0.0022 (6)	0.0018 (6)	0.0049 (6)
C2	0.0179 (7)	0.0138 (8)	0.0156 (8)	0.0026 (6)	0.0056 (6)	0.0029 (6)
C16	0.0185 (7)	0.0166 (8)	0.0126 (7)	0.0028 (6)	0.0038 (6)	0.0036 (6)
C13	0.0238 (8)	0.0173 (9)	0.0138 (8)	0.0047 (7)	0.0050 (6)	0.0007 (6)
C3	0.0250 (8)	0.0211 (9)	0.0138 (8)	0.0044 (7)	0.0041 (6)	0.0017 (7)
C14	0.0212 (8)	0.0148 (8)	0.0196 (8)	0.0054 (6)	0.0044 (7)	0.0033 (7)
C18	0.0300 (9)	0.0223 (9)	0.0156 (8)	0.0090 (7)	0.0026 (7)	0.0070 (7)
C17	0.0211 (8)	0.0196 (9)	0.0177 (8)	0.0052 (7)	0.0040 (6)	0.0074 (7)
C7	0.0234 (8)	0.0170 (9)	0.0176 (8)	0.0059 (7)	0.0055 (7)	0.0038 (7)
C8	0.0261 (9)	0.0232 (10)	0.0229 (9)	0.0069 (7)	0.0028 (7)	0.0098 (7)
C9	0.0238 (9)	0.0181 (9)	0.0336 (10)	0.0086 (7)	0.0051 (7)	0.0096 (8)
C4	0.0270 (9)	0.0180 (9)	0.0191 (8)	0.0062 (7)	0.0068 (7)	−0.0023 (7)
C10	0.0235 (8)	0.0135 (8)	0.0291 (9)	0.0060 (7)	0.0085 (7)	0.0015 (7)
C5	0.0183 (8)	0.0139 (8)	0.0215 (8)	0.0027 (6)	0.0071 (6)	0.0026 (7)

Geometric parameters (Å, º)

Br1—C12	1.8968 (16)	C13—H13	0.9300
O1—C1	1.221 (2)	C13—C14	1.379 (2)
O2—C17	1.213 (2)	C3—H3	0.9300
N2—H2	0.8600	C3—C4	1.363 (3)
N2—C11	1.395 (2)	C14—H14	0.9300
N2—C1	1.363 (2)	C18—H18A	0.9600
N1—C6	1.365 (2)	C18—H18B	0.9600
N1—C2	1.320 (2)	C18—H18C	0.9600
C11—C12	1.401 (2)	C18—C17	1.505 (2)
C11—C16	1.397 (2)	C7—H7	0.9300
C1—C2	1.506 (2)	C7—C8	1.366 (3)
C6—C7	1.413 (2)	C8—H8	0.9300
C6—C5	1.423 (2)	C8—C9	1.415 (3)
C15—C16	1.388 (2)	C9—H9	0.9300
C15—C14	1.395 (2)	C9—C10	1.365 (3)

C15—C17	1.501 (2)	C4—H4	0.9300
C12—C13	1.392 (2)	C4—C5	1.413 (3)
C2—C3	1.414 (2)	C10—H10	0.9300
C16—H16	0.9300	C10—C5	1.419 (3)

C11—N2—H2	116.0	C15—C14—H14	120.1
C1—N2—H2	116.0	C13—C14—C15	119.79 (16)
C1—N2—C11	128.05 (14)	C13—C14—H14	120.1
C2—N1—C6	117.86 (14)	H18A—C18—H18B	109.5
N2—C11—C12	119.73 (14)	H18A—C18—H18C	109.5
N2—C11—C16	122.69 (14)	H18B—C18—H18C	109.5
C16—C11—C12	117.58 (15)	C17—C18—H18A	109.5
O1—C1—N2	125.78 (16)	C17—C18—H18B	109.5
O1—C1—C2	121.70 (15)	C17—C18—H18C	109.5
N2—C1—C2	112.53 (14)	O2—C17—C15	120.30 (16)
N1—C6—C7	118.71 (15)	O2—C17—C18	121.59 (16)
N1—C6—C5	122.01 (15)	C15—C17—C18	118.10 (15)
C7—C6—C5	119.28 (16)	C6—C7—H7	119.7
C16—C15—C14	120.08 (15)	C8—C7—C6	120.57 (16)
C16—C15—C17	120.76 (15)	C8—C7—H7	119.7
C14—C15—C17	119.14 (15)	C7—C8—H8	119.9
C11—C12—Br1	120.33 (13)	C7—C8—C9	120.21 (17)
C13—C12—Br1	118.19 (12)	C9—C8—H8	119.9
C13—C12—C11	121.48 (15)	C8—C9—H9	119.7
N1—C2—C1	116.81 (14)	C10—C9—C8	120.64 (17)
N1—C2—C3	124.47 (16)	C10—C9—H9	119.7
C3—C2—C1	118.73 (15)	C3—C4—H4	119.9
C11—C16—H16	119.4	C3—C4—C5	120.19 (16)
C15—C16—C11	121.17 (15)	C5—C4—H4	119.9
C15—C16—H16	119.4	C9—C10—H10	119.8
C12—C13—H13	120.1	C9—C10—C5	120.48 (16)
C14—C13—C12	119.84 (15)	C5—C10—H10	119.8
C14—C13—H13	120.1	C4—C5—C6	117.53 (16)
C2—C3—H3	121.0	C4—C5—C10	123.66 (16)
C4—C3—C2	117.93 (16)	C10—C5—C6	118.80 (16)
C4—C3—H3	121.0		

Br1—C12—C13—C14	178.46 (13)	C2—N1—C6—C7	−178.60 (15)
O1—C1—C2—N1	−173.05 (15)	C2—N1—C6—C5	1.4 (2)
O1—C1—C2—C3	7.2 (2)	C2—C3—C4—C5	1.1 (3)
N2—C11—C12—Br1	2.1 (2)	C16—C11—C12—Br1	−177.52 (12)
N2—C11—C12—C13	−177.97 (15)	C16—C11—C12—C13	2.5 (2)
N2—C11—C16—C15	179.08 (15)	C16—C15—C14—C13	1.7 (2)
N2—C1—C2—N1	7.0 (2)	C16—C15—C17—O2	175.63 (17)
N2—C1—C2—C3	−172.76 (15)	C16—C15—C17—C18	−5.1 (2)
N1—C6—C7—C8	−179.06 (16)	C3—C4—C5—C6	0.0 (3)
N1—C6—C5—C4	−1.3 (2)	C3—C4—C5—C10	179.32 (17)
N1—C6—C5—C10	179.38 (15)	C14—C15—C16—C11	−0.7 (2)

N1—C2—C3—C4	−1.0 (3)	C14—C15—C17—O2	−5.5 (2)
C11—N2—C1—O1	−0.7 (3)	C14—C15—C17—C18	173.78 (16)
C11—N2—C1—C2	179.29 (14)	C17—C15—C16—C11	178.22 (14)
C11—C12—C13—C14	−1.5 (3)	C17—C15—C14—C13	−177.24 (15)
C1—N2—C11—C12	178.73 (15)	C7—C6—C5—C4	178.70 (15)
C1—N2—C11—C16	−1.7 (3)	C7—C6—C5—C10	−0.7 (2)
C1—C2—C3—C4	178.68 (15)	C7—C8—C9—C10	0.1 (3)
C6—N1—C2—C1	−179.91 (14)	C8—C9—C10—C5	0.2 (3)
C6—N1—C2—C3	−0.2 (2)	C9—C10—C5—C6	0.1 (3)
C6—C7—C8—C9	−0.7 (3)	C9—C10—C5—C4	−179.22 (17)
C12—C11—C16—C15	−1.4 (2)	C5—C6—C7—C8	1.0 (3)
C12—C13—C14—C15	−0.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1	0.86	2.19	2.629 (2)	112
C3—H3···O1^{i}	0.93	2.55	3.410 (2)	154
C18—H18···O2^{ii}	0.96	2.49	3.444 (2)	171
N2—H2···Br1	0.86	2.58	3.081 (1)	118

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

(III) *N*-(5-Acetyl-2-ethynylphenyl)quinoline-2-carboxamide

Crystal data

$C_{20}H_{14}N_2O_2$
M_r = 314.33
Triclinic, $P\overline{1}$
a = 7.3075 (6) Å
b = 8.2605 (4) Å
c = 13.8196 (9) Å
α = 92.734 (5)°
β = 100.608 (6)°
γ = 108.989 (6)°
V = 770.11 (10) Å^3

Z = 2
$F(000)$ = 328
D_x = 1.356 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5519 reflections
θ = 3.1–32.0°
μ = 0.09 mm^{-1}
T = 123 K
Block, colourless
0.19 × 0.08 × 0.05 mm

Data collection

Agilent SuperNova Single source at offset, Eos diffractometer
Radiation source: micro-focus sealed X-ray tube, SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 7.9851 pixels mm^{-1}
ω scans
Absorption correction: analytical [CrysAlis PRO (Rigaku OD, 2015), based on expressions derived by Clark & Reid (1995)]

T_{min} = 0.987, T_{max} = 0.996
20693 measured reflections
5173 independent reflections
3687 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 32.3°, θ_{min} = 3.0°
h = −10→10
k = −12→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.151$
$S = 1.04$
5173 reflections
218 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.282P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.81853 (17)	0.81639 (13)	0.58241 (8)	0.0298 (3)
O1	0.69300 (18)	0.80001 (15)	1.00770 (8)	0.0344 (3)
N1	0.73126 (17)	0.52751 (15)	0.59954 (8)	0.0204 (2)
H1	0.7132	0.4296	0.5678	0.025*
N2	0.76917 (16)	0.45956 (15)	0.41516 (8)	0.0204 (2)
C11	0.7866 (2)	0.66691 (18)	0.54929 (10)	0.0211 (3)
C16	0.78375 (19)	0.41914 (18)	0.32020 (10)	0.0205 (3)
C8	0.6340 (2)	0.49494 (18)	0.88964 (10)	0.0225 (3)
H8	0.6117	0.4859	0.9536	0.027*
C3	0.69438 (19)	0.65661 (18)	0.85563 (9)	0.0199 (3)
C9	0.6242 (2)	0.20816 (18)	0.66981 (10)	0.0235 (3)
C4	0.72565 (19)	0.67055 (17)	0.75912 (9)	0.0201 (3)
H4	0.7637	0.7782	0.7364	0.024*
C6	0.64210 (19)	0.36039 (17)	0.73190 (9)	0.0200 (3)
C5	0.69995 (19)	0.52316 (17)	0.69665 (9)	0.0190 (3)
C15	0.8349 (2)	0.54711 (19)	0.25516 (10)	0.0226 (3)
C12	0.80629 (19)	0.62324 (17)	0.44536 (9)	0.0198 (3)
C2	0.7259 (2)	0.81339 (19)	0.92427 (10)	0.0238 (3)
C13	0.8613 (2)	0.75994 (18)	0.38704 (10)	0.0235 (3)
H13	0.8881	0.8734	0.4126	0.028*
C7	0.6074 (2)	0.34872 (18)	0.82831 (10)	0.0227 (3)
H7	0.5661	0.2413	0.8511	0.027*
C17	0.7457 (2)	0.24391 (19)	0.28605 (11)	0.0264 (3)
H17	0.7138	0.1593	0.3282	0.032*
C10	0.6224 (2)	0.0885 (2)	0.61968 (12)	0.0305 (3)
H10	0.6210	−0.0063	0.5800	0.037*
C14	0.8738 (2)	0.72010 (19)	0.29172 (10)	0.0249 (3)
H14	0.9079	0.8069	0.2511	0.030*
C20	0.8445 (2)	0.4964 (2)	0.15714 (10)	0.0283 (3)
H20	0.8776	0.5790	0.1140	0.034*

C18	0.7560 (2)	0.2000 (2)	0.19069 (12)	0.0309 (3)
H18	0.7302	0.0851	0.1685	0.037*
C19	0.8051 (2)	0.3267 (2)	0.12586 (11)	0.0315 (3)
H19	0.8108	0.2945	0.0614	0.038*
C1	0.8052 (3)	0.9875 (2)	0.89000 (11)	0.0326 (4)
H1A	0.8080	1.0748	0.9392	0.049*
H1B	0.7214	0.9926	0.8288	0.049*
H1C	0.9369	1.0066	0.8801	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0459 (7)	0.0218 (5)	0.0232 (5)	0.0113 (5)	0.0114 (5)	0.0015 (4)
O1	0.0440 (7)	0.0339 (6)	0.0211 (5)	0.0056 (5)	0.0126 (5)	−0.0035 (4)
N1	0.0256 (6)	0.0189 (5)	0.0162 (5)	0.0063 (4)	0.0057 (4)	0.0002 (4)
N2	0.0197 (5)	0.0215 (5)	0.0187 (5)	0.0054 (4)	0.0043 (4)	0.0001 (4)
C11	0.0238 (6)	0.0227 (6)	0.0167 (6)	0.0079 (5)	0.0042 (5)	0.0012 (5)
C16	0.0180 (6)	0.0240 (7)	0.0180 (6)	0.0060 (5)	0.0034 (5)	−0.0014 (5)
C8	0.0225 (6)	0.0279 (7)	0.0173 (6)	0.0077 (5)	0.0062 (5)	0.0034 (5)
C3	0.0189 (6)	0.0236 (6)	0.0161 (5)	0.0064 (5)	0.0032 (5)	−0.0011 (5)
C9	0.0234 (7)	0.0252 (7)	0.0224 (6)	0.0072 (5)	0.0071 (5)	0.0070 (5)
C4	0.0207 (6)	0.0211 (6)	0.0173 (6)	0.0055 (5)	0.0039 (5)	0.0012 (5)
C6	0.0195 (6)	0.0214 (6)	0.0186 (6)	0.0061 (5)	0.0041 (5)	0.0015 (5)
C5	0.0182 (6)	0.0231 (6)	0.0158 (5)	0.0067 (5)	0.0047 (4)	0.0026 (5)
C15	0.0192 (6)	0.0308 (7)	0.0164 (6)	0.0072 (5)	0.0031 (5)	0.0014 (5)
C12	0.0201 (6)	0.0217 (6)	0.0165 (5)	0.0058 (5)	0.0036 (5)	0.0006 (5)
C2	0.0241 (7)	0.0273 (7)	0.0184 (6)	0.0083 (6)	0.0027 (5)	−0.0022 (5)
C13	0.0280 (7)	0.0209 (6)	0.0196 (6)	0.0057 (5)	0.0045 (5)	0.0016 (5)
C7	0.0238 (7)	0.0225 (6)	0.0219 (6)	0.0066 (5)	0.0071 (5)	0.0044 (5)
C17	0.0250 (7)	0.0247 (7)	0.0278 (7)	0.0068 (6)	0.0061 (6)	−0.0023 (5)
C10	0.0358 (8)	0.0276 (7)	0.0272 (7)	0.0098 (6)	0.0065 (6)	0.0020 (6)
C14	0.0266 (7)	0.0266 (7)	0.0202 (6)	0.0059 (6)	0.0066 (5)	0.0063 (5)
C20	0.0256 (7)	0.0418 (9)	0.0177 (6)	0.0119 (6)	0.0048 (5)	0.0020 (6)
C18	0.0285 (8)	0.0317 (8)	0.0302 (8)	0.0103 (6)	0.0038 (6)	−0.0090 (6)
C19	0.0295 (8)	0.0453 (9)	0.0197 (6)	0.0152 (7)	0.0037 (6)	−0.0059 (6)
C1	0.0483 (10)	0.0241 (7)	0.0223 (7)	0.0107 (7)	0.0044 (6)	−0.0023 (6)

Geometric parameters (Å, º)

O2—C11	1.2279 (17)	C6—C7	1.4033 (18)
O1—C2	1.2231 (17)	C15—C14	1.411 (2)
N1—H1	0.8600	C15—C20	1.4195 (19)
N1—C11	1.3595 (18)	C12—C13	1.4130 (19)
N1—C5	1.4025 (16)	C2—C1	1.501 (2)
N2—C16	1.3704 (17)	C13—H13	0.9300
N2—C12	1.3197 (17)	C13—C14	1.3692 (19)
C11—C12	1.5082 (18)	C7—H7	0.9300
C16—C15	1.422 (2)	C17—H17	0.9300

C16—C17	1.421 (2)	C17—C18	1.372 (2)
C8—H8	0.9300	C10—H10	0.9300
C8—C3	1.397 (2)	C14—H14	0.9300
C8—C7	1.3799 (19)	C20—H20	0.9300
C3—C4	1.3979 (18)	C20—C19	1.367 (2)
C3—C2	1.4962 (19)	C18—H18	0.9300
C9—C6	1.4435 (19)	C18—C19	1.411 (2)
C9—C10	1.175 (2)	C19—H19	0.9300
C4—H4	0.9300	C1—H1A	0.9600
C4—C5	1.3979 (18)	C1—H1B	0.9600
C6—C5	1.4115 (18)	C1—H1C	0.9600

C11—N1—H1	115.9	O1—C2—C3	120.60 (13)
C11—N1—C5	128.21 (12)	O1—C2—C1	120.68 (13)
C5—N1—H1	115.9	C3—C2—C1	118.69 (12)
C12—N2—C16	117.64 (12)	C12—C13—H13	121.0
O2—C11—N1	125.11 (12)	C14—C13—C12	117.90 (13)
O2—C11—C12	121.14 (12)	C14—C13—H13	121.0
N1—C11—C12	113.75 (11)	C8—C7—C6	120.69 (13)
N2—C16—C15	121.91 (12)	C8—C7—H7	119.7
N2—C16—C17	118.75 (13)	C6—C7—H7	119.7
C17—C16—C15	119.33 (12)	C16—C17—H17	120.1
C3—C8—H8	120.0	C18—C17—C16	119.78 (14)
C7—C8—H8	120.0	C18—C17—H17	120.1
C7—C8—C3	119.98 (12)	C9—C10—H10	180.0
C8—C3—C4	120.17 (12)	C15—C14—H14	120.0
C8—C3—C2	118.92 (12)	C13—C14—C15	119.92 (13)
C4—C3—C2	120.92 (12)	C13—C14—H14	120.0
C10—C9—C6	175.76 (16)	C15—C20—H20	119.8
C3—C4—H4	119.9	C19—C20—C15	120.33 (15)
C3—C4—C5	120.21 (12)	C19—C20—H20	119.8
C5—C4—H4	119.9	C17—C18—H18	119.5
C5—C6—C9	119.94 (12)	C17—C18—C19	120.92 (14)
C7—C6—C9	120.52 (12)	C19—C18—H18	119.5
C7—C6—C5	119.51 (12)	C20—C19—C18	120.49 (14)
N1—C5—C6	117.23 (12)	C20—C19—H19	119.8
C4—C5—N1	123.36 (12)	C18—C19—H19	119.8
C4—C5—C6	119.41 (12)	C2—C1—H1A	109.5
C14—C15—C16	117.90 (12)	C2—C1—H1B	109.5
C14—C15—C20	122.96 (14)	C2—C1—H1C	109.5
C20—C15—C16	119.14 (13)	H1A—C1—H1B	109.5
N2—C12—C11	117.50 (12)	H1A—C1—H1C	109.5
N2—C12—C13	124.71 (12)	H1B—C1—H1C	109.5
C13—C12—C11	117.78 (12)		

O2—C11—C12—N2	−179.91 (13)	C9—C6—C5—C4	−177.04 (12)
O2—C11—C12—C13	−0.5 (2)	C9—C6—C7—C8	176.73 (13)
N1—C11—C12—N2	−0.07 (18)	C4—C3—C2—O1	177.96 (13)

N1—C11—C12—C13	179.34 (12)	C4—C3—C2—C1	−4.1 (2)
N2—C16—C15—C14	0.9 (2)	C5—N1—C11—O2	−0.2 (2)
N2—C16—C15—C20	−179.00 (12)	C5—N1—C11—C12	180.00 (12)
N2—C16—C17—C18	178.87 (13)	C5—C6—C7—C8	−1.6 (2)
N2—C12—C13—C14	1.2 (2)	C15—C16—C17—C18	−0.9 (2)
C11—N1—C5—C4	−1.0 (2)	C15—C20—C19—C18	−0.5 (2)
C11—N1—C5—C6	179.84 (13)	C12—N2—C16—C15	−0.63 (19)
C11—C12—C13—C14	−178.19 (12)	C12—N2—C16—C17	179.63 (12)
C16—N2—C12—C11	178.94 (11)	C12—C13—C14—C15	−0.8 (2)
C16—N2—C12—C13	−0.4 (2)	C2—C3—C4—C5	178.53 (12)
C16—C15—C14—C13	−0.1 (2)	C7—C8—C3—C4	0.8 (2)
C16—C15—C20—C19	−0.1 (2)	C7—C8—C3—C2	−178.82 (13)
C16—C17—C18—C19	0.4 (2)	C7—C6—C5—N1	−179.53 (12)
C8—C3—C4—C5	−1.1 (2)	C7—C6—C5—C4	1.28 (19)
C8—C3—C2—O1	−2.4 (2)	C17—C16—C15—C14	−179.36 (13)
C8—C3—C2—C1	175.51 (13)	C17—C16—C15—C20	0.7 (2)
C3—C8—C7—C6	0.5 (2)	C17—C18—C19—C20	0.3 (2)
C3—C4—C5—N1	−179.10 (12)	C14—C15—C20—C19	−179.97 (14)
C3—C4—C5—C6	0.04 (19)	C20—C15—C14—C13	179.78 (13)
C9—C6—C5—N1	2.14 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2	0.86	2.23	2.666 (2)	111
C10—H10···O2^{i}	0.93	2.36	3.103 (2)	136

Symmetry code: (i) *x*, *y*−1, *z*.