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8-[*N*-(*tert*-Butoxycarbonyl)-L-glycyl]-quinolin-8-amine

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Key indicators

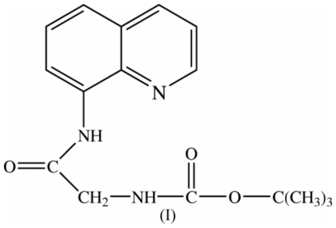
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.178
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{16}H_{19}N_3O_3$, has two crystallographically independent molecules in the asymmetric unit. There are two intermolecular (N—H···O) and two intramolecular hydrogen bonds (N—H···N) in the crystal structure. The crystal packing is stabilized by π–π-stacking interactions.

Comment

Aminoquinoline-based ligands possess a strong fluorescence which could be used as a potential probe for zinc ion detection (Jiang *et al.*, 2002). Moreover, some novel quinoline carboxamide ligands and their copper complexes, as well as platinum complexes with pyridine carboxamide ligands (Zhang, Liu *et al.*, 2002), have shown potent cytotoxicity against human leukaemia, murine leukaemia, human hepatoma and human lung adenocarcinoma cell lines (Zhang *et al.*, 2003). Compound (I) and its Cu^{II} complex have been synthesized and reported previously (Zhang *et al.*, 2003). In this work, we report the crystal structure of (I).



(I)

The X-ray crystallographic study shows that the bond lengths and angles are within the normal ranges. The N2*A*—C10*A* and N2*A*—C8*A* bond distances in (I) are comparable with those in *N*-(8-quinolyl)pyridine-2-carboxamide [1.357 (2) and 1.401 (2) Å; Zhang *et al.*, 2001] and *N*-(8-quinolyl)-pyridine-3-carboxamide [1.349 (3) and 1.405 (3) Å; Zhang, Tu *et al.*, 2002]; the C—C and C═O bond lengths are similar to those reported in [*N*-(8-quinolyl)-L-alanine-*N*′-BOC-carboxamide]copper(II) (Zhang *et al.*, 2003). The torsion angle C12*A*—N3*A*—C11*A*—C10*A* is 77.7 (3)° and N2*A*—C10*A*—C11*A*—N3*A* is −137.2 (2)°. There are two intermolecular hydrogen bonds (N3*A*—H3*AA*···O1*B* and N3*B*—H3*BA*···O1*A*) and two intramolecular hydrogen bonds (N2*B*—H2*BA*···N1*B* and N2*A*—H2*AA*···N1*A*) in the crystal structure.

The crystal packing of compound (I) is shown in Fig. 2. There is a π–π-stacking interaction between adjacent molecules, related by inversion symmetry. The distance between the two adjacent quinoline rings is 3.524 (3) Å and the angle between the two planes is 2.1 (3)°. This interaction keeps the quinoline planes in a face-to-face disposition, giving rise to alternating hydrophilic and hydrophobic layers.

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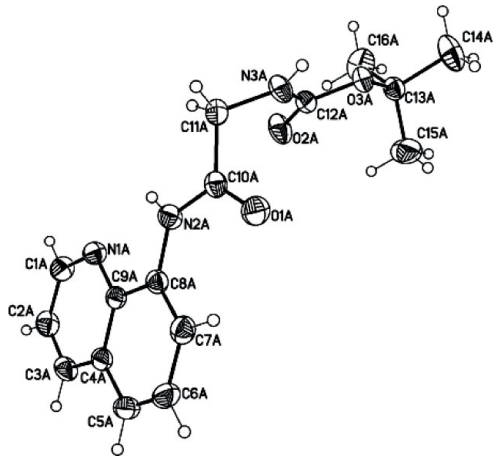

Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

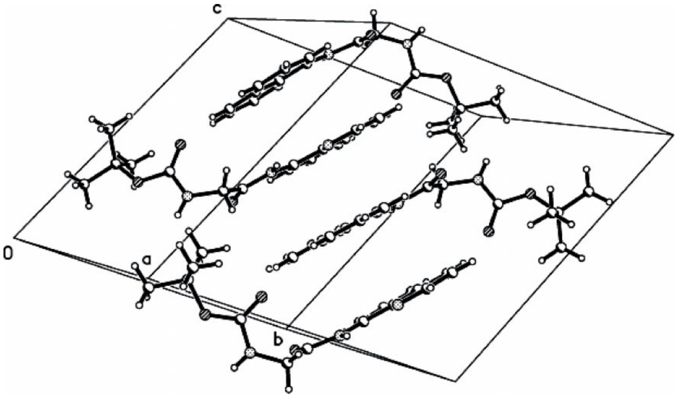

Figure 2
The packing in the crystal structure.

Experimental

The title compound was obtained by the reaction of one molar equivalent of 8-aminoquinoline and *N*-(*tert*-butoxycarbonyl)glycine in THF at 258 K for 1 h (Zhang *et al.*, 2003). Single crystals suitable for X-ray diffraction were recrystallized from THF and ethanol.

Crystal data

$C_{16}H_{19}N_3O_3$
$M_r = 301.34$
Triclinic, $P\overline{1}$
$a = 11.430$ (2) Å
$b = 12.240$ (2) Å
$c = 12.960$ (3) Å
$\alpha = 65.33$ (3)°
$\beta = 80.60$ (3)°
$\gamma = 69.44$ (3)°
$V = 1542.4$ (7) Å^3

$Z = 4$
$D_x = 1.298$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 5698 reflections
$\theta = 1.7$–25.0°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Block, brown
0.40 × 0.30 × 0.30 mm

Data collection

Siemens *P*4 diffractometer
$2\theta/\omega$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.968$, $T_{\max} = 0.973$
5698 measured reflections
5401 independent reflections
3476 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.023$
$\theta_{\max} = 25.0°$
$h = 0 \rightarrow 13$
$k = -13 \rightarrow 14$
$l = -15 \rightarrow 15$
3 standard reflections every 97 reflections
intensity decay: 7.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.178$
$S = 1.00$
5401 reflections
397 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.4212P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.32$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1*A*—C10*A*	1.221 (3)	O1*B*—C10*B*	1.221 (3)
O2*A*—C12*A*	1.213 (3)	O2*B*—C12*B*	1.206 (3)
O3*A*—C12*A*	1.338 (3)	O3*B*—C12*B*	1.351 (3)
O3*A*—C13*A*	1.475 (3)	O3*B*—C13*B*	1.472 (3)
N1*A*—C1*A*	1.319 (3)	N1*B*—C1*B*	1.316 (3)
N1*A*—C9*A*	1.360 (3)	N1*B*—C9*B*	1.359 (3)
N2*A*—C10*A*	1.356 (3)	N2*B*—C10*B*	1.346 (3)
N2*A*—C8*A*	1.403 (3)	N2*B*—C8*B*	1.400 (3)
N3*A*—C12*A*	1.334 (3)	N3*B*—C12*B*	1.336 (3)
N3*A*—C11*A*	1.439 (3)	N3*B*—C11*B*	1.441 (3)
C12*A*—O3*A*—C13*A*	121.4 (2)	C12*B*—O3*B*—C13*B*	121.6 (2)
C10*A*—N2*A*—C8*A*	128.7 (2)	C10*B*—N2*B*—C8*B*	130.1 (2)
C12*A*—N3*A*—C11*A*	120.5 (2)	C12*B*—N3*B*—C11*B*	118.8 (2)
N2*A*—C8*A*—C9*A*	115.0 (2)	N2*B*—C8*B*—C9*B*	114.6 (2)
O1*A*—C10*A*—N2*A*	123.6 (2)	O1*B*—C10*B*—N2*B*	123.5 (2)
O1*A*—C10*A*—C11*A*	121.1 (2)	O1*B*—C10*B*—C11*B*	122.6 (2)
N2*A*—C10*A*—C11*A*	115.3 (2)	N2*B*—C10*B*—C11*B*	113.9 (2)
N3*A*—C11*A*—C10*A*	112.1 (2)	N3*B*—C11*B*—C10*B*	113.1 (2)
O2*A*—C12*A*—N3*A*	122.9 (2)	O2*B*—C12*B*—N3*B*	124.6 (3)
O2*A*—C12*A*—O3*A*	125.7 (2)	O2*B*—C12*B*—O3*B*	125.5 (3)
N3*A*—C12*A*—O3*A*	111.5 (2)	N3*B*—C12*B*—O3*B*	109.9 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2*A*—H2*AA*···N1*A*	0.78 (3)	2.26 (3)	2.669 (3)	113 (2)
N3*A*—H3*AA*···O1*B*	0.86	2.16	2.949 (3)	153
N2*B*—H2*BA*···N1*B*	0.86	2.22	2.647 (3)	111
N3*B*—H3*BA*···O1*A*	0.86	2.20	2.991 (3)	153

All H atoms were placed in geometrically calculated positions, except for H2*AA*, which was located from a different Fourier map and refined isotropically [C—H = 0.93 Å and N—H 0.86 Å; $U_{\rm iso} = 1.2U_{\rm eq}$(parent atom)].

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 1997); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Jiang, P. J., Chen, L. Z., Lin, J., Liu, Q., Ding, J., Gao, X. & Guo, Z. J. (2002) *Chem. Commun.* pp. 1424–1425.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Sheldrick, G. M. (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens (1994). *XSCANS*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison. Wisconsin, USA.

Zhang, J. Y., Ke, X. K., Tu, C., Lin, J., Ding, J., Lin, L. P., Fun, H.-K., You, X. Z. & Guo, Z. J. (2003). *Biometals*. In the press.

Zhang, J. Y., Liu, Q., Duan, C. Y, Shao, Y., Ding, *j.* Miao, Z. H, You, X. Z. & Guo, Z. J. (2002). *J. Chem. Soc. Dalton Trans.* pp. 591–597.

Zhang, J. Y., Liu, Q., Xu, Y., Zhang, Y., You, X. Z. & Guo, Z. J. (2001). *Acta Cryst.* C**57**, 109–110.

Zhang, J. Y., Tu, C., Lin, J., Fun, H.-K., Chantrapromma, S., You, X. Z. & Guo, Z. J. (2002). *Chin. J. Inorg. Chem.* **18**, 554–558.