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N,*N*′-Di-8-quinolyladipamide

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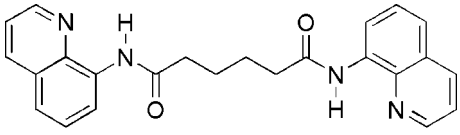
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.120; data-to-parameter ratio = 14.6.

The complete molecule of the title compound, $C_{24}H_{22}N_4O_2$, is generated by a crystallographic inversion centre located at the mid-point of the central C—C bond. The quinoline ring system and the hexyl chain are both essentially planar, and the dihedral angle between them is 46.30 (2)°. Intramolecular N—H···N and C—H···O hydrogen bonds form five- and six-numbered rings, respectively. The crystal packing is stabilized by short C—H···O interactions.

Related literature

For details of the synthesis, see: Chen *et al.* (2007). For related structures, see: Chen *et al.* (2007); Wen *et al.* (2006).



Experimental

Crystal data

$C_{24}H_{22}N_4O_2$
M_r = 398.46
Monoclinic, $P2_1/n$
a = 9.923 (2) Å
b = 9.184 (2) Å
c = 11.722 (3) Å
β = 110.530 (4)°
V = 1000.4 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 K
0.24 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick,1996)
T_{min} = 0.980, T_{max} = 0.990
5622 measured reflections
2048 independent reflections
1274 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
S = 1.00
2048 reflections
140 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1	0.892 (9)	2.23 (2)	2.676 (2)	110.4 (15)
C7—H7···O1	0.93	2.33	2.902 (2)	119
C11—H11B···O1^{i}	0.97	2.66	3.134 (2)	111

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

Data collection: *SMART* (Bruker 2001); cell refinement: *SAINT* (Bruker 2001); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2250).

References

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supporting information

Acta Cryst. (2009). E**65**, o1399 [doi:10.1107/S1600536809017541]

N,*N*′-Di-8-quinolyladipamide

Shi-Ying Wang, Xing-Lei Xie, Qing-Hua Huang and Yu-Sheng Lin

S1. Comment

Recently, Chen *et al.* (2007) reported the syntheses and crystal structures of the flexible ligand *N*,*N*′-di(2-pyridyl)-adipamide and its several Ag(I) complexes. Theses complexes form topologically promising zigzag, helical or sinusoidal chain architectures because the flexible ligand can adopt three different conformations. To investigate the influence of the terminal groups on crystal structure, and to obtain a more topologically promising coordination framework, we synthesized and carried out the structure determination of the title compound, (I) (Fig. 1).

The molecule sits on a center of symmetry passing through the central C12—C12^{ii} bond [symmetry code: (ii): -*x*, -*y*, -*z*] (Fig. 1). All bond lengths and angles in (I) show normal values and are comparable to those of the related compounds, *N*,*N*′-di(2-pyridyl)adipamide (Chen *et al.*, 2007), and *N*-(quinolin-8-yl)-2-(quinolin-8-yloxy)acetamide (Wen *et al.*, 2006). The quinoline group is essentially planar, with a dihedral angle of 1.70 (3)° between the benzene ring (C4—C9) and pyridine ring (C1—C4/C9/N1). The C10—C12/C10A—C12A unit is also planar, with the dihedral angle to the quinoline system of 46.30 (2)°. Two intramolecular hydrogen bonds, *viz.* N2—H2A···N1 and C7—H7···O1 (Fig. 1 and Table 1), form five- and six-membered rings, respectively, and affect the conformation of the molecule. The crystal packing is stabilized by short C11—H11B···O1 interactions (Fig. 2 and Table 1).

S2. Experimental

The title compound was synthesized by a reaction of adipoyl chloride and 8-aminoquinoline according to literature method (Chen *et al.*, 2007). Colourless single cystals suitable for X-ray diffraction were obtained by slow evaporation from a methanol solution over a period of 7 d.

S3. Refinement

H atoms were positioned geometrically, with N—H = 0.86 Å and C—H = 0.95–0.99 Å, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C,*N*).

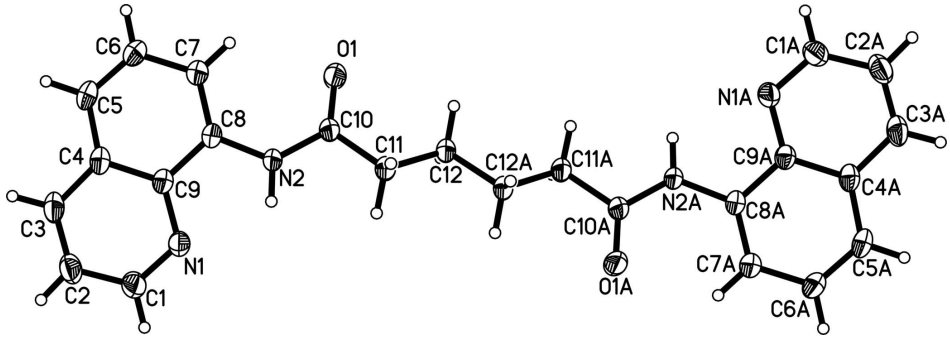

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids.

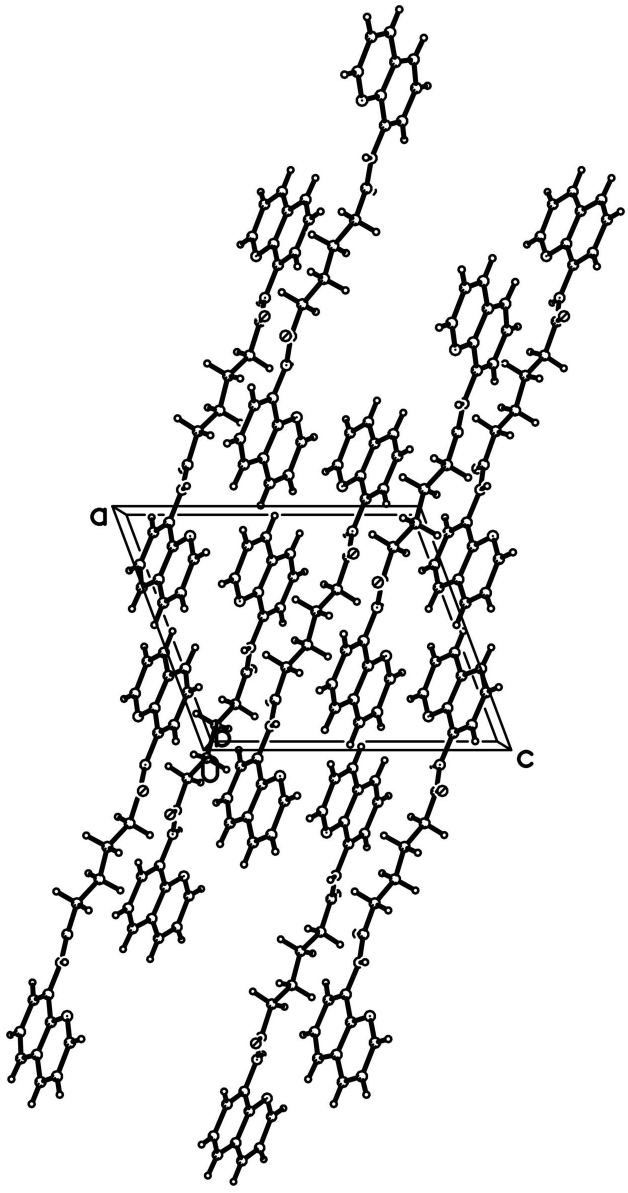

Figure 2

The packing diagram of (I), viewed down the *b* axis.

N,*N*′-Di-8-quinolyladipamide

Crystal data

$C_{24}H_{22}N_4O_2$
M_r = 398.46
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 9.923 (2) Å
b = 9.184 (2) Å
c = 11.722 (3) Å
β = 110.530 (4)°
V = 1000.4 (4) Å^3
Z = 2
F(000) = 420
D_x = 1.323 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1501 reflections

θ = 2.9–25.3°
μ = 0.09 mm^{-1}
T = 294 K

Column, colourless
0.24 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick,1996)
T_{min} = 0.980, T_{max} = 0.990

5622 measured reflections
2048 independent reflections
1274 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 26.4°, θ_{min} = 2.3°
h = −11→12
k = −11→9
l = −9→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
S = 1.00
2048 reflections
140 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.1339P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.31418 (15)	−0.13777 (14)	0.23248 (14)	0.0793 (5)
N1	0.61637 (15)	0.28926 (17)	0.28795 (13)	0.0498 (4)
N2	0.41475 (15)	0.08554 (16)	0.26119 (14)	0.0440 (4)
C1	0.7142 (2)	0.3904 (2)	0.30187 (19)	0.0626 (6)
H1	0.6886	0.4723	0.2522	0.075*
C2	0.8543 (2)	0.3835 (3)	0.38633 (19)	0.0649 (6)
H2	0.9192	0.4585	0.3917	0.078*
C3	0.8942 (2)	0.2662 (2)	0.46005 (17)	0.0559 (5)
H3	0.9869	0.2602	0.5172	0.067*
C4	0.79507 (17)	0.1532 (2)	0.45011 (15)	0.0438 (5)
C5	0.82757 (19)	0.0257 (2)	0.52156 (17)	0.0518 (5)
H5	0.9178	0.0148	0.5816	0.062*

C6	0.72814 (19)	−0.0807 (2)	0.50313 (17)	0.0529 (5)
H6	0.7518	−0.1654	0.5494	0.063*
C7	0.59014 (19)	−0.0659 (2)	0.41559 (16)	0.0475 (5)
H7	0.5236	−0.1407	0.4044	0.057*
C8	0.55222 (17)	0.05739 (19)	0.34647 (15)	0.0390 (4)
C9	0.65611 (17)	0.16955 (18)	0.36128 (14)	0.0391 (4)
C10	0.30407 (18)	−0.0079 (2)	0.21278 (16)	0.0455 (5)
C11	0.16598 (18)	0.06244 (19)	0.13495 (17)	0.0477 (5)
H11A	0.1883	0.1489	0.0975	0.057*
H11B	0.1132	0.0930	0.1866	0.057*
C12	0.07120 (17)	−0.03564 (19)	0.03641 (16)	0.0447 (5)
H12A	0.0526	−0.1245	0.0731	0.054*
H12B	0.1214	−0.0618	−0.0183	0.054*
H2A	0.4032 (19)	0.1789 (11)	0.2388 (17)	0.057 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0648 (10)	0.0370 (8)	0.0939 (12)	−0.0048 (7)	−0.0250 (8)	0.0065 (8)
N1	0.0425 (9)	0.0574 (10)	0.0425 (9)	−0.0107 (8)	0.0061 (7)	0.0051 (8)
N2	0.0328 (8)	0.0376 (9)	0.0489 (9)	−0.0033 (6)	−0.0017 (7)	0.0043 (7)
C1	0.0590 (13)	0.0706 (14)	0.0506 (12)	−0.0212 (11)	0.0096 (10)	0.0115 (10)
C2	0.0532 (13)	0.0802 (15)	0.0543 (12)	−0.0290 (11)	0.0100 (10)	−0.0005 (11)
C3	0.0382 (10)	0.0782 (14)	0.0444 (11)	−0.0126 (10)	0.0058 (8)	−0.0063 (11)
C4	0.0344 (10)	0.0587 (12)	0.0354 (9)	−0.0033 (8)	0.0087 (8)	−0.0069 (9)
C5	0.0343 (10)	0.0684 (13)	0.0427 (10)	0.0058 (9)	0.0012 (8)	0.0007 (10)
C6	0.0446 (11)	0.0561 (12)	0.0479 (11)	0.0067 (9)	0.0037 (9)	0.0073 (9)
C7	0.0396 (10)	0.0478 (11)	0.0475 (11)	−0.0017 (8)	0.0060 (9)	0.0023 (9)
C8	0.0315 (9)	0.0452 (10)	0.0363 (9)	−0.0001 (7)	0.0068 (7)	−0.0019 (8)
C9	0.0347 (9)	0.0476 (10)	0.0334 (9)	−0.0005 (8)	0.0099 (8)	−0.0023 (8)
C10	0.0393 (10)	0.0374 (10)	0.0478 (10)	−0.0042 (8)	0.0005 (8)	−0.0004 (8)
C11	0.0379 (10)	0.0404 (10)	0.0521 (11)	−0.0023 (8)	0.0000 (9)	−0.0006 (9)
C12	0.0333 (10)	0.0419 (10)	0.0485 (10)	−0.0030 (7)	0.0014 (8)	0.0006 (8)

Geometric parameters (Å, º)

O1—C10	1.213 (2)	C5—C6	1.351 (3)
N1—C1	1.312 (2)	C5—H5	0.9300
N1—C9	1.366 (2)	C6—C7	1.400 (2)
N2—C10	1.352 (2)	C6—H6	0.9300
N2—C8	1.404 (2)	C7—C8	1.366 (2)
N2—H2A	0.892 (9)	C7—H7	0.9300
C1—C2	1.397 (3)	C8—C9	1.424 (2)
C1—H1	0.9300	C10—C11	1.500 (2)
C2—C3	1.350 (3)	C11—C12	1.506 (2)
C2—H2	0.9300	C11—H11A	0.9700
C3—C4	1.407 (2)	C11—H11B	0.9700
C3—H3	0.9300	C12—C12^{i}	1.519 (3)

C4—C5	1.410 (3)	C12—H12A	0.9700
C4—C9	1.415 (2)	C12—H12B	0.9700
C1—N1—C9	117.01 (16)	C8—C7—H7	119.7
C10—N2—C8	128.73 (15)	C6—C7—H7	119.7
C10—N2—H2A	119.0 (12)	C7—C8—N2	124.88 (16)
C8—N2—H2A	112.2 (12)	C7—C8—C9	119.34 (15)
N1—C1—C2	124.37 (19)	N2—C8—C9	115.76 (15)
N1—C1—H1	117.8	N1—C9—C4	122.70 (15)
C2—C1—H1	117.8	N1—C9—C8	117.95 (15)
C3—C2—C1	119.07 (18)	C4—C9—C8	119.36 (15)
C3—C2—H2	120.5	O1—C10—N2	122.93 (16)
C1—C2—H2	120.5	O1—C10—C11	122.42 (15)
C2—C3—C4	119.71 (18)	N2—C10—C11	114.63 (15)
C2—C3—H3	120.1	C10—C11—C12	113.62 (15)
C4—C3—H3	120.1	C10—C11—H11A	108.8
C3—C4—C5	123.78 (17)	C12—C11—H11A	108.8
C3—C4—C9	117.12 (17)	C10—C11—H11B	108.8
C5—C4—C9	119.08 (16)	C12—C11—H11B	108.8
C6—C5—C4	120.26 (17)	H11A—C11—H11B	107.7
C6—C5—H5	119.9	C11—C12—C12^{i}	112.39 (18)
C4—C5—H5	119.9	C11—C12—H12A	109.1
C5—C6—C7	121.21 (17)	C12^{i}—C12—H12A	109.1
C5—C6—H6	119.4	C11—C12—H12B	109.1
C7—C6—H6	119.4	C12^{i}—C12—H12B	109.1
C8—C7—C6	120.70 (17)	H12A—C12—H12B	107.9
C9—N1—C1—C2	−0.3 (3)	C1—N1—C9—C8	−179.10 (17)
N1—C1—C2—C3	−0.3 (3)	C3—C4—C9—N1	−0.7 (2)
C1—C2—C3—C4	0.5 (3)	C5—C4—C9—N1	−179.61 (16)
C2—C3—C4—C5	178.89 (19)	C3—C4—C9—C8	179.22 (16)
C2—C3—C4—C9	0.0 (3)	C5—C4—C9—C8	0.3 (2)
C3—C4—C5—C6	−177.26 (18)	C7—C8—C9—N1	177.82 (16)
C9—C4—C5—C6	1.6 (3)	N2—C8—C9—N1	−3.5 (2)
C4—C5—C6—C7	−1.7 (3)	C7—C8—C9—C4	−2.1 (2)
C5—C6—C7—C8	−0.2 (3)	N2—C8—C9—C4	176.61 (15)
C6—C7—C8—N2	−176.52 (17)	C8—N2—C10—O1	−5.4 (3)
C6—C7—C8—C9	2.1 (3)	C8—N2—C10—C11	173.11 (17)
C10—N2—C8—C7	−14.2 (3)	O1—C10—C11—C12	−30.0 (3)
C10—N2—C8—C9	167.19 (17)	N2—C10—C11—C12	151.44 (17)
C1—N1—C9—C4	0.8 (3)	C10—C11—C12—C12^{i}	176.88 (18)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···N1	0.89 (1)	2.23 (2)	2.676 (2)	110 (2)

C7—H7···O1	0.93	2.33	2.902 (2)	119
C11—H11*B*···O1^{ii}	0.97	2.66	3.134 (2)	111

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