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N,*N*′-Bis(2-pyridyl)naphthalene-1,4-carboxamide

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Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.168
Data-to-parameter ratio = 15.3

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

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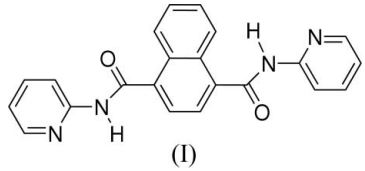
The title compound, $C_{22}H_{16}N_4O_2$, crystallizes in an *anti* C═O conformation. The two amide groups are twisted away from the attached ring by 69.94 (6) and 62.99 (7)°. The crystal packing is stabilized by N—H···N and C—H···O hydrogen bonds, and also by C—H···π interactions.

Comment

Naphthalene-1,4-dicarboxylic acid derivatives are a class of intermediates important for applications as monomers in the preparation of polymers (Fukuzumi *et al.*, 1994; Tsukada *et al.*, 1994). Previously, we have reported the crystal structures of *N*,*N*′-bis(4-nitrophenyl)naphthalene-1,4-dicarboxamide dimethyl sulfoxide disolvate (Jing, Qin, Gu, Zhang & Mao, 2006), *N*,*N*′-bis(2-methoxyphenyl)naphthalene-1,4-dicarboxamide (Jing, Qin, Gu, Zhang & Lei, 2006) and 1,1′-(naphthalene-1,4-diyldicarbonyl)bis(1*H*-imidazole) (Jing, Gu & Zhang, 2006). We now report the crystal structure of the title compound, (I).



(I)

The bond lengths and angles in (I) are normal. The naphthalene ring system is planar, with a maximum deviation of 0.032 (2) Å for atom C6. The two C═O groups are in an *anti* conformation. As a result of steric effects, the substituent groups at atoms C1 and C4 are twisted away from the plane of the naphthalene ring system (Fig. 1). The O1/N1/C11/C12 and O2/N3/C17/C18 planes form dihedral angles of 69.94 (6) and 62.99 (7)°, respectively, with the C1–C4/C9/C10 plane. The O1/N1/C11/C12 and N2/C12–C16 planes are inclined at an angle of 20.63 (9)°, while the O2/N3/C17/C18 and N4/C18–C22 planes make a dihedral angle of 12.87 (11)°. The crystal packing is stabilized by N—H···N and C—H···O hydrogen bonds, and C—H···π interactions (Table 2) involving the N2/C12–C16 (centroid *Cg*1), N4/C18–C22 (centroid *Cg*2) and C1–C4/C9/C10 (centroid *Cg*3) rings.

Experimental

Naphthalene-1,4-dicarboxylic acid (2 mmol) and an excess of thionyl chloride (8 mmol) in dioxane (20 ml) were boiled under reflux for 6 h. The solution was distilled under reduced pressure and a yellow solid was obtained. 2-Aminopyridine (4 mmol) in tetrahydrofuran (20 ml) was added to the yellow solid and boiled under reflux for 1 d. The

solution was then cooled to ambient temperature and filtered to remove the tetrahydrofuran. The precipitate was dissolved in dimethylsulfoxide and allowed to stand for one month at ambient temperature, after which time colourless single crystals of (I) suitable for X-ray diffraction were obtained.

Crystal data

$C_{22}H_{16}N_4O_2$	$Z = 4$
$M_r = 368.39$	$D_x = 1.393$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 13.6987$ (3) Å	$\mu = 0.09$ mm^{-1}
$b = 9.2100$ (2) Å	$T = 153$ (2) K
$c = 15.1404$ (4) Å	Block, colourless
$\beta = 113.091$ (1)°	0.54 × 0.46 × 0.43 mm
$V = 1757.15$ (7) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	4020 independent reflections
ω scans	3685 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.019$
26983 measured reflections	$\theta_{max} = 27.5°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0892P)^2 + 1.7P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.048$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.168$	$\Delta\rho_{max} = 0.33$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.23$ e Å^{-3}
4020 reflections	Extinction correction: *SHELXL97*
262 parameters	Extinction coefficient: 0.016 (2)
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···N4^{i}	0.96 (3)	2.16 (3)	3.105 (2)	172 (2)
N3—H3N···N2^{ii}	0.94 (3)	2.14 (3)	3.066 (2)	169 (2)
C20—H20···O2^{iii}	0.95	2.36	3.303 (2)	170
C3—H3···*Cg*2^{iv}	0.95	2.74	3.404 (2)	128
C16—H16···*Cg*3^{i}	0.95	2.51	3.296 (2)	140
C21—H21···*Cg*1^{v}	0.95	2.80	3.351 (2)	118
C22—H22···*Cg*3^{ii}	0.95	2.62	3.396 (2)	139

Symmetry codes: (i) $x, y+1, z$; (ii) $x, y-1, z$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, -y, -z+1$; (v) $x-\frac{3}{2}, -y-\frac{1}{2}, z-\frac{3}{2}$.

N-bound H atoms were located in a difference Fourier map and refined isotropically [N—H = 0.96 (3) and 0.94 (3) Å]. The C-bound H atoms were placed in calculated positions, with C—H = 0.95 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

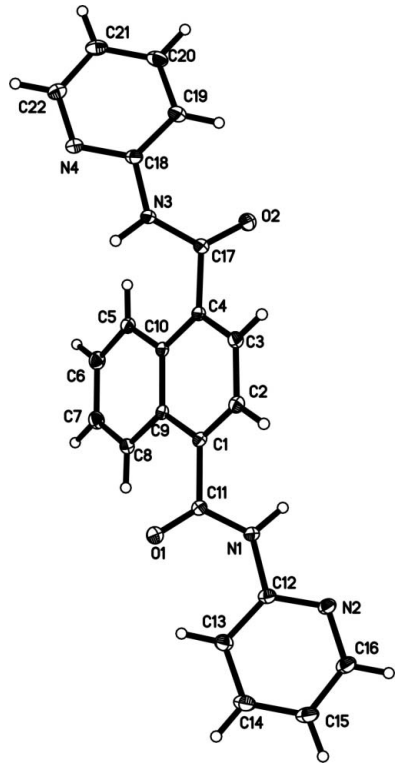


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

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