

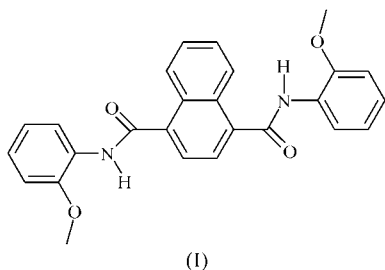
N,N'-Bis(2-methoxyphenyl)- naphthalene-1,4-dicarboxamide

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The title compound, $C_{26}H_{22}N_2O_4$, crystallizes in an *anti*-C=O orientation, with the two *N*-substituted benzene rings in different conformations relative to the naphthalene ring. These conformations allow two strong N—H...O hydrogen bonds and one C—H... π interaction to generate molecular chains in the cell.

Comment

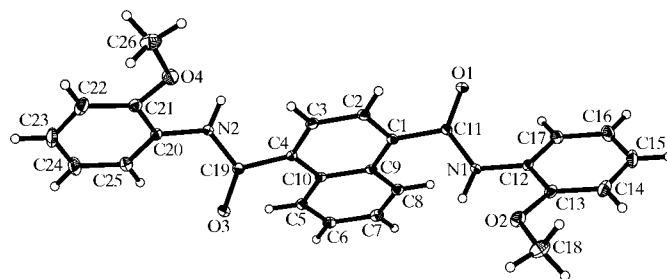
Non-covalent interactions, such as hydrogen-bonding, π - π stacking and C—H... π interactions, play a dominant role in supramolecular self-assembly (Casnati *et al.*, 2003; Ghosh & Bharadwaj, 2004; Glidewell *et al.*, 2005; Jennings *et al.*, 2001). Moreover, the conformations of the molecular building blocks have an important influence on the supramolecular structure. In order to further understanding of supramolecular self-assembly through non-covalent interactions, we have designed and synthesized an *N*-substituted aromatic acylamide, the title compound, (I), a member of the naphthalene-1,4-dicarboxamide family. These compounds are used as optical brightening agents (Hoechst, 1965), optical whiteners (Hoechst, 1969), chemotherapeutic agents (Wander, 1965; Cain *et al.*, 1969) and reagents for oligomers and polymers (Masu *et al.*, 2005; Hsiao & Chang, 2004). We report here the structure of (I) (Fig. 1).



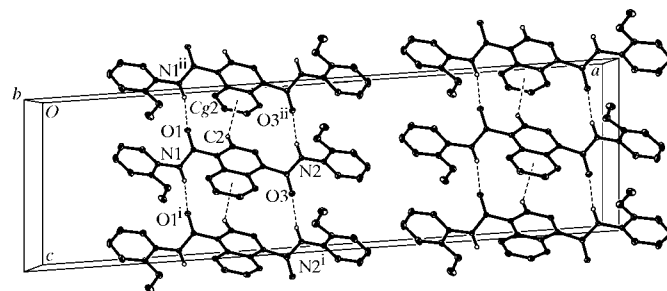
As in the case of the related compounds *N,N'*-dimethyl-1,4-naphthalenedicarboxamide [Cambridge Structural database (CSD, Version 5.27; Allen 2002) refcode ROPYUC (Lewis *et al.*, 1996)], and 8-methoxy-*N*-phenyl-1-naphthamide

and 8-(dimethylamino)-*N*-phenyl-1-naphthamide (refcodes TAWRIT02 and TAWROZ, respectively; O'Leary *et al.*, 2005), the naphthalene ring system of (I), containing two planar benzene rings, C1–C4/C9/C10 and C5–C10, with maximum deviations of 0.031 (2) and -0.007 (3) Å for atoms C4 and C8, respectively, is slightly distorted from planarity, with an interplanar angle of 3.4 (1)°. The corresponding angles for ROPYUC, TAWRIT02 and TAWROZ are 1.72 (7), 4.8 (1) and 4.6 (1)°, respectively. In (I), consistent with intermolecular packing interactions (see below), the substituent groups at atoms C1 and C4 are twisted away from the naphthalene ring system. Thus, the planes C12–C17 and C1–C4/C9/C10 form a dihedral angle of 72.5 (1)°, while the planes C20–C25 and C1–C4/C9/C10 are almost parallel, with a dihedral angle of 5.0 (1)°.

The O1/N1/C11/C12 and O3/N2/C19/C20 planes form dihedral angles of 60.4 (1) and 43.8 (1)°, respectively, with the naphthalene plane. The other two benzene rings of (I), *viz.* C12–C17 and C20–C25, are coplanar, with maximum deviations of -0.005 (2) and 0.011 (1) Å for atoms C13 and C21, respectively. These two benzene planes have an interplanar angle of 72.0 (1)°, quite different from the crystallographically enforced parallel ring planes (0°) found in the related structures *N,N'*-diphenylterephthalamide (CSD refcode DPTPAM; Harkema *et al.*, 1979) and 2,4,2',4'-tetranitro-*N,N'*-diphenylterephthalamide (CSD refcode FENPET; Novozhilova *et al.*, 1986). The two planes O1/N1/C11/C12 and C12–C17 subtend a dihedral angle of 48.1 (1)°, while the two planes O3/N2/C19/

**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

**Figure 2**

Part of the crystal structure of (I), viewed along the *b* axis, with displacement ellipsoids drawn at the 30% probability level. Dashed lines depict the intermolecular hydrogen bonds (see Table 1 for symmetry codes). H atoms not involved in hydrogen bonding have been omitted for clarity.

C20 and C20–C25 make a dihedral angle of 42.5 (1)° (Fig. 1). Because of the sp^2 hybridization of atoms N1 and N2, partial double-bond character is observed in the identical N1–C11/N2–C19 and N1–C12/N2–C20 linkages [average N–C bond lengths = 1.353 (2) and 1.421 (2) Å, respectively].

The observed *anti*-C=O orientation of (I) (Fig. 1) differs from the reported *cis*-C=O orientation in the closest related structure, *i.e.* ROPYUC. The packing structure of (I) involves two strong intermolecular N–H···O hydrogen bonds (Steiner, 2002) (Table 1), which link adjacent molecules into a one-dimensional chain, running parallel to the [001] direction, with a graph-set motif of $R_2^2(18)$ (Bernstein *et al.*, 1995) (Fig. 2). A similar hydrogen-bond network is found in *N,N'*-dimethyl-1,4'-phenylenediacetamide, *N,N'*-dimethyl-4,4'-biphenyldicarboxamide, *N,N'*-dimethyl-4,4'-stilbenedicarboxamide and *N,N'*-dimethyl-4,4'-diphenylacetylenedicarboxamide (CSD refcodes ROPYIQ, ZUKJUK10, ZUKJOE10 and ZUKKAR10, respectively; Lewis *et al.*, 1996). Within the chain between adjacent molecules, there is also a classical intermolecular C–H··· π hydrogen bond (Desiraju & Steiner, 1999) (Fig. 2 and Table 1). There are no significant interactions between adjacent chains.

Experimental

Naphthalene-1,4-dicarboxylic acid (2 mmol) and an excess of thionyl chloride in dioxane (20 ml) were boiled under reflux for 6 h. The solution was distilled at reduced pressure and a yellow solid was obtained. *o*-Anisidine (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 dimethyl sulfoxide 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

$C_{26}H_{22}N_2O_4$	$Z = 4$
$M_r = 426.46$	$D_x = 1.352 \text{ Mg m}^{-3}$
Monoclinic, Cc	Mo $K\alpha$ radiation
$a = 34.7194$ (9) Å	$\mu = 0.09 \text{ mm}^{-1}$
$b = 6.04620$ (10) Å	$T = 153$ (2) K
$c = 10.0042$ (3) Å	Column, colourless
$\beta = 93.9750$ (10)°	$0.35 \times 0.21 \times 0.14 \text{ mm}$
$V = 2095.03$ (9) Å ³	

Data collection

Rigaku R-Axis RAPID diffractometer	2074 independent reflections
ω scans	2049 reflections with $I > 2\sigma(I)$
8696 measured reflections	$R_{\text{int}} = 0.014$
	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.5976P]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.080$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
2074 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
292 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	(Sheldrick, 1997)
	Extinction coefficient: 0.0042 (8)

Table 1

Hydrogen-bond geometry (Å, °).

Cg_2 is the centroid of the C5–C10 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1N···O1 ⁱ	0.88	1.99	2.845 (2)	164
N2–H2N···O3 ⁱⁱ	0.88	2.05	2.917 (2)	168
C2–H2··· Cg_2 ⁱⁱ	0.95	2.55	3.353 (2)	142

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

All H atoms were placed in calculated positions and included in the final cycles of refinement using a riding model, with N–H = 0.88 Å and C–H = 0.95 or 0.98 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N,C})$.

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: *SHELXTL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GA3018). Services for accessing these data are described at the back of the journal.

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