organic papers

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Key indicators

Single-crystal X-ray study
$T = 296$ K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.038
wR factor = 0.090
Data-to-parameter ratio = 10.1

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

4-Bromo-N-(3,4,5-trimethoxyphenyl)benzamide

In the molecule of the title compound, $C_{16}H_{16}BrNO_4$, the dihedral angle between the planes of the two rings is 16.6 (2)°.

Comment

Benzanilide derivatives attract the attention of scientists for their widely known biological activities. They have been reported as arginine vasopressin receptor antagonists (Kakefuda *et al.*, 2002), dual acting agents with α_1-adrenoceptor antagonistic action and steroid 5-α reductase inhibitory activity (Yoshida *et al.*, 1998), potassium channel activators (Biagi *et al.*, 2004) and anticancer agents (Cushman *et al.*, 1991). We were interested in benzanilide derivatives on account of their antitumour activities. The title compound, (I), was chosen for crystallographic study in order to better understand its biological profile. The central carboxyl O atom is disordered over two sites (O11 and O12). The O11—C1 distance of 1.251 (10) Å suggests a double bond. The *N*-3,4,5-trimethoxyphenylformamide fragment is twisted from the mean plane of the 4-bromophenyl group by 9.9 (4)°. The dihedral angle between the planes of the 3,4,5-trimethoxy-aniline and 4-bromophenyl groups is 16.6 (2)°.


(I)
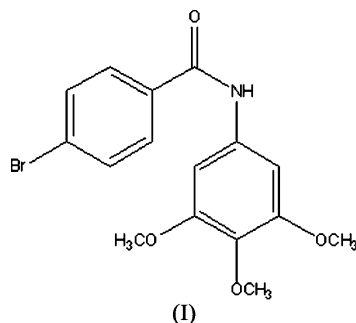
Experimental

The title compound was obtained from 3,4,5-trimethoxyaniline and *p*-bromobenzoyl chloride *via* the Schotten–Baumann reaction (Gao & Kawabatal, 2005). A crystal suitable for crystallographic study was obtained by slow crystallization from ethyl acetate at room temperature.

Crystal data

$C_{16}H_{16}BrNO_4$	$Z = 4$
$M_r = 366.21$	$D_x = 1.537$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 7.121$ (3) Å	$\mu = 2.62$ mm^{-1}
$b = 8.492$ (3) Å	$T = 296$ (1) K
$c = 26.171$ (7) Å	Block, colourless
$V = 1582.6$ (9) Å^3	$0.30 \times 0.30 \times 0.28$ mm
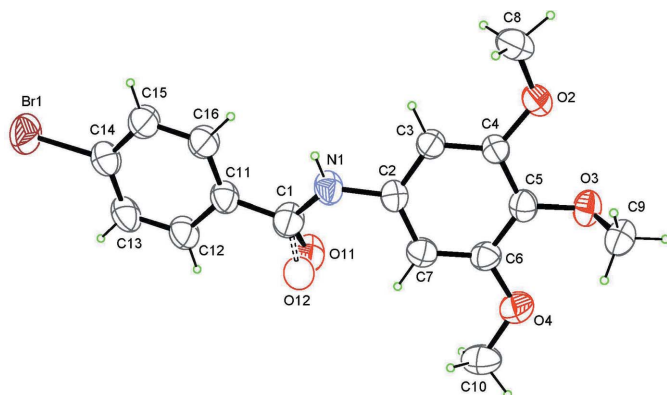
Figure 1
View of the molecule of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 40% probability level and both disordered carboxyl oxygen atoms (O11 and O12) are shown.

The carboxyl O atom is disordered over two sites with equal occupancy. All H atoms were positioned geometrically. The methyl H atoms were then constrained to an ideal geometry with C—H distances of 0.96 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93 Å, N—H = 0.84 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2004); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97*; program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

Data collection

Rigaku R-AXIS RAPID diffractometer	15633 measured reflections
ω scans	2107 independent reflections
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	1154 reflections with $F^2 > 2\sigma(F^2)$
$T_{min} = 0.456$, $T_{max} = 0.480$	$R_{int} = 0.060$
	$\theta_{max} = 27.5°$

Refinement

Refinement on F^2	$w = 2/[1.09\sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.090$	$\Delta\rho_{max} = 0.55$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.51$ e Å^{-3}
2107 reflections	Extinction correction: Larson (1970), equation 22
209 parameters	Extinction coefficient: 1.7 (3) × 10^2
H-atom parameters constrained	

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