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Crystal structure of 2-pentyloxybenzamide

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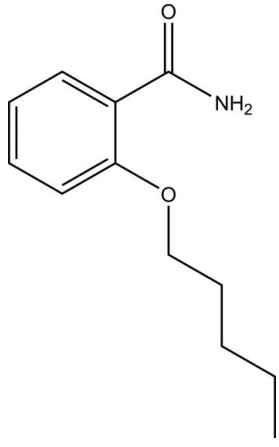
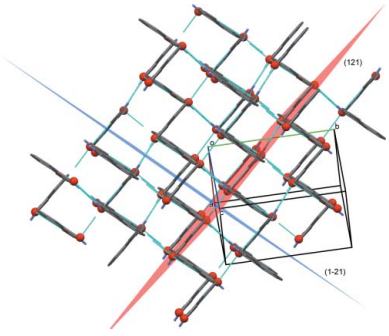
In the title molecule, $C_{12}H_{17}NO_2$, the amide NH_2 group is oriented toward the pentyloxy substituent and an intramolecular N—H···O hydrogen bond is formed with the pentyloxy O atom. The benzene ring forms dihedral angles of 2.93 (2) and 5.60 (2)° with the amide group and the pentyloxy group mean planes, respectively. In the crystal, molecules are linked by pairs of N—H···O hydrogen bonds, forming inversion dimers with their molecular planes parallel, but at an offset of 0.45 (1) Å to each other. These dimers are ordered into two types of symmetry-related columns extended along the *a* axis, with the mean plane of one set of dimers in a column approximately parallel to (121) and the other in a column approximately parallel to $(1\bar{2}1)$. The two planes form a dihedral angle of 85.31 (2)°, and are linked *via* C—H···O hydrogen bonds and C—H···π interactions, forming a three-dimensional framework structure.

1. Chemical context

2-Alkoxybenzamide moieties can be found as structural units in medicinally active compounds, such in dopamine (DA) receptor antagonists (van de Waterbeemd & Testa, 1983). Typically such components are Sulpiride®, Metoclopramide® and Tiapride®. Other substituted 2-alkoxybenzamides have been found to be antagonists of chemotherapy-induced nausea (Monkovic *et al.*, 1988). Also, 2-alkoxybenzamides have been proposed as agonists of the α7 nicotinic receptor (Bodnar *et al.*, 2005) and as neuroleptic compounds (Florvall & Oegren, 1982). 2-Ethoxybenzamide, under the name ethenzamide, is a commonly used analgesicum (Darias *et al.*, 1992).





In our efforts to use 2-alkoxybenzamides as components in co-crystal formation (Aitipamula *et al.*, 2012), we prepared the title compound, 2-pentyloxybenzamide, and report herein on its crystal structure. 2-Pentyloxybenzamide was first studied for its antipyretic and analgesic properties (Bavin *et al.*, 1952;

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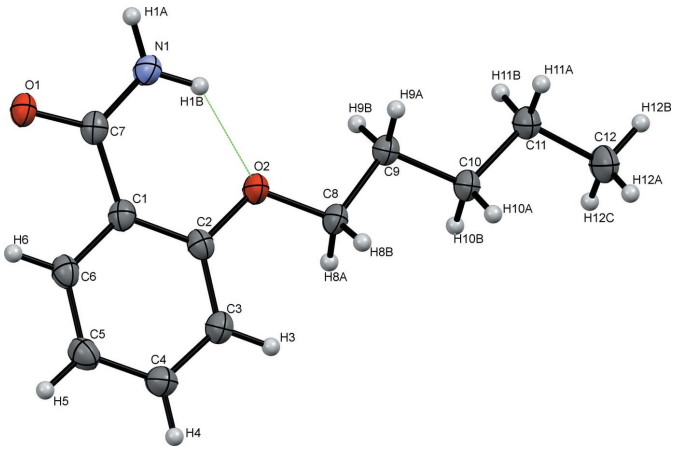

Figure 1
A view of the molecular structure of the title molecule, with atom labelling. Displacement ellipsoids are shown at the 50% probability level. The intramolecular N—H···O hydrogen bond is shown as a green dashed line (see Table 1 for details).

Macrae & Seymour, 1956). Afterwards, it was found to have antifungal activity and to be useful in the treatment of dermatomycosis (Simmonite & Tattersall, 1962; Coates *et al.*, 1957). Under the name pentalamide, it is still used as an ingredient in antifungal agents for topical use.

2. Structural commentary

In the title molecule, Fig. 1, the benzene ring is nearly coplanar with the amide group [C6—C1—C7—O1 = −2.48 (18)°] and the pentyloxy group [C3—C2—O2—C8 = 0.37 (18)°]. The amide NH_2 group is oriented towards the ether group allowing for an intramolecular hydrogen bond (N1—H1*B*···O2; Fig. 1 and Table 1). The latter is also present in analogous compounds, such as 3-hydroxy-2-methoxybenzamide (Wilbrand *et al.*, 2012), 2-propoxybenzamide (Al Jasem *et al.*, 2012) and 2-(prop-2-enyloxy)benzamide (Bugenhagen *et al.*, 2012). 2-Ethoxybenzamide is the only studied 2-alkoxybenzamide that does not exhibit an intramolecular hydrogen bond in the single component crystal (Pagola & Stephens, 2009). However, it shows a similar conformation to the other 2-alkoxybenzamides in the co-crystal form with thiourea (Moribe *et al.*, 2004), and with salicylic acid (Back *et al.*, 2012).

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

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O2	0.915 (17)	1.921 (18)	2.6510 (15)	135.4 (15)
N1—H1*A*···O1^{i}	0.919 (19)	1.964 (19)	2.8824 (15)	177.8 (17)
C3—H3···O1^{ii}	0.93	2.62	3.546 (2)	178
C4—H4···O1^{iii}	0.93	2.53	3.306 (2)	141
C11—H11*A*···*Cg*1^{iv}	0.97	2.90	3.7283 (16)	141

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

3. Supramolecular features

In the crystal, molecules are linked by pairs of N-H···O (N1—H1*A*···O1) hydrogen bonds forming inversion dimers (Fig. 2 and Table 1). These dimers form a nested network of molecules, made of two layers, (121) and (1$\bar{2}$1), which form an angle of 85.31 (2)° between their planes (Fig. 3). The dimers in the layers are linked by C—H···O (C4—H4···O1) hydrogen bonds and C—H···π interactions, forming a three-dimensional framework (Fig. 3 and Table 1). Within two parallel layers, pairs of molecules lie with an offset to each other without any noticeable, direct interaction between them; the

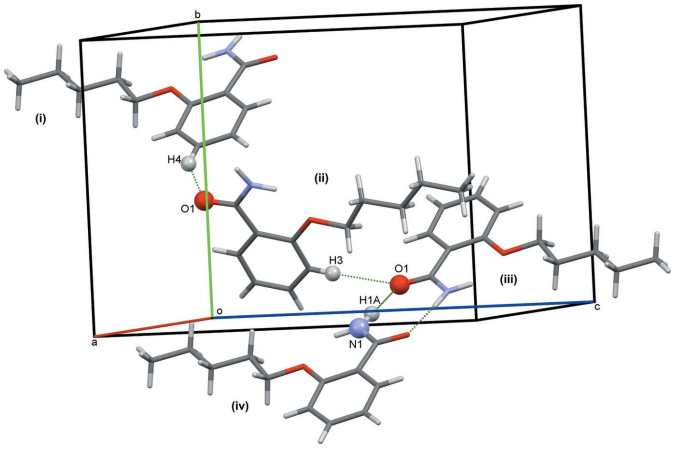

Figure 2
A partial view of the crystal packing of the title compound. The hydrogen bonds are shown as green dashed lines [see Table 1 for details; symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) x, y, z; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$]

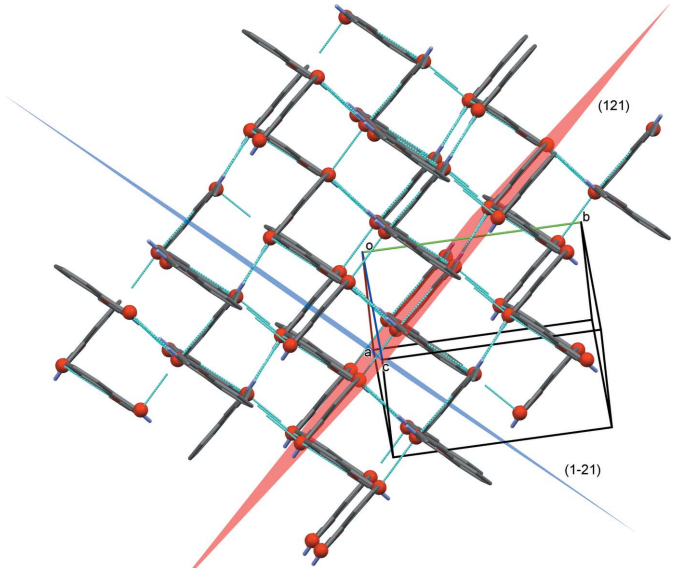

Figure 3
A view of the crystal network formed by the layers of inversion dimers in the planes (121) in red, and (1$\bar{2}$1) in blue. The hydrogen bonds are shown as green dashed lines (see Table 1 for details; H atoms have been omitted for clarity).

parallel layers are at a distance of 3.81 (3) Å from each other. Along the *a* axis the pairs are ordered in two symmetry-related columns. The plane of the benzene ring (C1–C6) of the 2-pentyloxybenzamide forms an angle of 25.29 (2)° with the column axis.

4. Database survey

From a database survey (Cambridge Structural Database, Version 5.35, last update May 2014; Allen, 2002), the following were picked as relevant comparable structures: 3-hydroxy-2-methoxybenzamide (Wilbrand *et al.*, 2012), 2-methoxybenzamide (Moribe *et al.*, 2006), 2-ethoxybenzamide (Pagola & Stephens, 2009; Back *et al.*, 2012), 2-propoxybenzamide (Al Jasem *et al.*, 2012) and 2-(prop-2-enyloxy)benzamide (Bugenhagen *et al.*, 2012). For 2-propoxybenzamide, a homologue of the title compound, a similar formation of inversion-related molecular pairs in the crystal was reported, hence the two compounds exhibit a similar packing. The noticeable difference between the two compounds is the larger dihedral angle between the carboxamide group and the benzene ring in 2-propoxybenzamide, 12.41 (2)° compared to 3.30 (15)° in the title compound, 2-pentyloxybenzamide. Also, the parallel layers of molecules in the title compound are further apart [separated by 3.81 (3) Å] than is found for a similar packing of 2-propoxybenzamide [3.69 (2) Å]. Similarly, inversion-related pairs of molecules are formed by intermolecular (amide–amide) hydrogen bonding in 2-ethoxybenzamide and 3-hydroxy-2-methoxybenzamide. As 2-ethoxybenzamide exhibits no intramolecular hydrogen bonding, the freed acceptor–donor sites are used for additional intermolecular hydrogen bonding with the adjacent molecule.

In contrast, in 2-methoxybenzamide and in 2-(prop-2-enyloxy)benzamide the intermolecular N—H···O hydrogen bonds involving the amide groups do not lead to pair formation but generate $C(4)$ and $R_3^2(7)$ motifs.

5. Synthesis and crystallization

The preparation of the title compound follows a Williamson ether synthesis using DMSO as solvent, analogous to a general procedure (Johnstone & Rose, 1979): To powdered KOH (1.12 g, 20.0 mmol) in DMSO (18 ml) was added salicylamide (1.37 g, 10.0 mmol), and the resulting mixture was stirred for 10 min. at rt. Then, *n*-amyl iodide (4.2 g, mmol, 21.2 mmol) was added dropwise. The solution was stirred for 12 h at rt. It was then poured into water (200 ml) and extracted with chloroform (3 × 75 ml). The organic phase was dried over anhydrous $MgSO_4$, concentrated *in vacuo*, and the residue was subjected to column chromatography on silica gel ($CHCl_3$/M^{t}BE/hexane *v/v/v* 1:1:1) to give the title compound (1.55 g, 75%) as colourless crystals (m.p. 362 K). IR (KBr, cm^{-1}) νmax 3434, 3168, 2948, 2868, 1664, 1593, 1387, 1232, 1164, 1018, 832, 788, 765, 575; ^{1}H NMR (400 MHz, $CDCl_3$, δ_H) 0.93 (3H, *t*, ^3J = 7.2 Hz, CH_3), 1.38–1.48 (4H, *m*), 1.84–1.89 (2H, *m*), 4.11 (2*H*, *d*, ^3J = 6.4 Hz); 6.03 (1H, *bs*, NH), 6.96 (1H, *d*, ^3J = 8.4 Hz), 7.03–7.07 (1H, *m*), 7.42–7.46 (1H, *m*), 7.85 (1H, *bs*, NH), 8.20 (1H, *dd*, ^3J = 7.6 Hz, ^4J = 2.0 Hz), ^{13}C NMR (100.5 MHz, $CDCl_3$, δ_C) 14.0 (CH_3), 22.4 (CH_2), 28.2 (CH_2), 28.9 (CH_2), 69.1 (OCH_2), 112.2 (CH), 120.7 (C_{quat}), 121.0 (CH), 132.5 (CH), 133.3 (C_{quat}), 157.4 (C_{quat}), 167.2 (C_{quat}, CO).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{17}NO_2$
M_r	207.27
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, *b*, *c* (Å)	8.1830 (2), 11.2706 (2), 14.5386 (4)
β (°)	119.696 (2)
V (Å^3)	1164.76 (5)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	0.64
Crystal size (mm)	0.25 × 0.19 × 0.10
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min}, T_{max}	0.854, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6112, 2268, 1900
R_{int}	0.022
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.621
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.115, 1.03
No. of reflections	2268
No. of parameters	145
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.22

Computer programs: *CrysAlis PRO* (Agilent, 2012), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) within *OLEX2* (Dolomanov *et al.*, 2009), *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All C-bound H atoms were placed in calculated positions and refined as riding atoms: C—H distances of 0.95 − 1.00 Å with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl and = 1.2 for other H-atoms. The N-bound H atoms were located in a difference electron-density map and freely refined.

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supporting information

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Crystal structure of 2-pentyloxybenzamide

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Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) within OLEX2 (Dolomanov *et al.*, 2009); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

2-pentyloxybenzamide

Crystal data

$C_{12}H_{17}NO_2$
M_r = 207.27
Monoclinic, $P2_1/c$
a = 8.1830 (2) Å
b = 11.2706 (2) Å
c = 14.5386 (4) Å
β = 119.696 (2)°
V = 1164.76 (5) Å^3
Z = 4
$F(000)$ = 448
D_x = 1.182 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.5418 Å
Cell parameters from 2743 reflections
θ = 3.9–73.1°
μ = 0.64 mm^{-1}
T = 100 K
Block, colourless
0.25 × 0.19 × 0.10 mm

Data collection

SuperNova, Dual, Cu at zero, Atlas diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.4127 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.854, T_{max} = 1.000
6112 measured reflections
2268 independent reflections
1900 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 73.3°, θ_{min} = 5.3°
$h = -10 \rightarrow 5$
$k = -13 \rightarrow 14$
$l = -16 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.03
2268 reflections
145 parameters
0 restraints
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

$w = 1/[\sigma^2(F_o^2) + (0.0645P)^2 + 0.2593P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.25614 (18)	0.29076 (11)	0.20599 (10)	0.0233 (3)
C10	−0.14119 (19)	0.33945 (13)	0.46481 (11)	0.0269 (3)
C11	−0.29380 (19)	0.41079 (13)	0.47067 (11)	0.0294 (3)
C12	−0.3051 (2)	0.37915 (16)	0.56955 (12)	0.0389 (4)
C2	0.21475 (18)	0.25854 (12)	0.28594 (10)	0.0240 (3)
C3	0.31443 (19)	0.16670 (12)	0.35597 (11)	0.0279 (3)
C4	0.45350 (19)	0.10654 (13)	0.34698 (11)	0.0303 (3)
C5	0.49609 (19)	0.13709 (13)	0.26885 (11)	0.0301 (3)
C6	0.39777 (18)	0.22849 (12)	0.19968 (10)	0.0266 (3)
C7	0.15680 (18)	0.38484 (11)	0.12366 (10)	0.0232 (3)
C8	0.03619 (19)	0.28821 (12)	0.37434 (10)	0.0263 (3)
C9	−0.11424 (18)	0.36885 (12)	0.37063 (10)	0.0256 (3)
H10A	−0.1714	0.2558	0.4618	0.032*
H10B	−0.0229	0.3526	0.5295	0.032*
H11A	−0.4142	0.3950	0.4082	0.035*
H11B	−0.2672	0.4948	0.4717	0.035*
H12A	−0.3329	0.2962	0.5683	0.058*
H12B	−0.4027	0.4250	0.5710	0.058*
H12C	−0.1869	0.3963	0.6315	0.058*
H1A	−0.056 (2)	0.4934 (17)	0.0658 (14)	0.042 (5)*
H1B	−0.021 (2)	0.4242 (16)	0.1713 (14)	0.041 (5)*
H3	0.2873	0.1458	0.4089	0.033*
H4	0.5188	0.0452	0.3937	0.036*
H5	0.5896	0.0967	0.2630	0.036*
H6	0.4270	0.2490	0.1475	0.032*
H8A	0.1495	0.2950	0.4427	0.032*
H8B	−0.0062	0.2065	0.3650	0.032*
H9A	−0.2313	0.3570	0.3049	0.031*
H9B	−0.0767	0.4511	0.3742	0.031*
N1	0.01348 (16)	0.44361 (11)	0.12198 (9)	0.0282 (3)
O1	0.20767 (12)	0.40558 (9)	0.05777 (7)	0.0264 (2)
O2	0.07616 (13)	0.32058 (8)	0.29182 (7)	0.0271 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0293 (5)	0.0312 (5)	0.0239 (5)	−0.0023 (4)	0.0171 (4)	0.0000 (4)
O2	0.0312 (5)	0.0313 (5)	0.0271 (5)	0.0063 (4)	0.0207 (4)	0.0059 (4)
N1	0.0343 (6)	0.0299 (6)	0.0271 (6)	0.0063 (5)	0.0204 (5)	0.0060 (5)
C1	0.0233 (6)	0.0263 (6)	0.0213 (6)	−0.0034 (5)	0.0116 (5)	−0.0028 (5)
C2	0.0227 (6)	0.0269 (7)	0.0250 (6)	−0.0002 (5)	0.0139 (5)	−0.0021 (5)
C3	0.0293 (7)	0.0316 (7)	0.0266 (7)	0.0015 (5)	0.0168 (6)	0.0028 (5)
C4	0.0302 (7)	0.0313 (7)	0.0300 (7)	0.0060 (6)	0.0153 (6)	0.0045 (6)
C5	0.0279 (7)	0.0347 (8)	0.0309 (7)	0.0044 (6)	0.0169 (6)	−0.0018 (6)
C6	0.0259 (7)	0.0331 (7)	0.0244 (6)	−0.0013 (5)	0.0153 (6)	−0.0028 (5)
C7	0.0252 (7)	0.0244 (6)	0.0224 (6)	−0.0053 (5)	0.0135 (5)	−0.0046 (5)
C8	0.0303 (7)	0.0300 (7)	0.0250 (6)	0.0035 (5)	0.0186 (6)	0.0055 (5)
C9	0.0260 (7)	0.0296 (7)	0.0247 (6)	0.0022 (5)	0.0152 (5)	0.0034 (5)
C10	0.0281 (7)	0.0318 (7)	0.0259 (7)	0.0031 (6)	0.0173 (6)	0.0039 (5)
C11	0.0290 (7)	0.0357 (7)	0.0284 (7)	0.0037 (6)	0.0180 (6)	0.0032 (6)
C12	0.0405 (9)	0.0513 (10)	0.0375 (8)	0.0100 (7)	0.0288 (7)	0.0064 (7)

Geometric parameters (Å, º)

O1—C7	1.2412 (15)	C6—H6	0.9300
O2—C2	1.3706 (15)	C8—H8A	0.9700
O2—C8	1.4381 (14)	C8—H8B	0.9700
N1—C7	1.3366 (17)	C8—C9	1.5095 (18)
N1—H1A	0.919 (19)	C9—H9A	0.9700
N1—H1B	0.915 (17)	C9—H9B	0.9700
C1—C2	1.4099 (17)	C9—C10	1.5272 (17)
C1—C6	1.3962 (18)	C10—H10A	0.9700
C1—C7	1.5013 (18)	C10—H10B	0.9700
C2—C3	1.3966 (19)	C10—C11	1.5227 (18)
C3—H3	0.9300	C11—H11A	0.9700
C3—C4	1.3853 (19)	C11—H11B	0.9700
C4—H4	0.9300	C11—C12	1.5278 (18)
C4—C5	1.3866 (19)	C12—H12A	0.9600
C5—H5	0.9300	C12—H12B	0.9600
C5—C6	1.385 (2)	C12—H12C	0.9600
C1—C6—H6	119.0	C6—C1—C7	116.23 (11)
C10—C11—C12	111.28 (12)	C6—C1—C2	118.09 (12)
C10—C11—H11B	109.4	C7—N1—H1B	118.2 (11)
C10—C11—H11A	109.4	C7—N1—H1A	118.0 (10)
C10—C9—H9B	110.0	C8—C9—C10	108.35 (11)
C10—C9—H9A	110.0	C8—C9—H9B	110.0
C11—C12—H12C	109.5	C8—C9—H9A	110.0
C11—C12—H12B	109.5	C9—C10—H10B	108.5
C11—C12—H12A	109.5	C9—C10—H10A	108.5
C11—C10—H10B	108.5	C9—C8—H8B	109.7

C11—C10—H10A	108.5	C9—C8—H8A	109.7
C11—C10—C9	114.98 (11)	H10A—C10—H10B	107.5
C12—C11—H11B	109.4	H11A—C11—H11B	108.0
C12—C11—H11A	109.4	H12A—C12—H12C	109.5
C2—C3—H3	119.9	H12A—C12—H12B	109.5
C2—C1—C7	125.65 (12)	H12B—C12—H12C	109.5
C2—O2—C8	117.38 (10)	H1A—N1—H1B	123.2 (14)
C3—C4—C5	120.48 (13)	H8A—C8—H8B	108.2
C3—C4—H4	119.8	H9A—C9—H9B	108.4
C3—C2—C1	119.99 (12)	N1—C7—C1	119.22 (11)
C4—C5—H5	120.4	O1—C7—C1	119.48 (11)
C4—C3—H3	119.9	O1—C7—N1	121.29 (12)
C4—C3—C2	120.29 (12)	O2—C8—C9	109.63 (10)
C5—C6—H6	119.0	O2—C8—H8B	109.7
C5—C6—C1	121.92 (12)	O2—C8—H8A	109.7
C5—C4—H4	119.8	O2—C2—C3	122.35 (11)
C6—C5—H5	120.4	O2—C2—C1	117.66 (11)
C6—C5—C4	119.22 (12)		

C1—C2—C3—C4	−0.3 (2)	C6—C1—C2—O2	179.67 (11)
C2—C3—C4—C5	0.3 (2)	C7—C1—C6—C5	−177.98 (12)
C2—C1—C7—N1	−1.4 (2)	C7—C1—C2—C3	178.07 (12)
C2—C1—C7—O1	179.44 (12)	C7—C1—C2—O2	−2.27 (19)
C2—C1—C6—C5	0.3 (2)	C8—C9—C10—C11	−178.10 (12)
C2—O2—C8—C9	177.89 (11)	C8—O2—C2—C3	0.37 (18)
C3—C4—C5—C6	−0.1 (2)	C8—O2—C2—C1	−179.28 (11)
C4—C5—C6—C1	−0.2 (2)	C9—C10—C11—C12	−177.64 (12)
C6—C1—C7—N1	176.66 (12)	O2—C8—C9—C10	−175.11 (10)
C6—C1—C7—O1	−2.48 (18)	O2—C2—C3—C4	−179.95 (12)
C6—C1—C2—C3	0.02 (19)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O2	0.915 (17)	1.921 (18)	2.6510 (15)	135.4 (15)
N1—H1*A*···O1^{i}	0.919 (19)	1.964 (19)	2.8824 (15)	177.8 (17)
C3—H3···O1^{ii}	0.93	2.62	3.546 (2)	178
C4—H4···O1^{iii}	0.93	2.53	3.306 (2)	141
C11—H11*A*···*Cg*1^{iv}	0.97	2.90	3.7283 (16)	141

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*+1, *y*−1/2, −*z*+1/2; (iv) *x*−1, *y*, *z*.