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6-(4-Bromophenyl)-2-ethoxy-4-(4-ethoxyphenyl)nicotinonitrile

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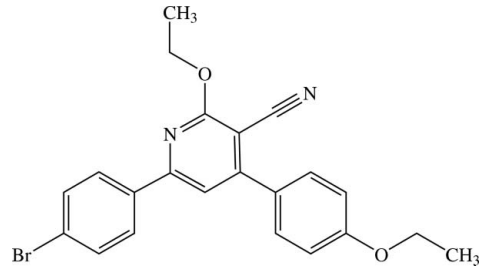
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.084; data-to-parameter ratio = 22.3.

The molecule of the title nicotinonitrile derivative, $C_{22}H_{19}BrN_2O_2$, is non-planar, the central pyridine ring making dihedral angles of 7.34 (14) and 43.56 (15)° with the 4-bromophenyl and 4-ethoxyphenyl rings, respectively. The ethoxy group of the 4-ethoxyphenyl is slightly twisted from the attached benzene ring [C—O—C—C = 174.2 (3)°], whereas the ethoxy group attached to the pyridine ring is in a (+)*syn*-clinal conformation [C—O—C—C = 83.0 (3)°]. A weak intramolecular C—H···N interaction generates an S(5) ring motif. In the crystal structure, the molecules are linked by weak intermolecular C—H···N interactions into screw chains along the b axis. These chains stacked along the a axis. π–π interactions with centroid–centroid distances of 3.8724 (16) and 3.8727 (16) Å are also observed.

Related literature

For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the synthesis and applications of nicotinonitrile derivatives, see: Borgna *et al.* (1993); Fun *et al.* (2008); Goda *et al.* (2004); Kamal *et al.* (2007); Malinka *et al.* (1998). For related structures, see: Chantrapromma *et al.* (2009). For the stability of the temperature controller used in the data collection, see Cosier & Glazer (1986).



Experimental

Crystal data

$C_{22}H_{19}BrN_2O_2$
M_r = 423.29
Orthorhombic, $P2_12_12_1$
a = 4.3414 (2) Å
b = 14.7392 (6) Å
c = 29.4409 (13) Å
V = 1883.89 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.20 mm^{-1}
T = 100 K
0.57 × 0.05 × 0.03 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.368, T_{max} = 0.931
18389 measured reflections
5477 independent reflections
4081 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.084
S = 0.99
5477 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}
Absolute structure: Flack (1983), 2269 Friedel pairs
Flack parameter: 0.008 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···N1	0.93	2.41	2.758 (4)	102
C5—H5A···N2^{i}	0.93	2.58	3.446 (4)	156
C13—H13A···N2^{ii}	0.93	2.53	3.206 (4)	130

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2683).

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6-(4-Bromophenyl)-2-ethoxy-4-(4-ethoxyphenyl)nicotinonitrile

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S1. Comment

A large number of substituted pyridines have been claimed to exhibit biological activities in a number of areas (Borgna *et al.*, 1993; Goda *et al.*, 2004; Kamal *et al.*, 2007; Malinka *et al.*, 1998). The pyridine ring is among the most common heterocyclic compounds found in the naturally occurring heterocycles and in various therapeutic agents. Our research is aimed at the synthesis and preliminary pharmacological screening (*in vivo*) of the nicotinonitrile derivatives. Therefore the title nicotinonitrile derivative, which is a substituted pyridine compound, was synthesized by cyclization of a chalcone derivative (Fun *et al.*, 2008) and malononitrile in order to investigate its analgesic and anti-inflammatory activities. Our results of these pharmacological studies showed that the title compound is a promising candidate for analgesic and anti-inflammatory activities. The analgesic and anti-inflammatory profiles of the title compound together with some other related nicotinonitrile derivatives will be reported elsewhere.

The title compound (I), $C_{22}H_{19}BrN_2O_2$ is a non-planar molecule (Fig. 1). The central pyridine ring is nearly coplanar with the 4-bromophenyl ring with the dihedral angle of 7.34 (14)° whereas it is inclined to the 4-ethoxyphenyl unit with the dihedral angle of 43.56 (15)°. The ethoxy substituent of the 4-ethoxyphenyl is slightly twisted from the mean plane of the attached benzene ring with the torsion angle C15–O2–C20–C21 = 174.2 (3)° whereas the ethoxy group attached to the pyridine ring is in a (+)*syn*-clinal conformation with a C11–O1–C18–C19 torsion angle of 83.0 (3)°. The orientation of the cyano group can be indicated by the torsion angle C8–C9–C10–C22 = 177.0 (3)°. A weak intramolecular C1—H1A···N1 interaction generates an S(5) ring motif (Bernstein *et al.*, 1995). The bond distances agree with the literature values (Allen *et al.*, 1987) and are comparable with those for a related structure (Chantrapromma *et al.*, 2009).

In the crystal structure (Fig. 2), the molecules are linked by weak intermolecular C—H···N interactions (Table 1) into screw chains along the *b* axis. These chains stacked along the *a* axis. The crystal is further stabilized by $\pi\cdots\pi$ interactions with the $Cg_1\cdots Cg_2$ distances of 3.8724 (16) Å (symmetry code: -1 + *x*, *y*, *z*) and 3.8727 (16) Å (symmetry code: 1 + *x*, *y*, *z*); Cg_1 and Cg_2 are the centroids of C7–C11/N1 and C1–C6 rings, respectively.

S2. Experimental

(*E*-1-(4-Bromophenyl)-3-(4-ethoxyphenyl)prop-2-en-1-one (0.50 g, 0.0015 mole) were added with continuous stirring to a freshly prepared sodium alkoxide (0.0014 mole of sodium in 100 ml of ethanol). Malononitrile (1.30 g, 0.02 mol) was then added with continuous stirring at room temperature until the precipitate separated out. The resulting solid was filtered (yield 65%). Colorless needle-shaped single crystals of the title compound suitable for *x*-ray structure determination were recrystalized from acetone/ethanol (1:1 *v*/*v*) by the slow evaporation of the solvent at room temperature over several days, Mp. 418–419 K.

S3. Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with d(C—H) = 0.93 Å for aromatic, 0.97 for CH_2 and 0.96 Å for CH_3 atoms. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 1.07 Å from Br1 and the deepest hole is located at 0.96 Å from Br1.

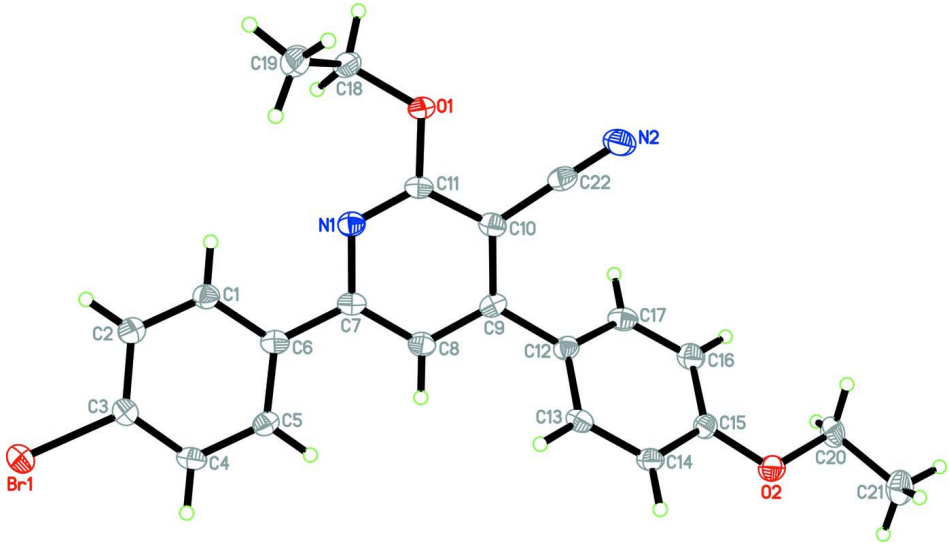

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

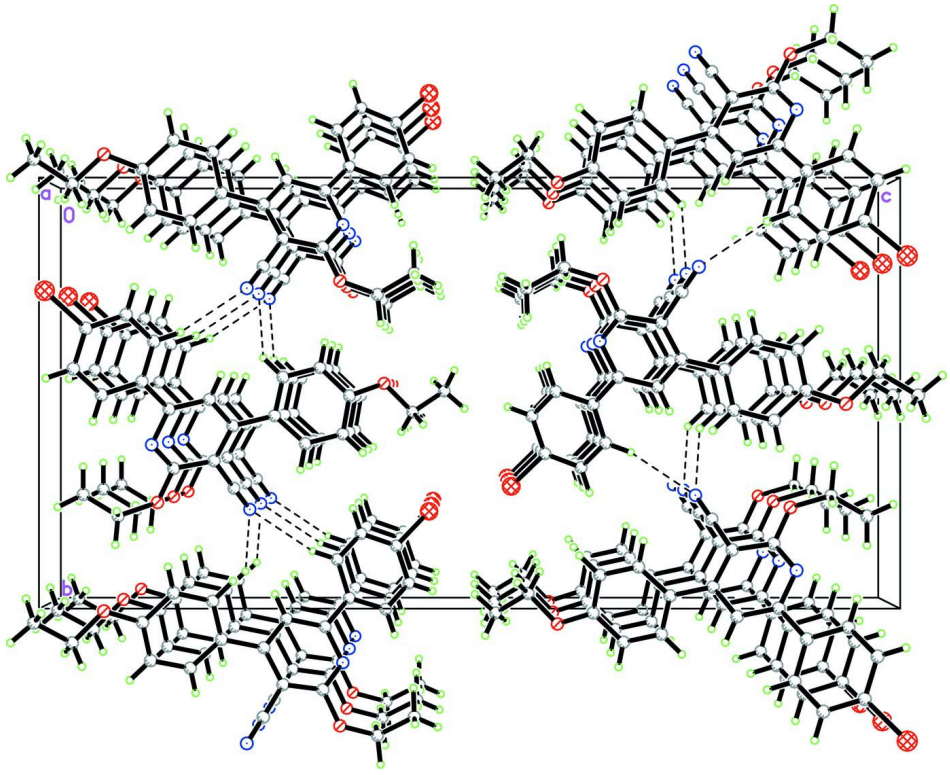

Figure 2

The crystal packing of the title compound viewed along the *a* axis, showing chains stacked down the *a* axis. Hydrogen bonds are shown as dashed lines.

6-(4-Bromophenyl)-2-ethoxy-4-(4-ethoxyphenyl)nicotinonitrile

Crystal data

$C_{22}H_{19}BrN_2O_2$
$M_r = 423.29$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 4.3414\ (2)$ Å
$b = 14.7392\ (6)$ Å
$c = 29.4409\ (13)$ Å
$V = 1883.89\ (14)$ Å^3
$Z = 4$
$F(000) = 864$
$D_x = 1.492$ Mg m^{-3}
Melting point = 418–419 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5478 reflections
$\theta = 1.4$–$30.0°$
$\mu = 2.20$ mm^{-1}
$T = 100$ K
Needle, colourless
0.57 × 0.05 × 0.03 mm

Data collection

Bruker APEXII CCD area detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.368$, $T_{max} = 0.931$
18389 measured reflections
5477 independent reflections
4081 reflections with $I > 2\sigma(I)$
$R_{int} = 0.076$
$\theta_{max} = 30.0°$, $\theta_{min} = 1.6°$
$h = -6 \rightarrow 6$
$k = -20 \rightarrow 20$
$l = -41 \rightarrow 41$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.084$
$S = 0.99$
5477 reflections
246 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0276P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-3}
Absolute structure: Flack (1983), 2269 Friedel pairs
Absolute structure parameter: 0.008 (9)

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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}
Br1	1.58148 (8)	0.282863 (19)	0.048491 (10)	0.02362 (8)
O1	0.4205 (6)	0.74788 (11)	0.14589 (6)	0.0216 (4)
O2	−0.0548 (6)	0.47728 (13)	0.40035 (6)	0.0252 (5)
N2	0.0125 (7)	0.76955 (17)	0.24500 (8)	0.0298 (7)
N1	0.7019 (6)	0.61534 (15)	0.14495 (8)	0.0196 (5)
C1	1.0999 (8)	0.50365 (18)	0.09800 (9)	0.0197 (6)
H1A	1.0551	0.5618	0.0877	0.024*
C2	1.2818 (8)	0.44749 (19)	0.07176 (10)	0.0214 (7)
H2A	1.3606	0.4679	0.0442	0.026*
C3	1.3459 (7)	0.36055 (18)	0.08677 (9)	0.0191 (7)
C4	1.2361 (8)	0.32993 (19)	0.12783 (10)	0.0220 (7)
H4A	1.2821	0.2716	0.1377	0.026*
C5	1.0564 (8)	0.38691 (17)	0.15427 (9)	0.0204 (6)
H5A	0.9838	0.3665	0.1822	0.025*
C6	0.9818 (7)	0.47489 (18)	0.13976 (9)	0.0185 (7)
C7	0.7817 (7)	0.53544 (18)	0.16580 (10)	0.0178 (6)
C8	0.6704 (7)	0.51430 (19)	0.20904 (10)	0.0195 (7)
H8A	0.7262	0.4597	0.2226	0.023*
C9	0.4766 (7)	0.57403 (18)	0.23214 (9)	0.0170 (6)
C10	0.3912 (8)	0.65388 (18)	0.20974 (9)	0.0189 (6)
C11	0.5132 (7)	0.67004 (18)	0.16607 (9)	0.0186 (7)

C12	0.3562 (8)	0.55145 (19)	0.27789 (9)	0.0189 (7)
C13	0.2478 (8)	0.46338 (18)	0.28616 (10)	0.0197 (7)
H13A	0.2680	0.4192	0.2638	0.024*
C14	0.1114 (9)	0.44126 (18)	0.32705 (9)	0.0200 (7)
H14A	0.0369	0.3829	0.3318	0.024*
C15	0.0855 (9)	0.50606 (18)	0.36103 (9)	0.0199 (6)
C16	0.1977 (8)	0.5937 (2)	0.35411 (10)	0.0230 (7)
H16A	0.1834	0.6371	0.3769	0.028*
C17	0.3314 (7)	0.61494 (19)	0.31246 (10)	0.0222 (7)
H17A	0.4061	0.6733	0.3077	0.027*
C18	0.5818 (8)	0.7761 (2)	0.10480 (8)	0.0230 (6)
H18A	0.7994	0.7626	0.1081	0.028*
H18B	0.5605	0.8412	0.1012	0.028*
C19	0.4616 (8)	0.7296 (2)	0.06258 (9)	0.0284 (7)
H19A	0.5543	0.7564	0.0362	0.043*
H19B	0.2420	0.7366	0.0610	0.043*
H19C	0.5123	0.6662	0.0637	0.043*
C20	−0.1371 (8)	0.5444 (2)	0.43323 (10)	0.0243 (8)
H20A	−0.2638	0.5911	0.4195	0.029*
H20B	0.0460	0.5726	0.4458	0.029*
C21	−0.3148 (8)	0.4952 (2)	0.46998 (11)	0.0306 (8)
H21A	−0.3648	0.5368	0.4939	0.046*
H21B	−0.1911	0.4467	0.4819	0.046*
H21C	−0.5011	0.4707	0.4574	0.046*
C22	0.1818 (7)	0.7186 (2)	0.22906 (9)	0.0210 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02481 (15)	0.02126 (12)	0.02480 (13)	0.00135 (15)	−0.00071 (16)	−0.00381 (13)
O1	0.0280 (11)	0.0181 (9)	0.0186 (9)	0.0039 (10)	0.0014 (12)	0.0043 (7)
O2	0.0376 (14)	0.0207 (9)	0.0173 (9)	0.0022 (11)	0.0044 (11)	−0.0004 (8)
N2	0.040 (2)	0.0236 (13)	0.0260 (12)	0.0087 (13)	−0.0018 (12)	0.0006 (10)
N1	0.0204 (14)	0.0189 (11)	0.0195 (12)	−0.0008 (11)	−0.0024 (11)	0.0008 (9)
C1	0.0211 (16)	0.0187 (12)	0.0192 (13)	0.0005 (15)	−0.0017 (15)	0.0004 (10)
C2	0.0186 (16)	0.0227 (15)	0.0229 (15)	−0.0008 (14)	−0.0008 (14)	0.0022 (12)
C3	0.0169 (18)	0.0196 (13)	0.0209 (14)	−0.0009 (12)	−0.0019 (13)	−0.0023 (11)
C4	0.0259 (18)	0.0154 (13)	0.0246 (16)	0.0012 (13)	−0.0041 (15)	0.0017 (11)
C5	0.0233 (17)	0.0196 (13)	0.0184 (13)	0.0003 (15)	−0.0004 (15)	0.0035 (10)
C6	0.0169 (18)	0.0186 (13)	0.0199 (14)	−0.0010 (12)	−0.0061 (13)	0.0020 (11)
C7	0.0172 (16)	0.0152 (13)	0.0210 (15)	−0.0022 (12)	−0.0055 (13)	0.0014 (11)
C8	0.0186 (19)	0.0190 (14)	0.0208 (15)	0.0006 (13)	−0.0027 (13)	0.0010 (12)
C9	0.0161 (17)	0.0181 (12)	0.0167 (13)	−0.0037 (12)	−0.0049 (12)	0.0021 (10)
C10	0.0219 (16)	0.0165 (12)	0.0182 (13)	0.0004 (14)	−0.0045 (14)	−0.0016 (10)
C11	0.0203 (19)	0.0141 (12)	0.0213 (13)	−0.0008 (12)	−0.0040 (12)	0.0016 (10)
C12	0.023 (2)	0.0186 (13)	0.0157 (14)	−0.0007 (13)	−0.0018 (13)	0.0008 (10)
C13	0.0243 (17)	0.0159 (13)	0.0191 (15)	0.0034 (13)	−0.0033 (14)	−0.0017 (11)
C14	0.0243 (18)	0.0157 (13)	0.0199 (14)	0.0017 (14)	−0.0019 (15)	0.0015 (10)

C15	0.0240 (16)	0.0215 (13)	0.0140 (13)	0.0030 (16)	0.0007 (15)	0.0007 (10)
C16	0.0288 (19)	0.0214 (14)	0.0188 (15)	0.0010 (14)	−0.0027 (15)	−0.0025 (12)
C17	0.0260 (19)	0.0169 (13)	0.0237 (15)	−0.0011 (13)	−0.0053 (14)	0.0001 (11)
C18	0.0266 (15)	0.0221 (13)	0.0204 (13)	−0.0010 (18)	0.0012 (15)	0.0036 (11)
C19	0.0302 (19)	0.0321 (16)	0.0230 (13)	0.0023 (17)	0.0012 (14)	0.0030 (12)
C20	0.029 (2)	0.0276 (15)	0.0165 (13)	0.0029 (15)	0.0022 (14)	−0.0077 (11)
C21	0.033 (2)	0.0360 (18)	0.0228 (16)	−0.0011 (17)	0.0033 (15)	−0.0058 (14)
C22	0.0264 (17)	0.0196 (12)	0.0171 (13)	−0.0023 (16)	−0.0042 (12)	0.0026 (13)

Geometric parameters (Å, º)

Br1—C3	1.905 (3)	C10—C11	1.411 (4)
O1—C11	1.353 (3)	C10—C22	1.435 (4)
O1—C18	1.458 (3)	C12—C17	1.387 (4)
O2—C15	1.375 (3)	C12—C13	1.402 (4)
O2—C20	1.429 (3)	C13—C14	1.380 (4)
N2—C22	1.151 (4)	C13—H13A	0.9300
N1—C11	1.307 (4)	C14—C15	1.388 (4)
N1—C7	1.372 (3)	C14—H14A	0.9300
C1—C2	1.380 (4)	C15—C16	1.395 (4)
C1—C6	1.398 (4)	C16—C17	1.392 (4)
C1—H1A	0.9300	C16—H16A	0.9300
C2—C3	1.384 (4)	C17—H17A	0.9300
C2—H2A	0.9300	C18—C19	1.512 (4)
C3—C4	1.376 (4)	C18—H18A	0.9700
C4—C5	1.386 (4)	C18—H18B	0.9700
C4—H4A	0.9300	C19—H19A	0.9600
C5—C6	1.403 (4)	C19—H19B	0.9600
C5—H5A	0.9300	C19—H19C	0.9600
C6—C7	1.462 (4)	C20—C21	1.514 (4)
C7—C8	1.397 (4)	C20—H20A	0.9700
C8—C9	1.395 (4)	C20—H20B	0.9700
C8—H8A	0.9300	C21—H21A	0.9600
C9—C10	1.399 (4)	C21—H21B	0.9600
C9—C12	1.483 (4)	C21—H21C	0.9600
C11—O1—C18	117.6 (2)	C14—C13—H13A	119.5
C15—O2—C20	117.9 (2)	C12—C13—H13A	119.5
C11—N1—C7	118.4 (3)	C13—C14—C15	120.1 (3)
C2—C1—C6	121.4 (3)	C13—C14—H14A	120.0
C2—C1—H1A	119.3	C15—C14—H14A	120.0
C6—C1—H1A	119.3	O2—C15—C14	115.5 (2)
C1—C2—C3	119.4 (3)	O2—C15—C16	124.3 (2)
C1—C2—H2A	120.3	C14—C15—C16	120.2 (3)
C3—C2—H2A	120.3	C17—C16—C15	118.8 (3)
C4—C3—C2	121.0 (3)	C17—C16—H16A	120.6
C4—C3—Br1	120.6 (2)	C15—C16—H16A	120.6
C2—C3—Br1	118.4 (2)	C12—C17—C16	121.8 (3)

C3—C4—C5	119.3 (3)	C12—C17—H17A	119.1
C3—C4—H4A	120.3	C16—C17—H17A	119.1
C5—C4—H4A	120.3	O1—C18—C19	112.8 (3)
C4—C5—C6	121.3 (3)	O1—C18—H18A	109.0
C4—C5—H5A	119.4	C19—C18—H18A	109.0
C6—C5—H5A	119.4	O1—C18—H18B	109.0
C1—C6—C5	117.6 (3)	C19—C18—H18B	109.0
C1—C6—C7	119.6 (2)	H18A—C18—H18B	107.8
C5—C6—C7	122.8 (3)	C18—C19—H19A	109.5
N1—C7—C8	120.8 (3)	C18—C19—H19B	109.5
N1—C7—C6	116.1 (3)	H19A—C19—H19B	109.5
C8—C7—C6	123.2 (2)	C18—C19—H19C	109.5
C9—C8—C7	120.8 (3)	H19A—C19—H19C	109.5
C9—C8—H8A	119.6	H19B—C19—H19C	109.5
C7—C8—H8A	119.6	O2—C20—C21	106.2 (2)
C8—C9—C10	117.5 (3)	O2—C20—H20A	110.5
C8—C9—C12	120.9 (3)	C21—C20—H20A	110.5
C10—C9—C12	121.6 (3)	O2—C20—H20B	110.5
C9—C10—C11	118.2 (3)	C21—C20—H20B	110.5
C9—C10—C22	122.7 (3)	H20A—C20—H20B	108.7
C11—C10—C22	119.1 (2)	C20—C21—H21A	109.5
N1—C11—O1	120.1 (2)	C20—C21—H21B	109.5
N1—C11—C10	124.4 (3)	H21A—C21—H21B	109.5
O1—C11—C10	115.6 (2)	C20—C21—H21C	109.5
C17—C12—C13	118.1 (3)	H21A—C21—H21C	109.5
C17—C12—C9	122.9 (2)	H21B—C21—H21C	109.5
C13—C12—C9	118.9 (2)	N2—C22—C10	179.0 (3)
C14—C13—C12	120.9 (3)		

C6—C1—C2—C3	0.8 (5)	C7—N1—C11—C10	1.9 (4)
C1—C2—C3—C4	−1.3 (5)	C18—O1—C11—N1	−11.6 (4)
C1—C2—C3—Br1	177.1 (2)	C18—O1—C11—C10	168.9 (3)
C2—C3—C4—C5	0.6 (5)	C9—C10—C11—N1	−0.1 (5)
Br1—C3—C4—C5	−177.8 (2)	C22—C10—C11—N1	−179.0 (3)
C3—C4—C5—C6	0.6 (5)	C9—C10—C11—O1	179.4 (3)
C2—C1—C6—C5	0.4 (5)	C22—C10—C11—O1	0.5 (4)
C2—C1—C6—C7	−178.0 (3)	C8—C9—C12—C17	140.0 (3)
C4—C5—C6—C1	−1.1 (5)	C10—C9—C12—C17	−42.6 (5)
C4—C5—C6—C7	177.2 (3)	C8—C9—C12—C13	−43.3 (4)
C11—N1—C7—C8	−1.7 (4)	C10—C9—C12—C13	134.0 (3)
C11—N1—C7—C6	177.2 (3)	C17—C12—C13—C14	2.0 (5)
C1—C6—C7—N1	5.4 (4)	C9—C12—C13—C14	−174.8 (3)
C5—C6—C7—N1	−173.0 (3)	C12—C13—C14—C15	−1.3 (5)
C1—C6—C7—C8	−175.7 (3)	C20—O2—C15—C14	−169.1 (3)
C5—C6—C7—C8	5.9 (5)	C20—O2—C15—C16	10.8 (5)
N1—C7—C8—C9	−0.3 (4)	C13—C14—C15—O2	179.8 (3)
C6—C7—C8—C9	−179.1 (3)	C13—C14—C15—C16	−0.2 (5)
C7—C8—C9—C10	2.0 (4)	O2—C15—C16—C17	−179.1 (3)

C7—C8—C9—C12	179.5 (3)	C14—C15—C16—C17	0.9 (5)
C8—C9—C10—C11	−1.9 (4)	C13—C12—C17—C16	−1.3 (5)
C12—C9—C10—C11	−179.3 (3)	C9—C12—C17—C16	175.4 (3)
C8—C9—C10—C22	177.0 (3)	C15—C16—C17—C12	−0.1 (5)
C12—C9—C10—C22	−0.4 (5)	C11—O1—C18—C19	83.0 (3)
C7—N1—C11—O1	−177.6 (3)	C15—O2—C20—C21	174.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···N1	0.93	2.41	2.758 (4)	102
C5—H5*A*···N2^{i}	0.93	2.58	3.446 (4)	156
C13—H13*A*···N2^{ii}	0.93	2.53	3.206 (4)	130

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