organic compounds

2-Amino-4-(4-bromophenyl)-6-methoxy-4*H*-benzo[*h*]chromene-3-carbonitrile

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In the title compound, $C_{21}H_{15}BrN_2O_2$, the 14 non-H atoms of the 4*H*-benzo[*h*]chromene fused-ring system are approximately coplanar (r.m.s. deviation = 0.129 Å). Within this system, the 4*H*-pyran ring adopts a flattened half-chair conformation with the methine C atom lying 0.281 (4) Å above the plane of the remaining atoms (r.m.s. deviation = 0.0446 Å). The bromobenzene ring is almost perpendicular to the fused-ring system [dihedral angle = 85.34 (13)°]. In the crystal, supramolecular layers parallel to (101) are sustained by amine–cyano N—H⋯N and amine–methoxy N—H⋯O hydrogen bonds. The layers stack with interactions of the type (bromobenzene)C—H⋯π(outer-C_6 ring of the fused-ring system) connecting them.

Related literature

For background to biologically active molecules having the 4*H*-chromene or 4*H*-benzochromene residue, see: Sabry *et al.* (2011); Amin *et al.* (2010); Kidwai *et al.* (2010); Singh *et al.* (2010), For the structure of the fluoro derivative, see: Al-Dies *et al.* (2012).

Experimental

Crystal data

$C_{21}H_{15}BrN_2O_2$	$V = 1800.4$ (3) Å^3
$M_r = 407.26$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 6.0823$ (7) Å	$\mu = 2.30$ mm^{-1}
$b = 16.6918$ (18) Å	$T = 295$ K
$c = 17.7700$ (16) Å	$0.30 \times 0.10 \times 0.10$ mm
$\beta = 93.646$ (9)°	

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector	8976 measured reflections
	4144 independent reflections
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011) $T_{min} = 0.694$, $T_{max} = 1.000$	2250 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.041$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.150$	
$S = 1.03$	$\Delta\rho_{max} = 0.71$ e Å^{-3}
4144 reflections	$\Delta\rho_{min} = -0.78$ e Å^{-3}
243 parameters	
2 restraints	

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

*Cg*1 is the centroid of the C2–C7 ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯N2^i	0.88 (1)	2.22 (2)	3.059 (5)	159 (4)
N1—H2⋯O2^{ii}	0.87 (3)	2.56 (5)	3.324 (4)	147 (4)
C18—H18⋯*Cg*1^{iii}	0.93	2.87	3.528 (4)	129

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7048).

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supplementary materials

2-Amino-4-(4-bromophenyl)-6-methoxy-4*H*-benzo[*h*]chromene-3-carbonitrile

Al-anood M. Al-dies, Ahmed M. El-Agrody, Mohamed A. Al-Omar, Abd El-Galil E. Amr, Seik Weng Ng and Edward R. T. Tiekink

Comment

Nitrogen-containing heterocyclic compounds having a 4*H*-chromene or 4*H*-benzochromene residue are often found in biologically active molecules (Amin *et al.*, 2010; Kidwai *et al.*, 2010; Singh *et al.*, 2010). As part of our on-going program investigating the chemistry of 4*H*-pyran derivatives (Sabry *et al.*, 2011), we now report the synthesis of the title compound, (I), and its crystal structure.

In (I), Fig. 1, the 4*H*-pyran ring approximates a half-chair conformation with the methine-C11 atom lying 0.281 (4) Å out of the least-squares plane defined by the remaining atoms (O1,C1,C10,C12,C13) which has a r.m.s. deviation of 0.0446 Å. Nevertheless, the 14 non-hydrogen atoms comprising the sequence of three six-membered rings of the 4*H*-benzo[*h*]chromene residue approximate a plane with the r.m.s. deviation of the fitted atoms being 0.129 Å. The bromo-benzene ring forms a dihedral angle of 85.34 (13)° with this plane, indicating an almost perpendicular relationship. The methoxy group is co-planar with the ring to which it is connected as seen in the value of the C14—O2—C8—C7 torsion angle of 177.4 (3)°. The overall structure resembles closely the recently reported fluoro derivative (Al-Dies *et al.*, 2012).

In the crystal packing, amine-*N*—*H*···*N*(cyano) hydrogen bonds between centrosymmetrically related molecules lead to dimeric aggregates, stabilized by 12-membered {···HNC$_3$N}$_2$ synthons, which are connected into a supramolecular layer parallel to (1 0 1) by amine-*N*—*H*···*O*(methoxy) hydrogen bonds, Fig. 2 and Table 1. Layers stack with the main interactions between them being of the type (bromobenzene)C—H···π(outer-C$_6$ ring of the fused ring system), Fig. 3 and Table 1.

Experimental

A solution of 4-methoxy-1-naphthol (0.01 mol) in EtOH (30 ml) was treated with α-cyano-*p*-bromocinnamonitrile (0.01 mol) and piperidine (0.5 ml). The reaction mixture was heated until complete precipitation occurred (reaction time: 60 min). The solid product which formed was collected by filtration and recrystallized from ethanol to give the title compound as yellow prisms; *M*. pt: 503–504 K.

Refinement

The C-bound H atoms were geometrically placed (C—H = 0.93–0.98 Å) and refined as riding with U_{iso}(H) = 1.2–1.5U_{eq}(C). The N-bound H atoms were refined with the distance restraint N—H = 0.88±0.01 Å and with free U_{eq}.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).
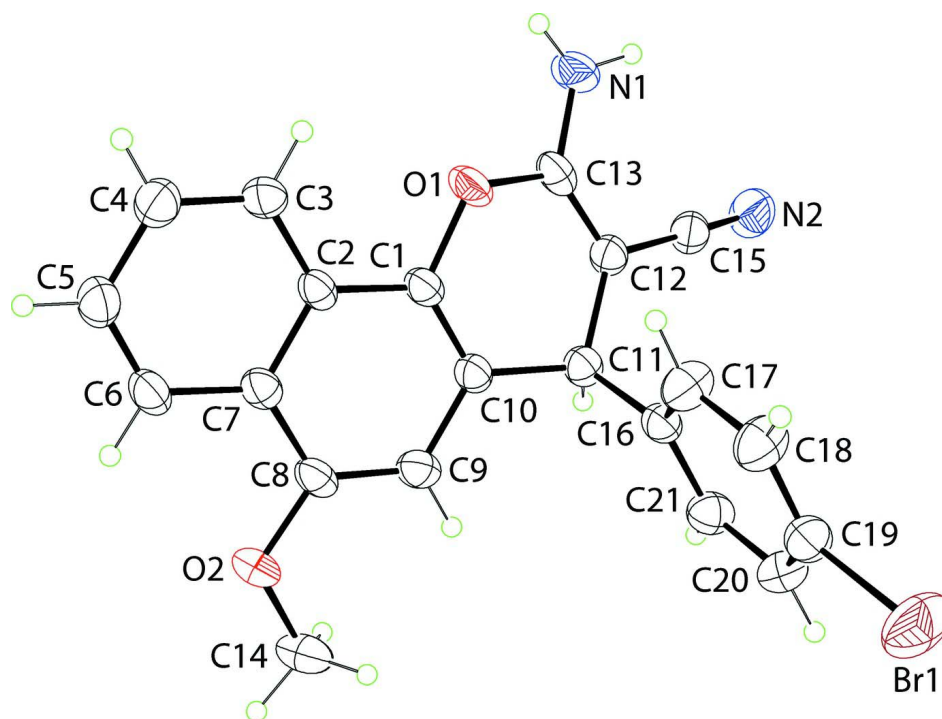
Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 35% probability level.
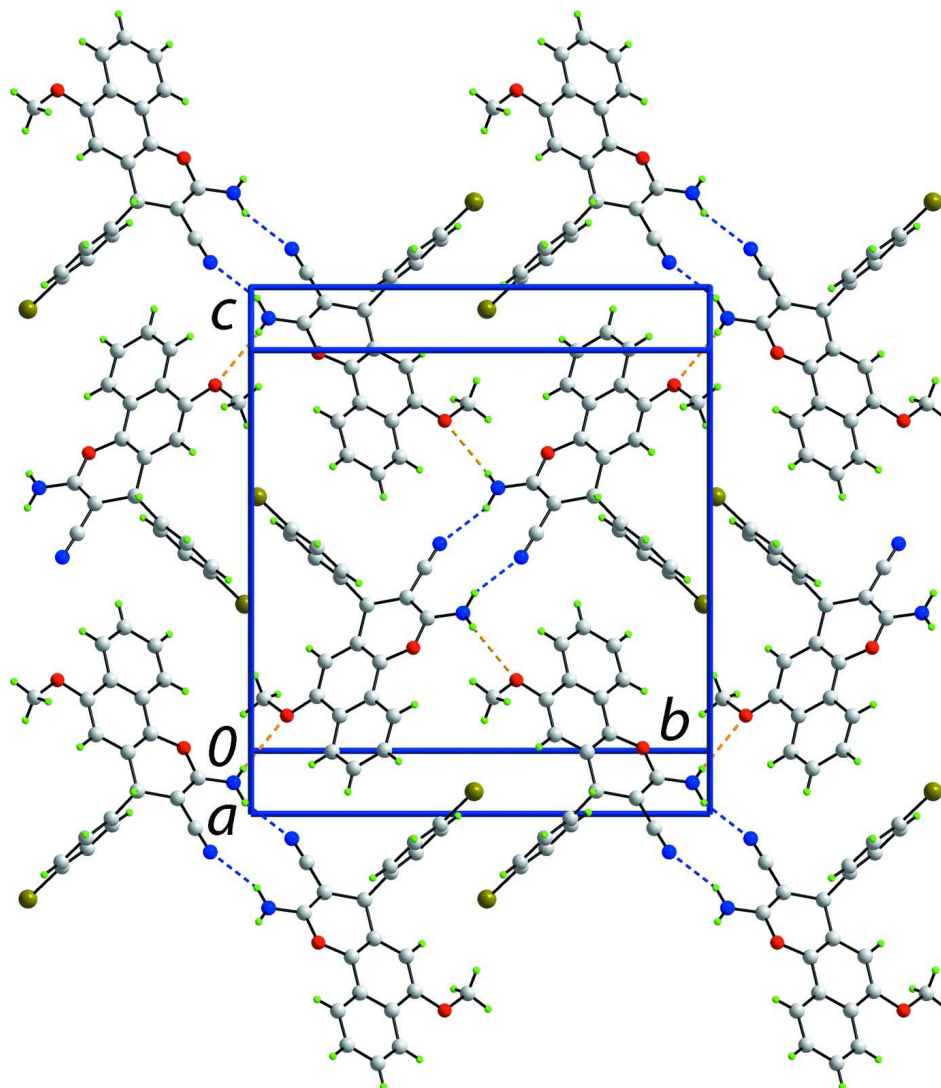
Figure 2

A view of the supramolecular layer parallel to (1 0 1) in (I). The N—H⋯N and N—H⋯O hydrogen bonds are shown as blue and orange dashed lines, respectively.

Figure 3

View in projection down the *b* axis of the crystal packing in (I). The N—H⋯N, N—H⋯O and C—H⋯π interactions are shown as blue, orange and purple dashed lines, respectively. One layer has been highlighted in space-filling mode.

2-Amino-4-(4-bromophenyl)-6-methoxy-4*H*-benzo[*h*]chromene-3-carbonitrile

Crystal data

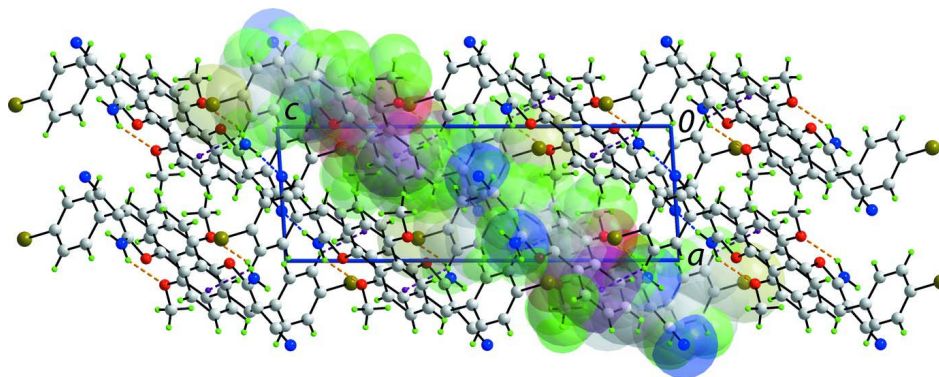|	
$C_{21}H_{15}BrN_2O_2$	$F(000) = 824$
$M_r = 407.26$	$D_x = 1.502$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1634 reflections
$a = 6.0823$ (7) Å	$\theta = 3.4$–$27.5°$
$b = 16.6918$ (18) Å	$\mu = 2.30$ mm^{-1}
$c = 17.7700$ (16) Å	$T = 295$ K
$\beta = 93.646$ (9)°	Prism, yellow
$V = 1800.4$ (3) Å^3	$0.30 \times 0.10 \times 0.10$ mm
$Z = 4$	

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector	$T_{min} = 0.694$, $T_{max} = 1.000$
	8976 measured reflections
Radiation source: SuperNova (Mo) X-ray Source	4144 independent reflections
	2250 reflections with $I > 2\sigma(I)$
Mirror monochromator	$R_{int} = 0.041$
Detector resolution: 10.4041 pixels mm^{-1}	$\theta_{max} = 27.6°$, $\theta_{min} = 3.4°$
ω scan	$h = -7 \rightarrow 7$
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)	$k = -15 \rightarrow 21$
	$l = -22 \rightarrow 23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.053$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.150$	
$S = 1.03$	H atoms treated by a mixture of independent and constrained refinement
4144 reflections	
243 parameters	$w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 0.4428P]$ where $P = (F_o^2 + 2F_c^2)/3$
2 restraints	
Primary atom site location: structure-invariant direct methods	$(\Delta/\sigma)_{max} < 0.001$
	$\Delta\rho_{max} = 0.71$ e Å^{-3}
	$\Delta\rho_{min} = -0.78$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	0.16537 (9)	0.98612 (4)	0.33868 (3)	0.0969 (3)
O1	0.0181 (4)	0.64654 (15)	0.64437 (13)	0.0504 (6)
O2	0.1773 (4)	0.92192 (15)	0.81237 (13)	0.0573 (7)
N1	0.1307 (6)	0.5382 (2)	0.5848 (2)	0.0582 (8)
H1	0.207 (7)	0.513 (3)	0.552 (2)	0.093 (17)*
H2	0.008 (4)	0.517 (3)	0.598 (3)	0.089 (17)*
N2	0.6286 (6)	0.5888 (2)	0.50299 (19)	0.0676 (9)
C1	0.0644 (5)	0.7191 (2)	0.68158 (16)	0.0393 (8)
C2	−0.0802 (5)	0.73721 (19)	0.73914 (16)	0.0375 (7)
C3	−0.2638 (6)	0.6894 (2)	0.75334 (18)	0.0453 (8)
H3	−0.2931	0.6437	0.7246	0.054*
C4	−0.3989 (6)	0.7094 (2)	0.80851 (19)	0.0520 (9)
H4	−0.5225	0.6783	0.8160	0.062*
C5	−0.3531 (6)	0.7762 (2)	0.8539 (2)	0.0547 (10)
H5	−0.4446	0.7887	0.8922	0.066*
C6	−0.1753 (6)	0.8235 (2)	0.84260 (18)	0.0500 (9)
H6	−0.1447	0.8672	0.8741	0.060*
C7	−0.0360 (5)	0.8068 (2)	0.78307 (17)	0.0405 (8)
C8	0.1447 (6)	0.8565 (2)	0.76620 (17)	0.0430 (8)
C9	0.2710 (5)	0.8382 (2)	0.70790 (18)	0.0446 (8)
H9	0.3847	0.8725	0.6964	0.054*
C10	0.2321 (5)	0.7680 (2)	0.66466 (16)	0.0390 (7)
C11	0.3774 (5)	0.7476 (2)	0.60075 (17)	0.0411 (8)
H11	0.5311	0.7556	0.6192	0.049*
C12	0.3481 (5)	0.6601 (2)	0.58086 (17)	0.0419 (8)
C13	0.1747 (6)	0.6157 (2)	0.60137 (18)	0.0455 (8)
C14	0.3613 (7)	0.9720 (2)	0.8004 (2)	0.0635 (11)
H14A	0.3620	1.0166	0.8345	0.095*
H14B	0.3509	0.9913	0.7494	0.095*
H14C	0.4949	0.9419	0.8092	0.095*
C15	0.5037 (6)	0.6215 (2)	0.53744 (19)	0.0479 (9)
C16	0.3287 (5)	0.8045 (2)	0.53448 (17)	0.0409 (8)
C17	0.1278 (6)	0.8030 (3)	0.4940 (2)	0.0577 (10)
H17	0.0232	0.7651	0.5058	0.069*
C18	0.0789 (6)	0.8566 (3)	0.4364 (2)	0.0627 (11)
H18	−0.0580	0.8551	0.4100	0.075*
C19	0.2331 (7)	0.9121 (2)	0.41810 (19)	0.0549 (10)

C20	0.4365 (6)	0.9136 (2)	0.4556 (2)	0.0581 (10)
H20	0.5421	0.9504	0.4423	0.070*
C21	0.4832 (6)	0.8596 (2)	0.51378 (19)	0.0505 (9)
H21	0.6214	0.8606	0.5394	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1155 (5)	0.0841 (4)	0.0888 (4)	−0.0019 (3)	−0.0114 (3)	0.0431 (3)
O1	0.0523 (13)	0.0429 (15)	0.0572 (13)	−0.0032 (11)	0.0139 (11)	−0.0239 (12)
O2	0.0760 (17)	0.0383 (15)	0.0578 (14)	−0.0057 (13)	0.0074 (12)	−0.0170 (12)
N1	0.063 (2)	0.0407 (19)	0.073 (2)	−0.0020 (17)	0.0213 (18)	−0.0202 (17)
N2	0.079 (2)	0.054 (2)	0.073 (2)	0.0104 (19)	0.0324 (18)	0.0012 (18)
C1	0.0484 (19)	0.0320 (18)	0.0372 (16)	0.0036 (15)	0.0016 (15)	−0.0055 (14)
C2	0.0478 (18)	0.0313 (17)	0.0333 (15)	0.0080 (15)	0.0011 (14)	−0.0027 (14)
C3	0.056 (2)	0.0330 (19)	0.0466 (19)	0.0026 (16)	0.0040 (16)	0.0014 (16)
C4	0.056 (2)	0.049 (2)	0.053 (2)	0.0027 (18)	0.0115 (18)	0.0047 (18)
C5	0.066 (2)	0.050 (2)	0.050 (2)	0.008 (2)	0.0177 (18)	−0.0008 (18)
C6	0.070 (2)	0.039 (2)	0.0417 (18)	0.0098 (19)	0.0078 (17)	−0.0074 (16)
C7	0.0516 (19)	0.0335 (18)	0.0361 (16)	0.0076 (16)	−0.0003 (15)	0.0001 (14)
C8	0.057 (2)	0.0304 (18)	0.0404 (17)	0.0094 (16)	−0.0021 (16)	−0.0060 (15)
C9	0.0510 (19)	0.0344 (19)	0.0482 (19)	0.0006 (16)	0.0011 (16)	−0.0017 (15)
C10	0.0486 (18)	0.0333 (18)	0.0353 (16)	0.0043 (16)	0.0041 (14)	−0.0009 (14)
C11	0.0445 (18)	0.040 (2)	0.0390 (17)	0.0029 (16)	0.0023 (14)	−0.0008 (15)
C12	0.0511 (19)	0.0356 (19)	0.0397 (17)	0.0065 (16)	0.0087 (15)	0.0006 (15)
C13	0.056 (2)	0.041 (2)	0.0400 (17)	0.0097 (18)	0.0032 (16)	−0.0114 (16)
C14	0.066 (2)	0.041 (2)	0.083 (3)	−0.005 (2)	0.000 (2)	−0.016 (2)
C15	0.063 (2)	0.037 (2)	0.0444 (18)	0.0100 (18)	0.0124 (17)	0.0034 (16)
C16	0.0457 (18)	0.0371 (19)	0.0399 (17)	0.0018 (16)	0.0032 (15)	−0.0047 (15)
C17	0.052 (2)	0.062 (3)	0.059 (2)	−0.0083 (19)	−0.0018 (18)	0.013 (2)
C18	0.057 (2)	0.071 (3)	0.059 (2)	−0.005 (2)	−0.0058 (19)	0.015 (2)
C19	0.076 (3)	0.043 (2)	0.0458 (19)	0.004 (2)	−0.0022 (19)	0.0060 (17)
C20	0.066 (2)	0.047 (2)	0.062 (2)	−0.014 (2)	0.008 (2)	0.0042 (19)
C21	0.051 (2)	0.047 (2)	0.053 (2)	−0.0032 (18)	−0.0037 (17)	−0.0006 (18)

Geometric parameters (Å, º)

Br1—C19	1.901 (3)	C8—C9	1.363 (5)
O1—C13	1.360 (4)	C9—C10	1.413 (4)
O1—C1	1.399 (4)	C9—H9	0.9300
O2—C8	1.372 (4)	C10—C11	1.521 (4)
O2—C14	1.423 (5)	C11—C12	1.510 (5)
N1—C13	1.349 (5)	C11—C16	1.528 (4)
N1—H1	0.877 (10)	C11—H11	0.9800
N1—H2	0.874 (10)	C12—C13	1.357 (5)
N2—C15	1.144 (4)	C12—C15	1.414 (5)
C1—C10	1.355 (5)	C14—H14A	0.9600
C1—C2	1.423 (4)	C14—H14B	0.9600
C2—C3	1.408 (5)	C14—H14C	0.9600
C2—C7	1.416 (4)	C16—C17	1.378 (5)

C3—C4	1.360 (5)	C16—C21	1.382 (5)
C3—H3	0.9300	C17—C18	1.378 (5)
C4—C5	1.395 (5)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.372 (5)
C5—C6	1.364 (5)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.368 (5)
C6—C7	1.424 (5)	C20—C21	1.387 (5)
C6—H6	0.9300	C20—H20	0.9300
C7—C8	1.424 (5)	C21—H21	0.9300
C13—O1—C1	117.8 (3)	C12—C11—C16	114.0 (3)
C8—O2—C14	117.6 (3)	C10—C11—C16	110.1 (3)
C13—N1—H1	120 (3)	C12—C11—H11	107.8
C13—N1—H2	120 (3)	C10—C11—H11	107.8
H1—N1—H2	118 (5)	C16—C11—H11	107.8
C10—C1—O1	123.2 (3)	C13—C12—C15	117.1 (3)
C10—C1—C2	122.6 (3)	C13—C12—C11	123.2 (3)
O1—C1—C2	114.1 (3)	C15—C12—C11	119.7 (3)
C3—C2—C7	119.4 (3)	N1—C13—C12	127.7 (3)
C3—C2—C1	122.8 (3)	N1—C13—O1	110.5 (3)
C7—C2—C1	117.8 (3)	C12—C13—O1	121.9 (3)
C4—C3—C2	120.9 (3)	O2—C14—H14A	109.5
C4—C3—H3	119.6	O2—C14—H14B	109.5
C2—C3—H3	119.6	H14A—C14—H14B	109.5
C3—C4—C5	120.3 (4)	O2—C14—H14C	109.5
C3—C4—H4	119.8	H14A—C14—H14C	109.5
C5—C4—H4	119.8	H14B—C14—H14C	109.5
C6—C5—C4	120.6 (3)	N2—C15—C12	178.6 (4)
C6—C5—H5	119.7	C17—C16—C21	117.9 (3)
C4—C5—H5	119.7	C17—C16—C11	120.8 (3)
C5—C6—C7	120.7 (3)	C21—C16—C11	121.2 (3)
C5—C6—H6	119.7	C18—C17—C16	121.2 (4)
C7—C6—H6	119.7	C18—C17—H17	119.4
C2—C7—C8	119.0 (3)	C16—C17—H17	119.4
C2—C7—C6	118.0 (3)	C19—C18—C17	119.8 (3)
C8—C7—C6	123.1 (3)	C19—C18—H18	120.1
C9—C8—O2	124.5 (3)	C17—C18—H18	120.1
C9—C8—C7	120.6 (3)	C20—C19—C18	120.5 (3)
O2—C8—C7	114.9 (3)	C20—C19—Br1	119.7 (3)
C8—C9—C10	121.1 (3)	C18—C19—Br1	119.7 (3)
C8—C9—H9	119.5	C19—C20—C21	119.1 (4)
C10—C9—H9	119.5	C19—C20—H20	120.4
C1—C10—C9	118.8 (3)	C21—C20—H20	120.4
C1—C10—C11	120.8 (3)	C16—C21—C20	121.4 (3)
C9—C10—C11	120.4 (3)	C16—C21—H21	119.3
C12—C11—C10	109.0 (3)	C20—C21—H21	119.3
C13—O1—C1—C10	14.6 (4)	C8—C9—C10—C11	−178.8 (3)
C13—O1—C1—C2	−165.3 (3)	C1—C10—C11—C12	−17.0 (4)

C10—C1—C2—C3	175.4 (3)	C9—C10—C11—C12	162.5 (3)
O1—C1—C2—C3	−4.7 (4)	C1—C10—C11—C16	108.7 (3)
C10—C1—C2—C7	−4.1 (4)	C9—C10—C11—C16	−71.8 (4)
O1—C1—C2—C7	175.8 (3)	C10—C11—C12—C13	17.6 (4)
C7—C2—C3—C4	0.1 (5)	C16—C11—C12—C13	−105.8 (3)
C1—C2—C3—C4	−179.4 (3)	C10—C11—C12—C15	−163.8 (3)
C2—C3—C4—C5	−2.3 (5)	C16—C11—C12—C15	72.8 (4)
C3—C4—C5—C6	1.5 (5)	C15—C12—C13—N1	−0.6 (5)
C4—C5—C6—C7	1.6 (5)	C11—C12—C13—N1	178.1 (3)
C3—C2—C7—C8	−177.4 (3)	C15—C12—C13—O1	178.7 (3)
C1—C2—C7—C8	2.1 (4)	C11—C12—C13—O1	−2.7 (5)
C3—C2—C7—C6	2.8 (4)	C1—O1—C13—N1	165.0 (3)
C1—C2—C7—C6	−177.7 (3)	C1—O1—C13—C12	−14.4 (4)
C5—C6—C7—C2	−3.7 (5)	C12—C11—C16—C17	56.2 (4)
C5—C6—C7—C8	176.6 (3)	C10—C11—C16—C17	−66.6 (4)
C14—O2—C8—C9	−2.8 (5)	C12—C11—C16—C21	−124.5 (3)
C14—O2—C8—C7	177.4 (3)	C10—C11—C16—C21	112.6 (4)
C2—C7—C8—C9	1.1 (5)	C21—C16—C17—C18	−2.2 (6)
C6—C7—C8—C9	−179.1 (3)	C11—C16—C17—C18	177.0 (3)
C2—C7—C8—O2	−179.0 (3)	C16—C17—C18—C19	0.7 (6)
C6—C7—C8—O2	0.7 (4)	C17—C18—C19—C20	1.3 (6)
O2—C8—C9—C10	177.5 (3)	C17—C18—C19—Br1	−179.9 (3)
C7—C8—C9—C10	−2.6 (5)	C18—C19—C20—C21	−1.7 (6)
O1—C1—C10—C9	−177.2 (3)	Br1—C19—C20—C21	179.6 (3)
C2—C1—C10—C9	2.7 (5)	C17—C16—C21—C20	1.9 (5)
O1—C1—C10—C11	2.3 (5)	C11—C16—C21—C20	−177.3 (3)
C2—C1—C10—C11	−177.8 (3)	C19—C20—C21—C16	0.0 (6)
C8—C9—C10—C1	0.7 (5)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N2[i]	0.88 (1)	2.22 (2)	3.059 (5)	159 (4)
N1—H2···O2[ii]	0.87 (3)	2.56 (5)	3.324 (4)	147 (4)
C18—H18···*Cg*1[iii]	0.93	2.87	3.528 (4)	129

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, *y*−1/2, −*z*+3/2; (iii) *x*, −*y*+3/2, *z*−1/2.