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#### Key indicators

Single-crystal X-ray study  
 $T = 120$  K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.032  
 $wR$  factor = 0.080  
 Data-to-parameter ratio = 16.6

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

## 4-Bromo- $\beta$ -(2-oxoquinolin-4-yloxy)cinnamionitrile: a three-dimensional framework structure built from $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, and bromo-carbonyl and aromatic $\pi-\pi$ stacking interactions

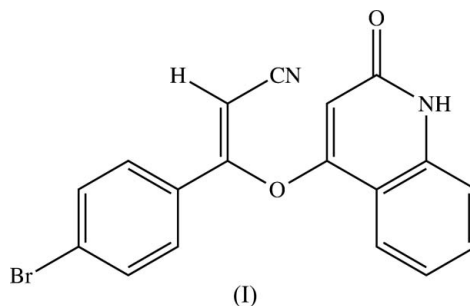
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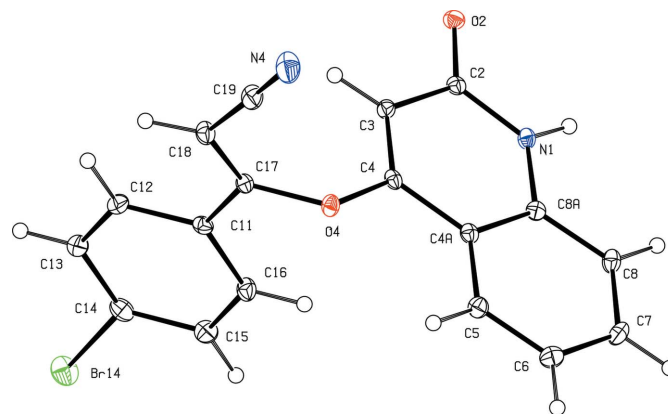
In the title compound,  $\text{C}_{18}\text{H}_{11}\text{BrN}_2\text{O}_2$ , the molecules are linked into sheets by a combination of one  $\text{N}-\text{H}\cdots\text{O}$  and two  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, and the sheets are linked by an aromatic  $\pi-\pi$  stacking interaction.

#### Comment

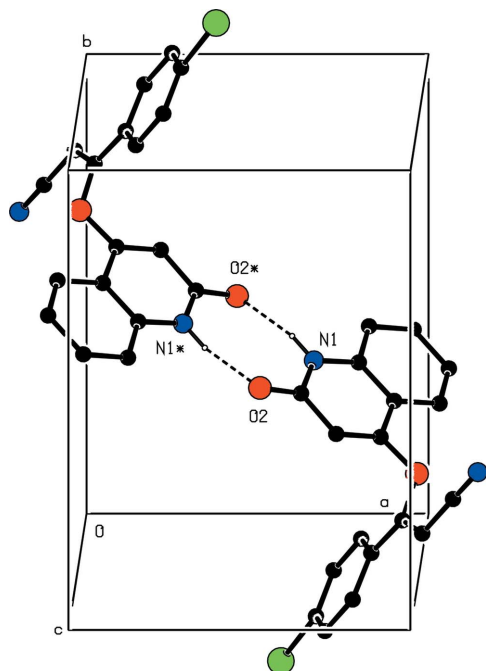
The title compound, (I), has been prepared from 2,4-dihydroxyquinoline and 4-bromo- $\beta$ -chlorocinnamionitrile as a potential intermediate for the synthesis of fused quinoline derivatives.



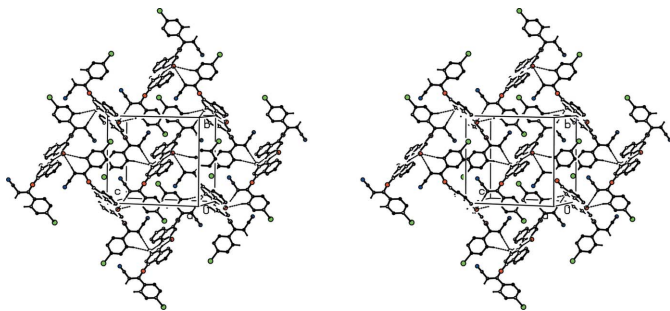
The molecules of compound (I) show a significant deviation from planarity, as shown by the key torsion angles (Table 1). The biggest deviation from planarity is associated with the rotation of the two effectively planar components of the molecule about the  $\text{O}4-\text{C}17$  bond, which is probably driven by the repulsive interaction between the cyano substituent and the H atom bonded to C3 (Fig. 1). Consistent with this, the bond angle at O4 is abnormally large.



**Figure 1**  
 The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.



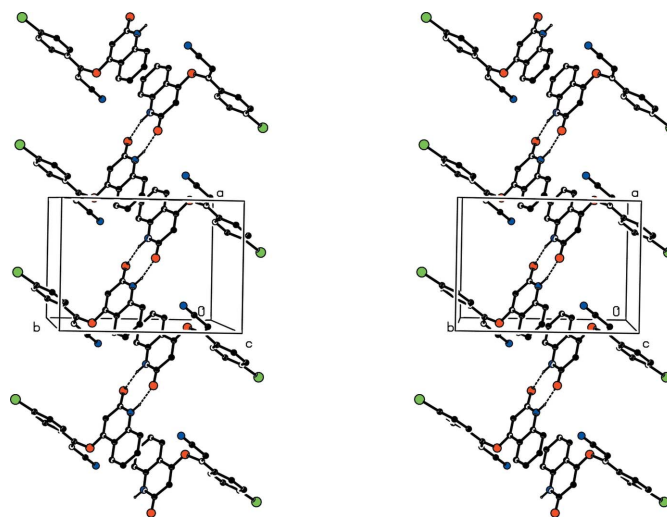
**Figure 2**  
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded  $R_2^2(8)$  dimer. Dashed lines indicate hydrogen bonds. For the sake of clarity, H atoms bonded to C atoms have been omitted. Atoms marked with an asterisk (\*) are at the symmetry position  $(1 - x, 1 - y, 1 - z)$ .



**Figure 3**  
A stereoscopic view of part of the crystal structure of (I), showing the formation of a hydrogen-bonded  $(10\bar{1})$  sheet. Dashed lines indicate hydrogen bonds. For the sake of clarity, H atoms not involved in the motifs shown have been omitted.

While the C—C distances within the brominated aryl ring span only a rather narrow range [1.383 (3) – 1.400 (3) Å with mean value 1.389 Å], the distances in the other carbocyclic ring show evidence of some bond fixation, with bonds C5—C6 and C7—C8 significantly shorter than the remainder.

The molecules of compound (I) are linked by paired N—H...O hydrogen bonds (Table 2) into centrosymmetric  $R_2^2(8)$  (Bernstein *et al.*, 1995) dimers, and the reference molecule was selected so that it forms part of a dimer centred at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  (Fig. 2). Atoms C12 and C18 in the molecule at  $(x, y, z)$  both act as hydrogen bond donors to atom O2 in the molecule at  $(\frac{3}{2} - x, -\frac{1}{2} + y, \frac{3}{2} - z)$ , in an  $R_1^1(7)$  motif. Propagation by the space group of these interactions then links the dimer centred at  $(1/2, 1/2, 1/2)$  as donor to those centred at  $(1, 0, 1)$  and  $(0, 1, 0)$ , and as acceptor from those centred at  $(0, 0, 0)$  and  $(1, 1, 1)$ ,



**Figure 4**  
A stereoscopic view of part of the crystal structure of (I), showing the formation of a  $\pi$ -stacked chain of hydrogen-bonded dimers along  $[100]$ , linking the  $(10\bar{1})$  sheets. Dashed lines indicate hydrogen bonds. For the sake of clarity, H atoms bonded to C atoms have been omitted.

thereby forming a  $(10\bar{1})$  sheet built from  $R_2^1(7)$ ,  $R_2^2(8)$  and  $R_6^6(36)$  rings (Fig. 3).

The rings C4A/C5–C8/C8A in the molecules at  $(x, y, z)$  and  $(2 - x, 1 - y, 1 - z)$  form parts of the  $R_2^2(8)$  dimers centred at  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  and  $(\frac{3}{2}, \frac{1}{2}, \frac{1}{2})$ , respectively. These rings are strictly parallel with an interplanar spacing of 3.439 (2) Å: the corresponding ring-centroid separation is 3.799 (2) and the ring offset is 1.614 (2) Å. The effect of this interaction is to link the sheets along the  $[100]$  direction (Fig. 4), so forming a continuous three-dimensional structure.

The Br atom at  $(x, y, z)$  makes a short contact with the amide atom O2 in the molecule at  $(1 - x, -y, 1 - z)$ , with  $\text{Br} \cdots \text{O}^{\text{iii}} = 3.078 (2)$  Å and  $\text{C} - \text{Br} \cdots \text{O}^{\text{iii}} = 164.3 (2)^\circ$  [symmetry code: (iii)  $1 - x, -y, 1 - z$ ] and this weakly attractive bromo–carbonyl interaction links the hydrogen-bonded dimers into a chain of edge-fused  $R_2^2(8)$  and  $R_2^2(22)$  rings (Bernstein *et al.*, 1995; Starbuck *et al.*, 1999) along  $[010]$ , further reinforcing the framework (Fig. 5).

## Experimental

A solution containing 4-bromo- $\beta$ -chlorocinnamionitrile (1 mmol), 2,4-dihydroxyquinoline (1 mmol) and triethylamine (0.5 ml) in anhydrous ethanol (10 ml) was heated under reflux for 10 h. The resulting solid product was collected by filtration, washed with ethanol and recrystallized from ethanol to give pale-yellow crystals suitable for single-crystal X-ray diffraction (m.p. 582 K, yield 60%).

### Crystal data

$\text{C}_{18}\text{H}_{11}\text{BrN}_2\text{O}_2$   
 $M_r = 367.20$   
 Monoclinic,  $P2_1/n$   
 $a = 8.9860 (2)$  Å  
 $b = 12.4111 (3)$  Å  
 $c = 13.6138 (3)$  Å  
 $\beta = 92.006 (2)^\circ$   
 $V = 1517.36 (6)$  Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.607 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 $\mu = 2.72 \text{ mm}^{-1}$   
 $T = 120 (2)$  K  
 Block, pale yellow  
 $0.70 \times 0.50 \times 0.30$  mm

Data collection

Bruker–Nonius KappaCCD diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.224$ ,  $T_{\max} = 0.441$

17684 measured reflections  
 3463 independent reflections  
 2907 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.034$   
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.080$   
 $S = 1.16$   
 3463 reflections  
 208 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 1.024P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.36 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.68 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

C4–C5	1.404 (3)	C7–C8	1.375 (3)
C5–C6	1.372 (3)	C8–C8A	1.404 (3)
C6–C7	1.403 (3)	C8A–C4A	1.400 (3)
C4–O4–C17	119.34 (15)		
C3–C4–O4–C17	26.0 (3)	C4–O4–C17–C11	68.3 (2)
C4–O4–C17–C18	−118.0 (2)	O4–C17–C11–C12	−176.79 (18)

Table 2

Hydrogen-bond geometry (Å, °).

D–H...A	D–H	H...A	D...A	D–H...A
N1–H1...O2 <sup>i</sup>	0.88	1.96	2.814 (2)	164
C12–H12...O2 <sup>ii</sup>	0.95	2.52	3.435 (2)	163
C18–H18...O2 <sup>ii</sup>	0.95	2.44	3.389 (3)	178

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

All H atoms were located in difference maps and then treated as riding atoms with C–H = 0.95 Å and N–H = 0.88 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ .

Data collection: COLLECT (Hooft, 1999); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SIR2004 (Burla et al., 2005); program(s) used to refine structure: OSCAIL (McArdle, 2003) and SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PRPKAPPA (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. JC and JT thanks the Consejería de Innovación, Ciencia y

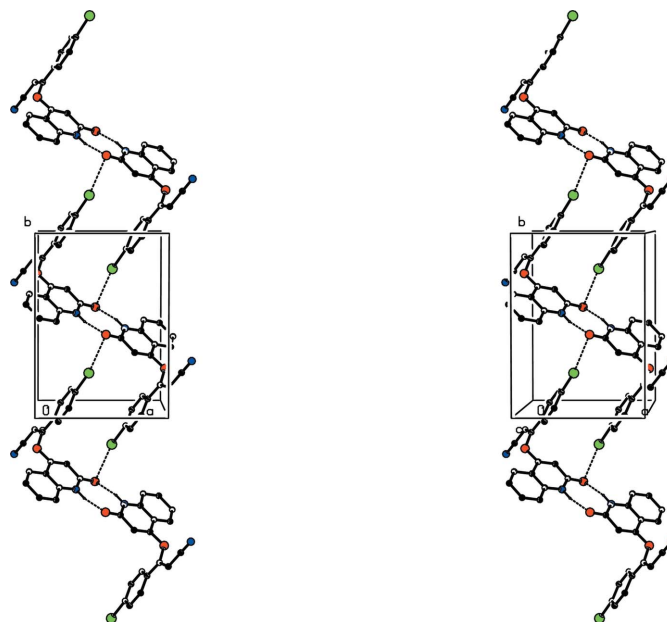


Figure 5

A stereoscopic view of part of the crystal structure of (I), showing the formation of a [010] chain of edge-fused rings formed by hydrogen-bonded dimers linked by the Br...O contact. Dashed lines indicate hydrogen bonds and Br...O contacts. For the sake of clarity, H atoms bonded to C atoms have been omitted.

Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. JT also thanks the Universidad de Jaén for a research scholarship supporting a short stay at the EPSRC X-ray Crystallographic Service, University of Southampton, England. SC thanks UDENAR (Universidad de Nariño, Colombia) for financial support.

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## supporting information

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## 4-Bromo- $\beta$ -(2-oxoquinolin-4-yloxy)cinnamionitrile: a three-dimensional framework structure built from N—H $\cdots$ O and C—H $\cdots$ O hydrogen bonds, and bromo–carbonyl and aromatic $\pi$ – $\pi$ stacking interactions

Silvia Cruz, José M. de la Torre, Justo Cobo, John N. Low and Christopher Glidewell

### 4-Bromo- $\beta$ -(2-oxoquinolin-4-yloxy)cinnamionitrile

#### Crystal data

C<sub>18</sub>H<sub>11</sub>BrN<sub>2</sub>O<sub>2</sub>

$M_r = 367.20$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 8.9860$  (2) Å

$b = 12.4111$  (3) Å

$c = 13.6138$  (3) Å

$\beta = 92.006$  (2)°

$V = 1517.36$  (6) Å<sup>3</sup>

$Z = 4$

$F(000) = 736$

$D_x = 1.607$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3463 reflections

$\theta = 3.1$ – $27.5$ °

$\mu = 2.72$  mm<sup>-1</sup>

$T = 120$  K

Block, colourless

$0.70 \times 0.50 \times 0.30$  mm

#### Data collection

Bruker–Nonius KappaCCD  
diffractometer

Radiation source: Bruker–Nonius FR591  
rotating anode

Graphite monochromator

Detector resolution: 9.091 pixels mm<sup>-1</sup>

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 2003)

$T_{\min} = 0.224$ ,  $T_{\max} = 0.441$

17684 measured reflections

3463 independent reflections

2907 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 3.1$ °

$h = -11 \rightarrow 11$

$k = -16 \rightarrow 15$

$l = -17 \rightarrow 17$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.080$

$S = 1.16$

3463 reflections

208 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

$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 1.024P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.36$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.68$  e Å<sup>-3</sup>

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.69050 (18)	0.45629 (14)	0.48541 (12)	0.0153 (3)
C2	0.6573 (2)	0.40615 (16)	0.57075 (14)	0.0145 (4)
O2	0.53963 (15)	0.42863 (12)	0.61305 (10)	0.0175 (3)
C3	0.7623 (2)	0.32710 (16)	0.60798 (15)	0.0152 (4)
C4	0.8893 (2)	0.30846 (16)	0.56033 (14)	0.0140 (4)
O4	0.99737 (15)	0.23650 (12)	0.59192 (10)	0.0163 (3)
C4A	0.9243 (2)	0.36467 (16)	0.47165 (15)	0.0145 (4)
C5	1.0543 (2)	0.34596 (17)	0.42009 (15)	0.0179 (4)
C6	1.0770 (2)	0.40041 (18)	0.33419 (16)	0.0217 (5)
C7	0.9722 (2)	0.47594 (18)	0.29849 (15)	0.0204 (4)
C8	0.8443 (2)	0.49569 (17)	0.34809 (15)	0.0180 (4)
C8A	0.8191 (2)	0.43912 (16)	0.43525 (14)	0.0146 (4)
C11	0.8644 (2)	0.06677 (16)	0.60203 (15)	0.0155 (4)
C12	0.8128 (2)	-0.02104 (17)	0.65539 (15)	0.0193 (4)
C13	0.7290 (3)	-0.10121 (18)	0.60951 (16)	0.0225 (5)
C14	0.6977 (2)	-0.09451 (18)	0.50928 (17)	0.0213 (5)
Br14	0.59176 (3)	-0.207817 (19)	0.445430 (18)	0.02971 (9)
C15	0.7466 (2)	-0.00827 (18)	0.45473 (16)	0.0212 (5)
C16	0.8295 (2)	0.07214 (17)	0.50110 (16)	0.0192 (4)
C17	0.9581 (2)	0.14977 (16)	0.64989 (15)	0.0155 (4)
C18	1.0206 (2)	0.14423 (17)	0.74090 (16)	0.0195 (4)
C19	1.1128 (3)	0.22890 (18)	0.77929 (16)	0.0235 (5)
H1	0.6256	0.5028	0.4605	0.018*
H3	0.7423	0.2880	0.6661	0.018*
H5	1.1264	0.2958	0.4446	0.021*
H6	1.1642	0.3869	0.2986	0.026*
H7	0.9898	0.5139	0.2394	0.025*
H8	0.7739	0.5470	0.3237	0.022*
H12	0.8354	-0.0257	0.7239	0.023*
H13	0.6934	-0.1603	0.6463	0.027*
H15	0.7236	-0.0043	0.3862	0.025*
H16	0.8630	0.1317	0.4640	0.023*
H18	1.0030	0.0827	0.7804	0.023*
N4	1.1869 (3)	0.29569 (16)	0.81204 (16)	0.0334 (5)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0154 (8)	0.0145 (8)	0.0157 (8)	0.0024 (7)	-0.0023 (7)	0.0027 (7)
C2	0.0162 (9)	0.0134 (9)	0.0138 (10)	-0.0011 (8)	-0.0018 (7)	-0.0023 (8)
O2	0.0176 (7)	0.0191 (7)	0.0158 (7)	0.0037 (6)	0.0005 (6)	-0.0010 (6)
C3	0.0189 (10)	0.0141 (9)	0.0125 (10)	-0.0004 (8)	-0.0010 (8)	0.0004 (8)
C4	0.0165 (10)	0.0107 (9)	0.0146 (10)	-0.0001 (7)	-0.0045 (8)	-0.0014 (7)
O4	0.0151 (7)	0.0164 (7)	0.0171 (7)	0.0026 (6)	-0.0016 (6)	0.0044 (6)
C4A	0.0156 (10)	0.0124 (9)	0.0153 (10)	-0.0019 (8)	-0.0023 (8)	-0.0011 (8)

C5	0.0180 (10)	0.0185 (10)	0.0170 (10)	0.0014 (8)	-0.0015 (8)	0.0009 (8)
C6	0.0199 (10)	0.0247 (11)	0.0208 (11)	-0.0005 (9)	0.0035 (8)	-0.0004 (9)
C7	0.0246 (11)	0.0225 (11)	0.0141 (10)	-0.0058 (9)	0.0007 (8)	0.0041 (8)
C8	0.0192 (10)	0.0167 (10)	0.0179 (10)	-0.0018 (8)	-0.0038 (8)	0.0034 (8)
C8A	0.0151 (9)	0.0146 (9)	0.0138 (10)	-0.0029 (8)	-0.0027 (7)	-0.0020 (8)
C11	0.0151 (9)	0.0164 (10)	0.0148 (10)	0.0045 (8)	-0.0015 (8)	-0.0018 (8)
C12	0.0234 (10)	0.0203 (11)	0.0141 (10)	-0.0005 (9)	0.0010 (8)	0.0001 (8)
C13	0.0278 (11)	0.0186 (11)	0.0214 (11)	-0.0013 (9)	0.0056 (9)	0.0001 (9)
C14	0.0181 (10)	0.0191 (11)	0.0267 (12)	0.0005 (8)	-0.0016 (8)	-0.0047 (9)
Br14	0.02947 (14)	0.02552 (14)	0.03352 (15)	-0.00713 (10)	-0.00755 (10)	-0.00544 (10)
C15	0.0231 (11)	0.0231 (11)	0.0170 (11)	0.0021 (9)	-0.0057 (8)	-0.0016 (9)
C16	0.0212 (10)	0.0171 (10)	0.0191 (11)	0.0020 (8)	-0.0031 (8)	0.0031 (8)
C17	0.0168 (10)	0.0139 (10)	0.0159 (10)	0.0045 (8)	0.0008 (8)	0.0020 (8)
C18	0.0238 (11)	0.0156 (10)	0.0187 (11)	0.0000 (8)	-0.0039 (8)	0.0014 (8)
C19	0.0321 (12)	0.0218 (11)	0.0162 (11)	0.0031 (10)	-0.0071 (9)	0.0023 (9)
N4	0.0487 (13)	0.0248 (11)	0.0256 (11)	-0.0043 (10)	-0.0136 (10)	0.0017 (9)

*Geometric parameters (Å, °)*

N1—C2	1.360 (3)	C8A—C4A	1.400 (3)
N1—C8A	1.379 (3)	C8—H8	0.95
N1—H1	0.88	C11—C12	1.398 (3)
C2—O2	1.253 (2)	C11—C16	1.400 (3)
C2—C3	1.441 (3)	C11—C17	1.468 (3)
C3—C4	1.352 (3)	C12—C13	1.383 (3)
C3—H3	0.95	C12—H12	0.95
C4—O4	1.377 (2)	C13—C14	1.386 (3)
C4—C4A	1.439 (3)	C13—H13	0.95
O4—C17	1.388 (2)	C14—C15	1.383 (3)
C4A—C5	1.404 (3)	C14—Br14	1.892 (2)
C5—C6	1.372 (3)	C15—C16	1.384 (3)
C5—H5	0.95	C15—H15	0.95
C6—C7	1.403 (3)	C16—H16	0.95
C6—H6	0.95	C17—C18	1.344 (3)
C7—C8	1.375 (3)	C18—C19	1.426 (3)
C7—H7	0.95	C18—H18	0.95
C8—C8A	1.404 (3)	C19—N4	1.144 (3)
C2—N1—C8A	124.39 (17)	N1—C8A—C4A	119.59 (18)
C2—N1—H1	117.8	N1—C8A—C8	120.28 (18)
C8A—N1—H1	117.8	C4A—C8A—C8	120.13 (19)
O2—C2—N1	120.30 (18)	C12—C11—C16	118.67 (19)
O2—C2—C3	122.87 (19)	C12—C11—C17	120.80 (18)
N1—C2—C3	116.83 (18)	C16—C11—C17	120.49 (19)
C4—C3—C2	120.07 (19)	C13—C12—C11	120.76 (19)
C4—C3—H3	120.0	C13—C12—H12	119.6
C2—C3—H3	120.0	C11—C12—H12	119.6
C3—C4—O4	123.99 (18)	C12—C13—C14	119.3 (2)

C3—C4—C4A	122.18 (18)	C12—C13—H13	120.3
O4—C4—C4A	113.83 (17)	C14—C13—H13	120.3
C4—O4—C17	119.34 (15)	C15—C14—C13	121.2 (2)
C8A—C4A—C5	119.73 (19)	C15—C14—Br14	119.51 (16)
C8A—C4A—C4	116.89 (18)	C13—C14—Br14	119.29 (17)
C5—C4A—C4	123.35 (18)	C14—C15—C16	119.3 (2)
C6—C5—C4A	119.72 (19)	C14—C15—H15	120.4
C6—C5—H5	120.1	C16—C15—H15	120.4
C4A—C5—H5	120.1	C15—C16—C11	120.8 (2)
C5—C6—C7	120.4 (2)	C15—C16—H16	119.6
C5—C6—H6	119.8	C11—C16—H16	119.6
C7—C6—H6	119.8	C18—C17—O4	117.23 (18)
C8—C7—C6	120.7 (2)	C18—C17—C11	125.99 (19)
C8—C7—H7	119.6	O4—C17—C11	116.43 (17)
C6—C7—H7	119.6	C17—C18—C19	121.3 (2)
C7—C8—C8A	119.24 (19)	C17—C18—H18	119.4
C7—C8—H8	120.4	C19—C18—H18	119.4
C8A—C8—H8	120.4	N4—C19—C18	178.5 (2)
C8A—N1—C2—O2	178.04 (18)	C4—C4A—C8A—C8	-178.90 (18)
C8A—N1—C2—C3	-2.5 (3)	C7—C8—C8A—N1	-178.94 (18)
O2—C2—C3—C4	-178.26 (18)	C7—C8—C8A—C4A	0.9 (3)
N1—C2—C3—C4	2.3 (3)	C16—C11—C12—C13	0.1 (3)
C2—C3—C4—O4	178.32 (17)	C17—C11—C12—C13	-177.63 (19)
C2—C3—C4—C4A	-0.6 (3)	C11—C12—C13—C14	0.7 (3)
C3—C4—O4—C17	26.0 (3)	C12—C13—C14—C15	-1.0 (3)
C4A—C4—O4—C17	-155.03 (17)	C12—C13—C14—Br14	176.84 (16)
C3—C4—C4A—C8A	-1.1 (3)	C13—C14—C15—C16	0.6 (3)
O4—C4—C4A—C8A	179.95 (16)	Br14—C14—C15—C16	-177.29 (16)
C3—C4—C4A—C5	-179.20 (19)	C14—C15—C16—C11	0.2 (3)
O4—C4—C4A—C5	1.8 (3)	C12—C11—C16—C15	-0.6 (3)
C8A—C4A—C5—C6	-0.3 (3)	C17—C11—C16—C15	177.18 (19)
C4—C4A—C5—C6	177.78 (19)	C4—O4—C17—C18	-118.0 (2)
C4A—C5—C6—C7	1.1 (3)	C4—O4—C17—C11	68.3 (2)
C5—C6—C7—C8	-0.9 (3)	C12—C11—C17—C18	10.1 (3)
C6—C7—C8—C8A	-0.1 (3)	C16—C11—C17—C18	-167.6 (2)
C2—N1—C8A—C4A	0.9 (3)	O4—C17—C11—C12	-176.79 (18)
C2—N1—C8A—C8	-179.29 (18)	C16—C11—C17—O4	5.5 (3)
C5—C4A—C8A—N1	179.16 (18)	O4—C17—C18—C19	5.5 (3)
C4—C4A—C8A—N1	0.9 (3)	C11—C17—C18—C19	178.5 (2)
C5—C4A—C8A—C8	-0.7 (3)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ O2 <sup>i</sup>	0.88	1.96	2.814 (2)	164

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C12—H12···O2 <sup>ii</sup>	0.95	2.52	3.435 (2)	163
C18—H18···O2 <sup>ii</sup>	0.95	2.44	3.389 (3)	178

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Symmetry codes: (i)  $-x+1, -y+1, -z+1$ ; (ii)  $-x+3/2, y-1/2, -z+3/2$ .