Synthesis, crystal structure and computational studies of a new Schiff base compound: (E)-4-bromo-2-ethoxy-6-{[(2-methoxyphenyl)-imino]methyl}phenol

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The title compound, $C_{16}H_{16}BrNO_3$, which shows enol–imine tautomerism, crystallizes in the monoclinic $P2_1/c$ space group. All non-H atoms of the molecule are nearly coplanar, with a maximum deviation of 0.274 (3) Å. In the crystal, molecules are held together by weak C—H$\cdots$O, π–π and C—H$\cdots$$\pi$ interactions. The E/Z isomerism and enol/keto tautomerism energy barriers of the compound have been calculated by relaxed potential energy surface scan calculations with DFT methods. To observe the changes in the aromatic ring, HOMA aromaticity indexes were calculated during the scan process. Total energy and HOMA change curves were obtained to visualize results of the scan calculations.

1. Chemical context

The synthesis and chemistry of Schiff bases have received considerable attention over the last several decades, primarily owing to their remarkable potential pharmacological (Hu *et al.*, 2012), anti-tumor (Kamel *et al.*, 2010) and biological properties (Lozier *et al.*, 1975). Furthermore, Schiff bases can display photo-chromic and thermo-chromic effect (Hadjoudis & Mavridis, 2004). These effects depend on the prototropic tautomerism and molecular planarity in Schiff bases (Moustakali-Mavridis *et al.*, 1978; Hadjoudis *et al.*, 1987). Prototropic tautomerism emerges from the intramolecular H-atom transfer between an enol–imine (Özdemir Tarı *et al.*, 2016) and a keto–amine tautomer (Özek *et al.*, 2006). The present work is part of our ongoing studies on Schiff bases (Özek Yıldırım *et al.*, 2016, 2017; Albayrak *et al.*, 2012). We report herein the synthesis, crystal structure and computational studies of the title compound, (*E*)-4-bromo-2-ethoxy-6-{[(2-methoxyphenyl)imino]methyl}phenol, obtained from the condensation of 5-bromo-3-ethoxy-2-hydroxybenzaldehyde with 2-methoxyaniline.
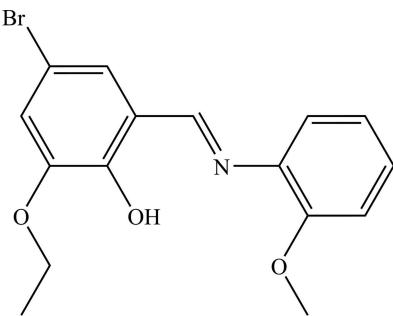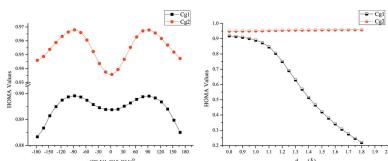

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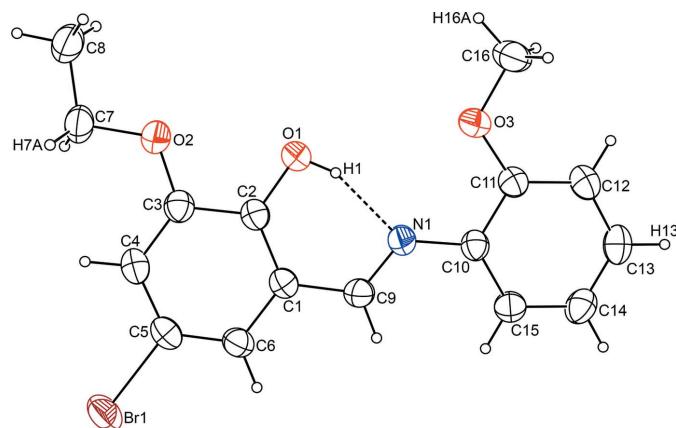
Figure 1
The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms. The dashed line indicates the intramolecular hydrogen bond.

2. Structural commentary

Fig. 1 represents the molecular structure of the title compound. All non-H atoms lie in the plane formed by the aromatic rings with a maximum deviation of 0.274 (3) Å. The dihedral angle between the aromatic rings C1–C6 and C10–C15 is 2.25 (13)°. In the chelate moiety, which comprises atoms C1, C2, O1, H1, N1 and C9, C9=N1 [1.281 (3)] is a typical double bond while C2—O1 [1.333 (3)] is a typical single bond; these are similar to those in related structures (Petek *et al.*, 2010; Gül *et al.*, 2007). The harmonic oscillator model of aromaticity (HOMA; Kruszewski & Krygowski, 1972) values were calculated [0.88 for C1–C6 and 0.98 for the C10–C15 ring] to observe the effect of substituent groups on the rings. There are no significant deformations of the rings when compared to those in (*E*)-2-ethoxy-6-[(2-methoxyphenyl-

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C10–C15 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$\cdots$N1	0.81 (5)	1.80 (5)	2.566 (3)	157 (5)
C16—H16$A\cdots$O1^i	0.96	2.55	3.293 (3)	135
C7—H7$A\cdots Cg$1^{ii}	0.97	2.80	3.662 (3)	149
C13—H13$\cdots Cg$2^{iii}	0.93	2.79	3.629 (3)	150

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

imino)methyl]phenol (Petek *et al.*, 2010). The chelate moiety forms an *S*(6) graph-set motif through a strong intramolecular O1—H1$\cdots$N1 hydrogen bond (Table 1).

3. Supramolecular features

In the crystal, inversion dimers with an R_2^2 motif are generated by the weak C16—H16$A\cdots$O1($-x+1, -y, -z+1$) hydrogen bonds (Table 1). As shown in Fig. 2, these dimers are connected to each other by π–π interactions [Cg1$\cdots Cg$2($x, y+1, z$) = 3.6237 (16) Å; Cg1 and Cg2 are the centroids of the C1–C6 and C10–C15 rings, respectively]. C—H$\cdots\pi$ interactions (Table 1) generate zigzag chains along the [100] direction as shown in Fig. 3.

4. Computational Studies

Relaxed potential energy surface scan calculations were performed using the DFT/B3LYP/6-311G++(d,p) method with *Gaussian 09W* software (Frisch *et al.*, 2009) to investigate the connection between the molecular conformation and physical properties of a Schiff base. The results of a torsional angle scan and a proton-transfer scan on the O—H$\cdots$N pathway are given in Fig. 4. The torsional barrier between the *E/Z* isomers was found to be 1.94 kcal mol^{-1} and the enol–keto tauto-
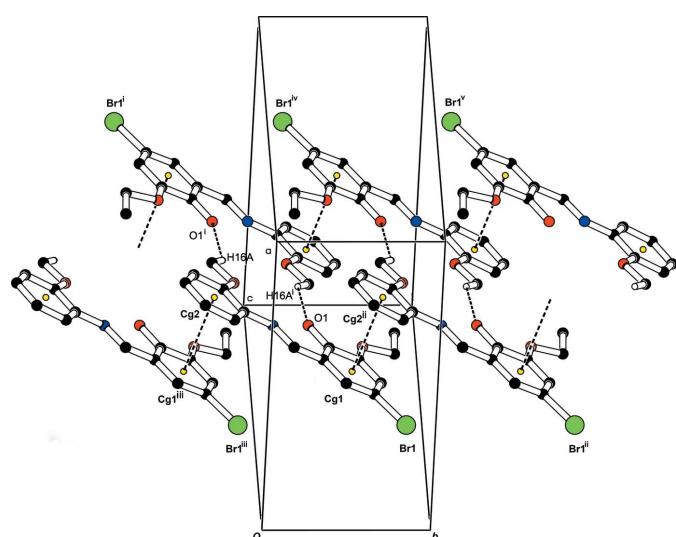
Figure 2
View of the inversion dimers, which are connected by π–π interactions, propagating along the *c*-axis direction. [Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x, y+1, z$; (iii) $x, y-1, z$; (iv) $-x+1, -y+1, -z+1$; (v) $-x+1, -y+2, -z+1$.]
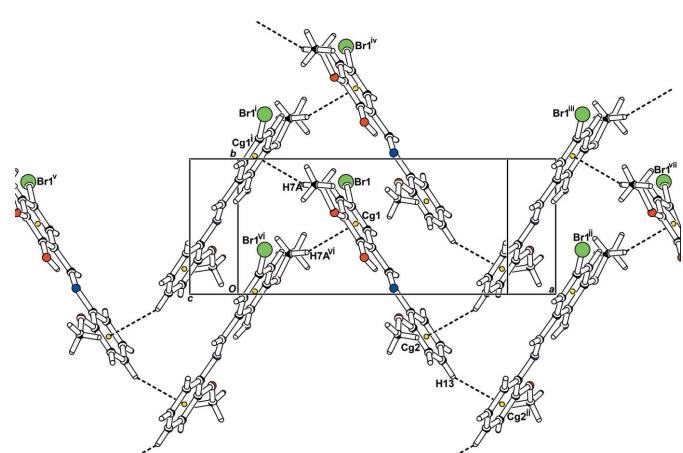
**Figure 3**
The packing, viewed down the *c* axis, showing molecules connected by C—H$\cdots\pi$ interactions [Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x, y+1, z$; (v) $x-1, y, z$; (vi) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (vii) $x+1, y, z$.]
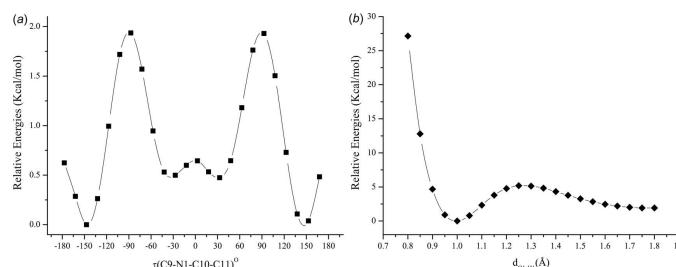
Figure 4
The potential energy curves for the torsional scan (*a*) and the O—H bond scan (*b*). Relative energies are calculated with respect to the global minimum of each curve.

merism barrier was 1.92 kcal mol^{-1}. The effects of the conformational changes on the aromatic ring can be visualized by calculating HOMA values during the scan calculations. Fig. 5*a* shows that changes in the HOMA indices are very limited with an average fluctuation of 2%. As can be seen in Fig. 5*b*, the aromaticity of the C1–C6 ring depends strongly on the prototropic tautomerism.

5. Database survey

A survey of the Cambridge Structural Database (CSD, Version 5.37, update May 2017; Groom *et al.*, 2016) for the (*E*)-4-bromo-2-ethoxy-6-[(methylimino)methyl]phenol unit of the title compound reveals five compounds, *viz.* OCOVEK (Kaştaş *et al.*, 2017*a*), OCOVIO (Kaştaş *et al.*, 2017*b*), OCOVOU (Kaştaş *et al.*, 2017*c*), OCOVUA (Kaştaş *et al.*, 2017*d*) and LUWZIO (Özek Yıldırım *et al.*, 2016). The molecular structures of the latter two compounds are planar, in which they are similar to the title compound, while the others are not planar.

6. Synthesis and crystallization

The title compound was prepared by refluxing a mixture of a solution containing 5-bromo-3-ethoxy-2-hydroxy-benzaldehyde (0.5 g, 2 mmol) in 20 ml ethanol and a solution containing 2-methoxyaniline (0.25 g, 2 mmol) in 20 ml ethanol. The reaction mixture was stirred for 1 h under reflux. Crystals suitable for X-ray analysis were obtained from an ethanol solution by slow evaporation (yield 70%).
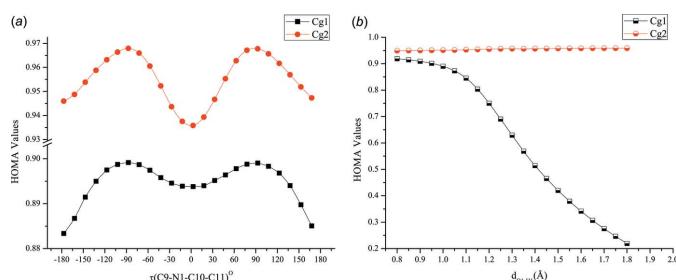

Figure 5
Graphics showing the variation of HOMA values with scan coordinate.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{16}BrNO_3$
M_r	350.21
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	15.3405 (8), 6.5204 (2), 15.3612 (10)
β (°)	98.716 (5)
V (Å^3)	1518.78 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.72
Crystal size (mm)	$0.56 \times 0.28 \times 0.05$
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.437, 0.893
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18156, 3491, 2754
R_{int}	0.042
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.042, 0.091, 1.06
No. of reflections	3491
No. of parameters	194
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.28, −0.38

Computer programs: *X-AREA* and *X-RED32* (Stoe & Cie, 2002), *SHELXS97* (Sheldrick, 2015), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydroxyl atom H1 was refined freely. All the other H atoms were located geometrically and refined using a riding model with C—H = 0.93–0.97 Å U_{iso}(H) = 1.2U_{eq}(C).

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supporting information

Synthesis, crystal structure and computational studies of a new Schiff base compound: (*E*)-4-bromo-2-ethoxy-6-{[(2-methoxyphenyl)imino]methyl}phenol

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2015); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

(*E*)-4-Bromo-2-ethoxy-6-{[(2-methoxyphenyl)imino]methyl}phenol

Crystal data

$C_{16}H_{16}BrNO_3$	$F(000) = 712$
$M_r = 350.21$	$D_x = 1.532$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 15.3405$ (8) Å	Cell parameters from 3491 reflections
$b = 6.5204$ (2) Å	$\theta = 2.0–28.1°$
$c = 15.3612$ (10) Å	$\mu = 2.72$ mm^{-1}
$\beta = 98.716$ (5)°	$T = 296$ K
$V = 1518.78$ (14) Å^3	Prism, orange
$Z = 4$	$0.56 \times 0.28 \times 0.05$ mm

Data collection

Stoe IPDS 2 diffractometer	18156 measured reflections
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus	3491 independent reflections
	2754 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.042$
rotation method scans	$\theta_{max} = 27.5°$, $\theta_{min} = 2.0°$
Absorption correction: integration	$h = -19 \rightarrow 19$
(X-RED32; Stoe & Cie, 2002)	$k = -8 \rightarrow 8$
$T_{min} = 0.437$, $T_{max} = 0.893$	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.042$	
$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 0.5265P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
3491 reflections	$(\Delta/\sigma)_{max} = 0.001$
194 parameters	$\Delta\rho_{max} = 0.28$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.38$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.44857 (16)	0.3446 (4)	0.18253 (15)	0.0403 (5)
C2	0.42497 (17)	0.3902 (4)	0.26511 (16)	0.0417 (5)
C3	0.37588 (17)	0.5714 (4)	0.27491 (17)	0.0440 (6)
C4	0.35124 (17)	0.6978 (4)	0.20324 (18)	0.0469 (6)
H4	0.318414	0.815670	0.208919	0.056*
C5	0.37596 (17)	0.6473 (4)	0.12266 (17)	0.0456 (6)
C6	0.42285 (18)	0.4758 (4)	0.11072 (16)	0.0457 (6)
H6	0.437777	0.445619	0.055674	0.055*
C7	0.3190 (2)	0.7984 (4)	0.3743 (2)	0.0574 (7)
H7A	0.260045	0.809407	0.341291	0.069*
H7B	0.354488	0.909669	0.356734	0.069*
C8	0.3155 (2)	0.8097 (5)	0.4713 (2)	0.0640 (8)
H8A	0.290087	0.938248	0.484727	0.077*
H8B	0.280127	0.699194	0.487896	0.077*
H8C	0.374171	0.799032	0.503274	0.077*
C9	0.50092 (17)	0.1655 (4)	0.17069 (16)	0.0442 (5)
H9	0.516428	0.138217	0.115620	0.053*
C10	0.57777 (16)	−0.1337 (4)	0.22892 (16)	0.0406 (5)
C11	0.59676 (16)	−0.2499 (4)	0.30608 (16)	0.0420 (5)
C12	0.64681 (19)	−0.4279 (4)	0.30608 (19)	0.0513 (6)
H12	0.659509	−0.505656	0.357194	0.062*
C13	0.67759 (18)	−0.4892 (5)	0.2304 (2)	0.0550 (7)
H13	0.711082	−0.608217	0.230857	0.066*
C14	0.6594 (2)	−0.3766 (5)	0.1542 (2)	0.0552 (7)
H14	0.680358	−0.419005	0.103432	0.066*
C15	0.60944 (19)	−0.1994 (4)	0.15371 (18)	0.0508 (6)
H15	0.596978	−0.123232	0.102130	0.061*
C16	0.5727 (2)	−0.2971 (5)	0.45460 (19)	0.0622 (8)
H16A	0.546330	−0.227372	0.499090	0.075*
H16B	0.544000	−0.426840	0.441808	0.075*
H16C	0.634215	−0.319190	0.475376	0.075*
N1	0.52630 (14)	0.0438 (3)	0.23498 (13)	0.0423 (5)
O1	0.44838 (15)	0.2719 (3)	0.33548 (12)	0.0536 (5)
O2	0.35740 (14)	0.6041 (3)	0.35724 (12)	0.0546 (5)
O3	0.56318 (14)	−0.1756 (3)	0.37679 (12)	0.0558 (5)
Br1	0.34398 (2)	0.82939 (5)	0.02613 (2)	0.06603 (13)
H1	0.479 (3)	0.186 (8)	0.316 (3)	0.119 (18)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0405 (12)	0.0374 (12)	0.0424 (12)	−0.0003 (11)	0.0041 (10)	0.0031 (10)
C2	0.0433 (13)	0.0374 (13)	0.0443 (12)	0.0007 (10)	0.0064 (10)	0.0027 (10)
C3	0.0429 (14)	0.0415 (13)	0.0483 (13)	0.0002 (11)	0.0092 (11)	0.0009 (11)
C4	0.0441 (14)	0.0383 (14)	0.0583 (15)	0.0045 (11)	0.0081 (11)	0.0060 (11)
C5	0.0446 (14)	0.0415 (14)	0.0493 (13)	−0.0018 (11)	0.0021 (11)	0.0109 (11)
C6	0.0492 (14)	0.0476 (15)	0.0403 (12)	0.0025 (12)	0.0070 (11)	0.0067 (11)
C7	0.0640 (18)	0.0433 (16)	0.0674 (18)	0.0125 (13)	0.0184 (14)	0.0005 (13)
C8	0.074 (2)	0.0519 (17)	0.0698 (19)	0.0103 (15)	0.0230 (16)	−0.0074 (15)
C9	0.0514 (14)	0.0430 (13)	0.0387 (12)	−0.0004 (12)	0.0087 (10)	0.0010 (11)
C10	0.0404 (13)	0.0363 (13)	0.0458 (12)	−0.0001 (10)	0.0089 (10)	0.0016 (10)
C11	0.0392 (13)	0.0422 (13)	0.0450 (12)	−0.0001 (11)	0.0080 (10)	0.0031 (10)
C12	0.0491 (15)	0.0465 (15)	0.0576 (15)	0.0062 (12)	0.0061 (12)	0.0089 (13)
C13	0.0458 (15)	0.0433 (15)	0.0764 (19)	0.0074 (12)	0.0106 (14)	−0.0017 (14)
C14	0.0555 (17)	0.0534 (17)	0.0607 (16)	0.0041 (13)	0.0217 (13)	−0.0073 (13)
C15	0.0580 (16)	0.0498 (16)	0.0475 (14)	0.0037 (13)	0.0170 (12)	0.0037 (12)
C16	0.070 (2)	0.070 (2)	0.0473 (15)	0.0027 (16)	0.0107 (13)	0.0152 (14)
N1	0.0467 (12)	0.0375 (11)	0.0436 (10)	0.0035 (9)	0.0092 (9)	0.0030 (9)
O1	0.0730 (14)	0.0473 (11)	0.0425 (10)	0.0160 (10)	0.0152 (9)	0.0081 (8)
O2	0.0703 (13)	0.0445 (10)	0.0519 (10)	0.0137 (9)	0.0184 (9)	0.0025 (8)
O3	0.0709 (13)	0.0559 (11)	0.0434 (9)	0.0145 (10)	0.0176 (9)	0.0106 (9)
Br1	0.0763 (2)	0.05858 (19)	0.06202 (19)	0.01265 (16)	0.00668 (14)	0.02361 (15)

Geometric parameters (Å, º)

C1—C2	1.403 (3)	C9—N1	1.281 (3)
C1—C6	1.405 (3)	C9—H9	0.9300
C1—C9	1.444 (4)	C10—C15	1.387 (4)
C2—O1	1.333 (3)	C10—C11	1.400 (3)
C2—C3	1.421 (4)	C10—N1	1.412 (3)
C3—O2	1.354 (3)	C11—O3	1.360 (3)
C3—C4	1.381 (4)	C11—C12	1.392 (4)
C4—C5	1.388 (4)	C12—C13	1.379 (4)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.356 (4)	C13—C14	1.373 (4)
C5—Br1	1.905 (2)	C13—H13	0.9300
C6—H6	0.9300	C14—C15	1.386 (4)
C7—O2	1.438 (3)	C14—H14	0.9300
C7—C8	1.500 (4)	C15—H15	0.9300
C7—H7A	0.9700	C16—O3	1.423 (3)
C7—H7B	0.9700	C16—H16A	0.9600
C8—H8A	0.9600	C16—H16B	0.9600
C8—H8B	0.9600	C16—H16C	0.9600
C8—H8C	0.9600	O1—H1	0.81 (5)
C2—C1—C6	120.0 (2)	N1—C9—H9	119.5

C2—C1—C9	120.7 (2)	C1—C9—H9	119.5
C6—C1—C9	119.3 (2)	C15—C10—C11	118.9 (2)
O1—C2—C1	122.4 (2)	C15—C10—N1	125.3 (2)
O1—C2—C3	118.5 (2)	C11—C10—N1	115.8 (2)
C1—C2—C3	119.1 (2)	O3—C11—C12	125.0 (2)
O2—C3—C4	125.4 (2)	O3—C11—C10	115.3 (2)
O2—C3—C2	114.8 (2)	C12—C11—C10	119.7 (2)
C4—C3—C2	119.8 (2)	C13—C12—C11	120.1 (3)
C3—C4—C5	119.4 (2)	C13—C12—H12	120.0
C3—C4—H4	120.3	C11—C12—H12	120.0
C5—C4—H4	120.3	C14—C13—C12	120.8 (3)
C6—C5—C4	122.6 (2)	C14—C13—H13	119.6
C6—C5—Br1	119.2 (2)	C12—C13—H13	119.6
C4—C5—Br1	118.23 (19)	C13—C14—C15	119.5 (3)
C5—C6—C1	119.2 (2)	C13—C14—H14	120.3
C5—C6—H6	120.4	C15—C14—H14	120.3
C1—C6—H6	120.4	C14—C15—C10	121.1 (3)
O2—C7—C8	107.6 (2)	C14—C15—H15	119.5
O2—C7—H7A	110.2	C10—C15—H15	119.5
C8—C7—H7A	110.2	O3—C16—H16A	109.5
O2—C7—H7B	110.2	O3—C16—H16B	109.5
C8—C7—H7B	110.2	H16A—C16—H16B	109.5
H7A—C7—H7B	108.5	O3—C16—H16C	109.5
C7—C8—H8A	109.5	H16A—C16—H16C	109.5
C7—C8—H8B	109.5	H16B—C16—H16C	109.5
H8A—C8—H8B	109.5	C9—N1—C10	124.4 (2)
C7—C8—H8C	109.5	C2—O1—H1	102 (3)
H8A—C8—H8C	109.5	C3—O2—C7	117.3 (2)
H8B—C8—H8C	109.5	C11—O3—C16	118.0 (2)
N1—C9—C1	120.9 (2)		
C6—C1—C2—O1	−179.4 (2)	N1—C10—C11—O3	−0.2 (3)
C9—C1—C2—O1	−0.7 (4)	C15—C10—C11—C12	0.1 (4)
C6—C1—C2—C3	−0.7 (4)	N1—C10—C11—C12	179.7 (2)
C9—C1—C2—C3	177.9 (2)	O3—C11—C12—C13	180.0 (3)
O1—C2—C3—O2	−0.3 (4)	C10—C11—C12—C13	0.1 (4)
C1—C2—C3—O2	−179.0 (2)	C11—C12—C13—C14	−0.1 (4)
O1—C2—C3—C4	179.5 (2)	C12—C13—C14—C15	0.0 (5)
C1—C2—C3—C4	0.8 (4)	C13—C14—C15—C10	0.1 (5)
O2—C3—C4—C5	179.0 (2)	C11—C10—C15—C14	−0.2 (4)
C2—C3—C4—C5	−0.9 (4)	N1—C10—C15—C14	−179.8 (3)
C3—C4—C5—C6	0.9 (4)	C1—C9—N1—C10	−179.8 (2)
C3—C4—C5—Br1	−178.1 (2)	C15—C10—N1—C9	1.3 (4)
C4—C5—C6—C1	−0.7 (4)	C11—C10—N1—C9	−178.3 (2)
Br1—C5—C6—C1	178.21 (19)	C4—C3—O2—C7	−8.4 (4)
C2—C1—C6—C5	0.7 (4)	C2—C3—O2—C7	171.4 (2)
C9—C1—C6—C5	−178.0 (2)	C8—C7—O2—C3	−172.8 (2)
C2—C1—C9—N1	0.6 (4)	C12—C11—O3—C16	−6.0 (4)

| C6—C1—C9—N1 | 179.3 (2) | C10—C11—O3—C16 | 173.9 (2) |
| C15—C10—C11—O3 | −179.8 (2) | | |

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the C1–C6 and C10–C15 rings, respectively.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1—H1⋯N1	0.81 (5)	1.80 (5)	2.566 (3)	157 (5)
C16—H16*A*⋯O1[i]	0.96	2.55	3.293 (3)	135
C7—H7*A*⋯*Cg*1[ii]	0.97	2.80	3.662 (3)	149
C13—H13⋯*Cg*2[iii]	0.93	2.79	3.629 (3)	150

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