



Crystal structure, Hirshfeld surface analysis and HOMO–LUMO analysis of (*E*)-4-bromo-*N'*-(4-methoxybenzylidene)benzohydrazide

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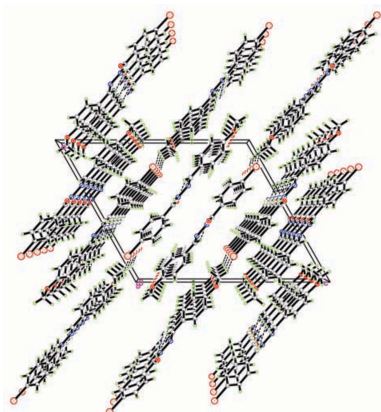
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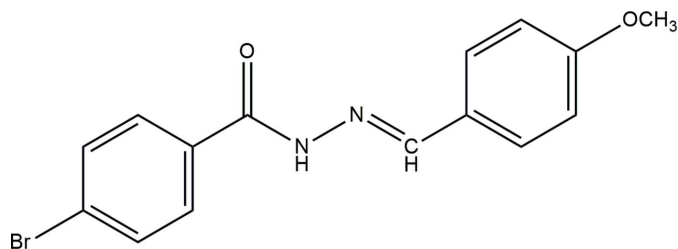
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The title Schiff base compound, C₁₅H₁₃BrN₂O₂, displays an *E* configuration with respect to the C=N double bond, which forms a dihedral angle of 58.06 (9)° with the benzene ring. In the crystal, the molecules are linked into chains parallel to the *b* axis by N–H···O and C–H···O hydrogen bonds, giving rise to rings with an R₂¹(6) graph-set motif. The chains are further linked into a three-dimensional network by C–H···π interactions. A Hirshfeld surface analysis indicates that the most important contributions to the crystal packing are from C···H (33.2%), H···H (27.7%), Br···H/H···Br (14.2%) and O···H/H···O (13.6%) interactions. The title compound has also been characterized by frontier molecular orbital analysis.

1. Chemical context

Schiff bases are nitrogen-containing compounds that were first obtained by the condensation reactions of aromatic amines and aldehydes (Schiff *et al.*, 1864). A wide range of these compounds with the general formula RHC=NR₁ (*R* and *R*₁ can be alkyl, aryl, cycloalkyl or heterocyclic groups) have been synthesized. Schiff bases are of great importance in the field of coordination chemistry because they are able to form stable complexes with metal ions (Souza *et al.*, 1985). The chemical and biological significance of Schiff bases can be attributed to the presence of a lone electron pair in the sp²-hybridized orbital of the nitrogen atom of the azomethine group (Singh *et al.*, 1975). These compounds are used in the fields of organic synthesis, chemical catalysis and medicine, pharmacy, as well as other new technologies (Tanaka *et al.*, 2010). Schiff bases are also used as probes in investigating the structure of DNA (Tiwari *et al.*, 2011), and have gained special attention in pharmacophore research and in the development of several bioactive lead molecules (Muralisankar *et al.*, 2016). Schiff bases showing photochromic and thermochromic properties have been used in information storage, electronic display systems, optical switching devices and ophthalmic glasses (Amimoto *et al.*, 2005). Herein the crystal structure of the title compound, (*E*)-4-bromo-*N'*-(4-methoxybenzylidene)benzohydrazide is reported.





2. Structural commentary

The asymmetric unit of the title compound (Fig. 1) consists of one independent molecule displaying an *E* configuration about the C=N double bond. All the bond lengths are within the normal ranges. The values of the C8=N2 [1.281 (3) Å] and C7=O2 [1.222 (3) Å] bond lengths confirm their double-bond character. The C7–N1, N1–N2 and C3–Br1 bond lengths are 1.354 (3), 1.379 (3) and 1.894 (3) Å, respectively. The central O2/C7/N1/N2 fragment is approximately planar (r.m.s. deviation 0.0141 Å) and forms dihedral angles of 32.5 (2) and 27.2 (2)° with the C1–C6 and C9–C14 rings, respectively. The dihedral angle formed by the aromatic rings is 58.06 (9)°.

3. Supramolecular features

In the crystal structure, the molecules are linked into chains extending along the *b*-axis direction by N1–H1N···O2 and C8–H8···O2 hydrogen-bonding interactions (Table 1)

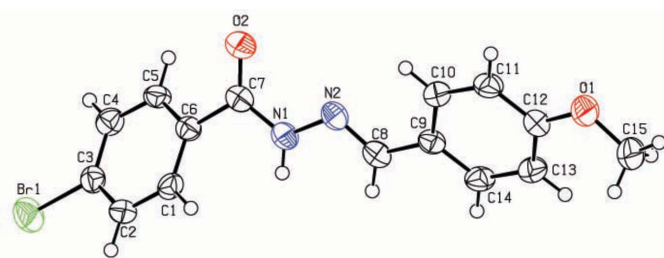


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

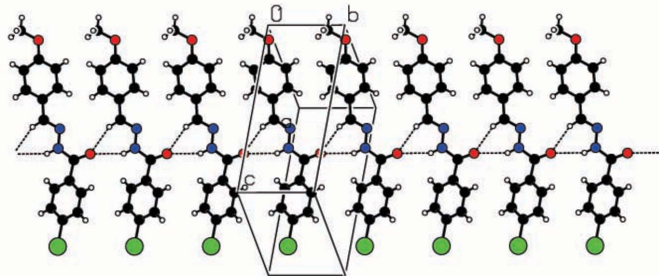


Figure 2
Partial packing diagram of the title compound showing the formation of a molecular chain parallel to the *b* axis through N–H···O and C–H···O hydrogen bonds (dashed lines).

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

Cg1 and Cg2 are the centroids of the C1–C6 and C9–C14 rings, respectively.

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1–H1N···O2 ⁱ	0.86	2.40	3.193 (3)	154
C8–H8···O2 ⁱ	0.93	2.43	3.240 (3)	146
C2–H2···Cg2 ⁱⁱ	0.93	2.81	3.531 (4)	135
C5–H5···Cg1 ⁱⁱⁱ	0.93	2.89	3.553 (4)	130
C10–H10···Cg1 ^{iv}	0.93	2.86	3.549 (4)	132

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

forming rings with an $R_2^1(6)$ graph-set motif (Fig. 2). The chains are further connected by C–H··· π interactions, forming a three-dimensional network (Fig. 3).

4. Hirshfeld surface analysis

The three-dimensional d_{norm} surface is a useful tool for analysing and visualizing the intermolecular interactions. d_{norm} takes negative or positive values depending on whether the intermolecular contact is shorter or longer, respectively, than the van der Waals radii (Spackman & Jayatilaka, 2009; McKinnon *et al.*, 2007). The three-dimensional d_{norm} surface of the title compound is shown in Fig. 4. The red points, which represent closer contacts and negative d_{norm} values on the surface, correspond to the N–H···O and C–H···O interactions. Two-dimensional fingerprint plots from Hirshfeld surface analysis (Fig. 5) provide information about the intermolecular contacts and their percentage contributions to the Hirshfeld surface. The percentage contributions from the

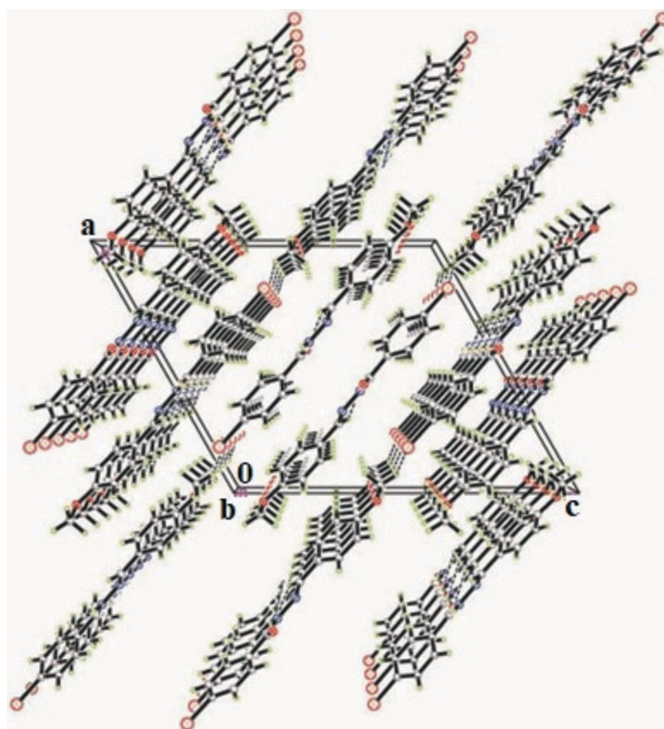


Figure 3
Packing diagram of the title compound viewed down the *b* axis.

Table 2

Calculated frontier molecular orbital energies (eV).

FMO	Energy
E_{HOMO}	-6.0275
E_{LUMO}	-1.9434
$E_{\text{HOMO}-1}$	-7.0785
$E_{\text{LUMO}+1}$	-1.2582
$(E_{\text{HOMO}} - E_{\text{LUMO}})$ gap	4.0841
$(E_{\text{HOMO}-1} - E_{\text{LUMO}+1})$ gap	5.8203
Chemical hardness	2.0420
Chemical potential	3.9854
Electronegativity	-3.9854
Electrophilicity index	3.8892

different interatomic contacts to the Hirshfeld surface in the title compound are as follows: C...H (33.2%), H...H (27.7%), Br...H/H...Br (14.2%), O...H/H...O (13.6%), N...H/H...N (4.6%), Br...O/O...Br (2.4%), C...N/N...C (1.6%), O...N/N...O (1.3%), O...C/C...O (0.6%), Br...N/N...Br (0.5%) and Br...C/C...Br (0.3%).

5. Frontier molecular orbitals

The HOMO (highest occupied molecular orbital) acts as an electron donor and the LUMO (lowest occupied molecular orbital) acts as an electron acceptor. If the energy gap is small then the molecule is highly polarizable and has high chemical reactivity. The energy levels were computed by the DFT-B3LYP/6-311G++(d,p) method (Becke, 1993) as implemented in GAUSSIAN09 (Frisch *et al.*, 2009). The electron distribution of the HOMO-1, HOMO, LUMO and LUMO+1 energy levels, which determines the chemical stability, chemical hardness, chemical potential, electronegativity and electrophilicity index (Table 2), are shown in Fig. 6. The frontier molecular orbital LUMO is located over the whole of the molecule. The energy gap of the molecule clearly shows the charge-transfer interaction involving donor and acceptor groups. From the HOMO-LUMO energy gap, information on whether or not the molecule is difficult (hard) or delicate (soft) can be derived. If the molecule has a large energy gap, then the molecule can be defined as a hard molecule whereas the presence of a small energy gap classifies the molecule as soft. The soft molecules are more polarizable than the hard

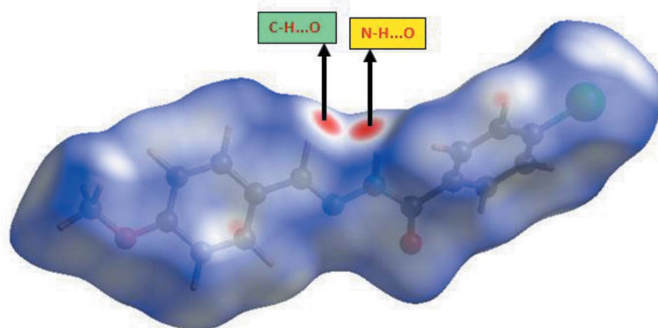


Figure 4
Hirshfeld surfaces of the title compound mapped over d_{norm} .

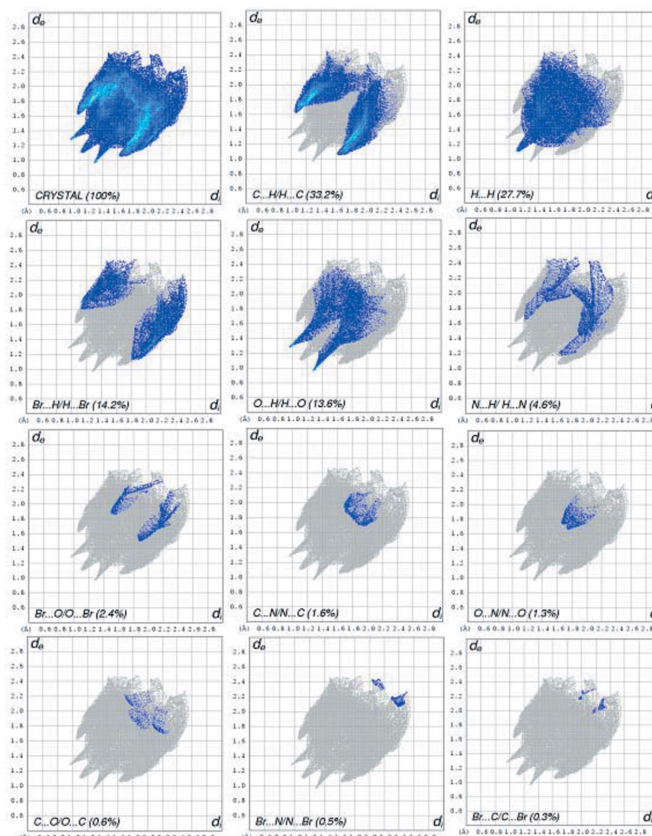


Figure 5

Two-dimensional fingerprint plots of the title compound and relative contributions of the atom pairs to the Hirshfeld surface.

ones because they only need a small energy for excitation. Therefore, from the data reported in Table 2, we conclude that the molecule of the title compound belongs to the really hard materials.

6. Database survey

A search of the Cambridge Structural Database (Version 5.39, update May 2018; Groom *et al.*, 2016) for uncoordinated molecules containing the 4-bromobenzohydrazide fragment

E_{HOMO} (eV)	E_{LUMO} (eV)	$E_{\text{HOMO}} - E_{\text{LUMO}}$ gap (eV)
-6.0275 eV	-1.9434 eV	4.0841 eV
$E_{\text{HOMO}-1}$ (eV)	$E_{\text{LUMO}+1}$ (eV)	$E_{\text{HOMO}-1} - E_{\text{LUMO}+1}$ gap (eV)
-7.0785 eV	-1.2582 eV	5.8203 eV

Figure 6
Molecular orbital energy levels of the title compound.

Table 3

Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₃ BrN ₂ O ₂
<i>M_r</i>	333.18
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	15.6963 (14), 5.4121 (4), 18.6224 (16)
β (°)	119.609 (6)
<i>V</i> (Å ³)	1375.4 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	2.99
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffraction	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2004)
<i>T_{min}</i> , <i>T_{max}</i>	0.467, 0.586
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	9456, 2563, 1923
<i>R_{int}</i>	0.030
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.606
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.032, 0.073, 1.02
No. of reflections	2563
No. of parameters	182
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.46, -0.49

Computer programs: *APEX2*, *SAINTE* and *XPREP* (Bruker, 2004), *SIR92* (Altomare *et al.*, 1999), *SHELXL2017/1* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

yielded 17 hits. Similar to the crystal structure of the title compound, in seven of them the carbonyl oxygen atom is engaged in intermolecular N—H···O and C—H···O hydrogen bonds as a bifurcated acceptor [4-bromo-*N'*-(2,4-dihydroxybenzylidene)benzohydrazide (Mohanraj *et al.*, 2016; Arunagiri *et al.*, 2018); 4-bromo-*N'*-(2-nitrobenzylidene)benzohydrazide (Zhang *et al.* 2009); 4-bromo-*N'*-(2-hydroxy-5-methoxybenzylidene)benzohydrazide (Wang *et al.*, 2017)] or trifurcated acceptor [4-bromo-*N'*-(2-chlorobenzylidene)benzohydrazide (Shu *et al.*, 2009); 4-bromo-*N'*-(5-methylfuran-2-yl)methylene)benzohydrazide (Bai & Jing, 2007); 4-bromo-*N'*-(4-methyl-1,2,3-thiadiazole-5-yl)methylidenebenzohydrazine (Zhang *et al.*, 2017); (2-fluoro-2-methyl-2-phenylethylidene) 4-bromobenzoyl hydrazone (Brandes *et al.*, 2006)], forming molecular chains.

7. Synthesis and crystallization

The title compound was synthesized by the reaction of a 1:1 molar ratio mixture of a hot ethanolic solution (20 mL) of 4-bromobenzohydrazide (0.213 mg) and a hot ethanolic solution of 4-methoxybenzaldehyde (0.136 mg). The mixture was refluxed for 8 h, then it was cooled and kept at room temperature. The powder formed was recrystallized from DMSO. Colourless block-shaped crystals suitable for X-ray analysis were obtained after a few days on slow evaporation of the solvent.

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atoms were positioned geometrically (C—H = 0.93–0.9 Å, N—H = 0.86 Å) and were refined as riding with *U*_{iso}(H) = 1.2*U*_{eq}(C, N) or 1.5*U*_{eq}(C) for methyl H atoms. A rotating model was used for the methyl H atoms. Three outliers (100, $\bar{1}$ 02, 002) were omitted in the last cycles of refinement.

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Crystal structure, Hirshfeld surface analysis and HOMO–LUMO analysis of (*E*)-4-bromo-*N'*-(4-methoxybenzylidene)benzohydrazide

**Kasthuri Balasubramani, Ganesan Premkumar, Palaniyappan Sivajeyanthi, Muthaiah Jeevaraj,
Bellarmin Edison and Toka Swu**

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2017/1* (Sheldrick, 2015).

(*E*)-4-Bromo-*N'*-(4-methoxybenzylidene)benzohydrazide

Crystal data

$C_{15}H_{13}BrN_2O_2$

$M_r = 333.18$

Monoclinic, $P2_1/c$

$a = 15.6963$ (14) Å

$b = 5.4121$ (4) Å

$c = 18.6224$ (16) Å

$\beta = 119.609$ (6)°

$V = 1375.4$ (2) Å³

$Z = 4$

$F(000) = 672$

$D_x = 1.609$ Mg m⁻³

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

Cell parameters from 3040 reflections

$\theta = 6.0$ – 48.0 °

$\mu = 2.99$ mm⁻¹

$T = 296$ K

Block, colourless

$0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEX2 CCD
diffractometer

Radiation source: fine-focus sealed tube

ω and ϕ scan

Absorption correction: multi-scan
(SADABS; Bruker, 2004)

$T_{\min} = 0.467$, $T_{\max} = 0.586$

9456 measured reflections

2563 independent reflections

1923 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 25.5$ °, $\theta_{\min} = 2.8$ °

$h = -19 \rightarrow 18$

$k = -6 \rightarrow 6$

$l = -20 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.073$

$S = 1.02$

2563 reflections

182 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 1.0475P]$

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

$$(\Delta/\sigma)_{\max} = 0.002$$

$$\Delta\rho_{\max} = 0.46 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.49 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.79167 (2)	0.30890 (7)	0.92827 (2)	0.05897 (14)
O1	-0.00864 (14)	0.0494 (4)	0.09196 (11)	0.0533 (5)
O2	0.43709 (15)	0.7268 (4)	0.55090 (12)	0.0549 (5)
N1	0.41072 (16)	0.3124 (4)	0.53160 (13)	0.0409 (5)
H1N	0.427566	0.168774	0.554028	0.049*
N2	0.33475 (16)	0.3322 (4)	0.45146 (13)	0.0407 (6)
C1	0.59886 (19)	0.2470 (5)	0.67875 (17)	0.0372 (6)
H1	0.586962	0.133251	0.637387	0.045*
C2	0.67360 (19)	0.2047 (5)	0.75843 (16)	0.0381 (6)
H2	0.712459	0.064141	0.770697	0.046*
C3	0.68987 (18)	0.3718 (5)	0.81921 (15)	0.0355 (6)
C4	0.63465 (19)	0.5837 (5)	0.80198 (16)	0.0382 (6)
H4	0.646969	0.696761	0.843605	0.046*
C5	0.56079 (19)	0.6261 (5)	0.72216 (16)	0.0365 (6)
H5	0.523578	0.769580	0.710036	0.044*
C6	0.54134 (18)	0.4582 (5)	0.65996 (15)	0.0322 (6)
C7	0.45937 (19)	0.5147 (5)	0.57559 (16)	0.0379 (7)
C8	0.28735 (19)	0.1307 (5)	0.42189 (16)	0.0390 (7)
H8	0.304278	-0.008120	0.455644	0.047*
C9	0.20794 (19)	0.1129 (5)	0.33719 (16)	0.0342 (6)
C10	0.19274 (19)	0.2921 (5)	0.27816 (16)	0.0379 (6)
H10	0.232143	0.432276	0.293687	0.046*
C11	0.1207 (2)	0.2643 (5)	0.19783 (16)	0.0410 (7)
H11	0.112410	0.384465	0.159190	0.049*
C12	0.05982 (19)	0.0593 (5)	0.17324 (16)	0.0379 (6)
C13	0.0727 (2)	-0.1177 (5)	0.23154 (17)	0.0411 (7)
H13	0.031518	-0.254468	0.216485	0.049*
C14	0.1471 (2)	-0.0895 (5)	0.31222 (16)	0.0407 (7)
H14	0.156194	-0.210907	0.350718	0.049*
C15	-0.0603 (2)	-0.1750 (6)	0.06035 (19)	0.0606 (9)
H15A	-0.014576	-0.309608	0.077155	0.091*
H15B	-0.096720	-0.167091	0.001142	0.091*
H15C	-0.104507	-0.200227	0.081334	0.091*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0530 (2)	0.0698 (2)	0.03805 (19)	0.00375 (18)	0.01023 (14)	0.00735 (16)
O1	0.0519 (12)	0.0497 (13)	0.0362 (11)	-0.0031 (11)	0.0050 (10)	0.0048 (10)
O2	0.0543 (13)	0.0428 (13)	0.0510 (13)	0.0078 (10)	0.0132 (10)	0.0112 (10)
N1	0.0423 (13)	0.0417 (14)	0.0299 (12)	0.0040 (12)	0.0113 (10)	0.0069 (11)
N2	0.0389 (13)	0.0491 (16)	0.0274 (12)	0.0054 (12)	0.0112 (10)	0.0062 (11)
C1	0.0391 (15)	0.0326 (15)	0.0418 (16)	-0.0027 (12)	0.0213 (13)	-0.0107 (12)
C2	0.0346 (14)	0.0325 (15)	0.0426 (16)	0.0040 (13)	0.0156 (13)	0.0017 (13)
C3	0.0316 (14)	0.0403 (16)	0.0324 (15)	-0.0032 (12)	0.0142 (12)	0.0038 (12)
C4	0.0415 (16)	0.0362 (15)	0.0395 (16)	-0.0032 (14)	0.0218 (13)	-0.0060 (13)
C5	0.0377 (15)	0.0280 (14)	0.0460 (16)	0.0063 (12)	0.0224 (13)	0.0035 (12)
C6	0.0319 (14)	0.0319 (14)	0.0356 (15)	0.0010 (12)	0.0187 (12)	0.0034 (12)
C7	0.0363 (15)	0.0397 (18)	0.0395 (16)	0.0043 (14)	0.0202 (13)	0.0045 (13)
C8	0.0400 (16)	0.0409 (17)	0.0359 (15)	0.0065 (14)	0.0185 (13)	0.0065 (13)
C9	0.0361 (15)	0.0344 (15)	0.0336 (14)	0.0059 (12)	0.0184 (12)	0.0019 (12)
C10	0.0394 (15)	0.0317 (14)	0.0429 (16)	-0.0008 (13)	0.0205 (13)	0.0015 (13)
C11	0.0464 (17)	0.0343 (16)	0.0382 (16)	0.0039 (13)	0.0179 (14)	0.0099 (12)
C12	0.0361 (15)	0.0385 (16)	0.0384 (16)	0.0043 (14)	0.0178 (13)	0.0022 (13)
C13	0.0435 (17)	0.0345 (15)	0.0442 (17)	-0.0034 (13)	0.0208 (14)	0.0013 (13)
C14	0.0520 (18)	0.0333 (15)	0.0377 (16)	0.0033 (14)	0.0229 (14)	0.0084 (13)
C15	0.0538 (19)	0.055 (2)	0.0473 (19)	-0.0075 (17)	0.0054 (16)	-0.0005 (16)

Geometric parameters (Å, °)

Br1—C3	1.894 (3)	C5—H5	0.9300
O1—C12	1.357 (3)	C6—C7	1.490 (4)
O1—C15	1.416 (3)	C8—C9	1.452 (4)
O2—C7	1.222 (3)	C8—H8	0.9300
N1—C7	1.354 (3)	C9—C14	1.375 (4)
N1—N2	1.379 (3)	C9—C10	1.395 (4)
N1—H1N	0.8600	C10—C11	1.367 (4)
N2—C8	1.281 (3)	C10—H10	0.9300
C1—C2	1.382 (4)	C11—C12	1.386 (4)
C1—C6	1.390 (3)	C11—H11	0.9300
C1—H1	0.9300	C12—C13	1.386 (4)
C2—C3	1.371 (4)	C13—C14	1.382 (4)
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.376 (4)	C14—H14	0.9300
C4—C5	1.380 (4)	C15—H15A	0.9600
C4—H4	0.9300	C15—H15B	0.9600
C5—C6	1.382 (4)	C15—H15C	0.9600
C12—O1—C15	118.2 (2)	N2—C8—H8	119.1
C7—N1—N2	121.3 (2)	C9—C8—H8	119.1
C7—N1—H1N	119.4	C14—C9—C10	117.9 (2)
N2—N1—H1N	119.3	C14—C9—C8	120.0 (2)

C8—N2—N1	114.0 (2)	C10—C9—C8	122.0 (2)
C2—C1—C6	120.5 (2)	C11—C10—C9	120.9 (3)
C2—C1—H1	119.7	C11—C10—H10	119.6
C6—C1—H1	119.7	C9—C10—H10	119.6
C3—C2—C1	119.3 (2)	C10—C11—C12	120.8 (2)
C3—C2—H2	120.3	C10—C11—H11	119.6
C1—C2—H2	120.3	C12—C11—H11	119.6
C2—C3—C4	121.2 (2)	O1—C12—C13	125.1 (3)
C2—C3—Br1	118.7 (2)	O1—C12—C11	115.9 (2)
C4—C3—Br1	120.0 (2)	C13—C12—C11	119.0 (2)
C3—C4—C5	119.1 (2)	C14—C13—C12	119.5 (3)
C3—C4—H4	120.4	C14—C13—H13	120.2
C5—C4—H4	120.4	C12—C13—H13	120.2
C4—C5—C6	120.9 (2)	C9—C14—C13	121.9 (2)
C4—C5—H5	119.6	C9—C14—H14	119.1
C6—C5—H5	119.6	C13—C14—H14	119.1
C5—C6—C1	118.9 (2)	O1—C15—H15A	109.5
C5—C6—C7	117.8 (2)	O1—C15—H15B	109.5
C1—C6—C7	123.3 (2)	H15A—C15—H15B	109.5
O2—C7—N1	124.1 (3)	O1—C15—H15C	109.5
O2—C7—C6	121.8 (3)	H15A—C15—H15C	109.5
N1—C7—C6	114.0 (2)	H15B—C15—H15C	109.5
N2—C8—C9	121.9 (2)		

Hydrogen-bond geometry (Å, °)

Cg1 and Cg2 are the centroids of the C1–C6 and C9–C14 rings, respectively.

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1N \cdots O2 ⁱ	0.86	2.40	3.193 (3)	154
C8—H8 \cdots O2 ⁱ	0.93	2.43	3.240 (3)	146
C2—H2 \cdots Cg2 ⁱⁱ	0.93	2.81	3.531 (4)	135
C5—H5 \cdots Cg1 ⁱⁱⁱ	0.93	2.89	3.553 (4)	130
C10—H10 \cdots Cg1 ^{iv}	0.93	2.86	3.549 (4)	132

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