Crystal and geometry-optimized structure, and Hirshfeld surface analysis of 1-(2-bromoethyl)-indoline-2,3-dione

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In the title compound, $C_{10}H_8BrNO_2$, the isatin ($1H$-indole-2,3-dione) moiety is nearly planar (r.m.s. deviation = 0.026 Å). In the crystal, molecules are linked by C—H···O hydrogen bonds, forming layers parallel to the ab plane, and enclosing $R_4^4(24)$ loops. There are a low percentage (19.3%) of intermolecular H···H contacts in the structure, as estimated by the analysis of Hirshfeld surfaces. This could be due to the presence of the Br atom, present in the bromoethylene group, which makes ca 18.7% Br···H contacts.

1. Chemical context

Isatin ($1H$-indole-2,3-dione) is an endogenous compound that has been identified in humans and possesses a wide range of biological activities, such as anxiogenic and sedative activities. It serves as a synthetically useful substrate which can be used to prepare a broad range of heterocyclic compounds, including molecules of pharmacological significance (Bekircan & Bektas, 2008). A variety of biological activities are associated with isatin, including central nervous system (CNS) activities (Raj, 2012). As part of our interest in the identification of bioactive compounds, we report herein on the synthesis, the crystal structure, and the geometry optimization and Hirshfeld surface analysis of the title isatin derivative, (I).
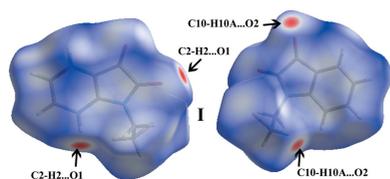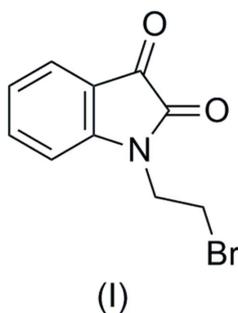
2. Structural commentary

The molecular structure of the title isatin derivative, (I), is illustrated in Fig. 1. It crystallized in the orthorhombic space group $P2_12_12_1$ with an absolute structure parameter of 0.015 (8). The bond lengths and angles of the isatin moiety are comparable with those reported for similar N-substituted isatin derivatives (Qachchachi et al., 2016a,b).

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C2—H2⋯O1[i]	0.93	2.41	3.286 (6)	156
C10—H10A⋯O2[ii]	0.97	2.42	3.309 (6)	151

Symmetry codes: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$.
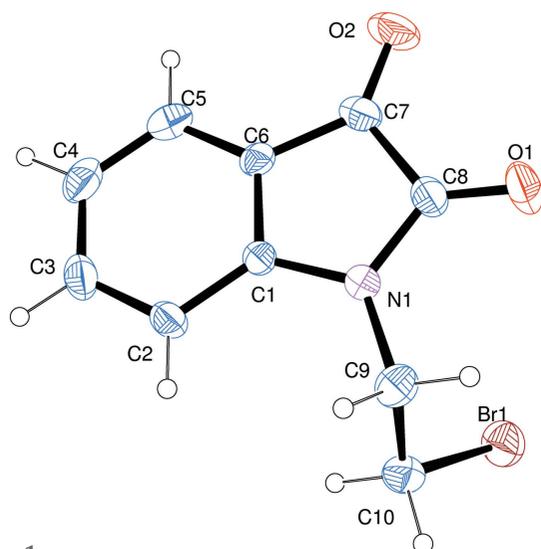
In compound (I), the isatin ring system is almost planar, with an r.m.s. deviation of the fitted atoms C1–C8/N1/O1/O2 of 0.026 Å. The sum of the bond angles around atom N1 is *ca* 360°, indicating little evidence for the presence of an sp^3 lone pair.

3. Supramolecular features
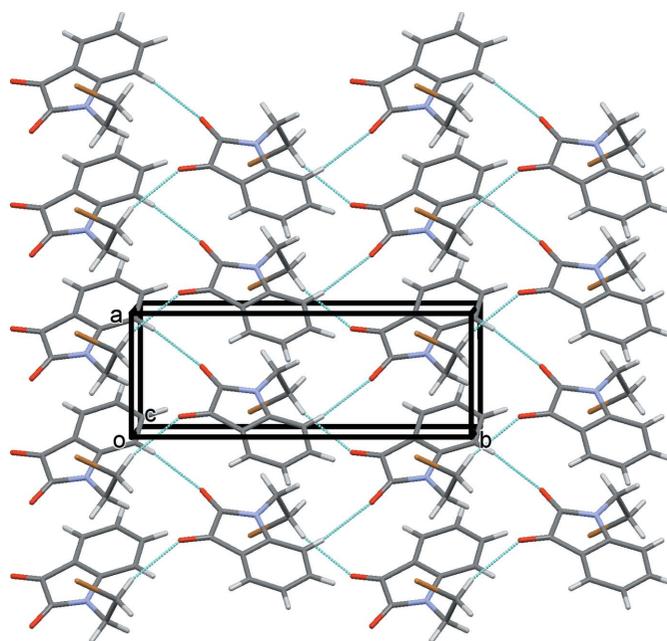
In the crystal of (I), molecules are linked by C—H⋯O hydrogen bonds, *viz* C2—H2⋯O1 and C10—H10A⋯O2 (Table 1), which individually form $C(6)$ and $C(7)$ chains, respectively. Together they form layers parallel to the *ab* plane and enclose $R_4^4(24)$ loops (Table 1 and Fig. 2). An analysis of the crystal packing of (I) indicated that no further significant intermolecular interactions were present (*PLATON*; Spek, 2009).

4. Database survey

A search of the Cambridge Structural Database (Version 5.37, update May 2016; Groom *et al.*, 2016) for *N*-substituted isatin derivatives yielded 58 hits. These include five reports of the structure of isatin itself and four reports of the structure of *N*-methylisatin. 13 of the structures involve an alkyl chain of two or more C atoms. The compound most similar to the title compound is 1-(3-bromopropyl)-1*H*-indole-2,3-dione (AKO-BIN), whose structure was published very recently (Qach-
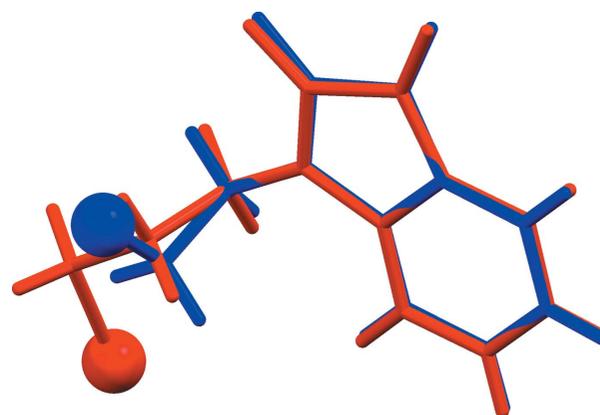

Figure 2
A view along the *c* axis of the crystal packing of compound (I). The hydrogen bonds are shown as dashed lines (see Table 1) and, for clarity, only H atoms H2 and H10A have been included.

chachi *et al.*, 2016*a*). A view of the structural overlap of this compound with that of compound (I) is shown in Fig. 3.

5. Geometry optimization

The geometry optimization of compound (I) was performed using the density functional theory (DFT) method with a 6-311++G** basis set. The crystal structure in the solid state was used as the starting structure for the calculations. The DFT calculations are performed with the *GAUSSIAN09* program package (Frisch *et al.*, 2013). The resulting geometrical parameters are compared with those obtained from an X-ray crystallography study. A superimposed analysis of (I) with its optimized structure gives an r.m.s. deviation of 0.068 Å

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

Figure 3
The structural fit of compound (I) and 1-(3-bromopropyl)-1*H*-indole-2,3-dione (AKOBIN; Qachchachi *et al.*, 2016*a*); molecules are shown in blue and red, respectively.
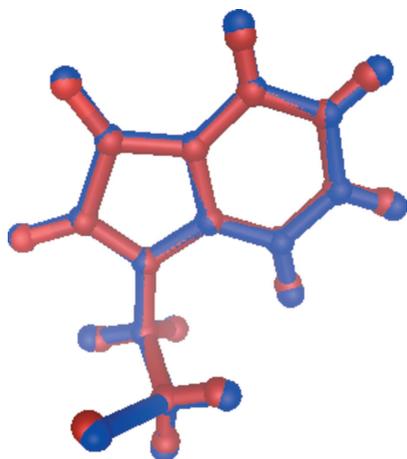
Figure 4
Superimposed fit of the molecule of compound (I) in the crystalline state (red) and after energy minimization (blue).
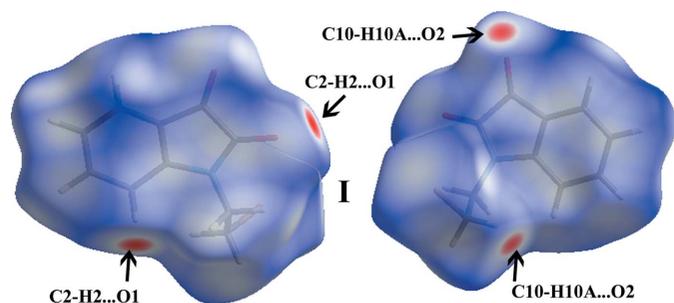
(Fig. 4). This indicates a twist leading to further separation between the isatin moiety and the benzene ring. Also, this suggests that the crystal packing could be influenced by the collective effect of the intermolecular interactions. To probe further, structure-based theoretical parameters, *viz.* HOMO and LUMO energy levels, total energy and dipole moment, were calculated and found to be −6.860 eV, −3.091 eV, −86134.81 eV and 7.2176 Debye, respectively. As a further structure-based test, semi-empirical molecular orbital calculations are carried out using the PM7 method in *MOPAC2012* (Stewart, 2012; Maia *et al.*, 2012). The PM7 method gave the HOMO and LUMO energy levels, total energy and dipole moment as −9.276 eV, −1.271 eV, −2334.96 eV and 5.8952 Debye, respectively. Also, the superimposed analysis of the X-ray structure with the isolated molecule in the gas phase by the PM7 method gave an r.m.s. deviation of 0.211 Å. Further, the N1—C8 and N1—C1 (X-ray: 1.367 Å; DFT: 1.392 Å; PM7: 1.424 Å) bond lengths increased, while the bond angles O2—C7—C6 (X-ray: 131.3°; DFT: 130.8°; PM7: 131.2°) and O1—C8—N1 (X-ray: 127.4°; DFT: 126.8°; PM7: 123.8°) decreased. These confirm the influence of the packing interactions in the solid state of the molecule. The relative conformation about the bond joining the isatin and bromoethylene moieties of (I) is defined by the N1—C9—C10—Br1 torsion angle of

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_8BrNO_2$
M_r	254.08
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, b, c (Å)	4.6834 (2), 12.9567 (7), 16.1130 (8)
V (Å^3)	977.76 (8)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	4.18
Crystal size (mm)	$0.25 \times 0.20 \times 0.20$
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.419, 0.498
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8226, 3150, 1663
R_{int}	0.037
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.762
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.055, 0.084, 1.02
No. of reflections	3150
No. of parameters	127
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.70, −0.59
Absolute structure	Flack x determined using 503 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.015 (8)

Computer programs: *APEX2*, *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *QMOL* (Gans & Shalloway, 2001), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

62.0 (5)°. This indicates that the conformation of the molecule is (+)-synclinal.

6. Hirshfeld surface analysis

A detailed Hirshfeld surface analysis is useful for identifying the various intermolecular interactions and intermolecular contacts present in crystal structures, with the aid of decomposed two-dimensional fingerprint plots. The Hirshfeld surface (HS) and the two-dimensional fingerprint plots were generated based on the d_i and d_e distances using *Crystal Explorer* (Wolff *et al.*, 2012); d_i is the distance from the nearest atom inside the surface, while d_e is the distance from the HS to the nearest atom outside the surface. This analysis identified the various intermolecular contacts (O—H, H—H, C—H, C—C and H—Br) and their relative contributions in the crystal structure. The bond lengths (C—H = 1.083 Å, N—H = 1.009 Å and O—H = 0.983 Å) were adjusted to typical neutron diffraction values before the HS calculation (Venkatesan *et al.*, 2015, 2016a,b). In Hirshfeld surface diagrams, the contacts with distances shorter than the sum of the van der Waals radii are indicated as red and the contacts with distances longer than the van der Waals radii are represented as blue, whereas the contacts with distances equal to the sum of the van der Waals radii are indicated as white. The HS area of compound

Figure 5
Views of the Hirshfeld surfaces mapped with d_{norm} in two different orientations for compound (I). The represented interactions are labelled (see Table 1).

Figure 6
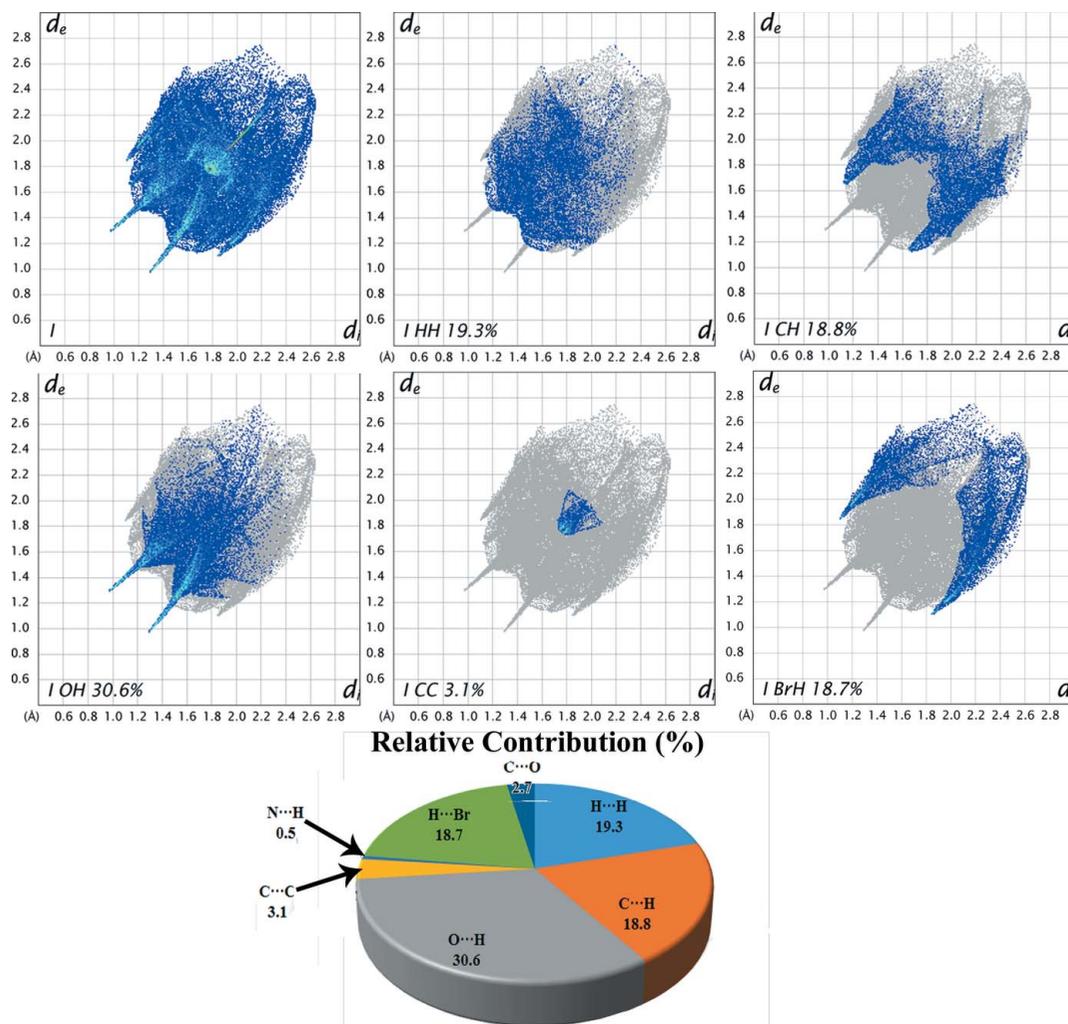Decomposed two-dimensional fingerprint plots for compound (I). Various close contacts and their relative contributions are indicated.

(I) is shown in Fig. 5, and the respective points of inter-molecular interactions are labelled.

Two-dimensional fingerprint plots are used to quantify and visualize the intermolecular interactions present in the crystal structure and the same for the title compound is shown in Fig. 6. The result suggests that the share of intermolecular H···H contacts in (I) is about 19.3%. The low percentage could be attributed to the presence of the Br atom in the bromoethylene group, which makes *ca* 18.7% contacts with H atoms (Br···H). The next significant intermolecular contacts observed in the structure, *i.e.* O···H, C···H and C···C, have relative contributions of 30.6, 18.8 and 3.1%, respectively.

7. Synthesis and crystallization

To a solution of 1-{2-[(2-bromoethyl)amino]phenyl}ethanone (1 equivalent) in DMSO were added I_2 (0.1 equivalents) and TBHP (1 equivalent, 70% in H_2O) at ambient temperature, and the mixture was heated to 353 K. The progress of the reaction was monitored by thin-layer chromatography. Upon completion, the reaction mixture was allowed to cool to ambient temperature and was quenched with aqueous sodium thiosulfate and ethyl acetate. The organic phase was separated, dried over Na_2SO_4, filtered and concentrated. The crude product was purified by silica-gel column chromatography using hexane–ethyl acetate (9:1 *v/v*) as eluent. The title compound was obtained as a red solid (yield: 71%, 74.5 mg; m.p. 404–406 K). It was dissolved in a mixture of hexane–ethyl acetate (9:1 *v/v*) and left to slowly evaporate at room temperature, yielding brown block-like crystals after a period of 3 d.

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were included in calculated positions and treated as riding, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

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References

Bekircan, O. & Bektas, H. (2008). *Molecules*, **13**, 2126–2135.

Bruker (2004). *APEX2*, *SAINT*, *XPREP* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., *et al.* (2013). *GAUSSIAN09*. Gaussian, Inc., Wallingford, CT, USA.

Gans, J. & Shalloway, D. (2001). *J. Mol. Graph. Model.* **19**, 557–559.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.

Maia, J. D. C., Carvalho, G. A. U., Mangueira, C. P. Jr, Santana, S. R., Cabral, L. A. F. & Rocha, G. B. (2012). *J. Chem. Theory Comput.* **8**, 3072–3081.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Qachchachi, F. Z., Kandri Rodi, Y., Haoudi, H., Essassi, E. M., Capet, F. & Zouihri, H. (2016*a*). *IUCrData*, **1**, x160593.

Qachchachi, F. Z., Kandri Rodi, Y., Haoudi, H., Essassi, E. M., Capet, F. & Zouihri, H. (2016*b*). *IUCrData*, **1**, x160609.

Raj, V. (2012). *Int. J. Curr. Pharm. Res.* **4**, 1–9.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Stewart, J. J. P. (2012). *MOPAC2012*. http://OpenMOPAC.net.

Venkatesan, P., Rajakannan, V., Venkataramanan, N. S., Ilangovan, A., Sundius, T. & Thamotharan, S. (2016*a*). *J. Mol. Struct.* **1119**, 259–268.

Venkatesan, P., Thamotharan, S., Ilangovan, A., Liang, H. & Sundius, T. (2016*b*). *Spectrochim. Acta A Mol. Biomol. Spectrosc.* **153**, 625–636.

Venkatesan, P., Thamotharan, S., Kumara, R. G. & Ilangovan, A. (2015). *CrystEngComm*, **17**, 904–915.

Wolff, S. K., Grimwood, D. J., McKinnon, J. J., Turner, M. J., Jayatilaka, D. & Spackman, M. A. (2012). *Crystal Explorer*. University of Western Australia.

supporting information

Crystal and geometry-optimized structure, and Hirshfeld surface analysis of 1-(2-bromoethyl)indoline-2,3-dione

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Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* (Bruker, 2004) and *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004) and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: QMOL (Gans & Shalloway, 2001) and *Mercury* (Macrae *et al.*, 2008).; software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

1-(2-Bromoethyl)indoline-2,3-dione

Crystal data

$C_{10}H_8BrNO_2$	$D_x = 1.726$ Mg m^{-3}
$M_r = 254.08$	Melting point: 406 K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 4.6834$ (2) Å	Cell parameters from 2844 reflections
$b = 12.9567$ (7) Å	$\theta = 2.5$–26.7°
$c = 16.1130$ (8) Å	$\mu = 4.18$ mm^{-1}
$V = 977.76$ (8) Å^3	$T = 293$ K
$Z = 4$	Block, brown
$F(000) = 504$	$0.25 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	3150 independent reflections
Radiation source: fine-focus sealed tube	1663 reflections with $I > 2\sigma(I)$
ω and φ scan	$R_{int} = 0.037$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$\theta_{max} = 32.8°$, $\theta_{min} = 2.0°$
$T_{min} = 0.419$, $T_{max} = 0.498$	$h = -7 \rightarrow 6$
8226 measured reflections	$k = -19 \rightarrow 17$
	$l = -22 \rightarrow 18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.055$	
$wR(F^2) = 0.084$	Hydrogen site location: inferred from neighbouring sites
$S = 1.02$	
3150 reflections	H-atom parameters constrained
127 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0167P)^2 + 0.3638P]$
0 restraints	where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.70$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

Absolute structure: Flack x determined using 503 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.015 (8)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.83217 (12)	0.83821 (4)	0.06227 (4)	0.0609 (2)
O1	0.4527 (9)	0.7005 (3)	0.2349 (3)	0.0719 (13)
O2	0.8447 (9)	0.6409 (2)	0.3684 (2)	0.0688 (10)
N1	0.6516 (8)	0.8607 (2)	0.2584 (2)	0.0378 (8)
C1	0.8490 (10)	0.9005 (3)	0.3156 (3)	0.0326 (9)
C2	0.9288 (9)	1.0020 (3)	0.3268 (3)	0.0429 (12)
H2	0.8520	1.0548	0.2947	0.051*
C3	1.1289 (12)	1.0218 (4)	0.3883 (3)	0.0538 (14)
H3	1.1896	1.0894	0.3966	0.065*
C4	1.2414 (10)	0.9446 (4)	0.4377 (4)	0.0572 (14)
H4	1.3755	0.9606	0.4783	0.069*
C5	1.1551 (10)	0.8445 (4)	0.4267 (3)	0.0503 (11)
H5	1.2276	0.7920	0.4599	0.060*
C6	0.9592 (9)	0.8233 (4)	0.3656 (3)	0.0362 (11)
C7	0.8222 (12)	0.7276 (3)	0.3414 (3)	0.0447 (12)
C8	0.6167 (11)	0.7569 (4)	0.2703 (3)	0.0458 (13)
C9	0.4985 (10)	0.9198 (4)	0.1964 (3)	0.0464 (12)
H9A	0.4179	0.9805	0.2227	0.056*
H9B	0.3412	0.8784	0.1757	0.056*
C10	0.6765 (12)	0.9533 (3)	0.1248 (3)	0.0499 (12)
H10A	0.8325	0.9956	0.1451	0.060*
H10B	0.5612	0.9955	0.0881	0.060*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0714 (3)	0.0570 (3)	0.0543 (3)	−0.0008 (3)	0.0059 (3)	−0.0069 (3)
O1	0.090 (3)	0.055 (2)	0.071 (3)	−0.036 (2)	−0.003 (2)	−0.012 (2)
O2	0.102 (3)	0.0323 (18)	0.072 (3)	0.005 (2)	0.013 (3)	0.0138 (17)
N1	0.042 (2)	0.035 (2)	0.036 (2)	−0.0055 (19)	−0.001 (2)	0.0022 (16)
C1	0.038 (2)	0.032 (2)	0.028 (2)	−0.001 (2)	0.007 (2)	−0.0028 (18)
C2	0.057 (3)	0.029 (2)	0.043 (3)	−0.001 (2)	0.006 (2)	0.000 (2)
C3	0.069 (4)	0.045 (3)	0.047 (3)	−0.016 (3)	0.011 (3)	−0.015 (3)
C4	0.060 (3)	0.078 (4)	0.034 (3)	−0.011 (2)	0.003 (3)	−0.007 (3)
C5	0.053 (2)	0.063 (3)	0.036 (3)	0.006 (3)	0.004 (3)	0.008 (3)

C6	0.045 (2)	0.038 (3)	0.026 (3)	0.002 (2)	0.006 (2)	−0.001 (2)
C7	0.060 (3)	0.032 (2)	0.043 (3)	0.003 (3)	0.017 (3)	0.002 (2)
C8	0.058 (3)	0.038 (3)	0.041 (3)	−0.011 (3)	0.010 (3)	−0.005 (2)
C9	0.041 (3)	0.053 (3)	0.045 (3)	0.004 (2)	−0.004 (3)	0.000 (3)
C10	0.061 (3)	0.040 (2)	0.048 (3)	0.005 (3)	−0.005 (3)	0.005 (2)

Geometric parameters (Å, º)

Br1—C10	1.942 (5)	C4—C5	1.370 (7)
O1—C8	1.204 (6)	C4—H4	0.9300
O2—C7	1.210 (5)	C5—C6	1.373 (6)
N1—C8	1.367 (5)	C5—H5	0.9300
N1—C1	1.404 (6)	C6—C7	1.449 (6)
N1—C9	1.449 (6)	C7—C8	1.544 (7)
C1—C2	1.380 (6)	C9—C10	1.488 (7)
C1—C6	1.384 (6)	C9—H9A	0.9700
C2—C3	1.388 (7)	C9—H9B	0.9700
C2—H2	0.9300	C10—H10A	0.9700
C3—C4	1.382 (7)	C10—H10B	0.9700
C3—H3	0.9300		
C8—N1—C1	110.4 (4)	C1—C6—C7	107.2 (4)
C8—N1—C9	123.9 (4)	O2—C7—C6	131.3 (5)
C1—N1—C9	125.7 (4)	O2—C7—C8	123.3 (5)
C2—C1—C6	120.7 (4)	C6—C7—C8	105.4 (4)
C2—C1—N1	128.0 (4)	O1—C8—N1	127.4 (5)
C6—C1—N1	111.2 (4)	O1—C8—C7	126.9 (5)
C1—C2—C3	116.9 (4)	N1—C8—C7	105.7 (4)
C1—C2—H2	121.5	N1—C9—C10	114.3 (4)
C3—C2—H2	121.5	N1—C9—H9A	108.7
C4—C3—C2	122.3 (5)	C10—C9—H9A	108.7
C4—C3—H3	118.8	N1—C9—H9B	108.7
C2—C3—H3	118.8	C10—C9—H9B	108.7
C5—C4—C3	119.9 (5)	H9A—C9—H9B	107.6
C5—C4—H4	120.1	C9—C10—Br1	112.9 (3)
C3—C4—H4	120.1	C9—C10—H10A	109.0
C4—C5—C6	118.6 (5)	Br1—C10—H10A	109.0
C4—C5—H5	120.7	C9—C10—H10B	109.0
C6—C5—H5	120.7	Br1—C10—H10B	109.0
C5—C6—C1	121.5 (4)	H10A—C10—H10B	107.8
C5—C6—C7	131.3 (5)		
C8—N1—C1—C2	−175.9 (5)	C5—C6—C7—O2	−0.3 (9)
C9—N1—C1—C2	2.7 (7)	C1—C6—C7—O2	−178.2 (6)
C8—N1—C1—C6	2.1 (5)	C5—C6—C7—C8	178.1 (5)
C9—N1—C1—C6	−179.4 (4)	C1—C6—C7—C8	0.2 (5)
C6—C1—C2—C3	1.9 (7)	C1—N1—C8—O1	175.8 (5)
N1—C1—C2—C3	179.7 (4)	C9—N1—C8—O1	−2.8 (8)

C1—C2—C3—C4	−1.2 (7)	C1—N1—C8—C7	−1.8 (5)
C2—C3—C4—C5	−0.1 (8)	C9—N1—C8—C7	179.6 (4)
C3—C4—C5—C6	0.7 (8)	O2—C7—C8—O1	2.0 (8)
C4—C5—C6—C1	0.0 (7)	C6—C7—C8—O1	−176.6 (5)
C4—C5—C6—C7	−177.6 (5)	O2—C7—C8—N1	179.6 (5)
C2—C1—C6—C5	−1.4 (7)	C6—C7—C8—N1	1.0 (5)
N1—C1—C6—C5	−179.5 (4)	C8—N1—C9—C10	−107.9 (5)
C2—C1—C6—C7	176.8 (4)	C1—N1—C9—C10	73.7 (6)
N1—C1—C6—C7	−1.3 (5)	N1—C9—C10—Br1	62.0 (5)

Hydrogen-bond geometry (Å, °)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C2—H2⋯O1[i]	0.93	2.41	3.286 (6)	156
C10—H10*A*⋯O2[ii]	0.97	2.42	3.309 (6)	151

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