research communications

Crystal structure, Hirshfeld surface analysis and DFT studies of 5-bromo-1-{2-[2-(2-chloroethoxy)-ethoxy]ethyl}indoline-2,3-dione

Omar Abdellaoui,[a]* Tuncer Hökelek,[b] Frédéric Capet,[c] Catherine Renard,[c] Amal Haoudi,[a] Mohamed Khalid Skalli[a] and Youssef Kandri Rodi[a]

[a]Laboratoire de Chimie Organique Appliquée, Université Sidi Mohamed Ben Abdallah, Faculté des Sciences et Techniques, Route d'immouzzer, BP 2202, Fez, Morocco, [b]Department of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey, and [c]Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181–UCCS–Unité de Catalyse et Chimie du Solide, F-59000 Lille, France. *Correspondence e-mail: abdellaouiomar10@gmail.com

The title compound, $C_{14}H_{15}BrClNO_4$, consists of a 5-bromoindoline-2,3-dione unit linked to a 1-{2-[2-(2-chloroethoxy)ethoxy]ethyl} moiety. In the crystal, a series of C—H···O hydrogen bonds link the molecules to form a supramolecular three-dimensional structure, enclosing $R_2^2(8)$, $R_2^2(12)$, $R_2^2(18)$ and $R_2^2(22)$ ring motifs. π–π contacts between the five-membered dione rings may further stabilize the structure, with a centroid–centroid distance of 3.899 (2) Å. The Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing are from H···H (28.1%), H···O/O···H (23.5%), H···Br/Br···H (13.8%), H···Cl/Cl···H (13.0%) and H···C/C···H (10.2%) interactions. Hydrogen bonding and van der Waals interactions are the dominant interactions in the crystal packing. Density functional theory (DFT) optimized structures at the B3LYP/6-311G(d,p) level are compared with the experimentally determined molecular structure in the solid state. The HOMO—LUMO behaviour was elucidated to determine the energy gap. The chloroethoxyethoxyethyl side chain atoms are disordered over two sets of sites with an occupancy ratio of 0.665 (8):0.335 (6).

1. Chemical context

Heterocycles are a class of chemical compounds in which one atom or more than one carboxyl group is replaced by a heteroatom such as oxygen, nitrogen, phosphorus or sulfur. They are very interesting chemical compounds because of their potential applications in different fields. The most common heterocycles contain nitrogen and oxygen (Pathak & Bahel, 1980; Naik & Malik, 2010; Srivalli *et al.*, 2011). The chemistry of nitrogen compounds is the preferred source for a large number of study subjects in the laboratory. The N atom is present in several natural molecules of pharmacological interest, so many methods have been developed to access nitrogen compounds, especially heterocyclic compounds. Given the biological interest of heterocyclic compounds, we have been interested in synthesizing new polyfunctional heterocyclic systems capable of presenting potential applications. The chemistry of isatin is already well documented due to its wide range of applications, especially in organic synthetic chemistry and medicinal chemistry. The first reports on the syntheses of isatin and isatin-based derivatives can be traced back to the first half of the 19th century, and almost one hundred years after those publications, the review 'The Chemistry of Isatin' showed the versatility of this molecular fragment. This reaction is also used for the synthesis of natural
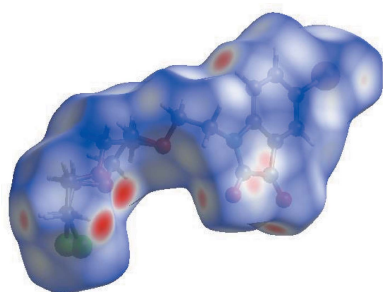
Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots$O1^{vii}	0.93	2.47	3.392 (4)	174
C5—H5$\cdots$O3^{v}	0.93	2.47	3.352 (4)	158
C14—H14$A\cdots$O2^{iii}	0.97	2.50	3.455 (5)	168
C14—H14$B\cdots$O4^{iii}	0.97	2.38	3.302 (6)	161

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

products, such as sugar derivatives (DeShong *et al.*, 1986), β-lactams (Kametani *et al.*, 1988), amino acids (Annuziata *et al.*, 1986) and alkaloids (Asrof Ali *et al.*, 1988), and products with pharmacological interest, such as pyrazolines, which have several biological activities (Araino *et al.*, 1996; Harrison *et al.*, 1996). As a continuation of our research devoted to the development of substituted 5-bromoindoline-2,3-dione derivatives, we report herein the synthesis and molecular and crystal structures, along with the Hirshfeld surface analysis and the density functional theory (DFT) computational calculations carried out at the B3LYP/6-311G(d,p) level, of a 5-bromoindoline-2,3-dione derivative by the alkylation reaction of 5-bromo-1*H*-indole-2,3-dione under phase-transfer catalysis conditions using tetra-*n*-butylammonium bromide (TBAB) as catalyst and potassium carbonate as base, leading to the title compound, (I).
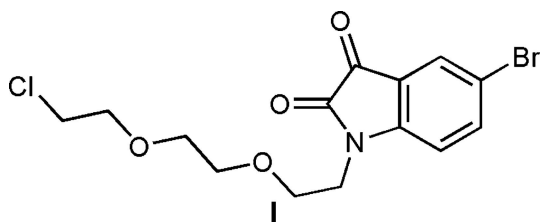
2. Structural commentary

The title compound, (I), consists of an 5-bromoindoline-2,3-dione unit linked to a 1-{2-[2-(2-chloroethoxy)ethoxy]ethyl} moiety (Fig. 1). The planar six- and five-membered benzene and dione rings, *i.e.* A (atoms C1–C6) and B (N1/C1/C6–C8), are oriented at a dihedral angle of A/B = 2.78 (6)°. Atoms Br1, O1 and C9 are at distances of 0.0415 (4), 0.0464 (8) and −0.0244 (7) Å, respectively, from the best plane of the bromoindoline unit. The 1-{2-[2-(2-chloroethoxy)ethoxy]ethyl} moiety is oriented with respect to the bromoindoline unit by 77.7 (2)°, as defined by the C10—C9—N1—C1 torsion angle.
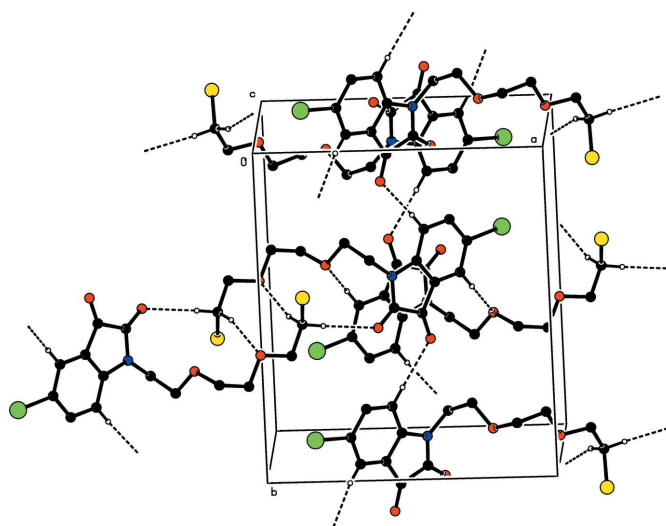
3. Supramolecular features

In the crystal, intermolecular C—H$_{Brmind}\cdots$O$_{Dio}$, C—H$_{Brmind}\cdots$O$_{Ethy}$, C—H$_{Chlethy}\cdots$O$_{Dio}$ and C—H$_{Chlethy}\cdots$O$_{Chlethy}$ (Brmind = bromoindoline, Dio = dione, Ethy = ethoxy and Chlethy = chloroethoxy) hydrogen bonds (Table 1) link the molecules into a three-dimensional structure, enclosing
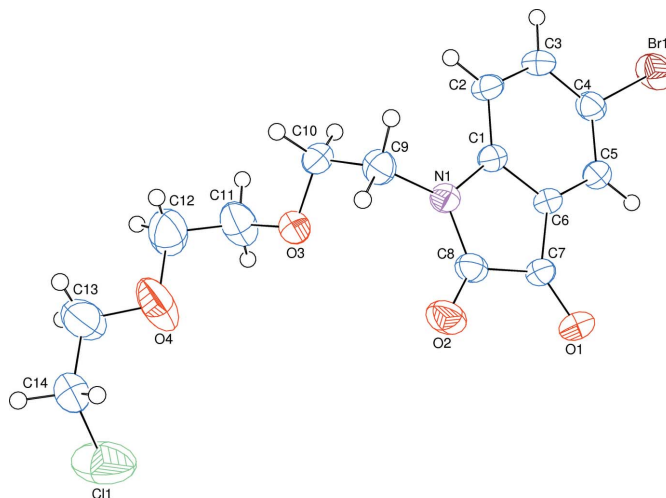
Figure 1
The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Only the major component of disorder is shown for clarity.

$R_2^2(8)$, $R_2^2(12)$, $R_2^2(18)$ and $R_2^2(22)$ ring motifs (Fig. 2). π–π contacts between the five-membered rings, $Cg1-Cg1^i$ [symmetry code: (i) $-x+1, -y+1, -z+1$, where $Cg1$ is the centroid of ring A (atoms N1/C1/C6–C8)], may further stabilize the structure, with a centroid–centroid distance of 3.899 (2) Å. The Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing are from H$\cdots$H (28.1%), H$\cdots$O/O$\cdots$H (23.5%), H$\cdots$Br/Br$\cdots$H (13.8%), H$\cdots$Cl/Cl$\cdots$H (13.0%) and H$\cdots$C/C$\cdots$H (10.2%) interactions. Hydrogen bonding and van der Waals interactions are the dominant interactions in the crystal packing.

Figure 2
A partial packing diagram, viewed down the *c*-axis direction. C—H$_{Brmind}\cdots$O$_{Dio}$, C—H$_{Brmind}\cdots$O$_{Ethy}$, C—H$_{Chlethy}\cdots$O$_{Dio}$ and C—H$_{Chlethy}\cdots$O$_{Chlethy}$ (Brmind = bromoindoline, Dio = dione, Ethy = ethoxy and Chlethy = chloroethoxy) hydrogen bonds are indicated by dashed lines. Only the major component of disorder is shown for clarity.

Table 2
Summary of short interatomic contacts (Å).

Br1···H12C^{i}	3.05	O4···H14B^{iii}	2.38
Cl1···O4	3.188 (5)	O4A···H14D^{iii}	2.48
Cl1A···C11A^{ii}	3.553 (4)	C1···$C7^{v}$	3.542 (4)
Cl1A···O4A	2.720 (14)	C2···C10	3.537 (4)
Cl1···H9B^{iii}	2.92	C5···$C7^{v}$	3.356 (5)
Cl1A···H11D^{ii}	2.99	C5···$C8^{v}$	3.290 (2)
O1···$C2^{iv}$	3.392 (4)	C6···$C7^{v}$	3.251 (4)
O1···O2	2.951 (4)	C6···$C6^{v}$	3.327 (2)
O1···$C10^{iv}$	3.294 (5)	C8···$C8^{vi}$	3.324 (4)
O1···$C1^{v}$	3.397 (4)	C10···C2	3.537 (4)
O2···$C8^{vi}$	3.093 (4)	C12A···O3	2.355 (5)
O2···$N1^{vi}$	3.191 (2)	C2···H9A	2.89
O3···$C5^{v}$	3.352 (5)	C4···H13C^{i}	2.93
O3···$C14^{iii}$	3.415 (4)	C5···H13C^{i}	2.89
O3···O4	2.953 (4)	C9···H2	2.86
O3···N1	2.949 (5)	C10···H12A	2.99
O3A···$C5^{v}$	3.352 (5)	C11···$H5^{v}$	2.84
O3A···N1	2.949 (5)	H2···H9A	2.48
O3A···O4A	2.866 (4)	H2···H10B	2.59
O4···$C14^{iii}$	3.302 (4)	H5···H12D^{v}	2.58
O4A···C14A^{iii}	3.37 (2)	H5···H11A^{v}	2.41
O1···$H2^{iv}$	2.47	H10A···H12A	2.52
O1···H9A^{iv}	2.77	H10A···H11D	2.09
O2···H9B	2.60	H10B···H11B	2.35
O2···$H3^{iv}$	2.85	H10B···H11C	2.34
O2···H14C^{iii}	2.66	H12A···H13B	2.53
O2···H14A^{iii}	2.50	H12B···H13A	2.39
O3···$H5^{v}$	2.47	H12C···H13C	2.07
O3A···$H5^{v}$	2.47	H14B···H14B^{iii}	2.37

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

4. Hirshfeld surface analysis

In order to visualize the intermolecular interactions in the crystal of the title compound, a Hirshfeld surface (HS) analysis (Hirshfeld, 1977; Spackman & Jayatilaka, 2009) was carried out using *CrystalExplorer17.5* (Turner *et al.*, 2017). In the HS plotted over d_{norm} (Fig. 3), the white surface indicates contacts with distances equal to the sum of the van der Waals
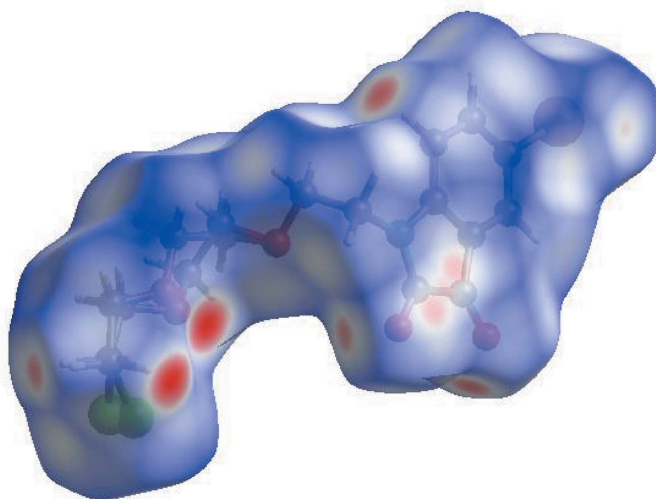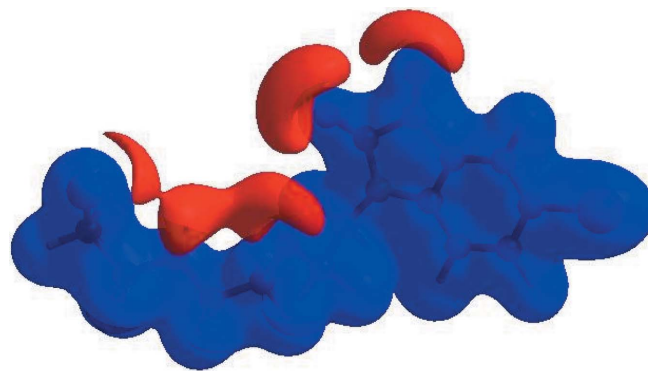

Figure 4
View of the three-dimensional Hirshfeld surface of the title compound plotted over electrostatic potential energy in the range -0.0500 to 0.0500 a.u. using the STO-3G basis set at the Hartree–Fock level of theory. Hydrogen-bond donors and acceptors are shown as blue and red regions around the atoms corresponding to positive and negative potentials, respectively.

radii, and the red and blue colours indicate distances shorter (in close contact) or longer (distinct contact) than the van der Waals radii, respectively (Venkatesan *et al.*, 2016). The bright-red spots appearing near atoms O1, O2 and O4, and H atoms H2, H14A and H14B, indicate their roles as the respective donors and/or acceptors; they also appear as blue and red regions corresponding to positive and negative potentials on the HS mapped over electrostatic potential (Spackman *et al.*, 2008; Jayatilaka *et al.*, 2005), as shown in Fig. 4. The blue regions indicate the positive electrostatic potential (hydrogen-bond donors), while the red regions indicate the negative electrostatic potential (hydrogen-bond acceptors). The shape-index of the HS is a tool to visualize the π–π stacking by the presence of adjacent red and blue triangles; if there are no adjacent red and/or blue triangles, then there are no π–π interactions. Fig. 5 clearly suggests that there is a π–π interaction in (I). The overall two-dimensional fingerprint plot

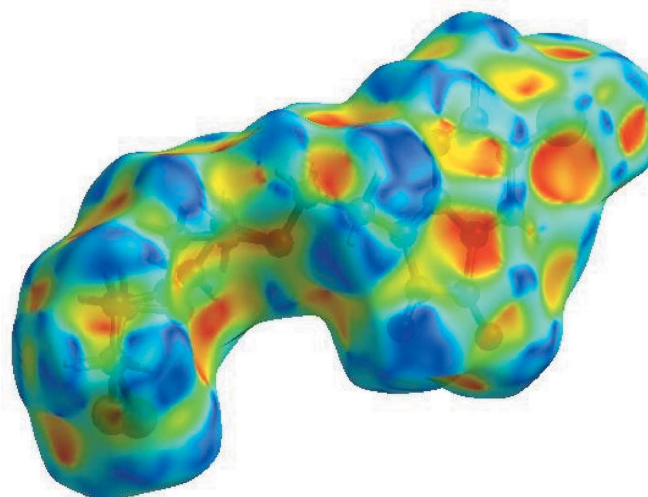**Figure 3**
View of the three-dimensional Hirshfeld surface of the title compound plotted over d_{norm} in the range -0.3481 to 1.0316 a.u.

Figure 5
Hirshfeld surface of the title compound plotted over shape-index.

(Fig. 6*a*) and those delineated into H$\cdots$H, H$\cdots$O/O$\cdots$H, H$\cdots$Br/Br$\cdots$H, H$\cdots$Cl/Cl$\cdots$H, H$\cdots$C/C$\cdots$H, O$\cdots$C/C$\cdots$O, C$\cdots$C and O$\cdots$Cl/Cl$\cdots$O contacts (McKinnon *et al.*, 2007) are illustrated in Figs. 6(*b*)–(*i*), respectively, together with their relative contributions to the Hirshfeld surface. The most important interaction is H$\cdots$H, contributing 28.1% to the overall crystal packing, which is reflected in Fig. 6(*b*) as widely scattered points of high density due to the large hydrogen content of the molecule with the tip at $d_e = d_i \sim 1.08$ Å, due to the short interatomic H$\cdots$H contacts (Table 2). The pair of characteristic wings resulting in the fingerprint plot delineated into H$\cdots$O/O$\cdots$H contacts (Fig. 6*c*), with a 23.5% contribution to the HS, arises from the H$\cdots$O/O$\cdots$H contacts (Table 2) and is viewed as a pair of spikes with the tips at $d_e + d_i = 2.10$ Å. The pairs of scattered points of wings resulting in the fingerprint plots delineated into H$\cdots$Br/Br$\cdots$H (Fig. 6*d*) and H$\cdots$Cl/Cl$\cdots$H (Fig. 6*e*) contacts, with 13.8 and 13.0% contributions to the HS, have nearly symmetrical distributions of points with the edges at $d_e + d_i = 2.92$ (for thin edge) and

3.20 Å (for thick edge) and $d_e + d_i = 2.78$ Å, respectively, arising from the H$\cdots$Br/Br$\cdots$H and H$\cdots$Cl/Cl$\cdots$H contacts (Table 2). In the absence of C—H$\cdots\pi$ interactions, with a pair of characteristic wings resulting in the fingerprint plot delineated into H$\cdots$C/C$\cdots$H contacts (Fig. 6*f*), a 10.2% contribution to the HS, arises from the H$\cdots$C/C$\cdots$H contacts (Table 2) and is seen as a thick pair of spikes with the tips at $d_e + d_i = 2.82$ Å. The pair of characteristic wings resulting in the fingerprint plot delineated into O$\cdots$C/C$\cdots$O contacts (Fig. 6*g*), with a 4.0% contribution to the HS, arises from the O$\cdots$C/C$\cdots$O contacts (Table 2) and is seen as a pair of spikes with the tips at $d_e + d_i = 3.05$ Å. The C$\cdots$C contacts (Fig. 6*h*), with a 2.6% contribution to the HS, have a nearly arrow-shaped distribution of points arising from the C$\cdots$C contacts (Table 2) and is seen with the tip at $d_e = d_i \sim 1.62$ Å. Finally, the pair of scattered points of wings resulting in the fingerprint plot delineated into O$\cdots$Cl/Cl$\cdots$O (Fig. 6*i*) contacts, with a 1.1% contribution to the HS, have nearly symmetrical distributions of points with the edge at $d_e + d_i = 3.50$ Å.
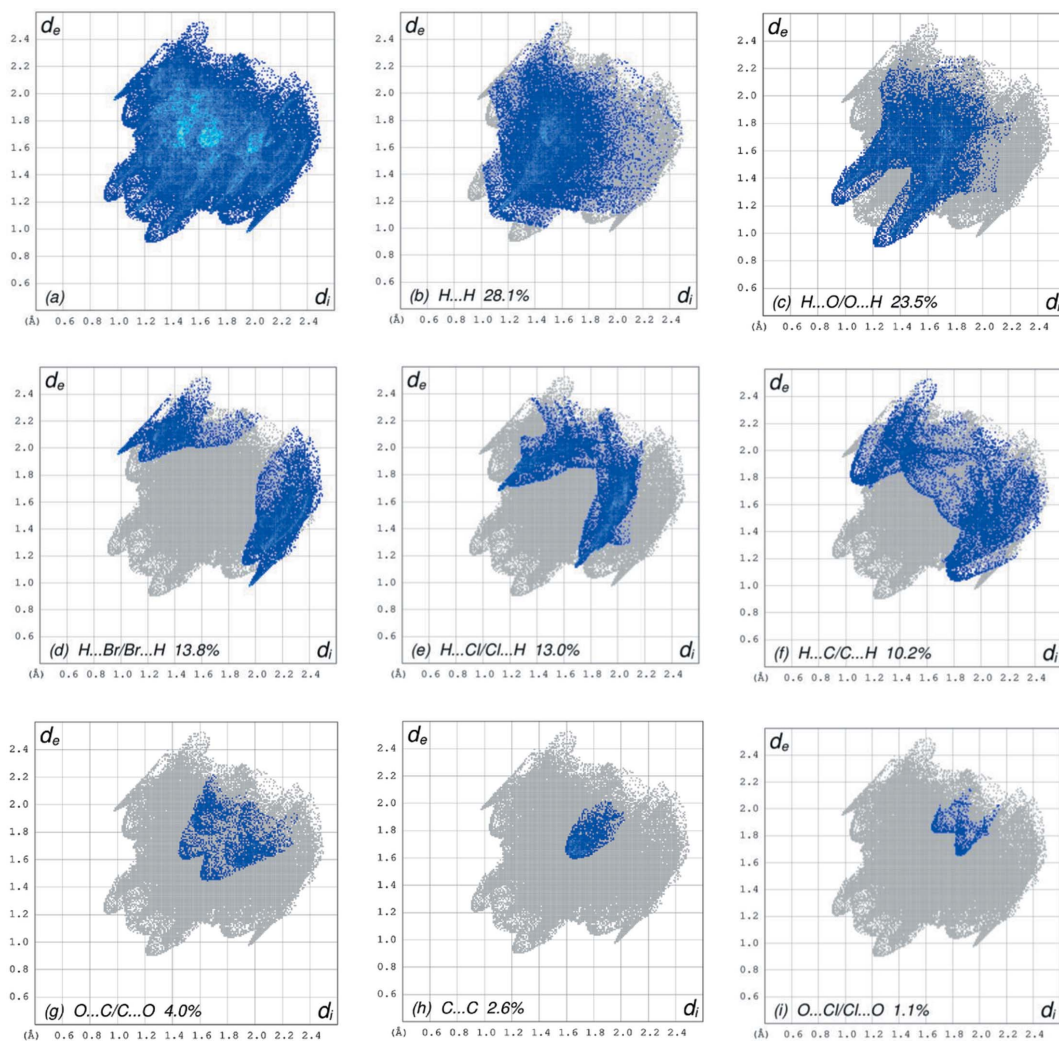
Figure 6
The full two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) H$\cdots$H, (*c*) H$\cdots$O/O$\cdots$H, (*d*) H$\cdots$Br/Br$\cdots$H, (*e*) H$\cdots$Cl/Cl$\cdots$H, (*f*) H$\cdots$C/C$\cdots$H, (*g*) O$\cdots$C/C$\cdots$O, (*h*) C$\cdots$C and (*i*) O$\cdots$Cl/Cl$\cdots$O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface contacts.

The Hirshfeld surface representations with the function d_{norm} plotted onto the surface are shown for the H···H, H···O/O···H, H···Br/Br···H, H···Cl/Cl···H and H···C/C···H interactions in Figs. 7(a)–(e), respectively.

The Hirshfeld surface analysis confirms the importance of H-atom contacts in establishing the packing. The large number of H···H, H···C/C···H and H···O/O···H interactions suggest that van der Waals interactions and hydrogen bonding play the major roles in the crystal packing (Hathwar *et al.*, 2015).

5. DFT calculations

The optimized structure of the title compound, (I), in the gas phase was generated theoretically *via* density functional theory (DFT) using standard B3LYP functional and 6-311G(d,p) basis-set calculations (Becke, 1993), as implemented in *GAUSSIAN09* (Frisch *et al.*, 2009). The theoretical and experimental results were in good agreement (Table 4). The highest-occupied molecular orbital (HOMO), acting as an electron donor, and the lowest-unoccupied molecular orbital (LUMO), acting as an electron acceptor, are very important
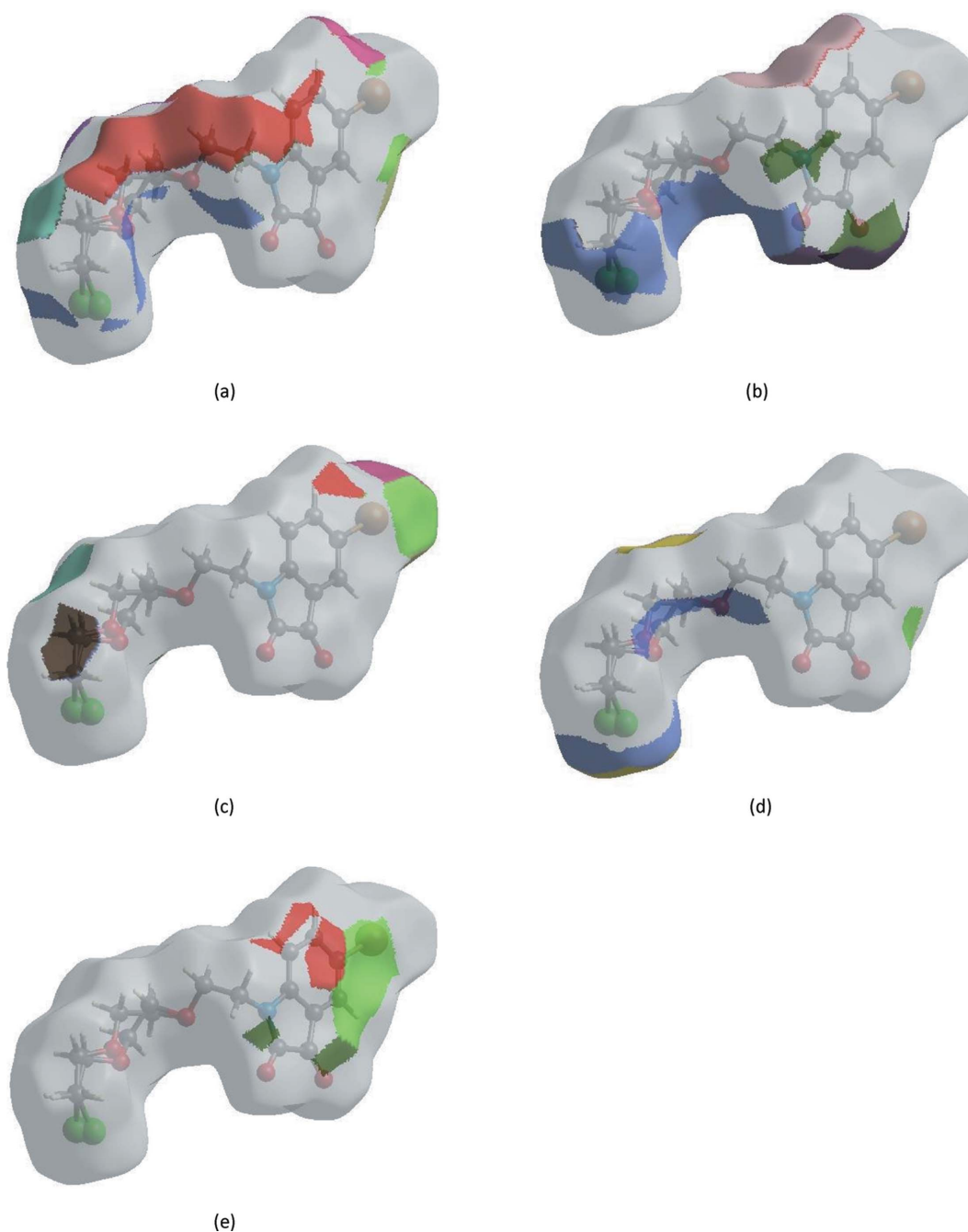

Figure 7
The Hirshfeld surface representations with the function d_{norm} plotted onto the surface for (a) H···H, (b) H···O/O···H, (c) H···Br/Br···H, (d) H···Cl/Cl···H and (e) H···C/C···H interactions.

parameters for quantum chemistry. When the energy gap is small, the molecule is highly polarizable and has high chemical reactivity. The electron transition from the HOMO to the LUMO energy level is shown in Fig. 8. The HOMO and LUMO are localized in the plane extending from the whole 1-{2-[2-(2-chloroethoxy)ethoxy]ethyl}-5-bromoindoline-2,3-dione ring. The energy band gap ($\Delta E = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}$) of the molecule was about 6.5402 eV, and the frontier molecular orbital energies, *i.e.* E_{HOMO} and E_{LUMO}, were −7.4517 and −0.9115 eV, respectively.

6. Database survey

A non-alkylated analogue, namely 5-chloroindoline-2,3-dione has been reported (Wei *et al.*, 2010), as well as three similar structures, namely 1-tetradecylindoline-2,3-dione (Mamari *et al.*, 2010), 5-fluoro-1-(prop-2-en-1-yl)-2,3-dihydro-1*H*-indole-2,3-dione (Qachchachi *et al.*, 2017) and 1-(morpholinomethyl)indoline-2,3-dione (Tang *et al.*, 2010).

7. Synthesis and crystallization

1,2-Bis(2-chloroethoxy)ethane (0.26 ml, 1.86 mmol) was added dropwise to a solution of 5-bromo-1*H*-indole-2,3-dione (0.4 g, 1.76 mmol) and dimethylformamide (DMF, 20 ml) in potassium carbonate (0.6 g, 4.4 mmol) and tetra-*n*-butylammonium bromide (0.1 g, 4.4 mmol). The mixture was stirred at 353 K for 48 h. The reaction was controlled by CCM. The solution was filtered and the DMF was removed under vacuum. The product obtained was separated by chromatography on a column of silica gel with hexane–ethyl acetate (4:1
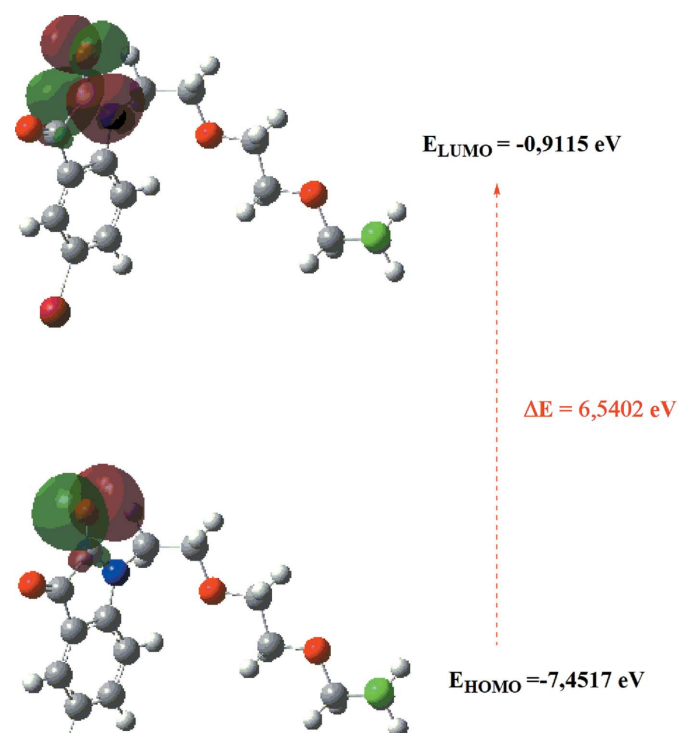
Figure 8
The energy band gap of the title compound.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{15}BrClNO_4$
M_r	376.63
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	300
a, b, c (Å)	12.4682 (4), 14.6397 (5), 8.3524 (3)
β (°)	91.392 (2)
V (Å^3)	1524.12 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.89
Crystal size (mm)	0.25 × 0.22 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
$T_{\min}, T_{\max}$	0.573, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36235, 4608, 3442
R_{int}	0.030
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.713
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.099, 1.04
No. of reflections	4608
No. of parameters	245
No. of restraints	11
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å^{-3})	0.77, −0.69

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

v/v) as eluent. The isolated solid was recrystallized from ethanol to afford red crystals (yield 48%, m.p. 349 K).

8. Refinement

The experimental details, including the crystal data, data collection and refinement, are summarized in Table 3. H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{C})$. During the refinement process, the disordered chloroethoxyethoxyethyl side-chain atoms were refined with a major–minor occupancy ratio of 0.665 (8):0.335 (6).

References

Araino, N., Miura, J., Oda, Y. & Nishioka, H. (1996). *Chem. Abstr.* **125**, 300995.

research communications

Asrof Ali, S., Khan, J. H. & Wazeer, M. I. M. (1988). *Tetrahedron*, **44**, 5911–5920.

Becke, A. D. (1993). *J. Chem. Phys.* **98**, 5648–5652.

Bruker (2016). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

DeShong, P., Leginus, J. M. & Lander, S. W. (1986). *J. Org. Chem.* **51**, 574–576.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Frisch, M. J., *et al.* (2009). *GAUSSIAN09*. Gaussian Inc., Wallingford, CT, USA.

Harrison, C. R., Lett, R. M., Mccann, S. F., Shapiro, R. & Stevenson, T. M. (1996). *Chem. Abstr.* **124**, 202246.

Hathwar, V. R., Sist, M., Jørgensen, M. R. V., Mamakhel, A. H., Wang, X., Hoffmann, C. M., Sugimoto, K., Overgaard, J. & Iversen, B. B. (2015). *IUCrJ*, **2**, 563–574.

Hirshfeld, H. L. (1977). *Theor. Chim. Acta*, **44**, 129–138.

Jayatilaka, D., Grimwood, D. J., Lee, A., Lemay, A., Russel, A. J., Taylor, C., Wolff, S. K., Cassam-Chenai, P. & Whitton, A. (2005). *TONTO – A System for Computational Chemistry*. http://hirshfeldsurface.net/.

Kametani, T., Chu, S. D. & Honda, T. (1988). *J. Chem. Soc. Perkin Trans. 1*, pp. 1593–1597.

Mamari, K., Zouihri, H., Essassi, E. M. & Ng, S. W. (2010). *Acta Cryst.* E**66**, o1410.

McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2007). *Chem. Commun.* pp. 3814–3816.

Naik, C. G. & Malik, C. M. (2010). *Orient. J. Chem.* **26**, 113–116.

Pathak, R. B. & Bahel, S. C. (1980). *J. Indian Chem. Soc.* **57**, 1108–1111.

Qachchachi, F.-Z., Mague, J. T., Kandri Rodi, Y., Haoudi, A., Ouzidan, Y. & Essassi, E. M. (2017). *IUCrData*, **2**, x170028.

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

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

Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.

Spackman, M. A., McKinnon, J. J. & Jayatilaka, D. (2008). *CrystEngComm*, **10**, 377–388.

Srivalli, T., Satish, K. & Suthakaran, R. (2011). *Int. J. Innov. Pharm. Res.* **2**, 172–174.

Tang, Y., Zhang, J., Miao, Y. & Chen, G. (2010). *Acta Cryst.* E**66**, o1748.

Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17*. The University of Western Australia.

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

Wei, W.-B., Tian, S., Zhou, H., Sun, J. & Wang, H.-B. (2010). *Acta Cryst.* E**66**, o3024.

supporting information

Crystal structure, Hirshfeld surface analysis and DFT studies of 5-bromo-1-{2-[2-(2-chloroethoxy)ethoxy]ethyl}indoline-2,3-dione

Omar Abdellaoui, Tuncer Hökelek, Frédéric Capet, Catherine Renard, Amal Haoudi, Mohamed Khalid Skalli and Youssef Kandri Rodi

Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

5-Bromo-1-{2-[2-(2-chloroethoxy)ethoxy]ethyl}indoline-2,3-dione

Crystal data

$C_{14}H_{15}BrClNO_4$	$F(000) = 760$
$M_r = 376.63$	$D_x = 1.641$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 12.4682$ (4) Å	Cell parameters from 9939 reflections
$b = 14.6397$ (5) Å	$\theta = 2.8$–$26.1°$
$c = 8.3524$ (3) Å	$\mu = 2.89$ mm^{-1}
$\beta = 91.392$ (2)°	$T = 300$ K
$V = 1524.12$ (9) Å^3	Plate, red
$Z = 4$	$0.25 \times 0.22 \times 0.07$ mm

Data collection

Bruker APEXII CCD diffractometer	4608 independent reflections
φ and ω scans	3442 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2016)	$R_{int} = 0.030$
	$\theta_{max} = 30.5°$, $\theta_{min} = 1.6°$
$T_{min} = 0.573$, $T_{max} = 0.746$	$h = -17 \rightarrow 17$
	$k = -20 \rightarrow 20$
36235 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Primary atom site location: dual
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.038$	
$wR(F^2) = 0.099$	Hydrogen site location: inferred from neighbouring sites
$S = 1.04$	
4608 reflections	H-atom parameters constrained
245 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.8377P]$
11 restraints	where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{min} = -0.69$ e Å^{-3}

$\Delta\rho_{max} = 0.77$ 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.

Refinement. At the end of the refinement, it remained some residual electronic density pics around O4 and C12. suggesting a disorder. We modeled this disorder considering two positions with following occupancies : 0.665 (7) and 0.335 (7). The R1(Fo > 4sig(Fo)) factor decreased from 5.96% to 3.76%.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.82107 (2)	0.34602 (2)	0.67781 (3)	0.06075 (11)	
O1	0.57179 (13)	0.62280 (10)	0.3141 (2)	0.0521 (4)	
O2	0.40213 (12)	0.55268 (11)	0.09446 (18)	0.0497 (4)	
N1	0.45304 (12)	0.41469 (10)	0.21008 (18)	0.0339 (3)	
C1	0.53610 (14)	0.38646 (12)	0.3166 (2)	0.0308 (3)	
C2	0.56401 (15)	0.29844 (12)	0.3613 (2)	0.0355 (4)	
H2	0.526977	0.248176	0.320193	0.043*	
C3	0.64948 (16)	0.28779 (13)	0.4700 (2)	0.0380 (4)	
H3	0.670281	0.229390	0.501726	0.046*	
C4	0.70420 (15)	0.36307 (13)	0.5319 (2)	0.0380 (4)	
C5	0.67705 (15)	0.45129 (13)	0.4869 (2)	0.0366 (4)	
H5	0.713826	0.501486	0.528804	0.044*	
C6	0.59299 (14)	0.46176 (12)	0.3772 (2)	0.0320 (3)	
C7	0.54778 (15)	0.54334 (12)	0.3003 (2)	0.0364 (4)	
C8	0.45658 (15)	0.50726 (13)	0.1861 (2)	0.0364 (4)	
C9	0.38069 (16)	0.35247 (14)	0.1244 (2)	0.0410 (4)	
H9A	0.422101	0.302168	0.082394	0.049*	
H9B	0.347871	0.384527	0.034163	0.049*	
C10	0.29340 (17)	0.31449 (14)	0.2271 (3)	0.0439 (4)	
H10A	0.253843	0.267628	0.168553	0.053*	0.665 (6)
H10B	0.324814	0.287076	0.322966	0.053*	0.665 (6)
H10C	0.253843	0.267628	0.168553	0.053*	0.335 (6)
H10D	0.324814	0.287076	0.322966	0.053*	0.335 (6)
Cl1	−0.1661 (2)	0.5843 (2)	0.1862 (3)	0.0789 (6)	0.665 (6)
O3	0.22328 (11)	0.38602 (10)	0.26936 (19)	0.0453 (3)	0.665 (6)
O4	−0.0082 (4)	0.4132 (3)	0.2056 (7)	0.0581 (10)	0.665 (6)
C11	0.1364 (4)	0.3629 (5)	0.3717 (7)	0.0464 (14)	0.665 (6)
H11A	0.120622	0.414886	0.439200	0.056*	0.665 (6)
H11B	0.158212	0.312658	0.440759	0.056*	0.665 (6)
C12	0.0374 (3)	0.3365 (2)	0.2790 (5)	0.0488 (10)	0.665 (6)
H12A	0.055106	0.291674	0.198247	0.059*	0.665 (6)
H12B	−0.013752	0.309075	0.350326	0.059*	0.665 (6)
C13	−0.1129 (5)	0.4046 (4)	0.1457 (8)	0.0532 (13)	0.665 (6)
H13A	−0.160649	0.392928	0.233262	0.064*	0.665 (6)

H13B	−0.117164	0.353052	0.072902	0.064*	0.665 (6)
C14	−0.1476 (9)	0.4885 (4)	0.0601 (12)	0.0487 (18)	0.665 (6)
H14A	−0.214573	0.476017	0.002703	0.058*	0.665 (6)
H14B	−0.094475	0.503776	−0.018419	0.058*	0.665 (6)
Cl1A	−0.1226 (6)	0.5970 (5)	0.1705 (9)	0.110 (2)	0.335 (6)
O3A	0.22328 (11)	0.38602 (10)	0.26936 (19)	0.0453 (3)	0.335 (6)
O4A	0.0068 (7)	0.4519 (9)	0.2390 (14)	0.085 (4)	0.335 (6)
C11A	0.1332 (8)	0.3392 (7)	0.3356 (18)	0.054 (4)	0.335 (6)
H11C	0.155056	0.306519	0.432005	0.064*	0.335 (6)
H11D	0.103552	0.295654	0.258975	0.064*	0.335 (6)
C12A	0.0522 (6)	0.4099 (7)	0.3732 (10)	0.074 (3)	0.335 (6)
H12C	−0.004449	0.381799	0.433809	0.089*	0.335 (6)
H12D	0.085853	0.456161	0.440578	0.089*	0.335 (6)
C13A	−0.0955 (10)	0.4210 (10)	0.199 (2)	0.074 (4)	0.335 (6)
H13C	−0.137940	0.416172	0.294477	0.089*	0.335 (6)
H13D	−0.091764	0.361186	0.149635	0.089*	0.335 (6)
C14A	−0.145 (2)	0.4874 (8)	0.086 (2)	0.074 (7)	0.335 (6)
H14C	−0.221538	0.475691	0.072880	0.089*	0.335 (6)
H14D	−0.112602	0.483019	−0.018129	0.089*	0.335 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.05356 (15)	0.06387 (18)	0.06366 (17)	0.01132 (11)	−0.02226 (11)	0.00047 (11)
O1	0.0518 (9)	0.0271 (7)	0.0773 (11)	−0.0023 (6)	0.0000 (8)	0.0077 (7)
O2	0.0477 (8)	0.0477 (8)	0.0536 (9)	0.0116 (7)	−0.0019 (7)	0.0146 (7)
N1	0.0340 (7)	0.0309 (8)	0.0368 (8)	0.0009 (6)	−0.0028 (6)	0.0022 (6)
C1	0.0325 (8)	0.0280 (8)	0.0319 (8)	0.0007 (6)	0.0024 (6)	0.0000 (6)
C2	0.0425 (10)	0.0245 (8)	0.0395 (9)	0.0003 (7)	−0.0007 (7)	−0.0035 (7)
C3	0.0445 (10)	0.0277 (8)	0.0418 (10)	0.0067 (7)	0.0006 (8)	0.0018 (7)
C4	0.0350 (9)	0.0396 (10)	0.0392 (9)	0.0051 (7)	−0.0035 (7)	0.0001 (8)
C5	0.0335 (8)	0.0312 (9)	0.0450 (10)	−0.0016 (7)	−0.0004 (7)	−0.0046 (7)
C6	0.0325 (8)	0.0245 (8)	0.0389 (9)	−0.0001 (6)	0.0023 (7)	0.0012 (7)
C7	0.0352 (9)	0.0280 (9)	0.0462 (10)	0.0007 (7)	0.0063 (7)	0.0044 (7)
C8	0.0359 (9)	0.0344 (9)	0.0392 (9)	0.0046 (7)	0.0051 (7)	0.0067 (7)
C9	0.0412 (10)	0.0429 (11)	0.0386 (10)	0.0024 (8)	−0.0072 (8)	−0.0078 (8)
C10	0.0411 (10)	0.0328 (9)	0.0575 (12)	−0.0031 (8)	−0.0088 (9)	−0.0027 (9)
Cl1	0.0912 (14)	0.0695 (10)	0.0751 (9)	0.0155 (10)	−0.0128 (9)	−0.0087 (7)
O3	0.0370 (7)	0.0433 (8)	0.0554 (9)	0.0009 (6)	−0.0002 (6)	0.0048 (7)
O4	0.0359 (19)	0.058 (2)	0.080 (2)	−0.0108 (15)	−0.0116 (14)	0.0262 (18)
C11	0.040 (2)	0.058 (3)	0.041 (2)	−0.0012 (19)	−0.0017 (15)	0.002 (2)
C12	0.0380 (16)	0.046 (2)	0.062 (2)	−0.0052 (13)	−0.0049 (14)	0.0137 (16)
C13	0.040 (2)	0.057 (3)	0.062 (3)	−0.0020 (19)	−0.010 (2)	0.007 (2)
C14	0.039 (3)	0.048 (3)	0.058 (3)	0.007 (2)	−0.009 (2)	0.004 (2)
Cl1A	0.113 (4)	0.077 (3)	0.138 (4)	0.023 (3)	−0.023 (3)	−0.047 (2)
O3A	0.0370 (7)	0.0433 (8)	0.0554 (9)	0.0009 (6)	−0.0002 (6)	0.0048 (7)
O4A	0.030 (3)	0.127 (9)	0.098 (7)	0.001 (5)	−0.001 (3)	0.064 (7)
C11A	0.059 (6)	0.046 (6)	0.056 (8)	0.010 (4)	0.012 (5)	0.016 (5)

C12A	0.051 (4)	0.097 (7)	0.075 (6)	0.015 (4)	0.016 (4)	0.027 (5)
C13A	0.061 (8)	0.074 (8)	0.087 (10)	−0.007 (6)	−0.009 (6)	0.027 (7)
C14A	0.052 (9)	0.102 (14)	0.068 (10)	−0.014 (8)	−0.007 (7)	0.006 (8)

Geometric parameters (Å, º)

Br1—C4	1.8934 (19)	O3—C11	1.436 (5)
O1—C7	1.206 (2)	O4—C12	1.394 (5)
O2—C8	1.210 (2)	O4—C13	1.392 (5)
N1—C1	1.411 (2)	C11—H11A	0.9700
N1—C8	1.371 (2)	C11—H11B	0.9700
N1—C9	1.457 (2)	C11—C12	1.493 (6)
C1—C2	1.384 (2)	C12—H12A	0.9700
C1—C6	1.399 (2)	C12—H12B	0.9700
C2—H2	0.9300	C13—H13A	0.9700
C2—C3	1.392 (3)	C13—H13B	0.9700
C3—H3	0.9300	C13—C14	1.480 (6)
C3—C4	1.389 (3)	C14—H14A	0.9700
C4—C5	1.385 (3)	C14—H14B	0.9700
C5—H5	0.9300	Cl1A—C14A	1.773 (9)
C5—C6	1.384 (2)	O3A—C11A	1.438 (8)
C6—C7	1.463 (2)	O4A—C12A	1.387 (8)
C7—C8	1.558 (3)	O4A—C13A	1.385 (8)
C9—H9A	0.9700	C11A—H11C	0.9700
C9—H9B	0.9700	C11A—H11D	0.9700
C9—C10	1.508 (3)	C11A—C12A	1.485 (9)
C10—H10A	0.9700	C12A—H12C	0.9700
C10—H10B	0.9700	C12A—H12D	0.9700
C10—H10C	0.9700	C13A—H13C	0.9700
C10—H10D	0.9700	C13A—H13D	0.9700
C10—O3	1.415 (3)	C13A—C14A	1.481 (9)
C10—O3A	1.415 (3)	C14A—H14C	0.9700
Cl1—C14	1.772 (6)	C14A—H14D	0.9700
Br1···H12C[i]	3.05	O4···H14B[iii]	2.38
Cl1···O4	3.188 (5)	O4A···H14D[iii]	2.48
Cl1A···C11A[ii]	3.553 (4)	C1···C7[v]	3.542 (4)
Cl1A···O4A	2.720 (14)	C2···C10	3.537 (4)
Cl1···H9B[iii]	2.92	C5···C7[v]	3.356 (5)
Cl1A···H11D[ii]	2.99	C5···C8[v]	3.290 (2)
O1···C2[iv]	3.392 (4)	C6···C7[v]	3.251 (4)
O1···O2	2.951 (4)	C6···C6[v]	3.327 (2)
O1···C10[iv]	3.294 (5)	C8···C8[vi]	3.324 (4)
O1···C1[v]	3.397 (4)	C10···C2	3.537 (4)
O2···C8[vi]	3.093 (4)	C12A···O3	2.355 (5)
O2···N1[vi]	3.191 (2)	C2···H9A	2.89
O3···C5[v]	3.352 (5)	C4···H13C[i]	2.93
O3···C14[iii]	3.415 (4)	C5···H13C[i]	2.89

O3···O4	2.953 (4)	C9···H2	2.86
O3···N1	2.949 (5)	C10···H12A	2.99
O3A···C5ᵛ	3.352 (4)	C11···H5ᵛ	2.84
O3A···N1	2.949 (5)	H2···H9A	2.48
O3A···O4A	2.866 (4)	H2···H10B	2.59
O4···C14ⁱⁱⁱ	3.302 (4)	H5···H12Dᵛ	2.58
O4A···C14Aⁱⁱⁱ	3.37 (2)	H5···H11Aᵛ	2.41
O1···H2ⁱᵛ	2.47	H10A···H12A	2.52
O1···H9Aⁱᵛ	2.77	H10A···H11D	2.09
O2···H9B	2.60	H10B···H11B	2.35
O2···H3ⁱᵛ	2.85	H10B···H11C	2.34
O2···H14Cⁱⁱⁱ	2.66	H12A···H13B	2.53
O2···H14Aⁱⁱⁱ	2.50	H12B···H13A	2.39
O3···H5ᵛ	2.47	H12C···H13C	2.07
O3A···H5ᵛ	2.47	H14B···H14Bⁱⁱⁱ	2.37
C1—N1—C9	124.25 (15)	O3—C11—C12	112.3 (4)
C8—N1—C1	110.85 (15)	H11A—C11—H11B	107.9
C8—N1—C9	124.61 (16)	C12—C11—H11A	109.2
C2—C1—N1	128.23 (16)	C12—C11—H11B	109.2
C2—C1—C6	120.95 (16)	O4—C12—C11	110.0 (4)
C6—C1—N1	110.81 (15)	O4—C12—H12A	109.7
C1—C2—H2	121.2	O4—C12—H12B	109.7
C1—C2—C3	117.63 (16)	C11—C12—H12A	109.7
C3—C2—H2	121.2	C11—C12—H12B	109.7
C2—C3—H3	119.5	H12A—C12—H12B	108.2
C4—C3—C2	121.00 (17)	O4—C13—H13A	109.4
C4—C3—H3	119.5	O4—C13—H13B	109.4
C3—C4—Br1	119.88 (14)	O4—C13—C14	111.1 (6)
C5—C4—Br1	118.47 (14)	H13A—C13—H13B	108.0
C5—C4—C3	121.64 (17)	C14—C13—H13A	109.4
C4—C5—H5	121.3	C14—C13—H13B	109.4
C6—C5—C4	117.33 (17)	Cl1—C14—H14A	108.7
C6—C5—H5	121.3	Cl1—C14—H14B	108.7
C1—C6—C7	107.34 (15)	C13—C14—Cl1	114.2 (6)
C5—C6—C1	121.43 (16)	C13—C14—H14A	108.7
C5—C6—C7	131.22 (17)	C13—C14—H14B	108.7
O1—C7—C6	130.79 (19)	H14A—C14—H14B	107.6
O1—C7—C8	124.15 (18)	C10—O3A—C11A	103.7 (4)
C6—C7—C8	105.05 (15)	C13A—O4A—C12A	113.9 (10)
O2—C8—N1	128.03 (19)	O3A—C11A—H11C	110.3
O2—C8—C7	126.21 (18)	O3A—C11A—H11D	110.3
N1—C8—C7	105.74 (15)	O3A—C11A—C12A	106.9 (7)
N1—C9—H9A	108.9	H11C—C11A—H11D	108.6
N1—C9—H9B	108.9	C12A—C11A—H11C	110.3
N1—C9—C10	113.45 (17)	C12A—C11A—H11D	110.3
H9A—C9—H9B	107.7	O4A—C12A—C11A	113.8 (10)
C10—C9—H9A	108.9	O4A—C12A—H12C	108.8

C10—C9—H9B	108.9	O4A—C12A—H12D	108.8
C9—C10—H10A	109.9	C11A—C12A—H12C	108.8
C9—C10—H10B	109.9	C11A—C12A—H12D	108.8
C9—C10—H10C	109.9	H12C—C12A—H12D	107.7
C9—C10—H10D	109.9	O4A—C13A—H13C	110.1
H10A—C10—H10B	108.3	O4A—C13A—H13D	110.1
H10C—C10—H10D	108.3	O4A—C13A—C14A	108.0 (12)
O3—C10—C9	109.14 (17)	H13C—C13A—H13D	108.4
O3—C10—H10A	109.9	C14A—C13A—H13C	110.1
O3—C10—H10B	109.9	C14A—C13A—H13D	110.1
O3A—C10—C9	109.14 (17)	Cl1A—C14A—H14C	110.5
O3A—C10—H10C	109.9	Cl1A—C14A—H14D	110.5
O3A—C10—H10D	109.9	C13A—C14A—Cl1A	106.2 (10)
C10—O3—C11	117.0 (3)	C13A—C14A—H14C	110.5
C13—O4—C12	117.0 (4)	C13A—C14A—H14D	110.5
O3—C11—H11A	109.2	H14C—C14A—H14D	108.7
O3—C11—H11B	109.2		

Br1—C4—C5—C6	178.48 (14)	C6—C1—C2—C3	0.9 (3)
O1—C7—C8—O2	2.9 (3)	C6—C7—C8—O2	−176.38 (18)
O1—C7—C8—N1	−178.03 (19)	C6—C7—C8—N1	2.66 (19)
N1—C1—C2—C3	−179.67 (18)	C8—N1—C1—C2	−174.80 (18)
N1—C1—C6—C5	178.66 (16)	C8—N1—C1—C6	4.7 (2)
N1—C1—C6—C7	−2.7 (2)	C8—N1—C9—C10	−109.2 (2)
N1—C9—C10—O3	67.1 (2)	C9—N1—C1—C2	−0.8 (3)
N1—C9—C10—O3A	67.1 (2)	C9—N1—C1—C6	178.69 (16)
C1—N1—C8—O2	174.61 (19)	C9—N1—C8—O2	0.7 (3)
C1—N1—C8—C7	−4.4 (2)	C9—N1—C8—C7	−178.36 (16)
C1—N1—C9—C10	77.7 (2)	C9—C10—O3—C11	−178.2 (3)
C1—C2—C3—C4	0.4 (3)	C9—C10—O3A—C11A	168.1 (7)
C1—C6—C7—O1	−179.2 (2)	C10—O3—C11—C12	−91.0 (5)
C1—C6—C7—C8	0.04 (19)	C10—O3A—C11A—C12A	−176.3 (8)
C2—C1—C6—C5	−1.8 (3)	O3—C11—C12—O4	−71.5 (6)
C2—C1—C6—C7	176.82 (16)	O4—C13—C14—Cl1	−69.5 (9)
C2—C3—C4—Br1	−179.34 (15)	C12—O4—C13—C14	−175.5 (6)
C2—C3—C4—C5	−0.8 (3)	C13—O4—C12—C11	−165.7 (5)
C3—C4—C5—C6	−0.1 (3)	O3A—C11A—C12A—O4A	67.7 (13)
C4—C5—C6—C1	1.4 (3)	O4A—C13A—C14A—Cl1A	−48 (2)
C4—C5—C6—C7	−176.87 (19)	C12A—O4A—C13A—C14A	164.5 (14)
C5—C6—C7—O1	−0.8 (4)	C13A—O4A—C12A—C11A	102.8 (13)
C5—C6—C7—C8	178.46 (19)		

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

Hydrogen-bond geometry (Å, º)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C2—H2⋯O1[vii]	0.93	2.47	3.392 (4)	174

C5—H5⋯O3ᵛ	0.93	2.47	3.352 (4)	158
C14—H14A⋯O2ⁱⁱⁱ	0.97	2.50	3.455 (5)	168
C14—H14B⋯O4ⁱⁱⁱ	0.97	2.38	3.302 (6)	161

Symmetry codes: (iii) −x, −y+1, −z; (v) −x+1, −y+1, −z+1; (vii) −x+1, y−1/2, −z+1/2.

Table 4. Comparison of the selected (X-ray and DFT) geometric data (Å, °).

Bonds/angles	X-ray	B3LYP/6-311G(d,p)
Br1—C4	1.8934 (19)	1.94411
Cl1—C14	1.772 (6)	1.88948
O3—C10	1.415 (3)	1.45191
O3—C11	1.436 (5)	1.45378
O2—C8	1.210 (2)	1.23688
O1—C7	1.206 (2)	1.23522
N1—C1	1.411 (2)	1.41761
N1—C8	1.371 (2)	1.39446
N1—C9	1.457 (2)	1.46194
C10—O3—C11	117.0 (3)	116.04457
C1—N1—C9	124.25(15	125.11525
C8—N1—C1	110.8 (2)	110.73581
C8—N1—C9	124.61 (16)	126.01387
C6—C1—N1	110.81 (15)	109.99463
C2—C1—N1	128.23 (16)	129.11525
C2—C1—C6	120.95 (16)	120.88664

Table 5. Calculated energies.

Molecular Energy (a.u.) (eV)	Compound (I)
Total Energy TE (eV)	-106925,446
E_{HOMO} (eV)	-7,4517
E_{LUMO} (eV)	-0,9115
Gap ΔE (eV)	6,5402
Dipole moment μ (Debye)	7,9257
Ionisation potential I (eV)	7,4517
Electron affinity A	0,9115
Electro negativity χ	4,1816
Hardness η	3,2701
Electrophilicity index ω	2,6736
Softness σ	0,3058
Fraction of electron transferred ΔN	0,4301