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Crystal structure and Hirshfeld surface analysis of 4-bromo-6-(4-chlorophenyl)-6,7-dihydro-5*H*-furo[2,3-*f*]isoindol-5-one

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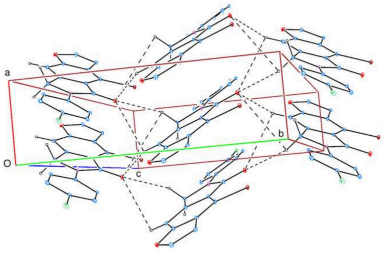
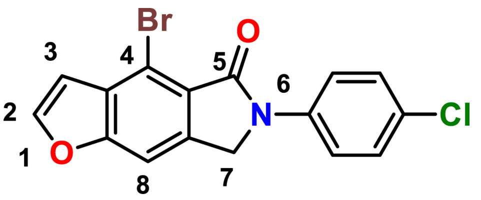
The molecule of the title compound, $C_{16}H_9BrClNO_2$, contains furan and phenyl rings and an isoindole ring system. The phenyl ring subtends a dihedral angle of 10.3 (2)° with the fused ring system. In the crystal, C—H⋯O hydrogen bonds link the molecules into a two-dimensional network nearly parallel to the *ab* plane, enclosing $R_2^2(6)$, $R_4^4(12)$, $R_4^4(14)$, $R_4^4(18)$ and $R_4^4(20)$ ring motifs. π–π stacking between the centroids of parallel rings [centroid–centroid distances = 3.919 (3)–3.695 (3) Å] helps to consolidate the packing. Hirshfeld surface analysis revealed that the most important contributions for the crystal packing are from H⋯H (21.2%), H⋯Cl/Cl⋯H (14.7%), H⋯O/O⋯H (13.9%), H⋯C/C⋯H (13.1%), H⋯Br/Br⋯H (12.3%) and C⋯C (11.6%) interactions.

1. Chemical context

Isoindoles have emerged as a significant class of heterocyclic compounds in organic chemistry due to their diverse biological activities as well as their utility in material science and organocatalysis (for recent reviews, see: Chen & Zou, 2021; Samandram *et al.*, 2025). Despite their importance, an efficient strategy for their synthesis remains to be found. Building on our and other studies of intramolecular Diels–Alder reactions of vinylarenes (IMDAV) (Zaytsev *et al.*, 2021; Krishna *et al.*, 2022), we now investigate how 3-(aryl)allylamines undergo IMDAV reactions with halogenated maleic anhydride (Alekseeva *et al.*, 2020). As well as hydrogen bonds (Burkin *et al.*, 2024; Maharramov *et al.*, 2010, 2011; Pronina *et al.*, 2024), intermolecular halogen bonds can also be used in the supramolecular assembly of organic and coordination compounds and improve their functional properties (Gurbanov *et al.*, 2022; Shixaliyev *et al.*, 2013, 2014). We have recently reported a new synthetic strategy for constructing a condensed isoindole scaffold, arising from a cascade transformation between 3-(2-furyl)allylaniline and dibromomaleic anhydride (Alekseeva *et al.*, 2025). Remarkably, substitution on the benzene ring of the starting aniline leads to a decrease in product yield, yet the overall reaction pathway remains unaffected, proceeding through decarboxylation and dehydrobromination. The resulting 6,7-dihydro-5*H*-furo[2,3-*f*]-isoindol-5-ones represent versatile intermediates that can be further transformed to other isoindole derivatives through



Heck or Suzuki cross-coupling reactions, thereby providing a valuable entry into a broader class of functionalized isoindole derivatives (Bartolucci *et al.*, 2012; Kalari *et al.*, 2017; Alzweiri *et al.*, 2021; Kumar *et al.*, 2023). Herein, we report the synthesis and molecular and crystal structure of the title compound, **1**, together with a Hirshfeld surface analysis.



2. Structural commentary

The asymmetric unit contains one molecule comprising a pyrrole ring fused to a benzofuran ring system, and a phenyl ring with substitutions on each one of them (Fig. 1). The individually planar rings *A* (O1/C2/C3/C3*A*/C8*A*), *B* (C3*A*/C4/C4*A*/C7*A*/C8/C8*A*) and *C* (C4*A*/C5/N6/C7/C7*A*), which are fused, and *D* (C11–C16) are oriented at dihedral angles of *A*/*B* = 0.9 (3)°, *A*/*C* = 1.8 (3)°, *A*/*D* = 10.5 (3)°, *B*/*C* = 0.9 (3)°, *B*/*D* = 10.0 (3)° and *C*/*D* = 9.9 (3)°. Thus, the *A*, *B* and *C* rings are essentially coplanar. The substituent atoms Br1, O2 and Cl1 are located 0.007 (1), 0.012 (4) and 0.024 (2) Å, respectively, from the best least-squares planes of the corresponding rings. The phenyl ring subtends a dihedral angle of 10.3 (2)° with the fused ring system. An intramolecular C—H⋯O occurs (Table 1).

3. Supramolecular features

In the crystal, C—H⋯O hydrogen bonds (Table 1, Fig. 2) link the molecules into a two-dimensional network nearly parallel to the *ab* plane, enclosing $R_2^2(6)$, $R_4^4(12)$, $R_4^4(14)$, $R_4^4(18)$ and $R_4^4(20)$ ring motifs (Etter *et al.*, 1990). π–π interactions further consolidate the packing: between *A* rings [centroid-to-centroid distance = 3.919 (3) Å, α = 0.0 (3)° and slippage = 1.971 Å], *B* rings [centroid-to-centroid distance = 3.919 (3) Å, α = 0.0 (3)° and slippage = 1.871 Å], *C* rings [centroid-to-centroid distance = 3.920 (3) Å, α = 0.0 (3)° and slippage = 1.926 Å], *D* rings [centroid-to-centroid distance = 3.919 (3) Å, α = 0.0 (3)° and slippage = 2.022 Å], *A* and *C* rings [centroid-to-centroid distance = 3.642 (3) Å, α = 0.9 (3)° and slippage = 1.289 Å] and *B* and *C* rings [centroid-to-centroid distance = 3.695 (3) Å, α = 0.9 (3)° and slippage = 1.384 Å].

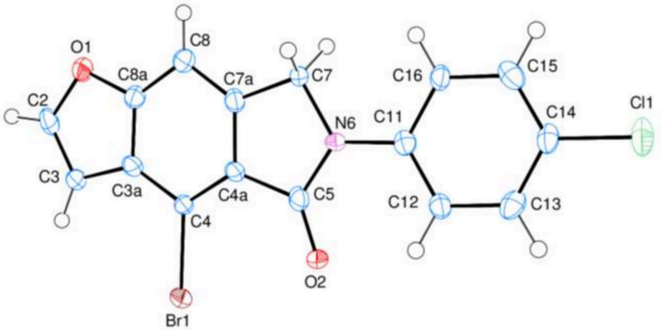


Figure 1
The asymmetric unit of the title compound with the atom-numbering scheme and 50% probability ellipsoids.

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C7—H7*B*⋯O2^{i}	0.99	2.48	3.387 (7)	152
C8—H8*A*⋯O2^{iii}	0.95	2.39	3.267 (7)	154
C12—H12*A*⋯O2	0.95	2.22	2.844 (6)	122

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

4. Hirshfeld surface analysis

To visualize the intermolecular interactions, a Hirshfeld surface (HS) analysis was carried out using *Crystal Explorer 17.5* (Spackman *et al.*, 2021). In the HS plotted over $d_{\rm norm}$ (Fig. 3), the contact distances equal, shorter and longer with respect to the sum of van der Waals radii are shown in white, red and blue, respectively. According to the two-dimensional

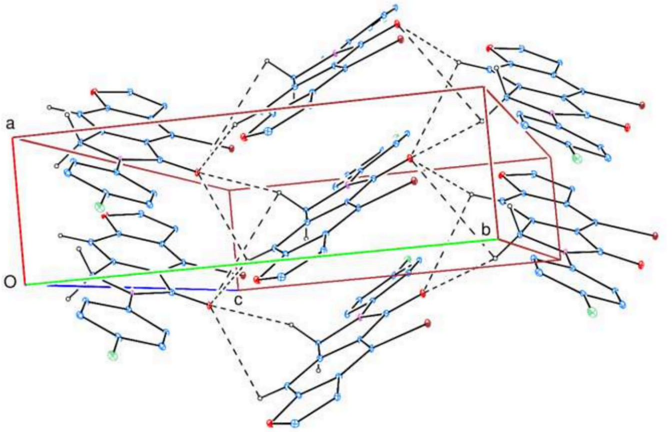


Figure 2
A partial packing diagram of the title compound with C—H⋯O hydrogen bonds shown as dashed lines. H atoms not involved in these interactions have been omitted for clarity.

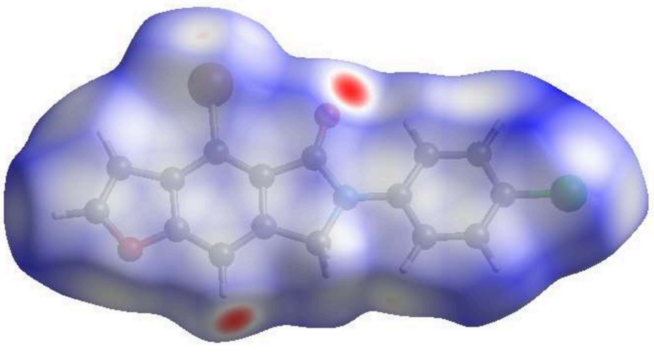


Figure 3
View of the three-dimensional Hirshfeld surface for title molecule plotted over $d_{\rm norm}$.

Table 2
Selected interatomic distances (Å).

Br1···O2	3.204 (4)	O2···H8A^{ii}	2.39
C16···$Br1^{i}$	3.424 (6)	C5···H12A	2.71
H16A···$Br1^{i}$	3.03	C7···H16A	2.46
Br1···H16A^{ii}	3.02	C16···H7A	2.72
O1···$C13^{iii}$	3.218 (7)	C16···H7B	2.90
O2···C12	2.844 (6)	H7A···H16A	2.16
H7B···$O2^{i}$	2.48		

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

fingerprint plots, H···H, H···Cl/Cl···H, H···O/O···H, H···C/C···H, H···Br/Br···H and C···C contacts make the most important contributions to the HS (Table 2, Fig. 4).

5. Synthesis and crystallization

4-Chloro-*N*-[(2*E*)-3-(furan-2-yl)prop-2-en-1-yl]aniline (0.30 g, 1.3 mmol) (**2**) was dissolved in dry CH_2Cl_2 (10 mL) and cooled to 251 K. Dibromomaleic anhydride (0.33 g, 1.3 mmol) was added, and the mixture was kept at 269 K for 1 d. The resulting precipitate was filtered off, dissolved in dry DMSO (10 mL), and stirred at 353 K for 10 h. The mixture was poured into water (50 mL), then resulting precipitate was filtered, and washed by water (3 × 3 mL). The product was dried in the air to constant weight to afford compound **1** as light-yellow solid (117.8 mg, 0.33 mmol, 25%, m.p.: 532-533 K). A single crystal suitable for X-ray analysis was obtained from DMSO-d_6 with heating to 353 K and following slow cooling to r.t. The reaction scheme is shown in Fig. 5). ^{1}H NMR (700.2 MHz, DMSO-d_6, 353 K) (J, Hz): δ 8.17 (d, J = 1.4, 1H, H-2-furyl), 7.91 (d, J = 8.6, 2H, H-2,6-C_6H_4Cl), 7.85 (s, 1H, H-8), 7.47 (d, J = 8.8, 2H, H-3,5-C_6H_4Cl), 7.06 ($br.s.$, 1H, H-3-furyl), 4.99 (s, 2H, H-7) ppm. $^{13}C\{^1H\}$NMR (176.1 MHz, DMSO-d_6, 353 K) δ 164.2 (C═O), 155.7, 147.9, 139.4, 138.0, 129.8, 128.4 (2C, C-2,6-C_6H_4Cl), 127.8, 124.0, 120.8 (2C, C-3,5-C_6H_4Cl), 110.0, 106.5, 105.5, 48.7 ppm. IR (KBr), ν (cm^{-1}) 3732, 3117, 3075, 2927, 1688, 1495, 1385, 1288, 1261, 1065, 825, 758. Analysis calculated for $C_{16}H_9BrClNO_2$: C 53.00, H 2.50, N 3.86; found C 52.81, H 2.38, N 3.69.

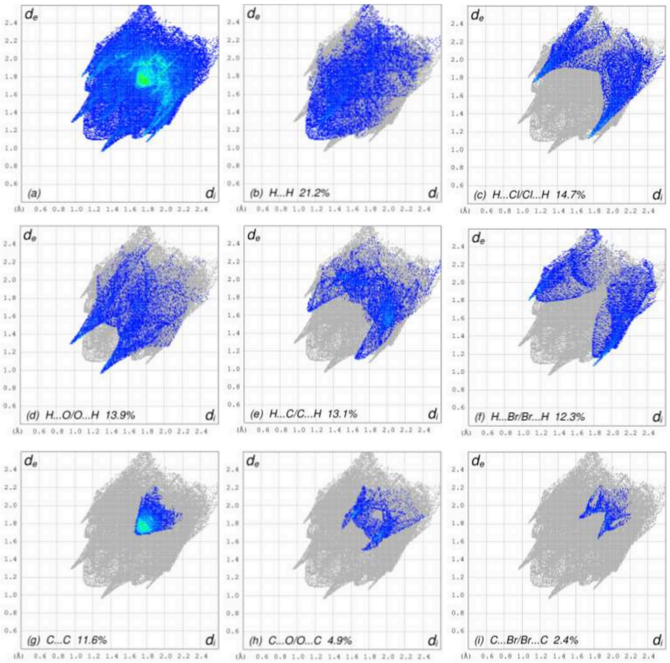


Figure 4
The full two-dimensional fingerprint plots for title molecule, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) H···Cl/Cl···H, (*d*) H···O/O···H, (*e*) H···C/C···H, (*f*) H···Br/Br···H, (*g*) C···C, (*h*) C···O/O···C, (*i*) C···Br/Br···C, (*j*) H···N/N···H, (*k*) Cl···Br/Br···Cl, (*l*) C···Cl/Cl···C, (*m*) Cl···Cl, (*n*) Br···Br, (*o*) C···N/N···C and (*p*) O···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.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_9BrClNO_2$
M_r	362.60
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	3.9194 (7), 12.594 (2), 26.858 (4)
β (°)	91.083 (6)
V (Å^3)	1325.5 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.31
Crystal size (mm)	0.50 × 0.08 × 0.02
Data collection	
Diffractometer	Bruker *KAPPA* APEXII area-detector diffractometer
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.556, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12749, 2992, 1967
R_{int}	0.132
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.144, 1.04
No. of reflections	2992
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.01, −0.99

Computer programs: *APEX3* and *SAINT* (Bruker, 2018), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* publication routines (Farrugia, 2012) and *PLATON* (Spek, 2020).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The C-bond hydrogen-atom positions were calculated geometrically at distances of 0.95 Å (for aromatic CH) and 0.99 Å (for methylene CH) and refined using a riding model by applying the constraint U_{iso}(H) = 1.2U_{eq}(C).

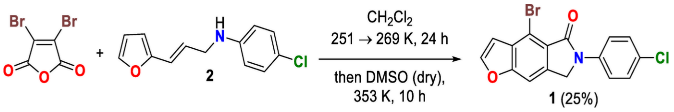


Figure 5
Reaction scheme for obtaining the title compound (**1**).

Acknowledgements

The authors' contributions are as follows. Conceptualization, AVG and TH; synthesis, KAA and EAS; X-ray analysis, AVG, MSG and TH; Hirshfeld surface analysis, TH; founding, KIH; writing (review and editing of the manuscript) AVG, IAK and TH, supervision, TH and MHAD.

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supporting information

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Kseniia A. Alekseeva, Atash V. Gurbanov, Mikhail S. Grigoriev, Elena A. Sorokina, Irina A. Kolesnik, Mohammed Hadi Al-Douh, Tuncer Hökelek and Khudayar I. Hasanov

Computing details

4-Bromo-6-(4-chlorophenyl)-6,7-dihydro-5*H*-furo[2,3-*f*]isoindol-5-one

Crystal data

$C_{16}H_9BrClNO_2$
$M_r = 362.60$
Monoclinic, $P2_1/n$
$a = 3.9194\ (7)$ Å
$b = 12.594\ (2)$ Å
$c = 26.858\ (4)$ Å
$\beta = 91.083\ (6)°$
$V = 1325.5\ (4)$ Å^3
$Z = 4$
$F(000) = 720$
$D_x = 1.817$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1710 reflections
$\theta = 3.0–28.1°$
$\mu = 3.31$ mm^{-1}
$T = 100$ K
Plate, colourless
0.50 × 0.08 × 0.02 mm

Data collection

Bruker KAPPA APEXII area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.556$, $T_{max} = 1.000$
12749 measured reflections
2992 independent reflections
1967 reflections with $I > 2\sigma(I)$
$R_{int} = 0.132$
$\theta_{max} = 27.5°$, $\theta_{min} = 4.1°$
$h = -5\rightarrow4$
$k = -16\rightarrow16$
$l = -34\rightarrow34$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.144$
$S = 1.04$
2992 reflections
190 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 0.5333P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.01$ e Å^{-3}
$\Delta\rho_{min} = -0.99$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Br1	0.49744 (14)	0.80459 (5)	0.13637 (2)	0.02236 (18)
Cl1	1.0284 (4)	0.67377 (13)	0.49698 (5)	0.0357 (4)
O1	−0.0949 (10)	0.4518 (3)	0.10290 (13)	0.0254 (9)
O2	0.7205 (10)	0.7699 (3)	0.25059 (13)	0.0228 (9)
N6	0.5883 (11)	0.6079 (4)	0.28682 (15)	0.0191 (10)
C2	−0.0979 (15)	0.5213 (5)	0.06345 (19)	0.0265 (14)
H2A	−0.200214	0.505380	0.031985	0.032*
C3	0.0575 (14)	0.6138 (5)	0.07363 (19)	0.0219 (13)
H3A	0.079676	0.673342	0.052237	0.026*
C3A	0.1838 (14)	0.6031 (5)	0.12427 (19)	0.0210 (12)
C4	0.3565 (14)	0.6695 (4)	0.15773 (19)	0.0191 (12)
C4A	0.4241 (14)	0.6307 (4)	0.20511 (18)	0.0197 (12)
C5	0.5962 (14)	0.6812 (5)	0.24847 (19)	0.0217 (13)
C7A	0.3151 (14)	0.5294 (5)	0.21916 (18)	0.0210 (12)
C7	0.4199 (14)	0.5088 (4)	0.27276 (18)	0.0202 (12)
H7A	0.218906	0.495166	0.293605	0.024*
H7B	0.578659	0.447864	0.275526	0.024*
C8A	0.0764 (14)	0.5035 (5)	0.14046 (19)	0.0216 (13)
C8	0.1392 (14)	0.4615 (5)	0.18745 (19)	0.0236 (13)
H8A	0.068007	0.392468	0.196964	0.028*
C11	0.7085 (14)	0.6249 (5)	0.33650 (19)	0.0203 (12)
C12	0.8993 (14)	0.7137 (4)	0.35026 (19)	0.0214 (12)
H12A	0.964013	0.763946	0.325817	0.026*
C13	0.9952 (15)	0.7287 (5)	0.4000 (2)	0.0258 (13)
H13A	1.121382	0.789909	0.409754	0.031*
C14	0.9054 (15)	0.6538 (5)	0.43502 (19)	0.0245 (13)
C15	0.7284 (15)	0.5643 (5)	0.4216 (2)	0.0272 (14)
H15A	0.675257	0.512542	0.445981	0.033*
C16	0.6270 (14)	0.5492 (5)	0.37244 (19)	0.0229 (13)
H16A	0.501947	0.487489	0.363146	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0309 (4)	0.0180 (4)	0.0183 (3)	−0.0014 (2)	0.00298 (19)	0.0033 (2)
Cl1	0.0482 (11)	0.0405 (12)	0.0181 (7)	0.0113 (7)	−0.0062 (6)	−0.0066 (6)
O1	0.029 (3)	0.028 (3)	0.019 (2)	−0.0065 (17)	0.0006 (16)	−0.0044 (17)
O2	0.036 (3)	0.014 (3)	0.0179 (19)	−0.0052 (16)	0.0019 (15)	0.0007 (15)
N6	0.029 (3)	0.012 (3)	0.016 (2)	−0.0013 (18)	0.0023 (18)	0.0014 (18)

C2	0.030 (4)	0.036 (4)	0.013 (3)	−0.001 (3)	0.000 (2)	0.001 (2)
C3	0.029 (4)	0.018 (4)	0.019 (3)	0.001 (2)	0.005 (2)	0.001 (2)
C3A	0.022 (4)	0.021 (4)	0.020 (3)	−0.001 (2)	0.007 (2)	0.001 (2)
C4	0.028 (4)	0.011 (3)	0.018 (3)	0.003 (2)	0.006 (2)	0.000 (2)
C4A	0.025 (4)	0.017 (4)	0.018 (3)	−0.001 (2)	0.008 (2)	0.000 (2)
C5	0.026 (4)	0.021 (4)	0.018 (3)	0.004 (2)	0.005 (2)	−0.002 (2)
C7A	0.025 (4)	0.022 (4)	0.016 (3)	0.002 (2)	0.002 (2)	0.000 (2)
C7	0.032 (4)	0.015 (4)	0.013 (2)	−0.002 (2)	0.002 (2)	−0.001 (2)
C8A	0.023 (4)	0.022 (4)	0.020 (3)	−0.002 (2)	0.000 (2)	−0.003 (2)
C8	0.028 (4)	0.020 (4)	0.023 (3)	0.003 (2)	0.004 (2)	−0.002 (2)
C11	0.022 (4)	0.020 (4)	0.019 (3)	0.005 (2)	0.001 (2)	0.000 (2)
C12	0.027 (4)	0.020 (4)	0.017 (3)	0.004 (2)	0.002 (2)	0.000 (2)
C13	0.030 (4)	0.019 (4)	0.028 (3)	0.006 (2)	−0.005 (2)	−0.005 (2)
C14	0.036 (4)	0.019 (4)	0.018 (3)	0.012 (2)	−0.004 (2)	−0.003 (2)
C15	0.031 (4)	0.028 (4)	0.022 (3)	0.008 (3)	0.004 (2)	0.006 (3)
C16	0.033 (4)	0.019 (4)	0.016 (3)	0.004 (2)	0.001 (2)	−0.003 (2)

Geometric parameters (Å, º)

Br1—C4	1.882 (5)	C7A—C8	1.381 (7)
Cl1—C14	1.742 (5)	C7A—C7	1.512 (7)
O1—C8A	1.367 (6)	C7—H7A	0.9900
O1—C2	1.375 (6)	C7—H7B	0.9900
O2—C5	1.219 (6)	C8A—C8	1.386 (7)
N6—C5	1.384 (7)	C8—H8A	0.9500
N6—C11	1.423 (6)	C11—C12	1.392 (8)
N6—C7	1.458 (7)	C11—C16	1.397 (7)
C2—C3	1.340 (8)	C12—C13	1.394 (7)
C2—H2A	0.9500	C12—H12A	0.9500
C3—C3A	1.445 (7)	C13—C14	1.383 (8)
C3—H3A	0.9500	C13—H13A	0.9500
C3A—C4	1.393 (7)	C14—C15	1.368 (8)
C3A—C8A	1.395 (8)	C15—C16	1.385 (7)
C4—C4A	1.384 (7)	C15—H15A	0.9500
C4A—C7A	1.399 (8)	C16—H16A	0.9500
C4A—C5	1.479 (7)		
Br1···O2	3.204 (4)	H7B···O2^{i}	2.48
C16···Br1^{i}	3.424 (6)	O2···H8A^{ii}	2.39
H16A···Br1^{i}	3.03	C5···H12A	2.71
Br1···H16A^{ii}	3.02	C7···H16A	2.46
O1···C13^{iii}	3.218 (7)	C16···H7A	2.72
O2···C12	2.844 (6)	C16···H7B	2.90
O2···H12A	2.23	H7A···H16A	2.16
C8A—O1—C2	105.2 (4)	N6—C7—H7B	111.3
C5—N6—C11	125.9 (5)	C7A—C7—H7B	111.3
C5—N6—C7	113.3 (4)	H7A—C7—H7B	109.2

C11—N6—C7	120.8 (4)	O1—C8A—C8	124.5 (5)
C3—C2—O1	113.5 (5)	O1—C8A—C3A	110.2 (5)
C3—C2—H2A	123.2	C8—C8A—C3A	125.3 (5)
O1—C2—H2A	123.2	C7A—C8—C8A	113.8 (5)
C2—C3—C3A	104.9 (5)	C7A—C8—H8A	123.1
C2—C3—H3A	127.5	C8A—C8—H8A	123.1
C3A—C3—H3A	127.5	C12—C11—C16	119.5 (5)
C4—C3A—C8A	119.0 (5)	C12—C11—N6	122.5 (5)
C4—C3A—C3	134.8 (5)	C16—C11—N6	118.0 (5)
C8A—C3A—C3	106.1 (5)	C11—C12—C13	119.8 (5)
C4A—C4—C3A	117.6 (5)	C11—C12—H12A	120.1
C4A—C4—Br1	123.2 (4)	C13—C12—H12A	120.1
C3A—C4—Br1	119.2 (4)	C14—C13—C12	119.5 (6)
C4—C4A—C7A	121.0 (5)	C14—C13—H13A	120.3
C4—C4A—C5	130.4 (5)	C12—C13—H13A	120.3
C7A—C4A—C5	108.5 (5)	C15—C14—C13	121.1 (5)
O2—C5—N6	126.2 (5)	C15—C14—Cl1	120.0 (5)
O2—C5—C4A	127.4 (5)	C13—C14—Cl1	118.8 (5)
N6—C5—C4A	106.4 (5)	C14—C15—C16	119.9 (5)
C8—C7A—C4A	123.3 (5)	C14—C15—H15A	120.0
C8—C7A—C7	127.2 (5)	C16—C15—H15A	120.0
C4A—C7A—C7	109.5 (4)	C15—C16—C11	120.0 (5)
N6—C7—C7A	102.3 (4)	C15—C16—H16A	120.0
N6—C7—H7A	111.3	C11—C16—H16A	120.0
C7A—C7—H7A	111.3		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*B*···O2$^{\text{i}}$	0.99	2.48	3.387 (7)	152
C8—H8*A*···O2$^{\text{iii}}$	0.95	2.39	3.267 (7)	154
C12—H12*A*···O2	0.95	2.22	2.844 (6)	122

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