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Crystal structure and Hirshfeld surface analysis of 4,5-dibromo-2-(4-methoxyphenyl)-2,3,4,4a,5,6,7,-7a-octahydro-1*H*-4,6-epoxy-1*H*-cyclopenta[*c*]pyridin-1-one

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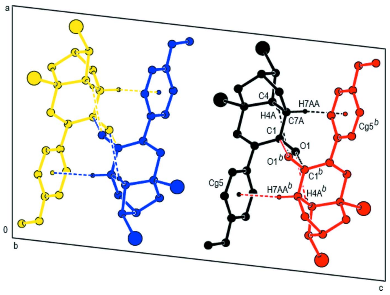
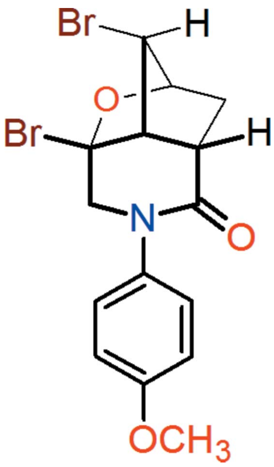
The molecule of the title compound, $C_{15}H_{15}Br_2NO_3$, comprises a fused tricyclic system consisting of two five-membered rings (cyclopentane and tetrahydrofuran) and one six-membered ring (tetrahydropyridinone). Both five-membered rings of the tricyclic system have envelope conformations, and the conformation of the six-membered cycle is intermediate between chair and half-chair. In the crystal, the molecules are linked by C—H⋯O hydrogen bonds and C—H⋯π, C—Br⋯π and C⋯O interactions into double layers. The layers are connected into a three-dimensional network by van der Waals interactions.



1. Chemical context

Isoindoles are important structural units of many natural products and are widely used as drugs and as building blocks for the construction of new *N*-containing heterocyclic compounds or functional materials (Nadirova *et al.*, 2019; Zubkov *et al.*, 2011, 2014, 2018). The biological and physical properties of isoindoles depend on the attached functional groups (Krishna *et al.*, 2021; Zaytsev *et al.*, 2017, 2019, 2020). Thus, the functionalization of isoindole moieties at the donor/acceptor sites for non-covalent bonding can improve their biological and photophysical properties as well as their coordination ability (Wicholas *et al.*, 2006).

On the other hand, non-covalent interactions, such as hydrogen, aerogen, halogen, chalcogen, pnictogen, tetrel and icosagen bonds, as well as n–π^*, π–π stacking, π–cation, π–anion, hydrophobic interactions, among others, have recently also attracted much attention and have been demonstrated to play a prominent role in synthesis, catalysis, supramolecular chemistry, molecular recognition, biological systems, functional materials, *etc.* (Asadov *et al.*, 2016; Gurbanov *et al.*, 2017, 2018; Karmakar *et al.*, 2017; Kopylovich *et al.*, 2011; Ma *et al.*, 2017*a*,*b*; 2020; Mahmudov *et al.*, 2010, 2012, 2013, 2019, 2020; Mizar *et al.*, 2012; Sutradhar *et al.*, 2015, 2016). Halogen bonding is a rather spread phenomenon since halogen atoms or ions can form short non-bonding contacts with electron acceptors, electron donors or be interconnected due to anisotropic charge distribution in halogen atoms (Afkhami *et* *al.*, 2017; Maharramov *et al.*, 2018; Mahmoudi *et al.*, 2017, 2019; Shixaliyev *et al.*, 2014). In fact, functionalization of isoindoles with donor or acceptor sites for non-covalent bonding greatly affects their supramolecular arrangements (Gurbanov *et al.*, 2021).



In a continuation of our work in this direction, we have functionalized a new isoindole (**1**) (Zaytsev *et al.*, 2020) by reaction with bromine yielding 4,5-dibromo-2-(4-methoxyphenyl)-2,3,4,4a,5,6,7,7a-octahydro-1*H*-4,6-epoxy-1*H*-cyclopenta[*c*]pyridin-1-one (**2**; Fig. 1), which provides examples of C—Br···O halogen bonds as well as of C—H···O and C—H···π types of intermolecular hydrogen bonds.

2. Structural commentary

As shown in Fig. 2, the molecule of the title compound, **2**, comprises a fused tricyclic system containing two five-membered rings (cyclopentane C4–C7/C7*A* and tetrahydrofuran C3*A*/C4–C6/O8) and one six-membered ring (tetrahydropyridinone C1/N2/C3/C3*A*/C4/C7*A*). Both five-membered rings of the tricyclic fragment have envelope conformations with the C5 atom as the flap, and the six-membered ring adopts a flattened chair conformation with the N2 and C4 atoms displaced by 0.276 (3) and −0.670 (4) Å, respectively, from the mean plane through the remaining four atoms. The environment of atom N2, being close to trigonal–planar, is slightly pyramidalized due to steric reasons [the sum of bond angles at N2 is 356.7 (5)°]. The dihedral angle between the mean planes of the tetrahydropyridinone and benzene rings is 82.82 (16)°.

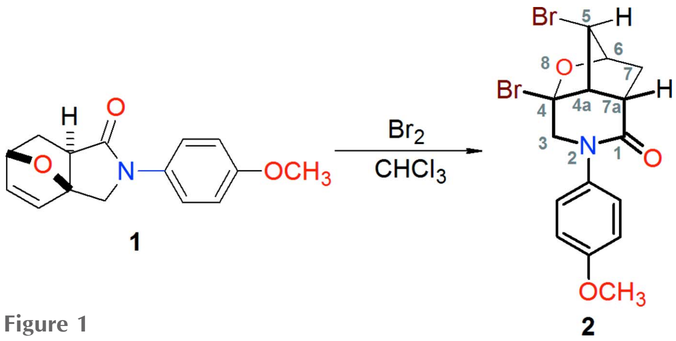


Figure 1
Synthesis of the title compound (**2**).

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

Cg is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O1^{i}	0.98	2.57	3.092 (3)	114
C7*A*—H7*AA*···*Cg*5^{i}	0.98	2.69	3.573 (4)	150

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

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked by intermolecular C—H···O hydrogen bonds, C—H···π, C—Br···π and C···O interactions into double layers parallel to (001) (Tables 1 and 2; Figs. 3, 4 and 5). The layers are further connected into a three-dimensional network by van der Waals interactions.

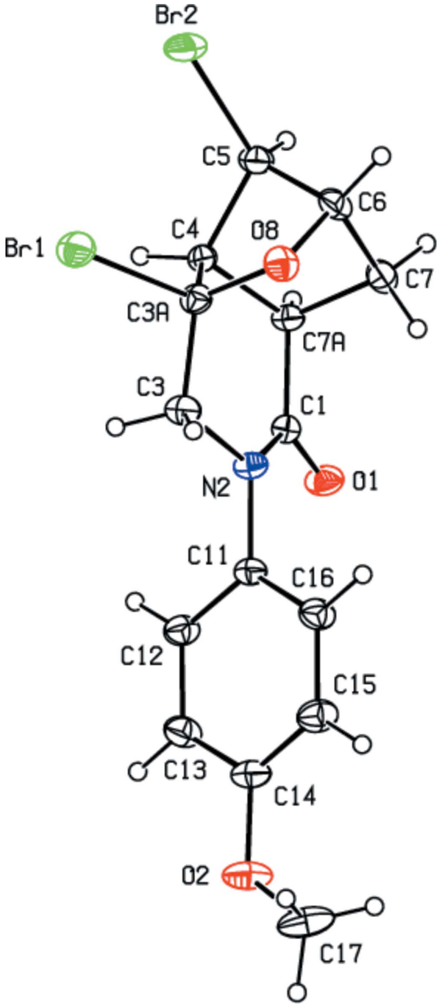


Figure 2
The molecular structure of **2**, with displacement ellipsoids for non-hydrogen atoms drawn at the 30% probability level.

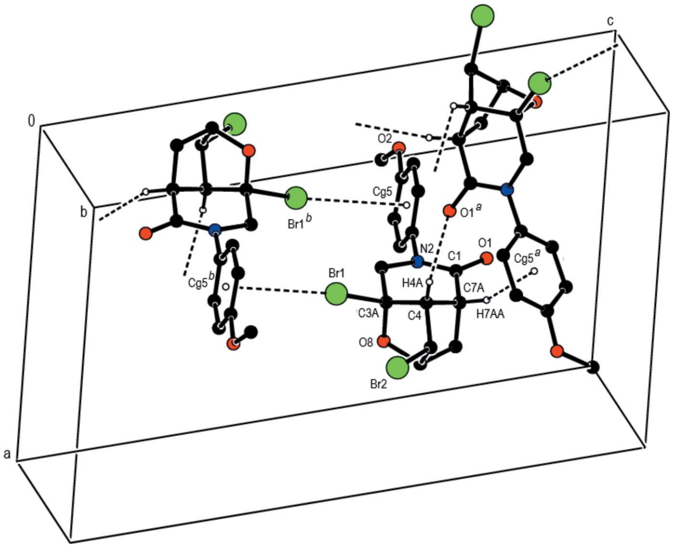


Figure 3
Intermolecular C—H$\cdots$O, C—H$\cdots\pi$ and C—Br$\cdots\pi$ interactions [symmetry codes: (a) $1 - x, -\frac{1}{2} + y, \frac{3}{2} - z$; ($b$) $1 - x, -y, 1 - z$].

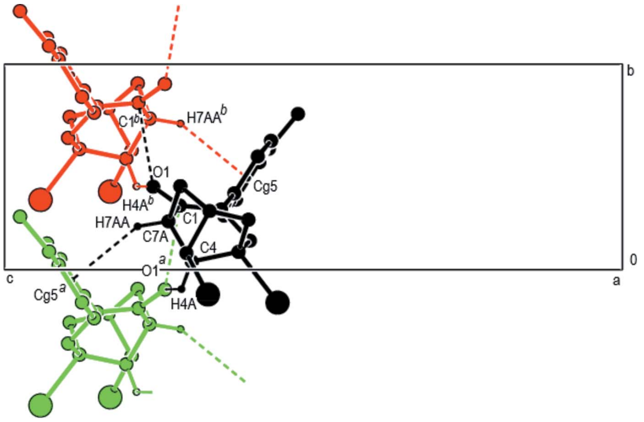


Figure 4
A fragment of the double layer in **2** formed by intermolecular C—H$\cdots$O, C$\cdots$O and C—H$\cdots\pi$ contacts [symmetry codes: (a) $1 - x, -\frac{1}{2} + y, \frac{3}{2} - z$; ($b$) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$].

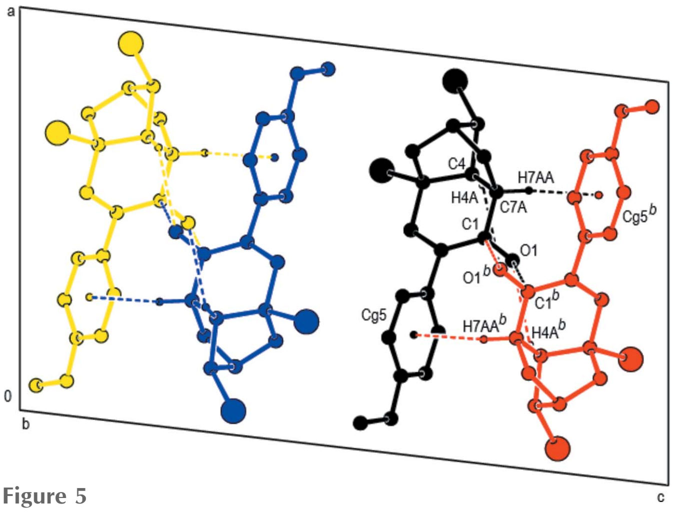
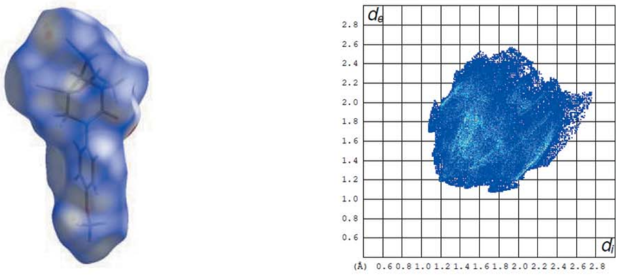
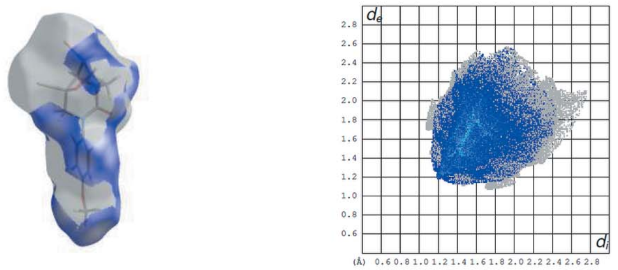


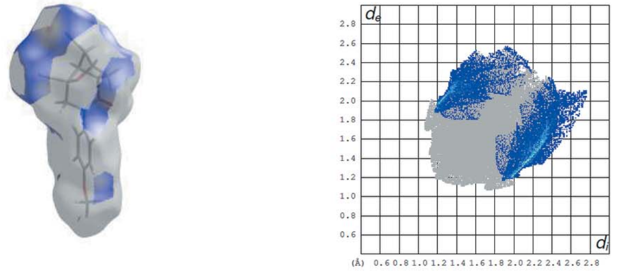
Figure 5
Packing diagram of **2** viewed along the b-axis direction showing the intermolecular C—H$\cdots$O and C—H$\cdots\pi$ contacts [symmetry code: (b) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$].



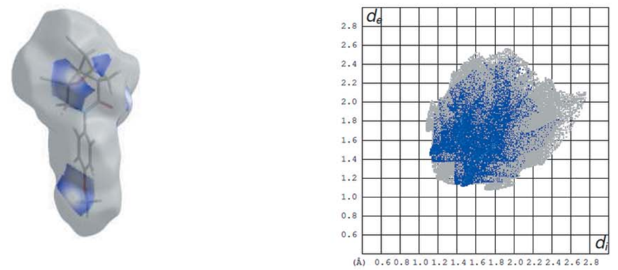
(a) All…All



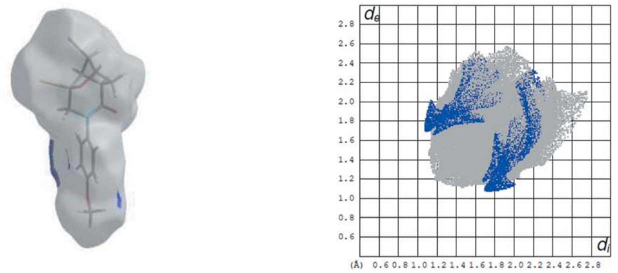
(b) H…H



(c) Br…H / H…Br



(d) O…H / H…O



(e) C…H / H…C

Figure 6
A view of the three-dimensional Hirshfeld surfaces and the two-dimensional fingerprint plots for **2**, showing (a) all interactions and delineated into (b) H$\cdots$H, (c) Br$\cdots$H/H$\cdots$Br, (d) O$\cdots$H/H$\cdots$O and (e) C$\cdots$H/H$\cdots$C interactions. The d_i and d_e values are the closest internal and external distances (Å) from given points on the Hirshfeld surface.

Table 2
Summary of shortest van der Waals contacts (Å) in the title compound.

Contact	Distance	Symmetry operation
Br1···*Cg*5	3.7132 (15)	$1 - x, -y, 1 - z$
Br2···O2	3.316 (3)	$1 + x, -1 + y, z$
Br2···H17*A*	3.13	$1 + x, -1 + y, z$
Br2···H5*A*	3.13	$2 - x, -\frac{1}{2} + y, \frac{3}{2} - z$
O1···C1	2.822 (4)	$1 - x, \frac{1}{2} + y, \frac{3}{2} - z$
O8···H17*C*	2.66	$1 - x, 1 - y, 1 - z$
H4*A*···H7*A*	2.54	$x, -1 + y, z$
H7*B*···H12*A*	2.55	$1 - x, \frac{1}{2} + y, \frac{3}{2} - z$

Table 3
Percentage contributions of interatomic contacts to the Hirshfeld surface for the title compound.

Contact	Percentage contribution
H···H	41.1
Br···H/H···Br	24.5
O···H/H···O	16.9
C···H/H···C	8.2
Br···C/C···Br	4.3
Br···O/O···Br	2.6
O···C/C···O	1.5
O···O	0.8
O···N/N···O	0.1

Table 4
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{15}Br_2NO_3$
M_r	417.10
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	12.0238 (12), 6.4316 (7), 19.463 (2)
β (°)	96.618 (4)
V (Å^3)	1495.1 (3)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	5.43
Crystal size (mm)	0.40 × 0.12 × 0.06
Data collection	
Diffractometer	Bruker Kappa APEXII area-detector diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.461, 0.736
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13519, 3429, 2522
R_{int}	0.043
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.037, 0.091, 1.01
No. of reflections	3429
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	1.30, −0.62

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

The Hirshfeld surface for **2** mapped over d_{norm} and the associated two-dimensional fingerprint plots are shown in Fig. 6. All of them were generated using *CrystalExplorer17* (Turner *et al.*, 2017). Red spots on the Hirshfeld surface mapped over d_{norm} in the colour range −0.2469 to 1.1913 a.u. confirm the intermolecular contacts (Tables 1 and 2). The fingerprint plots are given for all contacts and those delineated into H···H (41.1%; Fig. 6*b*), Br···H/H···Br (24.5%; Fig. 6*c*), O···H/H···O (16.9%; Fig. 6*d*) and C···H/H···C (8.2%; Fig. 6*e*) contacts. All contributions to the Hirshfeld surface are given in Table 3. The large number of H···H, Br···H/H···Br and O···H/H···O interactions suggest that van der Waals interactions and hydrogen bonding play the major roles in the crystal packing (Hathwar *et al.*, 2015).

4. Database survey

A survey of the Cambridge Structural Database (CSD version 5.41, update of March 2020; Groom *et al.*, 2016) reveals two compounds containing the octahydro-1*H*-4,6-epoxycyclopenta[c]pyridin-1-one skeleton, *viz*. methyl *rac*-(1*S**,3*R**,7*R**,8*R**,9*R**,10*S**)-3,9-diacetoxy-6-oxo-5-phenyl-2-oxa-5-azatricyclo[5.2.1.0^{3,8}]decane-10-carboxylate ethanol solvate (refcode RUJJUC; Gurbanov *et al.*, 2009) and methyl *rac*-(1*S**,2*R**,4*R**,13*S**,14*R**,15*R**,16*S**,117*S**)-1,16-diacetoxy-12-oxo-4-(2-oxopyrrolidin-1-yl)-18-oxa-11-azapentacyclo[13.2.1.0^{2,11}.0^{5,10}.0^{13,17}]octadeca-5,7,9-triene-14-carboxylate sesquihydrate (HUGJUP; Gurbanov *et al.*, 2010).

The racemic crystal of RUJJUC consists of enantiomeric pairs with the configurations *rac*-4*R**,4a*R**,5*R**,6*S**,7*S**,7a*R**. The ethanol solvate molecule is bound to the molecule of RUJJUC by a strong O—H···O hydrogen bond. In the crystal of HUGJUP, there are three O—H···O hydrogen bonds, which link the organic molecules and water molecules into layers parallel to (001). The layers are further linked into a three-dimensional framework by attractive intermolecular carbonyl–carbonyl interactions.

5. Synthesis and crystallization

A solution of isoindolone **1** (1.2 mmol) and bromine (1.75 mmol) in dry chloroform (3 mL) was stirred for 5 h (TLC control, EtOAc–hexane, 1:1). The reaction mixture was poured into H_2O (30 mL) and extracted with $CHCl_3$ (3 × 20 mL). The combined extracts were dried over anhydrous Na_2SO_4 and concentrated *in vacuo*. The obtained solid was recrystallized by slow evaporation from EtOH to give single crystals of dibromide **2** suitable for X-ray analysis. Colourless needles, yield 0.42 g (86%). M.p. > 478 K (decomposition). IR (KBr), ν (cm^{-1}): 1671 (N—C═O), 610 (C—Br). ^{1}H NMR (DMSO-d_6, 700.1 MHz, 298 K): δ = 7.19 (*d*, 2H, H2, H6 H-Ph, *J* = 8.8), 6.94 (*d*, 2H, H3, H5 H-Ph, *J* = 8.8), 4.92 (*s*, 1H, H-6), 4.62 (*d*, 1H, *J* = 13.1), 4.11 (*d*, 1H, H-3, *J* = 13.1), 4.61 (*d*, 1H, H-5), 3.57 (*s*, 3H, OCH_3), 3.67 (*d*, 1H, H-4a, *J* = 3.9), 2.93 (*dt*, 1H, H-7a, *J* = 3.9, *J* = 11.9), 2.41 (*t*, 1H, H-7exo, *J* = 11.9), 1.53 (*dd*, 1H, H-7endo, *J* = 3.9, *J* = 11.9). ^{13}C NMR (DMSO-d_6, 176.0 MHz, 298 K): δ = 169.7, 157.8, 133.7, 127.4 (2C), 114.1 (2C), 99.3, 86.0, 61.0, 55.3, 51.7, 48.5, 39.0, 36.4. MS (APCI): *m*/*z* = 420 $[M + H]^+$ (^{81}Br), 418 $[M + H]^+$ (^{81}Br, ^{79}Br), 416 $[M + H]^+$ (^{79}Br).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. All H atoms were positioned geometrically (C—H = 0.93 − 0.98 Å) and refined using a riding model, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C) or $1.5U_{\rm eq}$(C-methyl). Owing to poor agreement between observed and calculated intensities, four outliers (6 0 2, 1 2 0, 0 3 3 and 0 0 6) were omitted from the final cycles of refinement.

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Authors contributions are as follows. Conceptualization, MA and SM; methodology, STÇ and MA; investigation, DFM and NSS; writing (original draft), MA, STÇ and SM; writing (review and editing of the manuscript), MA, STÇ and SM; visualization, MA and SM; funding acquisition, DFM, NSS and EAS; resources, EAS; supervision, MA and SM.

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supporting information

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Crystal structure and Hirshfeld surface analysis of 4,5-dibromo-2-(4-methoxyphenyl)-2,3,4,4a,5,6,7,7a-octahydro-1*H*-4,6-epoxy-1*H*-cyclopenta[*c*]pyridin-1-one

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Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

4,5-Dibromo-2-(4-methoxyphenyl)-2,3,4,4a,5,6,7,7a-octahydro-1*H*-4,6-epoxy-1*H*-cyclopenta[*c*]pyridin-1-one

Crystal data

$C_{15}H_{15}Br_2NO_3$
$M_r = 417.10$
Monoclinic, $P2_1/c$
$a = 12.0238\ (12)$ Å
$b = 6.4316\ (7)$ Å
$c = 19.463\ (2)$ Å
$\beta = 96.618\ (4)°$
$V = 1495.1\ (3)$ Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.853$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2677 reflections
$\theta = 2.9–24.4°$
$\mu = 5.43$ mm^{-1}
$T = 296$ K
Needle, colourless
0.40 × 0.12 × 0.06 mm

Data collection

Bruker Kappa APEXII area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
$T_{min} = 0.461$, $T_{max} = 0.736$
13519 measured reflections
3429 independent reflections
2522 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -15 \rightarrow 15$
$k = -8 \rightarrow 8$
$l = -24 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.091$
$S = 1.01$
3429 reflections
190 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 0.868P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.30$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
Br1	0.69848 (3)	−0.16042 (6)	0.55820 (2)	0.04500 (13)
Br2	0.94126 (3)	−0.12067 (7)	0.67093 (2)	0.04941 (14)
O1	0.51267 (19)	0.4036 (4)	0.75946 (12)	0.0386 (6)
O2	0.0858 (2)	0.5884 (5)	0.57203 (14)	0.0504 (7)
O8	0.75480 (19)	0.2430 (4)	0.60541 (12)	0.0349 (5)
N2	0.5178 (2)	0.2933 (4)	0.64953 (13)	0.0284 (6)
C1	0.5603 (3)	0.3115 (5)	0.71658 (17)	0.0273 (7)
C3A	0.6814 (3)	0.0868 (5)	0.62134 (16)	0.0289 (7)
C3	0.5590 (3)	0.1411 (5)	0.60289 (17)	0.0323 (8)
H3A	0.548416	0.195612	0.556131	0.039*
H3B	0.514694	0.015166	0.603693	0.039*
C4	0.7156 (2)	0.0398 (5)	0.69685 (16)	0.0257 (6)
H4A	0.691323	−0.094568	0.713661	0.031*
C5	0.8414 (3)	0.0806 (5)	0.70565 (18)	0.0336 (8)
H5A	0.865966	0.106512	0.754666	0.040*
C6	0.8301 (3)	0.2855 (6)	0.66820 (19)	0.0358 (8)
H6A	0.901320	0.350442	0.660335	0.043*
C7A	0.6785 (3)	0.2352 (5)	0.73476 (17)	0.0279 (7)
H7AA	0.691219	0.210486	0.784733	0.033*
C7	0.7624 (3)	0.4062 (5)	0.71548 (19)	0.0355 (8)
H7A	0.723577	0.522331	0.691645	0.043*
H7B	0.808923	0.456851	0.756063	0.043*
C11	0.4066 (3)	0.3716 (5)	0.62824 (16)	0.0280 (7)
C12	0.3137 (3)	0.2636 (6)	0.64507 (18)	0.0342 (8)
H12A	0.322793	0.139531	0.669624	0.041*
C13	0.2078 (3)	0.3407 (6)	0.62528 (19)	0.0392 (8)
H13A	0.145407	0.270187	0.637376	0.047*
C14	0.1944 (3)	0.5227 (6)	0.58748 (17)	0.0351 (8)
C15	0.2861 (3)	0.6274 (6)	0.56874 (19)	0.0401 (9)
H15A	0.276873	0.747622	0.542168	0.048*
C16	0.3926 (3)	0.5508 (6)	0.59010 (18)	0.0362 (8)
H16A	0.455034	0.621952	0.578373	0.043*
C17	0.0658 (4)	0.7577 (8)	0.5251 (2)	0.0597 (12)
H17A	−0.012785	0.788516	0.518630	0.090*
H17B	0.106390	0.877628	0.543611	0.090*
H17C	0.090453	0.721139	0.481502	0.090*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0406 (2)	0.0497 (2)	0.0443 (2)	0.00670 (17)	0.00301 (16)	−0.01833 (18)
Br2	0.0286 (2)	0.0543 (3)	0.0653 (3)	0.01404 (17)	0.00518 (17)	−0.00677 (19)
O1	0.0321 (13)	0.0467 (14)	0.0370 (14)	0.0102 (11)	0.0042 (11)	−0.0118 (11)
O2	0.0300 (14)	0.0703 (19)	0.0501 (16)	0.0171 (13)	0.0013 (12)	0.0129 (14)
O8	0.0350 (13)	0.0375 (13)	0.0338 (13)	−0.0033 (11)	0.0102 (10)	0.0049 (10)
N2	0.0242 (14)	0.0339 (15)	0.0275 (14)	0.0068 (11)	0.0046 (11)	−0.0004 (11)
C1	0.0246 (16)	0.0260 (16)	0.0311 (17)	0.0002 (12)	0.0026 (13)	−0.0017 (13)
C3A	0.0286 (17)	0.0312 (17)	0.0276 (17)	0.0029 (14)	0.0058 (13)	−0.0043 (13)
C3	0.0279 (17)	0.042 (2)	0.0268 (17)	0.0045 (14)	0.0016 (13)	−0.0055 (14)
C4	0.0231 (16)	0.0246 (15)	0.0297 (16)	0.0016 (12)	0.0040 (12)	0.0018 (13)
C5	0.0240 (17)	0.0400 (19)	0.0364 (19)	0.0043 (14)	0.0017 (14)	−0.0062 (15)
C6	0.0236 (17)	0.0400 (19)	0.045 (2)	−0.0066 (14)	0.0069 (15)	−0.0020 (16)
C7A	0.0233 (16)	0.0329 (17)	0.0274 (16)	0.0052 (13)	0.0024 (13)	−0.0015 (13)
C7	0.0302 (18)	0.0354 (18)	0.041 (2)	−0.0062 (15)	0.0031 (15)	−0.0056 (15)
C11	0.0240 (16)	0.0323 (17)	0.0271 (16)	0.0041 (13)	0.0008 (13)	0.0003 (13)
C12	0.0299 (18)	0.0363 (19)	0.0368 (19)	0.0046 (15)	0.0051 (14)	0.0077 (15)
C13	0.0274 (18)	0.046 (2)	0.044 (2)	−0.0011 (16)	0.0053 (15)	0.0030 (17)
C14	0.0276 (18)	0.048 (2)	0.0287 (17)	0.0113 (15)	0.0003 (14)	−0.0031 (15)
C15	0.038 (2)	0.045 (2)	0.038 (2)	0.0084 (16)	0.0045 (16)	0.0124 (16)
C16	0.0285 (18)	0.039 (2)	0.041 (2)	−0.0003 (15)	0.0060 (15)	0.0107 (16)
C17	0.048 (2)	0.081 (3)	0.050 (3)	0.035 (2)	0.004 (2)	0.018 (2)

Geometric parameters (Å, º)

Br1—C3A	2.034 (3)	C6—C7	1.512 (5)
Br2—C5	1.940 (3)	C6—H6A	0.9800
O1—C1	1.219 (4)	C7A—C7	1.567 (5)
O2—C14	1.372 (4)	C7A—H7AA	0.9800
O2—C17	1.424 (5)	C7—H7A	0.9700
O8—C3A	1.395 (4)	C7—H7B	0.9700
O8—C6	1.461 (4)	C11—C16	1.371 (4)
N2—C1	1.351 (4)	C11—C12	1.386 (5)
N2—C11	1.443 (4)	C12—C13	1.380 (5)
N2—C3	1.460 (4)	C12—H12A	0.9300
C1—C7A	1.507 (4)	C13—C14	1.382 (5)
C3A—C4	1.510 (4)	C13—H13A	0.9300
C3A—C3	1.516 (4)	C14—C15	1.376 (5)
C3—H3A	0.9700	C15—C16	1.391 (5)
C3—H3B	0.9700	C15—H15A	0.9300
C4—C5	1.525 (4)	C16—H16A	0.9300
C4—C7A	1.549 (4)	C17—H17A	0.9600
C4—H4A	0.9800	C17—H17B	0.9600
C5—C6	1.505 (5)	C17—H17C	0.9600
C5—H5A	0.9800		

C14—O2—C17	117.5 (3)	C7—C6—H6A	114.7
C3A—O8—C6	107.2 (2)	C1—C7A—C4	117.9 (3)
C1—N2—C11	118.8 (3)	C1—C7A—C7	109.3 (3)
C1—N2—C3	122.8 (3)	C4—C7A—C7	103.1 (3)
C11—N2—C3	115.1 (3)	C1—C7A—H7AA	108.7
O1—C1—N2	123.3 (3)	C4—C7A—H7AA	108.7
O1—C1—C7A	120.1 (3)	C7—C7A—H7AA	108.7
N2—C1—C7A	116.1 (3)	C6—C7—C7A	101.1 (3)
O8—C3A—C4	104.6 (3)	C6—C7—H7A	111.6
O8—C3A—C3	113.8 (3)	C7A—C7—H7A	111.6
C4—C3A—C3	115.1 (3)	C6—C7—H7B	111.6
O8—C3A—Br1	108.6 (2)	C7A—C7—H7B	111.6
C4—C3A—Br1	113.4 (2)	H7A—C7—H7B	109.4
C3—C3A—Br1	101.5 (2)	C16—C11—C12	119.8 (3)
N2—C3—C3A	113.4 (3)	C16—C11—N2	120.1 (3)
N2—C3—H3A	108.9	C12—C11—N2	120.1 (3)
C3A—C3—H3A	108.9	C13—C12—C11	119.8 (3)
N2—C3—H3B	108.9	C13—C12—H12A	120.1
C3A—C3—H3B	108.9	C11—C12—H12A	120.1
H3A—C3—H3B	107.7	C12—C13—C14	120.0 (3)
C3A—C4—C5	103.3 (3)	C12—C13—H13A	120.0
C3A—C4—C7A	103.9 (2)	C14—C13—H13A	120.0
C5—C4—C7A	98.2 (2)	O2—C14—C15	124.2 (3)
C3A—C4—H4A	116.3	O2—C14—C13	115.3 (3)
C5—C4—H4A	116.3	C15—C14—C13	120.5 (3)
C7A—C4—H4A	116.3	C14—C15—C16	119.1 (3)
C6—C5—C4	93.7 (2)	C14—C15—H15A	120.5
C6—C5—Br2	116.1 (2)	C16—C15—H15A	120.5
C4—C5—Br2	119.5 (2)	C11—C16—C15	120.8 (3)
C6—C5—H5A	108.8	C11—C16—H16A	119.6
C4—C5—H5A	108.8	C15—C16—H16A	119.6
Br2—C5—H5A	108.8	O2—C17—H17A	109.5
O8—C6—C5	104.7 (3)	O2—C17—H17B	109.5
O8—C6—C7	106.2 (3)	H17A—C17—H17B	109.5
C5—C6—C7	100.3 (3)	O2—C17—H17C	109.5
O8—C6—H6A	114.7	H17A—C17—H17C	109.5
C5—C6—H6A	114.7	H17B—C17—H17C	109.5

C11—N2—C1—O1	−5.2 (5)	O1—C1—C7A—C4	151.2 (3)
C3—N2—C1—O1	−163.7 (3)	N2—C1—C7A—C4	−36.4 (4)
C11—N2—C1—C7A	−177.4 (3)	O1—C1—C7A—C7	−91.6 (4)
C3—N2—C1—C7A	24.1 (4)	N2—C1—C7A—C7	80.9 (3)
C6—O8—C3A—C4	0.7 (3)	C3A—C4—C7A—C1	50.2 (3)
C6—O8—C3A—C3	127.1 (3)	C5—C4—C7A—C1	156.1 (3)
C6—O8—C3A—Br1	−120.6 (2)	C3A—C4—C7A—C7	−70.3 (3)
C1—N2—C3—C3A	−29.3 (4)	C5—C4—C7A—C7	35.6 (3)
C11—N2—C3—C3A	171.5 (3)	O8—C6—C7—C7A	68.9 (3)
O8—C3A—C3—N2	−73.6 (4)	C5—C6—C7—C7A	−39.9 (3)

C4—C3A—C3—N2	47.1 (4)	C1—C7A—C7—C6	−124.2 (3)
Br1—C3A—C3—N2	169.9 (2)	C4—C7A—C7—C6	2.0 (3)
O8—C3A—C4—C5	−31.7 (3)	C1—N2—C11—C16	106.7 (4)
C3—C3A—C4—C5	−157.3 (3)	C3—N2—C11—C16	−93.2 (4)
Br1—C3A—C4—C5	86.4 (3)	C1—N2—C11—C12	−74.6 (4)
O8—C3A—C4—C7A	70.4 (3)	C3—N2—C11—C12	85.5 (4)
C3—C3A—C4—C7A	−55.3 (3)	C16—C11—C12—C13	−2.1 (5)
Br1—C3A—C4—C7A	−171.5 (2)	N2—C11—C12—C13	179.2 (3)
C3A—C4—C5—C6	47.1 (3)	C11—C12—C13—C14	1.4 (5)
C7A—C4—C5—C6	−59.3 (3)	C17—O2—C14—C15	9.8 (5)
C3A—C4—C5—Br2	−75.8 (3)	C17—O2—C14—C13	−171.3 (4)
C7A—C4—C5—Br2	177.8 (2)	C12—C13—C14—O2	−178.4 (3)
C3A—O8—C6—C5	31.2 (3)	C12—C13—C14—C15	0.6 (5)
C3A—O8—C6—C7	−74.4 (3)	O2—C14—C15—C16	177.0 (3)
C4—C5—C6—O8	−47.4 (3)	C13—C14—C15—C16	−1.9 (6)
Br2—C5—C6—O8	78.1 (3)	C12—C11—C16—C15	0.8 (5)
C4—C5—C6—C7	62.6 (3)	N2—C11—C16—C15	179.5 (3)
Br2—C5—C6—C7	−171.9 (2)	C14—C15—C16—C11	1.2 (6)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O1^{i}	0.98	2.57	3.092 (3)	114
C7*A*—H7*AA*···*Cg*5^{i}	0.98	2.69	3.573 (4)	150

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