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1,1′-[(2-Bromophenyl)methylene]-dipyrrolidin-2-one

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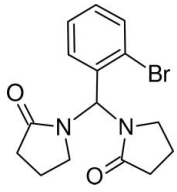
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.002 Å; R factor = 0.025; wR factor = 0.057; data-to-parameter ratio = 23.7.

In the title compound, $C_{15}H_{17}BrN_2O_2$, both pyrrolidinone rings adopt envelope conformations. The crystal packing is characterized by short C—Br···O=C interactions [Br···O = 3.1730 (13) Å], leading to supramolecular dimers. Intermolecular C—H···O and C—H···π interactions are also observed.

Related literature

For a related structure, see: Camus *et al.* (2001). For related references on Br···O interactions, see: Allen *et al.* (1997); Damodharan *et al.* (2004).



Experimental

Crystal data

$C_{15}H_{17}BrN_2O_2$
M_r = 337.22
Monoclinic, $P2_1/n$
a = 7.9734 (3) Å
b = 11.0788 (4) Å
c = 15.9456 (6) Å
β = 91.859 (1)°
V = 1407.82 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.92 mm^{-1}
T = 123 K
0.20 × 0.18 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.593, T_{max} = 0.621
15532 measured reflections
4296 independent reflections
3661 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.057
S = 1.01
4296 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

Cg is the centroid of the C10–C15 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2B···O2^{i}	0.97	2.40	3.363 (2)	174
C6—H6B···O2^{i}	0.97	2.59	3.528 (2)	163
C11—H11···O1^{i}	0.93	2.56	3.328 (2)	140
C13—H13···O2^{ii}	0.93	2.55	3.223 (2)	130
C8—H8B···Cg^{iii}	0.97	2.75	3.6405 (19)	152

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5471).

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supporting information

Acta Cryst. (2012). E**68**, o768 [doi:10.1107/S1600536812006277]

1,1′-[(2-Bromophenyl)methylene]dipyrrolidin-2-one

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S1. Comment

In the title compound, $C_{15}H_{17}BrN_2O_2$, both pyrrolidinone rings (N1/C2—C5; N2/C6—C9) adopt envelope conformation with C3 and C7 atoms at their flap, respectively (Fig. 1). Crystal packing is characterized by C15—Br1···O1—C5^{i} interaction [symmetry code (i): 2 - *x*,1 - *y*,-*z*; Br···O = 3.1730 (13) Å, C—Br···O = 170.33 (5)°] leading to molecular dimers (Fig. 2). Intermolecular C—H···O and C—H···π interactions additionally stabilize the packing (Table 1).

S2. Experimental

In a dry 100 ml Erlenmeyer flask 2-pyrrolidone (10 mmol), benzaldehyde (10 mmol), iodine (15 mol %) and dichloromethane (DCM; 15 ml) were taken. The reaction mixture was stirred at room temperature (25°C) for one hour. The reaction was monitored by TLC and after the completion of reaction iodine utilized was set free from the product by treating it with aqueous sodium thiosulfate solution and extracted into DCM (2 *X* 20 ml). The crude reaction mixture was purified by column chromatography on silica gel using ethyl acetate/hexane as the eluents. Final yields: 82%; m.p. 354 (1)°K. Suitable single crystals for data collection were grown from ethanol and tetrahydrofuran (THF) mixture (1:1).

S3. Refinement

H atoms were placed in the geometrically expected positions and refined with the riding options. The calculated distances with hydrogen atoms are: C(sp^2)—H = 0.93 Å, *C*(methylene)—H = 0.97 Å, C(methine)—H = 0.98 Å and U_{iso} = 1.2 U_{eq}(parent).

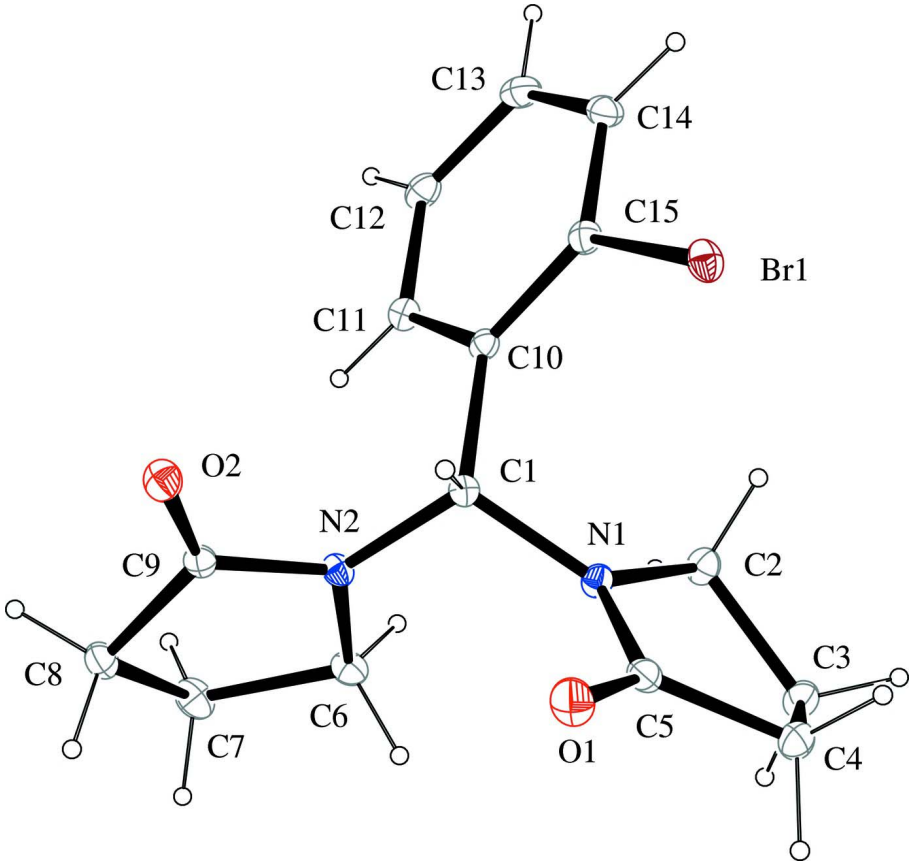

Figure 1

A view of (I) with non-H atoms shown as probability ellipsoids at 30% levels (Farrugia, 1997). H atoms radii are on an arbitrary scale.

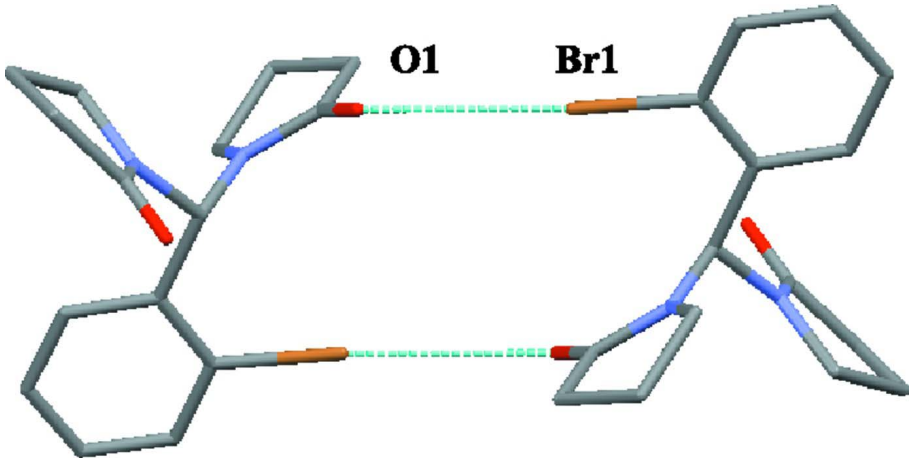

Figure 2

Molecular dimers *via* Br···O interaction.

1,1′-[(2-Bromophenyl)methylene]dipyrrolidin-2-one

Crystal data

$C_{15}H_{17}BrN_2O_2$
$M_r = 337.22$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.9734$ (3) Å
$b = 11.0788$ (4) Å
$c = 15.9456$ (6) Å
$\beta = 91.859$ (1)°
$V = 1407.82$ (9) Å^3
$Z = 4$
$F(000) = 688$
$D_x = 1.591$ Mg m^{-3}
Melting point: 354(1) K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 840 reflections
$\theta = 2.1$–$24.0°$
$\mu = 2.92$ mm^{-1}
$T = 123$ K
Block, colorless
0.20 × 0.18 × 0.18 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.593$, $T_{max} = 0.621$
15532 measured reflections
4296 independent reflections
3661 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 30.6°$, $\theta_{min} = 2.2°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 15$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.057$
$S = 1.01$
4296 reflections
181 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0228P)^2 + 0.7592P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.86332 (17)	0.68852 (12)	0.18659 (8)	0.0138 (3)
H1	0.9215	0.6106	0.1871	0.017*
C2	0.75434 (19)	0.81209 (13)	0.05820 (9)	0.0182 (3)
H2A	0.8600	0.8379	0.0356	0.022*

H2B	0.7103	0.8762	0.0925	0.022*
C3	0.62857 (19)	0.77622 (15)	−0.01195 (9)	0.0218 (3)
H3A	0.5146	0.7938	0.0037	0.026*
H3B	0.6515	0.8186	−0.0636	0.026*
C4	0.6548 (2)	0.64047 (14)	−0.02201 (9)	0.0223 (3)
H4A	0.5493	0.6001	−0.0355	0.027*
H4B	0.7329	0.6238	−0.0659	0.027*
C5	0.72546 (18)	0.60005 (14)	0.06225 (9)	0.0178 (3)
C6	0.58936 (18)	0.75537 (13)	0.25328 (9)	0.0180 (3)
H6A	0.5089	0.7226	0.2124	0.022*
H6B	0.6087	0.8398	0.2406	0.022*
C7	0.5283 (2)	0.73979 (15)	0.34296 (10)	0.0231 (3)
H7A	0.5544	0.8108	0.3765	0.028*
H7B	0.4080	0.7264	0.3425	0.028*
C8	0.62238 (18)	0.62932 (14)	0.37781 (9)	0.0191 (3)
H8A	0.6604	0.6428	0.4355	0.023*
H8B	0.5511	0.5584	0.3756	0.023*
C9	0.76951 (17)	0.61425 (12)	0.32157 (8)	0.0151 (3)
C10	0.99547 (17)	0.78631 (13)	0.19871 (8)	0.0139 (2)
C11	0.98318 (18)	0.87298 (13)	0.26151 (9)	0.0169 (3)
H11	0.8926	0.8708	0.2968	0.020*
C12	1.10341 (19)	0.96235 (14)	0.27229 (9)	0.0201 (3)
H12	1.0935	1.0188	0.3150	0.024*
C13	1.23820 (19)	0.96825 (14)	0.21989 (10)	0.0220 (3)
H13	1.3175	1.0293	0.2267	0.026*
C14	1.25446 (18)	0.88301 (14)	0.15741 (10)	0.0200 (3)
H14	1.3442	0.8867	0.1217	0.024*
C15	1.13587 (18)	0.79196 (13)	0.14840 (9)	0.0161 (3)
N1	0.77437 (15)	0.69982 (10)	0.10618 (7)	0.0147 (2)
N2	0.74562 (15)	0.68714 (10)	0.25438 (7)	0.0146 (2)
O1	0.73991 (15)	0.49624 (10)	0.08795 (7)	0.0253 (2)
O2	0.89131 (13)	0.54791 (10)	0.33318 (7)	0.0210 (2)
Br1	1.171997 (18)	0.670483 (13)	0.066302 (9)	0.01925 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0145 (6)	0.0132 (6)	0.0136 (6)	0.0009 (5)	0.0010 (5)	0.0000 (5)
C2	0.0219 (7)	0.0148 (7)	0.0178 (6)	0.0008 (5)	−0.0014 (5)	0.0013 (5)
C3	0.0200 (7)	0.0269 (8)	0.0184 (7)	0.0013 (6)	−0.0022 (5)	0.0011 (6)
C4	0.0262 (8)	0.0241 (8)	0.0166 (7)	−0.0066 (6)	0.0000 (6)	−0.0032 (6)
C5	0.0182 (6)	0.0188 (7)	0.0166 (6)	−0.0046 (5)	0.0040 (5)	−0.0032 (5)
C6	0.0148 (6)	0.0160 (7)	0.0233 (7)	0.0036 (5)	0.0030 (5)	0.0013 (5)
C7	0.0227 (7)	0.0219 (8)	0.0252 (8)	0.0032 (6)	0.0089 (6)	−0.0016 (6)
C8	0.0208 (7)	0.0197 (7)	0.0171 (6)	−0.0026 (6)	0.0044 (5)	−0.0004 (5)
C9	0.0175 (6)	0.0125 (6)	0.0154 (6)	−0.0029 (5)	0.0006 (5)	−0.0011 (5)
C10	0.0146 (6)	0.0133 (6)	0.0136 (6)	0.0007 (5)	−0.0014 (5)	0.0015 (5)
C11	0.0179 (7)	0.0174 (7)	0.0155 (6)	0.0002 (5)	0.0000 (5)	0.0000 (5)

C12	0.0238 (7)	0.0169 (7)	0.0191 (7)	−0.0015 (6)	−0.0049 (5)	−0.0020 (5)
C13	0.0181 (7)	0.0195 (7)	0.0279 (8)	−0.0034 (6)	−0.0049 (6)	0.0025 (6)
C14	0.0135 (6)	0.0227 (8)	0.0238 (7)	0.0003 (6)	0.0011 (5)	0.0049 (6)
C15	0.0157 (6)	0.0167 (6)	0.0160 (6)	0.0033 (5)	0.0000 (5)	0.0013 (5)
N1	0.0178 (6)	0.0123 (5)	0.0140 (5)	−0.0013 (4)	−0.0008 (4)	−0.0006 (4)
N2	0.0142 (5)	0.0140 (6)	0.0158 (5)	0.0018 (4)	0.0029 (4)	0.0015 (4)
O1	0.0359 (6)	0.0154 (5)	0.0246 (6)	−0.0066 (5)	0.0020 (5)	−0.0017 (4)
O2	0.0206 (5)	0.0194 (5)	0.0229 (5)	0.0047 (4)	0.0015 (4)	0.0052 (4)
Br1	0.02074 (8)	0.01928 (8)	0.01803 (7)	0.00452 (6)	0.00520 (5)	−0.00019 (6)

Geometric parameters (Å, º)

C1—N1	1.4504 (17)	C7—C8	1.531 (2)
C1—N2	1.4545 (17)	C7—H7A	0.9700
C1—C10	1.5192 (19)	C7—H7B	0.9700
C1—H1	0.9800	C8—C9	1.5088 (19)
C2—N1	1.4664 (18)	C8—H8A	0.9700
C2—C3	1.530 (2)	C8—H8B	0.9700
C2—H2A	0.9700	C9—O2	1.2272 (17)
C2—H2B	0.9700	C9—N2	1.3501 (18)
C3—C4	1.528 (2)	C10—C11	1.393 (2)
C3—H3A	0.9700	C10—C15	1.3997 (19)
C3—H3B	0.9700	C11—C12	1.385 (2)
C4—C5	1.508 (2)	C11—H11	0.9300
C4—H4A	0.9700	C12—C13	1.384 (2)
C4—H4B	0.9700	C12—H12	0.9300
C5—O1	1.2251 (19)	C13—C14	1.382 (2)
C5—N1	1.3589 (18)	C13—H13	0.9300
C6—N2	1.4569 (18)	C14—C15	1.387 (2)
C6—C7	1.535 (2)	C14—H14	0.9300
C6—H6A	0.9700	C15—Br1	1.9059 (14)
C6—H6B	0.9700		
N1—C1—N2	110.43 (11)	C8—C7—H7B	110.7
N1—C1—C10	111.61 (11)	C6—C7—H7B	110.7
N2—C1—C10	111.99 (11)	H7A—C7—H7B	108.8
N1—C1—H1	107.5	C9—C8—C7	104.72 (12)
N2—C1—H1	107.5	C9—C8—H8A	110.8
C10—C1—H1	107.5	C7—C8—H8A	110.8
N1—C2—C3	102.63 (11)	C9—C8—H8B	110.8
N1—C2—H2A	111.2	C7—C8—H8B	110.8
C3—C2—H2A	111.2	H8A—C8—H8B	108.9
N1—C2—H2B	111.2	O2—C9—N2	124.65 (13)
C3—C2—H2B	111.2	O2—C9—C8	127.11 (13)
H2A—C2—H2B	109.2	N2—C9—C8	108.25 (12)
C4—C3—C2	104.12 (12)	C11—C10—C15	117.22 (13)
C4—C3—H3A	110.9	C11—C10—C1	121.22 (12)
C2—C3—H3A	110.9	C15—C10—C1	121.55 (12)

C4—C3—H3B	110.9	C12—C11—C10	121.16 (13)
C2—C3—H3B	110.9	C12—C11—H11	119.4
H3A—C3—H3B	109.0	C10—C11—H11	119.4
C5—C4—C3	104.31 (12)	C13—C12—C11	120.45 (14)
C5—C4—H4A	110.9	C13—C12—H12	119.8
C3—C4—H4A	110.9	C11—C12—H12	119.8
C5—C4—H4B	110.9	C14—C13—C12	119.72 (14)
C3—C4—H4B	110.9	C14—C13—H13	120.1
H4A—C4—H4B	108.9	C12—C13—H13	120.1
O1—C5—N1	124.68 (14)	C13—C14—C15	119.48 (14)
O1—C5—C4	127.23 (13)	C13—C14—H14	120.3
N1—C5—C4	108.08 (12)	C15—C14—H14	120.3
N2—C6—C7	103.15 (12)	C14—C15—C10	121.90 (13)
N2—C6—H6A	111.1	C14—C15—Br1	117.84 (11)
C7—C6—H6A	111.1	C10—C15—Br1	120.24 (11)
N2—C6—H6B	111.1	C5—N1—C1	120.62 (12)
C7—C6—H6B	111.1	C5—N1—C2	113.36 (12)
H6A—C6—H6B	109.1	C1—N1—C2	125.19 (11)
C8—C7—C6	105.16 (11)	C9—N2—C1	121.21 (11)
C8—C7—H7A	110.7	C9—N2—C6	114.74 (11)
C6—C7—H7A	110.7	C1—N2—C6	123.90 (11)

N1—C2—C3—C4	−26.53 (15)	C1—C10—C15—Br1	−3.48 (18)
C2—C3—C4—C5	25.03 (15)	O1—C5—N1—C1	5.5 (2)
C3—C4—C5—O1	166.88 (15)	C4—C5—N1—C1	−173.64 (12)
C3—C4—C5—N1	−14.00 (16)	O1—C5—N1—C2	175.60 (14)
N2—C6—C7—C8	−19.18 (15)	C4—C5—N1—C2	−3.55 (16)
C6—C7—C8—C9	18.77 (16)	N2—C1—N1—C5	−91.10 (15)
C7—C8—C9—O2	168.80 (14)	C10—C1—N1—C5	143.64 (12)
C7—C8—C9—N2	−11.29 (16)	N2—C1—N1—C2	100.04 (15)
N1—C1—C10—C11	115.42 (14)	C10—C1—N1—C2	−25.22 (18)
N2—C1—C10—C11	−8.97 (18)	C3—C2—N1—C5	19.40 (16)
N1—C1—C10—C15	−65.71 (16)	C3—C2—N1—C1	−171.04 (12)
N2—C1—C10—C15	169.89 (12)	O2—C9—N2—C1	2.8 (2)
C15—C10—C11—C12	1.3 (2)	C8—C9—N2—C1	−177.13 (12)
C1—C10—C11—C12	−179.76 (13)	O2—C9—N2—C6	178.53 (13)
C10—C11—C12—C13	0.8 (2)	C8—C9—N2—C6	−1.39 (16)
C11—C12—C13—C14	−1.2 (2)	N1—C1—N2—C9	141.19 (13)
C12—C13—C14—C15	−0.5 (2)	C10—C1—N2—C9	−93.76 (15)
C13—C14—C15—C10	2.7 (2)	N1—C1—N2—C6	−34.15 (17)
C13—C14—C15—Br1	−175.86 (11)	C10—C1—N2—C6	90.89 (15)
C11—C10—C15—C14	−3.0 (2)	C7—C6—N2—C9	13.31 (16)
C1—C10—C15—C14	178.04 (13)	C7—C6—N2—C1	−171.07 (12)
C11—C10—C15—Br1	175.43 (10)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*B*···O2^{i}	0.97	2.40	3.363 (2)	174
C6—H6*B*···O2^{i}	0.97	2.59	3.528 (2)	163
C11—H11···O1^{i}	0.93	2.56	3.328 (2)	140
C13—H13···O2^{ii}	0.93	2.55	3.223 (2)	130
C8—H8*B*···*Cg*^{iii}	0.97	2.75	3.6405 (19)	152

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+1/2; (ii) −*x*+5/2, *y*+1/2, −*z*+1/2; (iii) −*x*+3/2, *y*−1/2, −*z*+1/2.