Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *N*-(2-Bromophenyl)-2-(naphthalen-1-yl)-acetamide

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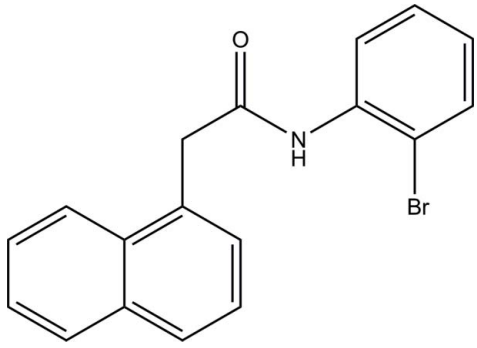
Received 31 July 2012; accepted 2 August 2012

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.029; $wR$ factor = 0.061; data-to-parameter ratio = 19.8.

In the title compound, $C_{18}H_{14}BrNO$, the naphthalene ring system [maximum deviation = 0.015 (3) Å] forms a dihedral angle of 67.70 (10)° with the benzene ring. In the crystal, molecules are linked by N—H···O hydrogen bonds into $C(4)$ chains propagating in [100]. A C—H···O interaction reinforces the chain connectivity, generating an $R_2^1(6)$ loop.

## Related literature

For general background to and related structures of the title compound, see: Fun *et al.* (2010, 2011*a*,*b*, 2012). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).




## Experimental

### *Crystal data*

$C_{18}H_{14}BrNO$
$M_r$ = 340.21
Orthorhombic, $P2_12_12_1$
$a$ = 4.7603 (1) Å
$b$ = 11.4614 (3) Å
$c$ = 26.6255 (6) Å
$V$ = 1452.68 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.83 mm$^{-1}$
$T$ = 100 K
0.32 × 0.16 × 0.13 mm

### *Data collection*

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.463, $T_{max}$ = 0.719
16642 measured reflections
3864 independent reflections
3516 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.061
$S$ = 1.03
3864 reflections
195 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.63 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$
Absolute structure: Flack (1983), 1587 Friedel pairs
Flack parameter: 0.001 (8)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*1···O1$^{i}$ | 0.86 (3) | 2.03 (3) | 2.855 (3) | 163 (2) |
| C11—H11*A*···O1$^{i}$ | 0.99 | 2.55 | 3.279 (3) | 130 |

Symmetry code: (i) $x-1, y, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

The authors thank Universiti Sains Malaysia (USM) for the Research University Grant (No. 1001/PFIZIK/811160). BN also thanks UGC, New Delhi, and the Government of India for the purchase of chemicals through the SAP-DRS-Phase 1 programme.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6923).

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‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5525-2009.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o2657 [doi:10.1107/S1600536812034423]

## *N*-(2-Bromophenyl)-2-(naphthalen-1-yl)acetamide

**Hoong-Kun Fun, Ching Kheng Quah, Prakash S. Nayak, B. Narayana and B. K. Sarojini**

### Comment

In continuation of our work on synthesis of amides (Fun *et al.*, 2010, 2011*a*, 2011*b*, 2012), we report herein the crystal structure of the title compound.

The molecular structure is shown in Fig. 1. Bond lengths are comparable to related structures (Fun *et al.*, 2010, 2011*a*, 2011*b*, 2012). The naphthalene ring system (C1-C10, maximum deviation of 0.015 (3) Å at atom C9) forms a dihedral angle of 67.70 (10)° with the benzene ring (C13-C18).

In the crystal structure, Fig. 2, molecules are linked *via* N1–H1N1···O1 and C11–H11A···O1 hydrogen bonds (Table 1) into one-dimensional [100] chains which contain $R_2^1$ (6) ring motifs (Bernstein *et al.*, 1995).

### Experimental

1-Naphthaleneacetic acid (0.186 g, 1 mmol), 2-bromoaniline (0.1 ml, 1 mmol) and 1-ethyl-3-(3-dimethylaminopropyl)-carbodiimide hydrochloride (1.0 g, 0.01 mol) were dissolved in dichloromethane (20 ml). The mixture was stirred in presence of triethylamine at 273 K for about 3 h. The contents were poured into 100 ml of ice-cold aqueous hydrochloric acid with stirring. The concotion was then extracted thrice with dichloromethane. The organic layer was washed with saturated $NaHCO_3$ solution and brine solution, dried and concentrated under reduced pressure to give the title compound. Colourless blocks were grown from toluene solution by the slow evaporation method (*m.p.*: 421K).

### Refinement

Atom H1N1 was located in a difference Fourier map and refined freely [N–H = 0.86 (3) Å]. The remaining H atoms were positioned geometrically and refined using a riding model with C–H = 0.95 or 0.99 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C). The reported Flack parameter was obtained by TWIN/BASF procedure in *SHELXL* (Sheldrick, 2008).

### Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

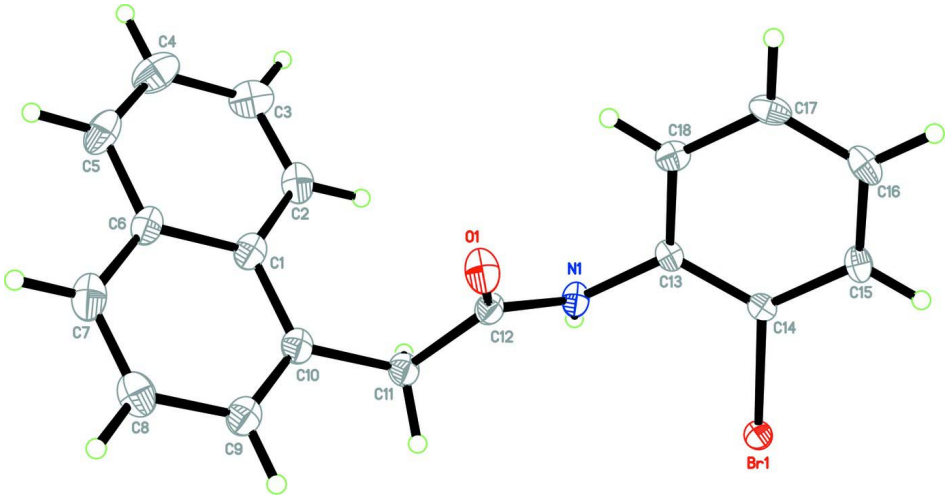


**Figure 1**

The molecular structure of the title compound showing 40% probability displacement ellipsoids for non-H atoms.

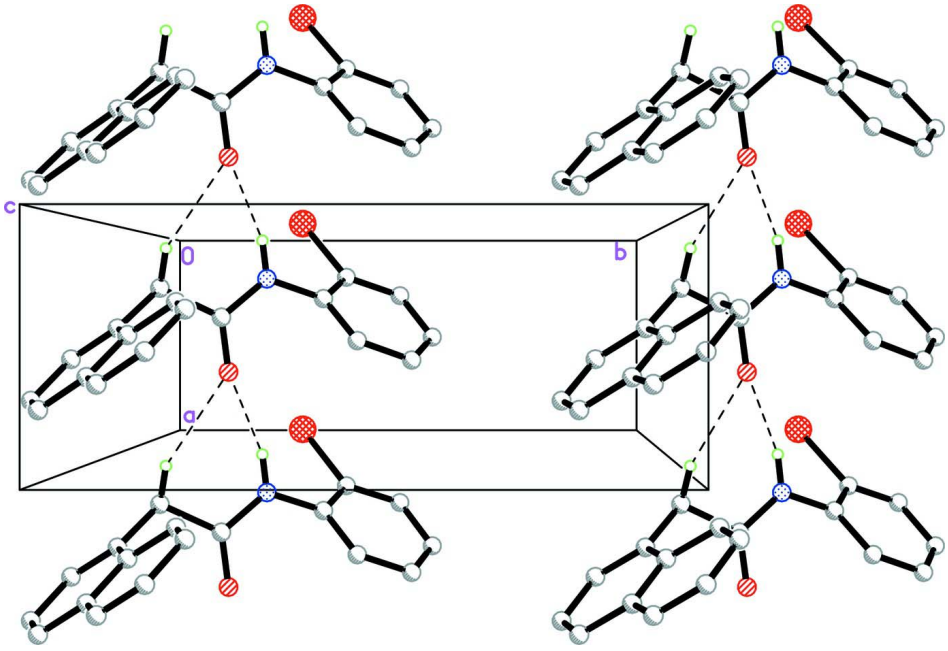


**Figure 2**

The crystal structure of the title compound, viewed along the *c* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

### *N*-(2-Bromophenyl)-2-(naphthalen-1-yl)acetamide

*Crystal data*

$C_{18}H_{14}BrNO$
$M_r$ = 340.21
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a$ = 4.7603 (1) Å
$b$ = 11.4614 (3) Å
$c$ = 26.6255 (6) Å
$V$ = 1452.68 (6) Å$^3$
$Z$ = 4
$F$(000) = 688
$D_x$ = 1.556 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å

Cell parameters from 8019 reflections
$\theta$ = 2.3–30.8°
$\mu$ = 2.83 mm$^{-1}$
$T$ = 100 K
Block, colourless
0.32 × 0.16 × 0.13 mm

*Data collection*

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.463, $T_{max}$ = 0.719
16642 measured reflections
3864 independent reflections
3516 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031
$\theta_{max}$ = 29.0°, $\theta_{min}$ = 1.5°
$h$ = −6→6
$k$ = −15→15
$l$ = −36→36

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.061
$S$ = 1.03
3864 reflections
195 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 0.2223P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.63 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$
Absolute structure: Flack (1983), 1587 Friedel pairs
Flack parameter: 0.001 (8)

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**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**. 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 $F^2 > 2$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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.44680 (5) | 0.197949 (18) | 0.766005 (8) | 0.01881 (6) |
| O1 | 1.1551 (4) | 0.32404 (15) | 0.64580 (7) | 0.0288 (4) |
| N1 | 0.7212 (5) | 0.25292 (18) | 0.66352 (8) | 0.0205 (4) |
| C1 | 0.9798 (6) | 0.4924 (2) | 0.54712 (8) | 0.0243 (5) |
| C2 | 0.8336 (6) | 0.3968 (2) | 0.52540 (10) | 0.0290 (6) |
| H2A | 0.7122 | 0.3512 | 0.5458 | 0.035* |
| C3 | 0.8643 (7) | 0.3692 (3) | 0.47576 (10) | 0.0362 (7) |
| H3A | 0.7616 | 0.3060 | 0.4618 | 0.043* |
| C4 | 1.0465 (8) | 0.4340 (3) | 0.44572 (10) | 0.0404 (7) |
| H4A | 1.0702 | 0.4133 | 0.4114 | 0.048* |

| | | | | |
|---|---|---|---|---|
| C5 | 1.1896 (7) | 0.5257 (3) | 0.46455 (10) | 0.0342 (7) |
| H5A | 1.3099 | 0.5691 | 0.4431 | 0.041* |
| C6 | 1.1646 (6) | 0.5586 (2) | 0.51556 (9) | 0.0254 (5) |
| C7 | 1.3132 (7) | 0.6544 (2) | 0.53578 (11) | 0.0327 (6) |
| H7A | 1.4370 | 0.6981 | 0.5151 | 0.039* |
| C8 | 1.2791 (6) | 0.6844 (2) | 0.58521 (10) | 0.0318 (6) |
| H8A | 1.3788 | 0.7488 | 0.5989 | 0.038* |
| C9 | 1.0935 (6) | 0.6184 (2) | 0.61591 (9) | 0.0274 (6) |
| H9A | 1.0688 | 0.6408 | 0.6500 | 0.033* |
| C10 | 0.9508 (6) | 0.52492 (19) | 0.59833 (8) | 0.0237 (5) |
| C11 | 0.7656 (6) | 0.45304 (19) | 0.63269 (9) | 0.0238 (5) |
| H11A | 0.5846 | 0.4374 | 0.6156 | 0.029* |
| H11B | 0.7254 | 0.4984 | 0.6635 | 0.029* |
| C12 | 0.9006 (6) | 0.3379 (2) | 0.64713 (8) | 0.0211 (6) |
| C13 | 0.8129 (5) | 0.14552 (19) | 0.68404 (8) | 0.0169 (5) |
| C14 | 0.7098 (5) | 0.10589 (17) | 0.73006 (8) | 0.0159 (4) |
| C15 | 0.7974 (5) | 0.00074 (19) | 0.75029 (8) | 0.0202 (5) |
| H15A | 0.7212 | −0.0260 | 0.7812 | 0.024* |
| C16 | 0.9963 (5) | −0.06519 (18) | 0.72528 (8) | 0.0244 (6) |
| H16A | 1.0604 | −0.1365 | 0.7394 | 0.029* |
| C17 | 1.1024 (5) | −0.0273 (2) | 0.67953 (9) | 0.0240 (6) |
| H17A | 1.2386 | −0.0729 | 0.6623 | 0.029* |
| C18 | 1.0100 (5) | 0.07691 (19) | 0.65886 (8) | 0.0207 (5) |
| H18A | 1.0815 | 0.1018 | 0.6273 | 0.025* |
| H1N1 | 0.543 (6) | 0.261 (2) | 0.6612 (8) | 0.015 (6)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.01624 (11) | 0.01879 (9) | 0.02138 (9) | 0.00023 (10) | 0.00331 (10) | 0.00085 (8) |
| O1 | 0.0139 (9) | 0.0299 (10) | 0.0427 (10) | 0.0035 (8) | 0.0034 (9) | 0.0116 (8) |
| N1 | 0.0126 (11) | 0.0246 (10) | 0.0244 (9) | 0.0045 (9) | 0.0025 (10) | 0.0081 (8) |
| C1 | 0.0171 (14) | 0.0310 (11) | 0.0249 (10) | 0.0080 (11) | −0.0005 (11) | 0.0072 (9) |
| C2 | 0.0178 (13) | 0.0312 (13) | 0.0380 (14) | 0.0009 (12) | −0.0006 (13) | 0.0094 (11) |
| C3 | 0.0269 (17) | 0.0460 (16) | 0.0359 (14) | 0.0036 (14) | −0.0049 (13) | −0.0062 (12) |
| C4 | 0.0273 (15) | 0.0627 (19) | 0.0312 (12) | 0.0067 (18) | 0.0001 (15) | −0.0022 (12) |
| C5 | 0.0229 (15) | 0.0514 (17) | 0.0282 (13) | 0.0013 (14) | 0.0047 (13) | 0.0095 (12) |
| C6 | 0.0188 (13) | 0.0313 (13) | 0.0261 (11) | 0.0052 (12) | 0.0023 (12) | 0.0084 (10) |
| C7 | 0.0226 (15) | 0.0352 (13) | 0.0404 (14) | 0.0043 (13) | 0.0041 (13) | 0.0134 (11) |
| C8 | 0.0249 (15) | 0.0285 (14) | 0.0419 (14) | −0.0021 (13) | −0.0034 (12) | 0.0033 (11) |
| C9 | 0.0242 (17) | 0.0307 (12) | 0.0271 (11) | 0.0073 (12) | 0.0011 (12) | 0.0060 (9) |
| C10 | 0.0189 (12) | 0.0245 (11) | 0.0278 (10) | 0.0071 (12) | 0.0013 (13) | 0.0058 (8) |
| C11 | 0.0214 (15) | 0.0234 (11) | 0.0264 (11) | 0.0057 (11) | 0.0021 (11) | 0.0045 (9) |
| C12 | 0.0202 (16) | 0.0237 (11) | 0.0195 (10) | 0.0030 (10) | 0.0020 (11) | 0.0028 (8) |
| C13 | 0.0116 (12) | 0.0168 (10) | 0.0222 (10) | −0.0002 (9) | −0.0031 (10) | 0.0016 (8) |
| C14 | 0.0123 (11) | 0.0158 (9) | 0.0197 (9) | −0.0006 (8) | −0.0020 (11) | −0.0013 (8) |
| C15 | 0.0157 (12) | 0.0187 (10) | 0.0262 (10) | −0.0041 (10) | −0.0027 (10) | 0.0052 (8) |
| C16 | 0.0170 (15) | 0.0169 (10) | 0.0393 (13) | −0.0006 (9) | −0.0036 (12) | 0.0034 (8) |
| C17 | 0.0140 (15) | 0.0231 (11) | 0.0349 (12) | 0.0026 (10) | −0.0006 (11) | −0.0088 (9) |
| C18 | 0.0146 (15) | 0.0267 (11) | 0.0210 (9) | 0.0031 (10) | −0.0019 (10) | −0.0022 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C14 | 1.896 (2) | C8—C9 | 1.422 (4) |
| O1—C12 | 1.223 (3) | C8—H8A | 0.9500 |
| N1—C12 | 1.367 (3) | C9—C10 | 1.352 (4) |
| N1—C13 | 1.416 (3) | C9—H9A | 0.9500 |
| N1—H1N1 | 0.86 (3) | C10—C11 | 1.514 (3) |
| C1—C10 | 1.420 (3) | C11—C12 | 1.517 (3) |
| C1—C2 | 1.421 (4) | C11—H11A | 0.9900 |
| C1—C6 | 1.434 (3) | C11—H11B | 0.9900 |
| C2—C3 | 1.367 (4) | C13—C18 | 1.396 (3) |
| C2—H2A | 0.9500 | C13—C14 | 1.396 (3) |
| C3—C4 | 1.394 (4) | C14—C15 | 1.384 (3) |
| C3—H3A | 0.9500 | C15—C16 | 1.382 (3) |
| C4—C5 | 1.349 (4) | C15—H15A | 0.9500 |
| C4—H4A | 0.9500 | C16—C17 | 1.388 (3) |
| C5—C6 | 1.415 (4) | C16—H16A | 0.9500 |
| C5—H5A | 0.9500 | C17—C18 | 1.386 (3) |
| C6—C7 | 1.412 (4) | C17—H17A | 0.9500 |
| C7—C8 | 1.370 (4) | C18—H18A | 0.9500 |
| C7—H7A | 0.9500 | | |

| | | | |
|---|---|---|---|
| C12—N1—C13 | 123.4 (2) | C9—C10—C1 | 119.4 (2) |
| C12—N1—H1N1 | 121.0 (16) | C9—C10—C11 | 121.0 (2) |
| C13—N1—H1N1 | 115.6 (16) | C1—C10—C11 | 119.6 (2) |
| C10—C1—C2 | 123.1 (2) | C10—C11—C12 | 112.3 (2) |
| C10—C1—C6 | 118.9 (2) | C10—C11—H11A | 109.1 |
| C2—C1—C6 | 118.0 (2) | C12—C11—H11A | 109.1 |
| C3—C2—C1 | 121.3 (3) | C10—C11—H11B | 109.1 |
| C3—C2—H2A | 119.3 | C12—C11—H11B | 109.1 |
| C1—C2—H2A | 119.3 | H11A—C11—H11B | 107.9 |
| C2—C3—C4 | 119.9 (3) | O1—C12—N1 | 122.4 (2) |
| C2—C3—H3A | 120.1 | O1—C12—C11 | 121.7 (2) |
| C4—C3—H3A | 120.1 | N1—C12—C11 | 115.8 (2) |
| C5—C4—C3 | 121.0 (3) | C18—C13—C14 | 118.3 (2) |
| C5—C4—H4A | 119.5 | C18—C13—N1 | 120.8 (2) |
| C3—C4—H4A | 119.5 | C14—C13—N1 | 120.9 (2) |
| C4—C5—C6 | 121.5 (3) | C15—C14—C13 | 121.2 (2) |
| C4—C5—H5A | 119.3 | C15—C14—Br1 | 119.14 (17) |
| C6—C5—H5A | 119.3 | C13—C14—Br1 | 119.61 (16) |
| C7—C6—C5 | 122.1 (2) | C16—C15—C14 | 119.7 (2) |
| C7—C6—C1 | 119.7 (2) | C16—C15—H15A | 120.2 |
| C5—C6—C1 | 118.2 (2) | C14—C15—H15A | 120.2 |
| C8—C7—C6 | 120.1 (3) | C15—C16—C17 | 120.1 (2) |
| C8—C7—H7A | 119.9 | C15—C16—H16A | 120.0 |
| C6—C7—H7A | 119.9 | C17—C16—H16A | 120.0 |
| C7—C8—C9 | 119.5 (3) | C18—C17—C16 | 120.2 (2) |
| C7—C8—H8A | 120.2 | C18—C17—H17A | 119.9 |
| C9—C8—H8A | 120.2 | C16—C17—H17A | 119.9 |
| C10—C9—C8 | 122.3 (2) | C17—C18—C13 | 120.5 (2) |

| | | | |
|---|---|---|---|
| C10—C9—H9A | 118.8 | C17—C18—H18A | 119.7 |
| C8—C9—H9A | 118.8 | C13—C18—H18A | 119.7 |
| | | | |
| C10—C1—C2—C3 | 179.1 (3) | C6—C1—C10—C11 | −177.6 (2) |
| C6—C1—C2—C3 | −0.9 (4) | C9—C10—C11—C12 | −104.1 (3) |
| C1—C2—C3—C4 | 1.4 (4) | C1—C10—C11—C12 | 74.6 (3) |
| C2—C3—C4—C5 | −1.5 (5) | C13—N1—C12—O1 | 5.2 (4) |
| C3—C4—C5—C6 | 1.1 (5) | C13—N1—C12—C11 | −172.3 (2) |
| C4—C5—C6—C7 | −180.0 (3) | C10—C11—C12—O1 | 23.2 (3) |
| C4—C5—C6—C1 | −0.6 (4) | C10—C11—C12—N1 | −159.3 (2) |
| C10—C1—C6—C7 | −0.1 (4) | C12—N1—C13—C18 | −50.8 (3) |
| C2—C1—C6—C7 | 179.9 (2) | C12—N1—C13—C14 | 128.9 (3) |
| C10—C1—C6—C5 | −179.5 (3) | C18—C13—C14—C15 | −0.6 (3) |
| C2—C1—C6—C5 | 0.4 (4) | N1—C13—C14—C15 | 179.7 (2) |
| C5—C6—C7—C8 | 178.9 (3) | C18—C13—C14—Br1 | 178.87 (17) |
| C1—C6—C7—C8 | −0.5 (4) | N1—C13—C14—Br1 | −0.8 (3) |
| C6—C7—C8—C9 | 0.0 (4) | C13—C14—C15—C16 | 1.7 (3) |
| C7—C8—C9—C10 | 1.1 (4) | Br1—C14—C15—C16 | −177.77 (17) |
| C8—C9—C10—C1 | −1.7 (4) | C14—C15—C16—C17 | −1.5 (3) |
| C8—C9—C10—C11 | 177.0 (2) | C15—C16—C17—C18 | 0.2 (4) |
| C2—C1—C10—C9 | −178.8 (2) | C16—C17—C18—C13 | 0.9 (4) |
| C6—C1—C10—C9 | 1.2 (4) | C14—C13—C18—C17 | −0.7 (3) |
| C2—C1—C10—C11 | 2.5 (4) | N1—C13—C18—C17 | 179.0 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*1···O1$^{i}$ | 0.86 (3) | 2.03 (3) | 2.855 (3) | 163 (2) |
| C11—H11*A*···O1$^{i}$ | 0.99 | 2.55 | 3.279 (3) | 130 |

Symmetry code: (i) *x*−1, *y*, *z*.