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## Structure Reports

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## 2-Bromo-2-methyl-*N*-(4-methyl-2-oxo-2*H*-chromen-7-yl)propanamide

N. Haridharan, V. Ramkumar and R. Dhamodharan\*

 Department of Chemistry, IIT Madras, Chennai, TamilNadu, India  
 Correspondence e-mail: damo@iitm.ac.in

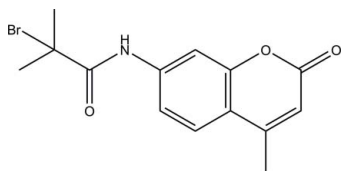
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 Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å;  $R$  factor = 0.057;  $wR$  factor = 0.174; data-to-parameter ratio = 14.0.

In the title compound  $\text{C}_{14}\text{H}_{14}\text{BrNO}_3$ , the coumarin ring system is almost planar (r.m.s. deviation = 0.008 Å) and an intramolecular  $\text{C}-\text{H}\cdots\text{O}$  interaction generates an  $S(6)$  ring. In the crystal, molecules are linked by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, with the  $\text{C}=\text{O}$  unit of the coumarin ring system acting as the acceptor group, generating [010]  $C(8)$  chains. The chain connectivity is reinforced by two  $\text{C}-\text{H}\cdots\text{O}$  interactions.

### Related literature

For background to the properties of coumarin derivatives, see: Sinkel *et al.* (2008); Matyjaszewski *et al.* (2008); Stenzel-Rosenbaum *et al.* (2001); Thaisrivongs *et al.* (1994). For a related structure, see: Haridharan *et al.* (2010)



### Experimental

#### Crystal data

$\text{C}_{14}\text{H}_{14}\text{BrNO}_3$   
 $M_r = 324.17$   
 Triclinic,  $P\bar{1}$   
 $a = 6.7054$  (8) Å  
 $b = 9.2415$  (11) Å  
 $c = 11.7612$  (15) Å  
 $\alpha = 105.255$  (5)°  
 $\beta = 100.630$  (5)°

$\gamma = 93.572$  (5)°  
 $V = 686.33$  (15) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 3.00$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.42 \times 0.20 \times 0.15$  mm

#### Data collection

Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2004)  
 $T_{\min} = 0.366$ ,  $T_{\max} = 0.662$

4624 measured reflections  
 2511 independent reflections  
 1716 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$   
 $wR(F^2) = 0.174$   
 $S = 1.09$   
 2511 reflections  
 179 parameters  
 1 restraint

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 1.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.53$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$                             | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{C}8-\text{H}8\cdots\text{O}3$             | 0.93         | 2.21               | 2.804 (6)   | 121                  |
| $\text{N}1-\text{H}1\text{N}\cdots\text{O}2^i$   | 0.91 (2)     | 2.12 (2)           | 3.016 (5)   | 168 (5)              |
| $\text{C}6-\text{H}6\cdots\text{O}2^i$           | 0.93         | 2.38               | 3.189 (6)   | 145                  |
| $\text{C}13-\text{H}13\text{C}\cdots\text{O}2^i$ | 0.96         | 2.51               | 3.347 (8)   | 146                  |

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

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.

The authors acknowledge the Department of Chemistry, IIT Madras, for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5522).

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## supporting information

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## 2-Bromo-2-methyl-*N*-(4-methyl-2-oxo-2*H*-chromen-7-yl)propanamide

N. Haridharan, V. Ramkumar and R. Dhamodharan

### S1. Comment

The title compound  $C_{14}H_{14}BrNO_3$ , is a monofunctional coumarin derivative, which is used as an initiator (Sinkel *et al.*, 2008) in Atom Transfer Radical Polymerization (ATRP). We have already reported a similar ATRP initiator (Haridharan *et al.*, 2010) with flourine containing coumarin derivative. The title compound reported here is a similiar derivative with bromo methyl propanamide and with a methyl substitution.

The synthesis of oxygen containing heterocyclic based initiators and their crystal structures are worth while to study due to their interesting properties and diverse bioactivities such as non peptidic HIV protease inhibition and tyrosine kinase inhibition (Thaisrivongs *et al.*, 1994).

In the title compound  $C_{14}H_{14}BrNO_3$ , the coumarin ring system is planar and the Br atom in the 2-bromo-2-methyl propanamide moiety is almost perpendicular to the ring.

The torsion angle of C6—C7—N1—C11 and C8—C7—N1—C11 are  $-177.89(2)^\circ$  and  $-2.75(2)^\circ$  respectively. The crystal is stabilized by intermolecular N—H $\cdots$ O hydrogen bond.

### S2. Experimental

7-Amino-4-methylcoumarin (4 g, 0.022 moles), triethylamine (5.08 g, 0.050 moles) and THF (200 ml) were placed in a 3-neck round bottomed flask. Bromoisobutyl bromide (11.54 g, 0.050 moles) was added slowly, using a syringe, with stirring, upon which a white precipitate of triethylammonium bromide was formed. The mixture was left to react for 6 h, with stirring. Subsequently, triethylammonium bromide, the precipitate was removed by filtration and the THF was removed by rotary evaporation. The resulting crude product was dissolved in ethyl acetate, washed with bicarbonate solution and then with water thrice followed by brine solution and dried over anhydrous sodium sulfate. The solvent was removed from the resulting solution by rotary evaporation. The product was purified by column chromatography technique using 10% ethyl acetate in hexane as the eluent to obtain pure initiator as a light yellow solid. Recrystallization of the compound from chloroform gave light yellow slabs of (I).

### S3. Refinement

The nitrogen H atom was located in a difference Fourier map and refined isotropically. All other hydrogen atoms were fixed geometrically and allowed to ride on the parent carbon atoms, with aromatic C—H = 0.93 Å and methyl C—H = 0.96 Å. The displacement parameters were set for phenyl H atoms at  $U_{iso}(H) = 1.2U_{eq}(C)$  and methyl H atoms at  $U_{iso}(H) = 1.5U_{eq}(C)$ .

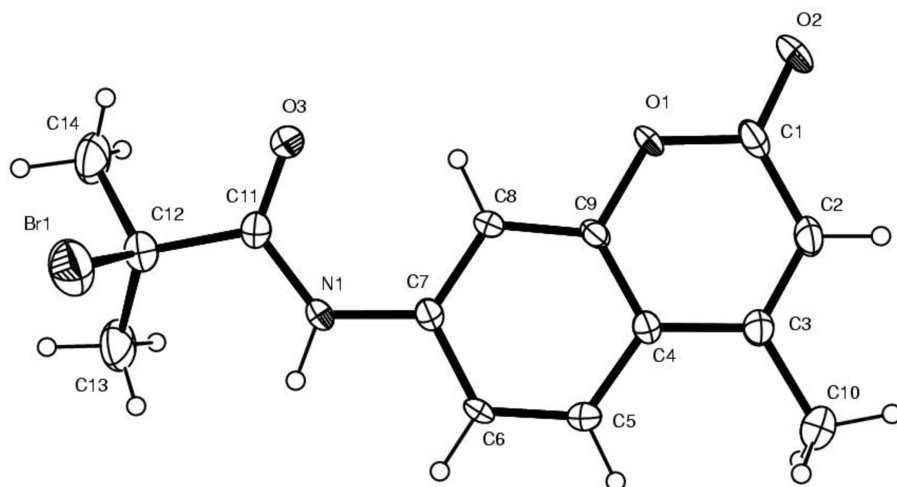


Figure 1

The molecular structure of (I) with atoms represented as 30% probability ellipsoids.

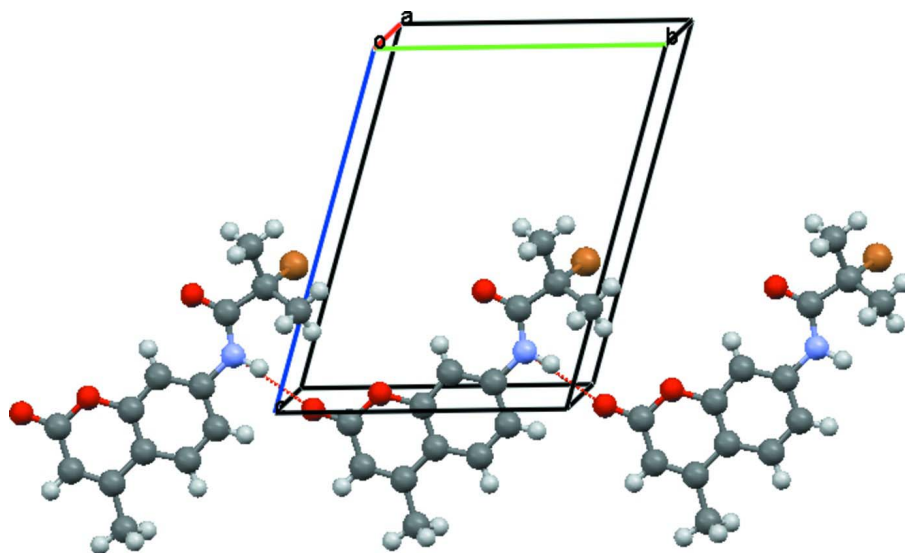


Figure 2

The packing diagram for (I) showing the N—H...O interaction along the *b* axis.

### 2-Bromo-2-methyl-*N*-(4-methyl-2-oxo-2*H*-chromen-7-yl)propanamide

#### Crystal data

$C_{14}H_{14}BrNO_3$

$M_r = 324.17$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 6.7054$  (8) Å

$b = 9.2415$  (11) Å

$c = 11.7612$  (15) Å

$\alpha = 105.255$  (5)°

$\beta = 100.630$  (5)°

$\gamma = 93.572$  (5)°

$V = 686.33$  (15) Å<sup>3</sup>

$Z = 2$

$F(000) = 328$

$D_x = 1.569$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1785 reflections

$\theta = 2.5$ – $24.5$ °

$\mu = 3.00$  mm<sup>-1</sup>

$T = 298$  K

Slab, light-yellow

$0.42 \times 0.20 \times 0.15$  mm

*Data collection*

|   |  |
|---|--|
| Bruker APEXII CCD diffractometer                            | 4624 measured reflections  |
| Radiation source: fine-focus sealed tube                    | 2511 independent reflections   |
| Graphite monochromator                                      | 1716 reflections with $I > 2\sigma(I)$                                 |
| phi and $\omega$ scans                                      | $R_{\text{int}} = 0.020$   |
| Absorption correction: multi-scan<br>(SADABS; Bruker, 2004) | $\theta_{\text{max}} = 28.3^\circ$ , $\theta_{\text{min}} = 1.8^\circ$ |
| $T_{\text{min}} = 0.366$ , $T_{\text{max}} = 0.662$         | $h = -8 \rightarrow 5$   |
|   | $k = -11 \rightarrow 10$   |
|   | $l = -11 \rightarrow 14$   |

*Refinement*

|  |  |
|--|--|
| Refinement on $F^2$  | Secondary atom site location: difference Fourier map                   |
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites               |
| $R[F^2 > 2\sigma(F^2)] = 0.057$                                | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.174$  | $w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.350P]$                          |
| $S = 1.09$   | where $P = (F_o^2 + 2F_c^2)/3$   |
| 2511 reflections   | $(\Delta/\sigma)_{\text{max}} < 0.001$                                 |
| 179 parameters   | $\Delta\rho_{\text{max}} = 1.16 \text{ e } \text{\AA}^{-3}$            |
| 1 restraint  | $\Delta\rho_{\text{min}} = -0.53 \text{ e } \text{\AA}^{-3}$           |
| Primary atom site location: structure-invariant direct methods |  |

*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 ( $\text{\AA}^2$ )*

|     | $x$         | $y$         | $z$         | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|-------------|----------------------------------|
| Br1 | 0.34908 (9) | 0.90419 (7) | 0.61854 (6) | 0.0714 (3)                       |
| C1  | 0.2652 (7)  | 0.2486 (5)  | 1.0477 (4)  | 0.0377 (11)                      |
| C2  | 0.3283 (7)  | 0.3307 (5)  | 1.1731 (4)  | 0.0388 (11)                      |
| H2  | 0.3551      | 0.2772      | 1.2299      | 0.047*                           |
| C3  | 0.3497 (6)  | 0.4824 (5)  | 1.2107 (4)  | 0.0352 (10)                      |
| C4  | 0.3086 (6)  | 0.5641 (5)  | 1.1221 (4)  | 0.0291 (10)                      |
| C5  | 0.3260 (7)  | 0.7225 (5)  | 1.1480 (4)  | 0.0362 (11)                      |
| H5  | 0.3639      | 0.7807      | 1.2279      | 0.043*                           |
| C6  | 0.2890 (7)  | 0.7927 (5)  | 1.0596 (4)  | 0.0347 (10)                      |
| H6  | 0.3042      | 0.8976      | 1.0795      | 0.042*                           |
| C7  | 0.2285 (6)  | 0.7087 (5)  | 0.9391 (4)  | 0.0291 (9)                       |

|      |              |            |            |             |
|------|--------------|------------|------------|-------------|
| C8   | 0.2092 (6)   | 0.5511 (4) | 0.9098 (4) | 0.0282 (9)  |
| H8   | 0.1700       | 0.4926     | 0.8301     | 0.034*      |
| C9   | 0.2497 (6)   | 0.4850 (4) | 1.0021 (4) | 0.0267 (9)  |
| C10  | 0.4152 (10)  | 0.5641 (7) | 1.3424 (5) | 0.0616 (15) |
| H10A | 0.3063       | 0.6170     | 1.3694     | 0.092*      |
| H10B | 0.5336       | 0.6349     | 1.3549     | 0.092*      |
| H10C | 0.4477       | 0.4925     | 1.3872     | 0.092*      |
| C11  | 0.1328 (7)   | 0.7309 (5) | 0.7300 (4) | 0.0394 (11) |
| C12  | 0.0809 (8)   | 0.8434 (6) | 0.6573 (4) | 0.0464 (12) |
| C13  | -0.0004 (12) | 0.9843 (7) | 0.7192 (6) | 0.0723 (18) |
| H13A | -0.1170      | 0.9573     | 0.7491     | 0.108*      |
| H13B | -0.0397      | 1.0413     | 0.6629     | 0.108*      |
| H13C | 0.1037       | 1.0443     | 0.7851     | 0.108*      |
| C14  | -0.0590 (10) | 0.7627 (8) | 0.5376 (5) | 0.0688 (17) |
| H14A | -0.1897      | 0.7310     | 0.5509     | 0.103*      |
| H14B | -0.0003      | 0.6760     | 0.4984     | 0.103*      |
| H14C | -0.0757      | 0.8300     | 0.4876     | 0.103*      |
| N1   | 0.1878 (5)   | 0.7900 (4) | 0.8526 (3) | 0.0344 (9)  |
| O1   | 0.2284 (4)   | 0.3286 (3) | 0.9663 (3) | 0.0340 (7)  |
| O2   | 0.2428 (6)   | 0.1122 (4) | 1.0081 (3) | 0.0560 (10) |
| O3   | 0.1211 (7)   | 0.5975 (4) | 0.6804 (3) | 0.0650 (12) |
| H1N  | 0.196 (7)    | 0.891 (3)  | 0.889 (4)  | 0.048 (14)* |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| Br1 | 0.0746 (4)  | 0.0678 (5)  | 0.0796 (6)  | 0.0004 (3)  | 0.0157 (3)  | 0.0365 (4)  |
| C1  | 0.044 (2)   | 0.024 (3)   | 0.050 (3)   | 0.0048 (18) | 0.007 (2)   | 0.020 (2)   |
| C2  | 0.048 (2)   | 0.035 (3)   | 0.039 (3)   | 0.0044 (19) | 0.0067 (19) | 0.022 (2)   |
| C3  | 0.041 (2)   | 0.034 (3)   | 0.032 (2)   | 0.0017 (18) | 0.0041 (18) | 0.014 (2)   |
| C4  | 0.035 (2)   | 0.026 (2)   | 0.029 (2)   | 0.0043 (16) | 0.0071 (16) | 0.012 (2)   |
| C5  | 0.049 (2)   | 0.026 (2)   | 0.028 (2)   | 0.0052 (18) | 0.0016 (18) | 0.002 (2)   |
| C6  | 0.059 (3)   | 0.012 (2)   | 0.030 (3)   | 0.0029 (17) | 0.0056 (19) | 0.0035 (19) |
| C7  | 0.036 (2)   | 0.024 (2)   | 0.030 (2)   | 0.0050 (16) | 0.0076 (16) | 0.011 (2)   |
| C8  | 0.038 (2)   | 0.018 (2)   | 0.026 (2)   | 0.0024 (16) | 0.0035 (16) | 0.0037 (19) |
| C9  | 0.0311 (18) | 0.017 (2)   | 0.032 (2)   | 0.0040 (14) | 0.0046 (16) | 0.0070 (19) |
| C10 | 0.091 (4)   | 0.055 (4)   | 0.037 (3)   | 0.006 (3)   | 0.001 (3)   | 0.020 (3)   |
| C11 | 0.055 (3)   | 0.035 (3)   | 0.031 (3)   | 0.009 (2)   | 0.0075 (19) | 0.015 (2)   |
| C12 | 0.060 (3)   | 0.041 (3)   | 0.042 (3)   | 0.008 (2)   | 0.008 (2)   | 0.018 (2)   |
| C13 | 0.112 (5)   | 0.063 (4)   | 0.062 (4)   | 0.045 (4)   | 0.028 (3)   | 0.037 (3)   |
| C14 | 0.080 (4)   | 0.074 (4)   | 0.051 (4)   | -0.003 (3)  | -0.012 (3)  | 0.036 (3)   |
| N1  | 0.053 (2)   | 0.020 (2)   | 0.031 (2)   | 0.0074 (15) | 0.0043 (16) | 0.0105 (18) |
| O1  | 0.0520 (17) | 0.0136 (15) | 0.0361 (18) | 0.0024 (12) | 0.0046 (13) | 0.0098 (14) |
| O2  | 0.088 (3)   | 0.0186 (18) | 0.061 (2)   | 0.0042 (16) | 0.0067 (19) | 0.0166 (17) |
| O3  | 0.129 (4)   | 0.031 (2)   | 0.0283 (19) | 0.016 (2)   | 0.0016 (19) | 0.0069 (16) |

*Geometric parameters (Å, °)*

|             |           |               |           |
|-------------|-----------|---------------|-----------|
| Br1—C12     | 2.017 (5) | C8—H8         | 0.9300    |
| C1—O2       | 1.213 (5) | C9—O1         | 1.385 (5) |
| C1—O1       | 1.353 (6) | C10—H10A      | 0.9600    |
| C1—C2       | 1.439 (7) | C10—H10B      | 0.9600    |
| C2—C3       | 1.344 (6) | C10—H10C      | 0.9600    |
| C2—H2       | 0.9300    | C11—O3        | 1.208 (6) |
| C3—C4       | 1.438 (7) | C11—N1        | 1.370 (6) |
| C3—C10      | 1.502 (7) | C11—C12       | 1.529 (7) |
| C4—C9       | 1.377 (6) | C12—C13       | 1.503 (8) |
| C4—C5       | 1.407 (6) | C12—C14       | 1.514 (7) |
| C5—C6       | 1.358 (7) | C13—H13A      | 0.9600    |
| C5—H5       | 0.9300    | C13—H13B      | 0.9600    |
| C6—C7       | 1.395 (6) | C13—H13C      | 0.9600    |
| C6—H6       | 0.9300    | C14—H14A      | 0.9600    |
| C7—C8       | 1.397 (6) | C14—H14B      | 0.9600    |
| C7—N1       | 1.414 (6) | C14—H14C      | 0.9600    |
| C8—C9       | 1.373 (6) | N1—H1N        | 0.91 (2)  |
| O2—C1—O1    | 116.6 (4) | H10A—C10—H10B | 109.5     |
| O2—C1—C2    | 125.3 (4) | C3—C10—H10C   | 109.5     |
| O1—C1—C2    | 118.1 (4) | H10A—C10—H10C | 109.5     |
| C3—C2—C1    | 122.1 (4) | H10B—C10—H10C | 109.5     |
| C3—C2—H2    | 119.0     | O3—C11—N1     | 123.0 (4) |
| C1—C2—H2    | 119.0     | O3—C11—C12    | 120.7 (4) |
| C2—C3—C4    | 118.5 (4) | N1—C11—C12    | 116.2 (4) |
| C2—C3—C10   | 120.5 (4) | C13—C12—C14   | 111.2 (5) |
| C4—C3—C10   | 121.0 (4) | C13—C12—C11   | 116.9 (4) |
| C9—C4—C5    | 116.0 (4) | C14—C12—C11   | 109.7 (4) |
| C9—C4—C3    | 119.2 (4) | C13—C12—Br1   | 108.2 (4) |
| C5—C4—C3    | 124.8 (4) | C14—C12—Br1   | 106.0 (4) |
| C6—C5—C4    | 121.8 (4) | C11—C12—Br1   | 104.1 (3) |
| C6—C5—H5    | 119.1     | C12—C13—H13A  | 109.5     |
| C4—C5—H5    | 119.1     | C12—C13—H13B  | 109.5     |
| C5—C6—C7    | 120.5 (4) | H13A—C13—H13B | 109.5     |
| C5—C6—H6    | 119.7     | C12—C13—H13C  | 109.5     |
| C7—C6—H6    | 119.7     | H13A—C13—H13C | 109.5     |
| C6—C7—C8    | 119.3 (4) | H13B—C13—H13C | 109.5     |
| C6—C7—N1    | 117.1 (4) | C12—C14—H14A  | 109.5     |
| C8—C7—N1    | 123.5 (4) | C12—C14—H14B  | 109.5     |
| C9—C8—C7    | 118.1 (4) | H14A—C14—H14B | 109.5     |
| C9—C8—H8    | 120.9     | C12—C14—H14C  | 109.5     |
| C7—C8—H8    | 120.9     | H14A—C14—H14C | 109.5     |
| C8—C9—C4    | 124.2 (4) | H14B—C14—H14C | 109.5     |
| C8—C9—O1    | 114.9 (3) | C11—N1—C7     | 126.8 (4) |
| C4—C9—O1    | 120.9 (4) | C11—N1—H1N    | 122 (3)   |
| C3—C10—H10A | 109.5     | C7—N1—H1N     | 111 (3)   |

|              |            |                |            |
|--------------|------------|----------------|------------|
| C3—C10—H10B  | 109.5      | C1—O1—C9       | 121.2 (3)  |
| O2—C1—C2—C3  | -179.9 (5) | C3—C4—C9—C8    | -179.1 (4) |
| O1—C1—C2—C3  | 0.5 (6)    | C5—C4—C9—O1    | 179.8 (3)  |
| C1—C2—C3—C4  | -0.2 (6)   | C3—C4—C9—O1    | 0.5 (6)    |
| C1—C2—C3—C10 | 179.8 (4)  | O3—C11—C12—C13 | 150.9 (6)  |
| C2—C3—C4—C9  | -0.3 (6)   | N1—C11—C12—C13 | -27.8 (7)  |
| C10—C3—C4—C9 | 179.7 (4)  | O3—C11—C12—C14 | 23.1 (7)   |
| C2—C3—C4—C5  | -179.5 (4) | N1—C11—C12—C14 | -155.6 (5) |
| C10—C3—C4—C5 | 0.5 (7)    | O3—C11—C12—Br1 | -89.9 (5)  |
| C9—C4—C5—C6  | -0.7 (6)   | N1—C11—C12—Br1 | 91.4 (4)   |
| C3—C4—C5—C6  | 178.6 (4)  | O3—C11—N1—C7   | -3.3 (7)   |
| C4—C5—C6—C7  | 1.1 (7)    | C12—C11—N1—C7  | 175.3 (4)  |
| C5—C6—C7—C8  | -1.0 (6)   | C6—C7—N1—C11   | 177.9 (4)  |
| C5—C6—C7—N1  | 178.4 (4)  | C8—C7—N1—C11   | -2.8 (6)   |
| C6—C7—C8—C9  | 0.5 (6)    | O2—C1—O1—C9    | -180.0 (4) |
| N1—C7—C8—C9  | -178.9 (4) | C2—C1—O1—C9    | -0.3 (6)   |
| C7—C8—C9—C4  | -0.1 (6)   | C8—C9—O1—C1    | 179.4 (4)  |
| C7—C8—C9—O1  | -179.7 (3) | C4—C9—O1—C1    | -0.2 (5)   |
| C5—C4—C9—C8  | 0.2 (6)    |                |            |

*Hydrogen-bond geometry (Å, °)*

| <i>D</i> —H $\cdots$ <i>A</i>     | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C8—H8 $\cdots$ O3                 | 0.93        | 2.21                | 2.804 (6)                  | 121                           |
| N1—H1N $\cdots$ O2 <sup>i</sup>   | 0.91 (2)    | 2.12 (2)            | 3.016 (5)                  | 168 (5)                       |
| C6—H6 $\cdots$ O2 <sup>i</sup>    | 0.93        | 2.38                | 3.189 (6)                  | 145                           |
| C13—H13C $\cdots$ O2 <sup>i</sup> | 0.96        | 2.51                | 3.347 (8)                  | 146                           |

Symmetry code: (i) *x*, *y*+1, *z*.