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## Structure Reports

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# 4-Bromo-2-[(E)-(2-fluoro-5-nitrophenyl)-iminomethyl]phenol

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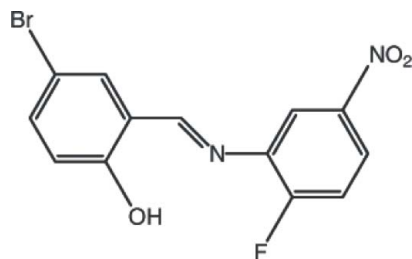
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.059; data-to-parameter ratio = 15.4.

The molecular conformation of the title compound,  $\text{C}_{13}\text{H}_8\text{BrFN}_2\text{O}_3$ , is essentially planar, with maximum deviations of 0.076 (1) and  $-0.080$  (2) Å for the O atoms of the  $\text{NO}_2$  group. The molecular conformation is stabilized by an intramolecular  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bond, forming an  $S(6)$  ring motif. In the crystal, pairs of molecules are linked *via* two pairs of  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, forming inversion dimers that enclose  $R_2^2(7)R_2^2(10)R_2^2(7)$  ring motifs.

## Related literature

For the synthesis and biological activity of azomethines, see: Przybylski *et al.* (2009); Kalaivani *et al.* (2012); Blair *et al.* (2000). For the synthesis of fluorinated azomethines, see: Mohamed *et al.* (2012). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For standard bond lengths, see: Allen *et al.* (1987).



## Experimental

### Crystal data

$\text{C}_{13}\text{H}_8\text{BrFN}_2\text{O}_3$   
 $M_r = 339.11$   
Monoclinic,  $P2_1/n$   
 $a = 4.5082$  (9) Å

$b = 19.815$  (4) Å  
 $c = 13.853$  (3) Å  
 $\beta = 95.484$  (5)°  
 $V = 1231.8$  (4) Å<sup>3</sup>

$Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 3.36$  mm<sup>-1</sup>

$T = 100$  K  
 $0.24 \times 0.04 \times 0.03$  mm

### Data collection

Rigaku AFC12 (Right) diffractometer  
Absorption correction: multi-scan (*CrystalClear-SM Expert*; Rigaku, 2012)  
 $T_{\min} = 0.500$ ,  $T_{\max} = 0.906$

8107 measured reflections  
2811 independent reflections  
2633 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.023$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.059$   
 $S = 1.05$   
2811 reflections

182 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.52$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.54$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$                            | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{O1}-\text{H1}\cdots\text{N1}$     | 0.84  | 1.86        | 2.601 (2)   | 146           |
| $\text{C7}-\text{H7}\cdots\text{O3}^i$   | 0.95  | 2.45        | 3.399 (3)   | 173           |
| $\text{C13}-\text{H13}\cdots\text{O3}^i$ | 0.95  | 2.48        | 3.430 (3)   | 173           |

 Symmetry code: (i)  $-x + 2, -y + 1, -z + 1$ .

Data collection: *CrystalClear-SM Expert* (Rigaku, 2012); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5665).

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## supporting information

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**4-Bromo-2-[(*E*)-(2-fluoro-5-nitrophenyl)iminomethyl]phenol**

**Shaaban K. Mohamed, Mehmet Akkurt, Peter N. Horton, Antar A. Abdelhamid and Adel A. Marzouk**

**S1. Comment**

Schiff bases have been shown to exhibit a broad range of biological activities, including antifungal, antibacterial, antimalarial, antiproliferative, anti-inflammatory, antiviral, and antipyretic properties (Przybylski *et al.*, 2009; Kalaivani *et al.*, 2012). Among such compounds, the fluorinated Schiff's bases were considered to possess a distinguished biological activity due to the dramatic affect of fluorine atom on the metabolism and distribution of drug molecules in the body (Blair *et al.*, 2000). Further to our on going study on synthesis of bioactive fluorinated compounds (Mohamed *et al.*, 2012) we herein report the synthesis and crystal structure of a new fluorinated azomethine derivative.

In the title compound (I), (Fig. 1), the molecular conformation is essentially planar, with maximum deviations of 0.076 (1) and -0.080 (2) Å, respectively, for O2 and O3. The C1–C7–N1–C8 torsion angle is 179.92 (16)°. The bond lengths and angles in (I) are within the normal range (Allen *et al.*, 1987).

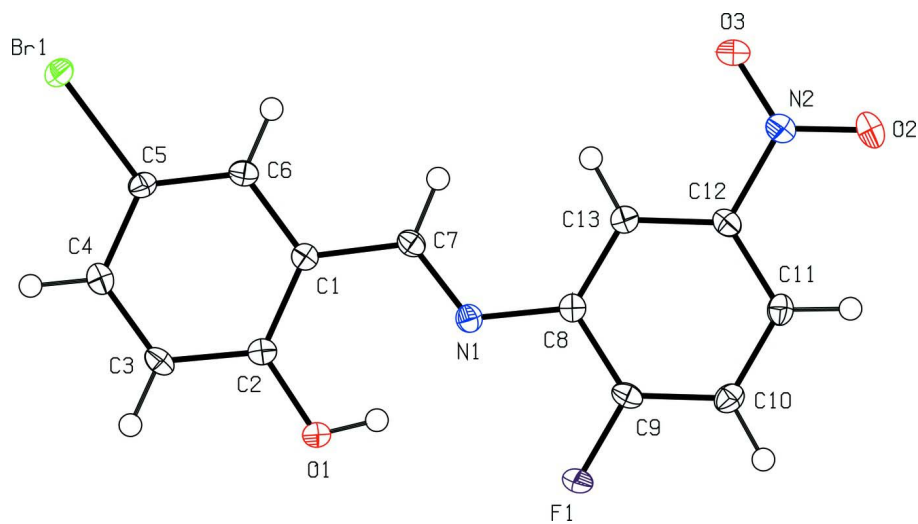
Molecular conformation is stabilized by O—H···N hydrogen bond (Table 1), forming an S(6) ring motif. In the crystal, the pairs of molecules are linked by C—H···O interactions (Table 1, Fig. 2), generating  $R^2_2(7)R^2_2(10)R^2_2(7)$  ring motifs (Bernstein *et al.*, 1995) along the [001] direction.

**S2. Experimental**

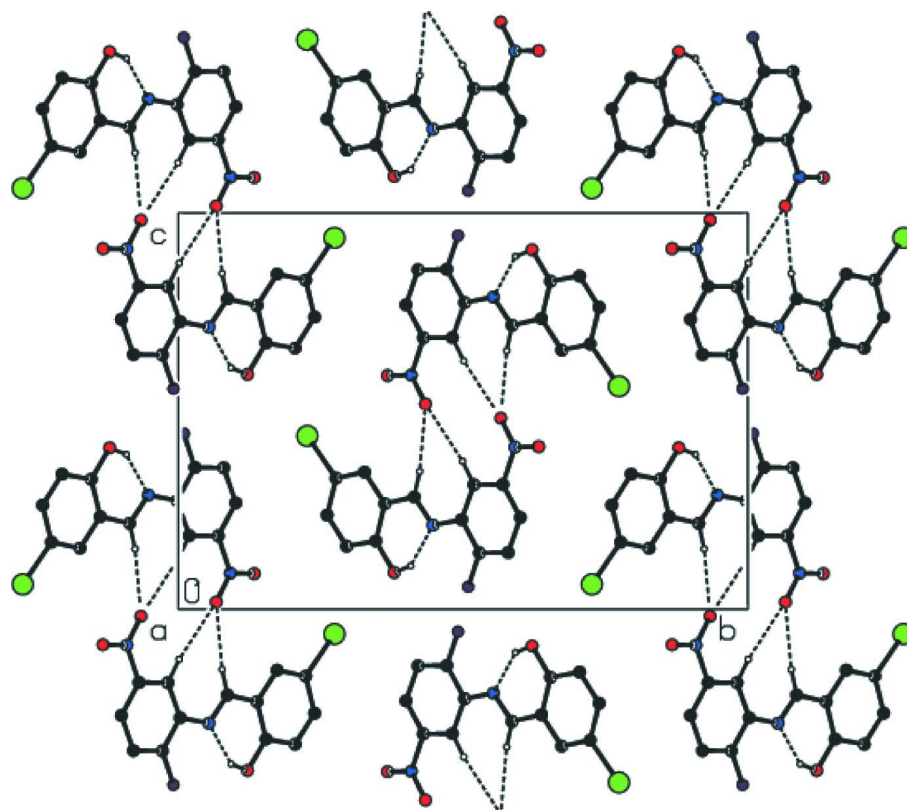
A mixture of 1 mmol (156 mg) 2-fluoro-5-nitroaniline and 1 mmol (201 mg) 5-bromo-2-hydroxybenzaldehyde in 50 ml ethanol was heated at 350 K and monitored by TLC till completion after 12 h. A mass solid product was deposited once the reaction mixture was allowed to cool at room temperature. The crude product was filtered dried under vacuum and washed by ethanol. Pure yellow rods (m.p. 465 K) suitable for X-ray diffraction were obtained in an excellent yield (92%) by crystallization of crude product from ethanol.

**S3. Refinement**

H atoms were positioned geometrically and refined using a riding model, with O—H = 0.84 Å, C—H = 0.95 Å, and with  $U_{iso}(H) = 1.5U_{eq}(O)$  for hydroxyl and  $U_{iso}(H) = 1.2 U_{eq}(C)$  for the other H atoms.

**Figure 1**

The molecular structure of (I) with ellipsoids drawn at the 50% probability level.

**Figure 2**

Crystal packing of (I) viewed along the *a* axis. The hydrogen atoms not involved in the hydrogen bonds have been omitted for clarity.

## 4-Bromo-2-[(E)-(2-fluoro-5-nitrophenyl)iminomethyl]phenol

## Crystal data

|                                |   |
|--------------------------------|---|
| $C_{13}H_8BrFN_2O_3$           | $F(000) = 672$  |
| $M_r = 339.11$                 | $D_x = 1.829 \text{ Mg m}^{-3}$                         |
| Monoclinic, $P2_1/n$           | Mo $K\alpha$ radiation, $\lambda = 0.71075 \text{ \AA}$ |
| Hall symbol: $-P 2_1n$         | Cell parameters from 4566 reflections                   |
| $a = 4.5082 (9) \text{ \AA}$   | $\theta = 2.5\text{--}31.2^\circ$                       |
| $b = 19.815 (4) \text{ \AA}$   | $\mu = 3.36 \text{ mm}^{-1}$                            |
| $c = 13.853 (3) \text{ \AA}$   | $T = 100 \text{ K}$                                     |
| $\beta = 95.484 (5)^\circ$     | Rod, yellow   |
| $V = 1231.8 (4) \text{ \AA}^3$ | $0.24 \times 0.04 \times 0.03 \text{ mm}$               |
| $Z = 4$                        |   |

## Data collection

|   |  |
|---|--|
| Rigaku AFC12 (Right) diffractometer                   | 8107 measured reflections  |
| Radiation source: Rotating Anode                      | 2811 independent reflections   |
| Detector resolution: $28.5714 \text{ pixels mm}^{-1}$ | 2633 reflections with $I > 2\sigma(I)$                                 |
| profile data from $\omega$ -scans                     | $R_{\text{int}} = 0.023$   |
| Absorption correction: multi-scan                     | $\theta_{\text{max}} = 27.5^\circ$ , $\theta_{\text{min}} = 3.0^\circ$ |
| ( <i>CrystalClear-SM Expert</i> ; Rigaku, 2012)       | $h = -5 \rightarrow 5$   |
| $T_{\text{min}} = 0.500$ , $T_{\text{max}} = 0.906$   | $k = -25 \rightarrow 24$   |
|   | $l = -17 \rightarrow 14$   |

## Refinement

|  |  |
|--|--|
| Refinement on $F^2$  | Secondary atom site location: difference Fourier map     |
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.025$                                | H-atom parameters constrained                            |
| $wR(F^2) = 0.059$  | $w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 1.1447P]$        |
| $S = 1.05$   | where $P = (F_o^2 + 2F_c^2)/3$                           |
| 2811 reflections   | $(\Delta/\sigma)_{\text{max}} = 0.001$                   |
| 182 parameters   | $\Delta\rho_{\text{max}} = 0.52 \text{ e \AA}^{-3}$      |
| 0 restraints   | $\Delta\rho_{\text{min}} = -0.54 \text{ e \AA}^{-3}$     |
| Primary atom site location: structure-invariant direct methods |  |

## Special details

**Geometry.** Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement.** Refinement on  $F^2$  for ALL reflections except those flagged by the user for potential systematic errors. Weighted  $R$ -factors  $wR$  and all goodnesses 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 observed criterion of  $F^2 > \sigma(F^2)$  is used only for calculating  $-R$ -factor-obs *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 | -0.15532 (4) | 0.22619 (1) | 0.43736 (1)  | 0.0188 (1)                       |
| F1  | 0.7510 (2)   | 0.50903 (6) | 0.05672 (7)  | 0.0202 (3)                       |
| O1  | 0.2171 (3)   | 0.37891 (7) | 0.09274 (9)  | 0.0171 (4)                       |
| O2  | 1.5039 (3)   | 0.63282 (8) | 0.41030 (11) | 0.0290 (4)                       |

|     |             |              |              |            |
|-----|-------------|--------------|--------------|------------|
| O3  | 1.2227 (5)  | 0.56614 (11) | 0.48212 (12) | 0.0614 (8) |
| N1  | 0.5847 (3)  | 0.44689 (7)  | 0.21201 (11) | 0.0140 (4) |
| N2  | 1.3057 (4)  | 0.59101 (9)  | 0.40914 (12) | 0.0227 (5) |
| C1  | 0.2662 (4)  | 0.36222 (8)  | 0.26646 (12) | 0.0123 (5) |
| C2  | 0.1398 (4)  | 0.34652 (9)  | 0.17204 (12) | 0.0135 (5) |
| C3  | -0.0742 (4) | 0.29535 (9)  | 0.15895 (13) | 0.0157 (5) |
| C4  | -0.1635 (4) | 0.26099 (9)  | 0.23746 (13) | 0.0159 (5) |
| C5  | -0.0389 (4) | 0.27669 (9)  | 0.33084 (12) | 0.0140 (5) |
| C6  | 0.1728 (4)  | 0.32683 (9)  | 0.34603 (12) | 0.0145 (5) |
| C7  | 0.4936 (4)  | 0.41399 (9)  | 0.28338 (13) | 0.0138 (5) |
| C8  | 0.8050 (4)  | 0.49730 (9)  | 0.22592 (13) | 0.0136 (5) |
| C9  | 0.8877 (4)  | 0.52873 (9)  | 0.14215 (12) | 0.0150 (5) |
| C10 | 1.0992 (4)  | 0.57931 (9)  | 0.14290 (13) | 0.0165 (5) |
| C11 | 1.2365 (4)  | 0.60049 (9)  | 0.23159 (13) | 0.0157 (5) |
| C12 | 1.1566 (4)  | 0.56969 (9)  | 0.31484 (13) | 0.0156 (5) |
| C13 | 0.9451 (4)  | 0.51880 (9)  | 0.31435 (13) | 0.0154 (5) |
| H1  | 0.34830     | 0.40790      | 0.10930      | 0.0260*    |
| H3  | -0.15830    | 0.28430      | 0.09540      | 0.0190*    |
| H4  | -0.31010    | 0.22660      | 0.22810      | 0.0190*    |
| H6  | 0.25500     | 0.33730      | 0.41000      | 0.0170*    |
| H7  | 0.57530     | 0.42350      | 0.34770      | 0.0170*    |
| H10 | 1.14920     | 0.59910      | 0.08410      | 0.0200*    |
| H11 | 1.38190     | 0.63530      | 0.23510      | 0.0190*    |
| H13 | 0.89690     | 0.49900      | 0.37330      | 0.0180*    |

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

|     | $U^{11}$    | $U^{22}$    | $U^{33}$   | $U^{12}$     | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|------------|--------------|-------------|-------------|
| Br1 | 0.0189 (1)  | 0.0213 (1)  | 0.0161 (1) | -0.0045 (1)  | 0.0003 (1)  | 0.0053 (1)  |
| F1  | 0.0209 (6)  | 0.0273 (6)  | 0.0115 (5) | -0.0064 (5)  | -0.0028 (4) | 0.0011 (4)  |
| O1  | 0.0208 (7)  | 0.0184 (6)  | 0.0119 (6) | -0.0042 (5)  | 0.0007 (5)  | 0.0008 (5)  |
| O2  | 0.0326 (8)  | 0.0292 (8)  | 0.0243 (7) | -0.0159 (7)  | -0.0022 (6) | -0.0043 (6) |
| O3  | 0.0880 (16) | 0.0804 (15) | 0.0135 (8) | -0.0628 (13) | -0.0074 (9) | 0.0082 (8)  |
| N1  | 0.0128 (7)  | 0.0141 (7)  | 0.0150 (7) | 0.0001 (6)   | 0.0013 (6)  | -0.0005 (5) |
| N2  | 0.0290 (9)  | 0.0228 (8)  | 0.0156 (8) | -0.0085 (7)  | -0.0011 (7) | -0.0008 (6) |
| C1  | 0.0110 (8)  | 0.0124 (8)  | 0.0136 (8) | 0.0021 (6)   | 0.0011 (6)  | -0.0003 (6) |
| C2  | 0.0137 (8)  | 0.0135 (8)  | 0.0133 (8) | 0.0026 (6)   | 0.0015 (6)  | 0.0004 (6)  |
| C3  | 0.0156 (9)  | 0.0171 (8)  | 0.0140 (8) | 0.0000 (7)   | -0.0011 (6) | -0.0047 (7) |
| C4  | 0.0145 (8)  | 0.0144 (8)  | 0.0186 (9) | -0.0005 (7)  | 0.0001 (7)  | -0.0018 (7) |
| C5  | 0.0144 (8)  | 0.0148 (8)  | 0.0127 (8) | 0.0009 (7)   | 0.0015 (6)  | 0.0021 (6)  |
| C6  | 0.0147 (8)  | 0.0160 (8)  | 0.0125 (8) | 0.0014 (7)   | 0.0000 (6)  | 0.0002 (6)  |
| C7  | 0.0123 (8)  | 0.0151 (8)  | 0.0137 (8) | 0.0012 (7)   | -0.0005 (6) | -0.0014 (6) |
| C8  | 0.0129 (8)  | 0.0129 (8)  | 0.0151 (8) | 0.0007 (6)   | 0.0016 (7)  | -0.0003 (6) |
| C9  | 0.0139 (8)  | 0.0179 (8)  | 0.0125 (8) | 0.0022 (7)   | -0.0023 (6) | -0.0014 (6) |
| C10 | 0.0164 (9)  | 0.0166 (8)  | 0.0167 (9) | 0.0011 (7)   | 0.0022 (7)  | 0.0036 (7)  |
| C11 | 0.0155 (8)  | 0.0126 (8)  | 0.0191 (9) | -0.0009 (7)  | 0.0017 (7)  | 0.0007 (7)  |
| C12 | 0.0163 (9)  | 0.0155 (8)  | 0.0145 (8) | -0.0004 (7)  | -0.0010 (7) | -0.0021 (6) |
| C13 | 0.0160 (9)  | 0.0159 (8)  | 0.0143 (8) | -0.0009 (7)  | 0.0012 (7)  | 0.0007 (6)  |

*Geometric parameters (Å, °)*

|               |              |               |              |
|---------------|--------------|---------------|--------------|
| Br1—C5        | 1.8980 (18)  | C5—C6         | 1.380 (3)    |
| F1—C9         | 1.339 (2)    | C8—C13        | 1.390 (3)    |
| O1—C2         | 1.347 (2)    | C8—C9         | 1.399 (2)    |
| O2—N2         | 1.218 (2)    | C9—C10        | 1.383 (3)    |
| O3—N2         | 1.215 (3)    | C10—C11       | 1.387 (3)    |
| O1—H1         | 0.8400       | C11—C12       | 1.383 (3)    |
| N1—C7         | 1.284 (2)    | C12—C13       | 1.387 (3)    |
| N1—C8         | 1.409 (2)    | C3—H3         | 0.9500       |
| N2—C12        | 1.473 (2)    | C4—H4         | 0.9500       |
| C1—C6         | 1.405 (2)    | C6—H6         | 0.9500       |
| C1—C7         | 1.453 (2)    | C7—H7         | 0.9500       |
| C1—C2         | 1.411 (2)    | C10—H10       | 0.9500       |
| C2—C3         | 1.399 (3)    | C11—H11       | 0.9500       |
| C3—C4         | 1.376 (3)    | C13—H13       | 0.9500       |
| C4—C5         | 1.395 (2)    |               |              |
| C2—O1—H1      | 109.00       | F1—C9—C10     | 118.47 (15)  |
| C7—N1—C8      | 121.86 (16)  | C8—C9—C10     | 123.70 (16)  |
| O2—N2—C12     | 118.63 (16)  | C9—C10—C11    | 118.36 (16)  |
| O3—N2—C12     | 118.09 (18)  | C10—C11—C12   | 118.40 (17)  |
| O2—N2—O3      | 123.29 (18)  | N2—C12—C11    | 118.69 (16)  |
| C2—C1—C7      | 121.43 (15)  | C11—C12—C13   | 123.40 (17)  |
| C6—C1—C7      | 119.05 (15)  | N2—C12—C13    | 117.91 (16)  |
| C2—C1—C6      | 119.52 (16)  | C8—C13—C12    | 118.76 (16)  |
| O1—C2—C3      | 117.94 (15)  | C2—C3—H3      | 120.00       |
| C1—C2—C3      | 119.50 (16)  | C4—C3—H3      | 120.00       |
| O1—C2—C1      | 122.56 (16)  | C3—C4—H4      | 120.00       |
| C2—C3—C4      | 120.43 (16)  | C5—C4—H4      | 120.00       |
| C3—C4—C5      | 120.02 (17)  | C1—C6—H6      | 120.00       |
| Br1—C5—C4     | 119.11 (13)  | C5—C6—H6      | 120.00       |
| Br1—C5—C6     | 119.98 (13)  | N1—C7—H7      | 120.00       |
| C4—C5—C6      | 120.88 (16)  | C1—C7—H7      | 120.00       |
| C1—C6—C5      | 119.65 (15)  | C9—C10—H10    | 121.00       |
| N1—C7—C1      | 120.45 (16)  | C11—C10—H10   | 121.00       |
| N1—C8—C9      | 116.27 (16)  | C10—C11—H11   | 121.00       |
| N1—C8—C13     | 126.35 (16)  | C12—C11—H11   | 121.00       |
| C9—C8—C13     | 117.38 (16)  | C8—C13—H13    | 121.00       |
| F1—C9—C8      | 117.83 (16)  | C12—C13—H13   | 121.00       |
| C8—N1—C7—C1   | -179.92 (16) | C3—C4—C5—C6   | 0.4 (3)      |
| C7—N1—C8—C9   | 179.13 (17)  | C3—C4—C5—Br1  | -177.66 (14) |
| C7—N1—C8—C13  | -1.3 (3)     | Br1—C5—C6—C1  | 177.55 (13)  |
| O3—N2—C12—C13 | -4.7 (3)     | C4—C5—C6—C1   | -0.5 (3)     |
| O2—N2—C12—C11 | -3.3 (3)     | N1—C8—C9—C10  | 179.72 (16)  |
| O2—N2—C12—C13 | 175.80 (17)  | C13—C8—C9—F1  | -179.08 (16) |
| O3—N2—C12—C11 | 176.20 (19)  | C13—C8—C9—C10 | 0.1 (3)      |

|             |              |                 |              |
|-------------|--------------|-----------------|--------------|
| C7—C1—C2—C3 | 178.71 (17)  | N1—C8—C9—F1     | 0.5 (2)      |
| C7—C1—C6—C5 | -178.80 (17) | N1—C8—C13—C12   | -179.49 (17) |
| C2—C1—C7—N1 | 0.1 (3)      | C9—C8—C13—C12   | 0.1 (3)      |
| C2—C1—C6—C5 | 0.7 (3)      | F1—C9—C10—C11   | 178.83 (16)  |
| C6—C1—C2—C3 | -0.8 (3)     | C8—C9—C10—C11   | -0.4 (3)     |
| C7—C1—C2—O1 | -1.2 (3)     | C9—C10—C11—C12  | 0.4 (3)      |
| C6—C1—C7—N1 | 179.58 (16)  | C10—C11—C12—N2  | 178.83 (16)  |
| C6—C1—C2—O1 | 179.35 (16)  | C10—C11—C12—C13 | -0.3 (3)     |
| O1—C2—C3—C4 | -179.43 (16) | N2—C12—C13—C8   | -179.08 (16) |
| C1—C2—C3—C4 | 0.7 (3)      | C11—C12—C13—C8  | 0.0 (3)      |
| C2—C3—C4—C5 | -0.5 (3)     |                 |              |

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> |
|----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O1—H1 $\cdots$ N1                | 0.84        | 1.86                | 2.601 (2)                  | 146                           |
| C7—H7 $\cdots$ O3 <sup>i</sup>   | 0.95        | 2.45                | 3.399 (3)                  | 173                           |
| C13—H13 $\cdots$ O3 <sup>i</sup> | 0.95        | 2.48                | 3.430 (3)                  | 173                           |

Symmetry code: (i)  $-x+2, -y+1, -z+1$ .