

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

***N'*-(*E*)-1-(4-Bromophenyl)ethylidene]-2-(2-methyl-4-nitro-1*H*-imidazol-1-yl)-acetohydrazide**

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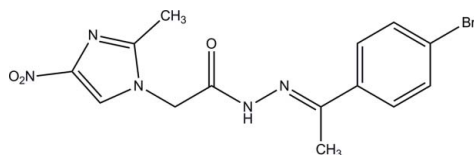
Received 11 June 2012; accepted 20 June 2012

Key indicators: single-crystal X-ray study; *T* = 100 K; mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$ ; *R* factor = 0.032; *wR* factor = 0.082; data-to-parameter ratio = 29.5.

In the title compound,  $\text{C}_{14}\text{H}_{14}\text{BrN}_5\text{O}_3$ , the mean plane of the imidazole ring (r.m.s deviation =  $0.004 \text{ \AA}$ ) forms a dihedral angle of  $58.13(7)^\circ$  with the benzene ring. In the crystal, molecules are linked *via*  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bonds into a three-dimensional network. A short  $\text{Br}\cdots\text{Br}$  contact of  $3.4932(2) \text{ \AA}$  also occurs.

Related literature

For general background to and applications of imidazole derivatives, see: Priya & Kalluraya (2005); Krapcho & Turk (1966); Chu *et al.* (2004); Khalafi-Nezhad *et al.* (2005). For standard bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see Cosier & Glazer (1986).



Experimental

Crystal data

$\text{C}_{14}\text{H}_{14}\text{BrN}_5\text{O}_3$   $a = 8.4176(1) \text{ \AA}$   
 $M_r = 380.21$   $b = 10.6541(1) \text{ \AA}$   
 Monoclinic,  $P2_1/c$   $c = 17.4933(2) \text{ \AA}$

$\beta = 90.100(1)^\circ$   $\mu = 2.64 \text{ mm}^{-1}$   
 $V = 1568.83(3) \text{ \AA}^3$   $T = 100 \text{ K}$   
 $Z = 4$   $0.37 \times 0.33 \times 0.15 \text{ mm}$   
 Mo  $K\alpha$  radiation

Data collection

Bruker SMART APEXII CCD 45099 measured reflections  
 area-detector diffractometer 6320 independent reflections  
 Absorption correction: multi-scan 5026 reflections with  $I > 2\sigma(I)$   
 (SADABS; Bruker, 2009)  $R_{\text{int}} = 0.040$   
 $T_{\text{min}} = 0.441, T_{\text{max}} = 0.701$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$  H atoms treated by a mixture of independent and constrained refinement  
 $wR(F^2) = 0.082$   $\Delta\rho_{\text{max}} = 0.88 \text{ e \AA}^{-3}$   
 $S = 1.02$   $\Delta\rho_{\text{min}} = -0.66 \text{ e \AA}^{-3}$   
 6320 reflections  
 214 parameters

Table 1  
Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
$\text{N2}-\text{H1N2}\cdots\text{O1}^{\text{i}}$	0.81 (2)	2.04 (2)	2.8318 (14)	166.6 (18)
$\text{C9}-\text{H9A}\cdots\text{O3}^{\text{ii}}$	0.99	2.31	3.1818 (16)	147
$\text{C9}-\text{H9B}\cdots\text{N4}^{\text{iii}}$	0.99	2.40	3.3462 (16)	160
$\text{C10}-\text{H10A}\cdots\text{O2}^{\text{ii}}$	0.95	2.56	3.4488 (16)	155

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

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). CKQ also thanks USM for an Incentive Grant.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2774).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.  
 Bruker (2009). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Chu, T., Hu, S., Wei, B., Wang, Y., Liu, X. & Wang, X. (2004). *Bioorg. Med. Chem.* **14**, 747–749.  
 Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.  
 Khalafi-Nezhad, A., Rad, M. N. S., Mohabatkar, H., Asrari, Z. & Hemmateenejad, B. (2005). *Bioorg. Med. Chem.* **13**, 1931–1938.  
 Krapcho, J. & Turk, C. F. (1966). *J. Med. Chem.* **9**, 191–195.  
 Priya, V. F. & Kalluraya, B. (2005). *Indian J. Chem. Sect. B*, **44**, 1456–1459.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

\* Thomson Reuters ResearcherID: A-3561-2009.  
 § Thomson Reuters ResearcherID: A-5525-2009.

## supporting information

*Acta Cryst.* (2012). E68, o2192 [https://doi.org/10.1107/S160053681202795X]

## *N'*-[(*E*)-1-(4-Bromophenyl)ethylidene]-2-(2-methyl-4-nitro-1*H*-imidazol-1-yl)acetohydrazide

Hoong-Kun Fun, Ching Kheng Quah, Priya V. Frank, N. Damodara and Balakrishna Kalluraya

### S1. Comment

The chemistry of imidazole derivatives has been the subject of much interest due to their importance in various applications and also due to their widespread potential as well as proven biological and pharmacological activities (Priya & Kalluraya, 2005). Various applications of imidazoles have been listed in the literature with functions as widely divergent as antidepressant agents (Krapcho & Turk, 1966), as a marker for imaging tumor hypoxia (Chu *et al.*, 2004), and in antibacterial activity (Khalafi-Nezhad *et al.*, 2005). In view of the obvious importance of imidazole derivatives as potential pharmacological agents, herein we report the crystal structure of the above imidazole derivative.

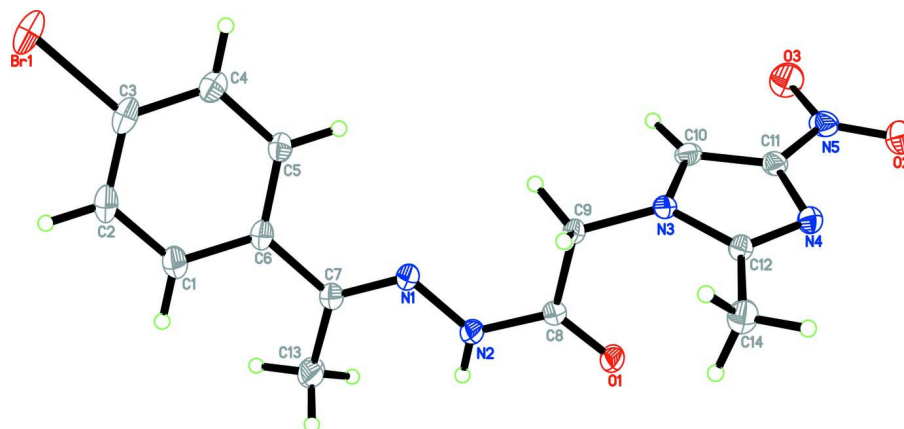
In the title molecule, Fig. 1, the mean plane of the imidazole ring (N3/N4/C10-C12, r.m.s deviation = 0.004 Å) forms a dihedral angle of 58.13 (7)° with the phenyl ring (C1-C6). Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. A short Br1...Br1 contact of 3.4932 (2) Å also occurs. In the crystal (Fig. 2), molecules are linked *via* intermolecular N2–H1N2...O1, C9–H9A...O3, C9–H9B...N4 and C10–H10A...O2 hydrogen bonds (Table 1) into a three-dimensional network.

### S2. Experimental

The title compound was synthesized by refluxing a mixture of 2-(2-methyl-4-nitro-1*H*-imidazol-1-yl)acethydrazide (0.1 mol) and 1-(4-bromophenyl)ethanone (0.1 mol) in glacial acetic acid for 1 hour. After cooling the reaction mixture to room temperature and evaporation of the solvent under reduced pressure, the solid separated was filtered, washed with water and dried. The recrystallization of the sample was done using an ethanol-dioxane (1:1 *v/v*) mixture. The melting point of the compound was found to be 549 K. The slow evaporation of the ethanol-dioxane mixture of the compound gave crystals suitable for X-ray analysis.

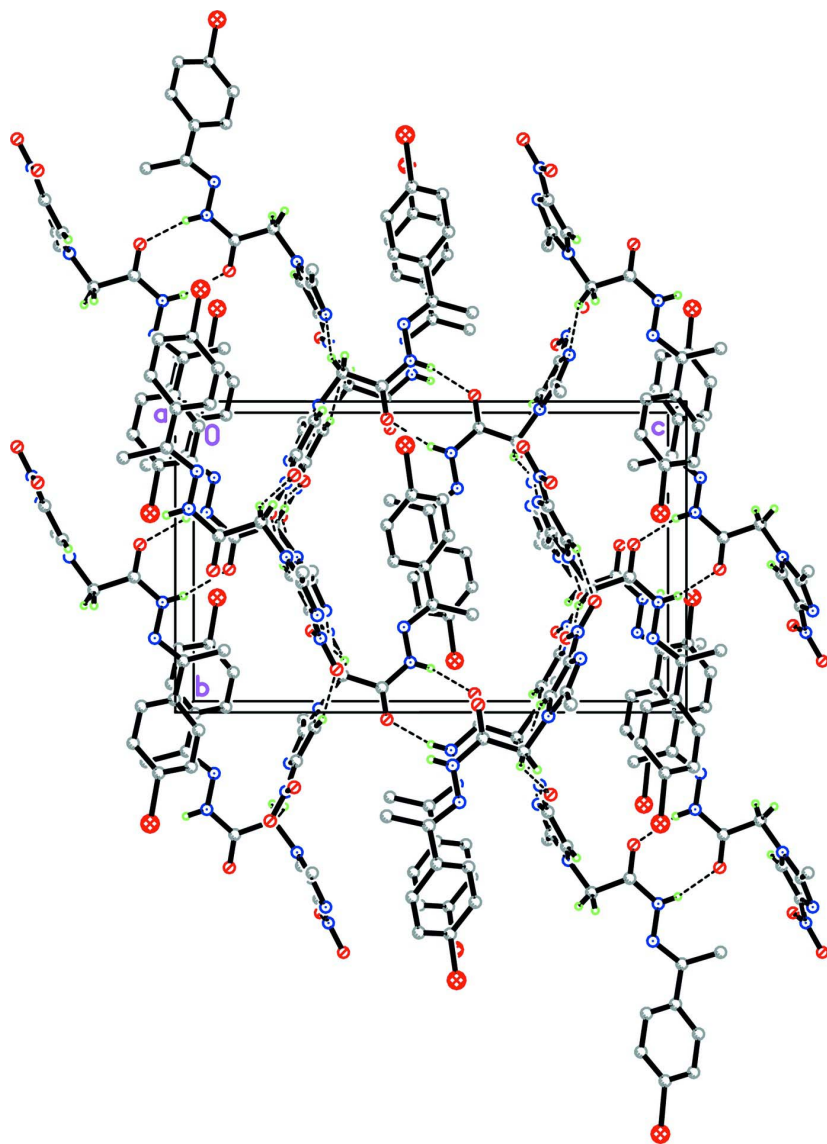
### S3. Refinement

Atom H1N2 was located in a difference Fourier map and refined freely [N–H = 0.81 (2) Å]. All other hydrogen atoms were positioned geometrically and refined using a riding model with C–H = 0.95–0.99 Å and  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5 U_{\text{eq}}(\text{C})$ . A rotating-group model was applied for the methyl groups.



**Figure 1**

The molecular structure of the title compound showing 50% probability displacement ellipsoids for non-H atoms.



**Figure 2**

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

*N'*-[(*E*)-1-(4-Bromophenyl)ethylidene]-2-(2-methyl-4-nitro-1*H*-imidazol-1-yl)acetohydrazide

*Crystal data*

$C_{14}H_{14}BrN_5O_3$

$M_r = 380.21$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 8.4176$  (1) Å

$b = 10.6541$  (1) Å

$c = 17.4933$  (2) Å

$\beta = 90.100$  (1)°

$V = 1568.83$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 768$

$D_x = 1.610$  Mg m<sup>-3</sup>

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

Cell parameters from 9969 reflections

$\theta = 2.3$ – $33.5$ °

$\mu = 2.64$  mm<sup>-1</sup>

$T = 100$  K

Block, yellow

$0.37 \times 0.33 \times 0.15$  mm

*Data collection*

Bruker SMART APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.441$ ,  $T_{\max} = 0.701$

45099 measured reflections

6320 independent reflections

5026 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\max} = 33.9^\circ$ ,  $\theta_{\min} = 2.2^\circ$

$h = -13 \rightarrow 13$

$k = -16 \rightarrow 16$

$l = -27 \rightarrow 27$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.032$

$wR(F^2) = 0.082$

$S = 1.02$

6320 reflections

214 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

$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.4612P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.88 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.66 \text{ e } \text{\AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.021322 (19)	-0.359303 (13)	0.050226 (9)	0.03144 (5)
O1	0.45656 (12)	0.54105 (9)	0.08914 (5)	0.02360 (19)
O2	0.13283 (13)	0.85764 (9)	0.31753 (6)	0.0269 (2)
O3	-0.04787 (11)	0.73832 (11)	0.26628 (7)	0.0345 (3)
N1	0.33805 (12)	0.23194 (9)	0.05430 (6)	0.01687 (18)
N2	0.40021 (13)	0.34967 (10)	0.04122 (6)	0.01891 (19)
N3	0.31916 (11)	0.50038 (9)	0.22432 (6)	0.01478 (17)
N4	0.36372 (12)	0.68190 (10)	0.28408 (6)	0.01722 (18)
N5	0.09082 (13)	0.76031 (10)	0.28541 (7)	0.0215 (2)
C1	0.29424 (16)	-0.06979 (12)	-0.03559 (7)	0.0221 (2)
H1A	0.3658	-0.0588	-0.0770	0.026*
C2	0.22669 (16)	-0.18701 (12)	-0.02307 (8)	0.0241 (2)
H2A	0.2518	-0.2559	-0.0553	0.029*
C3	0.12217 (16)	-0.20161 (12)	0.03723 (8)	0.0229 (2)

C4	0.08571 (16)	-0.10281 (12)	0.08621 (7)	0.0212 (2)
H4A	0.0153	-0.1149	0.1280	0.025*
C5	0.15433 (14)	0.01392 (11)	0.07288 (7)	0.0184 (2)
H5A	0.1300	0.0822	0.1058	0.022*
C6	0.25865 (14)	0.03226 (11)	0.01173 (7)	0.0181 (2)
C7	0.32849 (15)	0.15744 (11)	-0.00367 (7)	0.0182 (2)
C8	0.40582 (14)	0.43392 (11)	0.09867 (7)	0.0168 (2)
C9	0.35054 (14)	0.39082 (11)	0.17701 (7)	0.0163 (2)
H9A	0.2528	0.3399	0.1719	0.020*
H9B	0.4335	0.3382	0.2012	0.020*
C10	0.17458 (14)	0.55668 (11)	0.23059 (7)	0.0171 (2)
H10A	0.0746	0.5263	0.2134	0.021*
C11	0.20643 (14)	0.66705 (11)	0.26741 (7)	0.0172 (2)
C12	0.43050 (13)	0.57897 (11)	0.25673 (6)	0.01558 (19)
C13	0.38107 (18)	0.19047 (14)	-0.08367 (7)	0.0267 (3)
H13A	0.3421	0.2744	-0.0969	0.040*
H13B	0.3378	0.1290	-0.1198	0.040*
H13C	0.4974	0.1894	-0.0862	0.040*
C14	0.60238 (15)	0.54790 (13)	0.26074 (8)	0.0226 (2)
H14A	0.6556	0.6059	0.2959	0.034*
H14B	0.6494	0.5557	0.2098	0.034*
H14C	0.6155	0.4616	0.2792	0.034*
H1N2	0.436 (2)	0.3704 (17)	0.0004 (12)	0.028 (5)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Br1	0.03837 (9)	0.01604 (7)	0.03988 (9)	-0.00786 (5)	-0.01265 (6)	0.00296 (5)
O1	0.0347 (5)	0.0166 (4)	0.0195 (4)	-0.0089 (4)	0.0077 (4)	-0.0024 (3)
O2	0.0300 (5)	0.0167 (4)	0.0342 (5)	0.0039 (3)	0.0041 (4)	-0.0044 (4)
O3	0.0162 (4)	0.0334 (6)	0.0537 (7)	0.0041 (4)	0.0052 (4)	-0.0103 (5)
N1	0.0189 (4)	0.0138 (4)	0.0179 (4)	-0.0020 (3)	0.0007 (3)	-0.0014 (3)
N2	0.0244 (5)	0.0161 (4)	0.0162 (4)	-0.0052 (4)	0.0044 (4)	-0.0017 (4)
N3	0.0153 (4)	0.0130 (4)	0.0160 (4)	-0.0008 (3)	0.0029 (3)	-0.0008 (3)
N4	0.0176 (4)	0.0152 (4)	0.0189 (4)	0.0000 (3)	0.0009 (4)	-0.0017 (3)
N5	0.0204 (5)	0.0181 (5)	0.0261 (5)	0.0030 (4)	0.0068 (4)	0.0003 (4)
C1	0.0245 (6)	0.0194 (5)	0.0222 (5)	0.0008 (4)	-0.0012 (5)	-0.0056 (4)
C2	0.0272 (6)	0.0159 (5)	0.0291 (6)	0.0019 (5)	-0.0055 (5)	-0.0065 (5)
C3	0.0255 (6)	0.0147 (5)	0.0284 (6)	-0.0028 (4)	-0.0095 (5)	0.0003 (4)
C4	0.0241 (6)	0.0183 (5)	0.0212 (5)	-0.0036 (4)	-0.0030 (4)	0.0009 (4)
C5	0.0213 (5)	0.0156 (5)	0.0183 (5)	-0.0013 (4)	-0.0020 (4)	-0.0024 (4)
C6	0.0201 (5)	0.0149 (5)	0.0192 (5)	-0.0007 (4)	-0.0024 (4)	-0.0030 (4)
C7	0.0200 (5)	0.0168 (5)	0.0176 (5)	-0.0017 (4)	0.0007 (4)	-0.0028 (4)
C8	0.0182 (5)	0.0154 (5)	0.0168 (5)	-0.0018 (4)	0.0030 (4)	-0.0012 (4)
C9	0.0199 (5)	0.0116 (4)	0.0175 (5)	-0.0016 (4)	0.0035 (4)	-0.0016 (4)
C10	0.0145 (5)	0.0167 (5)	0.0201 (5)	-0.0011 (4)	0.0033 (4)	0.0007 (4)
C11	0.0172 (5)	0.0148 (5)	0.0197 (5)	0.0011 (4)	0.0040 (4)	-0.0004 (4)
C12	0.0165 (5)	0.0140 (4)	0.0163 (5)	-0.0002 (4)	0.0002 (4)	-0.0004 (4)

C13	0.0371 (7)	0.0252 (6)	0.0178 (5)	-0.0095 (5)	0.0034 (5)	-0.0032 (5)
C14	0.0162 (5)	0.0221 (6)	0.0296 (6)	0.0026 (4)	-0.0041 (5)	-0.0036 (5)

*Geometric parameters (Å, °)*

Br1—C3	1.8962 (13)	C3—C4	1.3919 (19)
O1—C8	1.2302 (14)	C4—C5	1.3912 (17)
O2—N5	1.2310 (15)	C4—H4A	0.9500
O3—N5	1.2363 (15)	C5—C6	1.3989 (17)
N1—C7	1.2901 (15)	C5—H5A	0.9500
N1—N2	1.3783 (14)	C6—C7	1.4824 (17)
N2—C8	1.3483 (15)	C7—C13	1.5102 (18)
N2—H1N2	0.81 (2)	C8—C9	1.5190 (16)
N3—C10	1.3614 (15)	C9—H9A	0.9900
N3—C12	1.3779 (15)	C9—H9B	0.9900
N3—C9	1.4554 (15)	C10—C11	1.3671 (17)
N4—C12	1.3223 (15)	C10—H10A	0.9500
N4—C11	1.3644 (16)	C12—C14	1.4857 (16)
N5—C11	1.4264 (15)	C13—H13A	0.9800
C1—C2	1.3898 (19)	C13—H13B	0.9800
C1—C6	1.3992 (17)	C13—H13C	0.9800
C1—H1A	0.9500	C14—H14A	0.9800
C2—C3	1.383 (2)	C14—H14B	0.9800
C2—H2A	0.9500	C14—H14C	0.9800
C7—N1—N2	116.91 (10)	C6—C7—C13	119.67 (10)
C8—N2—N1	119.67 (10)	O1—C8—N2	121.89 (11)
C8—N2—H1N2	117.7 (13)	O1—C8—C9	120.65 (10)
N1—N2—H1N2	122.6 (13)	N2—C8—C9	117.44 (10)
C10—N3—C12	107.86 (9)	N3—C9—C8	109.07 (9)
C10—N3—C9	124.22 (10)	N3—C9—H9A	109.9
C12—N3—C9	126.68 (10)	C8—C9—H9A	109.9
C12—N4—C11	103.86 (10)	N3—C9—H9B	109.9
O2—N5—O3	123.61 (11)	C8—C9—H9B	109.9
O2—N5—C11	119.47 (11)	H9A—C9—H9B	108.3
O3—N5—C11	116.91 (11)	N3—C10—C11	104.02 (10)
C2—C1—C6	121.13 (12)	N3—C10—H10A	128.0
C2—C1—H1A	119.4	C11—C10—H10A	128.0
C6—C1—H1A	119.4	N4—C11—C10	112.94 (10)
C3—C2—C1	118.82 (12)	N4—C11—N5	122.29 (11)
C3—C2—H2A	120.6	C10—C11—N5	124.74 (11)
C1—C2—H2A	120.6	N4—C12—N3	111.32 (10)
C2—C3—C4	121.70 (12)	N4—C12—C14	125.61 (11)
C2—C3—Br1	118.46 (10)	N3—C12—C14	123.07 (10)
C4—C3—Br1	119.80 (11)	C7—C13—H13A	109.5
C5—C4—C3	118.74 (12)	C7—C13—H13B	109.5
C5—C4—H4A	120.6	H13A—C13—H13B	109.5
C3—C4—H4A	120.6	C7—C13—H13C	109.5

C4—C5—C6	120.96 (11)	H13A—C13—H13C	109.5
C4—C5—H5A	119.5	H13B—C13—H13C	109.5
C6—C5—H5A	119.5	C12—C14—H14A	109.5
C5—C6—C1	118.63 (11)	C12—C14—H14B	109.5
C5—C6—C7	120.95 (11)	H14A—C14—H14B	109.5
C1—C6—C7	120.41 (11)	C12—C14—H14C	109.5
N1—C7—C6	115.78 (11)	H14A—C14—H14C	109.5
N1—C7—C13	124.54 (11)	H14B—C14—H14C	109.5
C7—N1—N2—C8	176.66 (12)	C12—N3—C9—C8	-73.37 (14)
C6—C1—C2—C3	0.25 (19)	O1—C8—C9—N3	18.68 (16)
C1—C2—C3—C4	-1.2 (2)	N2—C8—C9—N3	-162.77 (10)
C1—C2—C3—Br1	176.42 (10)	C12—N3—C10—C11	-0.47 (13)
C2—C3—C4—C5	1.3 (2)	C9—N3—C10—C11	-168.42 (10)
Br1—C3—C4—C5	-176.37 (9)	C12—N4—C11—C10	0.27 (14)
C3—C4—C5—C6	-0.28 (19)	C12—N4—C11—N5	-178.11 (11)
C4—C5—C6—C1	-0.66 (18)	N3—C10—C11—N4	0.13 (14)
C4—C5—C6—C7	178.40 (11)	N3—C10—C11—N5	178.47 (11)
C2—C1—C6—C5	0.68 (19)	O2—N5—C11—N4	-0.47 (18)
C2—C1—C6—C7	-178.39 (12)	O3—N5—C11—N4	178.49 (12)
N2—N1—C7—C6	-178.98 (10)	O2—N5—C11—C10	-178.65 (12)
N2—N1—C7—C13	0.29 (18)	O3—N5—C11—C10	0.30 (19)
C5—C6—C7—N1	24.91 (17)	C11—N4—C12—N3	-0.58 (13)
C1—C6—C7—N1	-156.05 (12)	C11—N4—C12—C14	-179.49 (12)
C5—C6—C7—C13	-154.40 (12)	C10—N3—C12—N4	0.69 (13)
C1—C6—C7—C13	24.64 (18)	C9—N3—C12—N4	168.26 (11)
N1—N2—C8—O1	-178.13 (11)	C10—N3—C12—C14	179.63 (11)
N1—N2—C8—C9	3.34 (17)	C9—N3—C12—C14	-12.80 (18)
C10—N3—C9—C8	92.28 (13)		

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H1N2 $\cdots$ O1 <sup>i</sup>	0.81 (2)	2.04 (2)	2.8318 (14)	166.6 (18)
C9—H9A $\cdots$ O3 <sup>ii</sup>	0.99	2.31	3.1818 (16)	147
C9—H9B $\cdots$ N4 <sup>iii</sup>	0.99	2.40	3.3462 (16)	160
C10—H10A $\cdots$ O2 <sup>ii</sup>	0.95	2.56	3.4488 (16)	155

Symmetry codes: (i)  $-x+1, -y+1, -z$ ; (ii)  $-x, y-1/2, -z+1/2$ ; (iii)  $-x+1, y-1/2, -z+1/2$ .