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2-Bromo-*N'*-[(2*Z*)-butan-2-ylidene]-5-methoxybenzohydrazideJerry P. Jasinski,^a Ray J. Butcher,^{b*} L. P. Suchitra,^c
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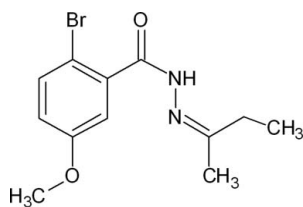
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Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.044; wR factor = 0.122; data-to-parameter ratio = 16.4.

In the title compound, $\text{C}_{12}\text{H}_{15}\text{BrN}_2\text{O}_2$, the dihedral angle between the benzene ring and the mean plane of the amide grouping is $77.7(8)^\circ$. In the crystal, inversion dimers linked by pairs of $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds occur, and the packing is further supported by $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Br}$ interactions and weak $\pi-\pi$ ring stacking interactions.

Related literature

Hydrazides and their corresponding Schiff bases are useful precursors in the synthesis of several heterocyclic systems, see: Narayana *et al.* (2005; 2005*a*). For the biological activity of substituted hydrazides, see: Cajocorius *et al.* (1977). Hydrazides are intermediates in the production of many pharmaceutically important compounds, see: Liu *et al.* (2006). For related structures, see: Butcher *et al.* (2007); Hou (2009); Li & Ban (2009); Sarojini *et al.* (2007*a,b,c,d*). For the MOPAC AM1 calculations, see: Schmidt & Polik (2007).



Experimental

Crystal data

$\text{C}_{12}\text{H}_{15}\text{BrN}_2\text{O}_2$ $c = 11.2974(2)$ Å
 $M_r = 299.17$ $\beta = 91.1519(13)^\circ$
 Monoclinic, $P2_1/c$ $V = 1302.58(3)$ Å³
 $a = 8.0942(1)$ Å $Z = 4$
 $b = 14.2475(2)$ Å Cu $K\alpha$ radiation

$\mu = 4.25$ mm⁻¹
 $T = 200$ K

 $0.56 \times 0.47 \times 0.35$ mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer 7962 measured reflections
 2577 independent reflections
 Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007) 2484 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $T_{\text{min}} = 0.452$, $T_{\text{max}} = 1.000$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$ 157 parameters
 $wR(F^2) = 0.122$ H-atom parameters constrained
 $S = 1.07$ $\Delta\rho_{\text{max}} = 0.73$ e Å⁻³
 2577 reflections $\Delta\rho_{\text{min}} = -1.07$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C7}-\text{H7B}\cdots\text{O2}^{\text{i}}$	0.98	2.60	3.561 (4)	166
$\text{C10}-\text{H10A}\cdots\text{Br}^{\text{iii}}$	0.98	3.07	3.949 (5)	151
$\text{C10}-\text{H10A}\cdots\text{O2}^{\text{iii}}$	0.98	2.55	3.231 (4)	127
$\text{C11}-\text{H11A}\cdots\text{O1}^{\text{iv}}$	0.99	2.55	3.373 (4)	141
$\text{N1}-\text{H1A}\cdots\text{O2}^{\text{iii}}$	0.88	2.07	2.932 (3)	165

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

Data collection: *CrysAlis Pro* (Oxford Diffraction, 2007); cell refinement: *CrysAlis Pro*; data reduction: *CrysAlis Pro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2010).

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supporting information

Acta Cryst. (2009). E65, o2968–o2969 [https://doi.org/10.1107/S1600536809044869]

2-Bromo-*N'*-[(2*Z*)-butan-2-ylidene]-5-methoxybenzohydrazide

Jerry P. Jasinski, Ray J. Butcher, L. P. Suchitra, H. S. Yathirajan and B. Narayana

S1. Comment

Hydrazides and the corresponding Schiff bases are useful precursors in the synthesis of several heterocyclic systems (Narayana *et al.* 2005; 2005*a*). Some substituted hydrazides are reported to exhibit carcinostatic activity against several types of tumors (Cajocorius *et al.* 1977) and also possess antimicrobial activity. It is also used as an intermediate in many pharmaceutically important compounds (Liu *et al.* 2006). In continuation with our studies on the structures of hydrazides and their Schiff bases (Sarojini *et al.* 2007*a*, 2007*b*, 2007*c*, 2007*d*; Butcher *et al.* 2007) a new Schiff base, (I), C₁₂H₁₅BrN₂O₂, has been synthesized and its crystal structure is now reported.

In the title compound, C₁₂H₁₅BrN₂O₂, (Fig. 1), the 2-bromo and 5-methoxy groups are in the plane of the benzene ring. The dihedral angle between the mean planes of the carbonyl group (–C6—C8(O2)—N1—N2–) and benzene ring is 77.7 (8)°. The C1—C6—C8—O2 and C1—C6—C8—N1 torsion angles (–101.1 (3)° & –103.7 (3)°) support this observation. Crystal packing is supported by a collection of intermediate N1—H1A—O2 (–*x*, –*y* + 2, –*z* + 1) intermolecular interactions (see Table 1) which produces a cooperative network of infinite O—H···O—H···O—H chains arranged diagonally along the (101) plane of the unit cell (Fig. 2). In addition, weak intermolecular C10—H10A···O2 (–*x*, –*y* + 2, –*z* + 1), C11—H11A···O1 (–*x* + 1, *y* – 1/2, –*z* + 1/2), C7—H7B···O2 (–*x*, –*y* + 2, –*z*) and C10—H10A···Br (*x*, –*y* + 3/2, *z*1/2) interactions (Table 1) along with C*g*1···C*g*1 π - π ring stacking interactions at 3.869 (1) Å (2 – *x*, 1 – *y*, 1 – *z*; slippage = 1.43 (2) Å, where C*g*1 = C1—C6), collectively, slightly influence crystal packing in this crystalline environment.

After a MOPAC AM1 computational calculation (Schmidt, 2007), the dihedral angle between the mean planes of the carbonyl group (–C6—C8(O2)—N1—N2–) and benzene ring becomes 84.0 (8)°, significantly greater than the 77.7 (8)° seen in the crystal. This supports the observation of a collective action of the intermediate and weak hydrogen bond interactions along with weak intermolecular π - π stacking interactions which influence crystal packing stability.

S2. Experimental

A mixture of 2-bromo-5-methoxybenzohydrazide (2.45 g, 0.01 mol) and ethyl methyl ketone (1.44 g, 0.02 mol) in 20 ml of ethanol containing a drop of dilute sulfuric acid was refluxed for about 2 h (Scheme 2). On cooling, the solid separated was filtered and recrystallized from ethyl methyl ketone. M.P.: 385 K. Analysis for C₁₂H₁₅BrN₂O₂: Found (Calculated): C: 48.14 (48.18); H: 5.02 (5.05%); N: 9.31 (9.36%).

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with N—H = 0.88, C—H = 0.95–0.99 Å, and with $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{C}, \text{N})$.

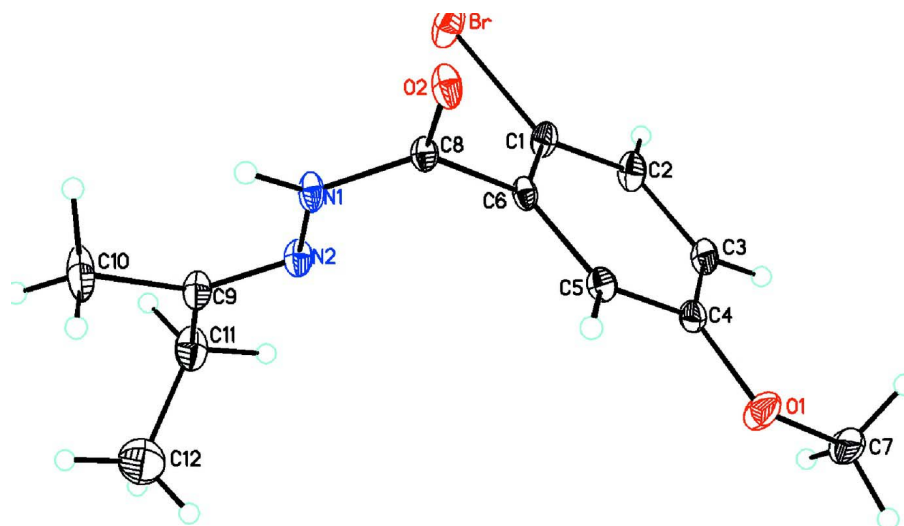


Figure 1

Molecular structure of $C_{12}H_{15}BrN_2O_2$ showing atom labeling scheme and 50% probability displacement ellipsoids.

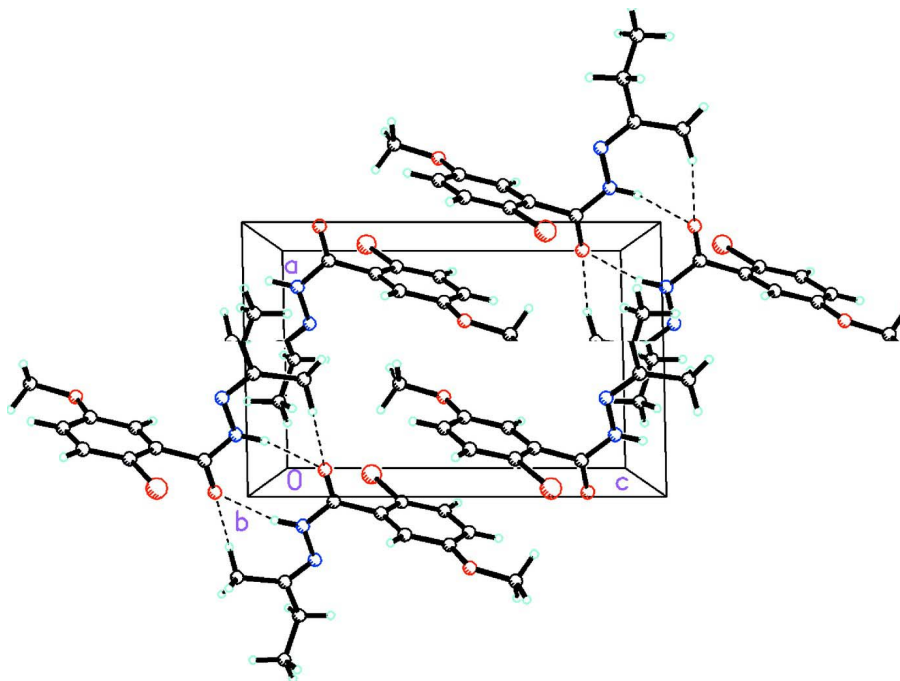


Figure 2

Packing diagram of the title compound, (I), viewed down the b axis. Dashed lines indicate intermediate intermolecular N—H \cdots O and C—H \cdots O interactions which produces a network of infinite O—H \cdots O—H chains arranged diagonally along the (101) plane of the unit cell.

2-Bromo- N' -[(2*Z*)-butan-2-ylidene]-5-methoxybenzohydrazide

Crystal data

$C_{12}H_{15}BrN_2O_2$
 $M_r = 299.17$

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

$a = 8.0942$ (1) Å
 $b = 14.2475$ (2) Å
 $c = 11.2974$ (2) Å
 $\beta = 91.1519$ (13)°
 $V = 1302.58$ (3) Å³
 $Z = 4$
 $F(000) = 608$
 $D_x = 1.526$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
 Cell parameters from 8517 reflections
 $\theta = 5.0$ – 73.4 °
 $\mu = 4.25$ mm⁻¹
 $T = 200$ K
 Chunk, colorless
 $0.56 \times 0.47 \times 0.35$ mm

Data collection

Oxford Diffraction Gemini R CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 10.5081 pixels mm⁻¹
 φ and ω scans
 Absorption correction: multi-scan
 (*CrysAlis RED*; Oxford Diffraction, 2007)
 $T_{\min} = 0.452$, $T_{\max} = 1.000$

7962 measured reflections
 2577 independent reflections
 2484 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\max} = 73.6$ °, $\theta_{\min} = 5.0$ °
 $h = -10 \rightarrow 9$
 $k = -16 \rightarrow 17$
 $l = -9 \rightarrow 13$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.122$
 $S = 1.07$
 2577 reflections
 157 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
 $w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 1.7115P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.73$ e Å⁻³
 $\Delta\rho_{\min} = -1.07$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Br	-0.00062 (5)	0.75926 (3)	0.23886 (3)	0.05362 (18)
O1	0.3113 (3)	1.07458 (17)	-0.03054 (18)	0.0478 (6)
O2	-0.0433 (2)	1.01275 (15)	0.35066 (16)	0.0358 (5)
N1	0.1775 (3)	0.93324 (16)	0.42004 (18)	0.0306 (5)
H1A	0.1550	0.9465	0.4941	0.037*
N2	0.3148 (3)	0.87860 (17)	0.39363 (19)	0.0318 (5)
C1	0.0954 (3)	0.85866 (18)	0.1528 (2)	0.0305 (5)
C2	0.1316 (4)	0.8445 (2)	0.0351 (2)	0.0361 (6)

H2A	0.1073	0.7858	-0.0012	0.043*
C3	0.2033 (3)	0.9154 (2)	-0.0303 (2)	0.0316 (6)
H3A	0.2285	0.9056	-0.1111	0.038*
C4	0.2379 (3)	1.00067 (19)	0.0234 (2)	0.0294 (5)
C5	0.1981 (3)	1.01479 (18)	0.1415 (2)	0.0285 (5)
H5A	0.2195	1.0739	0.1775	0.034*
C6	0.1282 (3)	0.94403 (17)	0.2066 (2)	0.0244 (5)
C7	0.3619 (4)	1.0618 (3)	-0.1501 (3)	0.0525 (9)
H7A	0.4202	1.1181	-0.1766	0.079*
H7B	0.2644	1.0512	-0.2012	0.079*
H7C	0.4357	1.0075	-0.1544	0.079*
C8	0.0802 (3)	0.96538 (18)	0.3318 (2)	0.0258 (5)
C9	0.4048 (3)	0.8504 (2)	0.4794 (2)	0.0357 (6)
C10	0.3829 (5)	0.8738 (3)	0.6083 (3)	0.0624 (12)
H10A	0.2676	0.8632	0.6295	0.094*
H10B	0.4118	0.9397	0.6221	0.094*
H10C	0.4551	0.8336	0.6570	0.094*
C11	0.5478 (4)	0.7880 (3)	0.4479 (3)	0.0485 (8)
H11A	0.5308	0.7253	0.4835	0.058*
H11B	0.5486	0.7800	0.3609	0.058*
C12	0.7109 (5)	0.8246 (4)	0.4882 (5)	0.0764 (13)
H12A	0.7969	0.7786	0.4702	0.115*
H12B	0.7097	0.8357	0.5738	0.115*
H12C	0.7339	0.8837	0.4472	0.115*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0949 (4)	0.0345 (2)	0.0315 (2)	-0.01786 (16)	0.00182 (18)	0.00284 (12)
O1	0.0666 (14)	0.0508 (13)	0.0261 (11)	-0.0214 (11)	0.0079 (9)	-0.0005 (9)
O2	0.0396 (10)	0.0467 (12)	0.0210 (9)	0.0198 (8)	-0.0009 (7)	-0.0063 (8)
N1	0.0373 (11)	0.0386 (12)	0.0159 (10)	0.0145 (9)	0.0007 (8)	-0.0042 (8)
N2	0.0371 (11)	0.0346 (12)	0.0238 (11)	0.0125 (9)	0.0026 (9)	-0.0023 (9)
C1	0.0452 (14)	0.0245 (12)	0.0219 (12)	0.0002 (10)	0.0004 (10)	-0.0003 (10)
C2	0.0576 (17)	0.0292 (13)	0.0212 (13)	0.0033 (12)	-0.0032 (11)	-0.0081 (10)
C3	0.0397 (13)	0.0395 (15)	0.0157 (11)	0.0066 (11)	0.0019 (9)	-0.0066 (10)
C4	0.0322 (12)	0.0352 (14)	0.0206 (12)	-0.0005 (10)	-0.0021 (10)	-0.0007 (10)
C5	0.0342 (12)	0.0283 (12)	0.0230 (12)	0.0015 (10)	-0.0020 (9)	-0.0070 (10)
C6	0.0281 (11)	0.0275 (12)	0.0175 (11)	0.0092 (9)	-0.0018 (8)	-0.0033 (9)
C7	0.0564 (19)	0.076 (2)	0.0250 (15)	-0.0218 (17)	0.0066 (13)	0.0033 (15)
C8	0.0327 (12)	0.0255 (12)	0.0192 (11)	0.0047 (9)	-0.0004 (9)	-0.0039 (9)
C9	0.0391 (14)	0.0418 (15)	0.0263 (13)	0.0132 (12)	0.0014 (10)	0.0018 (11)
C10	0.060 (2)	0.104 (3)	0.0233 (15)	0.040 (2)	-0.0041 (14)	0.0002 (17)
C11	0.0513 (18)	0.0549 (19)	0.0393 (17)	0.0250 (15)	0.0012 (13)	0.0036 (15)
C12	0.050 (2)	0.100 (4)	0.079 (3)	0.016 (2)	0.004 (2)	0.004 (3)

Geometric parameters (Å, °)

Br—C1	1.894 (3)	C5—H5A	0.9500
O1—C4	1.359 (3)	C6—C8	1.506 (3)
O1—C7	1.431 (4)	C7—H7A	0.9800
O2—C8	1.228 (3)	C7—H7B	0.9800
N1—C8	1.338 (3)	C7—H7C	0.9800
N1—N2	1.394 (3)	C9—C10	1.507 (4)
N1—H1A	0.8800	C9—C11	1.508 (4)
N2—C9	1.266 (4)	C10—H10A	0.9800
C1—C2	1.382 (4)	C10—H10B	0.9800
C1—C6	1.383 (3)	C10—H10C	0.9800
C2—C3	1.386 (4)	C11—C12	1.482 (6)
C2—H2A	0.9500	C11—H11A	0.9900
C3—C4	1.383 (4)	C11—H11B	0.9900
C3—H3A	0.9500	C12—H12A	0.9800
C4—C5	1.393 (4)	C12—H12B	0.9800
C5—C6	1.376 (4)	C12—H12C	0.9800
C4—O1—C7	117.4 (2)	H7A—C7—H7C	109.5
C8—N1—N2	119.4 (2)	H7B—C7—H7C	109.5
C8—N1—H1A	120.3	O2—C8—N1	121.9 (2)
N2—N1—H1A	120.3	O2—C8—C6	120.0 (2)
C9—N2—N1	117.5 (2)	N1—C8—C6	118.2 (2)
C2—C1—C6	120.6 (2)	N2—C9—C10	126.3 (3)
C2—C1—Br	118.8 (2)	N2—C9—C11	116.0 (3)
C6—C1—Br	120.59 (19)	C10—C9—C11	117.6 (3)
C1—C2—C3	120.3 (2)	C9—C10—H10A	109.5
C1—C2—H2A	119.9	C9—C10—H10B	109.5
C3—C2—H2A	119.9	H10A—C10—H10B	109.5
C4—C3—C2	119.4 (2)	C9—C10—H10C	109.5
C4—C3—H3A	120.3	H10A—C10—H10C	109.5
C2—C3—H3A	120.3	H10B—C10—H10C	109.5
O1—C4—C3	124.8 (2)	C12—C11—C9	113.8 (3)
O1—C4—C5	115.4 (2)	C12—C11—H11A	108.8
C3—C4—C5	119.8 (2)	C9—C11—H11A	108.8
C6—C5—C4	120.8 (2)	C12—C11—H11B	108.8
C6—C5—H5A	119.6	C9—C11—H11B	108.8
C4—C5—H5A	119.6	H11A—C11—H11B	107.7
C5—C6—C1	119.1 (2)	C11—C12—H12A	109.5
C5—C6—C8	118.1 (2)	C11—C12—H12B	109.5
C1—C6—C8	122.7 (2)	H12A—C12—H12B	109.5
O1—C7—H7A	109.5	C11—C12—H12C	109.5
O1—C7—H7B	109.5	H12A—C12—H12C	109.5
H7A—C7—H7B	109.5	H12B—C12—H12C	109.5
O1—C7—H7C	109.5		
C8—N1—N2—C9	179.2 (3)	Br—C1—C6—C5	179.97 (19)

C6—C1—C2—C3	0.8 (4)	C2—C1—C6—C8	175.6 (2)
Br—C1—C2—C3	-179.4 (2)	Br—C1—C6—C8	-4.2 (3)
C1—C2—C3—C4	-0.2 (4)	N2—N1—C8—O2	179.0 (3)
C7—O1—C4—C3	-2.5 (4)	N2—N1—C8—C6	-2.5 (4)
C7—O1—C4—C5	177.0 (3)	C5—C6—C8—O2	74.8 (3)
C2—C3—C4—O1	178.4 (3)	C1—C6—C8—O2	-101.1 (3)
C2—C3—C4—C5	-1.0 (4)	C5—C6—C8—N1	-103.7 (3)
O1—C4—C5—C6	-177.9 (2)	C1—C6—C8—N1	80.4 (3)
C3—C4—C5—C6	1.6 (4)	N1—N2—C9—C10	-3.0 (5)
C4—C5—C6—C1	-0.9 (4)	N1—N2—C9—C11	177.4 (3)
C4—C5—C6—C8	-177.0 (2)	N2—C9—C11—C12	122.5 (4)
C2—C1—C6—C5	-0.3 (4)	C10—C9—C11—C12	-57.1 (5)

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>
C7—H7B \cdots O2 ⁱ	0.98	2.60	3.561 (4)	166
C10—H10A \cdots Br ⁱⁱ	0.98	3.07	3.949 (5)	151
C10—H10A \cdots O2 ⁱⁱⁱ	0.98	2.55	3.231 (4)	127
C11—H11A \cdots O1 ^{iv}	0.99	2.55	3.373 (4)	141
N1—H1A \cdots O2 ⁱⁱⁱ	0.88	2.07	2.932 (3)	165

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x, -y+3/2, z+1/2$; (iii) $-x, -y+2, -z+1$; (iv) $-x+1, y-1/2, -z+1/2$.