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7-Bromo-1,4-dibutyl-1,2,3,4-tetrahydropyrido-[2,3-*b*]pyrazine-2,3-dione

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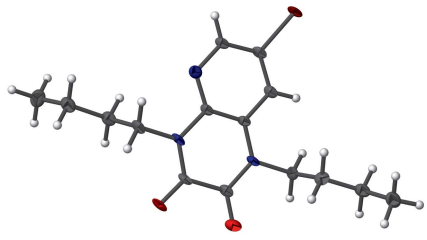
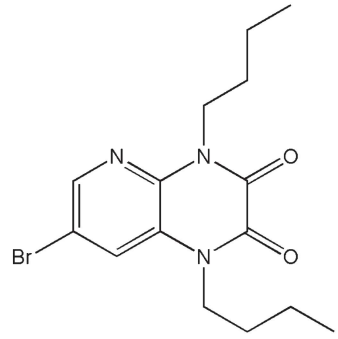
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{15}H_{20}BrN_3O_2$, the butyl substituents are in extended conformations on opposite sides of the bicyclic core. In the crystal, oblique stacks of molecules, formed by offset π-stacking interactions between pyridine and pyrazine rings in adjacent molecules, extend along the *b*-axis direction. The stacks are associated through a combination of C—H···O hydrogen bonds and C—Br···π(ring) interactions.

3D view



Chemical scheme



Structure description

Pyrido-pyrazine derivatives are a versatile class of nitrogen-containing heterocyclic compounds and they constitute useful intermediates in organic synthesis and medicinal chemistry. They possess a broad spectrum of biological activities including anti-cancer (Gong *et al.*, 2011), anti-inflammatory (Hodgetts *et al.*, 2010) and antimalarial (Richter *et al.*, 2006). They are also used as inhibitors of anaplastic lymphoma kinase (Milkiewicz *et al.*, 2010). As a continuation of our research in the field of substituted pyrido[2,3-*b*]-pyrazine derivatives (Hjouji *et al.*, 2014), we report here the synthesis of the title compound by the condensation of butyl bromide and 7-bromopyrido[2,3-*b*]pyrazine-2,3(1*H*,4*H*)-dione.

In the title molecule, the *n*-butyl substituents are both in extended conformations with one extending above and the other below the pyrazine ring (Fig. 1). The bicyclic core is planar within experimental error.

In the crystal, the molecules form oblique stacks along the *b*-axis direction through offset π-stacking interactions between the pyridine portion of one molecule and the

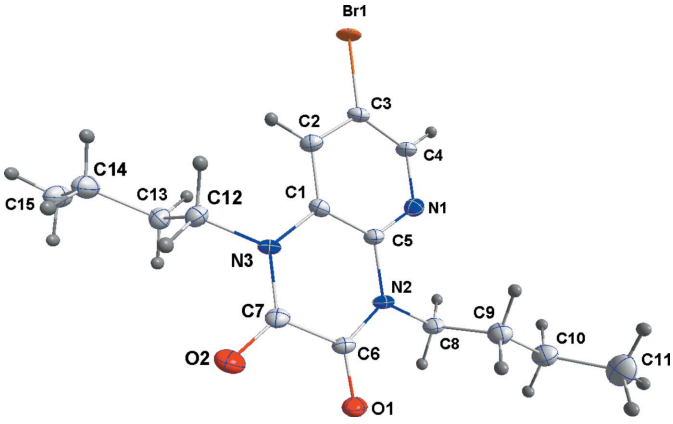


Figure 1
The title molecule with labeling scheme and 50% probability ellipsoids.

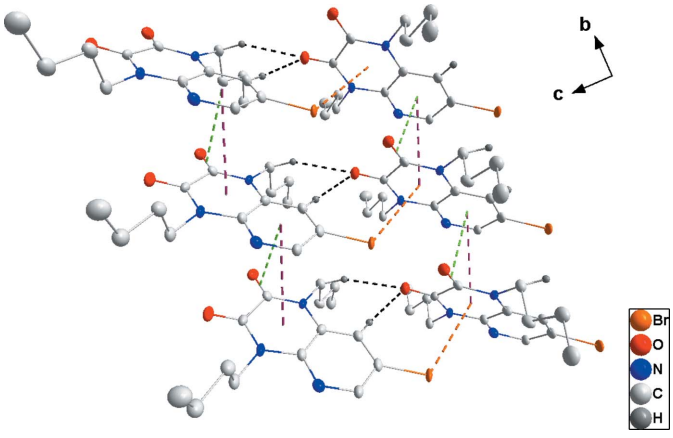


Figure 2
Detail of the intermolecular interactions (dashed lines), viewed along the *a*-axis direction (C—H···O hydrogen bonds (black), π-stacking (purple), C═O···π(ring) (green), C—Br···π(ring) (orange)).

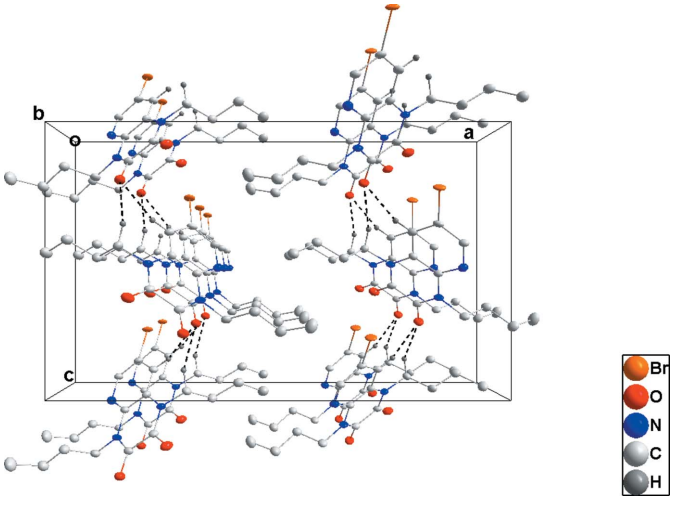


Figure 3
Packing viewed along the *b*-axis direction, with C—H···O hydrogen bonds shown as black dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.95	2.33	3.253 (12)	164
C12—H12*A*···O1^{i}	0.99	2.55	3.447 (11)	150

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{20}BrN_3O_2$
M_r	354.25
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	100
a, *b*, *c* (Å)	22.569 (6), 5.1097 (13), 13.497 (3)
V (Å^3)	1556.5 (7)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	2.65
Crystal size (mm)	0.22 × 0.21 × 0.02
Data collection	
Diffractometer	Bruker *SMART APEX* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.50, 0.96
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13413, 3859, 2916
R_{int}	0.091
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.676
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.068, 0.156, 1.06
No. of reflections	3859
No. of parameters	192
No. of restraints	94
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.33, −1.38
Absolute structure	Flack *x* determined using 1091 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.038 (15)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

pyrazine portion of the next (Fig. 2). In the stack, the centroid–centroid distance of the respective rings is 3.695 (5) Å and they are parallel within experimental error. Assisting these interactions in forming the stacks are π interactions between the C7O2 carbonyl group and the pyridine ring in adjacent molecules (Fig. 2) where the distance between the mid-point of the double bond and the ring centroid is 3.268 (8) Å. Finally, the stacks are associated through a combination of C2—H2···O1 and C12—H12*A*···O1 hydrogen bonds (Table 1 and Fig. 3) and C3—Br1···π(ring)^{i} interactions (Fig. 2) where Br1···*Cg*2 = 3.701 (4) Å, C3—Br1···*Cg*2 = 118.1 (3)° and *Cg*2 is the centroid of the pyrazine portion of the molecule with symmetry code (i) $\frac{1}{2}-x, -\frac{1}{2}+y, -\frac{1}{2}+z$).

Synthesis and crystallization

Butyl bromide (0.2 ml, 1.82 mmol) was added to a solution of 7-bromopyrido[2,3-*b*]pyrazine-2,3(1*H*,4*H*)-dione (0.2 g,

0.83 mmol), K_2CO_3 (0.28 g, 2.07 mmol) and tetra-*n*-butyl ammonium bromide (0.03 g, 0.1 mmol) in DMF (10 ml). The mixture was then stirred for 6 h at room temperature. The solvent was evaporated under reduced pressure and the product isolated by chromatography on a silica gel column with ethyl acetate/hexane (1/2) as eluent. The compound forms pale-blue plate-shaped crystals in 77% yield and was recrystallized from a solvent mixture (ethanol/dichloromethane: 2/1).

Refinement

Crystal and refinement details are presented in Table 2. The hydrogen atoms were included as riding contributions in idealized positions.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170984 [https://doi.org/10.1107/S2414314617009841]

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Crystal data

$C_{15}H_{20}BrN_3O_2$
M_r = 354.25
Orthorhombic, $Pna2_1$
a = 22.569 (6) Å
b = 5.1097 (13) Å
c = 13.497 (3) Å
V = 1556.5 (7) Å^3
Z = 4
$F(000)$ = 728
D_x = 1.512 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3677 reflections
θ = 2.4–26.1°
μ = 2.65 mm^{-1}
T = 100 K
Plate, pale blue
0.22 × 0.21 × 0.02 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.50, T_{max} = 0.96
13413 measured reflections
3859 independent reflections
2916 reflections with $I > 2\sigma(I)$
R_{int} = 0.091
θ_{max} = 28.7°, θ_{min} = 1.8°
h = −29→29
k = −6→6
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.156
S = 1.06
3859 reflections
192 parameters
94 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
$w = 1/[\sigma^2(F_o^2) + 6.1176P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.33 e Å^{-3}
$\Delta\rho_{min}$ = −1.38 e Å^{-3}
Absolute structure: Flack x determined using 1091 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.038 (15)

Special details

Experimental. The diffraction data were collected in three sets of 363 frames (0.5° width in ω) at φ = 0, 120 and 240°. A scan time of 80 sec/frame was used.

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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å). All were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.30633 (4)	−0.15545 (15)	0.26770 (7)	0.0209 (2)
O1	0.3211 (3)	0.8535 (14)	0.7274 (5)	0.0249 (16)
O2	0.2233 (3)	0.9499 (14)	0.6151 (5)	0.0249 (16)
N1	0.3741 (4)	0.1719 (16)	0.5238 (6)	0.0203 (16)
N2	0.3449 (4)	0.5053 (15)	0.6305 (5)	0.0180 (16)
N3	0.2463 (4)	0.6115 (14)	0.5112 (6)	0.0158 (15)
C1	0.2854 (4)	0.4141 (18)	0.4835 (7)	0.0168 (18)
C2	0.2764 (5)	0.259 (2)	0.4013 (7)	0.0191 (19)
H2	0.2422	0.2821	0.3612	0.023*
C3	0.3178 (4)	0.0675 (19)	0.3780 (6)	0.0193 (19)
C4	0.3653 (4)	0.0215 (19)	0.4425 (6)	0.0184 (19)
H4	0.3920	−0.1180	0.4289	0.022*
C5	0.3348 (5)	0.3572 (18)	0.5437 (6)	0.0172 (17)
C6	0.3103 (4)	0.7138 (17)	0.6563 (7)	0.0168 (18)
C7	0.2560 (5)	0.7737 (18)	0.5913 (7)	0.0185 (18)
C8	0.3954 (4)	0.4332 (19)	0.6961 (7)	0.021 (2)
H8A	0.4020	0.2419	0.6924	0.026*
H8B	0.3854	0.4776	0.7655	0.026*
C9	0.4524 (5)	0.576 (2)	0.6662 (7)	0.024 (2)
H9A	0.4622	0.5355	0.5963	0.029*
H9B	0.4464	0.7678	0.6717	0.029*
C10	0.5036 (5)	0.493 (2)	0.7330 (8)	0.028 (2)
H10A	0.4924	0.5245	0.8029	0.033*
H10B	0.5103	0.3028	0.7248	0.033*
C11	0.5613 (5)	0.637 (2)	0.7113 (10)	0.036 (3)
H11A	0.5737	0.6012	0.6431	0.055*
H11B	0.5921	0.5770	0.7572	0.055*
H11C	0.5552	0.8256	0.7198	0.055*
C12	0.1912 (4)	0.661 (2)	0.4538 (7)	0.0200 (19)
H12A	0.1987	0.6253	0.3827	0.024*
H12B	0.1799	0.8473	0.4605	0.024*
C13	0.1406 (4)	0.4884 (19)	0.4902 (7)	0.021 (2)

H13A	0.1526	0.3026	0.4847	0.026*
H13B	0.1331	0.5262	0.5610	0.026*
C14	0.0842 (5)	0.530 (2)	0.4327 (7)	0.025 (2)
H14A	0.0908	0.4771	0.3630	0.031*
H14B	0.0743	0.7186	0.4331	0.031*
C15	0.0318 (5)	0.377 (2)	0.4738 (8)	0.030 (2)
H15A	−0.0025	0.3997	0.4302	0.046*
H15B	0.0221	0.4411	0.5403	0.046*
H15C	0.0420	0.1905	0.4774	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0338 (5)	0.0191 (4)	0.0099 (3)	0.0011 (4)	0.0012 (6)	−0.0072 (5)
O1	0.035 (4)	0.027 (4)	0.012 (3)	−0.005 (3)	0.002 (3)	−0.013 (3)
O2	0.035 (4)	0.020 (4)	0.020 (4)	0.003 (3)	0.004 (3)	−0.002 (3)
N1	0.024 (4)	0.022 (4)	0.015 (3)	0.002 (3)	−0.002 (3)	0.000 (3)
N2	0.029 (4)	0.016 (4)	0.009 (3)	−0.003 (3)	−0.001 (3)	−0.005 (3)
N3	0.025 (4)	0.012 (3)	0.010 (3)	−0.001 (3)	0.001 (3)	−0.003 (3)
C1	0.023 (4)	0.016 (4)	0.011 (4)	0.001 (3)	0.002 (3)	−0.002 (3)
C2	0.028 (5)	0.019 (4)	0.010 (4)	−0.001 (4)	0.000 (4)	0.000 (3)
C3	0.030 (5)	0.021 (4)	0.007 (4)	−0.001 (3)	0.004 (3)	−0.002 (3)
C4	0.028 (5)	0.018 (4)	0.010 (4)	0.001 (4)	0.001 (3)	−0.002 (3)
C5	0.025 (4)	0.018 (4)	0.009 (3)	0.000 (3)	0.000 (3)	−0.002 (3)
C6	0.029 (4)	0.010 (4)	0.011 (3)	−0.004 (3)	0.001 (3)	−0.002 (3)
C7	0.029 (5)	0.018 (4)	0.009 (3)	−0.001 (3)	0.001 (3)	0.000 (3)
C8	0.030 (6)	0.025 (5)	0.009 (4)	−0.002 (4)	−0.002 (4)	−0.005 (4)
C9	0.031 (6)	0.023 (5)	0.017 (5)	0.000 (4)	−0.002 (4)	0.001 (4)
C10	0.036 (6)	0.024 (5)	0.023 (5)	−0.001 (4)	−0.005 (4)	−0.001 (4)
C11	0.031 (6)	0.031 (6)	0.047 (7)	0.001 (5)	−0.009 (5)	0.003 (5)
C12	0.023 (5)	0.025 (5)	0.013 (4)	0.002 (4)	−0.005 (4)	−0.001 (4)
C13	0.026 (6)	0.022 (5)	0.016 (5)	0.005 (4)	0.000 (4)	0.006 (4)
C14	0.034 (6)	0.025 (5)	0.017 (5)	0.002 (5)	0.001 (4)	−0.002 (4)
C15	0.031 (6)	0.036 (6)	0.024 (5)	−0.003 (5)	0.001 (5)	−0.006 (5)

Geometric parameters (Å, º)

Br1—C3	1.892 (9)	C9—C10	1.527 (15)
O1—C6	1.221 (11)	C9—H9A	0.9900
O2—C7	1.207 (12)	C9—H9B	0.9900
N1—C5	1.325 (12)	C10—C11	1.523 (15)
N1—C4	1.354 (12)	C10—H10A	0.9900
N2—C6	1.365 (12)	C10—H10B	0.9900
N2—C5	1.414 (11)	C11—H11A	0.9800
N2—C8	1.489 (12)	C11—H11B	0.9800
N3—C7	1.379 (12)	C11—H11C	0.9800
N3—C1	1.392 (11)	C12—C13	1.525 (14)
N3—C12	1.487 (12)	C12—H12A	0.9900

C1—C2	1.380 (13)	C12—H12B	0.9900
C1—C5	1.408 (14)	C13—C14	1.506 (14)
C2—C3	1.388 (14)	C13—H13A	0.9900
C2—H2	0.9500	C13—H13B	0.9900
C3—C4	1.402 (14)	C14—C15	1.523 (15)
C4—H4	0.9500	C14—H14A	0.9900
C6—C7	1.537 (14)	C14—H14B	0.9900
C8—C9	1.535 (14)	C15—H15A	0.9800
C8—H8A	0.9900	C15—H15B	0.9800
C8—H8B	0.9900	C15—H15C	0.9800

C5—N1—C4	118.2 (8)	C8—C9—H9B	109.6
C6—N2—C5	122.4 (8)	H9A—C9—H9B	108.1
C6—N2—C8	118.7 (7)	C11—C10—C9	113.5 (9)
C5—N2—C8	118.9 (8)	C11—C10—H10A	108.9
C7—N3—C1	123.1 (8)	C9—C10—H10A	108.9
C7—N3—C12	116.0 (8)	C11—C10—H10B	108.9
C1—N3—C12	120.9 (8)	C9—C10—H10B	108.9
C2—C1—N3	122.6 (9)	H10A—C10—H10B	107.7
C2—C1—C5	117.5 (9)	C10—C11—H11A	109.5
N3—C1—C5	119.7 (8)	C10—C11—H11B	109.5
C1—C2—C3	119.2 (9)	H11A—C11—H11B	109.5
C1—C2—H2	120.4	C10—C11—H11C	109.5
C3—C2—H2	120.4	H11A—C11—H11C	109.5
C2—C3—C4	119.5 (9)	H11B—C11—H11C	109.5
C2—C3—Br1	120.6 (7)	N3—C12—C13	111.1 (8)
C4—C3—Br1	119.5 (7)	N3—C12—H12A	109.4
N1—C4—C3	121.3 (9)	C13—C12—H12A	109.4
N1—C4—H4	119.3	N3—C12—H12B	109.4
C3—C4—H4	119.3	C13—C12—H12B	109.4
N1—C5—C1	124.0 (8)	H12A—C12—H12B	108.0
N1—C5—N2	116.3 (8)	C14—C13—C12	112.7 (8)
C1—C5—N2	119.7 (8)	C14—C13—H13A	109.0
O1—C6—N2	122.8 (9)	C12—C13—H13A	109.0
O1—C6—C7	119.4 (8)	C14—C13—H13B	109.0
N2—C6—C7	117.8 (8)	C12—C13—H13B	109.0
O2—C7—N3	124.0 (9)	H13A—C13—H13B	107.8
O2—C7—C6	118.9 (8)	C13—C14—C15	113.4 (9)
N3—C7—C6	117.0 (8)	C13—C14—H14A	108.9
N2—C8—C9	111.6 (8)	C15—C14—H14A	108.9
N2—C8—H8A	109.3	C13—C14—H14B	108.9
C9—C8—H8A	109.3	C15—C14—H14B	108.9
N2—C8—H8B	109.3	H14A—C14—H14B	107.7
C9—C8—H8B	109.3	C14—C15—H15A	109.5
H8A—C8—H8B	108.0	C14—C15—H15B	109.5
C10—C9—C8	110.3 (8)	H15A—C15—H15B	109.5
C10—C9—H9A	109.6	C14—C15—H15C	109.5
C8—C9—H9A	109.6	H15A—C15—H15C	109.5

C10—C9—H9B	109.6	H15B—C15—H15C	109.5
C7—N3—C1—C2	−177.7 (9)	C5—N2—C6—O1	−174.9 (9)
C12—N3—C1—C2	1.5 (14)	C8—N2—C6—O1	4.6 (14)
C7—N3—C1—C5	6.0 (14)	C5—N2—C6—C7	4.5 (13)
C12—N3—C1—C5	−174.8 (9)	C8—N2—C6—C7	−176.1 (8)
N3—C1—C2—C3	179.3 (9)	C1—N3—C7—O2	178.2 (9)
C5—C1—C2—C3	−4.3 (14)	C12—N3—C7—O2	−1.1 (14)
C1—C2—C3—C4	5.2 (15)	C1—N3—C7—C6	−5.1 (13)
C1—C2—C3—Br1	178.5 (7)	C12—N3—C7—C6	175.7 (8)
C5—N1—C4—C3	3.2 (13)	O1—C6—C7—O2	−3.9 (14)
C2—C3—C4—N1	−4.7 (14)	N2—C6—C7—O2	176.8 (9)
Br1—C3—C4—N1	−178.1 (7)	O1—C6—C7—N3	179.2 (9)
C4—N1—C5—C1	−2.4 (14)	N2—C6—C7—N3	−0.1 (12)
C4—N1—C5—N2	178.5 (8)	C6—N2—C8—C9	−89.8 (10)
C2—C1—C5—N1	3.0 (15)	C5—N2—C8—C9	89.6 (10)
N3—C1—C5—N1	179.5 (9)	N2—C8—C9—C10	−178.6 (8)
C2—C1—C5—N2	−177.9 (9)	C8—C9—C10—C11	−177.1 (9)
N3—C1—C5—N2	−1.4 (14)	C7—N3—C12—C13	−93.8 (10)
C6—N2—C5—N1	175.3 (8)	C1—N3—C12—C13	87.0 (10)
C8—N2—C5—N1	−4.1 (12)	N3—C12—C13—C14	−179.1 (8)
C6—N2—C5—C1	−3.8 (13)	C12—C13—C14—C15	−175.0 (8)
C8—N2—C5—C1	176.8 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.95	2.33	3.253 (12)	164
C12—H12*A*···O1^{i}	0.99	2.55	3.447 (11)	150

Symmetry code: (i) −*x*+1/2, *y*−1/2, *z*−1/2.