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3-Bromo-6-nitro-1-(prop-2-en-1-yl)-1*H*-indazole

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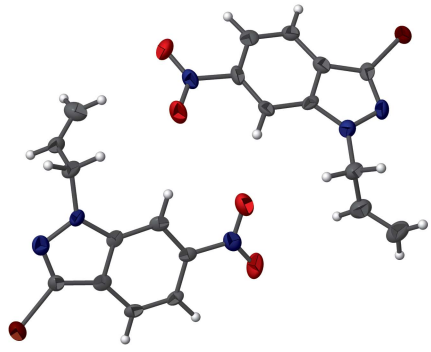
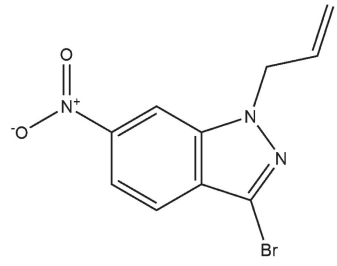
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{10}H_8BrN_3O_2$, contains two independent molecules differing primarily in the orientations of the allyl substituents [N—C—C═C torsion angles = −125.4 (16) and 116.0 (16)°]. The crystal packing involves slipped π–π stacking of indazole units, together with weak C—H···O and C—H···Br hydrogen bonds. The crystal studied was refined as a two-component twin.

3D view



Chemical scheme



Structure description

Studies of the structure and physicochemical properties of the indazole ring have been reviewed (Abbassi *et al.*, 2014; Li *et al.*, 2003). As a continuation of our studies of indazole derivatives (Mohamed Abdelahi *et al.*, 2017), we now report the synthesis and structure of the title compound (Fig. 1).

The asymmetric unit consists of two independent molecules differing primarily in the orientations of the allyl group. Thus, the torsion angles N2—N1—C8—C9 and N5—N4—C18—C19 are, respectively, −77.9 (15) and −71.9 (15)° while the N1—C8—C9—C10 and N4—C18—C19—C20 torsion angles are, respectively, −125.4 (16) and 116.0 (16)°.

In the crystal, offset π–π stacking interactions between the N1/N2/C1/C2/C7 ring and the N4/N5/C11/C12/C17 ring at $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$ form dimers with a dihedral angle between the ring planes of 3.9 (8)° and a centroid–centroid distance of 3.494 (8) Å. These dimers are arranged into two sets of oblique stacks, generally along the *a*-axis direction, by C4—H4···O1 and C18—H1*B*···O4 hydrogen bonds (Table 1 and Figs. 2–4). The normals to the stacks are inclined by +/-30.0 (8)° to [100] and by 44.7 (8)° to each other. Weak C—H···Br interactions are also observed (Table 1).

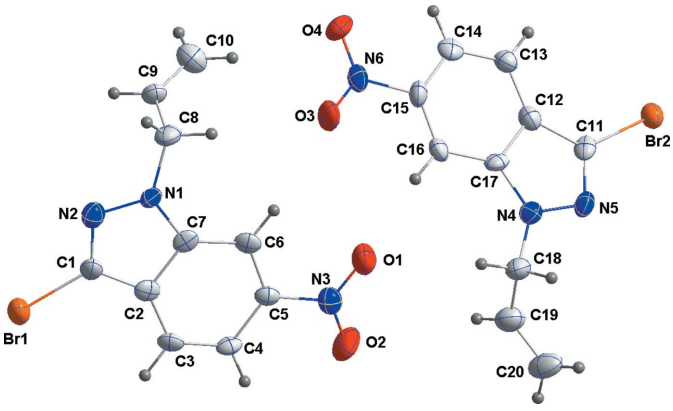


Figure 1
The asymmetric unit showing 50% probability ellipsoids.

Synthesis and crystallization

Allyl bromide (0.8 g, 5 mmol), potassium carbonate (1.24 g, 9 mmol) and a catalytic quantity of tetra-*n*-butylammonium iodide were added to a solution of 3-bromo-6-nitro-1*H*-indazole (0.6 g, 3 mmol) in tetrahydrofuran (30 ml). The mixture was stirred at room temperature for 48 h. The solution was then filtered and the solvent removed under reduced pressure. The residue was recrystallized from ethanol solution to afford the title compound as pale-orange plates (yield: 67%).

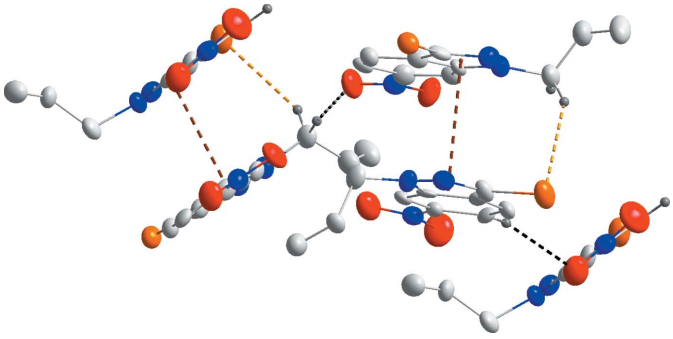


Figure 2
Detail of the intermolecular interactions. C—H···O and C—H···Br hydrogen bonds and the π-stacking interactions are shown, respectively, as black, light-orange and brown dashed lines.

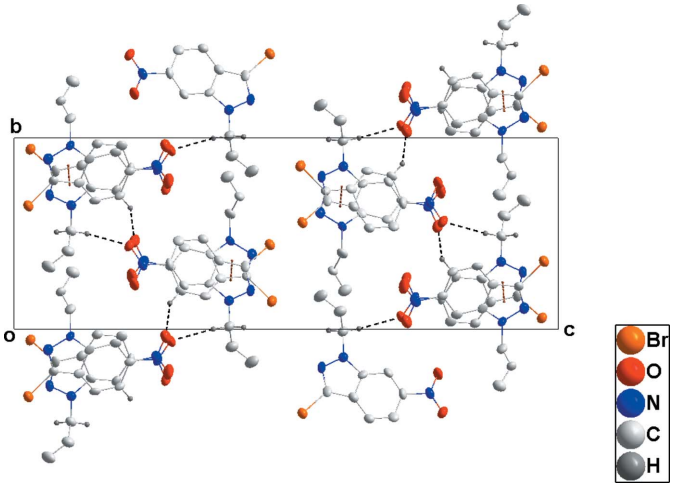


Figure 3
Packing viewed along the *a*-axis direction with intermolecular interactions shown as in Fig. 2

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1^{i}	0.95	2.46	3.304 (16)	147
C18—H18B···O4^{ii}	0.99	2.59	3.578 (16)	174
C9—H9···Br1^{iii}	0.95	3.09	3.814 (11)	134
C18—H18A···Br1^{iv}	0.99	2.91	3.770 (14)	146

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_8BrN_3O_2$
M_r	282.10
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	7.5971 (4), 9.9501 (5), 28.5690 (13)
β (°)	95.086 (2)
V (Å^3)	2151.08 (18)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	5.14
Crystal size (mm)	0.25 × 0.09 × 0.04
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.36, 0.82
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7880, 7639, 7050
R_{int}	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.079, 0.217, 1.19
No. of reflections	7639
No. of parameters	290
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.30, −1.22

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

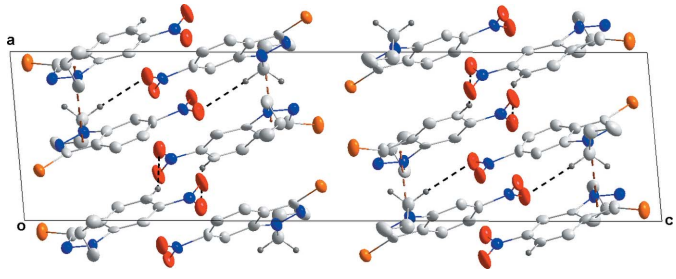


Figure 4
Packing viewed along the *b*-axis direction with intermolecular interactions shown as in Fig. 2

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The model was refined as a two-component twin. The largest residual peaks in the final difference map are not in chemically reasonable positions to represent additional atoms. Possible sources may be inadequacies in the absorption corrections due to the large absorption coefficient and difficulties in accurately measuring the dimensions of the small crystal or a small amount of 'whole molecule disorder' (*ca* 3%) with these peaks representing alternate locations of the bromine atoms but with peaks for the remainder of those molecules too small to be located confidently.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x171837 [https://doi.org/10.1107/S2414314617018375]

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Crystal data

$C_{10}H_8BrN_3O_2$
M_r = 282.10
Monoclinic, $P2_1/n$
a = 7.5971 (4) Å
b = 9.9501 (5) Å
c = 28.5690 (13) Å
β = 95.086 (2)°
V = 2151.08 (18) Å^3
Z = 8
$F(000)$ = 1120
D_x = 1.742 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 7120 reflections
θ = 3.1–72.2°
μ = 5.14 mm^{-1}
T = 150 K
Plate, pale orange
0.25 × 0.09 × 0.04 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.36, T_{max} = 0.82
7880 measured reflections
7639 independent reflections
7050 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 72.3°, θ_{min} = 3.1°
h = −9→9
k = −12→12
l = −34→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.217
S = 1.19
7639 reflections
290 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
$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 28.3909P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.30 e Å^{-3}
$\Delta\rho_{min}$ = −1.22 e Å^{-3}

Special details

Experimental. Analysis of 329 reflections having I/σ(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to be twinned by a 180° rotation about the *c** axis. The raw data were processed using the multi-component version of *SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

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. Refined as a 2-component twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.5670 (2)	0.14543 (15)	0.47380 (4)	0.0448 (5)
O1	0.4189 (17)	0.4609 (11)	0.2213 (3)	0.052 (3)
O2	0.2730 (18)	0.2752 (12)	0.2166 (3)	0.061 (3)
N1	0.6482 (14)	0.4618 (10)	0.3968 (3)	0.029 (3)
N2	0.6614 (15)	0.3910 (11)	0.4374 (3)	0.033 (3)
N3	0.3656 (16)	0.3548 (12)	0.2383 (3)	0.034 (3)
C1	0.582 (2)	0.2767 (12)	0.4274 (4)	0.031 (3)
C2	0.5133 (18)	0.2658 (12)	0.3802 (4)	0.026 (3)
C3	0.4215 (18)	0.1720 (13)	0.3514 (4)	0.028 (3)
H3	0.391544	0.087488	0.363954	0.033*
C4	0.3747 (17)	0.1995 (12)	0.3060 (4)	0.025 (3)
H4	0.312848	0.134651	0.286457	0.030*
C5	0.4187 (16)	0.3267 (13)	0.2873 (4)	0.024 (3)
C6	0.5098 (16)	0.4257 (12)	0.3134 (4)	0.026 (3)
H6	0.540098	0.509440	0.300322	0.031*
C7	0.5544 (15)	0.3920 (12)	0.3613 (4)	0.022 (3)
C8	0.703 (2)	0.6038 (13)	0.3969 (4)	0.036 (3)
H8A	0.816224	0.613203	0.416593	0.043*
H8B	0.724045	0.630139	0.364414	0.043*
C9	0.5749 (19)	0.6947 (12)	0.4142 (4)	0.030 (3)
H9	0.537239	0.676754	0.444368	0.036*
C10	0.508 (2)	0.7977 (14)	0.3921 (5)	0.044 (4)
H10A	0.541706	0.819364	0.361763	0.053*
H10B	0.424128	0.852263	0.406066	0.053*
Br2	0.29479 (19)	0.94236 (14)	0.02996 (4)	0.0338 (4)
O3	0.7297 (14)	0.7347 (10)	0.2791 (3)	0.044 (3)
O4	0.6462 (16)	0.9375 (10)	0.2877 (3)	0.047 (3)
N4	0.5227 (15)	0.6482 (11)	0.1051 (3)	0.032 (3)
N5	0.4444 (16)	0.7016 (11)	0.0653 (3)	0.032 (3)
N6	0.6590 (16)	0.8373 (12)	0.2639 (3)	0.032 (3)
C11	0.3999 (17)	0.8278 (14)	0.0754 (4)	0.028 (3)
C12	0.4494 (18)	0.8587 (13)	0.1237 (4)	0.030 (3)
C13	0.4325 (18)	0.9707 (13)	0.1528 (4)	0.029 (3)
H13	0.374507	1.050083	0.141120	0.035*
C14	0.5014 (17)	0.9617 (13)	0.1977 (4)	0.030 (3)
H14	0.494502	1.036167	0.218244	0.036*

C15	0.5842 (18)	0.8410 (14)	0.2143 (4)	0.031 (3)
C16	0.5987 (18)	0.7294 (13)	0.1879 (4)	0.027 (3)
H16	0.652562	0.649426	0.200420	0.033*
C17	0.5295 (18)	0.7390 (12)	0.1410 (4)	0.026 (3)
C18	0.598 (2)	0.5136 (13)	0.1044 (4)	0.035 (3)
H18A	0.673729	0.507640	0.078086	0.042*
H18B	0.673545	0.499252	0.133934	0.042*
C19	0.468 (2)	0.4073 (14)	0.0994 (5)	0.044 (4)
H19	0.392167	0.395215	0.123703	0.053*
C20	0.450 (2)	0.3270 (16)	0.0632 (5)	0.051 (4)
H20A	0.524262	0.336954	0.038349	0.061*
H20B	0.362454	0.258601	0.061658	0.061*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0687 (11)	0.0364 (8)	0.0294 (6)	0.0046 (9)	0.0052 (8)	0.0051 (5)
O1	0.071 (8)	0.051 (7)	0.033 (4)	0.008 (6)	0.006 (5)	0.007 (4)
O2	0.076 (9)	0.071 (8)	0.032 (5)	−0.014 (8)	−0.017 (6)	−0.008 (5)
N1	0.038 (7)	0.027 (6)	0.023 (4)	−0.007 (6)	0.004 (4)	−0.006 (4)
N2	0.034 (7)	0.037 (7)	0.029 (5)	0.005 (6)	0.005 (5)	−0.001 (4)
N3	0.030 (6)	0.038 (7)	0.033 (5)	0.006 (7)	0.002 (5)	0.004 (5)
C1	0.042 (8)	0.023 (7)	0.027 (5)	0.009 (7)	0.003 (6)	0.000 (5)
C2	0.021 (6)	0.025 (6)	0.035 (6)	0.003 (7)	0.014 (5)	−0.004 (5)
C3	0.028 (7)	0.017 (6)	0.038 (6)	0.005 (6)	0.002 (6)	−0.002 (5)
C4	0.019 (6)	0.023 (6)	0.032 (5)	−0.007 (6)	0.004 (5)	−0.008 (4)
C5	0.020 (7)	0.020 (6)	0.033 (6)	0.002 (6)	0.005 (5)	−0.003 (5)
C6	0.019 (7)	0.021 (6)	0.038 (6)	0.008 (6)	0.003 (5)	0.000 (5)
C7	0.010 (6)	0.027 (6)	0.030 (5)	0.009 (6)	0.004 (5)	−0.006 (4)
C8	0.042 (9)	0.029 (7)	0.035 (6)	−0.012 (7)	0.002 (6)	−0.008 (5)
C9	0.037 (8)	0.024 (6)	0.030 (5)	0.005 (7)	0.004 (6)	−0.005 (5)
C10	0.041 (9)	0.039 (9)	0.053 (8)	0.000 (8)	0.005 (8)	0.009 (6)
Br2	0.0371 (7)	0.0342 (7)	0.0288 (5)	−0.0009 (7)	−0.0042 (6)	0.0048 (5)
O3	0.058 (7)	0.045 (6)	0.028 (4)	0.022 (6)	−0.005 (5)	0.007 (4)
O4	0.070 (7)	0.041 (6)	0.031 (4)	−0.005 (6)	−0.001 (5)	−0.012 (4)
N4	0.037 (7)	0.030 (6)	0.028 (5)	−0.001 (6)	−0.003 (4)	−0.001 (4)
N5	0.038 (7)	0.039 (6)	0.020 (4)	−0.001 (6)	−0.001 (5)	−0.002 (4)
N6	0.032 (7)	0.039 (7)	0.025 (4)	−0.001 (6)	−0.006 (5)	0.008 (5)
C11	0.022 (6)	0.036 (8)	0.024 (5)	−0.014 (7)	−0.003 (5)	−0.001 (5)
C12	0.028 (7)	0.030 (7)	0.030 (5)	−0.003 (7)	0.000 (5)	0.006 (5)
C13	0.030 (7)	0.024 (6)	0.033 (6)	−0.002 (7)	0.000 (5)	0.003 (5)
C14	0.024 (7)	0.028 (7)	0.037 (6)	−0.012 (7)	0.004 (5)	0.001 (5)
C15	0.037 (8)	0.039 (8)	0.018 (5)	−0.005 (7)	0.002 (5)	0.004 (5)
C16	0.029 (7)	0.026 (6)	0.025 (5)	−0.005 (7)	0.001 (5)	0.008 (5)
C17	0.026 (7)	0.021 (6)	0.030 (5)	−0.010 (6)	0.005 (5)	−0.007 (5)
C18	0.044 (9)	0.028 (7)	0.033 (6)	−0.003 (7)	0.004 (6)	−0.005 (5)
C19	0.050 (10)	0.034 (8)	0.048 (7)	0.002 (8)	0.002 (7)	−0.006 (6)
C20	0.053 (10)	0.041 (8)	0.055 (8)	0.005 (10)	−0.018 (8)	−0.014 (7)

Geometric parameters (Å, º)

Br1—C1	1.872 (12)	Br2—C11	1.854 (12)
O1—N3	1.244 (15)	O3—N6	1.216 (14)
O2—N3	1.195 (15)	O4—N6	1.217 (14)
N1—N2	1.352 (13)	N4—N5	1.344 (14)
N1—C7	1.376 (14)	N4—C17	1.364 (15)
N1—C8	1.472 (16)	N4—C18	1.456 (17)
N2—C1	1.307 (16)	N5—C11	1.339 (17)
N3—C5	1.451 (15)	N6—C15	1.480 (13)
C1—C2	1.406 (17)	C11—C12	1.432 (15)
C2—C3	1.391 (18)	C12—C13	1.402 (17)
C2—C7	1.413 (17)	C12—C17	1.407 (18)
C3—C4	1.342 (16)	C13—C14	1.345 (16)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.424 (17)	C14—C15	1.418 (19)
C4—H4	0.9500	C14—H14	0.9500
C5—C6	1.383 (17)	C15—C16	1.352 (18)
C6—C7	1.420 (15)	C16—C17	1.399 (16)
C6—H6	0.9500	C16—H16	0.9500
C8—C9	1.448 (19)	C18—C19	1.44 (2)
C8—H8A	0.9900	C18—H18A	0.9900
C8—H8B	0.9900	C18—H18B	0.9900
C9—C10	1.285 (18)	C19—C20	1.304 (19)
C9—H9	0.9500	C19—H19	0.9500
C10—H10A	0.9500	C20—H20A	0.9500
C10—H10B	0.9500	C20—H20B	0.9500
N2—N1—C7	111.3 (10)	N5—N4—C17	111.0 (10)
N2—N1—C8	120.0 (9)	N5—N4—C18	119.7 (9)
C7—N1—C8	127.8 (10)	C17—N4—C18	129.1 (10)
C1—N2—N1	105.6 (9)	C11—N5—N4	106.8 (9)
O2—N3—O1	123.9 (11)	O3—N6—O4	122.8 (10)
O2—N3—C5	118.3 (11)	O3—N6—C15	119.0 (11)
O1—N3—C5	117.9 (11)	O4—N6—C15	118.2 (11)
N2—C1—C2	113.6 (11)	N5—C11—C12	111.1 (11)
N2—C1—Br1	120.6 (9)	N5—C11—Br2	121.8 (8)
C2—C1—Br1	125.8 (10)	C12—C11—Br2	127.1 (10)
C3—C2—C1	138.1 (12)	C13—C12—C17	121.7 (10)
C3—C2—C7	119.1 (11)	C13—C12—C11	135.4 (12)
C1—C2—C7	102.9 (11)	C17—C12—C11	102.9 (11)
C4—C3—C2	120.8 (12)	C14—C13—C12	117.6 (12)
C4—C3—H3	119.6	C14—C13—H13	121.2
C2—C3—H3	119.6	C12—C13—H13	121.2
C3—C4—C5	119.5 (11)	C13—C14—C15	119.9 (12)
C3—C4—H4	120.3	C13—C14—H14	120.0
C5—C4—H4	120.3	C15—C14—H14	120.0
C6—C5—C4	123.7 (11)	C16—C15—C14	124.4 (10)

C6—C5—N3	117.8 (11)	C16—C15—N6	118.0 (12)
C4—C5—N3	118.6 (11)	C14—C15—N6	117.6 (11)
C5—C6—C7	114.6 (11)	C15—C16—C17	115.8 (12)
C5—C6—H6	122.7	C15—C16—H16	122.1
C7—C6—H6	122.7	C17—C16—H16	122.1
N1—C7—C2	106.5 (10)	N4—C17—C16	131.4 (12)
N1—C7—C6	131.0 (11)	N4—C17—C12	108.1 (10)
C2—C7—C6	122.5 (11)	C16—C17—C12	120.5 (11)
C9—C8—N1	113.6 (12)	C19—C18—N4	114.3 (12)
C9—C8—H8A	108.8	C19—C18—H18A	108.7
N1—C8—H8A	108.8	N4—C18—H18A	108.7
C9—C8—H8B	108.8	C19—C18—H18B	108.7
N1—C8—H8B	108.8	N4—C18—H18B	108.7
H8A—C8—H8B	107.7	H18A—C18—H18B	107.6
C10—C9—C8	125.5 (13)	C20—C19—C18	123.5 (16)
C10—C9—H9	117.2	C20—C19—H19	118.3
C8—C9—H9	117.2	C18—C19—H19	118.3
C9—C10—H10A	120.0	C19—C20—H20A	120.0
C9—C10—H10B	120.0	C19—C20—H20B	120.0
H10A—C10—H10B	120.0	H20A—C20—H20B	120.0

C7—N1—N2—C1	1.8 (14)	C17—N4—N5—C11	−0.1 (15)
C8—N1—N2—C1	171.7 (12)	C18—N4—N5—C11	−175.7 (12)
N1—N2—C1—C2	0.3 (15)	N4—N5—C11—C12	−0.4 (15)
N1—N2—C1—Br1	−179.8 (9)	N4—N5—C11—Br2	177.7 (9)
N2—C1—C2—C3	179.7 (15)	N5—C11—C12—C13	−178.5 (15)
Br1—C1—C2—C3	0 (3)	Br2—C11—C12—C13	3 (2)
N2—C1—C2—C7	−2.0 (16)	N5—C11—C12—C17	0.7 (15)
Br1—C1—C2—C7	178.0 (10)	Br2—C11—C12—C17	−177.3 (10)
C1—C2—C3—C4	179.1 (16)	C17—C12—C13—C14	2 (2)
C7—C2—C3—C4	1.1 (19)	C11—C12—C13—C14	−178.6 (14)
C2—C3—C4—C5	0 (2)	C12—C13—C14—C15	−1 (2)
C3—C4—C5—C6	1 (2)	C13—C14—C15—C16	−1 (2)
C3—C4—C5—N3	−179.5 (12)	C13—C14—C15—N6	179.5 (12)
O2—N3—C5—C6	−173.3 (12)	O3—N6—C15—C16	−0.3 (18)
O1—N3—C5—C6	6.5 (17)	O4—N6—C15—C16	−180.0 (13)
O2—N3—C5—C4	6.8 (18)	O3—N6—C15—C14	179.4 (12)
O1—N3—C5—C4	−173.4 (12)	O4—N6—C15—C14	−0.2 (18)
C4—C5—C6—C7	−1.2 (18)	C14—C15—C16—C17	2 (2)
N3—C5—C6—C7	178.9 (10)	N6—C15—C16—C17	−178.6 (11)
N2—N1—C7—C2	−3.0 (13)	N5—N4—C17—C16	−179.5 (14)
C8—N1—C7—C2	−172.0 (12)	C18—N4—C17—C16	−4 (2)
N2—N1—C7—C6	−179.2 (12)	N5—N4—C17—C12	0.6 (15)
C8—N1—C7—C6	12 (2)	C18—N4—C17—C12	175.6 (13)
C3—C2—C7—N1	−178.4 (11)	C15—C16—C17—N4	179.5 (13)
C1—C2—C7—N1	2.9 (13)	C15—C16—C17—C12	−1 (2)
C3—C2—C7—C6	−1.8 (18)	C13—C12—C17—N4	178.6 (12)
C1—C2—C7—C6	179.5 (12)	C11—C12—C17—N4	−0.8 (14)

C5—C6—C7—N1	177.5 (12)	C13—C12—C17—C16	−1 (2)
C5—C6—C7—C2	1.8 (17)	C11—C12—C17—C16	179.3 (13)
N2—N1—C8—C9	−77.9 (15)	N5—N4—C18—C19	−71.9 (15)
C7—N1—C8—C9	90.1 (14)	C17—N4—C18—C19	113.4 (15)
N1—C8—C9—C10	−125.4 (16)	N4—C18—C19—C20	116.0 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1^{i}	0.95	2.46	3.304 (16)	147
C18—H18*B*···O4^{ii}	0.99	2.59	3.578 (16)	174
C9—H9···Br1^{iii}	0.95	3.09	3.814 (11)	134
C18—H18*A*···Br1^{iv}	0.99	2.91	3.770 (14)	146

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