Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

7-(4-Bromophenyl)-9-phenyl-7*H*-pyrrolo[3,2-e]tetrazolo[1,5-c]pyrimidine

Mukesh M. Jotani,[a] Rina D. Shah,[b] Jerry P. Jasinski[c]* and Ray J. Butcher[d]

[a]Department of Physics, Bhavan's Sheth R.A. College of Science, Ahmedabad, Gujarat, 380 001, India, [b]Department of Chemistry, M.G. Science Institute, Navrangpura, Navrangpura, Ahmedabad, Gujarat, 380 009, India, [c]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, and [d]Department of Chemistry, Howard University, 525 College Street NW, Washington DC 20059, USA
Correspondence e-mail: jjasinski@keene.edu

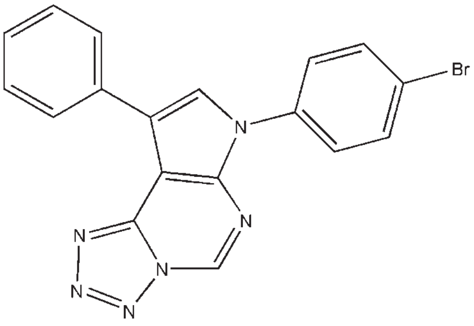
Received 2 February 2010; accepted 3 February 2010

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.090; data-to-parameter ratio = 22.2.

In the title compound, $C_{18}H_{11}BrN_6$, the phenyl ring is almost coplanar [dihedral angle 7.2 (1)°] with the planar (r.m.s. deviation 0.039 Å) tricyclic ring system while the 4-bromophenyl ring makes a dihedral angle of 33.98 (6)° with the ring system. Weak intermolecular C—H⋯N and C—H⋯Br hydrogen-bonding interactions and π–π stacking [centroid–centroid distances = 3.7971 (17) and 3.5599 (16) Å] stabilize the crystal packing. A comparison of the structure to a MOPAC PM3 geometry optimization calculation *in vacuo* supports these observations.

Related literature

For anticancer relationships, see: Hiedo & Yasuo (1960, 1961). For the synthesis of derivative compounds, see: Dave & Shukla (1997); Dave & Shah (1998). For graph-set motifs, see: Bernstein *et al.* (1995). For MOPAC PM3 calculations, see: Schmidt & Polik (2007).



Experimental

Crystal data

$C_{18}H_{11}BrN_6$
M_r = 391.24
Monoclinic, $P2_1/c$
a = 12.0173 (5) Å
b = 17.4007 (7) Å
c = 7.4201 (4) Å
β = 91.004 (4)°
V = 1551.37 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.66 mm^{-1}
T = 200 K
0.47 × 0.39 × 0.22 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.494, T_{max} = 1.000
13458 measured reflections
5032 independent reflections
2606 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.090
S = 1.14
5032 reflections
227 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C8—H8⋯N4^{i}	0.95	2.54	3.421 (3)	154
C4—H4⋯N5^{i}	0.95	2.60	3.532 (3)	166
C5—H5⋯Br^{ii}	0.95	2.87	3.667 (3)	142

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

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*.

RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase an X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5188).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Dave, C. G. & Shah, R. D. (1998). *J. Heterocycl. Chem.* **35**, 1295–1300.
Dave, C. G. & Shukla, M. C. (1997). *J. Heterocycl. Chem.* **34**, 1805–1808.
Hiedo, K. & Yasuo, M. (1960). Japan Patent 17,236.
Hiedo, K. & Yasuo, M. (1961). *Chem. Abstr.* **55**, 17664.
Oxford Diffraction (2007). *CrysAlis PRO* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
Schmidt, J. R. & Polik, W. F. (2007). *WebMO Pro*. WebMO, LLC: Holland, MI, USA, available from http://www.webmo.net.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, o574   [doi:10.1107/S1600536810004368]

7-(4-Bromophenyl)-9-phenyl-7*H*-pyrrolo[3,2-*e*]tetrazolo[1,5-*c*]pyrimidine

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S1. Comment

Fused tetrazoles are known to be related to a variety of biological activities including anticancer relationships (Hiedo & Yasuo, 1960, 1961). Moreover their reductive ring cleavage ability may result in the formation of synthetically important 4-aminopyrimidine derivatives which are building blocks for the construction of ring systems such as pyrimidine and imidazole (Dave & Shukla, 1997). Furthermore, nucleophilic substitution with NaN_3 results in either the formation of an azido group or tetrazole ring. An example of these reactions has been the synthesis of (7-Bromophenyl)-9-phenyl 7*H*-[1,2,3,4]tetrazolo[1,5-c]pyrrolo[3,2-e] pyrimidine by two different routes, either from 4-chloro-5-phenyl-(7-Bromophenyl)-7*H*-pyrrolo[2,3-d]pyrimidine or from 4-hydrazino-5-phenyl-(7-Bromophenyl)-7*H*-pyrrolo[2,3-d]pyrimidine (Dave & Shah, 1998) and then reduced to 4-amino-5-phenyl-(7-Bromophenyl)-7*H*-pyrrolo[2,3-d]pyrimidine. In view of the importance of these findings, we report the crystal structure of the title compound, $C_{18}H_{11}BrN_6$, (I).

The title compond, (I), contains a pyrrole ring with successively fused pyrimidine and tetrazole rings, together with bromophenyl and benzene rings bonded at the N1 and C3 positions in a nearly planar fashion (Fig. 1). The nearly planar conformation of the pyrimidine ring is significant in that it is often found to be puckered which may be affected by the tetrazole and pyrrole ring fusion here. The least squares planes of the pyrimidine and tetrazole rings are oriented at the angles of 2.62 (15)° and 3.15 (15)° with the best plane of the pyrrole ring, respectively. The ortho-substituted 4-bromophenyl ring is twisted considerably, whereas the benzene ring at C3 is almost co-planar with the mean plane of the pyrrole ring, each having dihedral angles of 32.62 (15)° and 9.97 (16)°, respectively.

The crystal sructure is supported by weak C—H···Br and C—H···N intermolecular and weak C—H···N intramolecular interactions which link the molecules into chains along the [011] (Fig. 2, Table 1). An R22(8) graph-set motif (Bernstein *et al.*, 1995) is established between the pyrrole, tetrazole and benzene rings resulting from these intermolecular interactions.

Crystal packing is also supported by two π-π stacking interactions (Fig. 3). One is between the centroids of two pyrrole rings [Cg2—Cg2; 3.7971 (17) Å; slippage = 1.318 Å; 1-x, 1-y, -z; Cg2 = N6/C3/C6/C5/C4]. The second is between the centroids of a pyrimidine (Cg3) and benzene (Cg4) ring [Cg3—Cg4: 3.5599 (16) Å; 1-x, 1-y, 1-z; Cg3 = N4/C1/C6/C3/N5/C2; Cg4 = C7—C12].

After a geometry optimized MOPAC PM3 computational calculation (Schmidt & Polik 2007) on (I), in vacuo, the angle between the mean planes of the pyrimidine, tetrazole and benzene groups become planar with the pyrrole ring in the local minimized structure. The dihedral angle between the ortho-substituted 4-bromophenyl ring and three planar tri-ring group becomes 42.28°. The separation of the H4A···H8A (2.111 Å) and H4A···H14A (2.301 Å) atoms between the pyrrole ring and the 4-bromophenyl and 9-phenyl rings before the calculations changed to 1.954 Å and 2.496 Å, respectively, after the calculation showing how the crystal packing effects significantly determine the twist of the 4-bromophenyl ring, in particular. In addition, the C3–C7 and N1–C13 bond lengths changed from 1.479 (3) Å and 1.430 (3) Å to 1.442 Å and 1.455 Å, respectively. It is clear that hydrogen bonding interactions and π-π stacking interactions significantly influence the twist angles for the molecule in this crystal.

S2. Experimental

The synthesis of (I) was carried out by two separate routes. Route 1: To a mixture of NaN_3 (0.011 m), NH_4Cl (0.011 m) and DMSO (20 ml) was added 4-chloro-5-phenyl-(7-bromophenyl)-7*H*-pyrrolo[2,3-d]pyrimidine (0.001 m) in portions and stirred for 2 hrs at 363 K to give the title compound. Route 2: 4-hydrazino-5-phenyl-(7-bromophenyl)-7*H*-pyrrolo-[2,3-d]pyrimidine (0.01 m) was diazotized with an aqueous solution of $NaNO_2$ (20% w/v, 4.2 ml) and glacial acetic acid (40 ml) at 273-278 K under stirring conditions for 2 hrs to give the title compound. Colorless, plate-like crystals of (I) were grown by slow evaporation from 1,4-dioxane solution.

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.95 Å, and with $U_{iso}(H) = 1.18\text{-}1.21U_{eq}(C)$.

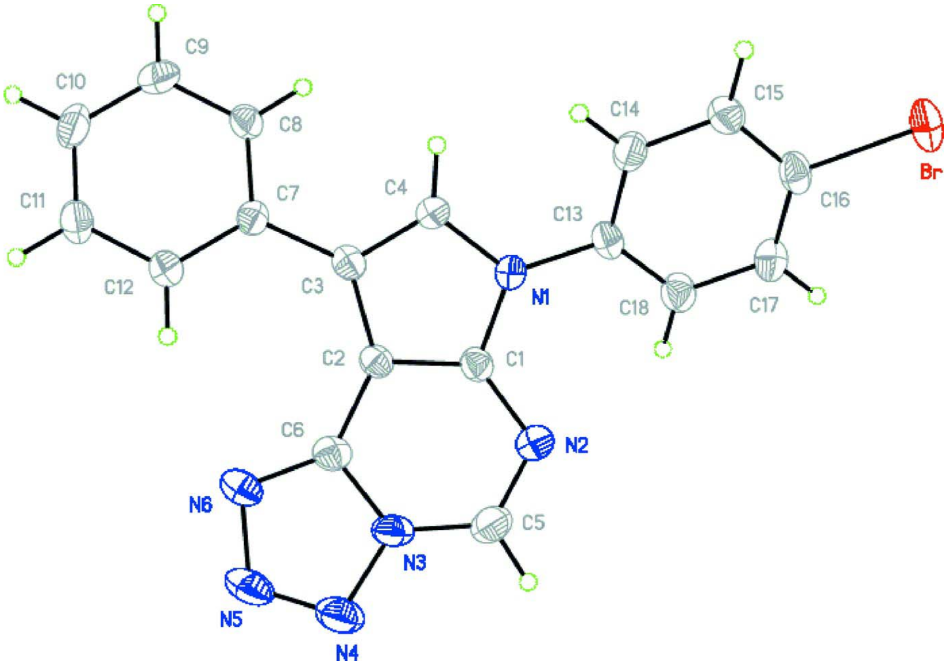

Figure 1

Molecular structure of $C_{18}H_{11}BrN_6$, (I), showing the atom labeling scheme and 50% probability displacement ellipsoids.

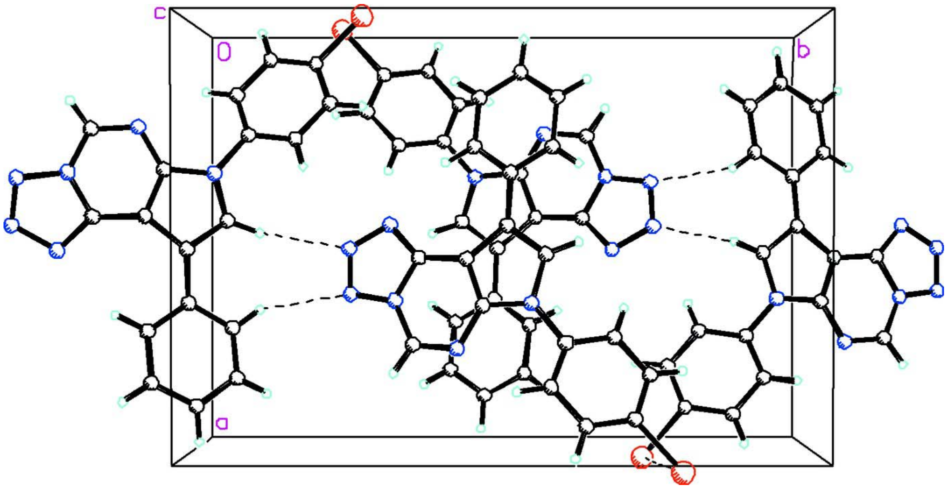

Figure 2

The molecular packing for (I) viewed down the *c* axis. Dashed lines indicate weak C—H···N intermolecular hydrogen bond interactions which link the molecule into chains propagating along the [011].

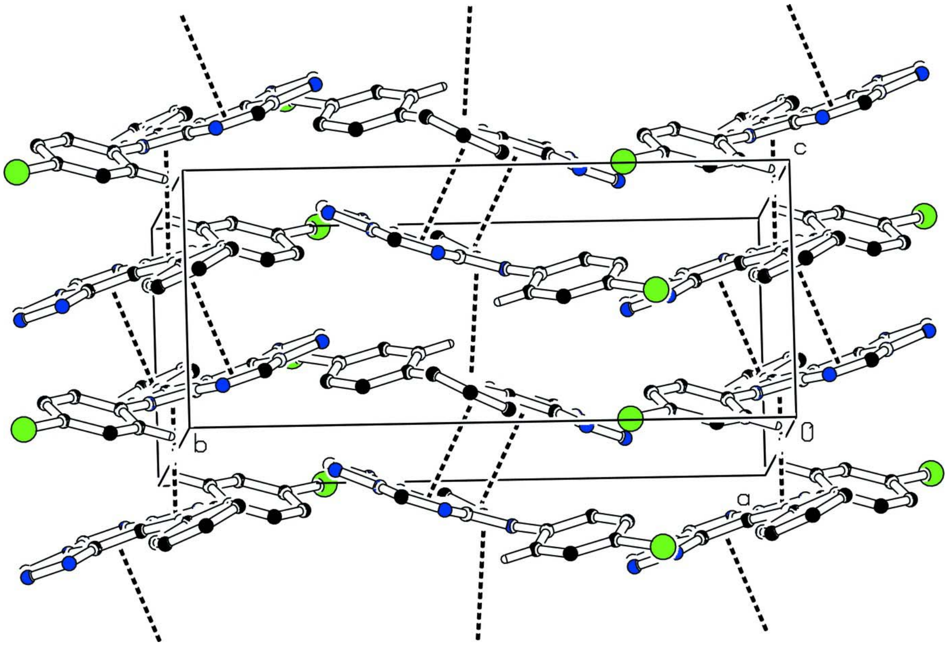

Figure 3

The molecular packing of (I), showing π—π stacking interactions along the *c* axis and forming a chain of molecules along [1 1 0].

7-(4-Bromophenyl)-9-phenyl-7*H*-pyrrolo[3,2-*e*]tetrazolo[1,5-*c*]pyrimidine

Crystal data

$C_{18}H_{11}BrN_6$	b = 17.4007 (7) Å
M_r = 391.24	c = 7.4201 (4) Å
Monoclinic, $P2_1/c$	β = 91.004 (4)°
Hall symbol: -P 2ybc	V = 1551.37 (12) Å^3
a = 12.0173 (5) Å	Z = 4

$F(000) = 784$	$\mu = 2.66\ \text{mm}^{-1}$
$D_x = 1.675$ Mg m^{-3}	$T = 200$ K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å	Plate, colorless
Cell parameters from 4168 reflections	0.47 × 0.39 × 0.22 mm
$\theta = 4.8–32.4°$	

Data collection

Oxford Diffraction Gemini diffractometer	13458 measured reflections
Radiation source: fine-focus sealed tube	5032 independent reflections
Graphite monochromator	2606 reflections with $I > 2\sigma(I)$
Detector resolution: 10.5081 pixels mm^{-1}	$R_{\text{int}} = 0.050$
φ and ω scans	$\theta_{\text{max}} = 32.5°$, $\theta_{\text{min}} = 4.8°$
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)	$h = -16 \rightarrow 18$
$T_{\text{min}} = 0.494$, $T_{\text{max}} = 1.000$	$k = -25 \rightarrow 26$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.090$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.14$	$\Delta\rho_{\text{max}} = 0.72$ e Å^{-3}
5032 reflections	$\Delta\rho_{\text{min}} = -0.71$ e Å^{-3}
227 parameters	Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
0 restraints	Extinction coefficient: 0.0033 (4)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Experimental. (CrysAlis RED; Oxford Diffraction, 2007)

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 $F^2 > \sigma(F^2)$ 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 (Å^2)

	x	y	z	$U_{\text{iso}}*/U_{\text{eq}}$
Br	−0.01667 (2)	0.226033 (17)	0.00063 (4)	0.03758 (11)
N1	0.35315 (14)	0.45391 (11)	0.1749 (3)	0.0245 (5)
N2	0.24838 (15)	0.57000 (12)	0.2186 (3)	0.0300 (5)
N3	0.35441 (16)	0.67017 (11)	0.3359 (3)	0.0292 (5)
N4	0.3685 (2)	0.74165 (13)	0.4080 (3)	0.0406 (6)
N5	0.4737 (2)	0.74487 (13)	0.4525 (4)	0.0432 (7)
N6	0.52928 (17)	0.67915 (12)	0.4136 (3)	0.0359 (6)
C1	0.34572 (18)	0.52985 (14)	0.2224 (3)	0.0235 (5)

C2	0.45169 (18)	0.55548 (13)	0.2756 (3)	0.0219 (5)
C3	0.52682 (19)	0.49222 (13)	0.2569 (3)	0.0230 (5)
C4	0.46260 (17)	0.43241 (14)	0.1955 (4)	0.0245 (6)
H4	0.4902	0.3825	0.1703	0.029*
C5	0.2555 (2)	0.63991 (16)	0.2741 (4)	0.0338 (7)
H5	0.1908	0.6713	0.2722	0.041*
C6	0.45368 (19)	0.63216 (14)	0.3404 (4)	0.0263 (6)
C7	0.64817 (18)	0.48691 (13)	0.2913 (3)	0.0225 (5)
C8	0.70547 (19)	0.42147 (14)	0.2367 (4)	0.0277 (6)
H8	0.6659	0.3814	0.1769	0.033*
C9	0.8188 (2)	0.41373 (15)	0.2680 (4)	0.0344 (7)
H9	0.8560	0.3687	0.2289	0.041*
C10	0.8778 (2)	0.47079 (17)	0.3551 (4)	0.0351 (7)
H10	0.9556	0.4654	0.3767	0.042*
C11	0.82296 (19)	0.53569 (16)	0.4107 (4)	0.0344 (7)
H11	0.8634	0.5752	0.4713	0.041*
C12	0.70894 (18)	0.54451 (14)	0.3794 (4)	0.0283 (6)
H12	0.6725	0.5899	0.4181	0.034*
C13	0.26457 (18)	0.40147 (14)	0.1343 (3)	0.0238 (6)
C14	0.16953 (19)	0.42519 (15)	0.0414 (4)	0.0301 (6)
H14	0.1623	0.4771	0.0035	0.036*
C15	0.08552 (19)	0.37323 (16)	0.0039 (4)	0.0308 (6)
H15	0.0195	0.3894	−0.0574	0.037*
C16	0.09811 (19)	0.29777 (15)	0.0561 (4)	0.0282 (6)
C17	0.19254 (19)	0.27285 (15)	0.1480 (4)	0.0294 (6)
H17	0.2005	0.2205	0.1822	0.035*
C18	0.27530 (18)	0.32577 (15)	0.1893 (4)	0.0293 (6)
H18	0.3397	0.3100	0.2556	0.035*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.03221 (15)	0.04452 (19)	0.03605 (18)	−0.01798 (12)	0.00207 (11)	−0.00499 (15)
N1	0.0192 (9)	0.0240 (11)	0.0302 (13)	−0.0015 (8)	−0.0006 (9)	−0.0010 (10)
N2	0.0265 (11)	0.0277 (12)	0.0361 (15)	0.0033 (9)	0.0021 (10)	−0.0018 (11)
N3	0.0332 (11)	0.0193 (11)	0.0354 (14)	0.0034 (9)	0.0050 (10)	−0.0002 (10)
N4	0.0478 (14)	0.0232 (13)	0.0509 (17)	0.0014 (10)	0.0049 (12)	−0.0054 (12)
N5	0.0527 (15)	0.0195 (12)	0.057 (2)	−0.0027 (10)	0.0016 (13)	−0.0071 (12)
N6	0.0398 (12)	0.0205 (12)	0.0473 (16)	−0.0030 (9)	−0.0007 (11)	−0.0038 (11)
C1	0.0236 (11)	0.0220 (12)	0.0250 (15)	−0.0031 (10)	0.0021 (10)	−0.0002 (11)
C2	0.0249 (12)	0.0186 (12)	0.0222 (15)	−0.0019 (9)	0.0009 (10)	0.0026 (11)
C3	0.0279 (13)	0.0211 (13)	0.0199 (13)	−0.0029 (9)	−0.0028 (10)	0.0028 (11)
C4	0.0215 (11)	0.0226 (13)	0.0295 (16)	0.0015 (9)	0.0001 (10)	−0.0001 (12)
C5	0.0281 (13)	0.0334 (16)	0.0399 (18)	0.0067 (11)	0.0029 (12)	−0.0003 (14)
C6	0.0299 (13)	0.0198 (13)	0.0294 (16)	−0.0005 (10)	0.0044 (11)	0.0061 (12)
C7	0.0206 (12)	0.0232 (13)	0.0237 (14)	−0.0020 (9)	−0.0001 (10)	0.0048 (11)
C8	0.0274 (12)	0.0210 (13)	0.0343 (17)	−0.0041 (10)	−0.0050 (11)	0.0037 (12)
C9	0.0342 (14)	0.0269 (15)	0.0418 (19)	0.0075 (11)	−0.0035 (13)	0.0054 (13)

C10	0.0237 (13)	0.0426 (16)	0.0388 (19)	0.0004 (12)	−0.0085 (12)	0.0022 (14)
C11	0.0291 (13)	0.0352 (15)	0.0387 (19)	−0.0065 (12)	−0.0077 (12)	−0.0027 (14)
C12	0.0261 (12)	0.0242 (14)	0.0346 (17)	−0.0022 (10)	−0.0022 (11)	−0.0011 (12)
C13	0.0243 (12)	0.0256 (13)	0.0216 (15)	−0.0063 (10)	0.0034 (10)	−0.0033 (11)
C14	0.0275 (12)	0.0294 (14)	0.0334 (17)	−0.0039 (10)	0.0003 (12)	0.0052 (13)
C15	0.0251 (13)	0.0369 (16)	0.0304 (16)	−0.0043 (11)	−0.0025 (11)	0.0022 (13)
C16	0.0255 (12)	0.0331 (15)	0.0263 (16)	−0.0093 (10)	0.0075 (11)	−0.0060 (12)
C17	0.0291 (13)	0.0252 (13)	0.0341 (16)	−0.0027 (11)	0.0036 (11)	0.0019 (13)
C18	0.0213 (12)	0.0313 (15)	0.0352 (17)	−0.0008 (10)	−0.0010 (11)	0.0036 (13)

Geometric parameters (Å, º)

Br—C16	1.900 (2)	C7—C12	1.396 (3)
N1—C1	1.371 (3)	C8—C9	1.383 (3)
N1—C4	1.373 (3)	C8—H8	0.9500
N1—C13	1.430 (3)	C9—C10	1.375 (4)
N2—C5	1.287 (3)	C9—H9	0.9500
N2—C1	1.362 (3)	C10—C11	1.374 (4)
N3—N4	1.363 (3)	C10—H10	0.9500
N3—C6	1.364 (3)	C11—C12	1.394 (3)
N3—C5	1.371 (3)	C11—H11	0.9500
N4—N5	1.301 (3)	C12—H12	0.9500
N5—N6	1.358 (3)	C13—C18	1.384 (3)
N6—C6	1.331 (3)	C13—C14	1.387 (3)
C1—C2	1.400 (3)	C14—C15	1.380 (3)
C2—C6	1.418 (3)	C14—H14	0.9500
C2—C3	1.432 (3)	C15—C16	1.377 (4)
C3—C4	1.369 (3)	C15—H15	0.9500
C3—C7	1.479 (3)	C16—C17	1.383 (3)
C4—H4	0.9500	C17—C18	1.386 (3)
C5—H5	0.9500	C17—H17	0.9500
C7—C8	1.394 (3)	C18—H18	0.9500

C1—N1—C4	107.48 (18)	C9—C8—H8	119.3
C1—N1—C13	128.14 (18)	C7—C8—H8	119.3
C4—N1—C13	123.9 (2)	C10—C9—C8	120.4 (2)
C5—N2—C1	115.2 (2)	C10—C9—H9	119.8
N4—N3—C6	109.3 (2)	C8—C9—H9	119.8
N4—N3—C5	125.7 (2)	C11—C10—C9	119.2 (2)
C6—N3—C5	125.1 (2)	C11—C10—H10	120.4
N5—N4—N3	104.6 (2)	C9—C10—H10	120.4
N4—N5—N6	112.9 (2)	C10—C11—C12	121.0 (2)
C6—N6—N5	105.6 (2)	C10—C11—H11	119.5
N2—C1—N1	123.28 (19)	C12—C11—H11	119.5
N2—C1—C2	128.2 (2)	C11—C12—C7	120.2 (2)
N1—C1—C2	108.47 (19)	C11—C12—H12	119.9
C1—C2—C6	113.9 (2)	C7—C12—H12	119.9
C1—C2—C3	107.4 (2)	C18—C13—C14	120.1 (2)

C6—C2—C3	138.5 (2)	C18—C13—N1	118.7 (2)
C4—C3—C2	105.3 (2)	C14—C13—N1	121.2 (2)
C4—C3—C7	123.9 (2)	C15—C14—C13	119.9 (2)
C2—C3—C7	130.7 (2)	C15—C14—H14	120.1
C3—C4—N1	111.3 (2)	C13—C14—H14	120.1
C3—C4—H4	124.3	C14—C15—C16	119.5 (2)
N1—C4—H4	124.3	C14—C15—H15	120.3
N2—C5—N3	121.5 (2)	C16—C15—H15	120.3
N2—C5—H5	119.2	C15—C16—C17	121.5 (2)
N3—C5—H5	119.2	C15—C16—Br	119.33 (19)
N6—C6—N3	107.6 (2)	C17—C16—Br	119.1 (2)
N6—C6—C2	136.3 (2)	C16—C17—C18	118.7 (2)
N3—C6—C2	116.0 (2)	C16—C17—H17	120.7
C8—C7—C12	117.7 (2)	C18—C17—H17	120.7
C8—C7—C3	119.4 (2)	C17—C18—C13	120.3 (2)
C12—C7—C3	122.8 (2)	C17—C18—H18	119.9
C9—C8—C7	121.4 (2)	C13—C18—H18	119.9

C6—N3—N4—N5	0.2 (3)	C1—C2—C6—N6	175.2 (3)
C5—N3—N4—N5	178.1 (3)	C3—C2—C6—N6	0.1 (6)
N3—N4—N5—N6	−0.1 (3)	C1—C2—C6—N3	−2.1 (3)
N4—N5—N6—C6	−0.1 (3)	C3—C2—C6—N3	−177.2 (3)
C5—N2—C1—N1	177.5 (2)	C4—C3—C7—C8	9.1 (4)
C5—N2—C1—C2	−1.3 (4)	C2—C3—C7—C8	−170.4 (3)
C4—N1—C1—N2	−179.8 (2)	C4—C3—C7—C12	−169.9 (3)
C13—N1—C1—N2	−7.7 (4)	C2—C3—C7—C12	10.6 (4)
C4—N1—C1—C2	−0.8 (3)	C12—C7—C8—C9	−0.2 (4)
C13—N1—C1—C2	171.3 (2)	C3—C7—C8—C9	−179.3 (2)
N2—C1—C2—C6	3.1 (4)	C7—C8—C9—C10	0.3 (4)
N1—C1—C2—C6	−175.8 (2)	C8—C9—C10—C11	−0.1 (4)
N2—C1—C2—C3	179.7 (2)	C9—C10—C11—C12	−0.2 (4)
N1—C1—C2—C3	0.8 (3)	C10—C11—C12—C7	0.3 (4)
C1—C2—C3—C4	−0.5 (3)	C8—C7—C12—C11	−0.1 (4)
C6—C2—C3—C4	174.9 (3)	C3—C7—C12—C11	178.9 (2)
C1—C2—C3—C7	179.1 (2)	C1—N1—C13—C18	−143.0 (3)
C6—C2—C3—C7	−5.6 (5)	C4—N1—C13—C18	27.9 (4)
C2—C3—C4—N1	0.0 (3)	C1—N1—C13—C14	37.2 (4)
C7—C3—C4—N1	−179.6 (2)	C4—N1—C13—C14	−151.9 (2)
C1—N1—C4—C3	0.5 (3)	C18—C13—C14—C15	0.1 (4)
C13—N1—C4—C3	−172.0 (2)	N1—C13—C14—C15	179.9 (2)
C1—N2—C5—N3	−1.4 (4)	C13—C14—C15—C16	−1.4 (4)
N4—N3—C5—N2	−175.5 (3)	C14—C15—C16—C17	1.0 (4)
C6—N3—C5—N2	2.1 (4)	C14—C15—C16—Br	−178.9 (2)
N5—N6—C6—N3	0.2 (3)	C15—C16—C17—C18	0.7 (4)
N5—N6—C6—C2	−177.2 (3)	Br—C16—C17—C18	−179.4 (2)
N4—N3—C6—N6	−0.3 (3)	C16—C17—C18—C13	−2.0 (4)
C5—N3—C6—N6	−178.2 (2)	C14—C13—C18—C17	1.6 (4)
N4—N3—C6—C2	177.8 (2)	N1—C13—C18—C17	−178.2 (2)

C5—N3—C6—C2	−0.1 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···N4^{i}	0.95	2.54	3.421 (3)	154
C4—H4···N5^{i}	0.95	2.60	3.532 (3)	166
C5—H5···Br^{ii}	0.95	2.87	3.667 (3)	142

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