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6-Bromo-2-(4-chlorophenyl)-3-[(1-octyl-1*H*-1,2,3-triazol-4-yl)methyl]-3*H*-imidazo[4,5-*b*]pyridine

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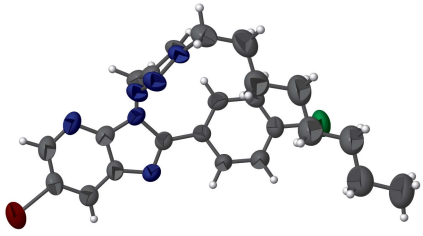
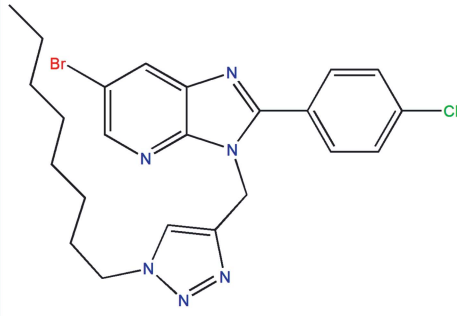
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{23}H_{26}BrClN_6$, the imidazo[4,5-*b*]pyridine ring system (r.m.s. deviation = 0.012 Å) is inclined at angles of 19.37 (12) and 89.27 (13)° to the phenyl and triazole rings, respectively, while the phenyl and triazole rings subtend a dihedral angle of 71.23 (15)°. In the crystal, the molecules are linked by C—H···N_I and bifurcated C—H···(N_T,N_T) (I = imidazo[4,5-*b*]pyridine and T = triazole) hydrogen bonds into a double-column structure propagating along the *b*-axis direction.

3D view



Chemical scheme



Structure description

Some imidazopyridine derivatives have a significant inhibitory effect on target enzymes (Palmer *et al.*, 2007; Katritzky *et al.*, 2003). The most popular synthetic approach to these compounds involves the cyclo-condensation of 2,3-pyridinediamine with carboxylic acid derivatives or with aldehydes (Dubey *et al.*, 2004). On the other hand, there is increasing interest in the design of new synthetic routes such as an eco-friendly synthesis by oxidation in aqueous medium (Kale *et al.*, 2009). As a continuation of our studies in this area (Bourichi *et al.*, 2016), we now report the synthesis and structure of the title compound (Fig. 1).

The imidazo[4,5-*b*]pyridine unit is planar to within 0.026 (5) Å (for atom C7), and the r.m.s. deviation of the fitted atoms is 0.012 Å. It is inclined by 19.37 (12) and 89.27 (13)° to the phenyl and triazole rings, respectively, while phenyl and triazole rings are oriented at a dihedral angle of 71.23 (15)°. Atoms Br1, Cl1 and C13 and C16 are displaced by

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···N4^{i}	0.93	2.60	3.452 (6)	153
C15—H15···N5^{i}	0.93	2.38	3.293 (6)	168
C16—H16B···N3^{ii}	0.97	2.53	3.444 (6)	157

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

−0.037 (1), 0.024 (2), −0.017 (4) and 0.031 (5) Å, respectively, away from their attached rings.

In the crystal, the molecules are linked *via* C—H···N hydrogen bonds (Table 1), enclosing $R_3^3(20)$, $R_3^3(21)$ and $R_3^3(22)$ ring motifs (Figs. 2 and 3) as part of a double-column structure (Fig. 2) running along the *b*-axis direction (Fig. 3). The Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing

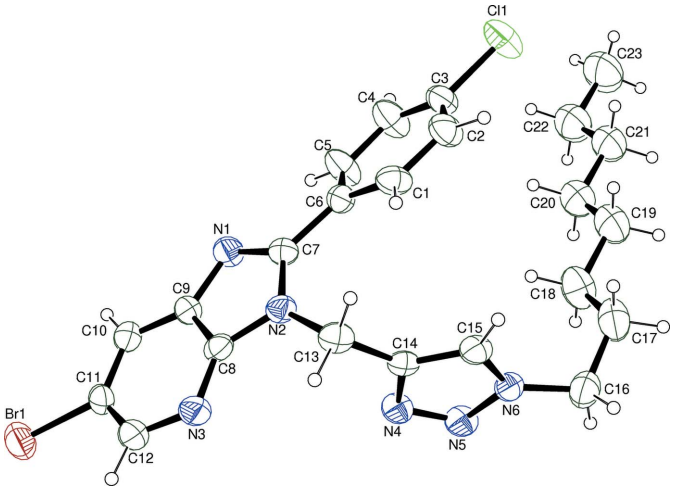


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

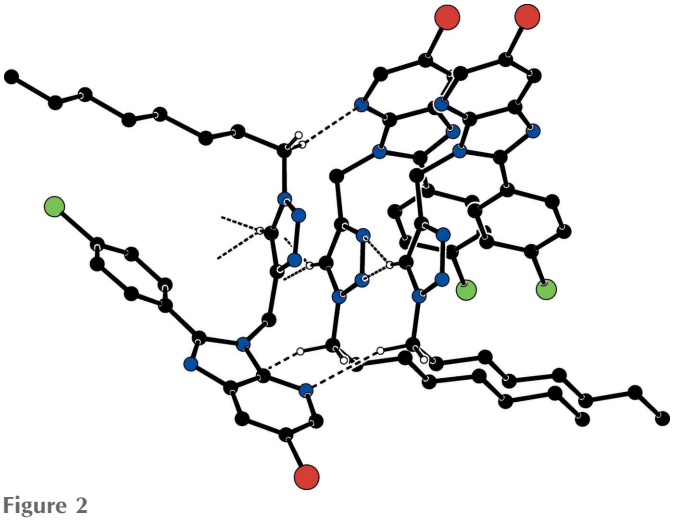


Figure 2
Detail of the crystal structure showing C—H···N_I and bifurcated C—H···(N_T,N_T) (I = imidazo[4,5-*b*]pyridine and T = triazole) hydrogen bonds, enclosing $R_3^3(20)$, $R_3^3(21)$ and $R_3^3(22)$ ring motifs, are shown as dashed lines. Non-bonding hydrogen atoms have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{26}BrClN_6$
M_r	501.86
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	16.252 (3), 5.3787 (9), 27.109 (4)
β (°)	90.551 (12)
V (Å^3)	2369.6 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.87
Crystal size (mm)	0.26 × 0.06 × 0.04
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.662, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26673, 4359, 2265
R_{int}	0.074
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.604
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.124, 1.01
No. of reflections	4359
No. of parameters	281
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.27

Computer programs: *APEX2* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018/1* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* publication routines (Farrugia, 2012) and *PLATON* (Spek, 2015).

are H···H (57.2%), H···N/N···H (17.6%), H···C/C···H (9.6%), H···Cl/Cl···H (7.9%) and H···Br/Br···H (7.0%) interactions. No significant π–π or C—H···π interactions are observed.

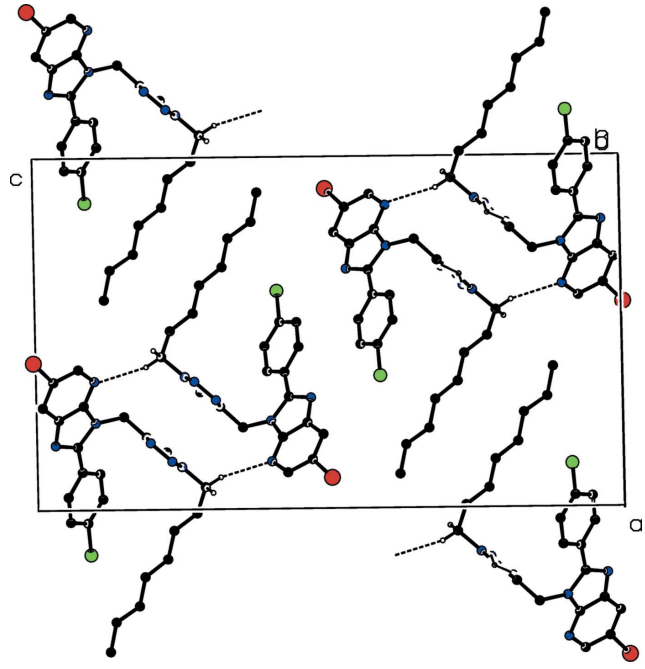


Figure 3
Packing viewed along the *b*-axis direction. C—H···N_I hydrogen bonds are shown by dashed lines.

Synthesis and crystallization

1-Azido-octane (0.18 mg, 1.16 mmol) was added to a solution of 6-bromo-2-(4-chlorophenyl)-3-(prop-2-yn-1-yl)-3*H*-imidazo[4,5-*b*] pyridine (0.2 g, 0.58 mmol) in ethanol (20 ml). The mixture was stirred under reflux for 48 h. After completion of reaction (monitored by TLC), the solution was concentrated and the residue was purified by column chromatography on silica gel by using a hexane/ethyl acetate (3/1) mixture. Colourless needles of the title compound were obtained when the solvent was allowed to evaporate.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

IUCrData (2019). **4**, x190053 [https://doi.org/10.1107/S2414314619000531]

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Crystal data

$C_{23}H_{26}BrClN_6$
M_r = 501.86
Monoclinic, $P2_1/n$
a = 16.252 (3) Å
b = 5.3787 (9) Å
c = 27.109 (4) Å
β = 90.551 (12)°
V = 2369.6 (7) Å^3
Z = 4
$F(000)$ = 1032
D_x = 1.407 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2998 reflections
θ = 2.5–17.9°
μ = 1.87 mm^{-1}
T = 296 K
Needle, colourless
0.26 × 0.06 × 0.04 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.662, T_{max} = 0.745
26673 measured reflections
4359 independent reflections
2265 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 25.4°, θ_{min} = 1.5°
h = −19→19
k = −6→6
l = −32→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.124
S = 1.01
4359 reflections
281 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 3.1135P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

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. The C-bound H-atoms were positioned geometrically with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methine and methyl hydrogen atoms and refined as riding with U_{iso}(H) = k × U_{eq}(C), where k = 1.2 for aromatic and methine H atoms and k = 1.5 for methyl H atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.91417 (3)	1.26424 (11)	0.49714 (2)	0.0850 (2)
Cl1	0.37541 (9)	−0.1921 (3)	0.58798 (6)	0.1026 (5)
N1	0.6829 (2)	0.5770 (8)	0.53176 (13)	0.0591 (10)
N2	0.7471 (2)	0.4450 (7)	0.60069 (12)	0.0515 (9)
N3	0.8640 (2)	0.7240 (8)	0.59990 (14)	0.0648 (11)
N4	0.6885 (2)	0.6629 (6)	0.69399 (14)	0.0567 (10)
N5	0.6355 (3)	0.6816 (7)	0.73019 (15)	0.0600 (11)
N6	0.6209 (2)	0.4516 (7)	0.74655 (13)	0.0529 (10)
C1	0.6048 (3)	0.0529 (9)	0.60623 (17)	0.0641 (14)
H1	0.6513	0.0047	0.6240	0.077*
C2	0.5331 (3)	−0.0841 (10)	0.61021 (18)	0.0729 (15)
H2	0.5316	−0.2218	0.6309	0.087*
C3	0.4649 (3)	−0.0182 (10)	0.58390 (19)	0.0642 (14)
C4	0.4666 (3)	0.1848 (11)	0.5548 (2)	0.0860 (18)
H4	0.4200	0.2305	0.5368	0.103*
C5	0.5372 (3)	0.3244 (10)	0.55179 (19)	0.0777 (17)
H5	0.5371	0.4675	0.5325	0.093*
C6	0.6082 (3)	0.2576 (9)	0.57660 (15)	0.0511 (11)
C7	0.6790 (3)	0.4233 (8)	0.56938 (16)	0.0503 (11)
C8	0.7946 (3)	0.6337 (9)	0.58096 (16)	0.0518 (12)
C9	0.7545 (3)	0.7123 (9)	0.53840 (16)	0.0535 (12)
C10	0.7887 (3)	0.9040 (9)	0.51141 (17)	0.0608 (13)
H10	0.7645	0.9638	0.4825	0.073*
C11	0.8606 (3)	0.9999 (9)	0.53016 (18)	0.0582 (13)
C12	0.8965 (3)	0.9066 (11)	0.57280 (19)	0.0682 (14)
H12	0.9463	0.9750	0.5833	0.082*
C13	0.7649 (3)	0.3372 (9)	0.64894 (16)	0.0588 (13)
H13A	0.8202	0.3842	0.6591	0.071*
H13B	0.7632	0.1574	0.6464	0.071*
C14	0.7059 (3)	0.4188 (8)	0.68720 (15)	0.0447 (11)
C15	0.6636 (3)	0.2859 (9)	0.72059 (17)	0.0580 (12)
H15	0.6641	0.1143	0.7247	0.070*
C16	0.5635 (3)	0.4089 (10)	0.78608 (18)	0.0769 (16)
H16A	0.5462	0.5681	0.7992	0.092*
H16B	0.5915	0.3194	0.8124	0.092*
C17	0.4894 (4)	0.2660 (13)	0.7708 (2)	0.105 (2)
H17A	0.5068	0.1010	0.7609	0.126*
H17B	0.4544	0.2469	0.7993	0.126*
C18	0.4402 (3)	0.3708 (12)	0.7310 (2)	0.0955 (19)
H18A	0.4732	0.3734	0.7014	0.115*
H18B	0.4273	0.5418	0.7393	0.115*

C19	0.3599 (4)	0.2355 (13)	0.7193 (2)	0.112 (2)
H19A	0.3726	0.0667	0.7093	0.134*
H19B	0.3276	0.2261	0.7491	0.134*
C20	0.3094 (4)	0.3534 (13)	0.6802 (2)	0.103 (2)
H20A	0.3408	0.3505	0.6499	0.124*
H20B	0.3017	0.5265	0.6890	0.124*
C21	0.2271 (4)	0.2445 (13)	0.6694 (2)	0.105 (2)
H21A	0.2340	0.0706	0.6609	0.126*
H21B	0.1944	0.2518	0.6991	0.126*
C22	0.1813 (4)	0.3678 (15)	0.6293 (3)	0.123 (2)
H22A	0.2136	0.3574	0.5994	0.148*
H22B	0.1756	0.5425	0.6374	0.148*
C23	0.0973 (4)	0.2647 (16)	0.6184 (3)	0.152 (3)
H23A	0.0753	0.3414	0.5892	0.227*
H23B	0.0617	0.2984	0.6457	0.227*
H23C	0.1011	0.0883	0.6135	0.227*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0782 (4)	0.0744 (4)	0.1029 (4)	−0.0149 (3)	0.0270 (3)	−0.0023 (4)
Cl1	0.0844 (11)	0.0859 (12)	0.1374 (14)	−0.0342 (9)	−0.0044 (9)	0.0181 (10)
N1	0.054 (3)	0.069 (3)	0.054 (2)	−0.006 (2)	−0.0109 (19)	0.008 (2)
N2	0.046 (2)	0.062 (3)	0.047 (2)	−0.001 (2)	−0.0078 (19)	−0.002 (2)
N3	0.049 (2)	0.084 (3)	0.062 (3)	−0.010 (2)	−0.003 (2)	−0.012 (2)
N4	0.073 (3)	0.033 (2)	0.064 (3)	0.0015 (19)	−0.002 (2)	0.0066 (19)
N5	0.082 (3)	0.031 (2)	0.067 (3)	0.006 (2)	−0.003 (2)	0.0022 (19)
N6	0.072 (3)	0.040 (2)	0.047 (2)	−0.001 (2)	−0.003 (2)	0.004 (2)
C1	0.072 (4)	0.054 (3)	0.066 (3)	−0.002 (3)	−0.019 (3)	0.002 (3)
C2	0.086 (4)	0.056 (3)	0.076 (4)	−0.015 (3)	−0.010 (3)	0.016 (3)
C3	0.060 (3)	0.060 (3)	0.073 (3)	−0.015 (3)	−0.005 (3)	0.001 (3)
C4	0.066 (4)	0.087 (5)	0.105 (4)	−0.018 (3)	−0.029 (3)	0.037 (4)
C5	0.058 (3)	0.076 (4)	0.099 (4)	−0.018 (3)	−0.029 (3)	0.040 (3)
C6	0.054 (3)	0.052 (3)	0.047 (3)	−0.003 (3)	−0.002 (2)	0.004 (3)
C7	0.048 (3)	0.049 (3)	0.053 (3)	0.000 (2)	−0.004 (2)	−0.003 (3)
C8	0.049 (3)	0.062 (3)	0.045 (3)	0.004 (3)	0.001 (2)	−0.012 (2)
C9	0.046 (3)	0.060 (3)	0.054 (3)	−0.006 (3)	0.004 (2)	−0.003 (3)
C10	0.057 (3)	0.072 (4)	0.053 (3)	−0.003 (3)	0.007 (2)	−0.005 (3)
C11	0.052 (3)	0.061 (3)	0.062 (3)	−0.008 (3)	0.019 (3)	−0.009 (3)
C12	0.052 (3)	0.086 (4)	0.067 (4)	−0.014 (3)	0.007 (3)	−0.015 (3)
C13	0.058 (3)	0.057 (3)	0.062 (3)	0.005 (2)	−0.017 (2)	0.003 (3)
C14	0.048 (3)	0.039 (3)	0.047 (3)	0.004 (2)	−0.018 (2)	0.002 (2)
C15	0.086 (4)	0.032 (3)	0.055 (3)	−0.002 (3)	−0.007 (3)	0.004 (3)
C16	0.097 (4)	0.074 (4)	0.060 (3)	0.001 (3)	0.011 (3)	0.006 (3)
C17	0.106 (5)	0.117 (6)	0.091 (4)	−0.025 (5)	0.019 (4)	0.021 (4)
C18	0.075 (4)	0.097 (5)	0.115 (5)	0.000 (4)	0.010 (4)	0.023 (4)
C19	0.100 (5)	0.126 (6)	0.110 (5)	−0.035 (5)	0.008 (4)	0.008 (5)
C20	0.097 (5)	0.110 (5)	0.103 (5)	−0.021 (4)	0.004 (4)	0.003 (4)

C21	0.096 (5)	0.120 (6)	0.100 (5)	−0.027 (5)	0.001 (4)	0.004 (4)
C22	0.115 (6)	0.135 (6)	0.120 (6)	−0.029 (5)	−0.005 (5)	0.008 (5)
C23	0.121 (6)	0.190 (9)	0.143 (6)	−0.060 (6)	−0.017 (5)	0.012 (6)

Geometric parameters (Å, º)

Br1—C11	1.896 (5)	C12—H12	0.9300
Cl1—C3	1.733 (5)	C13—H13A	0.9700
N1—C7	1.315 (5)	C13—H13B	0.9700
N1—C9	1.382 (5)	C14—C15	1.347 (6)
N2—C7	1.394 (5)	C14—C13	1.486 (6)
N2—C8	1.385 (5)	C15—H15	0.9300
N2—C13	1.457 (5)	C16—H16A	0.9700
N3—C8	1.327 (5)	C16—H16B	0.9700
N3—C12	1.338 (6)	C16—C17	1.485 (7)
N4—N5	1.317 (5)	C17—H17A	0.9700
N4—C14	1.356 (5)	C17—H17B	0.9700
N6—N5	1.336 (5)	C18—H18A	0.9700
N6—C15	1.334 (5)	C18—H18B	0.9700
N6—C16	1.446 (6)	C18—C17	1.450 (7)
C1—H1	0.9300	C18—C19	1.525 (8)
C1—C2	1.383 (6)	C19—H19A	0.9700
C2—H2	0.9300	C19—H19B	0.9700
C3—C2	1.361 (6)	C20—H20A	0.9700
C3—C4	1.347 (6)	C20—H20B	0.9700
C4—H4	0.9300	C20—C21	1.488 (8)
C5—H5	0.9300	C20—C19	1.477 (8)
C5—C4	1.375 (6)	C21—H21A	0.9700
C6—C1	1.365 (6)	C21—H21B	0.9700
C6—C5	1.378 (6)	C21—C22	1.471 (8)
C7—C6	1.469 (6)	C22—H22A	0.9700
C8—C9	1.386 (6)	C22—H22B	0.9700
C9—C10	1.384 (6)	C22—C23	1.499 (8)
C10—H10	0.9300	C23—H23A	0.9600
C11—C10	1.371 (6)	C23—H23B	0.9600
C11—C12	1.384 (6)	C23—H23C	0.9600
C7—N1—C9	106.0 (4)	C15—C14—N4	108.3 (4)
C7—N2—C13	131.5 (4)	C15—C14—C13	130.5 (4)
C8—N2—C7	105.6 (4)	N6—C15—C14	105.8 (4)
C8—N2—C13	122.1 (4)	N6—C15—H15	127.1
C8—N3—C12	113.2 (4)	C14—C15—H15	127.1
N5—N4—C14	108.3 (4)	N6—C16—H16A	108.8
N4—N5—N6	107.2 (3)	N6—C16—H16B	108.8
N5—N6—C16	120.7 (4)	N6—C16—C17	113.7 (4)
C15—N6—N5	110.4 (4)	H16A—C16—H16B	107.7
C15—N6—C16	128.9 (4)	C17—C16—H16A	108.8
C6—C1—H1	119.5	C17—C16—H16B	108.8

C6—C1—C2	121.0 (5)	C16—C17—H17A	108.2
C2—C1—H1	119.5	C16—C17—H17B	108.2
C1—C2—H2	119.9	C18—C17—C16	116.6 (5)
C3—C2—C1	120.2 (5)	C18—C17—H17A	108.2
C3—C2—H2	119.9	C18—C17—H17B	108.2
C2—C3—Cl1	120.4 (4)	H17A—C17—H17B	107.3
C4—C3—Cl1	119.8 (4)	H18A—C18—H18B	107.4
C4—C3—C2	119.8 (5)	C17—C18—H18A	108.4
C3—C4—C5	120.0 (5)	C17—C18—H18B	108.4
C3—C4—H4	120.0	C17—C18—C19	115.7 (6)
C5—C4—H4	120.0	C19—C18—H18A	108.4
C6—C5—H5	119.2	C19—C18—H18B	108.4
C4—C5—C6	121.6 (5)	C18—C19—H19A	108.7
C4—C5—H5	119.2	C18—C19—H19B	108.7
C1—C6—C7	127.2 (4)	C20—C19—C18	114.4 (6)
C1—C6—C5	117.3 (4)	C20—C19—H19A	108.7
C5—C6—C7	115.5 (4)	C20—C19—H19B	108.7
N2—C7—C6	126.0 (4)	H19A—C19—H19B	107.6
N1—C7—N2	112.1 (4)	H20A—C20—H20B	107.2
N1—C7—C6	121.9 (4)	C21—C20—H20A	107.9
N2—C8—C9	106.6 (4)	C21—C20—H20B	107.9
N3—C8—N2	126.4 (4)	C19—C20—H20A	107.9
N3—C8—C9	127.0 (5)	C19—C20—H20B	107.9
N1—C9—C8	109.7 (4)	C19—C20—C21	117.7 (6)
N1—C9—C10	131.7 (4)	C20—C21—H21A	108.6
C10—C9—C8	118.6 (4)	C20—C21—H21B	108.6
C9—C10—H10	122.3	H21A—C21—H21B	107.6
C11—C10—C9	115.4 (4)	C22—C21—C20	114.6 (6)
C11—C10—H10	122.3	C22—C21—H21A	108.6
C10—C11—Br1	120.0 (4)	C22—C21—H21B	108.6
C10—C11—C12	121.6 (5)	C21—C22—H22A	108.4
C12—C11—Br1	118.3 (4)	C21—C22—H22B	108.4
N3—C12—C11	124.0 (5)	C21—C22—C23	115.5 (6)
N3—C12—H12	118.0	H22A—C22—H22B	107.5
C11—C12—H12	118.0	C23—C22—H22A	108.4
N2—C13—C14	112.6 (4)	C23—C22—H22B	108.4
N2—C13—H13A	109.1	C22—C23—H23A	109.5
N2—C13—H13B	109.1	C22—C23—H23B	109.5
C14—C13—H13A	109.1	C22—C23—H23C	109.5
C14—C13—H13B	109.1	H23A—C23—H23B	109.5
H13A—C13—H13B	107.8	H23A—C23—H23C	109.5
N4—C14—C13	121.2 (4)	H23B—C23—H23C	109.5

C14—N4—N5—N6	1.1 (5)	C7—N1—C9—C8	0.8 (5)
N4—N5—N6—C15	−0.7 (5)	N3—C8—C9—N1	−178.3 (4)
N4—N5—N6—C16	−178.9 (4)	N2—C8—C9—N1	0.5 (5)
C6—C1—C2—C3	0.9 (8)	N3—C8—C9—C10	0.5 (7)
C1—C2—C3—C4	−1.6 (8)	N2—C8—C9—C10	179.2 (4)

C1—C2—C3—Cl1	179.0 (4)	N1—C9—C10—C11	178.2 (5)
C2—C3—C4—C5	0.0 (9)	C8—C9—C10—C11	−0.2 (6)
Cl1—C3—C4—C5	179.5 (4)	C9—C10—C11—C12	1.0 (7)
C3—C4—C5—C6	2.3 (9)	C9—C10—C11—Br1	−179.8 (3)
C2—C1—C6—C5	1.3 (7)	C8—N3—C12—C11	2.1 (7)
C2—C1—C6—C7	178.8 (4)	C10—C11—C12—N3	−2.1 (8)
C4—C5—C6—C1	−2.9 (8)	Br1—C11—C12—N3	178.7 (4)
C4—C5—C6—C7	179.3 (5)	C8—N2—C13—C14	105.9 (5)
C9—N1—C7—N2	−1.8 (5)	C7—N2—C13—C14	−62.4 (6)
C9—N1—C7—C6	176.4 (4)	N5—N4—C14—C15	−1.1 (5)
C8—N2—C7—N1	2.1 (5)	N5—N4—C14—C13	−179.4 (4)
C13—N2—C7—N1	171.8 (4)	N2—C13—C14—C15	131.6 (5)
C8—N2—C7—C6	−176.0 (4)	N2—C13—C14—N4	−50.5 (5)
C13—N2—C7—C6	−6.3 (7)	N5—N6—C15—C14	0.1 (5)
C1—C6—C7—N1	163.1 (5)	C16—N6—C15—C14	178.0 (4)
C5—C6—C7—N1	−19.4 (6)	N4—C14—C15—N6	0.6 (5)
C1—C6—C7—N2	−19.0 (7)	C13—C14—C15—N6	178.7 (4)
C5—C6—C7—N2	158.5 (4)	C15—N6—C16—C17	−63.3 (7)
C12—N3—C8—N2	−179.9 (4)	N5—N6—C16—C17	114.5 (5)
C12—N3—C8—C9	−1.4 (7)	N6—C16—C17—C18	−57.7 (7)
C7—N2—C8—N3	177.3 (4)	C16—C17—C18—C19	−174.1 (5)
C13—N2—C8—N3	6.4 (7)	C17—C18—C19—C20	177.3 (6)
C7—N2—C8—C9	−1.5 (5)	C18—C19—C20—C21	−175.2 (6)
C13—N2—C8—C9	−172.4 (4)	C19—C20—C21—C22	−178.6 (6)
C7—N1—C9—C10	−177.8 (5)	C20—C21—C22—C23	−178.7 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···N4^{i}	0.93	2.60	3.452 (6)	153
C15—H15···N5^{i}	0.93	2.38	3.293 (6)	168
C16—H16*B*···N3^{ii}	0.97	2.53	3.444 (6)	157

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