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4-(4-Bromophenyl)-6-(4-chlorophenyl)-pyrimidin-2-ylamine

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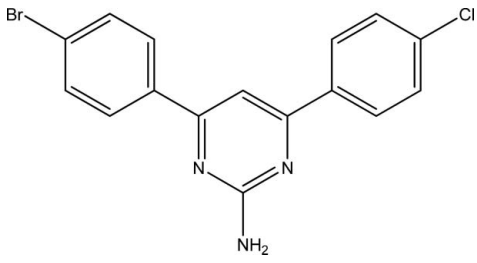
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.039; wR factor = 0.094; data-to-parameter ratio = 12.8.

The title compound, $C_{16}H_{11}BrClN_3$, contains pairs of molecules lying about inversion centers linked by amino–pyrimidine N—H···N hydrogen bonds. The eight-membered rings thus formed are represented by the $R_2^2(8)$ motif in graph-set notation. The second H atom of the amine group shows a rather weak interaction with two Br atoms, resulting in bifurcated N—H···(Br,Br) hydrogen bonds. The dihedral angles between the mean planes of the benzene rings and the mean plane of the heterocyclic ring are 8.98 (15) and 35.58 (10)°. The Br and Cl atoms show substitutional disorder, with site-occupancy factors of 0.599 (2) and 0.401 (2), respectively.

Related literature

For related structures, see: Bukhari *et al.* (2008); Fun *et al.* (2006); Gallagher *et al.* (2004). For pharmacological activities of pyrimidines, see: Gangjee *et al.* (1999); Grivsky *et al.* (1980); Malik *et al.* (2006); Rao *et al.* (2003). For graph-set notation, see: Bernstein *et al.* (1994).



Experimental

Crystal data

$C_{16}H_{11}BrClN_3$
M_r = 360.64
Monoclinic, $C2/c$
a = 39.343 (8) Å
b = 3.851 (2) Å
c = 22.620 (6) Å
β = 123.81 (2)°
V = 2847.6 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.07 mm^{-1}
T = 173 (2) K
0.20 × 0.03 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.579, T_{max} = 0.941
8088 measured reflections
2589 independent reflections
1944 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.094
S = 1.05
2589 reflections
203 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···Br1^{i}	0.92 (4)	2.97 (4)	3.803 (4)	153 (3)
N3—H3A···Br1^{ii}	0.92 (4)	3.11 (4)	3.540 (4)	111 (3)
N3—H3B···N2^{iii}	0.80 (4)	2.28 (5)	3.073 (5)	174 (4)

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2180).

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supporting information

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4-(4-Bromophenyl)-6-(4-chlorophenyl)pyrimidin-2-ylamine

Mujahid Hussain Bukhari, Hamid Latif Siddiqui, Naveed Ahmad, Waseeq Ahmad Siddiqui and Masood Parvez

S1. Comment

Pyrimidines are a class of biologically active compounds having utility in the pharmaceutical and the agrochemical industries. Compounds with the ring system show pharmacological activity such as antitumor (Gangjee *et al.*, 1999; Grivsky *et al.*, 1980), antiviral (Rao *et al.*, 2003), anti-HIV (Malik *et al.*, 2006), *etc*. In continuation of our research work (Bukhari *et al.*, 2008), we have prepared several pyrimidines. In this article, we report the crystal structure of the title compound, (I).

The structure of (I), (Fig. 1), contains dimeric pairs of molecules lying about inversion centers resulting from N3—H3B···N2^{iii} hydrogen bonds (N3···N2 = 3.071 (5) Å; Table 1 and Fig. 2). The 8-membered rings thus formed represent $R_2^2(8)$ motif in the graph set notation (Bernstein *et al.*, 1994). The second H-atom of the amine, N3A, shows rather week interactions with two Br atoms representing bifurcated hydrogen bonds (H3A···Br1 2.97 (4) and 3.11 (4) Å). The mean-planes of the two phenyl rings, C5—C10 and C11—C16, are oriented with respect to the mean-plane of the heterocyclic ring at 8.98 (15) and 35.58 (10)°, respectively. The molecular dimensions in (I) agree with the corresponding molecular dimensions reported for 4,6-(diphenyl)pyrimidin-2-amine (Gallagher *et al.*, 2004; Fun *et al.*, 2006). The structure is devoid of any C—H···π(arene) contacts observed in the structures reported above.

S2. Experimental

The title compound was synthesized by the procedure reported earlier (Bukhari *et al.*, 2008). Crystals of (I) suitable for crystallographic analysis were grown by slow evaporation at 313 K from a solutuion of $CHCl_3$ (Yield 58%; m.p. 512–514 K).

S3. Refinement

The Br and Cl atoms showed substitutional disorder with site occupancy factors refined for Br1 and Cl1 to 0.559 (2) and Br1′ and Cl1′ to 0.401 (2) values. C—Cl and C—Br distances were constrained using *DFIX* command in *SHELXL97* (Sheldrick, 2008). Though all the H atoms could be distinguished in the difference Fourier map the H-atoms bonded to C-atoms were included at geometrically idealized positions and refined in riding-model approximation with the following constraints: C—H distances were set to 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). H-atoms bonded to N3 were taken from the difference map and were allowed to refine with U_{iso} = 1.2 times U_{eq} of the parent atom. The final difference map was free of any chemically significant features.

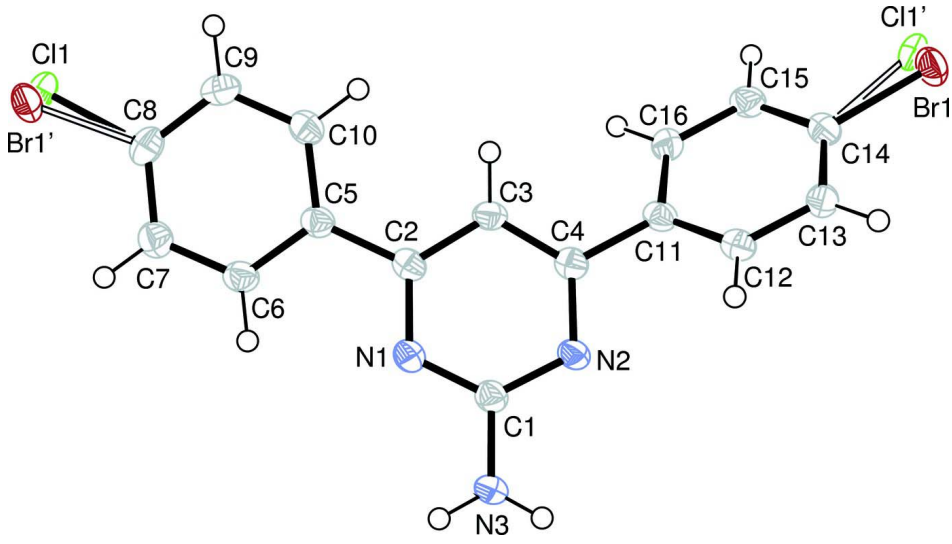

Figure 1

ORTEP-3 (Farrugia, 1997) drawing of (I) with displacement ellipsoids plotted at 50% probability level. Hollow bonds represent smaller fractions of the disordered Br and Cl atoms (Br1 and Cl1, respectively).

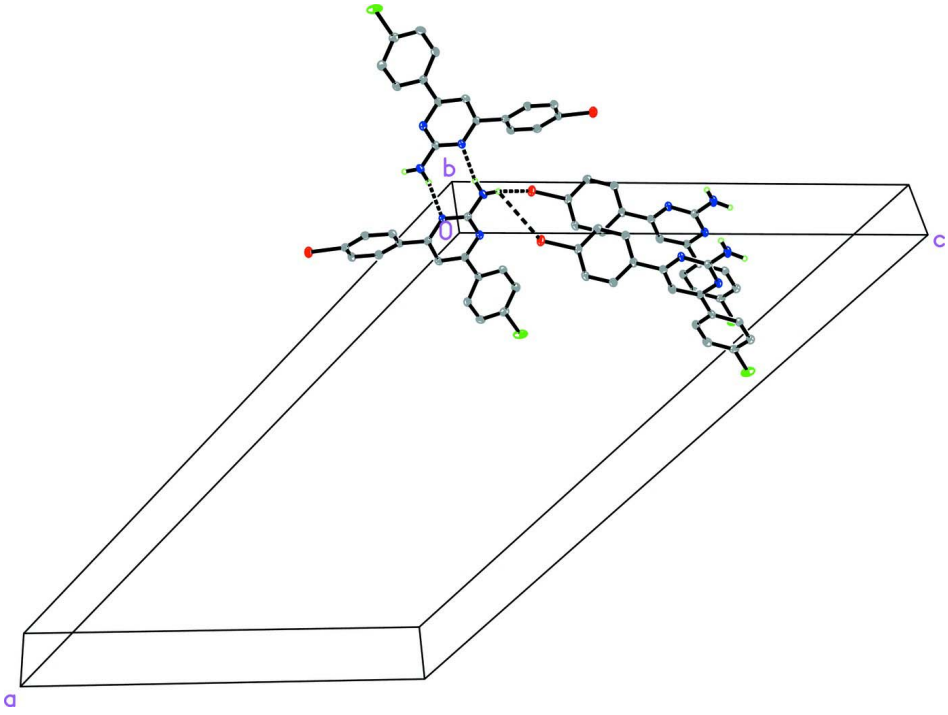

Figure 2

Unit cell packing of (I) showing hydrogen bonds with dashed lines; H-atoms not involved in H-bonds have been omitted.

4-(4-Bromophenyl)-6-(4-chlorophenyl)pyrimidin-2-ylamine

Crystal data

$C_{16}H_{11}BrClN_3$
M_r = 360.64

Monoclinic, *C*2/*c*
Hall symbol: -C 2yc

a = 39.343 (8) Å
b = 3.851 (2) Å
c = 22.620 (6) Å
β = 123.81 (2)°
V = 2847.6 (18) Å^3
Z = 8
F(000) = 1440
D_x = 1.682 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8088 reflections
θ = 3.1–25.3°
μ = 3.07 mm^{-1}
T = 173 K
Needle, colorless
0.20 × 0.03 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.579, T_{max} = 0.941

8088 measured reflections
2589 independent reflections
1944 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.3°, θ_{min} = 3.1°
h = −46→45
k = −4→4
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.094
S = 1.05
2589 reflections
203 parameters
4 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0319P)^2 + 9.7534P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Br1	0.07275 (3)	0.3788 (4)	−0.23596 (6)	0.0284 (2)	0.599 (2)
Cl1	0.28850 (8)	0.8754 (7)	0.45607 (13)	0.0257 (5)	0.599 (2)
Br1′	0.28731 (6)	0.8681 (5)	0.47100 (9)	0.0284 (2)	0.401 (2)
Cl1′	0.08059 (14)	0.3789 (17)	−0.2222 (2)	0.0257 (5)	0.401 (2)
N1	0.09743 (9)	0.9631 (7)	0.16544 (15)	0.0239 (6)	
N2	0.05683 (9)	0.8645 (8)	0.03909 (15)	0.0231 (6)	
N3	0.02841 (10)	1.0562 (9)	0.09907 (18)	0.0302 (8)	
H3A	0.0318 (12)	1.151 (11)	0.139 (2)	0.036*	

H3B	0.0070 (14)	1.073 (11)	0.061 (2)	0.036*
C1	0.06220 (11)	0.9592 (9)	0.10129 (18)	0.0239 (8)
C2	0.13100 (11)	0.8621 (9)	0.16862 (18)	0.0223 (7)
C3	0.12903 (11)	0.7667 (9)	0.10744 (18)	0.0249 (8)
H3	0.1529	0.6995	0.1095	0.030*
C4	0.09094 (11)	0.7729 (9)	0.04318 (18)	0.0223 (8)
C5	0.16972 (10)	0.8644 (9)	0.24074 (18)	0.0233 (7)
C6	0.17017 (11)	1.0069 (9)	0.29802 (19)	0.0261 (8)
H6	0.1458	1.1041	0.2901	0.031*
C7	0.20533 (11)	1.0093 (10)	0.3658 (2)	0.0291 (8)
H7	0.2053	1.1065	0.4044	0.035*
C8	0.24065 (9)	0.8673 (10)	0.37647 (15)	0.0283 (8)
C9	0.24130 (11)	0.7212 (10)	0.3213 (2)	0.0294 (8)
H9	0.2658	0.6224	0.3297	0.035*
C10	0.20581 (11)	0.7210 (9)	0.25364 (19)	0.0267 (8)
H10	0.2060	0.6216	0.2154	0.032*
C11	0.08642 (11)	0.6800 (9)	−0.02477 (18)	0.0233 (8)
C12	0.05169 (11)	0.5079 (9)	−0.07802 (19)	0.0244 (8)
H12	0.0308	0.4484	−0.0708	0.029*
C13	0.04712 (11)	0.4215 (9)	−0.14167 (18)	0.0245 (8)
H13	0.0233	0.3047	−0.1782	0.029*
C14	0.07789 (11)	0.5087 (9)	−0.15093 (16)	0.0239 (8)
C15	0.11279 (11)	0.6792 (9)	−0.09883 (19)	0.0270 (8)
H15	0.1336	0.7372	−0.1062	0.032*
C16	0.11689 (11)	0.7644 (9)	−0.03569 (19)	0.0255 (8)
H16	0.1408	0.8818	0.0006	0.031*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0312 (5)	0.0367 (4)	0.0141 (5)	0.0009 (4)	0.0106 (4)	−0.0020 (4)
Cl1	0.0220 (8)	0.0441 (11)	0.0050 (9)	0.0017 (7)	0.0039 (7)	−0.0014 (7)
Br1′	0.0312 (5)	0.0367 (4)	0.0141 (5)	0.0009 (4)	0.0106 (4)	−0.0020 (4)
Cl1′	0.0220 (8)	0.0441 (11)	0.0050 (9)	0.0017 (7)	0.0039 (7)	−0.0014 (7)
N1	0.0256 (16)	0.0279 (16)	0.0216 (14)	0.0007 (13)	0.0152 (13)	0.0007 (12)
N2	0.0241 (15)	0.0273 (15)	0.0228 (14)	0.0024 (13)	0.0161 (13)	0.0015 (13)
N3	0.0247 (16)	0.045 (2)	0.0243 (16)	0.0089 (16)	0.0157 (14)	0.0010 (16)
C1	0.0259 (18)	0.0262 (19)	0.0234 (18)	0.0024 (15)	0.0161 (16)	0.0030 (15)
C2	0.0280 (19)	0.0195 (17)	0.0249 (18)	0.0003 (15)	0.0181 (16)	0.0022 (15)
C3	0.0226 (18)	0.0301 (19)	0.0265 (19)	0.0036 (15)	0.0164 (17)	0.0014 (15)
C4	0.0260 (19)	0.0199 (17)	0.0246 (18)	0.0010 (14)	0.0163 (17)	0.0034 (14)
C5	0.0240 (18)	0.0244 (18)	0.0250 (18)	0.0002 (16)	0.0159 (16)	0.0019 (15)
C6	0.0246 (19)	0.0292 (19)	0.0298 (19)	0.0010 (15)	0.0184 (17)	0.0011 (16)
C7	0.029 (2)	0.030 (2)	0.0274 (19)	−0.0011 (16)	0.0154 (17)	−0.0020 (16)
C8	0.0229 (19)	0.0275 (19)	0.0270 (19)	−0.0033 (16)	0.0092 (16)	0.0027 (16)
C9	0.0251 (19)	0.030 (2)	0.035 (2)	0.0061 (16)	0.0181 (18)	0.0052 (16)
C10	0.029 (2)	0.029 (2)	0.0276 (19)	−0.0001 (16)	0.0193 (18)	0.0004 (15)
C11	0.0275 (19)	0.0218 (19)	0.0251 (18)	0.0054 (15)	0.0173 (16)	0.0033 (14)

C12	0.0262 (19)	0.0240 (18)	0.0267 (18)	0.0029 (15)	0.0169 (17)	0.0010 (15)
C13	0.0237 (18)	0.0240 (19)	0.0229 (17)	0.0021 (15)	0.0112 (16)	−0.0009 (15)
C14	0.032 (2)	0.0217 (17)	0.0219 (17)	0.0064 (15)	0.0171 (17)	0.0043 (14)
C15	0.0261 (19)	0.033 (2)	0.0278 (19)	0.0024 (16)	0.0190 (17)	0.0043 (16)
C16	0.0233 (18)	0.030 (2)	0.0228 (18)	0.0000 (16)	0.0126 (16)	−0.0004 (15)

Geometric parameters (Å, º)

Br1—C14	1.886 (3)	C6—C7	1.380 (5)
Cl1—C8	1.736 (3)	C6—H6	0.9500
Br1′—C8	1.891 (3)	C7—C8	1.384 (5)
Cl1′—C14	1.746 (4)	C7—H7	0.9500
N1—C1	1.337 (5)	C8—C9	1.382 (5)
N1—C2	1.340 (4)	C9—C10	1.384 (5)
N2—C4	1.340 (4)	C9—H9	0.9500
N2—C1	1.352 (4)	C10—H10	0.9500
N3—C1	1.354 (4)	C11—C12	1.388 (5)
N3—H3A	0.92 (4)	C11—C16	1.391 (5)
N3—H3B	0.80 (4)	C12—C13	1.388 (5)
C2—C3	1.392 (5)	C12—H12	0.9500
C2—C5	1.489 (5)	C13—C14	1.380 (5)
C3—C4	1.391 (5)	C13—H13	0.9500
C3—H3	0.9500	C14—C15	1.380 (5)
C4—C11	1.489 (5)	C15—C16	1.385 (5)
C5—C10	1.395 (5)	C15—H15	0.9500
C5—C6	1.398 (5)	C16—H16	0.9500
C1—N1—C2	116.8 (3)	C9—C8—Br1′	121.8 (3)
C4—N2—C1	115.4 (3)	C7—C8—Br1′	116.4 (3)
C1—N3—H3A	118 (3)	C10—C9—C8	119.0 (3)
C1—N3—H3B	119 (3)	C10—C9—H9	120.5
H3A—N3—H3B	121 (4)	C8—C9—H9	120.5
N1—C1—N2	126.8 (3)	C9—C10—C5	121.0 (3)
N1—C1—N3	116.1 (3)	C9—C10—H10	119.5
N2—C1—N3	117.0 (3)	C5—C10—H10	119.5
N1—C2—C3	121.0 (3)	C12—C11—C16	119.2 (3)
N1—C2—C5	115.7 (3)	C12—C11—C4	120.3 (3)
C3—C2—C5	123.2 (3)	C16—C11—C4	120.5 (3)
C4—C3—C2	117.8 (3)	C11—C12—C13	120.8 (3)
C4—C3—H3	121.1	C11—C12—H12	119.6
C2—C3—H3	121.1	C13—C12—H12	119.6
N2—C4—C3	122.1 (3)	C14—C13—C12	118.7 (3)
N2—C4—C11	116.9 (3)	C14—C13—H13	120.6
C3—C4—C11	121.0 (3)	C12—C13—H13	120.6
C10—C5—C6	118.4 (3)	C13—C14—C15	121.8 (3)
C10—C5—C2	121.9 (3)	C13—C14—Cl1′	125.4 (3)
C6—C5—C2	119.7 (3)	C15—C14—Cl1′	112.4 (3)
C7—C6—C5	121.4 (3)	C13—C14—Br1	119.0 (3)

C7—C6—H6	119.3	C15—C14—Br1	119.2 (3)
C5—C6—H6	119.3	C14—C15—C16	118.9 (3)
C6—C7—C8	118.6 (3)	C14—C15—H15	120.6
C6—C7—H7	120.7	C16—C15—H15	120.6
C8—C7—H7	120.7	C15—C16—C11	120.7 (3)
C9—C8—C7	121.7 (3)	C15—C16—H16	119.6
C9—C8—Cl1	112.9 (3)	C11—C16—H16	119.6
C7—C8—Cl1	125.3 (3)		

C2—N1—C1—N2	−0.1 (5)	C7—C8—C9—C10	0.8 (6)
C2—N1—C1—N3	178.9 (3)	Cl1—C8—C9—C10	−175.4 (3)
C4—N2—C1—N1	−1.5 (5)	Br1′—C8—C9—C10	178.3 (3)
C4—N2—C1—N3	179.5 (3)	C8—C9—C10—C5	−0.2 (6)
C1—N1—C2—C3	1.5 (5)	C6—C5—C10—C9	−0.4 (5)
C1—N1—C2—C5	−179.2 (3)	C2—C5—C10—C9	−179.0 (3)
N1—C2—C3—C4	−1.3 (5)	N2—C4—C11—C12	−35.5 (5)
C5—C2—C3—C4	179.5 (3)	C3—C4—C11—C12	145.1 (4)
C1—N2—C4—C3	1.7 (5)	N2—C4—C11—C16	144.5 (3)
C1—N2—C4—C11	−177.7 (3)	C3—C4—C11—C16	−34.9 (5)
C2—C3—C4—N2	−0.4 (5)	C16—C11—C12—C13	−0.3 (5)
C2—C3—C4—C11	179.0 (3)	C4—C11—C12—C13	179.7 (3)
N1—C2—C5—C10	170.9 (3)	C11—C12—C13—C14	0.3 (5)
C3—C2—C5—C10	−9.9 (5)	C12—C13—C14—C15	−0.2 (5)
N1—C2—C5—C6	−7.7 (5)	C12—C13—C14—Cl1′	172.1 (4)
C3—C2—C5—C6	171.5 (3)	C12—C13—C14—Br1	177.9 (3)
C10—C5—C6—C7	0.4 (5)	C13—C14—C15—C16	0.0 (5)
C2—C5—C6—C7	179.1 (3)	Cl1′—C14—C15—C16	−173.1 (4)
C5—C6—C7—C8	0.1 (5)	Br1—C14—C15—C16	−178.1 (3)
C6—C7—C8—C9	−0.7 (6)	C14—C15—C16—C11	0.0 (5)
C6—C7—C8—Cl1	174.9 (3)	C12—C11—C16—C15	0.1 (5)
C6—C7—C8—Br1′	−178.4 (3)	C4—C11—C16—C15	−179.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···Br1^{i}	0.92 (4)	2.97 (4)	3.803 (4)	153 (3)
N3—H3*A*···Br1^{ii}	0.92 (4)	3.11 (4)	3.540 (4)	111 (3)
N3—H3*B*···N2^{iii}	0.80 (4)	2.28 (5)	3.073 (5)	174 (4)

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