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2-Amino-4-(4-methoxyphenyl)-6-(4-methylphenyl)-pyrimidin-1-ium chloride

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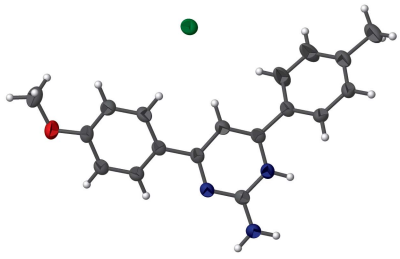
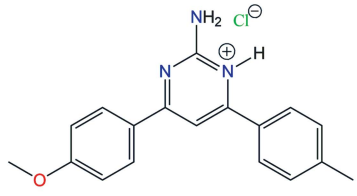
In the title salt, $C_{18}H_{18}N_3O^+\cdot Cl^-$, the aminopyrimidine molecule is protonated at one of the pyrimidine N atoms. The chloride anion interacts with the protonated pyrimidine N—H group and one of the amino N—H groups through two N—H···Cl hydrogen bonds, forming a six-membered ring. The chloride anion interacts further with the other amino N—H group to form an additional N—H···Cl hydrogen bond, which links the molecules along [001] in a helical manner.

3D view



Chemical scheme



Structure description

As a result of their being a natural component of nucleic acid, aminopyrimidine derivatives are biologically important and have shown a broad spectrum of biological activities including anti-platelet (Giridhar *et al.*, 2012), antitumor (Lee *et al.*, 2011), antibacterial (Nagarajan *et al.*, 2014) and anti-diabetic properties (Singh *et al.*, 2011). As a continuation of our research program to expand the use of novel synthetic chalcones (Lee *et al.* 2016), the title aminopyrimidine compound was synthesized from chalcone and its crystal structure was determined. Other examples of aminopyrimidinium salt structures have been published recently (Swinton Darious *et al.*, 2018; Jeevaraj *et al.*, 2016).

The molecular structure of the title compound is shown in Fig. 1. The aminopyrimidine molecule is protonated at one of the pyrimidine nitrogen atoms. As a result, the two C—N—C bond angles in the pyrimidine ring are different: the C1—N2—C4 angle at protonated atom N2 is 121.1 (2)°, while for the unprotonated atom N1, the C1—N1—C2 angle is 117.8 (2)°.

In the crystal, a six-membered ring is formed through N—H···Cl hydrogen bonds (aqua coloured dashed lines in Fig. 2, Table 1) involving one of the hydrogen atoms in the amino group (N3—H3*B*) and a hydrogen atom in the pyrimidium ring (N2—H2*A*) and the chlorine anion. An additional hydrogen bond is formed by the other hydrogen atom

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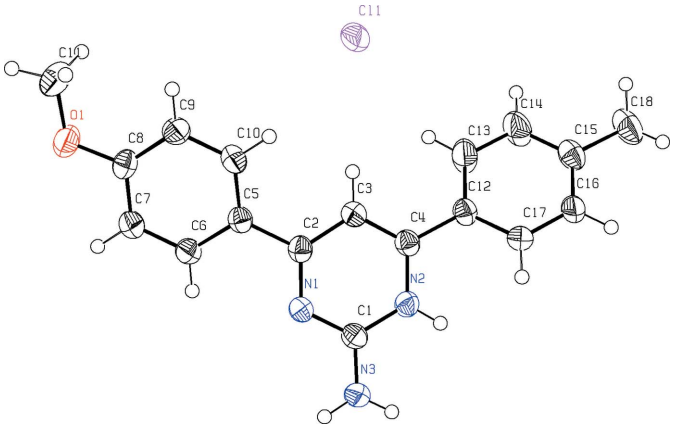

Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level.

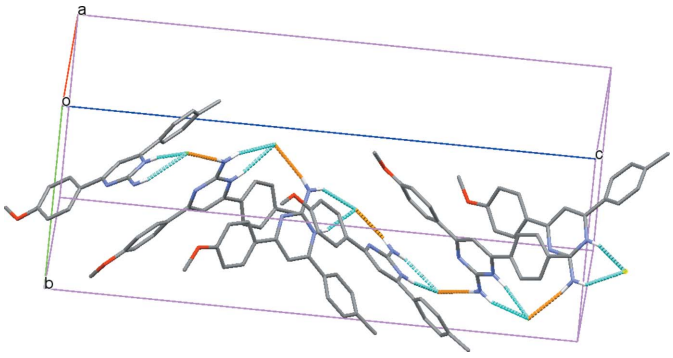

Figure 2
Part of the crystal structure with intermolecular hydrogen bonds are shown as red and blue dashed lines. For clarity, only those H atoms involved in hydrogen bonding are shown.

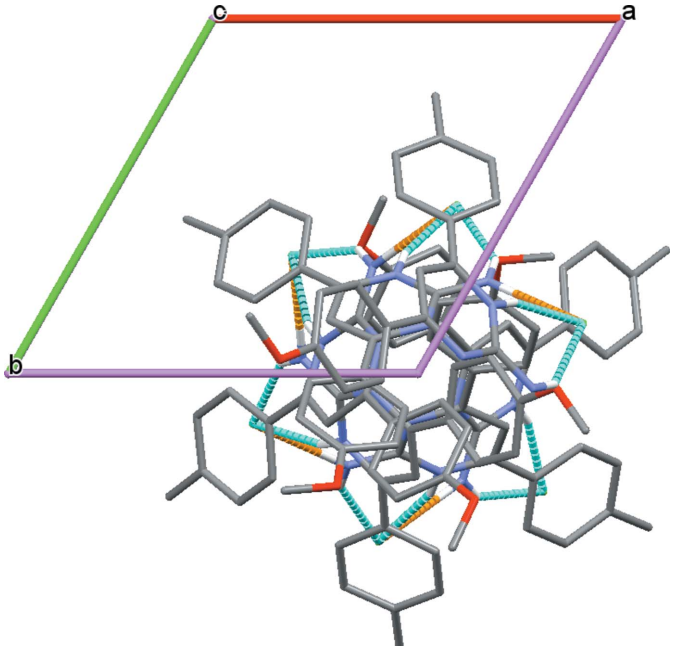

Figure 3
Part of the crystal structure shown along the *c* axis. The three N—H···Cl hydrogen bonds connect molecules in a helical manner along the *c* axis.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Cl1^{i}	0.87	2.27	3.106 (3)	160
N3—H3*A*···Cl1^{ii}	0.87	2.44	3.305 (3)	172
N3—H3*B*···Cl1^{i}	0.87	2.56	3.332 (3)	148
C14—H14···O1^{iii}	0.94	2.46	3.300 (4)	148

Symmetry codes: (i) $y+1, -x+y+1, z+\frac{1}{6}$; (ii) $x+1, y+1, z$; (iii) $-x+y, -x+1, z+\frac{1}{3}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{18}N_3O^+\cdot Cl^-$
M_r	327.80
Crystal system, space group	Hexagonal, $P6_5$
Temperature (K)	223
a, *c* (Å)	9.9013 (9), 28.981 (2)
V (Å^3)	2460.6 (5)
Z	6
Radiation type	Mo *Kα*
μ (mm^{-1})	0.24
Crystal size (mm)	0.18 × 0.10 × 0.07
Data collection	
Diffractometer	Bruker PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.721, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	135729, 4073, 3401
R_{int}	0.081
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.040, 0.083, 1.10
No. of reflections	4073
No. of parameters	228
No. of restraints	1
H-atom treatment	Only H-atom displacement parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.15
Absolute structure	Flack *x* determined using 1416 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter	0.016 (15)

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXS* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015)and *publCIF* (Westrip, 2010).

in the amino group (N3—H3*A*) and the chloride anion (orange dashed line in Fig. 2, Table 1), which links the molecules into a chain along [001]. The three N—H···Cl hydrogen bonds connect the molecules in helical manner along [001]. Six molecules are involved in one turn of the helix (Fig. 3).

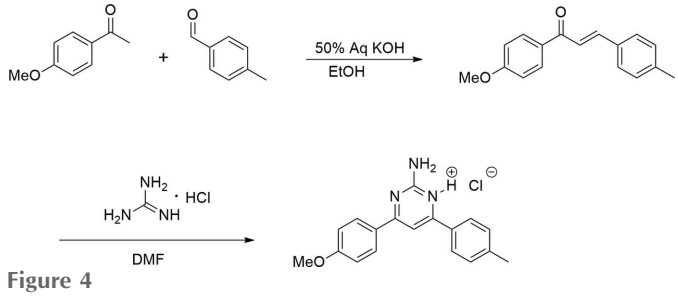

Figure 4
Synthetic scheme for the preparation of the title compound.

Synthesis and crystallization

The same synthetic procedures were used as described in our previous report (Koh & Lee, 2018), but starting from 4-methoxy acetophenone and 4-methyl benzaldehyde for the synthesis of the chalcone intermediate, as shown in Fig. 4.

Refinement

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

Funding information

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full crystallographic data

IUCrData (2018). **3**, x181152 [https://doi.org/10.1107/S2414314618011525]

2-Amino-4-(4-methoxyphenyl)-6-(4-methylphenyl)pyrimidin-1-ium chloride

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Crystal data

$C_{18}H_{18}N_3O^+\cdot Cl^-$
M_r = 327.80
Hexagonal, $P6_5$
a = 9.9013 (9) Å
c = 28.981 (2) Å
V = 2460.6 (5) Å^3
Z = 6
F(000) = 1032
D_x = 1.327 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9935 reflections
θ = 2.4–26.1°
μ = 0.24 mm^{-1}
T = 223 K
Block, colourless
0.18 × 0.10 × 0.07 mm

Data collection

Bruker PHOTON 100 CMOS diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2012)
T_{min} = 0.721, T_{max} = 0.746
135729 measured reflections
4073 independent reflections
3401 reflections with $I > 2\sigma(I)$
R_{int} = 0.081
θ_{max} = 28.3°, θ_{min} = 2.4°
h = −13→13
k = −13→13
l = −38→38

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.083
S = 1.10
4073 reflections
228 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
Only H-atom displacement parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2 + 0.7437P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack x determined using 1416 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)
Absolute structure parameter: 0.016 (15)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.1580 (3)	0.9339 (3)	0.12113 (9)	0.0327 (6)
N1	1.0866 (3)	0.9519 (3)	0.08454 (8)	0.0324 (5)
C2	0.9390 (3)	0.8427 (3)	0.07668 (9)	0.0317 (6)
C3	0.8602 (3)	0.7103 (3)	0.10505 (10)	0.0363 (6)
H3	0.7569	0.6335	0.0984	0.041 (9)*
C4	0.9356 (3)	0.6949 (3)	0.14220 (9)	0.0327 (6)
N2	1.0862 (3)	0.8080 (3)	0.14949 (8)	0.0335 (5)
H2A	1.1373	0.7995	0.1727	0.056 (11)*
N3	1.3025 (3)	1.0421 (3)	0.13150 (9)	0.0402 (6)
H3A	1.3512	1.1252	0.1145	0.050 (10)*
H3B	1.3488	1.0301	0.1554	0.052 (11)*
C5	0.8595 (3)	0.8685 (3)	0.03772 (9)	0.0314 (6)
C6	0.9184 (3)	1.0184 (3)	0.01960 (10)	0.0353 (6)
H6	1.0093	1.1017	0.0323	0.038 (8)*
C7	0.8450 (4)	1.0454 (3)	−0.01649 (10)	0.0385 (7)
H7	0.8863	1.1466	−0.0286	0.041 (9)*
C8	0.7090 (3)	0.9226 (4)	−0.03525 (10)	0.0355 (6)
C9	0.6482 (4)	0.7740 (3)	−0.01741 (10)	0.0373 (6)
H9	0.5561	0.6912	−0.0298	0.047 (9)*
C10	0.7234 (4)	0.7477 (3)	0.01875 (10)	0.0358 (6)
H10	0.6819	0.6464	0.0307	0.039 (8)*
O1	0.6439 (3)	0.9614 (3)	−0.07036 (8)	0.0485 (6)
C11	0.5094 (4)	0.8394 (4)	−0.09247 (12)	0.0523 (9)
H11A	0.5351	0.7651	−0.1058	0.076 (13)*
H11B	0.4752	0.8831	−0.1167	0.073 (12)*
H11C	0.4266	0.7869	−0.0700	0.066 (12)*
C12	0.8636 (3)	0.5676 (3)	0.17621 (9)	0.0337 (6)
C13	0.7053 (4)	0.4976 (5)	0.18546 (15)	0.0597 (10)
H13	0.6432	0.5276	0.1687	0.084 (14)*
C14	0.6380 (4)	0.3837 (5)	0.21918 (15)	0.0617 (11)
H14	0.5307	0.3381	0.2252	0.079 (13)*
C15	0.7247 (4)	0.3361 (4)	0.24390 (10)	0.0417 (7)
C16	0.8803 (4)	0.3997 (4)	0.23269 (11)	0.0474 (8)
H16	0.9402	0.3638	0.2479	0.059 (11)*
C17	0.9500 (4)	0.5155 (3)	0.19954 (11)	0.0406 (7)
H17	1.0567	0.5586	0.1930	0.062 (11)*
C18	0.6526 (5)	0.2185 (4)	0.28224 (12)	0.0597 (10)
H18A	0.7155	0.1703	0.2880	0.088 (16)*
H18B	0.5481	0.1391	0.2734	0.082 (14)*
H18C	0.6477	0.2704	0.3101	0.12 (2)*
Cl1	0.47413 (9)	0.33310 (8)	0.05723 (3)	0.0449 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0317 (15)	0.0354 (15)	0.0304 (13)	0.0165 (13)	0.0060 (11)	0.0016 (11)
N1	0.0319 (12)	0.0331 (13)	0.0304 (12)	0.0149 (10)	0.0030 (10)	0.0038 (10)
C2	0.0343 (15)	0.0355 (15)	0.0288 (13)	0.0201 (12)	0.0038 (11)	0.0026 (11)
C3	0.0316 (16)	0.0355 (15)	0.0392 (15)	0.0148 (13)	0.0015 (12)	0.0062 (12)
C4	0.0334 (15)	0.0339 (15)	0.0319 (15)	0.0177 (12)	0.0053 (11)	0.0033 (11)
N2	0.0328 (13)	0.0387 (13)	0.0294 (12)	0.0182 (11)	0.0019 (10)	0.0042 (10)
N3	0.0298 (13)	0.0434 (15)	0.0385 (14)	0.0117 (11)	0.0008 (11)	0.0092 (11)
C5	0.0338 (15)	0.0329 (14)	0.0293 (13)	0.0181 (12)	0.0038 (11)	0.0019 (11)
C6	0.0349 (15)	0.0331 (15)	0.0346 (15)	0.0145 (13)	−0.0005 (12)	0.0010 (12)
C7	0.0411 (17)	0.0331 (15)	0.0398 (16)	0.0174 (14)	0.0005 (13)	0.0050 (13)
C8	0.0410 (16)	0.0439 (17)	0.0281 (14)	0.0261 (14)	−0.0010 (12)	0.0004 (12)
C9	0.0387 (16)	0.0364 (16)	0.0334 (15)	0.0162 (13)	−0.0032 (12)	−0.0035 (12)
C10	0.0427 (16)	0.0297 (14)	0.0327 (14)	0.0163 (13)	0.0032 (12)	0.0022 (12)
O1	0.0548 (14)	0.0477 (13)	0.0455 (13)	0.0277 (12)	−0.0140 (10)	0.0018 (10)
C11	0.061 (2)	0.058 (2)	0.047 (2)	0.0364 (19)	−0.0178 (17)	−0.0105 (16)
C12	0.0370 (15)	0.0343 (15)	0.0317 (15)	0.0194 (13)	0.0047 (11)	0.0044 (11)
C13	0.0438 (19)	0.075 (3)	0.072 (2)	0.038 (2)	0.0222 (17)	0.041 (2)
C14	0.047 (2)	0.068 (3)	0.076 (3)	0.0336 (19)	0.0296 (19)	0.038 (2)
C15	0.0532 (19)	0.0341 (16)	0.0328 (15)	0.0181 (14)	0.0045 (13)	0.0022 (13)
C16	0.0474 (18)	0.0349 (16)	0.0466 (19)	0.0106 (14)	−0.0143 (15)	0.0093 (14)
C17	0.0335 (16)	0.0342 (15)	0.0455 (17)	0.0105 (13)	−0.0069 (13)	0.0048 (13)
C18	0.080 (3)	0.043 (2)	0.0413 (19)	0.019 (2)	0.0055 (18)	0.0100 (16)
Cl1	0.0498 (5)	0.0295 (3)	0.0452 (4)	0.0122 (3)	−0.0071 (3)	−0.0003 (3)

Geometric parameters (Å, º)

C1—N3	1.324 (4)	C9—C10	1.384 (4)
C1—N1	1.335 (4)	C9—H9	0.9400
C1—N2	1.360 (4)	C10—H10	0.9400
N1—C2	1.333 (4)	O1—C11	1.426 (4)
C2—C3	1.407 (4)	C11—H11A	0.9700
C2—C5	1.470 (4)	C11—H11B	0.9700
C3—C4	1.361 (4)	C11—H11C	0.9700
C3—H3	0.9400	C12—C17	1.377 (4)
C4—N2	1.361 (4)	C12—C13	1.387 (4)
C4—C12	1.473 (4)	C13—C14	1.385 (5)
N2—H2A	0.8700	C13—H13	0.9400
N3—H3A	0.8700	C14—C15	1.369 (5)
N3—H3B	0.8700	C14—H14	0.9400
C5—C10	1.391 (4)	C15—C16	1.380 (5)
C5—C6	1.397 (4)	C15—C18	1.506 (4)
C6—C7	1.374 (4)	C16—C17	1.386 (4)
C6—H6	0.9400	C16—H16	0.9400
C7—C8	1.396 (4)	C17—H17	0.9400
C7—H7	0.9400	C18—H18A	0.9700

C8—O1	1.359 (4)	C18—H18B	0.9700
C8—C9	1.381 (4)	C18—H18C	0.9700
N3—C1—N1	120.2 (3)	C9—C10—C5	121.2 (3)
N3—C1—N2	117.6 (3)	C9—C10—H10	119.4
N1—C1—N2	122.2 (3)	C5—C10—H10	119.4
C2—N1—C1	117.8 (2)	C8—O1—C11	118.1 (3)
N1—C2—C3	121.9 (3)	O1—C11—H11A	109.5
N1—C2—C5	117.1 (2)	O1—C11—H11B	109.5
C3—C2—C5	121.0 (3)	H11A—C11—H11B	109.5
C4—C3—C2	119.1 (3)	O1—C11—H11C	109.5
C4—C3—H3	120.4	H11A—C11—H11C	109.5
C2—C3—H3	120.4	H11B—C11—H11C	109.5
N2—C4—C3	117.9 (3)	C17—C12—C13	118.5 (3)
N2—C4—C12	117.5 (2)	C17—C12—C4	121.6 (3)
C3—C4—C12	124.6 (3)	C13—C12—C4	119.9 (3)
C1—N2—C4	121.1 (2)	C14—C13—C12	120.4 (3)
C1—N2—H2A	119.5	C14—C13—H13	119.8
C4—N2—H2A	119.5	C12—C13—H13	119.8
C1—N3—H3A	120.0	C15—C14—C13	121.4 (3)
C1—N3—H3B	120.0	C15—C14—H14	119.3
H3A—N3—H3B	120.0	C13—C14—H14	119.3
C10—C5—C6	118.3 (3)	C14—C15—C16	117.9 (3)
C10—C5—C2	121.8 (3)	C14—C15—C18	121.0 (3)
C6—C5—C2	119.9 (3)	C16—C15—C18	121.0 (3)
C7—C6—C5	120.8 (3)	C15—C16—C17	121.4 (3)
C7—C6—H6	119.6	C15—C16—H16	119.3
C5—C6—H6	119.6	C17—C16—H16	119.3
C6—C7—C8	120.0 (3)	C12—C17—C16	120.2 (3)
C6—C7—H7	120.0	C12—C17—H17	119.9
C8—C7—H7	120.0	C16—C17—H17	119.9
O1—C8—C9	124.4 (3)	C15—C18—H18A	109.5
O1—C8—C7	115.6 (3)	C15—C18—H18B	109.5
C9—C8—C7	120.0 (3)	H18A—C18—H18B	109.5
C8—C9—C10	119.6 (3)	C15—C18—H18C	109.5
C8—C9—H9	120.2	H18A—C18—H18C	109.5
C10—C9—H9	120.2	H18B—C18—H18C	109.5
N3—C1—N1—C2	−177.3 (3)	O1—C8—C9—C10	−179.4 (3)
N2—C1—N1—C2	1.2 (4)	C7—C8—C9—C10	−0.6 (4)
C1—N1—C2—C3	−1.4 (4)	C8—C9—C10—C5	0.2 (4)
C1—N1—C2—C5	176.8 (2)	C6—C5—C10—C9	0.5 (4)
N1—C2—C3—C4	1.6 (4)	C2—C5—C10—C9	178.9 (3)
C5—C2—C3—C4	−176.6 (3)	C9—C8—O1—C11	−4.4 (4)
C2—C3—C4—N2	−1.5 (4)	C7—C8—O1—C11	176.8 (3)
C2—C3—C4—C12	175.9 (3)	N2—C4—C12—C17	−32.0 (4)
N3—C1—N2—C4	177.3 (3)	C3—C4—C12—C17	150.6 (3)
N1—C1—N2—C4	−1.2 (4)	N2—C4—C12—C13	147.8 (3)

C3—C4—N2—C1	1.3 (4)	C3—C4—C12—C13	−29.6 (5)
C12—C4—N2—C1	−176.3 (2)	C17—C12—C13—C14	3.4 (6)
N1—C2—C5—C10	162.7 (3)	C4—C12—C13—C14	−176.4 (4)
C3—C2—C5—C10	−19.1 (4)	C12—C13—C14—C15	−0.6 (7)
N1—C2—C5—C6	−19.0 (4)	C13—C14—C15—C16	−3.1 (6)
C3—C2—C5—C6	159.2 (3)	C13—C14—C15—C18	176.7 (4)
C10—C5—C6—C7	−0.9 (4)	C14—C15—C16—C17	4.1 (5)
C2—C5—C6—C7	−179.3 (3)	C18—C15—C16—C17	−175.7 (3)
C5—C6—C7—C8	0.6 (5)	C13—C12—C17—C16	−2.4 (5)
C6—C7—C8—O1	179.1 (3)	C4—C12—C17—C16	177.4 (3)
C6—C7—C8—C9	0.2 (4)	C15—C16—C17—C12	−1.4 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···Cl1^{i}	0.87	2.27	3.106 (3)	160
N3—H3*A*···Cl1^{ii}	0.87	2.44	3.305 (3)	172
N3—H3*B*···Cl1^{i}	0.87	2.56	3.332 (3)	148
C14—H14···O1^{iii}	0.94	2.46	3.300 (4)	148

Symmetry codes: (i) *y*+1, −*x*+*y*+1, *z*+1/6; (ii) *x*+1, *y*+1, *z*; (iii) −*x*+*y*, −*x*+1, *z*+1/3.