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OPEN ACCESS

4-Amino-5-tetradecylamino-4*H*-1,2,4-triazol-1-ium chloride

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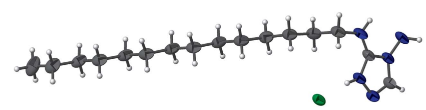
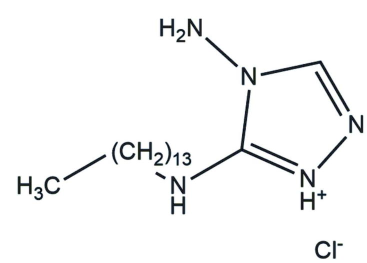
In the crystal of the title molecular salt, $C_{16}H_{34}N_5^+\cdot Cl^-$, (100) bilayers arise in which the tetradecylamino 'tails' (which adopt extended conformations) interdigitate and the triazolium 'heads' associate with the chloride anions through N—H$\cdots$Cl hydrogen bonds.

3D view



Chemical scheme



Structure description

As part of our ongoing synthetic and structural studies of triazole derivatives (El Bakri *et al.*, 2016*a*,*b*), we now describe the synthesis and crystal structure of the title salt, $C_{16}H_{34}N_5^+\cdot Cl^-$ (Fig. 1).

The alkyl chain of the cation adopts an extended conformation. In the crystal, the cations form bilayers with the tetradecylamino chains interdigitating to form the hydrophobic portion (Fig. 2). The triazolium 'heads' and the chloride ions form the hydrophilic portion and are connected through a network of N—H$\cdots$Cl hydrogen bonds (Table 1).

Synthesis and crystallization

A large excess of hydroxylammonium chloride was added to a solution of 6-methyl-7,9-ditetradecyl-7*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]triazepin-8(9*H*)-thione (0.3 g) in ethanol (10 ml). The reaction mixture was stirred for 72 h at room temperature. The solution was then concentrated to dryness under reduced pressure and the residue was recrystallized from ethanol solution to give crystals of the title compound in the form of colourless plates with a yield of 50%.

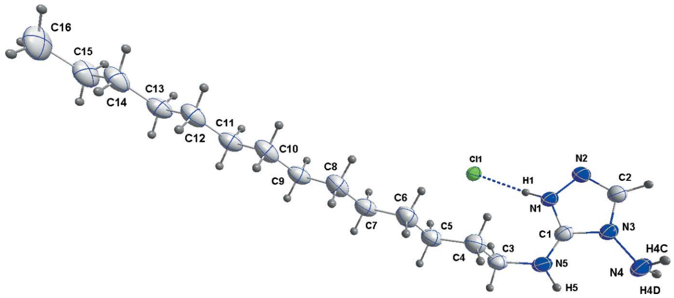


Figure 1
The title compound, showing 50% probability ellipsoids.

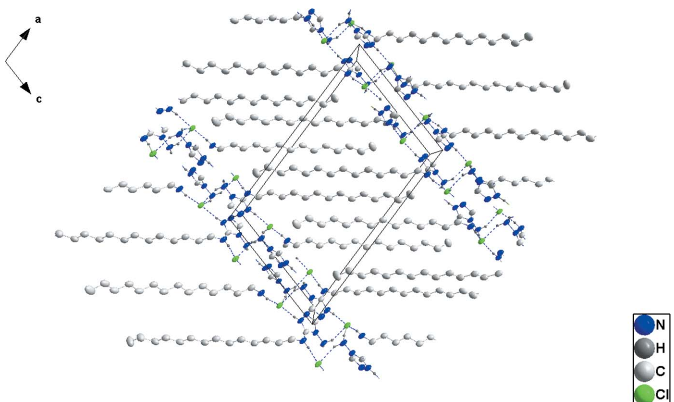


Figure 2
The packing of the title compound, viewed along the b axis, with N—H···Cl hydrogen bonds shown as dotted lines.

Refinement

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

Acknowledgements

The support of NSF–MRI Grant No. 1228232 for the purchase of the diffractometer and Tulane University for support of the Tulane Crystallography Laboratory are gratefully acknowledged.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1	0.86 (3)	2.19 (3)	3.0423 (17)	172 (2)
N4—H4C···Cl1^{i}	0.91 (3)	2.50 (3)	3.3301 (19)	153 (2)
N4—H4D···Cl1^{ii}	0.98 (3)	2.33 (3)	3.253 (2)	156 (3)
N5—H5···Cl1^{iii}	0.86 (3)	2.42 (3)	3.1700 (17)	146 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{34}N_5^+ \cdot Cl^+$
M_r	331.93
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	21.5980 (6), 7.0666 (2), 13.3909 (4)
β (°)	105.031 (2)
V (Å^3)	1973.85 (10)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.74
Crystal size (mm)	0.29 × 0.21 × 0.03
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.82, 0.95
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14321, 3808, 3006
R_{int}	0.048
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.121, 1.07
No. of reflections	3808
No. of parameters	335
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.19

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

References

Brandenburg, K. & Putz, H. (2012). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2016). *APEX3*, *SAINT* and *SADABS* . Bruker AXS Inc., Madison, Wisconsin, USA.
El Bakri, Y., Harmaoui, A., Essassi, E. M., Saadi, M. & El Ammari, L. (2016). *IUCrData*, **1**, x161229.
El Bakri, Y., Harmaoui, A., Sebhaoui, J., Ramli, Y., Essassi, E. M. & Mague, J. T. (2016). *IUCrData*, **1**, x161245.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2016). **1**, x161819 [https://doi.org/10.1107/S2414314616018198]

4-Amino-5-tetradecylamino-4*H*-1,2,4-triazol-1-ium chloride

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4-Amino-5-tetradecylamino-4*H*-1,2,4-triazol-1-ium chloride

Crystal data

$C_{16}H_{34}N_5^+\cdot Cl^+$	$F(000) = 728$
$M_r = 331.93$	$D_x = 1.117$ Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 21.5980$ (6) Å	Cell parameters from 8831 reflections
$b = 7.0666$ (2) Å	$\theta = 4.2–72.1°$
$c = 13.3909$ (4) Å	$\mu = 1.74$ mm^{-1}
$\beta = 105.031$ (2)°	$T = 150$ K
$V = 1973.85$ (10) Å^3	Plate, colourless
$Z = 4$	0.29 × 0.21 × 0.03 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer	$T_{min} = 0.82$, $T_{max} = 0.95$
Radiation source: INCOATEC IμS micro–focus source	14321 measured reflections
Mirror monochromator	3808 independent reflections
Detector resolution: 10.4167 pixels mm^{-1}	3006 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.048$
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)	$\theta_{max} = 72.2°$, $\theta_{min} = 4.2°$
	$h = -23\rightarrow26$
	$k = -8\rightarrow8$
	$l = -16\rightarrow15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	All H-atom parameters refined
$wR(F^2) = 0.121$	$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.6009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
3808 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
335 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
0 restraints	
Primary atom site location: structure-invariant direct methods	

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. 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.

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

	x	y	z	$U_{iso}*/U_{eq}$
N1	0.07493 (9)	0.5920 (2)	0.05555 (12)	0.0415 (4)
H1	0.0856 (11)	0.546 (3)	0.117 (2)	0.054 (7)*
N2	0.04242 (9)	0.7636 (2)	0.03771 (12)	0.0443 (4)
N3	0.05586 (8)	0.6421 (2)	−0.10682 (11)	0.0396 (4)
N4	0.05546 (11)	0.6121 (3)	−0.21102 (12)	0.0482 (5)
H4C	0.0739 (13)	0.716 (4)	−0.231 (2)	0.075 (8)*
H4D	0.0105 (15)	0.599 (4)	−0.251 (2)	0.084 (10)*
N5	0.11118 (10)	0.3574 (2)	−0.04370 (13)	0.0477 (5)
C1	0.08315 (10)	0.5171 (3)	−0.03142 (14)	0.0389 (4)
C2	0.03191 (11)	0.7888 (3)	−0.06109 (15)	0.0430 (5)
H2	0.0101 (12)	0.898 (4)	−0.100 (2)	0.058 (7)*
C3	0.14181 (12)	0.2353 (3)	0.04370 (16)	0.0488 (5)
H3A	0.1459 (11)	0.110 (4)	0.0142 (19)	0.056 (7)*
H3B	0.1142 (10)	0.228 (3)	0.0916 (17)	0.045 (6)*
C4	0.20681 (12)	0.3084 (3)	0.10316 (18)	0.0502 (5)
H4A	0.2357 (11)	0.312 (3)	0.0583 (19)	0.055 (7)*
H4B	0.2016 (10)	0.442 (3)	0.1237 (18)	0.049 (6)*
C5	0.23699 (12)	0.1955 (3)	0.20055 (18)	0.0501 (5)
H5A	0.2424 (12)	0.057 (4)	0.182 (2)	0.069 (8)*
H5B	0.2081 (11)	0.195 (3)	0.2432 (18)	0.047 (6)*
H5	0.1083 (12)	0.323 (4)	−0.106 (2)	0.062 (7)*
C6	0.30078 (12)	0.2777 (3)	0.26025 (19)	0.0530 (6)
H6A	0.3321 (13)	0.276 (4)	0.216 (2)	0.071 (8)*
H6B	0.2924 (12)	0.414 (4)	0.272 (2)	0.065 (7)*
C7	0.33079 (12)	0.1835 (3)	0.36325 (18)	0.0512 (5)
H7A	0.3350 (12)	0.048 (4)	0.352 (2)	0.066 (7)*
H7B	0.3016 (12)	0.197 (3)	0.408 (2)	0.060 (7)*
C8	0.39563 (12)	0.2647 (3)	0.41916 (19)	0.0514 (6)
H8A	0.4242 (12)	0.247 (4)	0.375 (2)	0.067 (8)*
H8B	0.3899 (11)	0.408 (4)	0.4251 (19)	0.057 (7)*
C9	0.42485 (12)	0.1812 (3)	0.52507 (18)	0.0493 (5)
H9A	0.4283 (12)	0.042 (4)	0.522 (2)	0.063 (7)*
H9B	0.3942 (11)	0.200 (3)	0.5684 (18)	0.051 (6)*
C10	0.48964 (12)	0.2627 (3)	0.57950 (19)	0.0517 (6)
H10A	0.5183 (12)	0.243 (3)	0.535 (2)	0.060 (7)*
H10B	0.4858 (12)	0.401 (4)	0.5840 (19)	0.058 (7)*
C11	0.51906 (12)	0.1806 (3)	0.68599 (19)	0.0500 (5)
H11A	0.5241 (13)	0.042 (4)	0.682 (2)	0.074 (8)*
H11B	0.4903 (12)	0.202 (3)	0.7273 (19)	0.055 (7)*
C12	0.58380 (12)	0.2617 (3)	0.7403 (2)	0.0518 (6)

H12A	0.6129 (12)	0.247 (4)	0.694 (2)	0.066 (7)*
H12B	0.5796 (12)	0.399 (4)	0.747 (2)	0.067 (8)*
C13	0.61347 (12)	0.1762 (3)	0.84547 (19)	0.0518 (5)
H13A	0.6157 (12)	0.037 (4)	0.837 (2)	0.063 (7)*
H13B	0.5853 (12)	0.198 (3)	0.889 (2)	0.062 (7)*
C14	0.67833 (12)	0.2564 (3)	0.9004 (2)	0.0544 (6)
H14A	0.7063 (12)	0.241 (4)	0.854 (2)	0.064 (7)*
H14B	0.6741 (12)	0.396 (4)	0.911 (2)	0.062 (7)*
C15	0.70822 (13)	0.1684 (4)	1.0053 (2)	0.0635 (7)
H15A	0.7103 (13)	0.030 (4)	0.995 (2)	0.073 (8)*
H15B	0.6784 (13)	0.185 (4)	1.049 (2)	0.069 (8)*
C16	0.77319 (15)	0.2468 (5)	1.0580 (3)	0.0826 (10)
H16A	0.7733 (14)	0.391 (5)	1.073 (2)	0.088 (10)*
H16B	0.7894 (15)	0.187 (5)	1.123 (3)	0.098 (11)*
H16C	0.8041 (16)	0.224 (4)	1.016 (2)	0.090 (10)*
Cl1	0.09950 (3)	0.43921 (6)	0.27475 (3)	0.04379 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0670 (12)	0.0325 (8)	0.0274 (8)	−0.0044 (7)	0.0165 (7)	−0.0009 (6)
N2	0.0657 (12)	0.0327 (9)	0.0367 (8)	−0.0027 (8)	0.0175 (8)	−0.0005 (6)
N3	0.0599 (10)	0.0343 (8)	0.0265 (7)	−0.0089 (7)	0.0148 (7)	−0.0013 (6)
N4	0.0803 (14)	0.0417 (10)	0.0252 (8)	−0.0128 (9)	0.0183 (8)	−0.0025 (7)
N5	0.0803 (13)	0.0352 (9)	0.0309 (9)	−0.0046 (8)	0.0204 (8)	−0.0054 (7)
C1	0.0566 (12)	0.0327 (10)	0.0293 (9)	−0.0112 (8)	0.0145 (8)	−0.0028 (7)
C2	0.0607 (13)	0.0339 (10)	0.0364 (10)	−0.0081 (9)	0.0159 (9)	−0.0002 (8)
C3	0.0783 (16)	0.0302 (11)	0.0424 (11)	−0.0016 (10)	0.0238 (11)	−0.0014 (8)
C4	0.0688 (15)	0.0392 (12)	0.0497 (12)	0.0012 (10)	0.0281 (11)	0.0033 (9)
C5	0.0690 (15)	0.0368 (12)	0.0512 (12)	0.0049 (10)	0.0277 (11)	0.0024 (9)
C6	0.0643 (15)	0.0448 (13)	0.0566 (13)	0.0088 (11)	0.0275 (11)	0.0079 (10)
C7	0.0701 (16)	0.0351 (12)	0.0564 (13)	0.0071 (10)	0.0311 (12)	0.0022 (9)
C8	0.0591 (14)	0.0414 (12)	0.0627 (14)	0.0105 (10)	0.0319 (12)	0.0098 (10)
C9	0.0664 (15)	0.0318 (11)	0.0577 (13)	0.0048 (9)	0.0304 (11)	0.0050 (9)
C10	0.0613 (15)	0.0377 (12)	0.0659 (14)	0.0121 (10)	0.0343 (12)	0.0115 (10)
C11	0.0645 (15)	0.0336 (11)	0.0606 (13)	0.0040 (9)	0.0320 (12)	0.0060 (9)
C12	0.0586 (14)	0.0367 (12)	0.0704 (15)	0.0084 (10)	0.0351 (12)	0.0098 (10)
C13	0.0647 (15)	0.0343 (11)	0.0644 (14)	0.0045 (10)	0.0312 (12)	0.0078 (9)
C14	0.0554 (14)	0.0369 (12)	0.0790 (16)	0.0094 (10)	0.0317 (12)	0.0141 (10)
C15	0.0630 (16)	0.0485 (15)	0.0837 (18)	0.0079 (12)	0.0273 (14)	0.0217 (13)
C16	0.0629 (19)	0.069 (2)	0.110 (3)	0.0094 (15)	0.0109 (18)	0.0388 (19)
Cl1	0.0688 (3)	0.0359 (3)	0.0283 (2)	0.0019 (2)	0.01565 (19)	0.00279 (16)

Geometric parameters (Å, º)

N1—C1	1.332 (2)	C8—C9	1.514 (3)
N1—N2	1.391 (2)	C8—H8A	0.97 (3)
N1—H1	0.86 (3)	C8—H8B	1.03 (3)

N2—C2	1.295 (3)	C9—C10	1.514 (4)
N3—C1	1.356 (2)	C9—H9A	0.98 (3)
N3—C2	1.372 (3)	C9—H9B	1.00 (2)
N3—N4	1.409 (2)	C10—C11	1.518 (3)
N4—H4C	0.91 (3)	C10—H10A	0.97 (3)
N4—H4D	0.98 (3)	C10—H10B	0.99 (3)
N5—C1	1.311 (3)	C11—C12	1.512 (4)
N5—C3	1.466 (3)	C11—H11A	0.99 (3)
N5—H5	0.86 (3)	C11—H11B	0.94 (3)
C2—H2	0.98 (3)	C12—C13	1.514 (3)
C3—C4	1.514 (3)	C12—H12A	0.99 (3)
C3—H3A	0.98 (2)	C12—H12B	0.98 (3)
C3—H3B	0.98 (2)	C13—C14	1.513 (4)
C4—C5	1.523 (3)	C13—H13A	0.99 (3)
C4—H4A	0.97 (2)	C13—H13B	0.96 (3)
C4—H4B	1.00 (2)	C14—C15	1.518 (4)
C5—C6	1.518 (4)	C14—H14A	0.98 (3)
C5—H5A	1.03 (3)	C14—H14B	1.01 (3)
C5—H5B	0.95 (2)	C15—C16	1.503 (4)
C6—C7	1.517 (3)	C15—H15A	0.99 (3)
C6—H6A	1.00 (3)	C15—H15B	0.98 (3)
C6—H6B	1.00 (3)	C16—H16A	1.04 (3)
C7—C8	1.519 (4)	C16—H16B	0.95 (4)
C7—H7A	0.97 (3)	C16—H16C	0.99 (3)
C7—H7B	0.98 (2)		

C1—N1—N2	111.84 (16)	C9—C8—H8B	109.9 (14)
C1—N1—H1	128.3 (16)	C7—C8—H8B	107.2 (13)
N2—N1—H1	119.8 (16)	H8A—C8—H8B	106 (2)
C2—N2—N1	104.02 (16)	C10—C9—C8	114.30 (19)
C1—N3—C2	107.54 (15)	C10—C9—H9A	109.2 (15)
C1—N3—N4	121.93 (17)	C8—C9—H9A	111.4 (16)
C2—N3—N4	130.53 (17)	C10—C9—H9B	109.8 (13)
N3—N4—H4C	106.2 (17)	C8—C9—H9B	108.4 (13)
N3—N4—H4D	107.8 (18)	H9A—C9—H9B	103.1 (19)
H4C—N4—H4D	111 (2)	C9—C10—C11	114.61 (19)
C1—N5—C3	122.27 (17)	C9—C10—H10A	107.9 (15)
C1—N5—H5	116.5 (17)	C11—C10—H10A	109.8 (15)
C3—N5—H5	121.1 (17)	C9—C10—H10B	109.0 (15)
N5—C1—N1	128.46 (18)	C11—C10—H10B	110.1 (15)
N5—C1—N3	126.38 (17)	H10A—C10—H10B	105 (2)
N1—C1—N3	105.16 (17)	C12—C11—C10	114.62 (19)
N2—C2—N3	111.45 (19)	C12—C11—H11A	107.6 (16)
N2—C2—H2	125.8 (15)	C10—C11—H11A	110.5 (17)
N3—C2—H2	122.8 (15)	C12—C11—H11B	109.0 (15)
N5—C3—C4	112.58 (17)	C10—C11—H11B	108.1 (14)
N5—C3—H3A	106.1 (14)	H11A—C11—H11B	107 (2)
C4—C3—H3A	110.5 (14)	C11—C12—C13	114.32 (19)

N5—C3—H3B	109.0 (13)	C11—C12—H12A	108.6 (15)
C4—C3—H3B	108.1 (13)	C13—C12—H12A	110.5 (15)
H3A—C3—H3B	110.6 (18)	C11—C12—H12B	108.9 (16)
C3—C4—C5	113.84 (18)	C13—C12—H12B	109.7 (16)
C3—C4—H4A	109.9 (14)	H12A—C12—H12B	104 (2)
C5—C4—H4A	110.0 (14)	C14—C13—C12	114.73 (19)
C3—C4—H4B	108.2 (13)	C14—C13—H13A	111.1 (15)
C5—C4—H4B	108.3 (13)	C12—C13—H13A	108.0 (16)
H4A—C4—H4B	106.3 (19)	C14—C13—H13B	107.1 (15)
C6—C5—C4	112.28 (19)	C12—C13—H13B	108.8 (15)
C6—C5—H5A	110.3 (15)	H13A—C13—H13B	107 (2)
C4—C5—H5A	110.3 (15)	C13—C14—C15	114.5 (2)
C6—C5—H5B	109.5 (14)	C13—C14—H14A	107.3 (15)
C4—C5—H5B	108.4 (14)	C15—C14—H14A	110.8 (15)
H5A—C5—H5B	106 (2)	C13—C14—H14B	109.3 (14)
C7—C6—C5	115.3 (2)	C15—C14—H14B	107.9 (15)
C7—C6—H6A	109.5 (16)	H14A—C14—H14B	107 (2)
C5—C6—H6A	110.2 (16)	C16—C15—C14	113.8 (2)
C7—C6—H6B	109.5 (15)	C16—C15—H15A	111.1 (16)
C5—C6—H6B	105.9 (15)	C14—C15—H15A	107.2 (17)
H6A—C6—H6B	106 (2)	C16—C15—H15B	110.8 (16)
C6—C7—C8	113.87 (19)	C14—C15—H15B	108.4 (16)
C6—C7—H7A	109.1 (16)	H15A—C15—H15B	105 (2)
C8—C7—H7A	109.5 (15)	C15—C16—H16A	114.1 (17)
C6—C7—H7B	108.8 (15)	C15—C16—H16B	110 (2)
C8—C7—H7B	108.6 (15)	H16A—C16—H16B	106 (3)
H7A—C7—H7B	107 (2)	C15—C16—H16C	111 (2)
C9—C8—C7	114.95 (19)	H16A—C16—H16C	108 (3)
C9—C8—H8A	110.1 (16)	H16B—C16—H16C	108 (3)
C7—C8—H8A	107.7 (16)		

C1—N1—N2—C2	−0.3 (2)	N5—C3—C4—C5	174.31 (18)
C3—N5—C1—N1	−2.9 (3)	C3—C4—C5—C6	−177.71 (19)
C3—N5—C1—N3	177.3 (2)	C4—C5—C6—C7	174.63 (19)
N2—N1—C1—N5	−179.6 (2)	C5—C6—C7—C8	177.98 (19)
N2—N1—C1—N3	0.3 (2)	C6—C7—C8—C9	176.51 (19)
C2—N3—C1—N5	179.7 (2)	C7—C8—C9—C10	179.65 (18)
N4—N3—C1—N5	−0.7 (3)	C8—C9—C10—C11	179.65 (19)
C2—N3—C1—N1	−0.1 (2)	C9—C10—C11—C12	179.90 (19)
N4—N3—C1—N1	179.50 (17)	C10—C11—C12—C13	−178.78 (19)
N1—N2—C2—N3	0.2 (2)	C11—C12—C13—C14	180.0 (2)
C1—N3—C2—N2	0.0 (2)	C12—C13—C14—C15	−179.3 (2)
N4—N3—C2—N2	−179.61 (19)	C13—C14—C15—C16	178.8 (3)
C1—N5—C3—C4	−77.5 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1	0.86 (3)	2.19 (3)	3.0423 (17)	172 (2)
N4—H4*C*···Cl1^{i}	0.91 (3)	2.50 (3)	3.3301 (19)	153 (2)
N4—H4*D*···Cl1^{ii}	0.98 (3)	2.33 (3)	3.253 (2)	156 (3)
N5—H5···Cl1^{iii}	0.86 (3)	2.42 (3)	3.1700 (17)	146 (2)

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