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2-Chloro-4,6-bis(1,1,3,3-tetramethylbutylamino)-*s*-triazine

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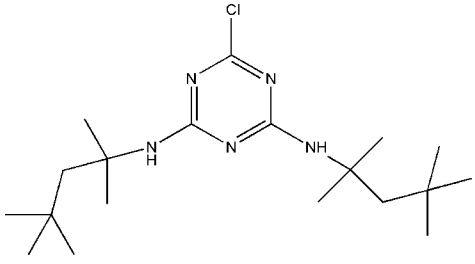
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.049; wR factor = 0.163; data-to-parameter ratio = 13.8.

In the title compound, $C_{19}H_{36}ClN_5$, intermolecular N—H···N hydrogen bonds link the molecules into zigzag chains.

Related literature

For general background, see Borzatta & Carrozza (1991). For related structures, see Deng *et al.* (2006). For related literature, see: Kaiser & Thurston (1951).



Experimental

Crystal data

$C_{19}H_{36}ClN_5$
M_r = 369.98
Orthorhombic, *Pbca*
a = 11.9729 (18) Å
b = 16.584 (2) Å
c = 22.581 (4) Å
V = 4483.6 (12) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 294 (2) K
0.22 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.982
21444 measured reflections
3904 independent reflections
1999 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.163
S = 1.04
3904 reflections
282 parameters
120 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···N3^{i}	0.86	2.39	3.245 (4)	174
N5—H5···N2^{ii}	0.86	2.29	3.147 (3)	179

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RN2026).

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supplementary materials

Acta Cryst. (2007). E**63**, o3327 [**doi:10.1107/S1600536807030334**]

2-Chloro-4,6-bis(1,1,3,3-tetramethylbutylamino)-*s*-triazine

F.-Y. Yan

Comment

The title compound, (I), has attracted much attention as an important intermediate in the synthesis of hindered light stabilizers (Borzatta & Carrozza, 1991). These triazine ring containing compounds are widely used (Deng *et al.*, 2006). Herein we report the crystal structure of the title compound (Fig. 1).

The triazine ring in (I) is essentially planar despite having two substituents. The r.m.s. deviation from the mean plane is 0.009 (7) Å.

Intermolecular N—H···N hydrogen bonds are observed which link the molecules into zigzag chains.

Experimental

The title compound was prepared according to the method of Kaiser & Thurston (1951). 2,4,6-Trichloro-1,3,5-triazine (40.0 g, 0.217 mol) was dissolved in toluene (120 ml) and then cooled to 278 K. With stirring, a solution of 2,4,4-trimethylpentan-2-amine (27.5 g, 0.213 mol) in toluene (50 ml) was then added dropwise to the mixture over a period of 0.5 h. A solution of Na_2CO_3 (23.02 g, 0.217 mol) in water (50 ml) was then added dropwise for 0.5 h. The mixture was stirred at 273–278 K for a further 3 h. Another portion of 2,4,4-trimethylpentan-2-amine (27.5 g, 0.213 mol) and solid Na_2CO_3 (23.02 g, 0.217 mol) were added to the mixture, maintaining the temperature at 338 k for 5 h. The organic layer was washed with water and then concentrated *in vacuo*. The title compound (67.9 g) was obtained in powder form in a yield of 85.5%. Crystals of (I) were obtained by slow evaporation of a solution of methanol (m.p. 427–429 K).

Refinement

All H atoms were constrained; positioned geometrically (C—H=0.96–0.97 Å) and refined as riding with U_{iso}(H)=1.2U_{eq}(carrier) or 1.5$_{eq}$(methyl groups). Atoms C9, C10 and C11 are disordered over two conformations with an occupancy ratio of 0.61 (3):0.39 (3) and atoms C17, C18 and C19 are disordered over two conformations in a 0.758 (9):0.242 (9) ratio.

Figures

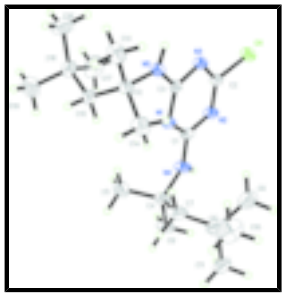


Fig. 1. A view of the molecule (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. The disordered methyl groups are omitted for clarity.

2-Chloro-4,6-bis(1,1,3,3-tetramethylbutylamino)-s-triazine

Crystal data

$C_{19}H_{36}ClN_5$	D_x = 1.096 Mg m^{-3}
M_r = 369.98	Melting point: 154-156 K
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
a = 11.9729 (18) Å	Cell parameters from 2903 reflections
b = 16.584 (2) Å	θ = 2.3–21.2º
c = 22.581 (4) Å	μ = 0.18 mm^{-1}
V = 4483.6 (12) Å^3	*T* = 294 (2) K
Z = 8	Block, colorless
F_{000} = 1616	0.22 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3904 independent reflections
Radiation source: fine-focus sealed tube	1999 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.086
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −10→14
T_{min} = 0.961, T_{max} = 0.982	*k* = −16→19
21444 measured reflections	*l* = −26→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H-atom parameters constrained
$wR(F^2)$ = 0.163	$w = 1/[\sigma^2(F_o^2) + (0.0711P)^2 + 1.3408P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
3904 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
282 parameters	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
120 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl1	0.06499 (7)	0.22660 (5)	0.33227 (4)	0.0512 (3)	
N1	0.0743 (2)	0.08356 (15)	0.16893 (10)	0.0354 (6)	
N3	0.1692 (2)	0.14722 (15)	0.25042 (11)	0.0367 (6)	
N2	−0.0295 (2)	0.14834 (16)	0.24687 (11)	0.0384 (7)	
N4	−0.1201 (2)	0.08910 (16)	0.16998 (11)	0.0438 (7)	
H4	−0.1780	0.1006	0.1908	0.053*	
N5	0.2677 (2)	0.08484 (14)	0.17770 (11)	0.0365 (6)	
H5	0.3233	0.1024	0.1981	0.044*	
C1	−0.0220 (3)	0.10610 (18)	0.19509 (13)	0.0349 (7)	
C2	0.0689 (3)	0.16651 (17)	0.26901 (13)	0.0347 (7)	
C3	0.1671 (2)	0.10456 (17)	0.19841 (13)	0.0328 (7)	
C4	−0.1430 (3)	0.0532 (2)	0.11131 (15)	0.0491 (9)	
C5	−0.0922 (3)	−0.0317 (2)	0.10735 (18)	0.0696 (12)	
H5A	−0.0122	−0.0279	0.1086	0.104*	
H5B	−0.1147	−0.0566	0.0709	0.104*	
H5C	−0.1179	−0.0636	0.1401	0.104*	
C6	−0.2708 (3)	0.0443 (3)	0.10853 (16)	0.0620 (11)	
H6A	−0.3049	0.0966	0.1106	0.093*	
H6B	−0.2959	0.0120	0.1412	0.093*	
H6C	−0.2914	0.0187	0.0720	0.093*	
C7	−0.0953 (3)	0.1046 (3)	0.06081 (16)	0.0636 (11)	
H7A	−0.0148	0.1034	0.0657	0.076*	
H7B	−0.1110	0.0752	0.0246	0.076*	
C8	−0.1256 (3)	0.1924 (3)	0.04815 (17)	0.0746 (12)	
C9	−0.1280 (13)	0.2466 (7)	0.1047 (4)	0.082 (3)	0.61 (3)
H9A	−0.1479	0.3007	0.0938	0.124*	0.61 (3)

H9B	−0.0555	0.2467	0.1229	0.124*	0.61 (3)
H9C	−0.1820	0.2258	0.1321	0.124*	0.61 (3)
C10	−0.0428 (10)	0.2347 (12)	0.0057 (7)	0.105 (4)	0.61 (3)
H10A	−0.0659	0.2895	−0.0003	0.157*	0.61 (3)
H10B	−0.0419	0.2069	−0.0316	0.157*	0.61 (3)
H10C	0.0306	0.2339	0.0227	0.157*	0.61 (3)
C11	−0.2464 (7)	0.1932 (10)	0.0228 (6)	0.068 (3)	0.61 (3)
H11A	−0.2684	0.2478	0.0147	0.103*	0.61 (3)
H11B	−0.2966	0.1701	0.0513	0.103*	0.61 (3)
H11C	−0.2487	0.1623	−0.0131	0.103*	0.61 (3)
C9'	−0.079 (3)	0.2461 (13)	0.0978 (9)	0.105 (6)	0.39 (3)
H9'A	−0.0983	0.3013	0.0902	0.158*	0.39 (3)
H9'B	0.0010	0.2409	0.0991	0.158*	0.39 (3)
H9'C	−0.1099	0.2296	0.1351	0.158*	0.39 (3)
C10'	−0.0550 (16)	0.2007 (15)	−0.0096 (7)	0.080 (5)	0.39 (3)
H10D	−0.0634	0.2541	−0.0254	0.119*	0.39 (3)
H10E	−0.0803	0.1620	−0.0382	0.119*	0.39 (3)
H10F	0.0223	0.1910	−0.0007	0.119*	0.39 (3)
C11'	−0.2416 (12)	0.2242 (16)	0.0303 (12)	0.082 (6)	0.39 (3)
H11D	−0.2384	0.2817	0.0256	0.123*	0.39 (3)
H11E	−0.2948	0.2109	0.0605	0.123*	0.39 (3)
H11F	−0.2638	0.1998	−0.0065	0.123*	0.39 (3)
C12	0.2972 (3)	0.03718 (19)	0.12475 (14)	0.0412 (8)	
C13	0.4244 (3)	0.0404 (2)	0.11983 (18)	0.0630 (11)	
H13A	0.4483	0.0956	0.1179	0.095*	
H13B	0.4478	0.0127	0.0846	0.095*	
H13C	0.4572	0.0150	0.1539	0.095*	
C14	0.2474 (3)	0.0762 (2)	0.06931 (14)	0.0589 (10)	
H14A	0.2739	0.1306	0.0660	0.088*	
H14B	0.1674	0.0763	0.0722	0.088*	
H14C	0.2697	0.0461	0.0350	0.088*	
C15	0.2529 (3)	−0.05055 (19)	0.12883 (15)	0.0472 (9)	
H15A	0.1725	−0.0471	0.1243	0.057*	
H15B	0.2806	−0.0782	0.0939	0.057*	
C16	0.2736 (3)	−0.1075 (2)	0.18095 (17)	0.0587 (10)	
C17	0.1935 (7)	−0.0847 (4)	0.2326 (3)	0.089 (2)	0.758 (9)
H17A	0.2063	−0.1200	0.2656	0.133*	0.758 (9)
H17B	0.1175	−0.0899	0.2196	0.133*	0.758 (9)
H17C	0.2072	−0.0299	0.2445	0.133*	0.758 (9)
C18	0.3921 (5)	−0.1080 (4)	0.2060 (3)	0.092 (2)	0.758 (9)
H18A	0.4437	−0.1229	0.1754	0.138*	0.758 (9)
H18B	0.3966	−0.1461	0.2379	0.138*	0.758 (9)
H18C	0.4103	−0.0551	0.2204	0.138*	0.758 (9)
C19	0.2426 (7)	−0.1919 (3)	0.1590 (4)	0.088 (2)	0.758 (9)
H19A	0.2918	−0.2072	0.1274	0.132*	0.758 (9)
H19B	0.1669	−0.1917	0.1450	0.132*	0.758 (9)
H19C	0.2496	−0.2297	0.1910	0.132*	0.758 (9)
C17'	0.277 (2)	−0.0737 (11)	0.2437 (5)	0.081 (6)	0.242 (9)
H17D	0.3526	−0.0601	0.2538	0.122*	0.242 (9)

H17E	0.2495	−0.1135	0.2709	0.122*	0.242 (9)
H17F	0.2312	−0.0263	0.2459	0.122*	0.242 (9)
C18'	0.3859 (13)	−0.1499 (13)	0.1679 (11)	0.094 (6)	0.242 (9)
H18D	0.3987	−0.1507	0.1259	0.141*	0.242 (9)
H18E	0.3833	−0.2042	0.1826	0.141*	0.242 (9)
H18F	0.4454	−0.1212	0.1871	0.141*	0.242 (9)
C19'	0.1904 (18)	−0.1786 (12)	0.1821 (11)	0.086 (7)	0.242 (9)
H19D	0.2102	−0.2168	0.1519	0.129*	0.242 (9)
H19E	0.1163	−0.1588	0.1748	0.129*	0.242 (9)
H19F	0.1929	−0.2042	0.2201	0.129*	0.242 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0463 (5)	0.0593 (6)	0.0481 (5)	0.0011 (4)	−0.0006 (4)	−0.0154 (4)
N1	0.0265 (14)	0.0436 (15)	0.0361 (14)	0.0013 (12)	−0.0037 (13)	−0.0017 (12)
N3	0.0291 (15)	0.0418 (15)	0.0391 (15)	−0.0026 (12)	−0.0005 (12)	−0.0017 (13)
N2	0.0276 (14)	0.0516 (17)	0.0360 (15)	0.0011 (12)	−0.0020 (12)	−0.0026 (13)
N4	0.0255 (14)	0.0683 (19)	0.0375 (15)	−0.0001 (13)	−0.0035 (13)	−0.0078 (14)
N5	0.0265 (14)	0.0413 (15)	0.0418 (16)	−0.0019 (12)	0.0007 (12)	−0.0049 (12)
C1	0.0309 (17)	0.0409 (18)	0.0329 (17)	−0.0001 (15)	−0.0005 (15)	0.0063 (15)
C2	0.0345 (18)	0.0383 (18)	0.0312 (16)	−0.0006 (16)	0.0012 (16)	0.0001 (14)
C3	0.0318 (18)	0.0301 (17)	0.0364 (18)	−0.0003 (14)	−0.0004 (15)	0.0055 (15)
C4	0.0330 (19)	0.071 (3)	0.044 (2)	0.0026 (18)	−0.0087 (16)	−0.0126 (18)
C5	0.053 (3)	0.076 (3)	0.080 (3)	0.007 (2)	−0.008 (2)	−0.031 (2)
C6	0.035 (2)	0.096 (3)	0.055 (2)	−0.002 (2)	−0.0122 (18)	−0.018 (2)
C7	0.039 (2)	0.108 (3)	0.044 (2)	0.007 (2)	−0.0056 (17)	−0.002 (2)
C8	0.061 (3)	0.106 (4)	0.056 (3)	−0.002 (3)	−0.007 (2)	0.026 (3)
C9	0.070 (7)	0.066 (5)	0.111 (6)	−0.007 (5)	−0.021 (5)	0.023 (4)
C10	0.087 (6)	0.120 (8)	0.107 (7)	−0.013 (6)	0.014 (5)	0.035 (6)
C11	0.063 (5)	0.075 (7)	0.067 (5)	0.024 (4)	−0.011 (4)	0.009 (5)
C9'	0.110 (10)	0.092 (8)	0.113 (8)	−0.014 (8)	−0.013 (8)	0.005 (7)
C10'	0.068 (7)	0.085 (9)	0.086 (8)	−0.007 (6)	0.005 (6)	0.029 (6)
C11'	0.074 (7)	0.084 (10)	0.088 (8)	0.007 (6)	0.004 (6)	0.006 (8)
C12	0.0330 (18)	0.0426 (19)	0.048 (2)	0.0004 (15)	0.0044 (16)	−0.0034 (16)
C13	0.039 (2)	0.071 (3)	0.080 (3)	−0.004 (2)	0.022 (2)	−0.023 (2)
C14	0.069 (3)	0.067 (3)	0.041 (2)	−0.001 (2)	0.0097 (19)	0.0026 (19)
C15	0.0397 (19)	0.044 (2)	0.058 (2)	0.0040 (16)	−0.0058 (17)	−0.0059 (17)
C16	0.063 (3)	0.043 (2)	0.071 (3)	0.0043 (19)	−0.010 (2)	0.0045 (19)
C17	0.115 (6)	0.074 (4)	0.077 (4)	0.009 (4)	0.017 (4)	0.035 (3)
C18	0.087 (4)	0.092 (5)	0.098 (5)	0.010 (4)	−0.039 (4)	0.018 (4)
C19	0.113 (6)	0.052 (3)	0.100 (5)	−0.013 (4)	−0.011 (4)	−0.001 (3)
C17'	0.096 (10)	0.074 (8)	0.074 (8)	0.004 (8)	−0.009 (8)	0.019 (7)
C18'	0.090 (9)	0.087 (9)	0.105 (10)	0.007 (8)	−0.013 (8)	0.013 (8)
C19'	0.098 (10)	0.068 (9)	0.093 (10)	−0.014 (8)	0.004 (8)	−0.008 (7)

Geometric parameters (Å, °)

Cl1—C2	1.742 (3)	C10'—H10D	0.9600

N1—C3	1.341 (4)	C10'—H10E	0.9600
N1—C1	1.349 (4)	C10'—H10F	0.9600
N3—C2	1.311 (3)	C11'—H11D	0.9600
N3—C3	1.371 (4)	C11'—H11E	0.9600
N2—C2	1.315 (4)	C11'—H11F	0.9600
N2—C1	1.366 (4)	C12—C13	1.528 (4)
N4—C1	1.334 (4)	C12—C14	1.530 (5)
N4—C4	1.478 (4)	C12—C15	1.551 (5)
N4—H4	0.8600	C13—H13A	0.9600
N5—C3	1.333 (4)	C13—H13B	0.9600
N5—C12	1.476 (4)	C13—H13C	0.9600
N5—H5	0.8600	C14—H14A	0.9600
C4—C7	1.534 (5)	C14—H14B	0.9600
C4—C5	1.537 (5)	C14—H14C	0.9600
C4—C6	1.538 (4)	C15—C16	1.530 (5)
C5—H5A	0.9600	C15—H15A	0.9700
C5—H5B	0.9600	C15—H15B	0.9700
C5—H5C	0.9600	C16—C17'	1.524 (9)
C6—H6A	0.9600	C16—C18	1.527 (6)
C6—H6B	0.9600	C16—C19	1.530 (6)
C6—H6C	0.9600	C16—C19'	1.543 (10)
C7—C8	1.529 (6)	C16—C18'	1.546 (9)
C7—H7A	0.9700	C16—C17	1.557 (6)
C7—H7B	0.9700	C17—H17A	0.9600
C8—C9'	1.536 (9)	C17—H17B	0.9600
C8—C11'	1.539 (9)	C17—H17C	0.9600
C8—C10	1.546 (8)	C18—H18A	0.9600
C8—C11	1.556 (7)	C18—H18B	0.9600
C8—C10'	1.560 (9)	C18—H18C	0.9600
C8—C9	1.561 (8)	C19—H19A	0.9600
C9—H9A	0.9600	C19—H19B	0.9600
C9—H9B	0.9600	C19—H19C	0.9600
C9—H9C	0.9600	C17'—H17D	0.9600
C10—H10A	0.9600	C17'—H17E	0.9600
C10—H10B	0.9600	C17'—H17F	0.9600
C10—H10C	0.9600	C18'—H18D	0.9600
C11—H11A	0.9600	C18'—H18E	0.9600
C11—H11B	0.9600	C18'—H18F	0.9600
C11—H11C	0.9600	C19'—H19D	0.9600
C9'—H9'A	0.9600	C19'—H19E	0.9600
C9'—H9'B	0.9600	C19'—H19F	0.9600
C9'—H9'C	0.9600		
C3—N1—C1	114.8 (2)	C8—C10'—H10F	109.5
C2—N3—C3	112.5 (2)	H10D—C10'—H10F	109.5
C2—N2—C1	112.6 (3)	H10E—C10'—H10F	109.5
C1—N4—C4	129.0 (3)	C8—C11'—H11D	109.5
C1—N4—H4	115.5	C8—C11'—H11E	109.5
C4—N4—H4	115.5	H11D—C11'—H11E	109.5
C3—N5—C12	129.2 (3)	C8—C11'—H11F	109.5

C3—N5—H5	115.4	H11D—C11'—H11F	109.5
C12—N5—H5	115.4	H11E—C11'—H11F	109.5
N4—C1—N1	120.5 (3)	N5—C12—C13	106.2 (3)
N4—C1—N2	114.5 (3)	N5—C12—C14	110.1 (3)
N1—C1—N2	125.0 (3)	C13—C12—C14	108.3 (3)
N3—C2—N2	130.0 (3)	N5—C12—C15	111.8 (3)
N3—C2—Cl1	115.3 (2)	C13—C12—C15	112.2 (3)
N2—C2—Cl1	114.8 (2)	C14—C12—C15	108.2 (3)
N5—C3—N1	120.7 (3)	C12—C13—H13A	109.5
N5—C3—N3	114.2 (3)	C12—C13—H13B	109.5
N1—C3—N3	125.1 (3)	H13A—C13—H13B	109.5
N4—C4—C7	111.9 (3)	C12—C13—H13C	109.5
N4—C4—C5	110.3 (3)	H13A—C13—H13C	109.5
C7—C4—C5	108.5 (3)	H13B—C13—H13C	109.5
N4—C4—C6	105.1 (3)	C12—C14—H14A	109.5
C7—C4—C6	113.2 (3)	C12—C14—H14B	109.5
C5—C4—C6	107.7 (3)	H14A—C14—H14B	109.5
C4—C5—H5A	109.5	C12—C14—H14C	109.5
C4—C5—H5B	109.5	H14A—C14—H14C	109.5
H5A—C5—H5B	109.5	H14B—C14—H14C	109.5
C4—C5—H5C	109.5	C16—C15—C12	124.7 (3)
H5A—C5—H5C	109.5	C16—C15—H15A	106.1
H5B—C5—H5C	109.5	C12—C15—H15A	106.1
C4—C6—H6A	109.5	C16—C15—H15B	106.1
C4—C6—H6B	109.5	C12—C15—H15B	106.1
H6A—C6—H6B	109.5	H15A—C15—H15B	106.3
C4—C6—H6C	109.5	C17'—C16—C18	68.4 (10)
H6A—C6—H6C	109.5	C17'—C16—C15	119.5 (8)
H6B—C6—H6C	109.5	C18—C16—C15	116.0 (4)
C8—C7—C4	125.4 (3)	C17'—C16—C19	130.1 (9)
C8—C7—H7A	106.0	C18—C16—C19	110.0 (4)
C4—C7—H7A	106.0	C15—C16—C19	106.0 (4)
C8—C7—H7B	106.0	C17'—C16—C19'	106.4 (13)
C4—C7—H7B	106.0	C18—C16—C19'	126.2 (10)
H7A—C7—H7B	106.3	C15—C16—C19'	112.3 (10)
C7—C8—C9'	109.2 (10)	C19—C16—C19'	31.8 (9)
C7—C8—C11'	126.1 (11)	C17'—C16—C18'	108.7 (13)
C9'—C8—C11'	108.8 (11)	C18—C16—C18'	42.3 (9)
C7—C8—C10	113.3 (8)	C15—C16—C18'	106.0 (9)
C9'—C8—C10	87.5 (9)	C19—C16—C18'	74.5 (10)
C11'—C8—C10	105.1 (11)	C19'—C16—C18'	102.6 (13)
C7—C8—C11	107.3 (7)	C17'—C16—C17	39.7 (9)
C9'—C8—C11	127.0 (11)	C18—C16—C17	107.2 (5)
C11'—C8—C11	20.2 (10)	C15—C16—C17	109.0 (3)
C10—C8—C11	111.4 (9)	C19—C16—C17	108.4 (5)
C7—C8—C10'	96.4 (9)	C19'—C16—C17	77.0 (10)
C9'—C8—C10'	111.2 (10)	C18'—C16—C17	142.2 (9)
C11'—C8—C10'	103.9 (12)	C16—C17—H17A	109.5
C10—C8—C10'	25.2 (8)	C16—C17—H17B	109.5

C11—C8—C10'	101.3 (10)	H17A—C17—H17B	109.5
C7—C8—C9	113.6 (5)	C16—C17—H17C	109.5
C9'—C8—C9	22.7 (10)	H17A—C17—H17C	109.5
C11'—C8—C9	90.1 (10)	H17B—C17—H17C	109.5
C10—C8—C9	104.9 (8)	C16—C18—H18A	109.5
C11—C8—C9	106.2 (7)	C16—C18—H18B	109.5
C10'—C8—C9	130.0 (9)	H18A—C18—H18B	109.5
C8—C9—H9A	109.5	C16—C18—H18C	109.5
C8—C9—H9B	109.5	H18A—C18—H18C	109.5
H9A—C9—H9B	109.5	H18B—C18—H18C	109.5
C8—C9—H9C	109.5	C16—C19—H19A	109.5
H9A—C9—H9C	109.5	C16—C19—H19B	109.5
H9B—C9—H9C	109.5	H19A—C19—H19B	109.5
C8—C10—H10A	109.5	C16—C19—H19C	109.5
C8—C10—H10B	109.5	H19A—C19—H19C	109.5
H10A—C10—H10B	109.5	H19B—C19—H19C	109.5
C8—C10—H10C	109.5	C16—C17'—H17D	109.5
H10A—C10—H10C	109.5	C16—C17'—H17E	109.5
H10B—C10—H10C	109.5	H17D—C17'—H17E	109.5
C8—C11—H11A	109.5	C16—C17'—H17F	109.5
C8—C11—H11B	109.5	H17D—C17'—H17F	109.5
H11A—C11—H11B	109.5	H17E—C17'—H17F	109.5
C8—C11—H11C	109.5	C16—C18'—H18D	109.5
H11A—C11—H11C	109.5	C16—C18'—H18E	109.5
H11B—C11—H11C	109.5	H18D—C18'—H18E	109.5
C8—C9'—H9'A	109.5	C16—C18'—H18F	109.5
C8—C9'—H9'B	109.5	H18D—C18'—H18F	109.5
H9'A—C9'—H9'B	109.5	H18E—C18'—H18F	109.5
C8—C9'—H9'C	109.5	C16—C19'—H19D	109.5
H9'A—C9'—H9'C	109.5	C16—C19'—H19E	109.5
H9'B—C9'—H9'C	109.5	H19D—C19'—H19E	109.5
C8—C10'—H10D	109.5	C16—C19'—H19F	109.5
C8—C10'—H10E	109.5	H19D—C19'—H19F	109.5
H10D—C10'—H10E	109.5	H19E—C19'—H19F	109.5
C4—N4—C1—N1	−6.4 (5)	C5—C4—C7—C8	178.9 (3)
C4—N4—C1—N2	172.2 (3)	C6—C4—C7—C8	59.5 (5)
C3—N1—C1—N4	179.7 (3)	C4—C7—C8—C9'	69.0 (13)
C3—N1—C1—N2	1.2 (4)	C4—C7—C8—C11'	−63.6 (14)
C2—N2—C1—N4	−177.6 (3)	C4—C7—C8—C10	164.7 (9)
C2—N2—C1—N1	1.0 (4)	C4—C7—C8—C11	−71.9 (7)
C3—N3—C2—N2	3.2 (4)	C4—C7—C8—C10'	−175.9 (10)
C3—N3—C2—Cl1	−175.90 (19)	C4—C7—C8—C9	45.1 (8)
C1—N2—C2—N3	−3.4 (5)	C3—N5—C12—C13	175.0 (3)
C1—N2—C2—Cl1	175.6 (2)	C3—N5—C12—C14	58.0 (4)
C12—N5—C3—N1	−2.9 (4)	C3—N5—C12—C15	−62.2 (4)
C12—N5—C3—N3	177.6 (3)	N5—C12—C15—C16	−52.4 (4)
C1—N1—C3—N5	179.0 (3)	C13—C12—C15—C16	66.8 (4)
C1—N1—C3—N3	−1.5 (4)	C14—C12—C15—C16	−173.7 (3)
C2—N3—C3—N5	179.1 (2)	C12—C15—C16—C17'	35.9 (13)

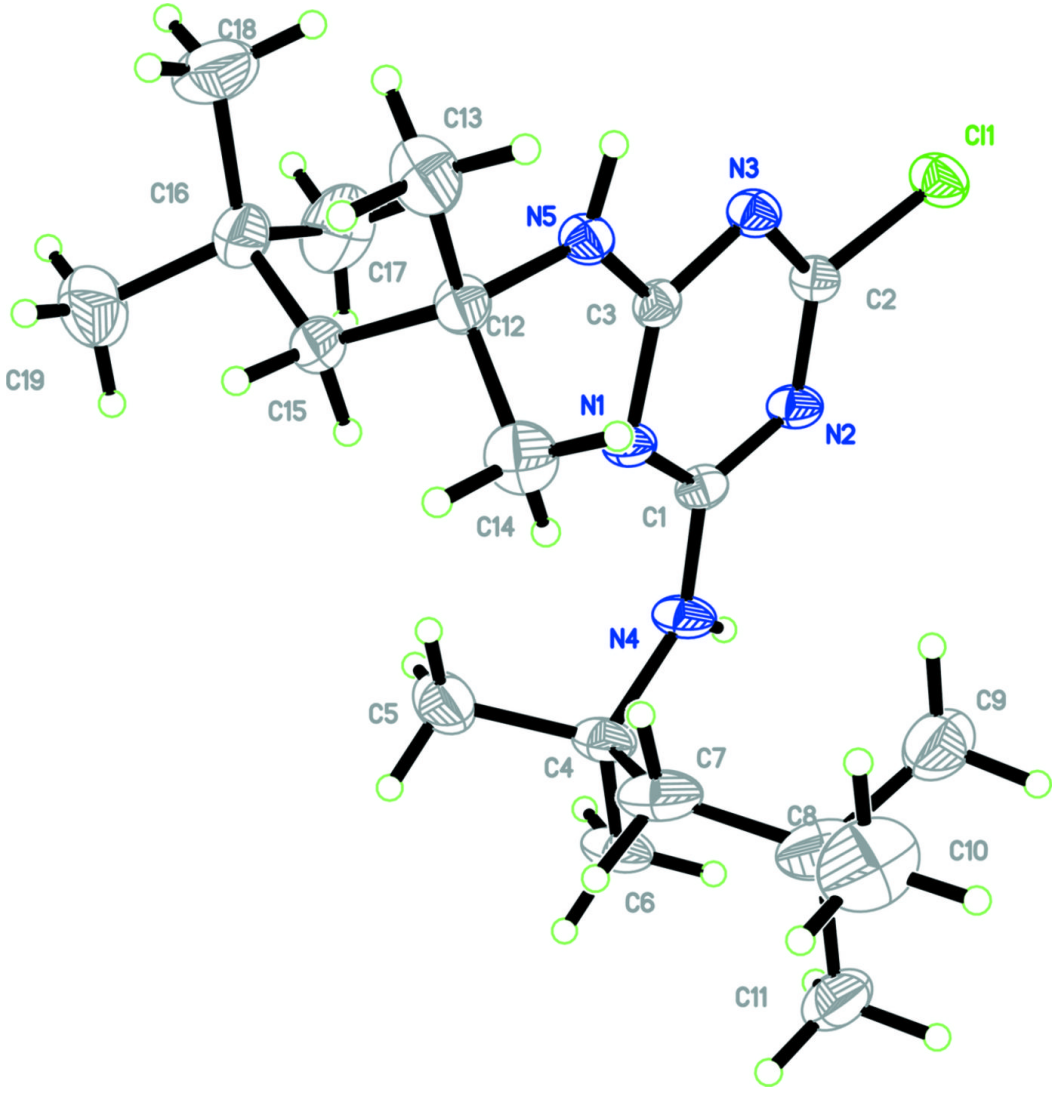
C2—N3—C3—N1	−0.4 (4)	C12—C15—C16—C18	−42.9 (6)
C1—N4—C4—C7	−59.6 (4)	C12—C15—C16—C19	−165.3 (5)
C1—N4—C4—C5	61.4 (4)	C12—C15—C16—C19'	161.6 (11)
C1—N4—C4—C6	177.2 (3)	C12—C15—C16—C18'	−87.2 (11)
N4—C4—C7—C8	−59.1 (4)	C12—C15—C16—C17	78.2 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···N3^{i}	0.86	2.39	3.245 (4)	174
N5—H5···N2^{ii}	0.86	2.29	3.147 (3)	179

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

Fig. 1


C18
C13
C16
N5
N3
Cl1
C17
C12
C3
C2
C19
C15
N1
N2
C14
C1
N4
C5
C9
C4
C7
C8
C10
C6
C11