Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6-Chloro-N^2-propyl-N^4-(2,4,4-trimethylpentan-2-yl)-1,3,5-triazine-2,4-diamine

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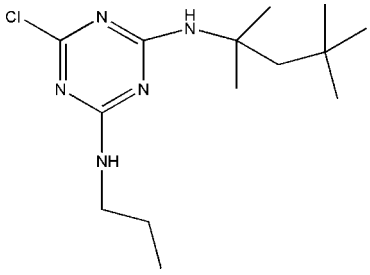
Received 28 May 2007; accepted 28 May 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.061; wR factor = 0.199; data-to-parameter ratio = 13.5.

In the title compound, $C_{14}H_{26}ClN_5$, the triazine ring is almost planar and both pendant alkyl chains are disordered; the site occupancy ratios are 0.5:0.5 for the *tert*-butyl chain and approximately 0.6:0.4 for the *n*-propyl chain. The crystal packing is consolidated by N—H···N hydrogen bonds, resulting in infinite chains propagating along [001].

Related literature

For a related structure, see: Deng *et al.* (2006). For background, see: Kaiser & Thurston (1951); Borzatta & Carrozza, (1991).



Experimental

Crystal data

$C_{14}H_{26}ClN_5$
M_r = 299.85
Monoclinic, $C2/c$
a = 19.354 (4) Å
b = 8.1265 (16) Å
c = 22.312 (4) Å
β = 98.211 (4)°
V = 3473.3 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 294 (2) K
0.24 × 0.20 × 0.14 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.949, T_{max} = 0.970
8715 measured reflections
3070 independent reflections
1927 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.200
S = 1.04
3070 reflections
227 parameters
124 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···N1^{i}	0.86	2.25	3.099 (4)	169
N5—H5···N2^{ii}	0.86	2.38	3.135 (4)	147

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

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: HB2437).

References

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  doi:10.1107/S1600536807025950

supplementary materials

Acta Cryst. (2007). E**63**, o3096 [**doi:10.1107/S1600536807025950**]

6-Chloro-N^2-propyl-N^4-(2,4,4-trimethylpentan-2-yl)-1,3,5-triazine-2,4-diamine

Y.-P. Jiang, T. Qiu, L.-E. Wang and J.-N. Wang

Comment

The title compound, (I), is an important intermediate of hindered light stabilizers (Borzatta & Carrozza, 1991). The triazine ring in (I) is essentially planar with an r.m.s. deviation from the mean plane of 0.0173 Å. Both alkyl side chains are disordered. The crystal packing is consolidated by N—H···N hydrogen bonds (Table 1).

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. Then 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. Propan-1-amine (12.80 g, 0.217 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 title compound (52.18 g) was obtained in powder form in a yield of 80.2%. Crystals of (I) were obtained by slow evaporation of a solution of methanol.

Refinement

Both alkyl side chains are disordered over two positions, in a 0.5:0.5 ratio for the *tert*-butyl containing side chain, and a 0.592 (8):0.408 (8) ratio for the n-propyl chain (occupancy sum for the latter constrained to unity).

The H atoms were positioned geometrically (N—H = 0.86 Å, C—H = 0.96–0.97 Å), and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5$_{eq}$(methyl C).

Figures

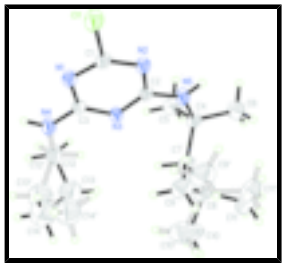


Fig. 1. A view of (I) with displacement ellopsoids drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radius.

6-Chloro-N^2-propyl-N^4-(2,4,4-trimethylpentan-2-yl)-1,3,5-triazine- 2,4-diamine

Crystal data

$C_{14}H_{26}ClN_5$	F_{000} = 1296
M_r = 299.85	D_x = 1.147 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: 427-429 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 19.354 (4) Å	Cell parameters from 2001 reflections
b = 8.1265 (16) Å	θ = 2.7–21.9º
c = 22.312 (4) Å	μ = 0.22 mm^{-1}
β = 98.211 (4)º	*T* = 294 (2) K
V = 3473.3 (11) Å^3	Prism, colorless
Z = 8	0.24 × 0.20 × 0.14 mm

Data collection

Bruker SMART 1000 CCD diffractometer	3070 independent reflections
Radiation source: fine-focus sealed tube	1927 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 294(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	*h* = −22→22
T_{min} = 0.949, T_{max} = 0.970	*k* = −9→9
8715 measured reflections	*l* = −26→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.061	H-atom parameters constrained
$wR(F^2)$ = 0.200	$w = 1/[\sigma^2(F_o^2) + (0.1008P)^2 + 4.0532P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
3070 reflections	$\Delta\rho_{max}$ = 0.82 e Å^{-3}
227 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
124 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	1.12154 (5)	0.54065 (15)	0.15428 (4)	0.0679 (4)	
N1	1.01263 (14)	0.5960 (3)	0.07597 (11)	0.0428 (7)	
N2	1.01295 (13)	0.7029 (3)	0.17513 (11)	0.0410 (7)	
N3	0.91505 (13)	0.7532 (3)	0.09899 (11)	0.0409 (7)	
N4	0.91928 (15)	0.6518 (4)	0.00350 (12)	0.0561 (9)	
H4	0.9410	0.5949	−0.0204	0.067*	
N5	0.91712 (13)	0.8346 (4)	0.19857 (12)	0.0438 (7)	
H5	0.9419	0.8406	0.2337	0.053*	
C1	1.03866 (16)	0.6232 (4)	0.13245 (15)	0.0409 (8)	
C2	0.94741 (16)	0.7621 (4)	0.15558 (14)	0.0366 (8)	
C3	0.94923 (17)	0.6693 (4)	0.06058 (14)	0.0407 (8)	
C4	0.84639 (17)	0.9060 (4)	0.19365 (16)	0.0441 (8)	
C5	0.79276 (19)	0.7711 (5)	0.1755 (2)	0.0646 (11)	
H5A	0.7965	0.7341	0.1353	0.097*	
H5B	0.7467	0.8136	0.1767	0.097*	
H5C	0.8013	0.6805	0.2032	0.097*	
C6	0.8389 (2)	0.9614 (6)	0.25784 (18)	0.0707 (12)	
H6A	0.8720	1.0470	0.2702	0.106*	
H6B	0.8474	0.8697	0.2850	0.106*	
H6C	0.7925	1.0021	0.2586	0.106*	
C7	0.83308 (19)	1.0435 (4)	0.14660 (17)	0.0529 (9)	
H7A	0.7848	1.0766	0.1461	0.063*	
H7B	0.8357	0.9926	0.1077	0.063*	
C8	0.8755 (2)	1.2031 (5)	0.1477 (2)	0.0786 (14)	
C9	0.9459 (5)	1.1708 (16)	0.1267 (5)	0.081 (3)	0.50
H9A	0.9720	1.2715	0.1280	0.122*	0.50
H9B	0.9386	1.1292	0.0861	0.122*	0.50
H9C	0.9714	1.0913	0.1530	0.122*	0.50
C10	0.8316 (8)	1.301 (2)	0.0956 (7)	0.111 (5)	0.50
H10A	0.8526	1.4068	0.0916	0.166*	0.50
H10B	0.7850	1.3154	0.1047	0.166*	0.50
H10C	0.8302	1.2413	0.0583	0.166*	0.50
C11	0.8522 (8)	1.3241 (19)	0.1929 (6)	0.110 (5)	0.50

H11A	0.8794	1.4230	0.1933	0.165*	0.50
H11B	0.8587	1.2757	0.2325	0.165*	0.50
H11C	0.8037	1.3500	0.1812	0.165*	0.50
C9'	0.9560 (5)	1.1719 (18)	0.1623 (6)	0.100 (4)	0.50
H9'A	0.9804	1.2749	0.1629	0.150*	0.50
H9'B	0.9706	1.1020	0.1317	0.150*	0.50
H9'C	0.9664	1.1196	0.2011	0.150*	0.50
C10'	0.8601 (9)	1.299 (3)	0.0881 (7)	0.133 (6)	0.50
H10D	0.8874	1.3978	0.0908	0.200*	0.50
H10E	0.8114	1.3264	0.0807	0.200*	0.50
H10F	0.8718	1.2321	0.0555	0.200*	0.50
C11'	0.8846 (7)	1.3011 (17)	0.2076 (5)	0.090 (4)	0.50
H11D	0.9120	1.3978	0.2033	0.135*	0.50
H11E	0.9078	1.2337	0.2396	0.135*	0.50
H11F	0.8396	1.3328	0.2170	0.135*	0.50
C12	0.8530 (2)	0.7219 (6)	−0.02092 (18)	0.0785 (15)	0.592 (8)
H12A	0.8196	0.6870	0.0051	0.094*	0.592 (8)
H12B	0.8389	0.6708	−0.0601	0.094*	0.592 (8)
C13	0.8442 (6)	0.8996 (11)	−0.0295 (5)	0.119 (3)	0.592 (8)
H13A	0.8581	0.9583	0.0081	0.143*	0.592 (8)
H13B	0.7961	0.9269	−0.0448	0.143*	0.592 (8)
C14	0.8909 (6)	0.9395 (18)	−0.0745 (5)	0.129 (3)	0.592 (8)
H14A	0.8929	1.0567	−0.0794	0.193*	0.592 (8)
H14B	0.8732	0.8896	−0.1126	0.193*	0.592 (8)
H14C	0.9368	0.8980	−0.0607	0.193*	0.592 (8)
C12'	0.8530 (2)	0.7219 (6)	−0.02092 (18)	0.0785 (15)	0.408 (8)
H12C	0.8317	0.7718	0.0115	0.094*	0.408 (8)
H12D	0.8222	0.6356	−0.0390	0.094*	0.408 (8)
C13'	0.8621 (9)	0.8539 (16)	−0.0695 (6)	0.122 (3)	0.408 (8)
H13C	0.8866	0.8072	−0.1005	0.146*	0.408 (8)
H13D	0.8167	0.8919	−0.0887	0.146*	0.408 (8)
C14'	0.9031 (9)	0.995 (2)	−0.0388 (9)	0.127 (4)	0.408 (8)
H14D	0.8821	1.0974	−0.0534	0.190*	0.408 (8)
H14E	0.9502	0.9909	−0.0475	0.190*	0.408 (8)
H14F	0.9032	0.9881	0.0042	0.190*	0.408 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0464 (6)	0.0923 (8)	0.0621 (7)	0.0296 (5)	−0.0018 (5)	−0.0159 (5)
N1	0.0408 (15)	0.0505 (18)	0.0374 (16)	0.0101 (13)	0.0058 (12)	−0.0052 (13)
N2	0.0356 (14)	0.0494 (17)	0.0384 (15)	0.0072 (13)	0.0063 (12)	−0.0056 (13)
N3	0.0414 (15)	0.0463 (17)	0.0348 (15)	0.0116 (13)	0.0042 (12)	−0.0024 (12)
N4	0.0573 (19)	0.073 (2)	0.0359 (16)	0.0262 (17)	−0.0011 (14)	−0.0091 (15)
N5	0.0354 (14)	0.0586 (19)	0.0375 (15)	0.0113 (13)	0.0054 (12)	−0.0083 (13)
C1	0.0343 (17)	0.043 (2)	0.045 (2)	0.0076 (15)	0.0056 (15)	−0.0022 (15)
C2	0.0341 (16)	0.0370 (19)	0.0390 (18)	0.0026 (14)	0.0061 (14)	−0.0030 (14)
C3	0.0436 (18)	0.042 (2)	0.0363 (18)	0.0059 (15)	0.0046 (15)	−0.0012 (14)

C4	0.0374 (18)	0.043 (2)	0.054 (2)	0.0100 (15)	0.0130 (16)	0.0000 (16)
C5	0.045 (2)	0.055 (3)	0.098 (3)	0.0007 (18)	0.020 (2)	0.007 (2)
C6	0.072 (3)	0.083 (3)	0.063 (3)	0.029 (2)	0.030 (2)	−0.001 (2)
C7	0.051 (2)	0.044 (2)	0.065 (2)	0.0107 (18)	0.0143 (18)	0.0011 (18)
C8	0.091 (3)	0.045 (3)	0.106 (4)	0.000 (2)	0.039 (3)	0.001 (2)
C9	0.085 (6)	0.064 (5)	0.102 (7)	−0.015 (5)	0.042 (5)	0.004 (6)
C10	0.122 (9)	0.081 (6)	0.135 (8)	0.001 (7)	0.039 (7)	0.051 (6)
C11	0.126 (9)	0.071 (7)	0.131 (8)	0.006 (7)	0.014 (7)	−0.027 (6)
C9'	0.102 (7)	0.079 (6)	0.125 (8)	−0.026 (5)	0.035 (6)	−0.001 (7)
C10'	0.150 (10)	0.111 (8)	0.146 (9)	−0.011 (8)	0.047 (7)	0.046 (7)
C11'	0.097 (8)	0.060 (6)	0.113 (7)	−0.012 (6)	0.016 (6)	−0.018 (5)
C12	0.075 (3)	0.107 (4)	0.048 (2)	0.038 (3)	−0.012 (2)	−0.015 (2)
C13	0.121 (4)	0.122 (4)	0.112 (4)	0.010 (3)	0.013 (3)	−0.005 (3)
C14	0.131 (5)	0.129 (5)	0.126 (5)	0.002 (4)	0.016 (4)	0.002 (4)
C12'	0.075 (3)	0.107 (4)	0.048 (2)	0.038 (3)	−0.012 (2)	−0.015 (2)
C13'	0.121 (4)	0.122 (4)	0.121 (4)	0.007 (4)	0.014 (4)	−0.001 (4)
C14'	0.129 (5)	0.128 (5)	0.122 (5)	0.003 (4)	0.016 (4)	−0.003 (4)

Geometric parameters (Å, °)

Cl1—C1	1.743 (3)	C9—H9B	0.9600
N1—C1	1.307 (4)	C9—H9C	0.9600
N1—C3	1.363 (4)	C10—H10A	0.9600
N2—C1	1.307 (4)	C10—H10B	0.9600
N2—C2	1.369 (4)	C10—H10C	0.9600
N3—C2	1.329 (4)	C11—H11A	0.9600
N3—C3	1.342 (4)	C11—H11B	0.9600
N4—C3	1.329 (4)	C11—H11C	0.9600
N4—C12	1.438 (5)	C9'—H9'A	0.9600
N4—H4	0.8600	C9'—H9'B	0.9600
N5—C2	1.331 (4)	C9'—H9'C	0.9600
N5—C4	1.476 (4)	C10'—H10D	0.9600
N5—H5	0.8600	C10'—H10E	0.9600
C4—C5	1.524 (5)	C10'—H10F	0.9600
C4—C6	1.528 (5)	C11'—H11D	0.9600
C4—C7	1.529 (5)	C11'—H11E	0.9600
C5—H5A	0.9600	C11'—H11F	0.9600
C5—H5B	0.9600	C12—C13	1.464 (8)
C5—H5C	0.9600	C12—H12A	0.9700
C6—H6A	0.9600	C12—H12B	0.9700
C6—H6B	0.9600	C13—C14	1.478 (9)
C6—H6C	0.9600	C13—H13A	0.9700
C7—C8	1.534 (6)	C13—H13B	0.9700
C7—H7A	0.9700	C14—H14A	0.9600
C7—H7B	0.9700	C14—H14B	0.9600
C8—C11	1.522 (9)	C14—H14C	0.9600
C8—C9	1.524 (8)	C13'—C14'	1.506 (10)
C8—C10'	1.533 (9)	C13'—H13C	0.9700
C8—C11'	1.543 (8)	C13'—H13D	0.9700

C8—C10	1.557 (9)	C14'—H14D	0.9600
C8—C9'	1.566 (9)	C14'—H14E	0.9600
C9—H9A	0.9600	C14'—H14F	0.9600
C1—N1—C3	112.2 (3)	C8—C9—H9A	109.5
C1—N2—C2	112.0 (3)	C8—C9—H9B	109.5
C2—N3—C3	115.2 (3)	H9A—C9—H9B	109.5
C3—N4—C12	124.4 (3)	C8—C9—H9C	109.5
C3—N4—H4	117.8	H9A—C9—H9C	109.5
C12—N4—H4	117.8	H9B—C9—H9C	109.5
C2—N5—C4	128.3 (3)	C8—C10—H10A	109.5
C2—N5—H5	115.9	C8—C10—H10B	109.5
C4—N5—H5	115.9	H10A—C10—H10B	109.5
N2—C1—N1	130.6 (3)	C8—C10—H10C	109.5
N2—C1—Cl1	114.7 (2)	H10A—C10—H10C	109.5
N1—C1—Cl1	114.6 (2)	H10B—C10—H10C	109.5
N3—C2—N5	120.8 (3)	C8—C11—H11A	109.5
N3—C2—N2	125.0 (3)	C8—C11—H11B	109.5
N5—C2—N2	114.2 (3)	H11A—C11—H11B	109.5
N4—C3—N3	118.6 (3)	C8—C11—H11C	109.5
N4—C3—N1	116.6 (3)	H11A—C11—H11C	109.5
N3—C3—N1	124.7 (3)	H11B—C11—H11C	109.5
N5—C4—C5	109.0 (3)	C8—C9'—H9'A	109.5
N5—C4—C6	104.9 (3)	C8—C9'—H9'B	109.5
C5—C4—C6	107.9 (3)	H9'A—C9'—H9'B	109.5
N5—C4—C7	113.7 (3)	C8—C9'—H9'C	109.5
C5—C4—C7	107.6 (3)	H9'A—C9'—H9'C	109.5
C6—C4—C7	113.5 (3)	H9'B—C9'—H9'C	109.5
C4—C5—H5A	109.5	C8—C10'—H10D	109.5
C4—C5—H5B	109.5	C8—C10'—H10E	109.5
H5A—C5—H5B	109.5	H10D—C10'—H10E	109.5
C4—C5—H5C	109.5	C8—C10'—H10F	109.5
H5A—C5—H5C	109.5	H10D—C10'—H10F	109.5
H5B—C5—H5C	109.5	H10E—C10'—H10F	109.5
C4—C6—H6A	109.5	C8—C11'—H11D	109.5
C4—C6—H6B	109.5	C8—C11'—H11E	109.5
H6A—C6—H6B	109.5	H11D—C11'—H11E	109.5
C4—C6—H6C	109.5	C8—C11'—H11F	109.5
H6A—C6—H6C	109.5	H11D—C11'—H11F	109.5
H6B—C6—H6C	109.5	H11E—C11'—H11F	109.5
C4—C7—C8	124.7 (3)	N4—C12—C13	121.4 (6)
C4—C7—H7A	106.1	N4—C12—H12A	107.0
C8—C7—H7A	106.1	C13—C12—H12A	107.0
C4—C7—H7B	106.1	N4—C12—H12B	107.0
C8—C7—H7B	106.1	C13—C12—H12B	107.0
H7A—C7—H7B	106.3	H12A—C12—H12B	106.7
C11—C8—C9	132.6 (9)	C12—C13—C14	103.6 (9)
C11—C8—C10'	102.0 (12)	C12—C13—H13A	111.0
C9—C8—C10'	83.9 (8)	C14—C13—H13A	111.0
C11—C8—C7	110.4 (8)	C12—C13—H13B	111.0

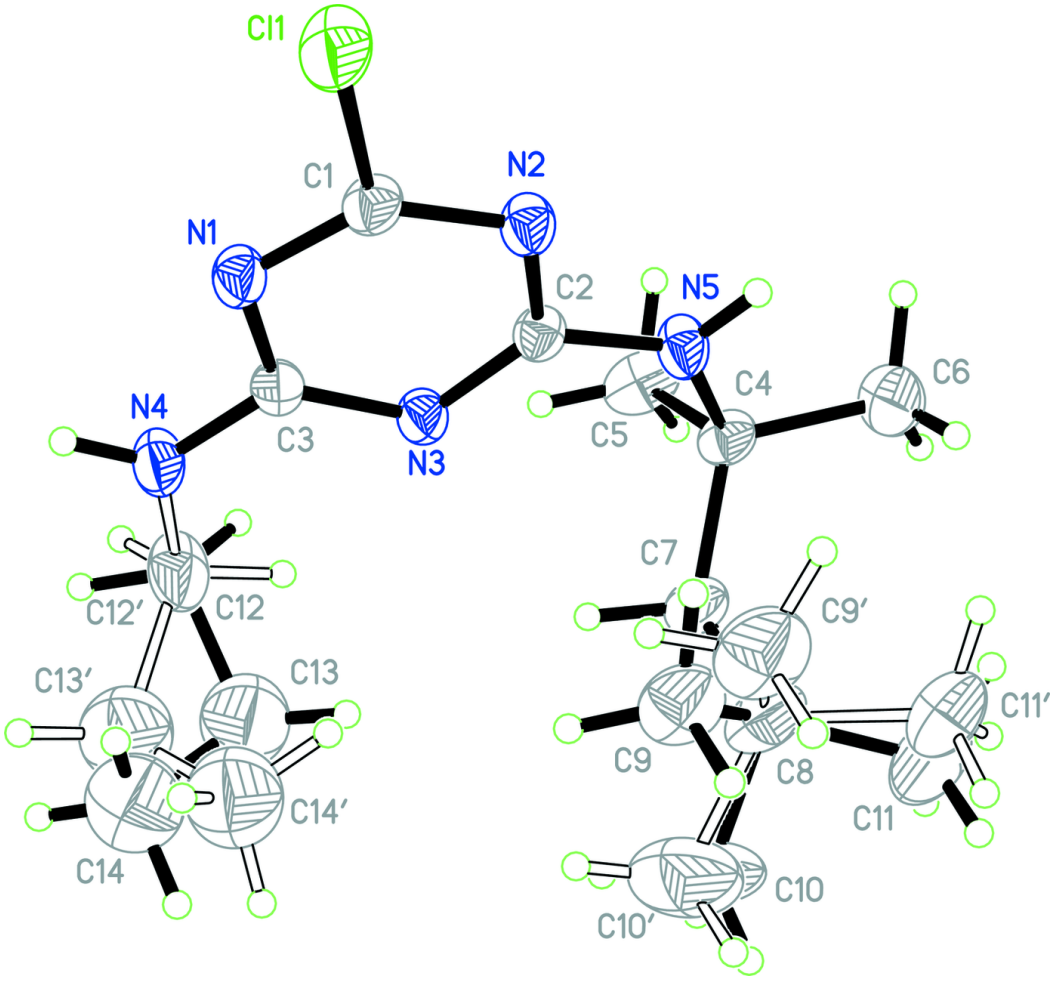
C9—C8—C7	110.4 (6)	C14—C13—H13B	111.0
C10'—C8—C7	112.2 (10)	H13A—C13—H13B	109.0
C11—C8—C11'	26.0 (7)	C13—C14—H14A	109.5
C9—C8—C11'	111.0 (8)	C13—C14—H14B	109.5
C10'—C8—C11'	118.2 (12)	H14A—C14—H14B	109.5
C7—C8—C11'	116.4 (6)	C13—C14—H14C	109.5
C11—C8—C10	89.0 (10)	H14A—C14—H14C	109.5
C9—C8—C10	106.0 (8)	H14B—C14—H14C	109.5
C10'—C8—C10	22.3 (10)	C14'—C13'—H13C	110.0
C7—C8—C10	100.7 (8)	C14'—C13'—H13D	110.0
C11'—C8—C10	111.4 (10)	H13C—C13'—H13D	108.4
C11—C8—C9'	110.3 (9)	C13'—C14'—H14D	109.5
C9—C8—C9'	29.6 (6)	C13'—C14'—H14E	109.5
C10'—C8—C9'	109.1 (8)	H14D—C14'—H14E	109.5
C7—C8—C9'	112.4 (6)	C13'—C14'—H14F	109.5
C11'—C8—C9'	85.3 (8)	H14D—C14'—H14F	109.5
C10—C8—C9'	131.2 (8)	H14E—C14'—H14F	109.5
C2—N2—C1—N1	1.6 (5)	C1—N1—C3—N3	−3.1 (5)
C2—N2—C1—Cl1	−178.9 (2)	C2—N5—C4—C5	61.2 (4)
C3—N1—C1—N2	2.2 (6)	C2—N5—C4—C6	176.6 (3)
C3—N1—C1—Cl1	−177.3 (2)	C2—N5—C4—C7	−58.9 (5)
C3—N3—C2—N5	−176.4 (3)	N5—C4—C7—C8	−59.1 (4)
C3—N3—C2—N2	4.6 (5)	C5—C4—C7—C8	−179.9 (3)
C4—N5—C2—N3	3.2 (5)	C6—C4—C7—C8	60.7 (4)
C4—N5—C2—N2	−177.7 (3)	C4—C7—C8—C11	−79.3 (8)
C1—N2—C2—N3	−5.3 (5)	C4—C7—C8—C9	76.1 (7)
C1—N2—C2—N5	175.7 (3)	C4—C7—C8—C10'	167.8 (9)
C12—N4—C3—N3	2.1 (6)	C4—C7—C8—C11'	−51.6 (8)
C12—N4—C3—N1	−179.3 (4)	C4—C7—C8—C10	−172.2 (8)
C2—N3—C3—N4	178.4 (3)	C4—C7—C8—C9'	44.4 (7)
C2—N3—C3—N1	−0.1 (5)	C3—N4—C12—C13	69.5 (7)
C1—N1—C3—N4	178.5 (3)	N4—C12—C13—C14	63.0 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···N1^{i}	0.86	2.25	3.099 (4)	169
N5—H5···N2^{ii}	0.86	2.38	3.135 (4)	147

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

Fig. 1


Cl1
C1
N2
N1
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C5
N4
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