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

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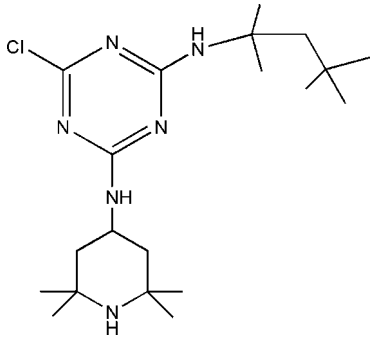
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.102; data-to-parameter ratio = 20.0.

In the title compound, $C_{20}H_{37}ClN_6$, the piperidine ring adopts a chair conformation. In the crystal structure, N—H···N hydrogen bonds link the molecules into chains along b.

Related literature

For the preparation and uses of the title compound and similar compounds, see: Borzatta & Carrozza (1991); Deng *et al.* (2006); Kaiser & Thurston (1951).



Experimental

Crystal data

$C_{20}H_{37}ClN_6$
M_r = 397.01
Monoclinic, $P2_1/n$
a = 7.9906 (7) Å
b = 20.5197 (16) Å
c = 13.6338 (10) Å
β = 97.273 (3)°
V = 2217.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 113 (2) K
0.26 × 0.22 × 0.20 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.943, T_{max} = 0.963
27567 measured reflections
5297 independent reflections
4972 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.102
S = 1.09
5297 reflections
265 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···N2^{i}	0.866 (17)	2.510 (17)	3.3531 (15)	164.7 (14)
N6—H6···N1^{ii}	0.893 (17)	2.337 (17)	3.1653 (15)	154.2 (14)
N4—H4···N6^{iii}	0.880 (17)	2.415 (17)	3.2470 (15)	157.9 (14)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *CrystalStructure* (Rigaku/MSC, 2005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2356).

References

Borzatta, V. & Carrozza, P. (1991). Eur. Patent EP 0 462 069.
Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Deng, Y., Wang, X.-J., Wen, F., Wang, L. & Zhang, Y. (2006). *Acta Cryst.* E**62**, o5207–o5208.
Kaiser, D. W. & Thurston, J. T. (1951). *J. Am. Chem. Soc.* **73**, 2984–2986.
Rigaku/MSC (2005). *CrystalClear* and *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA .
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

Acta Cryst. (2007). E**63**, o4113 [**doi:10.1107/S1600536807045035**]

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

J.-Y. Dong and P.-M. Huang

Comment

The title compound (I) is an important intermediate in the preparation of hindered light stabilizers (Borzatta & Carrozza, 1991). Compounds containing a triazine ring are widely used in polymers, dyes, drugs and hindered amine light stabilizers (Deng et al., 2006). We report here the crystal structure of the title compound (I) (Fig. 1). In (I) the piperidine ring adopts a chair conformation and the triazine ring is essentially planar with an r.m.s. deviation from the mean plane of 0.0115 Å. In the crystal structure N—H···N hydrogen bonds link the molecules into chains along b</>, Table 1.

Experimental

The title compound was prepared according to the method of Kaiser & Thurston (1951) in 74.5% yield. Crystals of (I) were obtained by slow evaporation of a solution in methanol (m.p. 473–475 K).

Refinement

The amine H atoms were located in a Fourier map and refined freely with isotropic displacement parameters. All other H atoms were positioned geometrically and refined using a riding model with d(C—H) = 1.00 Å, U_{iso} = 1.2U_{eq} (C) for CH, 0.99 Å, U_{iso} = 1.2U_{eq} (C) for CH_2 and 0.98 Å, U_{iso} = 1.5U_{eq} (C) for CH_3 atoms.

Figures

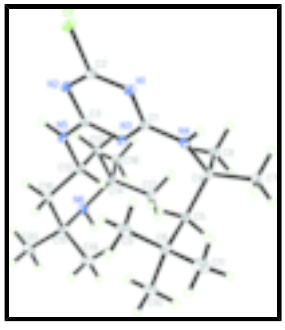


Fig. 1. A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres with arbitrary radii.

6-Chloro-N4-(2,2,6,6-tetramethylpiperidin-4-yl)-N2-(2,4,4- trimethylpentan-2-yl)-1,3,5-triazine-2,4-diamine

Crystal data

$C_{20}H_{37}ClN_6$	F_{000} = 864
M_r = 397.01	D_x = 1.189 Mg m^{-3}

Monoclinic, $P2_1/n$	Melting point: 473-475 K K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
$a = 7.9906$ (7) Å	Cell parameters from 7832 reflections
$b = 20.5197$ (16) Å	$\theta = 1.5–27.9°$
$c = 13.6338$ (10) Å	$\mu = 0.19$ mm^{-1}
$\beta = 97.273$ (3)°	$T = 113$ (2) K
$V = 2217.5$ (3) Å^3	Block, colorless
$Z = 4$	0.26 × 0.22 × 0.20 mm

Data collection

Rigaku Saturn CCD diffractometer	5297 independent reflections
Radiation source: rotating anode	4972 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{int} = 0.035$
Detector resolution: 14.63 pixels mm^{-1}	$\theta_{max} = 27.9°$
$T = 113(2)$ K	$\theta_{min} = 1.8°$
ω scans	$h = -10\rightarrow10$
Absorption correction: multi-scan (Crystalclear; Rigaku/MSC, 2005)	$k = -26\rightarrow27$
$T_{min} = 0.943$, $T_{max} = 0.963$	$l = -17\rightarrow17$
27567 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.6837P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = <0.001$
5297 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
265 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$sigma(F^2) is used only for calculat-

ing *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}
Cl1	0.01081 (4)	0.699625 (15)	0.47224 (2)	0.02317 (10)
N1	0.15950 (13)	0.66230 (5)	0.32523 (8)	0.0168 (2)
N2	0.09387 (13)	0.57989 (5)	0.43869 (8)	0.0173 (2)
N3	0.22982 (13)	0.55103 (5)	0.29729 (8)	0.0155 (2)
N4	0.28136 (14)	0.63301 (5)	0.18846 (8)	0.0170 (2)
N5	0.17778 (15)	0.47447 (5)	0.41161 (8)	0.0204 (2)
N6	0.28530 (14)	0.28875 (5)	0.29972 (8)	0.0175 (2)
C1	0.22279 (15)	0.61388 (6)	0.27161 (9)	0.0149 (2)
C2	0.09911 (16)	0.63977 (6)	0.40412 (9)	0.0162 (2)
C3	0.16769 (15)	0.53637 (6)	0.38127 (9)	0.0159 (2)
C4	0.33522 (16)	0.59015 (6)	0.11107 (9)	0.0173 (3)
C5	0.48819 (15)	0.54635 (6)	0.14791 (9)	0.0165 (2)
H5A	0.4449	0.5120	0.1890	0.020*
H5B	0.5207	0.5242	0.0886	0.020*
C6	0.65409 (16)	0.57120 (6)	0.20685 (10)	0.0197 (3)
C7	0.37084 (19)	0.63562 (7)	0.02693 (10)	0.0248 (3)
H7A	0.2657	0.6567	−0.0015	0.037*
H7B	0.4170	0.6103	−0.0244	0.037*
H7C	0.4526	0.6689	0.0528	0.037*
C8	0.18857 (17)	0.54531 (7)	0.07119 (10)	0.0228 (3)
H8A	0.1592	0.5172	0.1246	0.034*
H8B	0.2223	0.5183	0.0178	0.034*
H8C	0.0906	0.5718	0.0457	0.034*
C9	0.63165 (19)	0.59348 (8)	0.31157 (11)	0.0317 (3)
H9A	0.7423	0.6028	0.3485	0.048*
H9B	0.5762	0.5589	0.3452	0.048*
H9C	0.5620	0.6329	0.3080	0.048*
C10	0.77338 (18)	0.51252 (7)	0.21771 (11)	0.0271 (3)
H10A	0.7925	0.4971	0.1520	0.041*
H10B	0.7228	0.4775	0.2530	0.041*
H10C	0.8812	0.5254	0.2550	0.041*
C11	0.7392 (2)	0.62547 (8)	0.15494 (14)	0.0375 (4)
H11A	0.6733	0.6657	0.1562	0.056*
H11B	0.7459	0.6129	0.0862	0.056*
H11C	0.8532	0.6327	0.1890	0.056*
C12	0.24318 (17)	0.42220 (6)	0.35383 (9)	0.0187 (3)
H12	0.3114	0.4423	0.3051	0.022*
C13	0.09877 (17)	0.38406 (6)	0.29721 (10)	0.0200 (3)
H13A	0.0288	0.4142	0.2524	0.024*
H13B	0.0268	0.3662	0.3447	0.024*
C14	0.15876 (17)	0.32805 (6)	0.23626 (9)	0.0194 (3)
C15	0.42659 (16)	0.32117 (6)	0.36202 (10)	0.0187 (3)

C16	0.35639 (17)	0.37652 (6)	0.42026 (10)	0.0191 (3)
H16A	0.2913	0.3577	0.4705	0.023*
H16B	0.4514	0.4017	0.4553	0.023*
C17	0.2212 (2)	0.35397 (7)	0.14140 (10)	0.0279 (3)
H17A	0.3049	0.3884	0.1585	0.042*
H17B	0.1256	0.3717	0.0974	0.042*
H17C	0.2728	0.3183	0.1080	0.042*
C18	0.00934 (19)	0.28255 (7)	0.20586 (11)	0.0268 (3)
H18A	0.0459	0.2464	0.1668	0.040*
H18B	−0.0808	0.3068	0.1662	0.040*
H18C	−0.0327	0.2654	0.2652	0.040*
C19	0.56744 (18)	0.34602 (7)	0.30424 (12)	0.0293 (3)
H19A	0.6053	0.3104	0.2644	0.044*
H19B	0.6625	0.3616	0.3508	0.044*
H19C	0.5241	0.3818	0.2607	0.044*
C20	0.50283 (18)	0.26939 (7)	0.43525 (11)	0.0258 (3)
H20A	0.4158	0.2532	0.4737	0.039*
H20B	0.5953	0.2886	0.4801	0.039*
H20C	0.5462	0.2332	0.3989	0.039*
H4	0.2754 (19)	0.6750 (8)	0.1757 (11)	0.023 (4)*
H6	0.328 (2)	0.2611 (8)	0.2589 (12)	0.028 (4)*
H5	0.121 (2)	0.4641 (8)	0.4594 (12)	0.026 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.03026 (19)	0.01401 (16)	0.02806 (18)	0.00117 (12)	0.01467 (14)	−0.00363 (12)
N1	0.0180 (5)	0.0129 (5)	0.0204 (5)	0.0004 (4)	0.0057 (4)	−0.0004 (4)
N2	0.0212 (5)	0.0138 (5)	0.0183 (5)	0.0006 (4)	0.0073 (4)	−0.0011 (4)
N3	0.0178 (5)	0.0128 (5)	0.0167 (5)	0.0009 (4)	0.0051 (4)	0.0011 (4)
N4	0.0208 (5)	0.0124 (5)	0.0186 (5)	0.0018 (4)	0.0060 (4)	0.0022 (4)
N5	0.0312 (6)	0.0139 (5)	0.0188 (5)	0.0035 (5)	0.0135 (5)	0.0016 (4)
N6	0.0214 (6)	0.0127 (5)	0.0185 (5)	0.0032 (4)	0.0036 (4)	−0.0010 (4)
C1	0.0132 (6)	0.0148 (6)	0.0169 (6)	0.0001 (5)	0.0022 (5)	0.0000 (5)
C2	0.0164 (6)	0.0144 (6)	0.0184 (6)	0.0001 (5)	0.0040 (5)	−0.0029 (5)
C3	0.0173 (6)	0.0138 (6)	0.0171 (6)	0.0000 (5)	0.0037 (5)	−0.0006 (4)
C4	0.0195 (6)	0.0188 (6)	0.0143 (6)	0.0019 (5)	0.0044 (5)	0.0008 (5)
C5	0.0178 (6)	0.0161 (6)	0.0161 (6)	0.0010 (5)	0.0045 (5)	−0.0003 (5)
C6	0.0179 (6)	0.0200 (6)	0.0214 (6)	−0.0005 (5)	0.0039 (5)	−0.0004 (5)
C7	0.0284 (7)	0.0280 (7)	0.0192 (6)	0.0055 (6)	0.0074 (5)	0.0071 (5)
C8	0.0198 (6)	0.0284 (7)	0.0196 (6)	0.0013 (5)	0.0005 (5)	−0.0031 (5)
C9	0.0218 (7)	0.0440 (9)	0.0281 (8)	0.0038 (6)	−0.0022 (6)	−0.0143 (7)
C10	0.0205 (7)	0.0291 (8)	0.0307 (7)	0.0056 (6)	−0.0004 (6)	−0.0020 (6)
C11	0.0247 (8)	0.0372 (9)	0.0492 (10)	−0.0104 (7)	−0.0008 (7)	0.0141 (7)
C12	0.0276 (7)	0.0120 (6)	0.0183 (6)	0.0031 (5)	0.0100 (5)	−0.0003 (5)
C13	0.0250 (7)	0.0171 (6)	0.0184 (6)	0.0066 (5)	0.0041 (5)	0.0020 (5)
C14	0.0267 (7)	0.0156 (6)	0.0161 (6)	0.0043 (5)	0.0028 (5)	0.0012 (5)
C15	0.0187 (6)	0.0143 (6)	0.0236 (6)	0.0015 (5)	0.0048 (5)	−0.0004 (5)

C16	0.0212 (6)	0.0156 (6)	0.0210 (6)	−0.0008 (5)	0.0044 (5)	−0.0016 (5)
C17	0.0453 (9)	0.0215 (7)	0.0179 (6)	0.0063 (6)	0.0084 (6)	0.0019 (5)
C18	0.0296 (8)	0.0247 (7)	0.0245 (7)	0.0015 (6)	−0.0030 (6)	−0.0013 (6)
C19	0.0251 (7)	0.0248 (7)	0.0407 (8)	0.0007 (6)	0.0148 (6)	−0.0015 (6)
C20	0.0243 (7)	0.0201 (7)	0.0317 (7)	0.0037 (5)	−0.0012 (6)	0.0015 (6)

Geometric parameters (Å, °)

Cl1—C2	1.7420 (12)	C9—H9C	0.9800
N1—C2	1.3171 (16)	C10—H10A	0.9800
N1—C1	1.3679 (16)	C10—H10B	0.9800
N2—C2	1.3185 (16)	C10—H10C	0.9800
N2—C3	1.3695 (16)	C11—H11A	0.9800
N3—C1	1.3358 (16)	C11—H11B	0.9800
N3—C3	1.3386 (15)	C11—H11C	0.9800
N4—C1	1.3389 (16)	C12—C16	1.5198 (18)
N4—C4	1.4789 (16)	C12—C13	1.5212 (19)
N4—H4	0.880 (17)	C12—H12	1.0000
N5—C3	1.3351 (16)	C13—C14	1.5305 (17)
N5—C12	1.4658 (16)	C13—H13A	0.9900
N5—H5	0.866 (17)	C13—H13B	0.9900
N6—C15	1.4819 (17)	C14—C18	1.5310 (19)
N6—C14	1.4832 (16)	C14—C17	1.5387 (18)
N6—H6	0.893 (17)	C15—C20	1.5307 (18)
C4—C7	1.5331 (17)	C15—C16	1.5323 (17)
C4—C8	1.5343 (18)	C15—C19	1.5400 (18)
C4—C5	1.5487 (17)	C16—H16A	0.9900
C5—C6	1.5471 (18)	C16—H16B	0.9900
C5—H5A	0.9900	C17—H17A	0.9800
C5—H5B	0.9900	C17—H17B	0.9800
C6—C11	1.525 (2)	C17—H17C	0.9800
C6—C9	1.5312 (19)	C18—H18A	0.9800
C6—C10	1.5312 (19)	C18—H18B	0.9800
C7—H7A	0.9800	C18—H18C	0.9800
C7—H7B	0.9800	C19—H19A	0.9800
C7—H7C	0.9800	C19—H19B	0.9800
C8—H8A	0.9800	C19—H19C	0.9800
C8—H8B	0.9800	C20—H20A	0.9800
C8—H8C	0.9800	C20—H20B	0.9800
C9—H9A	0.9800	C20—H20C	0.9800
C9—H9B	0.9800		
C2—N1—C1	112.33 (10)	H10B—C10—H10C	109.5
C2—N2—C3	111.59 (10)	C6—C11—H11A	109.5
C1—N3—C3	115.68 (10)	C6—C11—H11B	109.5
C1—N4—C4	126.45 (11)	H11A—C11—H11B	109.5
C1—N4—H4	116.0 (10)	C6—C11—H11C	109.5
C4—N4—H4	117.1 (10)	H11A—C11—H11C	109.5
C3—N5—C12	122.77 (11)	H11B—C11—H11C	109.5
C3—N5—H5	116.8 (11)	N5—C12—C16	110.90 (10)

C12—N5—H5	118.7 (11)	N5—C12—C13	110.48 (10)
C15—N6—C14	120.26 (10)	C16—C12—C13	109.95 (10)
C15—N6—H6	108.5 (10)	N5—C12—H12	108.5
C14—N6—H6	105.6 (10)	C16—C12—H12	108.5
N3—C1—N4	119.83 (11)	C13—C12—H12	108.5
N3—C1—N1	124.57 (11)	C12—C13—C14	113.09 (11)
N4—C1—N1	115.60 (11)	C12—C13—H13A	109.0
N1—C2—N2	130.58 (11)	C14—C13—H13A	109.0
N1—C2—Cl1	113.76 (9)	C12—C13—H13B	109.0
N2—C2—Cl1	115.66 (9)	C14—C13—H13B	109.0
N5—C3—N3	117.67 (11)	H13A—C13—H13B	107.8
N5—C3—N2	117.18 (11)	N6—C14—C13	109.20 (10)
N3—C3—N2	125.15 (11)	N6—C14—C18	106.08 (10)
N4—C4—C7	105.68 (10)	C13—C14—C18	108.54 (11)
N4—C4—C8	109.35 (10)	N6—C14—C17	114.12 (11)
C7—C4—C8	107.80 (11)	C13—C14—C17	110.72 (11)
N4—C4—C5	113.75 (10)	C18—C14—C17	107.94 (11)
C7—C4—C5	112.47 (10)	N6—C15—C20	105.88 (10)
C8—C4—C5	107.63 (10)	N6—C15—C16	109.11 (10)
C6—C5—C4	124.50 (11)	C20—C15—C16	108.55 (11)
C6—C5—H5A	106.2	N6—C15—C19	114.11 (11)
C4—C5—H5A	106.2	C20—C15—C19	107.89 (11)
C6—C5—H5B	106.2	C16—C15—C19	111.03 (11)
C4—C5—H5B	106.2	C12—C16—C15	112.19 (10)
H5A—C5—H5B	106.4	C12—C16—H16A	109.2
C11—C6—C9	109.06 (13)	C15—C16—H16A	109.2
C11—C6—C10	108.07 (12)	C12—C16—H16B	109.2
C9—C6—C10	106.83 (12)	C15—C16—H16B	109.2
C11—C6—C5	113.76 (11)	H16A—C16—H16B	107.9
C9—C6—C5	112.89 (11)	C14—C17—H17A	109.5
C10—C6—C5	105.84 (11)	C14—C17—H17B	109.5
C4—C7—H7A	109.5	H17A—C17—H17B	109.5
C4—C7—H7B	109.5	C14—C17—H17C	109.5
H7A—C7—H7B	109.5	H17A—C17—H17C	109.5
C4—C7—H7C	109.5	H17B—C17—H17C	109.5
H7A—C7—H7C	109.5	C14—C18—H18A	109.5
H7B—C7—H7C	109.5	C14—C18—H18B	109.5
C4—C8—H8A	109.5	H18A—C18—H18B	109.5
C4—C8—H8B	109.5	C14—C18—H18C	109.5
H8A—C8—H8B	109.5	H18A—C18—H18C	109.5
C4—C8—H8C	109.5	H18B—C18—H18C	109.5
H8A—C8—H8C	109.5	C15—C19—H19A	109.5
H8B—C8—H8C	109.5	C15—C19—H19B	109.5
C6—C9—H9A	109.5	H19A—C19—H19B	109.5
C6—C9—H9B	109.5	C15—C19—H19C	109.5
H9A—C9—H9B	109.5	H19A—C19—H19C	109.5
C6—C9—H9C	109.5	H19B—C19—H19C	109.5
H9A—C9—H9C	109.5	C15—C20—H20A	109.5
H9B—C9—H9C	109.5	C15—C20—H20B	109.5

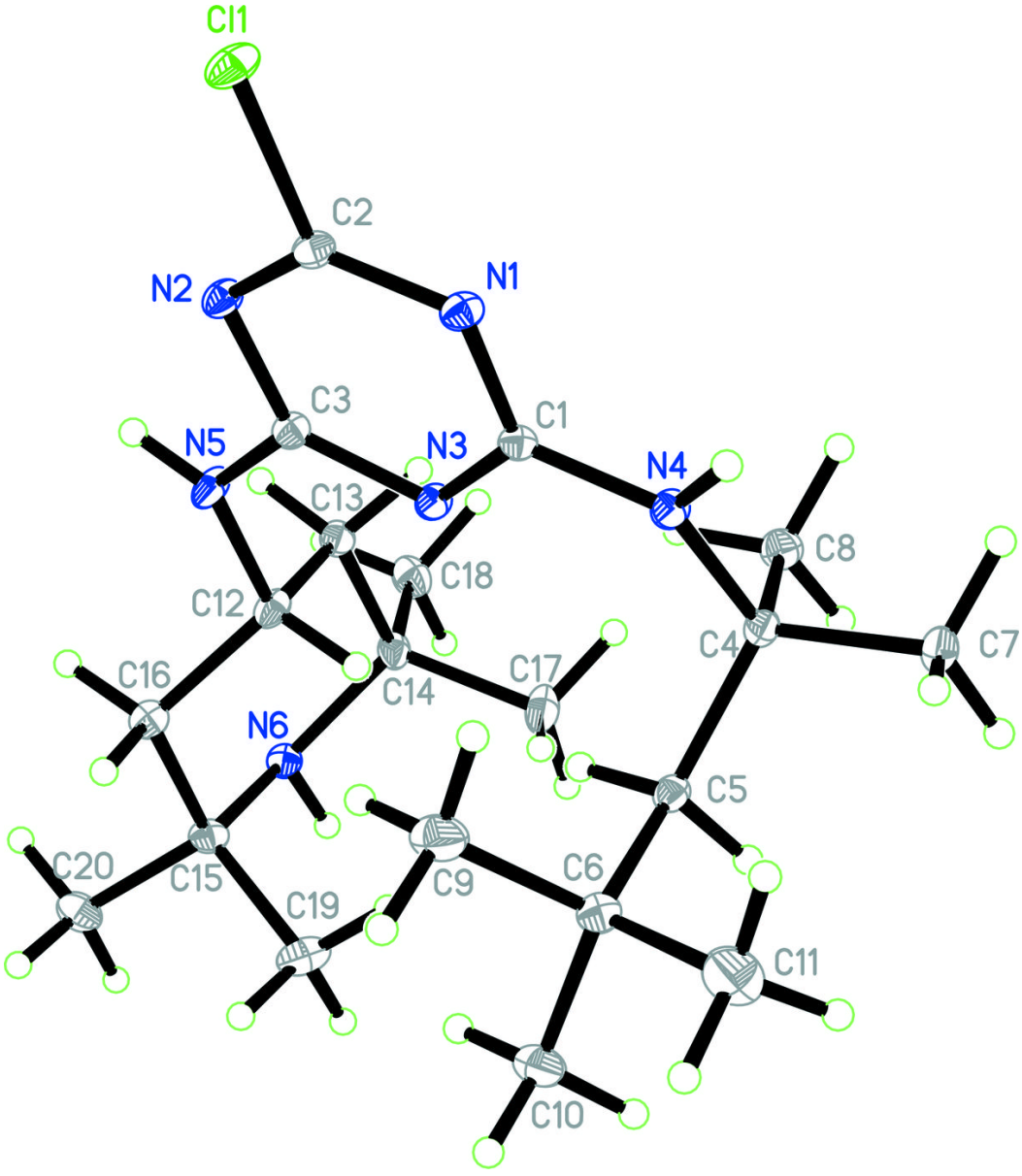
C6—C10—H10A	109.5	H20A—C20—H20B	109.5
C6—C10—H10B	109.5	C15—C20—H20C	109.5
H10A—C10—H10B	109.5	H20A—C20—H20C	109.5
C6—C10—H10C	109.5	H20B—C20—H20C	109.5
H10A—C10—H10C	109.5		
C3—N3—C1—N4	−179.70 (11)	C4—C5—C6—C11	−55.96 (17)
C3—N3—C1—N1	0.73 (18)	C4—C5—C6—C9	69.01 (16)
C4—N4—C1—N3	8.97 (19)	C4—C5—C6—C10	−174.47 (11)
C4—N4—C1—N1	−171.43 (11)	C3—N5—C12—C16	138.28 (13)
C2—N1—C1—N3	−2.54 (17)	C3—N5—C12—C13	−99.54 (14)
C2—N1—C1—N4	177.87 (11)	N5—C12—C13—C14	−179.25 (10)
C1—N1—C2—N2	1.44 (19)	C16—C12—C13—C14	−56.51 (14)
C1—N1—C2—Cl1	−177.96 (8)	C15—N6—C14—C13	−48.00 (15)
C3—N2—C2—N1	1.3 (2)	C15—N6—C14—C18	−164.79 (11)
C3—N2—C2—Cl1	−179.28 (9)	C15—N6—C14—C17	76.50 (15)
C12—N5—C3—N3	−4.09 (19)	C12—C13—C14—N6	49.64 (14)
C12—N5—C3—N2	175.73 (11)	C12—C13—C14—C18	164.86 (11)
C1—N3—C3—N5	−177.61 (11)	C12—C13—C14—C17	−76.83 (14)
C1—N3—C3—N2	2.58 (18)	C14—N6—C15—C20	165.88 (11)
C2—N2—C3—N5	176.71 (12)	C14—N6—C15—C16	49.23 (15)
C2—N2—C3—N3	−3.48 (18)	C14—N6—C15—C19	−75.61 (14)
C1—N4—C4—C7	173.46 (12)	N5—C12—C16—C15	179.88 (10)
C1—N4—C4—C8	57.68 (16)	C13—C12—C16—C15	57.39 (14)
C1—N4—C4—C5	−62.67 (16)	N6—C15—C16—C12	−51.79 (14)
N4—C4—C5—C6	−49.78 (16)	C20—C15—C16—C12	−166.74 (11)
C7—C4—C5—C6	70.32 (15)	C19—C15—C16—C12	74.83 (14)
C8—C4—C5—C6	−171.09 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···N2^{i}	0.866 (17)	2.510 (17)	3.3531 (15)	164.7 (14)
N6—H6···N1^{ii}	0.893 (17)	2.337 (17)	3.1653 (15)	154.2 (14)
N4—H4···N6^{iii}	0.880 (17)	2.415 (17)	3.2470 (15)	157.9 (14)

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

Fig. 1


Cl1
C2
N2
N1
C3
C1
N5
N3
N4
C13
C8
C18
C12
C4
C7
C16
C14
C17
N6
C5
C20
C15
C9
C6
C19
C11
C10