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

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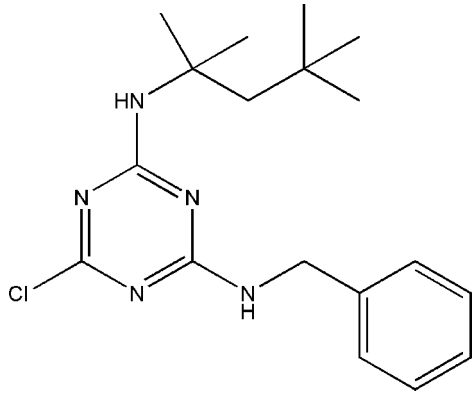
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.056; wR factor = 0.134; data-to-parameter ratio = 18.0.

In the title compound, $C_{18}H_{26}ClN_5$, there are four molecules in the asymmetric unit, two of which show disorder of their tert-butyl groups in 0.58 (2):0.42 (2) and 0.753 (4):0.247 (4) ratios. A complex network of N—H···N hydrogen bonds helps to establish the packing.

Related literature

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



Experimental

Crystal data

$C_{18}H_{26}ClN_5$
M_r = 347.89
Triclinic, $P\overline{1}$
a = 8.0987 (16) Å
b = 20.811 (4) Å
c = 23.984 (5) Å
α = 105.36 (3)°
β = 96.33 (3)°
γ = 96.46 (3)°
V = 3831.6 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 113 (2) K
0.34 × 0.32 × 0.18 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.932, T_{max} = 0.963
35937 measured reflections
17590 independent reflections
14508 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.134
S = 1.08
17590 reflections
979 parameters
96 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N20—H20···N3^{i}	0.87 (2)	2.14 (2)	3.007 (2)	179 (2)
N19—H19···N12^{ii}	0.87 (2)	2.22 (2)	3.085 (2)	174 (2)
N15—H15···N13^{iii}	0.89 (2)	2.06 (3)	2.953 (2)	176 (2)
N14—H14···N17^{ii}	0.84 (2)	2.24 (2)	3.078 (2)	172 (2)
N10—H10···N8^{ii}	0.93 (2)	2.06 (2)	2.989 (2)	171 (2)
N9—H9···N2	0.87 (2)	2.29 (2)	3.127 (2)	163.3 (19)
N5—H5···N18^{i}	0.85 (2)	2.14 (2)	2.984 (2)	172 (2)
N4—H4···N7	0.85 (2)	2.24 (2)	3.085 (2)	174 (2)

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

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* (Sheldrick, 1996); 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: HB2528).

References

Borzatta, V. & Carrozza, P. (1991). Eur. Patent EP 0 462 069.
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. (1996). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

Acta Cryst. (2007). E**63**, o3968 [**doi:10.1107/S1600536807042559**]

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

J.-L. Cui, J.-B. Cai and Y. Deng

Comment

The title compound, (I), is an important intermediate in the preparation of hindered light stabilizers (Borzatta & Carrozza, 1991; Deng *et al.*, 2006).

There are four molecules of (I) in the asymmetic unit, with simplar conformations, although two of the molecules show disorder of their *tert*-butyl groupings. In each case, the triazine ring is essentially planar (Fig. 1). The molecules are linked by strong, near-linear, intermolecular 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 (20.0 g, 0.109 mol) was dissolved in toluene (65 ml) and then cooled to 278 K. With stirring, a solution of 2,4,4-trimethylpentan-2-amine (13.75 g, 0.107 mol) in toluene (35 ml) was then added dropwise to the mixture over a period of 30 min. Then, a solution of Na_2CO_3 (11.51 g, 0.109 mol) in water (30 ml) was then added dropwise for 30 min. The mixture was stirred at 273–278 K for a further 3 h and phenylmethanamine (11.61 g, 0.109 mol) and solid Na_2CO_3 (11.51 g, 0.109 mol) were added to the mixture, maintaining the temperature at 358 K for 4.5 h. The organic layer was washed with water and then concentrated *in vacuo*. The title compound (28.47 g) was obtained in powder form in a yield of 75.4%. Colourles blocks (I) were obtained by slow evaporation of a solution of methanol (m.p. 421–423 K).

Refinement

The N-bound H atoms were located in a difference map and their positions and U_{iso} values were freely refined.

The C-bound H atoms were positioned geometrically (C—H = 0.98–0.99 Å), and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

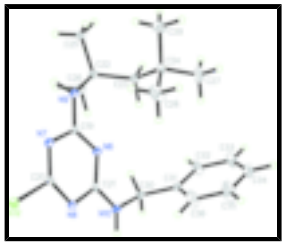


Fig. 1. A view of the structure of the Cl2 molecule in (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

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

Crystal data

$C_{18}H_{26}ClN_5$	$Z = 8$
$M_r = 347.89$	$F_{000} = 1488$
Triclinic, $P\overline{1}$	$D_x = 1.206$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 421-423 K
$a = 8.0987$ (16) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 20.811$ (4) Å	Cell parameters from 8593 reflections
$c = 23.984$ (5) Å	$\theta = 1.8$–27.9º
$\alpha = 105.36$ (3)º	$\mu = 0.21$ mm^{-1}
$\beta = 96.33$ (3)º	$T = 113$ (2) K
$\gamma = 96.46$ (3)º	Block, colorless
$V = 3831.6$ (13) Å^3	0.34 × 0.32 × 0.18 mm

Data collection

Rigaku Saturn diffractometer	17590 independent reflections
Radiation source: rotating anode	14508 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{int} = 0.035$
$T = 113$(2) K	$\theta_{max} = 27.8$º
ω scans	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	$h = -10 \rightarrow 10$
$T_{min} = 0.932$, $T_{max} = 0.963$	$k = -27 \rightarrow 27$
35937 measured reflections	$l = -31 \rightarrow 31$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.056$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.134$	$w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 1.4707P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} = 0.001$
17590 reflections	$\Delta\rho_{max} = 0.55$ e Å^{-3}
979 parameters	$\Delta\rho_{min} = -0.53$ e Å^{-3}
96 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	0.25176 (6)	0.22828 (2)	0.156778 (19)	0.02256 (11)	
N1	0.51718 (18)	0.39243 (7)	0.10231 (6)	0.0168 (3)	
N2	0.45024 (19)	0.34162 (7)	0.17781 (6)	0.0177 (3)	
N3	0.33144 (18)	0.28719 (7)	0.07868 (6)	0.0165 (3)	
N4	0.61749 (19)	0.44332 (7)	0.20073 (7)	0.0180 (3)	
N5	0.3981 (2)	0.33659 (8)	0.00755 (7)	0.0188 (3)	
C1	0.5267 (2)	0.39225 (9)	0.15850 (7)	0.0161 (4)	
C2	0.3578 (2)	0.29361 (9)	0.13527 (7)	0.0165 (4)	
C3	0.4182 (2)	0.33940 (9)	0.06421 (7)	0.0160 (3)	
C4	0.7199 (2)	0.50406 (9)	0.19479 (8)	0.0189 (4)	
C5	0.8540 (2)	0.48759 (9)	0.15411 (8)	0.0206 (4)	
H5A	0.9110	0.5314	0.1520	0.025*	
H5B	0.7919	0.4646	0.1146	0.025*	
C6	0.9950 (2)	0.44549 (10)	0.16437 (8)	0.0239 (4)	
C7	0.7949 (3)	0.54427 (10)	0.25749 (8)	0.0265 (4)	
H7A	0.7045	0.5594	0.2794	0.040*	
H7B	0.8729	0.5835	0.2568	0.040*	
H7C	0.8552	0.5156	0.2764	0.040*	
C8	0.6039 (3)	0.54624 (10)	0.16903 (9)	0.0266 (4)	
H8A	0.5523	0.5206	0.1293	0.040*	
H8B	0.6699	0.5882	0.1679	0.040*	
H8C	0.5158	0.5567	0.1935	0.040*	
C9	1.111 (2)	0.4693 (7)	0.2234 (4)	0.056 (4)	0.42 (2)
H9A	1.0492	0.4596	0.2539	0.084*	0.42 (2)
H9B	1.1479	0.5179	0.2328	0.084*	0.42 (2)
H9C	1.2086	0.4455	0.2210	0.084*	0.42 (2)
C10	0.9190 (13)	0.3714 (4)	0.1544 (9)	0.043 (3)	0.42 (2)
H10A	1.0095	0.3439	0.1542	0.065*	0.42 (2)
H10B	0.8450	0.3555	0.1168	0.065*	0.42 (2)
H10C	0.8541	0.3679	0.1859	0.065*	0.42 (2)
C11	1.108 (2)	0.4471 (9)	0.1174 (6)	0.043 (3)	0.42 (2)
H11A	1.1943	0.4182	0.1202	0.064*	0.42 (2)
H11B	1.1621	0.4935	0.1233	0.064*	0.42 (2)

H11C	1.0401	0.4308	0.0786	0.064*	0.42 (2)
C9'	1.1350 (11)	0.4899 (6)	0.2119 (5)	0.065 (3)	0.58 (2)
H9'1	1.0931	0.5009	0.2495	0.097*	0.58 (2)
H9'2	1.1703	0.5315	0.2018	0.097*	0.58 (2)
H9'3	1.2310	0.4655	0.2145	0.097*	0.58 (2)
C10'	0.9370 (13)	0.3817 (5)	0.1808 (5)	0.049 (2)	0.58 (2)
H10D	0.8428	0.3547	0.1517	0.073*	0.58 (2)
H10E	0.9008	0.3938	0.2194	0.073*	0.58 (2)
H10F	1.0299	0.3554	0.1817	0.073*	0.58 (2)
C11'	1.0693 (14)	0.4258 (6)	0.1073 (3)	0.0358 (18)	0.58 (2)
H11D	1.1653	0.4022	0.1129	0.054*	0.58 (2)
H11E	1.1064	0.4665	0.0961	0.054*	0.58 (2)
H11F	0.9836	0.3961	0.0764	0.054*	0.58 (2)
C12	0.4864 (2)	0.38653 (9)	−0.01533 (8)	0.0198 (4)	
H12A	0.4994	0.4311	0.0139	0.024*	
H12B	0.4166	0.3892	−0.0510	0.024*	
C13	0.6584 (2)	0.37214 (9)	−0.03011 (8)	0.0199 (4)	
C14	0.7036 (3)	0.30838 (11)	−0.03965 (10)	0.0302 (5)	
H14A	0.6266	0.2723	−0.0359	0.036*	
C15	0.8611 (3)	0.29648 (12)	−0.05476 (10)	0.0365 (5)	
H15A	0.8909	0.2525	−0.0610	0.044*	
C16	0.9740 (3)	0.34835 (12)	−0.06067 (9)	0.0327 (5)	
H16	1.0815	0.3403	−0.0708	0.039*	
C17	0.9296 (3)	0.41180 (12)	−0.05183 (10)	0.0348 (5)	
H17	1.0066	0.4475	−0.0561	0.042*	
C18	0.7725 (3)	0.42401 (11)	−0.03661 (9)	0.0299 (5)	
H18	0.7431	0.4680	−0.0306	0.036*	
Cl2	0.41948 (6)	0.53961 (2)	0.346225 (19)	0.02303 (11)	
N6	0.60553 (19)	0.36615 (7)	0.39037 (6)	0.0179 (3)	
N7	0.54407 (19)	0.42739 (7)	0.32025 (6)	0.0184 (3)	
N8	0.49763 (19)	0.47124 (7)	0.41881 (6)	0.0178 (3)	
N9	0.6442 (2)	0.32725 (8)	0.29300 (7)	0.0194 (3)	
N10	0.5585 (2)	0.41230 (8)	0.48486 (7)	0.0196 (3)	
C19	0.5968 (2)	0.37354 (9)	0.33635 (7)	0.0167 (4)	
C20	0.4964 (2)	0.47114 (9)	0.36373 (8)	0.0172 (4)	
C21	0.5555 (2)	0.41615 (9)	0.43003 (7)	0.0166 (4)	
C22	0.6925 (2)	0.26095 (9)	0.29462 (8)	0.0198 (4)	
C23	0.8450 (2)	0.26562 (10)	0.34155 (8)	0.0218 (4)	
H23A	0.8066	0.2822	0.3799	0.026*	
H23B	0.8645	0.2187	0.3381	0.026*	
C24	1.0196 (2)	0.30679 (11)	0.34632 (9)	0.0275 (4)	
C25	0.7218 (3)	0.22687 (10)	0.23221 (8)	0.0276 (4)	
H25A	0.6154	0.2173	0.2057	0.041*	
H25B	0.7656	0.1846	0.2312	0.041*	
H25C	0.8031	0.2569	0.2198	0.041*	
C26	0.5431 (2)	0.21836 (10)	0.30844 (9)	0.0262 (4)	
H26A	0.5190	0.2401	0.3476	0.039*	
H26B	0.5707	0.1733	0.3069	0.039*	
H26C	0.4442	0.2145	0.2796	0.039*	

C27	1.1306 (3)	0.29118 (16)	0.39577 (12)	0.0548 (8)
H27A	1.1360	0.2427	0.3858	0.082*
H27B	1.0828	0.3048	0.4322	0.082*
H27C	1.2441	0.3160	0.4009	0.082*
C28	1.0154 (3)	0.38242 (12)	0.36303 (14)	0.0533 (7)
H28A	1.1303	0.4065	0.3703	0.080*
H28B	0.9629	0.3955	0.3985	0.080*
H28C	0.9503	0.3940	0.3311	0.080*
C29	1.1032 (3)	0.28702 (15)	0.29119 (11)	0.0500 (7)
H29A	1.0451	0.3026	0.2603	0.075*
H29B	1.0968	0.2379	0.2781	0.075*
H29C	1.2212	0.3079	0.2999	0.075*
C30	0.6211 (2)	0.35846 (9)	0.50476 (8)	0.0195 (4)
H30A	0.5938	0.3163	0.4724	0.023*
H30B	0.5615	0.3518	0.5371	0.023*
C31	0.8088 (2)	0.37065 (9)	0.52564 (8)	0.0204 (4)
C32	0.8865 (3)	0.31716 (11)	0.53284 (11)	0.0358 (5)
H32	0.8220	0.2737	0.5235	0.043*
C33	1.0568 (3)	0.32539 (13)	0.55349 (11)	0.0403 (6)
H33	1.1073	0.2878	0.5585	0.048*
C34	1.1519 (3)	0.38748 (13)	0.56667 (11)	0.0426 (6)
H34	1.2688	0.3935	0.5802	0.051*
C35	1.0751 (3)	0.44103 (14)	0.55990 (16)	0.0713 (11)
H35	1.1399	0.4845	0.5692	0.086*
C36	0.9044 (3)	0.43288 (12)	0.53970 (14)	0.0537 (8)
H36	0.8537	0.4707	0.5356	0.064*
Cl3	1.14070 (7)	−0.03951 (2)	0.64751 (2)	0.02864 (12)
N11	0.90224 (19)	0.12914 (7)	0.61493 (6)	0.0176 (3)
N12	1.01421 (19)	0.07117 (8)	0.68179 (6)	0.0197 (3)
N13	1.01909 (19)	0.02732 (8)	0.57954 (6)	0.0189 (3)
N14	0.9165 (2)	0.17138 (8)	0.71538 (7)	0.0210 (3)
N15	0.9065 (2)	0.08231 (8)	0.51668 (6)	0.0187 (3)
C37	0.9436 (2)	0.12389 (9)	0.66904 (7)	0.0176 (4)
C38	1.0467 (2)	0.02792 (9)	0.63493 (8)	0.0191 (4)
C39	0.9421 (2)	0.08014 (9)	0.57184 (7)	0.0168 (4)
C40	0.8286 (2)	0.23066 (9)	0.71594 (8)	0.0210 (4)
C41	0.6431 (2)	0.20115 (9)	0.68843 (8)	0.0206 (4)
H41A	0.6479	0.1647	0.6527	0.025*
H41B	0.5947	0.1792	0.7161	0.025*
C42	0.5123 (2)	0.24412 (9)	0.67094 (8)	0.0227 (4)
C43	0.9193 (2)	0.27622 (10)	0.68524 (9)	0.0250 (4)
H43A	1.0387	0.2868	0.7017	0.038*
H43B	0.8702	0.3180	0.6908	0.038*
H43C	0.9076	0.2532	0.6434	0.038*
C44	0.8433 (3)	0.26835 (10)	0.78098 (8)	0.0303 (5)
H44A	0.7858	0.2393	0.8013	0.045*
H44B	0.7913	0.3094	0.7852	0.045*
H44C	0.9621	0.2804	0.7980	0.045*
C45	0.5010 (3)	0.30788 (10)	0.71917 (9)	0.0318 (5)

H45A	0.6040	0.3400	0.7252	0.048*	
H45B	0.4877	0.2962	0.7556	0.048*	
H45C	0.4042	0.3283	0.7076	0.048*	
C46	0.3414 (3)	0.19809 (11)	0.65819 (11)	0.0350 (5)	
H46A	0.3152	0.1879	0.6941	0.052*	
H46B	0.3469	0.1561	0.6284	0.052*	
H46C	0.2537	0.2211	0.6439	0.052*	
C47	0.5413 (3)	0.26333 (11)	0.61505 (9)	0.0291 (5)	
H47A	0.4463	0.2840	0.6024	0.044*	
H47B	0.5512	0.2228	0.5843	0.044*	
H47C	0.6449	0.2955	0.6227	0.044*	
C48	0.8381 (2)	0.13786 (9)	0.50105 (8)	0.0192 (4)	
H48A	0.8927	0.1473	0.4685	0.023*	
H48B	0.8674	0.1785	0.5349	0.023*	
C49	0.6487 (2)	0.12544 (9)	0.48282 (8)	0.0198 (4)	
C50	0.5413 (3)	0.08988 (10)	0.50896 (9)	0.0246 (4)	
H50	0.5864	0.0701	0.5376	0.029*	
C51	0.3679 (3)	0.08275 (10)	0.49370 (10)	0.0297 (5)	
H51	0.2954	0.0582	0.5118	0.036*	
C52	0.3012 (3)	0.11149 (12)	0.45208 (11)	0.0360 (5)	
H52	0.1829	0.1072	0.4420	0.043*	
C53	0.4066 (3)	0.14630 (13)	0.42534 (11)	0.0400 (6)	
H53	0.3610	0.1656	0.3965	0.048*	
C54	0.5797 (3)	0.15324 (11)	0.44046 (9)	0.0298 (5)	
H54	0.6517	0.1772	0.4217	0.036*	
Cl4	−0.31144 (6)	0.73479 (2)	0.15285 (2)	0.02536 (11)	
N16	−0.04068 (19)	0.89942 (7)	0.10058 (6)	0.0178 (3)	
N17	−0.11611 (19)	0.84876 (8)	0.17520 (6)	0.0189 (3)	
N18	−0.22056 (19)	0.79254 (7)	0.07524 (6)	0.0175 (3)	
N19	0.0458 (2)	0.95158 (8)	0.19963 (7)	0.0206 (3)	
N20	−0.1436 (2)	0.84117 (8)	0.00481 (6)	0.0186 (3)	
C55	−0.0378 (2)	0.89986 (9)	0.15664 (8)	0.0174 (4)	
C56	−0.2033 (2)	0.80012 (9)	0.13198 (8)	0.0178 (4)	
C57	−0.1327 (2)	0.84514 (9)	0.06163 (7)	0.0166 (4)	
C58	0.1483 (3)	1.01300 (9)	0.19478 (8)	0.0248 (4)	
C59	0.2904 (2)	0.99697 (10)	0.15752 (9)	0.0272 (4)	
H59A	0.3469	1.0408	0.1554	0.033*	
H59B	0.2346	0.9726	0.1174	0.033*	
C60	0.4322 (3)	0.95702 (12)	0.17192 (10)	0.0369 (5)	
C61	0.2131 (3)	1.05436 (12)	0.25774 (10)	0.0443 (6)	
H61A	0.1186	1.0697	0.2772	0.067*	
H61B	0.2928	1.0935	0.2578	0.067*	
H61C	0.2696	1.0264	0.2786	0.067*	
C62	0.0340 (3)	1.05308 (10)	0.16575 (10)	0.0329 (5)	
H62A	−0.0097	1.0266	0.1255	0.049*	
H62B	0.0990	1.0957	0.1656	0.049*	
H62C	−0.0598	1.0624	0.1877	0.049*	
C63	0.3762 (5)	0.8940 (2)	0.1873 (2)	0.0516 (10)	0.753 (4)
H63A	0.2909	0.8649	0.1559	0.077*	0.753 (4)

H63B	0.3283	0.9053	0.2238	0.077*	0.753 (4)
H63C	0.4725	0.8704	0.1922	0.077*	0.753 (4)
C64	0.5174 (5)	0.9369 (2)	0.11552 (16)	0.0456 (9)	0.753 (4)
H64A	0.6142	0.9146	0.1234	0.068*	0.753 (4)
H64B	0.5550	0.9774	0.1042	0.068*	0.753 (4)
H64C	0.4363	0.9060	0.0837	0.068*	0.753 (4)
C65	0.5730 (5)	1.0033 (2)	0.21834 (18)	0.0660 (12)	0.753 (4)
H65A	0.5355	1.0126	0.2568	0.099*	0.753 (4)
H65B	0.5999	1.0457	0.2086	0.099*	0.753 (4)
H65C	0.6733	0.9810	0.2192	0.099*	0.753 (4)
C63'	0.3532 (14)	0.8805 (4)	0.1520 (6)	0.0510 (15)	0.247 (4)
H63D	0.4395	0.8530	0.1592	0.076*	0.247 (4)
H63E	0.3095	0.8672	0.1101	0.076*	0.247 (4)
H63F	0.2614	0.8734	0.1741	0.076*	0.247 (4)
C64'	0.5729 (13)	0.9674 (6)	0.1397 (5)	0.0512 (14)	0.247 (4)
H64D	0.6533	0.9368	0.1446	0.077*	0.247 (4)
H64E	0.6291	1.0141	0.1550	0.077*	0.247 (4)
H64F	0.5301	0.9583	0.0981	0.077*	0.247 (4)
C65'	0.4932 (16)	0.9692 (7)	0.2389 (3)	0.0663 (16)	0.247 (4)
H65D	0.4008	0.9531	0.2572	0.099*	0.247 (4)
H65E	0.5294	1.0174	0.2574	0.099*	0.247 (4)
H65F	0.5876	0.9446	0.2438	0.099*	0.247 (4)
C66	−0.0526 (2)	0.89078 (9)	−0.01753 (8)	0.0189 (4)	
H66A	−0.0379	0.9352	0.0120	0.023*	
H66B	−0.1213	0.8942	−0.0531	0.023*	
C67	0.1189 (2)	0.87506 (9)	−0.03230 (8)	0.0195 (4)	
C68	0.1535 (3)	0.80974 (10)	−0.04905 (10)	0.0302 (5)	
H68	0.0697	0.7734	−0.0504	0.036*	
C69	0.3099 (3)	0.79679 (11)	−0.06397 (11)	0.0372 (5)	
H69	0.3322	0.7517	−0.0753	0.045*	
C70	0.4326 (3)	0.84886 (11)	−0.06239 (9)	0.0323 (5)	
H70	0.5399	0.8399	−0.0721	0.039*	
C71	0.3991 (3)	0.91358 (12)	−0.04675 (11)	0.0394 (6)	
H71	0.4826	0.9497	−0.0464	0.047*	
C72	0.2429 (3)	0.92689 (11)	−0.03128 (11)	0.0337 (5)	
H72	0.2214	0.9721	−0.0199	0.040*	
H4	0.605 (3)	0.4400 (10)	0.2346 (10)	0.024 (6)*	
H5	0.339 (3)	0.3010 (12)	−0.0155 (10)	0.035 (7)*	
H9	0.611 (3)	0.3310 (10)	0.2585 (9)	0.021 (5)*	
H10	0.534 (3)	0.4500 (12)	0.5119 (10)	0.037 (6)*	
H14	0.963 (3)	0.1670 (10)	0.7469 (9)	0.022 (6)*	
H15	0.931 (3)	0.0484 (12)	0.4890 (11)	0.039 (7)*	
H19	0.033 (3)	0.9481 (12)	0.2344 (11)	0.034 (7)*	
H20	−0.198 (3)	0.8040 (12)	−0.0189 (10)	0.030 (6)*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

Cl1	0.0266 (2)	0.0209 (2)	0.0187 (2)	−0.00383 (18)	0.00524 (17)	0.00532 (17)
N1	0.0178 (7)	0.0168 (7)	0.0149 (7)	0.0020 (6)	0.0026 (6)	0.0031 (6)
N2	0.0189 (8)	0.0175 (7)	0.0151 (7)	−0.0007 (6)	0.0026 (6)	0.0031 (6)
N3	0.0168 (7)	0.0171 (7)	0.0147 (7)	0.0007 (6)	0.0035 (6)	0.0030 (6)
N4	0.0217 (8)	0.0162 (7)	0.0142 (7)	−0.0009 (6)	0.0035 (6)	0.0023 (6)
N5	0.0199 (8)	0.0183 (8)	0.0157 (7)	−0.0026 (6)	0.0006 (6)	0.0038 (6)
C1	0.0158 (8)	0.0160 (8)	0.0157 (8)	0.0026 (7)	0.0020 (7)	0.0029 (7)
C2	0.0157 (8)	0.0170 (8)	0.0173 (8)	0.0033 (7)	0.0057 (7)	0.0038 (7)
C3	0.0141 (8)	0.0166 (8)	0.0167 (8)	0.0023 (7)	0.0023 (7)	0.0036 (7)
C4	0.0206 (9)	0.0130 (8)	0.0205 (9)	−0.0016 (7)	0.0028 (7)	0.0018 (7)
C5	0.0203 (9)	0.0194 (9)	0.0217 (9)	0.0012 (7)	0.0035 (7)	0.0057 (7)
C6	0.0182 (9)	0.0296 (10)	0.0231 (10)	0.0044 (8)	0.0020 (7)	0.0063 (8)
C7	0.0290 (11)	0.0214 (10)	0.0228 (10)	−0.0039 (8)	0.0045 (8)	−0.0019 (8)
C8	0.0290 (11)	0.0205 (10)	0.0312 (11)	0.0065 (8)	0.0068 (8)	0.0069 (8)
C9	0.068 (8)	0.051 (6)	0.038 (5)	0.035 (5)	−0.021 (5)	−0.004 (4)
C10	0.024 (3)	0.033 (4)	0.085 (8)	0.015 (3)	0.014 (5)	0.029 (5)
C11	0.035 (6)	0.052 (8)	0.048 (5)	0.022 (5)	0.018 (5)	0.014 (5)
C9'	0.020 (3)	0.093 (7)	0.060 (5)	0.020 (4)	−0.012 (3)	−0.011 (4)
C10'	0.044 (4)	0.061 (4)	0.064 (5)	0.032 (3)	0.021 (4)	0.041 (4)
C11'	0.031 (4)	0.048 (5)	0.039 (3)	0.020 (3)	0.017 (3)	0.019 (3)
C12	0.0228 (9)	0.0192 (9)	0.0168 (8)	−0.0002 (7)	0.0016 (7)	0.0058 (7)
C13	0.0226 (9)	0.0224 (9)	0.0144 (8)	0.0018 (7)	0.0020 (7)	0.0053 (7)
C14	0.0273 (11)	0.0243 (10)	0.0393 (12)	0.0045 (8)	0.0091 (9)	0.0075 (9)
C15	0.0358 (13)	0.0325 (12)	0.0438 (13)	0.0132 (10)	0.0122 (10)	0.0091 (10)
C16	0.0247 (11)	0.0465 (13)	0.0271 (11)	0.0078 (10)	0.0068 (8)	0.0086 (10)
C17	0.0268 (11)	0.0407 (13)	0.0398 (13)	−0.0001 (10)	0.0099 (9)	0.0162 (10)
C18	0.0295 (11)	0.0264 (11)	0.0370 (12)	0.0028 (9)	0.0081 (9)	0.0137 (9)
Cl2	0.0296 (2)	0.0206 (2)	0.0194 (2)	0.00947 (18)	0.00033 (18)	0.00568 (17)
N6	0.0208 (8)	0.0187 (8)	0.0141 (7)	0.0046 (6)	0.0032 (6)	0.0033 (6)
N7	0.0218 (8)	0.0183 (8)	0.0146 (7)	0.0033 (6)	0.0019 (6)	0.0037 (6)
N8	0.0196 (8)	0.0182 (7)	0.0151 (7)	0.0050 (6)	0.0014 (6)	0.0033 (6)
N9	0.0264 (8)	0.0175 (8)	0.0145 (7)	0.0064 (6)	0.0025 (6)	0.0040 (6)
N10	0.0252 (8)	0.0208 (8)	0.0149 (7)	0.0081 (7)	0.0047 (6)	0.0058 (6)
C19	0.0170 (8)	0.0168 (8)	0.0149 (8)	0.0013 (7)	0.0012 (7)	0.0029 (7)
C20	0.0165 (8)	0.0156 (8)	0.0183 (8)	0.0020 (7)	−0.0003 (7)	0.0040 (7)
C21	0.0163 (8)	0.0170 (8)	0.0149 (8)	0.0004 (7)	0.0004 (7)	0.0037 (7)
C22	0.0235 (9)	0.0169 (9)	0.0183 (9)	0.0051 (7)	0.0024 (7)	0.0033 (7)
C23	0.0235 (10)	0.0241 (10)	0.0191 (9)	0.0071 (8)	0.0042 (7)	0.0065 (8)
C24	0.0192 (10)	0.0355 (11)	0.0263 (10)	0.0056 (8)	0.0042 (8)	0.0051 (9)
C25	0.0372 (12)	0.0232 (10)	0.0199 (9)	0.0111 (9)	0.0027 (8)	−0.0002 (8)
C26	0.0255 (10)	0.0202 (10)	0.0308 (11)	0.0007 (8)	0.0018 (8)	0.0059 (8)
C27	0.0255 (12)	0.090 (2)	0.0485 (16)	−0.0002 (13)	−0.0087 (11)	0.0279 (15)
C28	0.0269 (12)	0.0358 (14)	0.086 (2)	−0.0069 (10)	0.0103 (13)	0.0010 (13)
C29	0.0297 (13)	0.0741 (19)	0.0410 (14)	−0.0010 (12)	0.0176 (11)	0.0059 (13)
C30	0.0246 (10)	0.0178 (9)	0.0163 (8)	0.0038 (7)	0.0031 (7)	0.0048 (7)
C31	0.0230 (10)	0.0217 (9)	0.0164 (8)	0.0053 (7)	0.0026 (7)	0.0043 (7)
C32	0.0278 (11)	0.0295 (11)	0.0550 (15)	0.0055 (9)	0.0019 (10)	0.0213 (11)
C33	0.0304 (12)	0.0454 (14)	0.0543 (15)	0.0130 (11)	0.0030 (11)	0.0278 (12)
C34	0.0259 (12)	0.0445 (14)	0.0484 (15)	0.0061 (10)	−0.0071 (10)	0.0026 (11)

C35	0.0333 (15)	0.0303 (14)	0.128 (3)	−0.0046 (11)	−0.0209 (17)	0.0017 (16)
C36	0.0322 (13)	0.0213 (11)	0.096 (2)	0.0017 (10)	−0.0116 (13)	0.0069 (13)
Cl3	0.0402 (3)	0.0260 (2)	0.0201 (2)	0.0180 (2)	−0.0017 (2)	0.00425 (18)
N11	0.0196 (8)	0.0164 (7)	0.0154 (7)	0.0038 (6)	0.0024 (6)	0.0015 (6)
N12	0.0221 (8)	0.0192 (8)	0.0164 (7)	0.0048 (6)	0.0007 (6)	0.0028 (6)
N13	0.0211 (8)	0.0186 (8)	0.0160 (7)	0.0055 (6)	0.0007 (6)	0.0028 (6)
N14	0.0267 (9)	0.0209 (8)	0.0145 (8)	0.0077 (7)	−0.0003 (6)	0.0028 (6)
N15	0.0250 (8)	0.0177 (8)	0.0139 (7)	0.0077 (6)	0.0019 (6)	0.0037 (6)
C37	0.0166 (8)	0.0185 (9)	0.0158 (8)	0.0019 (7)	0.0005 (7)	0.0028 (7)
C38	0.0202 (9)	0.0181 (9)	0.0176 (9)	0.0035 (7)	−0.0004 (7)	0.0034 (7)
C39	0.0165 (8)	0.0172 (9)	0.0152 (8)	0.0011 (7)	0.0016 (7)	0.0029 (7)
C40	0.0268 (10)	0.0176 (9)	0.0172 (9)	0.0066 (8)	0.0034 (7)	0.0010 (7)
C41	0.0227 (9)	0.0184 (9)	0.0223 (9)	0.0045 (7)	0.0078 (7)	0.0060 (7)
C42	0.0226 (10)	0.0205 (9)	0.0268 (10)	0.0056 (8)	0.0089 (8)	0.0066 (8)
C43	0.0238 (10)	0.0200 (9)	0.0299 (10)	0.0022 (8)	0.0041 (8)	0.0048 (8)
C44	0.0431 (13)	0.0254 (11)	0.0196 (10)	0.0114 (9)	0.0026 (9)	−0.0003 (8)
C45	0.0362 (12)	0.0264 (11)	0.0367 (12)	0.0141 (9)	0.0147 (10)	0.0077 (9)
C46	0.0236 (11)	0.0337 (12)	0.0494 (14)	0.0061 (9)	0.0093 (10)	0.0121 (10)
C47	0.0295 (11)	0.0308 (11)	0.0298 (11)	0.0086 (9)	0.0038 (9)	0.0116 (9)
C48	0.0232 (9)	0.0180 (9)	0.0179 (9)	0.0061 (7)	0.0022 (7)	0.0067 (7)
C49	0.0229 (9)	0.0165 (9)	0.0194 (9)	0.0058 (7)	0.0032 (7)	0.0025 (7)
C50	0.0270 (10)	0.0220 (10)	0.0254 (10)	0.0038 (8)	0.0037 (8)	0.0079 (8)
C51	0.0251 (10)	0.0256 (11)	0.0399 (12)	0.0004 (8)	0.0076 (9)	0.0118 (9)
C52	0.0215 (11)	0.0406 (13)	0.0487 (14)	0.0049 (9)	0.0002 (10)	0.0189 (11)
C53	0.0264 (12)	0.0508 (15)	0.0516 (15)	0.0071 (10)	−0.0016 (10)	0.0319 (12)
C54	0.0254 (11)	0.0365 (12)	0.0333 (11)	0.0069 (9)	0.0040 (9)	0.0193 (9)
Cl4	0.0315 (3)	0.0222 (2)	0.0201 (2)	−0.00605 (19)	0.00489 (19)	0.00582 (18)
N16	0.0177 (7)	0.0193 (8)	0.0150 (7)	0.0001 (6)	0.0011 (6)	0.0041 (6)
N17	0.0204 (8)	0.0188 (8)	0.0152 (7)	−0.0013 (6)	0.0006 (6)	0.0035 (6)
N18	0.0185 (8)	0.0182 (7)	0.0143 (7)	−0.0005 (6)	0.0025 (6)	0.0036 (6)
N19	0.0239 (8)	0.0191 (8)	0.0154 (8)	−0.0040 (6)	0.0014 (6)	0.0022 (6)
N20	0.0215 (8)	0.0185 (8)	0.0129 (7)	−0.0019 (6)	0.0012 (6)	0.0023 (6)
C55	0.0157 (8)	0.0188 (9)	0.0163 (8)	0.0020 (7)	0.0016 (7)	0.0031 (7)
C56	0.0194 (9)	0.0163 (8)	0.0178 (8)	0.0011 (7)	0.0039 (7)	0.0050 (7)
C57	0.0144 (8)	0.0180 (9)	0.0172 (8)	0.0036 (7)	0.0029 (7)	0.0040 (7)
C58	0.0279 (10)	0.0185 (9)	0.0228 (10)	−0.0068 (8)	0.0027 (8)	0.0017 (8)
C59	0.0216 (10)	0.0275 (10)	0.0321 (11)	−0.0030 (8)	0.0028 (8)	0.0109 (9)
C60	0.0231 (11)	0.0446 (14)	0.0434 (13)	0.0027 (10)	0.0001 (9)	0.0160 (11)
C61	0.0544 (16)	0.0348 (13)	0.0290 (12)	−0.0208 (11)	0.0066 (11)	−0.0054 (10)
C62	0.0352 (12)	0.0207 (10)	0.0449 (13)	0.0040 (9)	0.0109 (10)	0.0110 (9)
C63	0.0415 (17)	0.059 (2)	0.072 (2)	0.0204 (15)	0.0201 (19)	0.039 (2)
C64	0.0376 (18)	0.056 (2)	0.0485 (19)	0.0175 (15)	0.0118 (15)	0.0174 (16)
C65	0.0374 (19)	0.084 (3)	0.063 (2)	0.0076 (17)	−0.0108 (16)	0.0044 (19)
C63'	0.041 (2)	0.057 (2)	0.070 (3)	0.019 (2)	0.019 (3)	0.034 (3)
C64'	0.043 (2)	0.058 (3)	0.056 (3)	0.015 (2)	0.011 (2)	0.016 (2)
C65'	0.044 (2)	0.080 (3)	0.063 (3)	0.009 (2)	−0.013 (2)	0.009 (2)
C66	0.0221 (9)	0.0189 (9)	0.0171 (8)	0.0026 (7)	0.0037 (7)	0.0073 (7)
C67	0.0202 (9)	0.0220 (9)	0.0162 (8)	0.0039 (7)	0.0020 (7)	0.0054 (7)
C68	0.0258 (11)	0.0222 (10)	0.0408 (12)	0.0018 (8)	0.0078 (9)	0.0052 (9)

C69	0.0312 (12)	0.0275 (11)	0.0503 (14)	0.0106 (9)	0.0112 (10)	0.0016 (10)
C70	0.0243 (11)	0.0393 (12)	0.0343 (12)	0.0103 (9)	0.0079 (9)	0.0082 (10)
C71	0.0256 (11)	0.0326 (12)	0.0641 (16)	0.0034 (9)	0.0151 (11)	0.0175 (11)
C72	0.0263 (11)	0.0217 (10)	0.0554 (14)	0.0052 (8)	0.0117 (10)	0.0120 (10)

Geometric parameters (Å, °)

Cl1—C2	1.7489 (19)	Cl3—C38	1.7472 (19)
N1—C3	1.342 (2)	N11—C37	1.340 (2)
N1—C1	1.342 (2)	N11—C39	1.342 (2)
N2—C2	1.313 (2)	N12—C38	1.314 (2)
N2—C1	1.372 (2)	N12—C37	1.380 (2)
N3—C2	1.319 (2)	N13—C38	1.319 (2)
N3—C3	1.370 (2)	N13—C39	1.367 (2)
N4—C1	1.336 (2)	N14—C37	1.334 (2)
N4—C4	1.480 (2)	N14—C40	1.490 (2)
N4—H4	0.85 (2)	N14—H14	0.84 (2)
N5—C3	1.336 (2)	N15—C39	1.336 (2)
N5—C12	1.454 (2)	N15—C48	1.453 (2)
N5—H5	0.85 (2)	N15—H15	0.89 (2)
C4—C7	1.532 (3)	C40—C43	1.521 (3)
C4—C8	1.542 (3)	C40—C44	1.534 (3)
C4—C5	1.546 (3)	C40—C41	1.558 (3)
C5—C6	1.552 (3)	C41—C42	1.553 (3)
C5—H5A	0.9900	C41—H41A	0.9900
C5—H5B	0.9900	C41—H41B	0.9900
C6—C10'	1.522 (6)	C42—C45	1.531 (3)
C6—C11'	1.530 (6)	C42—C47	1.531 (3)
C6—C11	1.533 (8)	C42—C46	1.542 (3)
C6—C9	1.535 (7)	C43—H43A	0.9800
C6—C9'	1.536 (6)	C43—H43B	0.9800
C6—C10	1.540 (7)	C43—H43C	0.9800
C7—H7A	0.9800	C44—H44A	0.9800
C7—H7B	0.9800	C44—H44B	0.9800
C7—H7C	0.9800	C44—H44C	0.9800
C8—H8A	0.9800	C45—H45A	0.9800
C8—H8B	0.9800	C45—H45B	0.9800
C8—H8C	0.9800	C45—H45C	0.9800
C9—H9A	0.9800	C46—H46A	0.9800
C9—H9B	0.9800	C46—H46B	0.9800
C9—H9C	0.9800	C46—H46C	0.9800
C10—H10A	0.9800	C47—H47A	0.9800
C10—H10B	0.9800	C47—H47B	0.9800
C10—H10C	0.9800	C47—H47C	0.9800
C11—H11A	0.9800	C48—C49	1.522 (3)
C11—H11B	0.9800	C48—H48A	0.9900
C11—H11C	0.9800	C48—H48B	0.9900
C9'—H9'1	0.9800	C49—C50	1.385 (3)
C9'—H9'2	0.9800	C49—C54	1.392 (3)

C9'—H9'3	0.9800	C50—C51	1.392 (3)
C10'—H10D	0.9800	C50—H50	0.9500
C10'—H10E	0.9800	C51—C52	1.384 (3)
C10'—H10F	0.9800	C51—H51	0.9500
C11'—H11D	0.9800	C52—C53	1.376 (3)
C11'—H11E	0.9800	C52—H52	0.9500
C11'—H11F	0.9800	C53—C54	1.390 (3)
C12—C13	1.517 (3)	C53—H53	0.9500
C12—H12A	0.9900	C54—H54	0.9500
C12—H12B	0.9900	Cl4—C56	1.7480 (19)
C13—C14	1.384 (3)	N16—C55	1.340 (2)
C13—C18	1.393 (3)	N16—C57	1.342 (2)
C14—C15	1.395 (3)	N17—C56	1.311 (2)
C14—H14A	0.9500	N17—C55	1.376 (2)
C15—C16	1.381 (3)	N18—C56	1.317 (2)
C15—H15A	0.9500	N18—C57	1.370 (2)
C16—C17	1.376 (3)	N19—C55	1.332 (2)
C16—H16	0.9500	N19—C58	1.483 (2)
C17—C18	1.394 (3)	N19—H19	0.87 (2)
C17—H17	0.9500	N20—C57	1.336 (2)
C18—H18	0.9500	N20—C66	1.451 (2)
Cl2—C20	1.7475 (18)	N20—H20	0.87 (2)
N6—C19	1.340 (2)	C58—C61	1.527 (3)
N6—C21	1.344 (2)	C58—C62	1.541 (3)
N7—C20	1.315 (2)	C58—C59	1.546 (3)
N7—C19	1.374 (2)	C59—C60	1.552 (3)
N8—C20	1.319 (2)	C59—H59A	0.9900
N8—C21	1.365 (2)	C59—H59B	0.9900
N9—C19	1.340 (2)	C60—C64'	1.473 (7)
N9—C22	1.485 (2)	C60—C63	1.490 (4)
N9—H9	0.87 (2)	C60—C65	1.540 (4)
N10—C21	1.336 (2)	C60—C64	1.566 (4)
N10—C30	1.448 (2)	C60—C65'	1.572 (7)
N10—H10	0.93 (2)	C60—C63'	1.574 (8)
C22—C25	1.534 (3)	C61—H61A	0.9800
C22—C26	1.537 (3)	C61—H61B	0.9800
C22—C23	1.553 (3)	C61—H61C	0.9800
C23—C24	1.545 (3)	C62—H62A	0.9800
C23—H23A	0.9900	C62—H62B	0.9800
C23—H23B	0.9900	C62—H62C	0.9800
C24—C28	1.523 (3)	C63—H63A	0.9800
C24—C29	1.532 (3)	C63—H63B	0.9800
C24—C27	1.535 (3)	C63—H63C	0.9800
C25—H25A	0.9800	C64—H64A	0.9800
C25—H25B	0.9800	C64—H64B	0.9800
C25—H25C	0.9800	C64—H64C	0.9800
C26—H26A	0.9800	C65—H65A	0.9800
C26—H26B	0.9800	C65—H65B	0.9800
C26—H26C	0.9800	C65—H65C	0.9800

C27—H27A	0.9800	C63'—H63D	0.9800
C27—H27B	0.9800	C63'—H63E	0.9800
C27—H27C	0.9800	C63'—H63F	0.9800
C28—H28A	0.9800	C64'—H64D	0.9800
C28—H28B	0.9800	C64'—H64E	0.9800
C28—H28C	0.9800	C64'—H64F	0.9800
C29—H29A	0.9800	C65'—H65D	0.9800
C29—H29B	0.9800	C65'—H65E	0.9800
C29—H29C	0.9800	C65'—H65F	0.9800
C30—C31	1.518 (3)	C66—C67	1.520 (3)
C30—H30A	0.9900	C66—H66A	0.9900
C30—H30B	0.9900	C66—H66B	0.9900
C31—C36	1.370 (3)	C67—C68	1.382 (3)
C31—C32	1.378 (3)	C67—C72	1.382 (3)
C32—C33	1.389 (3)	C68—C69	1.389 (3)
C32—H32	0.9500	C68—H68	0.9500
C33—C34	1.367 (3)	C69—C70	1.375 (3)
C33—H33	0.9500	C69—H69	0.9500
C34—C35	1.373 (4)	C70—C71	1.366 (3)
C34—H34	0.9500	C70—H70	0.9500
C35—C36	1.390 (3)	C71—C72	1.394 (3)
C35—H35	0.9500	C71—H71	0.9500
C36—H36	0.9500	C72—H72	0.9500
C3—N1—C1	114.95 (15)	C37—N11—C39	115.23 (15)
C2—N2—C1	112.59 (15)	C38—N12—C37	112.49 (15)
C2—N3—C3	112.39 (15)	C38—N13—C39	112.45 (15)
C1—N4—C4	128.27 (16)	C37—N14—C40	127.89 (16)
C1—N4—H4	112.2 (15)	C37—N14—H14	112.3 (14)
C4—N4—H4	119.4 (14)	C40—N14—H14	119.7 (14)
C3—N5—C12	122.93 (15)	C39—N15—C48	123.26 (15)
C3—N5—H5	115.9 (16)	C39—N15—H15	116.7 (15)
C12—N5—H5	120.8 (16)	C48—N15—H15	120.0 (15)
N4—C1—N1	120.58 (17)	N14—C37—N11	120.34 (16)
N4—C1—N2	114.53 (16)	N14—C37—N12	115.08 (16)
N1—C1—N2	124.89 (16)	N11—C37—N12	124.58 (16)
N2—C2—N3	129.94 (17)	N12—C38—N13	129.98 (17)
N2—C2—Cl1	115.24 (14)	N12—C38—Cl3	115.36 (14)
N3—C2—Cl1	114.81 (13)	N13—C38—Cl3	114.66 (13)
N5—C3—N1	118.79 (16)	N15—C39—N11	118.75 (16)
N5—C3—N3	116.04 (15)	N15—C39—N13	116.09 (15)
N1—C3—N3	125.16 (16)	N11—C39—N13	125.16 (16)
N4—C4—C7	104.89 (15)	N14—C40—C43	110.35 (16)
N4—C4—C8	109.24 (15)	N14—C40—C44	104.19 (15)
C7—C4—C8	108.56 (15)	C43—C40—C44	108.77 (16)
N4—C4—C5	113.26 (14)	N14—C40—C41	105.76 (15)
C7—C4—C5	113.24 (16)	C43—C40—C41	115.28 (16)
C8—C4—C5	107.53 (15)	C44—C40—C41	111.89 (16)
C4—C5—C6	123.98 (16)	C42—C41—C40	123.57 (16)
C4—C5—H5A	106.3	C42—C41—H41A	106.4

C6—C5—H5A	106.3	C40—C41—H41A	106.4
C4—C5—H5B	106.3	C42—C41—H41B	106.4
C6—C5—H5B	106.3	C40—C41—H41B	106.4
H5A—C5—H5B	106.4	H41A—C41—H41B	106.5
C10'—C6—C11'	108.6 (4)	C45—C42—C47	109.11 (17)
C10'—C6—C11	123.2 (7)	C45—C42—C46	107.95 (17)
C11'—C6—C11	18.8 (5)	C47—C42—C46	107.61 (17)
C10'—C6—C9	87.4 (5)	C45—C42—C41	114.06 (17)
C11'—C6—C9	120.3 (8)	C47—C42—C41	112.53 (16)
C11—C6—C9	106.5 (7)	C46—C42—C41	105.22 (16)
C10'—C6—C9'	109.5 (4)	C40—C43—H43A	109.5
C11'—C6—C9'	107.6 (5)	C40—C43—H43B	109.5
C11—C6—C9'	90.5 (7)	H43A—C43—H43B	109.5
C9—C6—C9'	22.4 (6)	C40—C43—H43C	109.5
C10'—C6—C10	22.8 (4)	H43A—C43—H43C	109.5
C11'—C6—C10	89.9 (6)	H43B—C43—H43C	109.5
C11—C6—C10	107.2 (5)	C40—C44—H44A	109.5
C9—C6—C10	108.5 (5)	C40—C44—H44B	109.5
C9'—C6—C10	129.4 (5)	H44A—C44—H44B	109.5
C10'—C6—C5	114.8 (4)	C40—C44—H44C	109.5
C11'—C6—C5	106.8 (5)	H44A—C44—H44C	109.5
C11—C6—C5	106.5 (7)	H44B—C44—H44C	109.5
C9—C6—C5	117.6 (6)	C42—C45—H45A	109.5
C9'—C6—C5	109.3 (5)	C42—C45—H45B	109.5
C10—C6—C5	110.0 (4)	H45A—C45—H45B	109.5
C4—C7—H7A	109.5	C42—C45—H45C	109.5
C4—C7—H7B	109.5	H45A—C45—H45C	109.5
H7A—C7—H7B	109.5	H45B—C45—H45C	109.5
C4—C7—H7C	109.5	C42—C46—H46A	109.5
H7A—C7—H7C	109.5	C42—C46—H46B	109.5
H7B—C7—H7C	109.5	H46A—C46—H46B	109.5
C4—C8—H8A	109.5	C42—C46—H46C	109.5
C4—C8—H8B	109.5	H46A—C46—H46C	109.5
H8A—C8—H8B	109.5	H46B—C46—H46C	109.5
C4—C8—H8C	109.5	C42—C47—H47A	109.5
H8A—C8—H8C	109.5	C42—C47—H47B	109.5
H8B—C8—H8C	109.5	H47A—C47—H47B	109.5
C6—C9—H9A	109.5	C42—C47—H47C	109.5
C6—C9—H9B	109.5	H47A—C47—H47C	109.5
C6—C9—H9C	109.5	H47B—C47—H47C	109.5
C6—C10—H10A	109.5	N15—C48—C49	114.48 (16)
C6—C10—H10B	109.5	N15—C48—H48A	108.6
C6—C10—H10C	109.5	C49—C48—H48A	108.6
C6—C11—H11A	109.5	N15—C48—H48B	108.6
C6—C11—H11B	109.5	C49—C48—H48B	108.6
C6—C11—H11C	109.5	H48A—C48—H48B	107.6
C6—C9'—H9'1	109.5	C50—C49—C54	118.62 (18)
C6—C9'—H9'2	109.5	C50—C49—C48	122.09 (17)
H9'1—C9'—H9'2	109.5	C54—C49—C48	119.22 (18)

C6—C9'—H9'3	109.5	C49—C50—C51	120.71 (19)
H9'1—C9'—H9'3	109.5	C49—C50—H50	119.6
H9'2—C9'—H9'3	109.5	C51—C50—H50	119.6
C6—C10'—H10D	109.5	C52—C51—C50	120.0 (2)
C6—C10'—H10E	109.5	C52—C51—H51	120.0
H10D—C10'—H10E	109.5	C50—C51—H51	120.0
C6—C10'—H10F	109.5	C53—C52—C51	119.8 (2)
H10D—C10'—H10F	109.5	C53—C52—H52	120.1
H10E—C10'—H10F	109.5	C51—C52—H52	120.1
C6—C11'—H11D	109.5	C52—C53—C54	120.2 (2)
C6—C11'—H11E	109.5	C52—C53—H53	119.9
H11D—C11'—H11E	109.5	C54—C53—H53	119.9
C6—C11'—H11F	109.5	C53—C54—C49	120.7 (2)
H11D—C11'—H11F	109.5	C53—C54—H54	119.7
H11E—C11'—H11F	109.5	C49—C54—H54	119.7
N5—C12—C13	114.27 (15)	C55—N16—C57	115.08 (16)
N5—C12—H12A	108.7	C56—N17—C55	112.68 (15)
C13—C12—H12A	108.7	C56—N18—C57	112.29 (15)
N5—C12—H12B	108.7	C55—N19—C58	128.10 (17)
C13—C12—H12B	108.7	C55—N19—H19	113.4 (16)
H12A—C12—H12B	107.6	C58—N19—H19	118.4 (16)
C14—C13—C18	118.67 (18)	C57—N20—C66	123.28 (16)
C14—C13—C12	122.10 (18)	C57—N20—H20	115.8 (15)
C18—C13—C12	119.18 (17)	C66—N20—H20	120.4 (15)
C13—C14—C15	120.6 (2)	N19—C55—N16	121.02 (17)
C13—C14—H14A	119.7	N19—C55—N17	114.32 (16)
C15—C14—H14A	119.7	N16—C55—N17	124.66 (16)
C16—C15—C14	120.3 (2)	N17—C56—N18	130.00 (17)
C16—C15—H15A	119.9	N17—C56—Cl4	114.97 (14)
C14—C15—H15A	119.9	N18—C56—Cl4	115.02 (14)
C17—C16—C15	119.5 (2)	N20—C57—N16	118.83 (17)
C17—C16—H16	120.2	N20—C57—N18	115.96 (16)
C15—C16—H16	120.2	N16—C57—N18	125.21 (16)
C16—C17—C18	120.4 (2)	N19—C58—C61	105.07 (17)
C16—C17—H17	119.8	N19—C58—C62	109.08 (16)
C18—C17—H17	119.8	C61—C58—C62	108.82 (18)
C13—C18—C17	120.4 (2)	N19—C58—C59	112.79 (16)
C13—C18—H18	119.8	C61—C58—C59	113.11 (18)
C17—C18—H18	119.8	C62—C58—C59	107.85 (17)
C19—N6—C21	115.00 (15)	C58—C59—C60	124.08 (18)
C20—N7—C19	112.49 (15)	C58—C59—H59A	106.3
C20—N8—C21	112.58 (15)	C60—C59—H59A	106.3
C19—N9—C22	127.59 (16)	C58—C59—H59B	106.3
C19—N9—H9	113.5 (14)	C60—C59—H59B	106.3
C22—N9—H9	115.6 (14)	H59A—C59—H59B	106.4
C21—N10—C30	123.30 (15)	C64'—C60—C63	125.7 (5)
C21—N10—H10	116.1 (14)	C64'—C60—C65	75.0 (5)
C30—N10—H10	119.9 (14)	C63—C60—C65	111.7 (3)
N6—C19—N9	120.68 (16)	C64'—C60—C59	110.6 (5)

N6—C19—N7	124.97 (15)	C63—C60—C59	115.5 (2)
N9—C19—N7	114.34 (16)	C65—C60—C59	110.8 (2)
N7—C20—N8	129.78 (17)	C64'—C60—C64	30.0 (5)
N7—C20—Cl2	115.44 (14)	C63—C60—C64	107.6 (3)
N8—C20—Cl2	114.78 (13)	C65—C60—C64	104.2 (3)
N10—C21—N6	118.81 (16)	C59—C60—C64	106.2 (2)
N10—C21—N8	116.04 (15)	C64'—C60—C65'	112.0 (6)
N6—C21—N8	125.14 (16)	C63—C60—C65'	72.2 (5)
N9—C22—C25	105.41 (15)	C65—C60—C65'	43.3 (5)
N9—C22—C26	108.75 (15)	C59—C60—C65'	115.1 (5)
C25—C22—C26	107.91 (16)	C64—C60—C65'	134.1 (5)
N9—C22—C23	113.99 (15)	C64'—C60—C63'	109.6 (6)
C25—C22—C23	113.25 (16)	C63—C60—C63'	30.6 (4)
C26—C22—C23	107.34 (16)	C65—C60—C63'	137.7 (5)
C24—C23—C22	124.97 (17)	C59—C60—C63'	106.5 (5)
C24—C23—H23A	106.1	C64—C60—C63'	83.4 (5)
C22—C23—H23A	106.1	C65'—C60—C63'	102.4 (6)
C24—C23—H23B	106.1	C58—C61—H61A	109.5
C22—C23—H23B	106.1	C58—C61—H61B	109.5
H23A—C23—H23B	106.3	H61A—C61—H61B	109.5
C28—C24—C29	109.1 (2)	C58—C61—H61C	109.5
C28—C24—C27	108.0 (2)	H61A—C61—H61C	109.5
C29—C24—C27	107.4 (2)	H61B—C61—H61C	109.5
C28—C24—C23	112.44 (17)	C58—C62—H62A	109.5
C29—C24—C23	114.03 (18)	C58—C62—H62B	109.5
C27—C24—C23	105.61 (18)	H62A—C62—H62B	109.5
C22—C25—H25A	109.5	C58—C62—H62C	109.5
C22—C25—H25B	109.5	H62A—C62—H62C	109.5
H25A—C25—H25B	109.5	H62B—C62—H62C	109.5
C22—C25—H25C	109.5	C60—C63—H63A	109.5
H25A—C25—H25C	109.5	C60—C63—H63B	109.5
H25B—C25—H25C	109.5	C60—C63—H63C	109.5
C22—C26—H26A	109.5	C60—C64—H64A	109.5
C22—C26—H26B	109.5	C60—C64—H64B	109.5
H26A—C26—H26B	109.5	C60—C64—H64C	109.5
C22—C26—H26C	109.5	C60—C65—H65A	109.5
H26A—C26—H26C	109.5	C60—C65—H65B	109.5
H26B—C26—H26C	109.5	C60—C65—H65C	109.5
C24—C27—H27A	109.5	C60—C63'—H63D	109.5
C24—C27—H27B	109.5	C60—C63'—H63E	109.5
H27A—C27—H27B	109.5	H63D—C63'—H63E	109.5
C24—C27—H27C	109.5	C60—C63'—H63F	109.5
H27A—C27—H27C	109.5	H63D—C63'—H63F	109.5
H27B—C27—H27C	109.5	H63E—C63'—H63F	109.5
C24—C28—H28A	109.5	C60—C64'—H64D	109.5
C24—C28—H28B	109.5	C60—C64'—H64E	109.5
H28A—C28—H28B	109.5	H64D—C64'—H64E	109.5
C24—C28—H28C	109.5	C60—C64'—H64F	109.5
H28A—C28—H28C	109.5	H64D—C64'—H64F	109.5

H28B—C28—H28C	109.5	H64E—C64'—H64F	109.5
C24—C29—H29A	109.5	C60—C65'—H65D	109.5
C24—C29—H29B	109.5	C60—C65'—H65E	109.5
H29A—C29—H29B	109.5	H65D—C65'—H65E	109.5
C24—C29—H29C	109.5	C60—C65'—H65F	109.5
H29A—C29—H29C	109.5	H65D—C65'—H65F	109.5
H29B—C29—H29C	109.5	H65E—C65'—H65F	109.5
N10—C30—C31	114.48 (16)	N20—C66—C67	114.16 (15)
N10—C30—H30A	108.6	N20—C66—H66A	108.7
C31—C30—H30A	108.6	C67—C66—H66A	108.7
N10—C30—H30B	108.6	N20—C66—H66B	108.7
C31—C30—H30B	108.6	C67—C66—H66B	108.7
H30A—C30—H30B	107.6	H66A—C66—H66B	107.6
C36—C31—C32	118.1 (2)	C68—C67—C72	118.38 (18)
C36—C31—C30	123.17 (18)	C68—C67—C66	121.88 (18)
C32—C31—C30	118.71 (18)	C72—C67—C66	119.70 (17)
C31—C32—C33	121.5 (2)	C67—C68—C69	120.6 (2)
C31—C32—H32	119.2	C67—C68—H68	119.7
C33—C32—H32	119.2	C69—C68—H68	119.7
C34—C33—C32	120.0 (2)	C70—C69—C68	120.4 (2)
C34—C33—H33	120.0	C70—C69—H69	119.8
C32—C33—H33	120.0	C68—C69—H69	119.8
C33—C34—C35	118.7 (2)	C71—C70—C69	119.5 (2)
C33—C34—H34	120.6	C71—C70—H70	120.2
C35—C34—H34	120.6	C69—C70—H70	120.2
C34—C35—C36	121.2 (2)	C70—C71—C72	120.2 (2)
C34—C35—H35	119.4	C70—C71—H71	119.9
C36—C35—H35	119.4	C72—C71—H71	119.9
C31—C36—C35	120.4 (2)	C67—C72—C71	120.8 (2)
C31—C36—H36	119.8	C67—C72—H72	119.6
C35—C36—H36	119.8	C71—C72—H72	119.6
C4—N4—C1—N1	−1.5 (3)	C40—N14—C37—N11	5.8 (3)
C4—N4—C1—N2	177.59 (16)	C40—N14—C37—N12	−173.85 (17)
C3—N1—C1—N4	−178.05 (16)	C39—N11—C37—N14	177.08 (17)
C3—N1—C1—N2	3.0 (2)	C39—N11—C37—N12	−3.3 (3)
C2—N2—C1—N4	177.79 (15)	C38—N12—C37—N14	−176.42 (17)
C2—N2—C1—N1	−3.2 (2)	C38—N12—C37—N11	3.9 (3)
C1—N2—C2—N3	1.1 (3)	C37—N12—C38—N13	−1.5 (3)
C1—N2—C2—Cl1	−178.40 (12)	C37—N12—C38—Cl3	178.67 (13)
C3—N3—C2—N2	0.9 (3)	C39—N13—C38—N12	−1.2 (3)
C3—N3—C2—Cl1	−179.60 (12)	C39—N13—C38—Cl3	178.60 (13)
C12—N5—C3—N1	3.7 (3)	C48—N15—C39—N11	4.8 (3)
C12—N5—C3—N3	−177.45 (15)	C48—N15—C39—N13	−174.53 (16)
C1—N1—C3—N5	178.20 (15)	C37—N11—C39—N15	−179.27 (16)
C1—N1—C3—N3	−0.6 (2)	C37—N11—C39—N13	0.1 (3)
C2—N3—C3—N5	180.00 (15)	C38—N13—C39—N15	−178.64 (16)
C2—N3—C3—N1	−1.2 (2)	C38—N13—C39—N11	2.0 (3)
C1—N4—C4—C7	−179.82 (17)	C37—N14—C40—C43	−61.0 (2)
C1—N4—C4—C8	64.0 (2)	C37—N14—C40—C44	−177.59 (19)

C1—N4—C4—C5	−55.9 (2)	C37—N14—C40—C41	64.3 (2)
N4—C4—C5—C6	−58.9 (2)	N14—C40—C41—C42	−169.69 (16)
C7—C4—C5—C6	60.4 (2)	C43—C40—C41—C42	−47.5 (2)
C8—C4—C5—C6	−179.71 (16)	C44—C40—C41—C42	77.5 (2)
C4—C5—C6—C10'	45.1 (6)	C40—C41—C42—C45	−50.4 (2)
C4—C5—C6—C11'	165.5 (5)	C40—C41—C42—C47	74.6 (2)
C4—C5—C6—C11	−174.9 (7)	C40—C41—C42—C46	−168.54 (17)
C4—C5—C6—C9	−55.6 (9)	C39—N15—C48—C49	−98.3 (2)
C4—C5—C6—C9'	−78.3 (6)	N15—C48—C49—C50	36.4 (2)
C4—C5—C6—C10	69.3 (8)	N15—C48—C49—C54	−146.64 (18)
C3—N5—C12—C13	86.8 (2)	C54—C49—C50—C51	−0.8 (3)
N5—C12—C13—C14	20.3 (2)	C48—C49—C50—C51	176.20 (17)
N5—C12—C13—C18	−162.29 (17)	C49—C50—C51—C52	−0.1 (3)
C18—C13—C14—C15	0.8 (3)	C50—C51—C52—C53	0.9 (3)
C12—C13—C14—C15	178.20 (19)	C51—C52—C53—C54	−0.7 (4)
C13—C14—C15—C16	−0.3 (3)	C52—C53—C54—C49	−0.2 (4)
C14—C15—C16—C17	−0.3 (3)	C50—C49—C54—C53	0.9 (3)
C15—C16—C17—C18	0.4 (3)	C48—C49—C54—C53	−176.1 (2)
C14—C13—C18—C17	−0.7 (3)	C58—N19—C55—N16	−1.9 (3)
C12—C13—C18—C17	−178.15 (19)	C58—N19—C55—N17	177.43 (17)
C16—C17—C18—C13	0.0 (3)	C57—N16—C55—N19	−178.45 (16)
C21—N6—C19—N9	179.58 (16)	C57—N16—C55—N17	2.2 (2)
C21—N6—C19—N7	0.8 (3)	C56—N17—C55—N19	177.13 (16)
C22—N9—C19—N6	7.0 (3)	C56—N17—C55—N16	−3.5 (2)
C22—N9—C19—N7	−174.08 (16)	C55—N17—C56—N18	2.7 (3)
C20—N7—C19—N6	−2.1 (3)	C55—N17—C56—Cl4	−178.07 (12)
C20—N7—C19—N9	179.06 (16)	C57—N18—C56—N17	−0.6 (3)
C19—N7—C20—N8	2.3 (3)	C57—N18—C56—Cl4	−179.83 (12)
C19—N7—C20—Cl2	−177.57 (12)	C66—N20—C57—N16	3.8 (3)
C21—N8—C20—N7	−1.1 (3)	C66—N20—C57—N18	−177.05 (15)
C21—N8—C20—Cl2	178.76 (12)	C55—N16—C57—N20	179.26 (16)
C30—N10—C21—N6	3.2 (3)	C55—N16—C57—N18	0.2 (2)
C30—N10—C21—N8	−177.96 (16)	C56—N18—C57—N20	179.90 (15)
C19—N6—C21—N10	179.27 (16)	C56—N18—C57—N16	−1.0 (2)
C19—N6—C21—N8	0.6 (3)	C55—N19—C58—C61	179.9 (2)
C20—N8—C21—N10	−179.21 (16)	C55—N19—C58—C62	63.4 (2)
C20—N8—C21—N6	−0.5 (3)	C55—N19—C58—C59	−56.4 (3)
C19—N9—C22—C25	175.88 (18)	N19—C58—C59—C60	−59.4 (3)
C19—N9—C22—C26	60.4 (2)	C61—C58—C59—C60	59.7 (3)
C19—N9—C22—C23	−59.3 (2)	C62—C58—C59—C60	−179.89 (18)
N9—C22—C23—C24	−56.2 (2)	C58—C59—C60—C64'	−163.0 (6)
C25—C22—C23—C24	64.3 (2)	C58—C59—C60—C63	46.5 (3)
C26—C22—C23—C24	−176.73 (17)	C58—C59—C60—C65	−81.8 (3)
C22—C23—C24—C28	66.9 (3)	C58—C59—C60—C64	165.7 (2)
C22—C23—C24—C29	−58.0 (3)	C58—C59—C60—C65'	−34.8 (6)
C22—C23—C24—C27	−175.60 (19)	C58—C59—C60—C63'	77.9 (5)
C21—N10—C30—C31	87.3 (2)	C57—N20—C66—C67	90.7 (2)
N10—C30—C31—C36	16.8 (3)	N20—C66—C67—C68	28.2 (2)
N10—C30—C31—C32	−165.53 (18)	N20—C66—C67—C72	−154.30 (18)

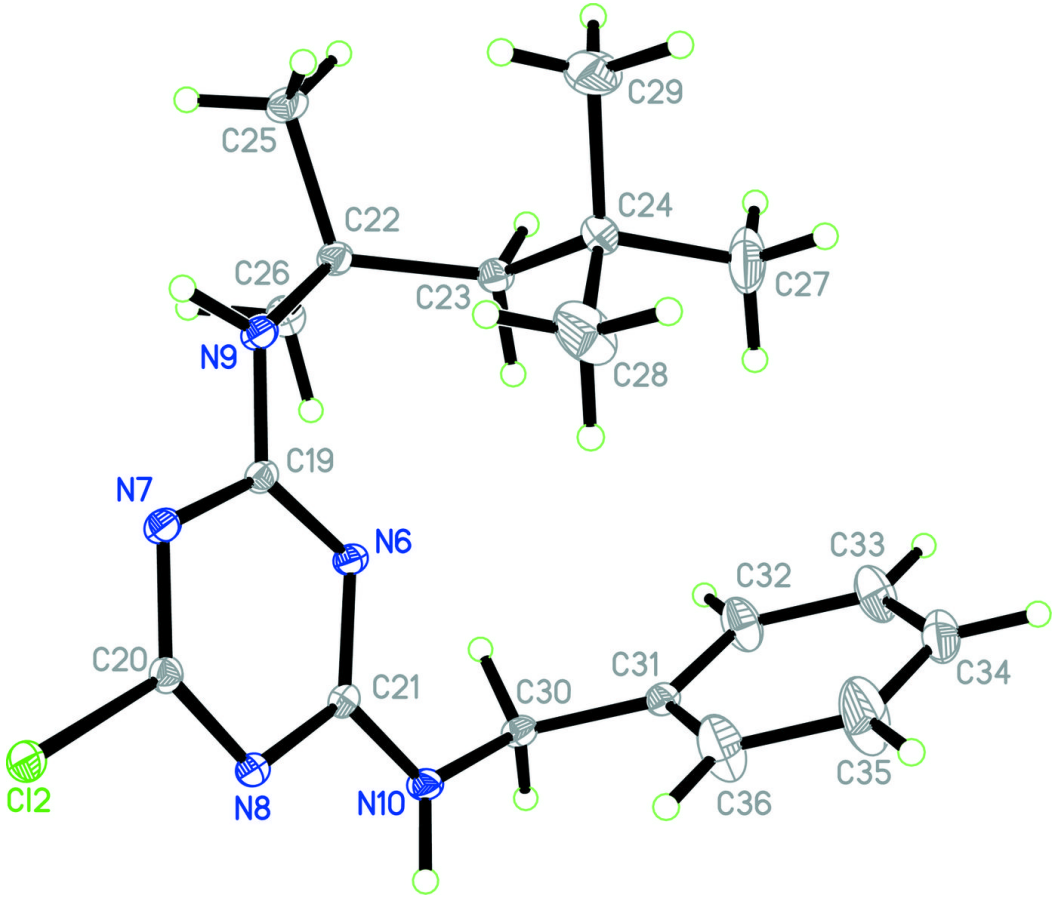
C36—C31—C32—C33	−0.3 (4)	C72—C67—C68—C69	0.6 (3)
C30—C31—C32—C33	−178.0 (2)	C66—C67—C68—C69	178.1 (2)
C31—C32—C33—C34	−0.6 (4)	C67—C68—C69—C70	−0.1 (4)
C32—C33—C34—C35	1.0 (4)	C68—C69—C70—C71	−0.8 (4)
C33—C34—C35—C36	−0.4 (5)	C69—C70—C71—C72	1.4 (4)
C32—C31—C36—C35	0.8 (4)	C68—C67—C72—C71	0.0 (3)
C30—C31—C36—C35	178.5 (3)	C66—C67—C72—C71	−177.6 (2)
C34—C35—C36—C31	−0.5 (5)	C70—C71—C72—C67	−0.9 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N20—H20···N3^{i}	0.87 (2)	2.14 (2)	3.007 (2)	179 (2)
N19—H19···N12^{ii}	0.87 (2)	2.22 (2)	3.085 (2)	174 (2)
N15—H15···N13^{iii}	0.89 (2)	2.06 (3)	2.953 (2)	176 (2)
N14—H14···N17^{ii}	0.84 (2)	2.24 (2)	3.078 (2)	172 (2)
N10—H10···N8^{ii}	0.93 (2)	2.06 (2)	2.989 (2)	171 (2)
N9—H9···N2	0.87 (2)	2.29 (2)	3.127 (2)	163.3 (19)
N5—H5···N18^{i}	0.85 (2)	2.14 (2)	2.984 (2)	172 (2)
N4—H4···N7	0.85 (2)	2.24 (2)	3.085 (2)	174 (2)

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

Fig. 1


C29
C25
C24
C22
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C28
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N7
N6
C33
C32
C20
C31
C34
C21
C30
C35
Cl2
N8
N10
C36