Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure and Hirshfeld surface analysis of 4-{2,2-dichloro-1-[(*E*)-2-(4-methylphenyl)diazen-1-yl]ethenyl}-*N*,*N*-dimethylaniline

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Received 18 May 2020
Accepted 6 June 2020

Edited by H. Ishida, Okayama University, Japan

Keywords: crystal structure; Hirshfeld surface analysis; non-covalent interactions; halogen and H-atom contacts.

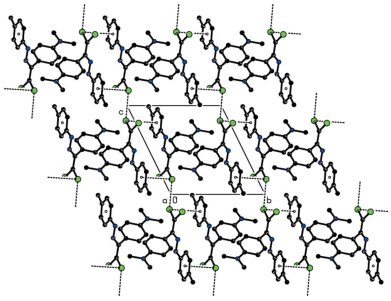
CCDC reference: 2008423

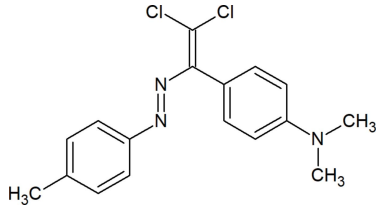
Supporting information: this article has supporting information at journals.iucr.org/e

In the tile compound, $C_{17}H_{17}Cl_2N_3$, the dihedral angle between the benzene rings is 62.73 (9)°. In the crystal, there are no classical hydrogen bonds. Molecules are linked by a pair of C—Cl···π interactions, forming an inversion dimer. A short intermolecular H*L*···H*L* contact [Cl···Cl = 3.2555 (9) Å] links the dimers, forming a ribbon along the *c*-axis direction. The Hirshfeld surface analysis and two-dimensional fingerprint plots reveal that the most important contributions for the crystal packing are from H···H (45.4%), Cl···H/H···Cl (21.0%) and C···H/H···C (19.0%) contacts.

1. Chemical context

Although non-covalent interactions are weaker than the covalent bonds, they are common and play critical roles in micellization, synthesis and catalysis as well as in forming supramolecular structures as a result of their significant contribution to the self-assembly process (Asadov *et al.*, 2016; Maharramov *et al.*, 2010; Mahmudov *et al.*, 2019). Similar to well-explored hydrogen bonds and π-interactions (Gurbanov *et al.*, 2018; Mahmoudi *et al.*, 2018), all aspects of chemistry and physics of halogen bonding have been subject to rapidly growing interest over the past decade. Thus, the attachment of halogen-bond donor site(s) to organic molecules can be used in the regulation of the solvatochromic, analytical, catalytic *etc*. properties of materials (Maharramov *et al.*, 2018; Mahmudov *et al.*, 2016). In a continuation of our work in this area we have functionalized the title compound, a new azo dye, which provides weak intermolecular interactions of the C—Cl···π and C—Cl···Cl types.





2. Structural commentary

In the title compound (Fig. 1), the dihedral angle between the C1–C6 and C8–C13 benzene rings is 62.73 (9)°. The amine N

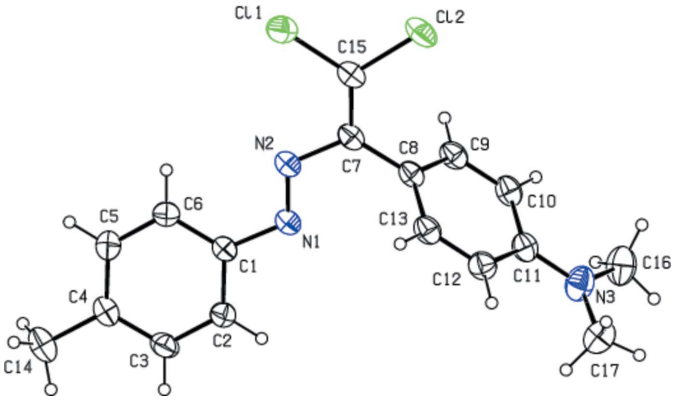


Figure 1
The molecular structure of the title compound with displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level.

atom (N3) displaced slightly from the C8–C13 benzene ring plane, with a deviation of 0.014 (2) Å. The N1/N2/C7/C15/Cl1/Cl2 unit is approximately planar with a maximum deviation of 0.0225 (19) Å, and makes dihedral angles of 6.46 (7) and 63.06 (7)°, respectively, with the C1–C6 and C8–C11 rings.

3. Supramolecular features

In the crystal, there are no classical hydrogen bonds observed. Molecules are linked by a pair of C—Cl···π interactions (Table 1), forming an inversion dimer. A short intermolecular H*L*···H*L* contact [Cl2···Cl2 (1 − *x*, 2 − *y*, 2 − *z*) = 3.2555 (9) Å] links the dimers to form a ribbon along the *c*-axis direction (Figs. 2 and 3). The molecular packing is further stabilized by van der Waals interactions between these ribbons.

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

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—Cl2···*Cg*1^{i}	1.71 (1)	3.60 (1)	4.065 (2)	93 (1)

Symmetry code: (i) $-x+1, -y+2, -z+1$.

Hirshfeld surfaces (McKinnon *et al.*, 2007) and their associated two-dimensional fingerprint plots (Spackman & McKinnon, 2002) were calculated using *CrystalExplorer17* (Turner *et al.*, 2017) to visualize the intermolecular interactions in the title compound. In the Hirshfeld surface mapped over d_{norm} (Fig. 4), a bright-red spot near atom Cl2 indicates the short Cl···Cl contact. Other contacts are equal to or longer than the sum of van der Walls radii.

The overall two-dimensional fingerprint plot and those delineated into H···H, Cl···H/H···Cl and C···H/H···C contacts (McKinnon *et al.*, 2007) are illustrated in Fig. 5. The most important interaction is H···H, contributing 45.4% to the overall crystal packing (Fig. 5*b*), which is reflected as widely scattered points of high density due to the large hydrogen content of the molecule with the tip at $d_e = d_i = 1.25$ Å. The Cl···H/H···Cl interactions appear as two symmetrical broad wings with $d_e + d_i \simeq 2.80$ Å and contribute 21.0% to the Hirshfeld surface (Fig. 5*c*). The pair of characteristic wings in the fingerprint plot delineated into H···C/C···H contacts (Fig. 5*d*; 19.0% contribution) have the tips at $d_e + d_i \simeq 2.80$ Å. The remaining contributions are from N···H/H···N (5.9%), Cl···C/C···Cl (3.8%), Cl···Cl (1.5%), C···C (1.5%), N···C/C···N (1.1%), N···Cl/Cl···N (0.5%) and N···N (0.4%) contacts, which have a negligible effect on the packing.

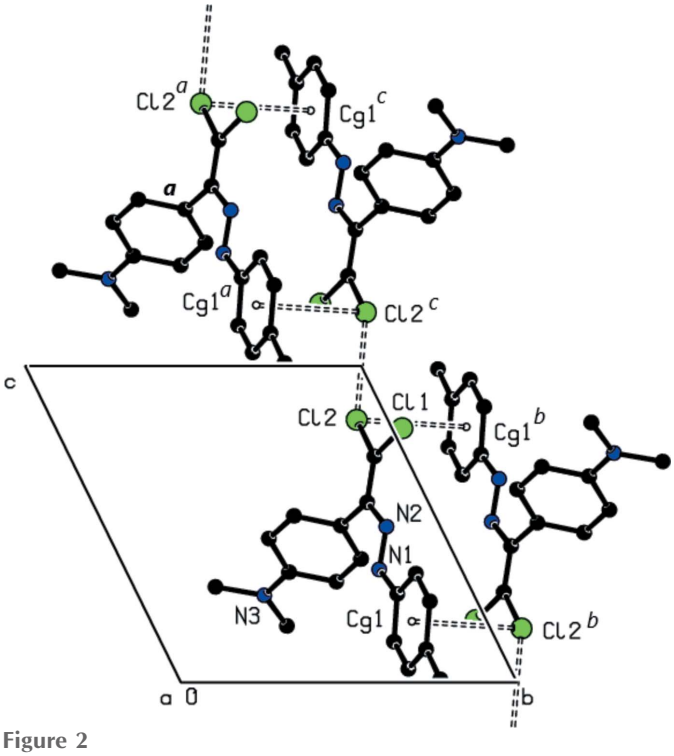


Figure 2
A view of the Cl···Cl short contacts and C—Cl···π interactions between the molecules. All hydrogen atoms were omitted for clarity. [Symmetry codes: (*a*) *x*, *y*, 1 + *z*; (*b*) 1 − *x*, 2 − *y*, 1 − *z*; (*c*) 1 − *x*, 2 − *y*, 2 − *z*.]

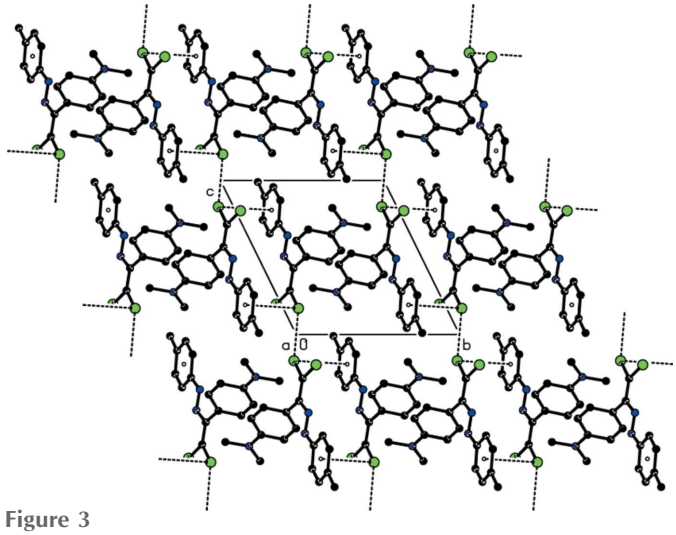


Figure 3
A packing diagram of the title compound, viewed along the *a*-axis direction. All hydrogen atoms were omitted for clarity.

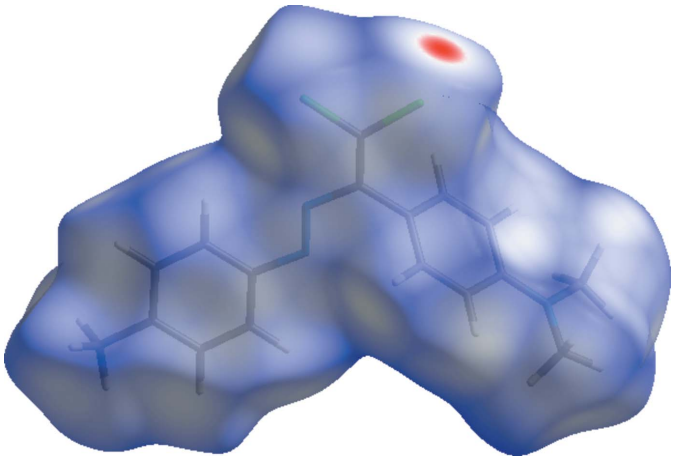


Figure 4
A view of the three-dimensional Hirshfeld surface for the title compound plotted over d_{norm} in the range −0.1388 to 1.4611 a.u.

4. Database survey

The title compound is similar to 4-{2,2-dichloro-1-[(*E*)-(4-fluorophenyl) diazenyl]ethenyl}-*N*,*N*-dimethylaniline (CSD refcode DULTAI; Özkaraca *et al.*, 2020), and closely resembles four other compounds, *viz*. 1-(4-bromophenyl)-2-[2,2-dichloro-1-(4-nitrophenyl)ethenyl]diazene (HONBOE; Akkurt *et al.*, 2019), 1-(4-chlorophenyl)-2-[2,2-dichloro-1-(4-nitrophenyl)ethenyl]diazene (HONBUK; Akkurt *et al.*, 2019), 1-(4-chlorophenyl)-2-[2,2-dichloro-1-(4-fluorophenyl)ethenyl]diazene (HODQAV; Shikhaliyev *et al.*, 2019) and 1-[2,2-dichloro-1-(4-nitrophenyl)ethenyl]-2-(4-fluorophenyl)diazene (XIZREG; Atioğlu *et al.*, 2019).

The crystal structure of DULTAI is stabilized by C—Cl···π and van der Waals interactions. In the crystals of HONBOE and HONBUK, molecules are linked through weak *X*···Cl contacts (*X* = Br for HONBOE and Cl for HONBUK), C—H···Cl and C—Cl···π interactions into sheets parallel to the *ab* plane. In HODQAV, molecules are stacked in columns along the *a* axis *via* weak C—H···Cl hydrogen bonds and face-to-face π–π stacking interactions. The crystal packing is further stabilized by short Cl···Cl contacts. In XIZREG, molecules are linked by C—H···O hydrogen bonds into zigzag chains running along the *c*-axis direction. The crystal packing is further stabilized by C—Cl···π, C—F···π and N—O···π interactions.

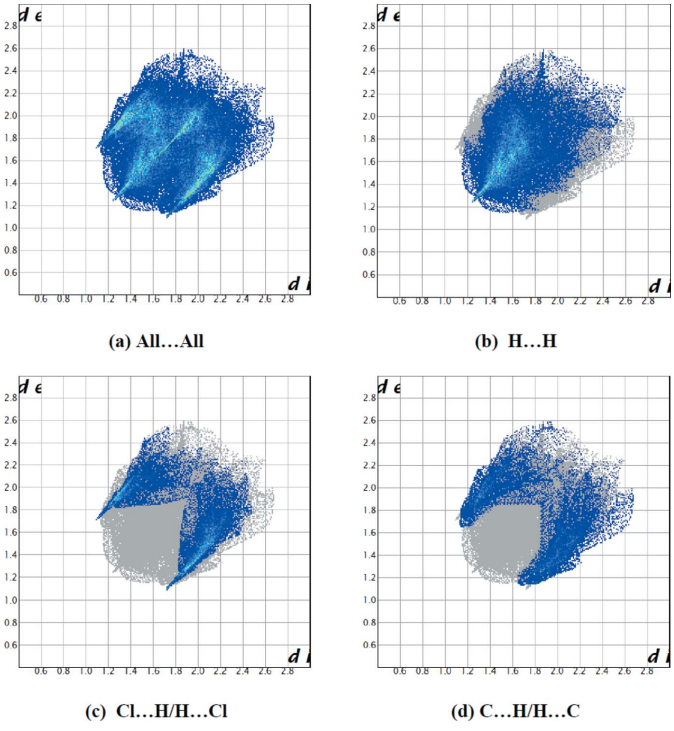


Figure 5
Two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) Cl···H/H···Cl and (*d*) C···H/H···C interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

5. Synthesis and crystallization

The title dye compound was synthesized according to the reported method (Atioğlu *et al.*, 2019). A 20 mL screw neck vial was charged with DMSO (10 mL), (*Z*)-*N*,*N*-dimethyl-4-{[2-(*p*-tolyl)hydrazineylidene]methyl}aniline (253 mg, 1 mmol), tetramethylethylenediamine (TMEDA) (295 mg, 2.5 mmol), CuCl (2 mg, 0.02 mmol) and CCl_4 (20 mmol, 10 equiv). After 1–3 h (when TLC analysis showed complete consumption of corresponding Schiff base), the reaction mixture was poured into 100 mL of dilute HCl (∼0.01 *M*, pH = 2–3), and extracted with dichloromethane (3 × 20 mL). The combined organic phase was washed with water (3 × 50 mL), brine (30 mL), dried over anhydrous Na_2SO_4 and concentrated *in vacuo* using a rotary evaporator. The residue was purified by column chromatography on silica gel using appropriate mixtures of hexane and dichloromethane (3:1–1:1). Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution. Orange solid (79%); m.p. 386 K. Analysis calculated for $C_{17}H_{17}Cl_2N_3$ (*M* = 334.24): C 61.09, H 5.13, N 12.57; found: C 61.03, H 5.07, N 12.53%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 2.34 (3H, ArMe), 3.06 (6H, NMe_2), 6.80–7.79 (8H, Ar). ^{13}C NMR (75MHz, $CDCl_3$) δ 152.33, 151.30, 150.28, 142.01, 133.28, 131.15, 129.71, 123.30, 119.47, 111.42, 40.30, 21.62. ESI–MS: *m*/*z*: 335.22 $[M + H]^+$.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.5 or 1.2U_{eq}(C).

Funding information

This work was funded by the Science Development Foundation under the President of the Republic of Azerbaijan grant No. EIF– BGM-4-RFTF-1/2017–21/13/4 and by RFBR grant No. 18–53-06006.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{17}Cl_2N_3$
M_r	334.23
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	9.5967 (15), 9.6767 (15), 10.8043 (17)
α, β, γ (°)	114.162 (5), 109.930 (5), 90.917 (6)
V (Å^3)	846.3 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.38
Crystal size (mm)	0.34 × 0.31 × 0.25
Data collection	
Diffractometer	Bruker APEXII PHOTON 100 detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2003)
T_{min}, T_{max}	0.875, 0.894
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13168, 3286, 2808
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.620
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.109, 1.05
No. of reflections	3286
No. of parameters	202
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.30

Computer programs: *APEX3* and *SAINT* (Bruker, 2007), *SHELXT2016/6* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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supporting information

Acta Cryst. (2020). E**76**, 1122-1125 [https://doi.org/10.1107/S2056989020007744]

Crystal structure and Hirshfeld surface analysis of 4-{2,2-dichloro-1-[(*E*)-2-(4-methylphenyl)diazen-1-yl]ethenyl}-*N*,*N*-dimethylaniline

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Computing details

Data collection: *APEX3* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXT2016/6* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

4-{2,2-Dichloro-1-[(*E*)-2-(4-methylphenyl)diazen-1-yl]ethenyl}-*N*,*N*-dimethylaniline

Crystal data

$C_{17}H_{17}Cl_2N_3$
$M_r = 334.23$
Triclinic, $P\overline{1}$
$a = 9.5967$ (15) Å
$b = 9.6767$ (15) Å
$c = 10.8043$ (17) Å
$\alpha = 114.162$ (5)°
$\beta = 109.930$ (5)°
$\gamma = 90.917$ (6)°
$V = 846.3$ (2) Å^3
$Z = 2$
$F(000) = 348$
$D_x = 1.312$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8175 reflections
$\theta = 2.2$–26.1°
$\mu = 0.38$ mm^{-1}
$T = 296$ K
Block, orange
0.34 × 0.31 × 0.25 mm

Data collection

Bruker APEXII PHOTON 100 detector diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2003)
$T_{min} = 0.875$, $T_{max} = 0.894$
13168 measured reflections
3286 independent reflections
2808 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 26.1°$, $\theta_{min} = 2.4°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.109$
$S = 1.05$
3286 reflections
202 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.2744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.62327 (18)	0.77347 (17)	0.27963 (16)	0.0430 (3)
C2	0.55622 (19)	0.69400 (19)	0.12860 (18)	0.0511 (4)
H2A	0.458599	0.638289	0.084781	0.061*
C3	0.6330 (2)	0.6968 (2)	0.04271 (18)	0.0556 (4)
H3A	0.586196	0.643088	−0.058810	0.067*
C4	0.7787 (2)	0.77812 (19)	0.1045 (2)	0.0524 (4)
C5	0.8437 (2)	0.8594 (2)	0.2560 (2)	0.0546 (4)
H5A	0.940803	0.916211	0.299537	0.065*
C6	0.76843 (19)	0.85845 (19)	0.34383 (18)	0.0504 (4)
H6A	0.814274	0.914147	0.445239	0.060*
C7	0.50704 (19)	0.81792 (18)	0.56909 (17)	0.0466 (4)
C8	0.36451 (18)	0.70537 (18)	0.49547 (17)	0.0459 (4)
C9	0.3511 (2)	0.58051 (19)	0.52632 (19)	0.0516 (4)
H9A	0.432363	0.569863	0.597144	0.062*
C10	0.2204 (2)	0.4724 (2)	0.4546 (2)	0.0533 (4)
H10A	0.215848	0.390240	0.477657	0.064*
C11	0.09506 (19)	0.48342 (19)	0.34826 (19)	0.0508 (4)
C12	0.1089 (2)	0.6101 (2)	0.3183 (2)	0.0553 (4)
H12A	0.027551	0.622051	0.248519	0.066*
C13	0.2401 (2)	0.7167 (2)	0.39000 (19)	0.0527 (4)
H13A	0.245451	0.798834	0.366953	0.063*
C14	0.8640 (3)	0.7763 (3)	0.0098 (3)	0.0783 (6)
H14A	0.889625	0.879225	0.023489	0.118*
H14B	0.802118	0.712384	−0.091347	0.118*
H14C	0.954396	0.736056	0.036936	0.118*
C15	0.5678 (2)	0.9067 (2)	0.71430 (18)	0.0517 (4)
C16	−0.0462 (3)	0.2427 (2)	0.3018 (3)	0.0794 (6)
H16A	0.034913	0.189498	0.288174	0.119*
H16B	−0.140759	0.175108	0.234394	0.119*
H16C	−0.039713	0.274646	0.400506	0.119*
C17	−0.1688 (2)	0.3981 (3)	0.1783 (3)	0.0790 (6)
H17A	−0.149409	0.401936	0.098146	0.118*
H17B	−0.196497	0.493105	0.230865	0.118*
H17C	−0.249623	0.314219	0.140945	0.118*
Cl1	0.73773 (6)	1.03097 (6)	0.80319 (5)	0.07071 (18)
Cl2	0.48299 (7)	0.90774 (6)	0.82988 (5)	0.07116 (18)
N1	0.53535 (15)	0.75555 (15)	0.35683 (14)	0.0473 (3)
N2	0.59263 (16)	0.83959 (15)	0.49225 (14)	0.0477 (3)
N3	−0.03590 (19)	0.37582 (19)	0.2751 (2)	0.0710 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0496 (8)	0.0432 (8)	0.0417 (7)	0.0113 (6)	0.0216 (6)	0.0203 (6)
C2	0.0529 (9)	0.0533 (9)	0.0430 (8)	0.0018 (7)	0.0187 (7)	0.0176 (7)
C3	0.0691 (11)	0.0580 (10)	0.0405 (8)	0.0085 (8)	0.0239 (8)	0.0201 (7)
C4	0.0623 (10)	0.0522 (9)	0.0586 (10)	0.0173 (8)	0.0346 (8)	0.0295 (8)
C5	0.0500 (9)	0.0553 (9)	0.0615 (10)	0.0073 (7)	0.0249 (8)	0.0258 (8)
C6	0.0524 (9)	0.0511 (9)	0.0422 (8)	0.0061 (7)	0.0166 (7)	0.0168 (7)
C7	0.0562 (9)	0.0502 (8)	0.0468 (8)	0.0194 (7)	0.0268 (7)	0.0277 (7)
C8	0.0526 (9)	0.0510 (8)	0.0468 (8)	0.0180 (7)	0.0279 (7)	0.0259 (7)
C9	0.0584 (10)	0.0587 (10)	0.0550 (9)	0.0246 (8)	0.0286 (8)	0.0349 (8)
C10	0.0627 (10)	0.0520 (9)	0.0665 (10)	0.0217 (8)	0.0348 (9)	0.0372 (8)
C11	0.0547 (9)	0.0504 (9)	0.0585 (9)	0.0183 (7)	0.0311 (8)	0.0264 (8)
C12	0.0539 (10)	0.0627 (10)	0.0604 (10)	0.0189 (8)	0.0223 (8)	0.0367 (9)
C13	0.0615 (10)	0.0551 (9)	0.0593 (10)	0.0200 (8)	0.0283 (8)	0.0369 (8)
C14	0.0881 (15)	0.0940 (15)	0.0805 (14)	0.0209 (12)	0.0559 (13)	0.0447 (12)
C15	0.0640 (10)	0.0548 (9)	0.0462 (8)	0.0167 (8)	0.0275 (8)	0.0259 (7)
C16	0.0795 (14)	0.0573 (11)	0.1090 (18)	0.0117 (10)	0.0443 (13)	0.0369 (12)
C17	0.0613 (12)	0.0817 (14)	0.0822 (14)	0.0056 (10)	0.0186 (11)	0.0327 (12)
Cl1	0.0783 (3)	0.0738 (3)	0.0505 (3)	−0.0015 (2)	0.0190 (2)	0.0236 (2)
Cl2	0.0960 (4)	0.0798 (3)	0.0523 (3)	0.0182 (3)	0.0452 (3)	0.0289 (2)
N1	0.0530 (8)	0.0512 (7)	0.0426 (7)	0.0111 (6)	0.0231 (6)	0.0212 (6)
N2	0.0563 (8)	0.0500 (7)	0.0440 (7)	0.0118 (6)	0.0248 (6)	0.0228 (6)
N3	0.0598 (9)	0.0643 (10)	0.0933 (12)	0.0091 (7)	0.0258 (9)	0.0415 (9)

Geometric parameters (Å, º)

C1—C2	1.382 (2)	C10—H10A	0.9300
C1—C6	1.391 (2)	C11—N3	1.377 (2)
C1—N1	1.4251 (19)	C11—C12	1.405 (2)
C2—C3	1.375 (2)	C12—C13	1.375 (3)
C2—H2A	0.9300	C12—H12A	0.9300
C3—C4	1.385 (3)	C13—H13A	0.9300
C3—H3A	0.9300	C14—H14A	0.9600
C4—C5	1.386 (3)	C14—H14B	0.9600
C4—C14	1.507 (2)	C14—H14C	0.9600
C5—C6	1.377 (2)	C15—Cl2	1.7046 (17)
C5—H5A	0.9300	C15—Cl1	1.7179 (19)
C6—H6A	0.9300	C16—N3	1.439 (3)
C7—C15	1.340 (2)	C16—H16A	0.9600
C7—N2	1.418 (2)	C16—H16B	0.9600
C7—C8	1.480 (2)	C16—H16C	0.9600
C8—C13	1.384 (2)	C17—N3	1.432 (3)
C8—C9	1.393 (2)	C17—H17A	0.9600
C9—C10	1.378 (3)	C17—H17B	0.9600
C9—H9A	0.9300	C17—H17C	0.9600
C10—C11	1.393 (2)	N1—N2	1.2520 (18)

C2—C1—C6	119.28 (14)	C13—C12—C11	121.43 (16)
C2—C1—N1	115.14 (14)	C13—C12—H12A	119.3
C6—C1—N1	125.54 (14)	C11—C12—H12A	119.3
C3—C2—C1	120.38 (16)	C12—C13—C8	121.84 (15)
C3—C2—H2A	119.8	C12—C13—H13A	119.1
C1—C2—H2A	119.8	C8—C13—H13A	119.1
C2—C3—C4	121.27 (16)	C4—C14—H14A	109.5
C2—C3—H3A	119.4	C4—C14—H14B	109.5
C4—C3—H3A	119.4	H14A—C14—H14B	109.5
C3—C4—C5	117.74 (15)	C4—C14—H14C	109.5
C3—C4—C14	120.93 (17)	H14A—C14—H14C	109.5
C5—C4—C14	121.33 (18)	H14B—C14—H14C	109.5
C6—C5—C4	121.83 (16)	C7—C15—Cl2	123.03 (14)
C6—C5—H5A	119.1	C7—C15—Cl1	123.91 (13)
C4—C5—H5A	119.1	Cl2—C15—Cl1	113.06 (10)
C5—C6—C1	119.47 (15)	N3—C16—H16A	109.5
C5—C6—H6A	120.3	N3—C16—H16B	109.5
C1—C6—H6A	120.3	H16A—C16—H16B	109.5
C15—C7—N2	114.01 (15)	N3—C16—H16C	109.5
C15—C7—C8	123.11 (15)	H16A—C16—H16C	109.5
N2—C7—C8	122.87 (14)	H16B—C16—H16C	109.5
C13—C8—C9	116.98 (16)	N3—C17—H17A	109.5
C13—C8—C7	121.61 (14)	N3—C17—H17B	109.5
C9—C8—C7	121.38 (15)	H17A—C17—H17B	109.5
C10—C9—C8	121.69 (16)	N3—C17—H17C	109.5
C10—C9—H9A	119.2	H17A—C17—H17C	109.5
C8—C9—H9A	119.2	H17B—C17—H17C	109.5
C9—C10—C11	121.48 (15)	N2—N1—C1	113.76 (13)
C9—C10—H10A	119.3	N1—N2—C7	113.53 (14)
C11—C10—H10A	119.3	C11—N3—C17	121.17 (17)
N3—C11—C10	122.12 (15)	C11—N3—C16	120.75 (18)
N3—C11—C12	121.30 (16)	C17—N3—C16	117.94 (18)
C10—C11—C12	116.58 (16)		

C6—C1—C2—C3	1.0 (2)	N3—C11—C12—C13	−179.23 (17)
N1—C1—C2—C3	−177.02 (15)	C10—C11—C12—C13	0.4 (3)
C1—C2—C3—C4	0.3 (3)	C11—C12—C13—C8	−0.4 (3)
C2—C3—C4—C5	−1.3 (3)	C9—C8—C13—C12	−0.1 (2)
C2—C3—C4—C14	177.94 (17)	C7—C8—C13—C12	178.13 (15)
C3—C4—C5—C6	1.1 (3)	N2—C7—C15—Cl2	177.33 (11)
C14—C4—C5—C6	−178.15 (17)	C8—C7—C15—Cl2	−3.6 (2)
C4—C5—C6—C1	0.2 (3)	N2—C7—C15—Cl1	−2.5 (2)
C2—C1—C6—C5	−1.3 (2)	C8—C7—C15—Cl1	176.56 (12)
N1—C1—C6—C5	176.59 (15)	C2—C1—N1—N2	−173.79 (14)
C15—C7—C8—C13	119.31 (18)	C6—C1—N1—N2	8.3 (2)
N2—C7—C8—C13	−61.7 (2)	C1—N1—N2—C7	−178.18 (12)
C15—C7—C8—C9	−62.6 (2)	C15—C7—N2—N1	179.64 (14)

N2—C7—C8—C9	116.43 (17)	C8—C7—N2—N1	0.6 (2)
C13—C8—C9—C10	0.4 (2)	C10—C11—N3—C17	172.96 (19)
C7—C8—C9—C10	−177.74 (15)	C12—C11—N3—C17	−7.4 (3)
C8—C9—C10—C11	−0.4 (3)	C10—C11—N3—C16	−2.6 (3)
C9—C10—C11—N3	179.61 (16)	C12—C11—N3—C16	177.03 (18)
C9—C10—C11—C12	0.0 (2)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—Cl2···*Cg*1^{i}	1.71 (1)	3.60 (1)	4.065 (2)	93 (1)

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+1.