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Crystal structures and Hirshfeld surface analyses of (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-phenyldiazene, (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-(4-methylphenyl)diazene, (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-(4-methoxyphenyl)diazene and (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-(3-methylphenyl)diazene

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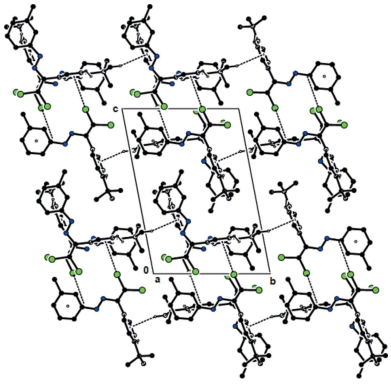
The crystal structures and Hirshfeld surface analyses of four similar azo compounds are reported. (*E*)-1-[1-(4-*tert*-Butylphenyl)-2,2-dichloroethenyl]-2-phenyldiazene, $C_{18}H_{18}Cl_2N_2$, (**I**), and (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-(4-methylphenyl)diazene, $C_{19}H_{20}Cl_2N_2$, (**II**), crystallize in the monoclinic space group $C2/c$ with Z = 8, and (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-(4-methoxyphenyl)diazene, $C_{19}H_{20}Cl_2N_2O$, (**III**), in the monoclinic space group $P2_1/c$ with Z = 4. (*E*)-1-[1-(4-*tert*-Butylphenyl)-2,2-dichloroethenyl]-2-(3-methylphenyl)diazene, $C_{19}H_{20}Cl_2N_2$, (**IV**), crystallizes in the triclinic space group $P\overline{1}$ with $Z = 4$ and comprises two molecules (**A** and **B**) in the asymmetric unit. In the crystal structures of (**I**) and (**II**), molecules are linked by C—H···π and C—Cl···π interactions, forming layers parallel to $(\overline{2}02)$, while molecules of (**III**) are linked by C—H···O contacts, C—H···π and C—Cl···π interactions forming layers parallel to $(\overline{3}02)$. The stability of the molecular packing is ensured by van der Waals forces between these layers. In the crystal structure of (**IV**), molecules are linked by C—H···π and C—Cl···π interactions, forming a tri-periodic network.



1. Chemical context

The synthesis of polyfunctional compounds and the study of their structures and properties are one of the directions in organic chemistry that have been studied in detail in recent years. In this regard, the synthesis of dihalogendiazabutadienes from the reaction of N-substituted hydrazones of benzaldehyde derivatives with polyhalomethanes (CCl_4, CBr_4) in the presence of a CuCl catalyst (Maharramov *et al.*, 2018; Shikhaliyev *et al.*, 2019*a*,*b*, 2021*a*,*b*; Nenajdenko *et al.*, 2020, 2022), the investigation of their structural features by the RQA method (Shikhaliyev *et al.*, 2021*c*,*d*,*e*; Atioğlu *et al.*, 2020) and the investigation of the factors affecting the direction of the reaction are distinguished by their relevance.

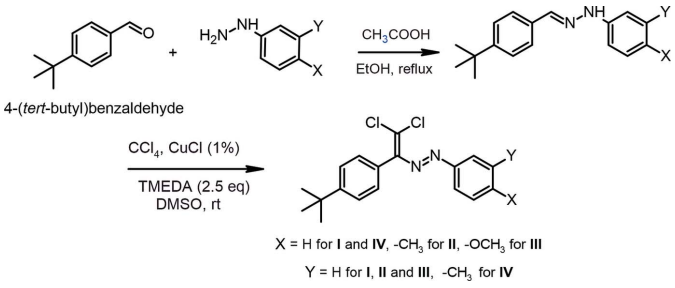
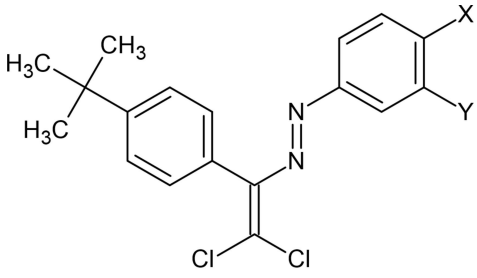


Figure 1
Reaction scheme for the synthesis of compounds (**I**), (**II**), (**III**) and (**IV**).

The presence of an attached diazadiene system in dihalogendiazabutadiene derivatives leads to their application as a new class of diazo dyes, and the reaction of heminal halogen atoms with various nucleophiles results in important compounds such as azidotriazoles, hydrozo derivatives of α-ketoethers and other nitrogen-containing heterocyclic compounds (Shikhaliyev *et al.*, 2021*f*; Tsyrenova *et al.*, 2021).



In this context, the corresponding azo dyes were synthesized based on 4-(*tert*-butyl)benzaldehyde (Fig. 1), their crystal structures determined and their Hirshfeld surface analysed, and the results of these studies are reported in the current communication.

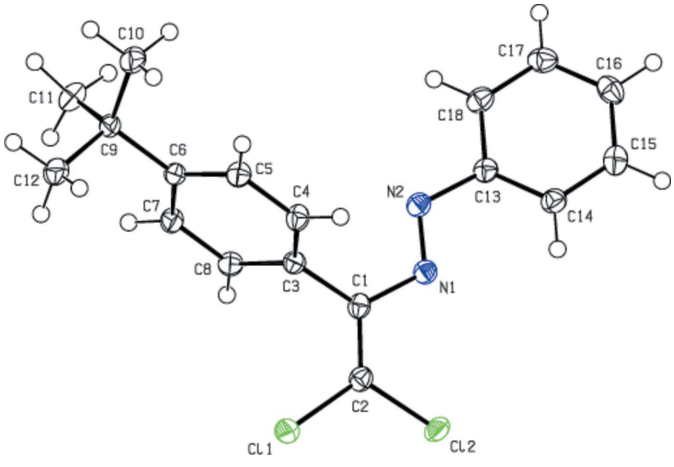


Figure 2
The molecular structure of (**I**) with displacement ellipsoids drawn at the 50% probability level.

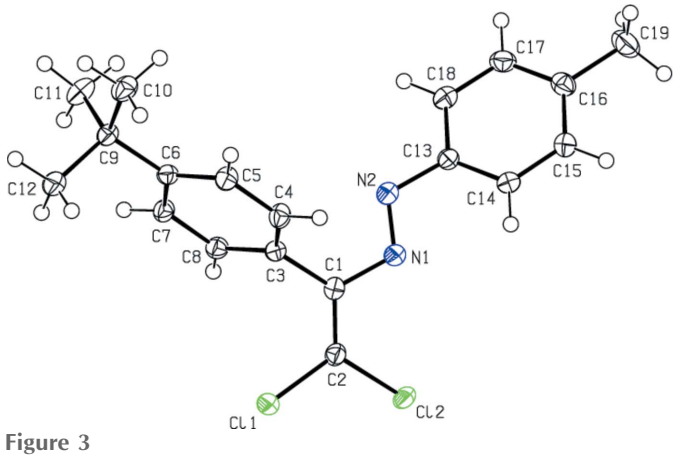


Figure 3
The molecular structure of (**II**) with displacement ellipsoids drawn at the 50% probability level.

2. Structural commentary

In the crystal structure of (**I**), the central fragment of the molecule, C1/C2/N1/N2/C3/C13/Cl1/Cl2, is almost planar (Fig. 2), with an r.m.s. deviation of fitted atoms of 0.0625 Å from the least-squares plane. This plane forms a dihedral angles of 26.86 (7) and 66.71 (5)° with the planes of the phenyl (C13–C18) and 4-*tert*-butylphenyl (C3–C8) rings, respectively. In the crystal structure of (**II**), the central fragment (C1/C2/N2/N1/C3/C13/Cl1/Cl2; r.m.s. deviation of fitted atoms = 0.0779 Å) of the molecule (Fig. 3) makes dihedral angles of 42.41 (5) and 65.31 (4)° with the planes of the 4-methylphenyl (C13–C18) and 4-*tert*-butylphenyl (C3–C8) rings, respectively. In the crystal structure of (**III**), the central fragment (C1/C2/N1/N2/C3/C13/Cl1/Cl2; r.m.s. deviation of fitted atoms = 0.0324 Å) of the molecule (Fig. 4) forms dihedral angles of 10.75 (3) and 82.00 (3)° with the planes of the 4-methoxyphenyl (C13–C18) and 4-*tert*-butylphenyl (C3–C8) rings, respectively.

In the crystal structure of (**IV**), the asymmetric unit comprises two molecules (**A** and **B**), Fig. 5. The central fragments (C1/C2/N1/N2/C3/C13/Cl1/Cl2 and C20/C21/N3/N4/C22/C32/Cl3/Cl4) of the molecules **A** and **B** are almost planar

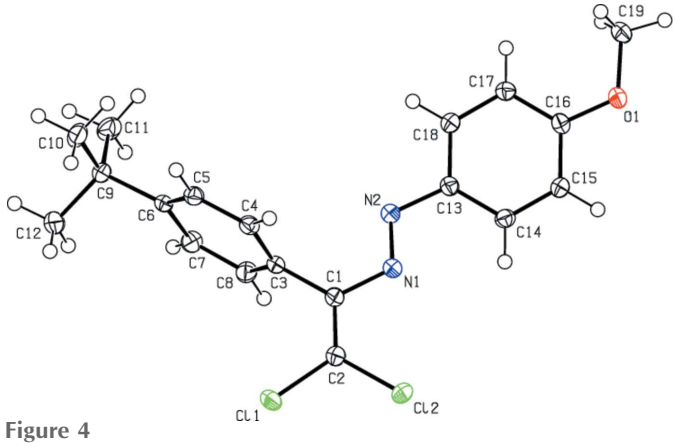


Figure 4
The molecular structure of (**III**) with displacement ellipsoids drawn at the 50% probability level.

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

*Cg*1 is the centroid of the 4-*tert*-butylphenyl ring (C3–C8).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···*Cg*1^{i}	0.95	2.95	3.476 (2)	116

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

Table 2
Hydrogen-bond geometry (Å, °) for (**II**).

*Cg*1 is the centroid of the 4-*tert*-butylphenyl ring (C3–C8).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···*Cg*1^{i}	0.95	2.88	3.675 (2)	142

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

Table 3
Hydrogen-bond geometry (Å, °) for (**III**).

*Cg*1 is the centroid of the 4-*tert*-butylphenyl ring (C3–C8).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···O1^{i}	0.95	2.39	3.2753 (17)	155
C19—H19*B*···*Cg*1^{ii}	0.98	2.87	3.4276 (17)	117

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 4
Hydrogen-bond geometry (Å, °) for (**IV**).

*Cg*1 and *Cg*2 are the centroids of the 4-*tert*-butylphenyl rings [(**IVA**: C3–C8 and (**IVB**): C13–C18]. *Cg*4 is the centroid of the 3-methylphenyl ring (C32–C37) of molecule (**IVB**).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···*Cg*4^{i}	0.95	2.91	3.768 (2)	151
C24—H24···*Cg*2^{ii}	0.95	2.97	3.824 (2)	150
C29—H29*B*···*Cg*1^{iii}	0.98	2.78	3.706 (2)	157

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

with the r.m.s. deviations of fitted atoms being 0.0336 for **A** and 0.0243 Å for **B**. The central fragment of molecule **A** forms dihedral angles of 13.45 (4) and 67.03 (5)°, respectively, with

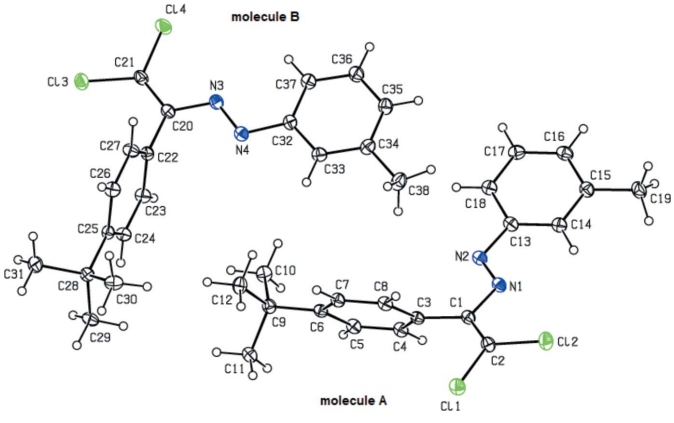


Figure 5
View of the two molecules (**A** and **B**) in the asymmetric unit of (**IV**) with displacement ellipsoids drawn at the 30% probability level.

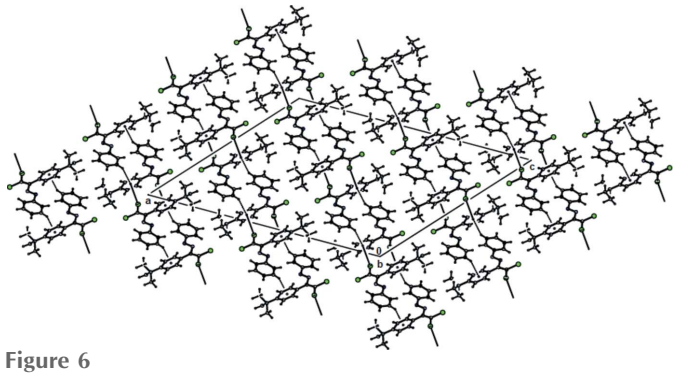


Figure 6
The C—Cl···π and C—H···π contacts (solid lines) of (**I**), shown along the *b* axis.

the planes of the 3-methylphenyl (C13–C18) and 4-*tert*-butylphenyl (C3–C8) rings. The central fragment of molecule **B** forms dihedral angles of 3.45 (2) and 84.00 (5)°, respectively, with the planes of the 3-methylphenyl (C32–C37) and 4-*tert*-butylphenyl (C22–C27) rings.

Bond lengths and angles in all compounds are in agreement with those reported for the related azo compounds discussed in the *Database survey* section.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal structures of (**I**) and (**II**), molecules are mainly connected by C—Cl···π interactions [for (**I**), C2—Cl1···*Cg*1^{i} = 3.5617 (8) Å; 158.39 (8)°; symmetry code: (i) $1-x, -y, 1-z$, and for (**II**), C2—Cl1···*Cg*1^{i} = 3.6343 (1) Å; 160.79 (1)°, with *Cg*1 being the centroid of the 4-*tert*-butylphenyl ring (C3–C8); symmetry code: (i) $1-x, -y, 1-z$]. These interactions, together with C—H···*Cg*1 interactions (Tables 1 and 2), lead

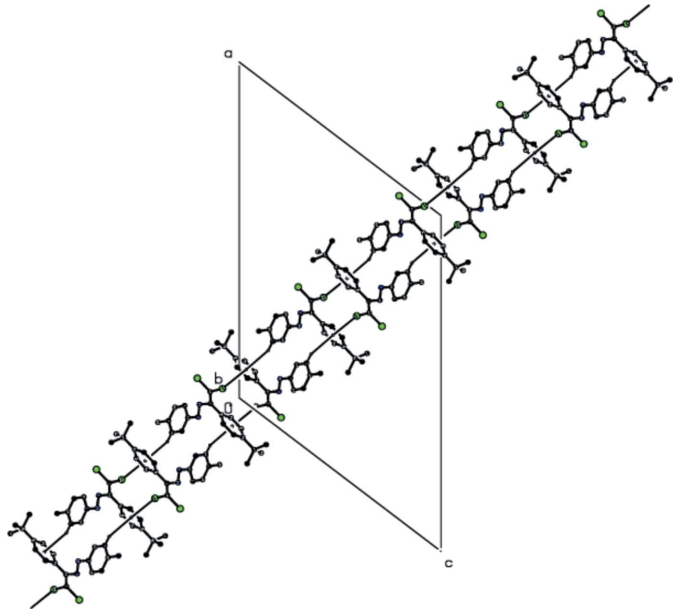


Figure 7
The C—Cl···π and C—H···π contacts (solid lines) of (**II**), shown along the *b* axis.

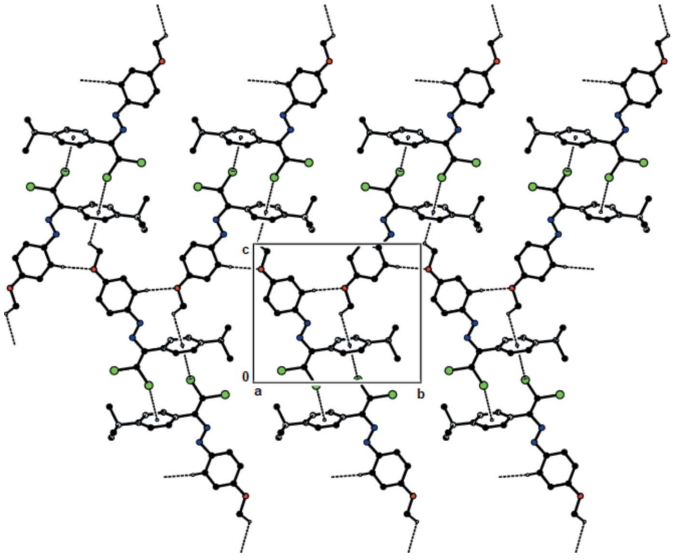


Figure 8
The C—H···O, C—Cl···π and C—H···π contacts (dashed lines) of (**III**), shown along the *a* axis.

to the formation of layers parallel to ($\bar{2}$02), Figs. 6 and 7. In the crystal structure of (**III**), molecules are connected by C—H···O and C—H···π interactions (Table 3) and additional C—Cl···π [C2—Cl1···*Cg*1^{i} = 3.7693 (1) Å; 146.35 (1) Å; *Cg*1 is the centroid of the 4-*tert*-butylphenyl ring (C3–C8); symmetry code: (i) $1-x, -y, 1-z$], forming layers parallel to ($\bar{3}$02) (Table 3, Fig. 8). van der Waals forces between these layers maintain the stability of the molecular packing. In the crystal structure of (**IV**), molecules are connected *via* C—H···π (Table 4) and C—Cl···π [C2—Cl2···*Cg*3^{ii} =

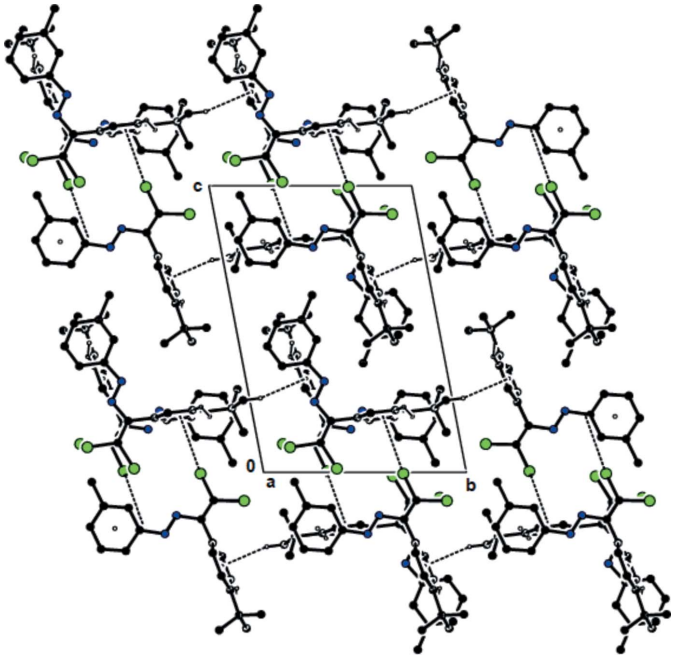


Figure 9
The C—Cl···π and C—H···π contacts (dashed lines) of (**IV**), shown along the *a* axis.

Table 5
Percentage contributions of interatomic contacts to the Hirshfeld surface in the crystal structure.

Contact	Percentage contribution				
	(**I**)	(**II**)	(**III**)	(**IVA**)	(**IVB**)
H···H	45.3	47.1	43.6	47.0	44.2
Cl···H/H···Cl	22.8	22.2	21.3	20.1	19.8
C···H/H···C	17.5	18.6	17.0	20.7	21.1
N···H/H···N	5.3	5.8	3.7	7.2	8.3
O···H/H···O	–	–	5.1	–	–
Cl···C/C···Cl	3.2	2.8	2.7	2.4	3.3
C···C	2.4	1.2	1.7	0.3	0.3
N···C/C···N	1.5	0.7	1.4	–	–
Cl···N/N···Cl	1.2	0.5	2.9	–	–
Cl···Cl	0.8	1.2	0.6	2.3	3.0

3.9515 (9) Å; C2—Cl2···*Cg*3^{ii} = 165.48 (1)°; symmetry code: (ii) $-x, y, -1+z$; *Cg*3 is the centroid of the 4-*tert*-butylphenyl ring (C22–C27) of molecule (**IVB**)] interactions, creating a tri-periodic network (Fig. 9).

To quantify intermolecular interactions between molecules (**I**), (**II**), (**III**), (**IVA**) and (**IVB**) in their respective crystal

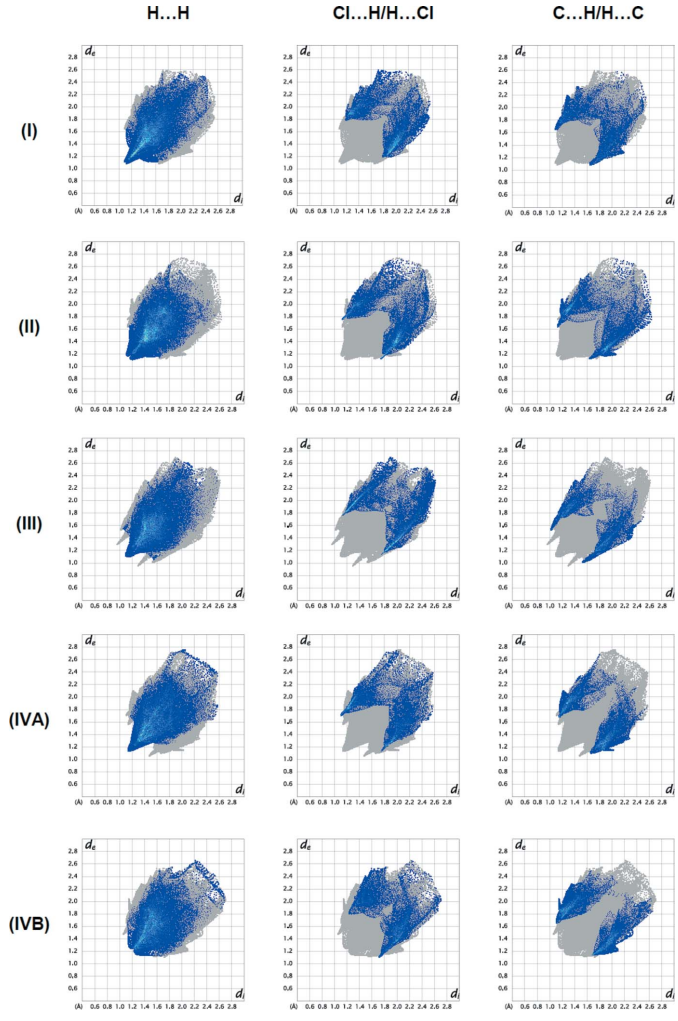


Figure 10
Two-dimensional fingerprint graphs showing the H···H, Cl···H/H···Cl and C···H/H···C interactions of (**I**), (**II**), (**III**), (**IVA**) and (**IV B**).

structures, Hirshfeld surface analyses were performed, and the two-dimensional fingerprint plots generated with *CrystalExplorer17* (Spackman *et al.*, 2021). The two-dimensional fingerprint plots are shown in Fig. 10. Comparative interactions calculated for each compound are given in Table 5. The dominant interactions of all compounds are H···H [(**I**): 45.3%, (**II**): 47.1%, (**III**): 43.6%, (**IVA**): 47.0% and (**IVB**): 44.2%], Cl···H/H···Cl [(**I**): 22.8%, (**II**): 22.2%, (**III**): 21.3%, (**IVA**): 20.1% and (**IVB**): 19.8%] and C···H/H···C [(**I**) 17.5%, (**II**): 18.6%, (**III**): 17.0%, (**IVA**): 20.7% and (**IVB**): 21.1%]. These interactions play a crucial role in the overall stabilization of the crystal packing. The presence of different functional groups in the compounds leads to some differences in the remaining weak interactions.

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom *et al.*, 2016) for the *(E)-1-(2,2-dichloro-1-phenylethenyl)-2-phenyldiazene* moiety resulted in 32 hits. Fourteen compounds are closely related to the title compound, *viz*. those with CSD refcodes TAZDIL (Atioğlu *et al.*, 2022*a*), HEHKEO (Akkurt *et al.*, 2022), ECUDAL (Atioğlu *et al.*, 2022*b*), PAXDOL (Çelikesir *et al.*, 2022), CANVUM, (Shikhaliyev *et al.*, 2021*d*), EBUCUD (Shikhaliyev *et al.*, 2021*d*), GUPHIL (Özkaraca *et al.*, 2020*a*), DULTAI (Özkaraca *et al.*, 2020*b*), XIZREG (Atioğlu *et al.*, 2019), HODQAV (Shikhaliyev *et al.*, 2019*c*), HONBUK (Akkurt *et al.*, 2019), HONBOE (Akkurt *et al.*, 2019), LEQXOX (Shikhaliyev *et al.*, 2018) and LEQXIR (Shikhaliyev *et al.*, 2018).

The molecules in TAZDIL are joined into layers parallel to (011) by C—H···O and C—H···F hydrogen bonds. C—Br···π and C—F···π contacts, as well as π–π stacking interactions strengthen the crystal packing. C—H···Br interactions connect the molecules in the crystal of the polymorph-1 of HEHKEO, resulting in zigzag *C*(8) chains along [100]. These chains are connected by C—Br···π interactions into layers parallel to (001). van der Waals interactions between the layers contribute to the crystal cohesion. In the crystals of ECUDAL, C—H···O hydrogen bonds link molecules into chains. These chains are linked by face-to-face π–π stacking interactions, resulting in a layered structure. Short intermolecular Br···O contacts and van der Waals interactions between the layers aid in the cohesion of the crystal packing. The molecules in the crystal of PAXDOL are connected into chains running parallel to [001] by C—H···O hydrogen bonds. C—F···π contacts and π–π stacking interactions help to consolidate the crystal packing, and short Br···O [2.9828 (13) Å] distances are also observed. In CANVUM, the molecules are linked by C—H···N interactions along [100], forming a *C*(6) chain. The molecules are further connected by C—Cl···π interactions and face-to-face π–π stacking interactions, resulting in ribbons along [100]. The crystal structure of EBUCUD features short C—H···Cl and C—H···O contacts and C—H···π and van der Waals interactions. In GUPHIL, molecules are associated into inversion dimers *via* short Cl···Cl contacts [3.3763 (9) Å]. In DULTAI, the crystal structure is stabilized by a short C—H···Cl contact, C—Cl···π and van der Waals interactions. In XIZREG, the molecules are linked by C—H···O hydrogen bonds into zigzag chains running along [001]. The crystal packing also features C—Cl···π, C—F···π and N—O···π interactions. In HODQAV, molecules are stacked in columns along [100] *via* weak C—H···Cl hydrogen bonds and face-to-face π–π stacking interactions. The crystal packing is further consolidated by short Cl···Cl contacts. In HONBUK and HONBOE, molecules are linked through weak *X*···Cl contacts (*X* = Cl for HONBUK and Br for HONBOE), C—H···Cl and C—Cl···π interactions into sheets parallel to (001). Additional van der Waals interactions consolidate the three-dimensional packing. In the crystals of LEQXOX, C—H···N and short Cl···Cl contacts are observed and in LEQXIR, C—H···N and C—H···O hydrogen bonds and short C—Cl···O contacts occur.

5. Synthesis and crystallization

Dyes (**I**), (**II**), (**III**) and (**IV**) were synthesized according to a literature protocol (Shikhaliyev *et al.*, 2018).

For (**I**), a 20 ml screw-neck vial was charged with DMSO (10 ml), (*E*)-1-(4-(*tert*-butyl)benzylidene)-2-phenylhydrazine (252 mg, 1 mmol), tetramethylethylenediamine (TMEDA) (295 mg, 2.5 mmol), CuCl (2 mg, 0.02 mmol) and CBr_4 (4.5 mmol). After 1–3 h (until TLC analysis showed complete consumption of the corresponding Schiff base), the reaction mixture was poured into a 0.01 *M* solution of HCl (100 ml, 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 (*v*/*v*: 3/1–1/1). Red solid (yield 69%); m.p. 361 K. Analysis calculated for $C_{18}H_{18}Cl_2N_2$ (*M* = 333.26): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (*dd*, *J* = 6.6, 2.9 Hz, 2H), 7.54–7.47 (*m*, 5H), 7.21 (*d*, *J* = 8.3 Hz, 2H), 1.44 (*s*, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.3, 153.0, 152.2, 151.6, 135.1, 131.5, 129.7, 129.3, 129.0, 125.1, 123.3, 31.4, 29.8.

For (**II**), the procedure was the same as that for (**I**) using (*E*)-1-(4-(*tert*-butyl)benzylidene)-2-(*p*-tolyl)hydrazine (266 mg, 1 mmol). A red solid was obtained (yield 71%); mp 369 K. Analysis calculated for $C_{19}H_{20}Cl_2N_2$ (*M* = 347.28): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.72 (*d*, *J* = 8.3 Hz, 2H), 7.46 (*d*, *J* = 8.3 Hz, 2H), 7.25 (*d*, *J* = 8.2 Hz, 2H), 7.15 (*d*, *J* = 8.3 Hz, 2H), 2.42 (*s*, 3H), 1.39 (*s*, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) 152.1, 151.5, 151.1, 142.2, 134.2, 129.7, 129.7, 129.4, 125.0, 123.3, 34.8, 31.3, 21.6.

For (**III**), the procedure was the same as that for (**I**) using (*E*)-1-(4-(*tert*-butyl)benzylidene)-2-(4-methoxyphenyl)hydrazine (276 mg, 1 mmol). An orange solid was obtained (yield 63%); mp 400 K. Analysis calculated for $C_{19}H_{20}Cl_2N_2O$ (*M* = 363.28): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (*d*, *J* = 9.0 Hz, 2H), 7.48 (*d*, *J* = 8.4 Hz, 2H), 7.17 (*d*, *J* = 8.3 Hz, 2H), 6.96 (*d*, *J*

Table 6
Experimental details.

	(I)	(II)	(III)	(IV)
Crystal data				
Chemical formula	$C_{18}H_{18}Cl_2N_2$	$C_{19}H_{20}Cl_2N_2$	$C_{19}H_{20}Cl_2N_2O$	$C_{19}H_{20}Cl_2N_2$
M_r	333.24	347.27	363.27	347.27
Crystal system, space group	Monoclinic, $C2/c$	Monoclinic, $C2/c$	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$
Temperature (K)	100	100	100	100
a, b, c (Å)	31.7847 (8), 6.0289 (1), 23.7220 (6)	30.9062 (6), 6.27248 (5), 23.3475 (4)	13.8738 (2), 12.5946 (2), 11.3013 (1)	9.8352 (2), 11.8401 (2), 16.3964 (2)
α, β, γ (°)	90, 132.669 (4), 90	90, 127.223 (3), 90	90, 112.505 (1), 90	98.397 (1), 96.189 (1), 107.149 (1)
V (Å^3)	3342.4 (2)	3604.08 (15)	1824.35 (4)	1781.77 (5)
Z	8	8	4	4
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	3.46	3.23	3.26	3.27
Crystal size (mm)	0.23 × 0.18 × 0.15	0.19 × 0.17 × 0.14	0.24 × 0.20 × 0.18	0.25 × 0.22 × 0.18
Data collection				
Diffractometer	XtaLAB Synergy, Dualflex, HyPix	XtaLAB Synergy, Dualflex, HyPix	XtaLAB Synergy, Dualflex, HyPix	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.339, 0.580	0.464, 0.630	0.431, 0.550	0.328, 0.550
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25151, 3543, 3242	28692, 3805, 3643	25894, 3843, 3603	53607, 7515, 6948
R_{int}	0.074	0.047	0.076	0.071
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.634	0.633	0.634	0.634
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.105, 1.08	0.033, 0.090, 1.10	0.043, 0.118, 1.06	0.058, 0.171, 1.04
No. of reflections	3543	3805	3843	7515
No. of parameters	202	213	221	423
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.34, −0.36	0.29, −0.30	0.53, −0.33	0.93, −0.63

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2016/6* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

= 9.0 Hz, 2H), 3.88 (*s*, 3H), 1.41 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.5, 152.0, 151.4, 147.4, 132.9, 129.7, 129.6, 125.2, 125.0, 114.1, 55.5, 34.7, 31.3.

For (**IV**), the procedure was the same as that for (**I**) using (*E*)-1-(4-(*tert*-butyl)benzylidene)-2-(m-tolyl)hydrazine (276 mg, 1 mmol). An orange solid was obtained (yield 63%); mp 339 K. Analysis calculated for $C_{19}H_{20}Cl_2N_2$ (M = 347.28): ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 (*s*, 2H), 7.50 (*d*, J = 8.3 Hz, 2H), 7.37 (*dd*, J = 9.7, 6.0 Hz, 1H), 7.31 (*s*, 1H), 7.19 (*d*, J = 8.3 Hz, 2H), 2.45 (*s*, 3H), 1.43 (*s*, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ δ 153.0, 152.2, 151.5, 138.9, 134.7, 132.3, 129.7, 129.3, 128.8, 125.1, 124.0, 120.3, 34.8, 31.3, 21.3.

Compounds (**I**), (**II**), (**III**) and (**IV**) were dissolved in dichloromethane and then left at room temperature for slow evaporation; red crystals of all compounds suitable for X-rays started to form after *ca* 2 d.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 6. For all structures, H atoms were positioned geometrically and treated as riding atoms, with C—H = 0.95–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C-methyl).

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supporting information

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Crystal structures and Hirshfeld surface analyses of (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-phenyldiazene, (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-(4-methylphenyl)diazene, (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-(4-methoxyphenyl)diazene and (*E*)-1-[1-(4-*tert*-butylphenyl)-2,2-dichloroethenyl]-2-(3-methylphenyl)diazene

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Computing details

For all structures, data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); 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).

(*E*)-1-[1-(4-*tert*-Butylphenyl)-2,2-dichloroethenyl]-2-phenyldiazene (I)

Crystal data

$C_{18}H_{18}Cl_2N_2$
M_r = 333.24
Monoclinic, *C*2/*c*
a = 31.7847 (8) Å
b = 6.0289 (1) Å
c = 23.7220 (6) Å
β = 132.669 (4)°
V = 3342.4 (2) Å^3
Z = 8
F(000) = 1392
D_x = 1.324 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 12999 reflections
θ = 3.7–77.3°
μ = 3.46 mm^{-1}
T = 100 K
Prism, red
0.23 × 0.18 × 0.15 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and *ω* scans
Absorption correction: multi-scan (*CrysAlisPro*; Rigaku OD, 2021)
T_{min} = 0.339, T_{max} = 0.580
25151 measured reflections
3543 independent reflections
3242 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 77.7°, θ_{min} = 3.7°
h = −40→33
k = −7→7
l = −30→30

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.105$
$S = 1.08$
3543 reflections
202 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 1.5568P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.41113 (6)	0.3707 (3)	0.34806 (7)	0.0190 (3)
C2	0.44632 (6)	0.2439 (3)	0.34891 (8)	0.0202 (3)
C3	0.40396 (6)	0.3436 (2)	0.40351 (8)	0.0181 (3)
C4	0.42175 (6)	0.5130 (3)	0.45571 (8)	0.0209 (3)
H4	0.439678	0.641238	0.456824	0.025*
C5	0.41349 (6)	0.4962 (2)	0.50612 (8)	0.0202 (3)
H5	0.426029	0.613327	0.541285	0.024*
C6	0.38719 (6)	0.3110 (2)	0.50615 (7)	0.0174 (3)
C7	0.37085 (6)	0.1406 (3)	0.45491 (8)	0.0202 (3)
H7	0.353829	0.010531	0.454639	0.024*
C8	0.37887 (6)	0.1563 (3)	0.40417 (8)	0.0202 (3)
H8	0.367082	0.037981	0.369712	0.024*
C9	0.37725 (6)	0.2913 (2)	0.56103 (8)	0.0190 (3)
C10	0.37583 (8)	0.5188 (3)	0.58853 (10)	0.0298 (4)
H10A	0.413067	0.591510	0.617926	0.045*
H10B	0.367473	0.499800	0.621133	0.045*
H10C	0.346043	0.610581	0.544116	0.045*
C11	0.32022 (7)	0.1755 (3)	0.52144 (9)	0.0276 (3)
H11A	0.289387	0.251751	0.473242	0.041*
H11B	0.312533	0.179721	0.555056	0.041*
H11C	0.322279	0.020866	0.510718	0.041*
C12	0.42652 (7)	0.1554 (3)	0.63116 (9)	0.0290 (4)
H12A	0.427998	0.009439	0.614365	0.044*
H12B	0.420195	0.136703	0.665981	0.044*
H12C	0.462777	0.233242	0.657860	0.044*
C13	0.31598 (6)	0.8111 (3)	0.23028 (8)	0.0190 (3)
C14	0.33920 (6)	0.9139 (3)	0.20375 (8)	0.0223 (3)
H14	0.373214	0.858034	0.217910	0.027*
C15	0.31215 (7)	1.0977 (3)	0.15666 (9)	0.0263 (3)
H15	0.327976	1.169410	0.138947	0.032*

C16	0.26201 (7)	1.1785 (3)	0.13505 (8)	0.0258 (3)
H16	0.243926	1.305662	0.103079	0.031*
C17	0.23826 (6)	1.0734 (3)	0.16015 (8)	0.0260 (3)
H17	0.203476	1.126355	0.144314	0.031*
C18	0.26553 (6)	0.8909 (3)	0.20839 (8)	0.0231 (3)
H18	0.249845	0.820563	0.226471	0.028*
Cl1	0.48464 (2)	0.02700 (6)	0.41131 (2)	0.02358 (12)
Cl2	0.45673 (2)	0.28133 (7)	0.28705 (2)	0.02385 (12)
N1	0.38241 (5)	0.5414 (2)	0.29193 (7)	0.0193 (3)
N2	0.34302 (5)	0.6330 (2)	0.28416 (6)	0.0199 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0203 (6)	0.0199 (7)	0.0164 (6)	−0.0021 (5)	0.0123 (5)	−0.0010 (5)
C2	0.0205 (7)	0.0230 (7)	0.0170 (6)	−0.0001 (5)	0.0127 (5)	0.0002 (5)
C3	0.0195 (6)	0.0190 (7)	0.0164 (6)	0.0016 (5)	0.0123 (5)	0.0006 (5)
C4	0.0251 (7)	0.0194 (7)	0.0208 (6)	−0.0038 (5)	0.0165 (6)	−0.0018 (6)
C5	0.0245 (7)	0.0186 (7)	0.0184 (6)	−0.0035 (5)	0.0149 (6)	−0.0044 (5)
C6	0.0193 (6)	0.0179 (7)	0.0161 (6)	0.0022 (5)	0.0124 (5)	0.0014 (5)
C7	0.0245 (7)	0.0177 (7)	0.0214 (6)	−0.0027 (5)	0.0168 (6)	−0.0021 (5)
C8	0.0246 (7)	0.0179 (7)	0.0198 (6)	−0.0018 (5)	0.0157 (6)	−0.0039 (5)
C9	0.0256 (7)	0.0175 (7)	0.0190 (6)	0.0018 (5)	0.0171 (6)	0.0012 (5)
C10	0.0499 (10)	0.0213 (8)	0.0375 (8)	0.0005 (7)	0.0373 (8)	−0.0022 (7)
C11	0.0296 (8)	0.0337 (9)	0.0284 (7)	−0.0040 (7)	0.0232 (7)	−0.0027 (7)
C12	0.0323 (8)	0.0366 (9)	0.0246 (7)	0.0103 (7)	0.0218 (7)	0.0099 (7)
C13	0.0204 (6)	0.0203 (7)	0.0154 (6)	−0.0014 (5)	0.0118 (5)	−0.0025 (5)
C14	0.0238 (7)	0.0233 (7)	0.0223 (6)	0.0001 (6)	0.0167 (6)	−0.0008 (6)
C15	0.0295 (8)	0.0250 (8)	0.0261 (7)	−0.0028 (6)	0.0196 (6)	0.0012 (6)
C16	0.0282 (8)	0.0217 (8)	0.0198 (6)	0.0029 (6)	0.0133 (6)	0.0017 (6)
C17	0.0223 (7)	0.0308 (8)	0.0216 (7)	0.0048 (6)	0.0136 (6)	−0.0002 (6)
C18	0.0218 (7)	0.0291 (8)	0.0197 (6)	−0.0007 (6)	0.0145 (6)	−0.0021 (6)
Cl1	0.0259 (2)	0.0243 (2)	0.02326 (19)	0.00553 (13)	0.01777 (16)	0.00450 (13)
Cl2	0.0253 (2)	0.0312 (2)	0.02177 (19)	0.00330 (13)	0.01869 (16)	0.00240 (13)
N1	0.0210 (6)	0.0201 (6)	0.0174 (5)	−0.0001 (5)	0.0132 (5)	−0.0006 (5)
N2	0.0212 (6)	0.0217 (6)	0.0181 (5)	−0.0003 (5)	0.0138 (5)	−0.0009 (5)

Geometric parameters (Å, º)

C1—C2	1.344 (2)	C10—H10C	0.9800
C1—N1	1.4205 (19)	C11—H11A	0.9800
C1—C3	1.4886 (19)	C11—H11B	0.9800
C2—Cl1	1.7146 (15)	C11—H11C	0.9800
C2—Cl2	1.7240 (15)	C12—H12A	0.9800
C3—C8	1.388 (2)	C12—H12B	0.9800
C3—C4	1.396 (2)	C12—H12C	0.9800
C4—C5	1.391 (2)	C13—C18	1.394 (2)
C4—H4	0.9500	C13—C14	1.398 (2)

C5—C6	1.395 (2)	C13—N2	1.4269 (19)
C5—H5	0.9500	C14—C15	1.383 (2)
C6—C7	1.396 (2)	C14—H14	0.9500
C6—C9	1.5381 (19)	C15—C16	1.390 (2)
C7—C8	1.393 (2)	C15—H15	0.9500
C7—H7	0.9500	C16—C17	1.391 (2)
C8—H8	0.9500	C16—H16	0.9500
C9—C11	1.532 (2)	C17—C18	1.388 (2)
C9—C10	1.532 (2)	C17—H17	0.9500
C9—C12	1.536 (2)	C18—H18	0.9500
C10—H10A	0.9800	N1—N2	1.2628 (18)
C10—H10B	0.9800		

C2—C1—N1	115.21 (13)	H10A—C10—H10C	109.5
C2—C1—C3	123.29 (13)	H10B—C10—H10C	109.5
N1—C1—C3	121.45 (13)	C9—C11—H11A	109.5
C1—C2—Cl1	122.94 (12)	C9—C11—H11B	109.5
C1—C2—Cl2	123.42 (12)	H11A—C11—H11B	109.5
Cl1—C2—Cl2	113.64 (9)	C9—C11—H11C	109.5
C8—C3—C4	118.41 (13)	H11A—C11—H11C	109.5
C8—C3—C1	122.15 (13)	H11B—C11—H11C	109.5
C4—C3—C1	119.42 (13)	C9—C12—H12A	109.5
C5—C4—C3	120.69 (14)	C9—C12—H12B	109.5
C5—C4—H4	119.7	H12A—C12—H12B	109.5
C3—C4—H4	119.7	C9—C12—H12C	109.5
C4—C5—C6	121.41 (13)	H12A—C12—H12C	109.5
C4—C5—H5	119.3	H12B—C12—H12C	109.5
C6—C5—H5	119.3	C18—C13—C14	120.28 (14)
C5—C6—C7	117.28 (13)	C18—C13—N2	115.83 (13)
C5—C6—C9	121.94 (13)	C14—C13—N2	123.75 (13)
C7—C6—C9	120.78 (13)	C15—C14—C13	119.32 (14)
C8—C7—C6	121.63 (14)	C15—C14—H14	120.3
C8—C7—H7	119.2	C13—C14—H14	120.3
C6—C7—H7	119.2	C14—C15—C16	120.54 (15)
C3—C8—C7	120.55 (13)	C14—C15—H15	119.7
C3—C8—H8	119.7	C16—C15—H15	119.7
C7—C8—H8	119.7	C15—C16—C17	120.12 (15)
C11—C9—C10	107.75 (13)	C15—C16—H16	119.9
C11—C9—C12	109.54 (13)	C17—C16—H16	119.9
C10—C9—C12	108.60 (13)	C18—C17—C16	119.81 (14)
C11—C9—C6	110.65 (12)	C18—C17—H17	120.1
C10—C9—C6	111.93 (12)	C16—C17—H17	120.1
C12—C9—C6	108.33 (12)	C17—C18—C13	119.91 (14)
C9—C10—H10A	109.5	C17—C18—H18	120.0
C9—C10—H10B	109.5	C13—C18—H18	120.0
H10A—C10—H10B	109.5	N2—N1—C1	113.43 (12)
C9—C10—H10C	109.5	N1—N2—C13	113.31 (12)

N1—C1—C2—Cl1	−179.36 (10)	C7—C6—C9—C11	−37.58 (18)
C3—C1—C2—Cl1	3.2 (2)	C5—C6—C9—C10	23.30 (19)
N1—C1—C2—Cl2	−0.05 (19)	C7—C6—C9—C10	−157.77 (14)
C3—C1—C2—Cl2	−177.52 (11)	C5—C6—C9—C12	−96.41 (16)
C2—C1—C3—C8	−67.0 (2)	C7—C6—C9—C12	82.52 (17)
N1—C1—C3—C8	115.67 (16)	C18—C13—C14—C15	1.1 (2)
C2—C1—C3—C4	114.42 (17)	N2—C13—C14—C15	−174.40 (14)
N1—C1—C3—C4	−62.90 (18)	C13—C14—C15—C16	−0.8 (2)
C8—C3—C4—C5	−1.2 (2)	C14—C15—C16—C17	−0.6 (2)
C1—C3—C4—C5	177.40 (13)	C15—C16—C17—C18	1.6 (2)
C3—C4—C5—C6	−0.2 (2)	C16—C17—C18—C13	−1.3 (2)
C4—C5—C6—C7	1.7 (2)	C14—C13—C18—C17	−0.1 (2)
C4—C5—C6—C9	−179.38 (13)	N2—C13—C18—C17	175.75 (13)
C5—C6—C7—C8	−1.8 (2)	C2—C1—N1—N2	169.00 (13)
C9—C6—C7—C8	179.25 (13)	C3—C1—N1—N2	−13.47 (19)
C4—C3—C8—C7	1.1 (2)	C1—N1—N2—C13	177.31 (11)
C1—C3—C8—C7	−177.48 (13)	C18—C13—N2—N1	168.30 (13)
C6—C7—C8—C3	0.4 (2)	C14—C13—N2—N1	−16.0 (2)
C5—C6—C9—C11	143.50 (14)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the 4-*tert*-butylphenyl ring (C3–C8).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···*Cg*1^{i}	0.95	2.95	3.476 (2)	116

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

(*E*)-1-[1-(4-*tert*-Butylphenyl)-2,2-dichloroethenyl]-2-\ (4-methylphenyl)diazene (II)

Crystal data

$C_{19}H_{20}Cl_2N_2$
M_r = 347.27
Monoclinic, *C*2/*c*
a = 30.9062 (6) Å
b = 6.27248 (5) Å
c = 23.3475 (4) Å
β = 127.223 (3)°
V = 3604.08 (15) Å^3
Z = 8
F(000) = 1456
D_x = 1.280 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 19033 reflections
θ = 3.6–77.1°
μ = 3.23 mm^{-1}
T = 100 K
Prism, red
0.19 × 0.17 × 0.14 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and *ω* scans
Absorption correction: multi-scan (*CrysAlisPro*; Rigaku OD, 2021)
T_{min} = 0.464, T_{max} = 0.630
28692 measured reflections
3805 independent reflections
3643 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 77.5°, θ_{min} = 3.6°
h = −38→38
k = −6→7
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.090$
$S = 1.10$
3805 reflections
213 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.047P)^2 + 2.8P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXL2016/6* (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00017 (5)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.48998 (2)	0.03552 (5)	0.41749 (2)	0.02454 (11)
Cl2	0.46363 (2)	0.25942 (5)	0.29246 (2)	0.02446 (11)
N1	0.39101 (4)	0.51844 (18)	0.30369 (6)	0.0208 (2)
N2	0.35039 (5)	0.59579 (18)	0.29674 (6)	0.0222 (2)
C1	0.41805 (5)	0.3591 (2)	0.35785 (7)	0.0201 (3)
C2	0.45276 (5)	0.2354 (2)	0.35637 (7)	0.0208 (3)
C3	0.40920 (5)	0.3421 (2)	0.41360 (7)	0.0195 (3)
C4	0.42254 (6)	0.5155 (2)	0.45907 (7)	0.0227 (3)
H4	0.438159	0.639440	0.455003	0.027*
C5	0.41316 (6)	0.5082 (2)	0.51023 (7)	0.0220 (3)
H5	0.422523	0.627803	0.540667	0.026*
C6	0.39028 (5)	0.3292 (2)	0.51781 (7)	0.0191 (3)
C7	0.37776 (5)	0.1560 (2)	0.47236 (7)	0.0211 (3)
H7	0.362819	0.030753	0.477002	0.025*
C8	0.38657 (5)	0.1621 (2)	0.42057 (7)	0.0209 (3)
H8	0.377088	0.042930	0.389929	0.025*
C9	0.38015 (5)	0.3145 (2)	0.57443 (7)	0.0206 (3)
C10	0.38607 (6)	0.5300 (2)	0.60923 (8)	0.0284 (3)
H10A	0.423263	0.582766	0.634072	0.043*
H10B	0.378300	0.513209	0.643923	0.043*
H10C	0.360454	0.632136	0.571982	0.043*
C11	0.32232 (6)	0.2333 (3)	0.53954 (8)	0.0295 (3)
H11A	0.296101	0.325794	0.499032	0.044*
H11B	0.315190	0.234963	0.575128	0.044*
H11C	0.318734	0.087345	0.522185	0.044*
C12	0.42191 (6)	0.1599 (3)	0.63358 (8)	0.0315 (3)
H12A	0.417802	0.019311	0.612496	0.047*
H12B	0.415934	0.147896	0.670170	0.047*

H12C	0.458667	0.213787	0.655851	0.047*
C13	0.32527 (5)	0.7652 (2)	0.24618 (7)	0.0199 (3)
C14	0.35328 (5)	0.8930 (2)	0.22966 (7)	0.0221 (3)
H14	0.390374	0.865296	0.250923	0.027*
C15	0.32646 (6)	1.0606 (2)	0.18195 (8)	0.0252 (3)
H15	0.345643	1.148864	0.171144	0.030*
C16	0.27186 (6)	1.1026 (2)	0.14946 (7)	0.0247 (3)
C17	0.24436 (6)	0.9736 (2)	0.16630 (8)	0.0263 (3)
H17	0.206996	0.999041	0.144008	0.032*
C18	0.27109 (6)	0.8078 (2)	0.21550 (8)	0.0261 (3)
H18	0.252413	0.723936	0.228125	0.031*
C19	0.24335 (7)	1.2860 (3)	0.09755 (9)	0.0361 (4)
H19A	0.204956	1.250175	0.061231	0.054*
H19B	0.260343	1.313112	0.073900	0.054*
H19C	0.246248	1.413799	0.123816	0.054*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02633 (18)	0.02606 (18)	0.02459 (17)	0.00732 (11)	0.01716 (14)	0.00613 (11)
Cl2	0.02460 (18)	0.03214 (19)	0.02356 (17)	0.00413 (12)	0.01819 (15)	0.00397 (11)
N1	0.0216 (5)	0.0219 (5)	0.0208 (5)	0.0017 (4)	0.0139 (4)	0.0011 (4)
N2	0.0225 (5)	0.0241 (5)	0.0229 (5)	0.0014 (4)	0.0153 (5)	0.0021 (4)
C1	0.0210 (6)	0.0207 (6)	0.0197 (6)	−0.0009 (5)	0.0129 (5)	0.0008 (5)
C2	0.0207 (6)	0.0241 (6)	0.0192 (6)	0.0006 (5)	0.0129 (5)	0.0022 (5)
C3	0.0192 (6)	0.0211 (6)	0.0194 (6)	0.0021 (5)	0.0123 (5)	0.0018 (5)
C4	0.0268 (7)	0.0202 (6)	0.0242 (6)	−0.0034 (5)	0.0170 (6)	−0.0009 (5)
C5	0.0256 (6)	0.0201 (6)	0.0229 (6)	−0.0030 (5)	0.0160 (5)	−0.0029 (5)
C6	0.0178 (6)	0.0210 (6)	0.0191 (6)	0.0023 (5)	0.0115 (5)	0.0014 (5)
C7	0.0246 (6)	0.0184 (6)	0.0253 (6)	−0.0019 (5)	0.0177 (5)	−0.0005 (5)
C8	0.0236 (6)	0.0190 (6)	0.0227 (6)	−0.0001 (5)	0.0153 (5)	−0.0016 (5)
C9	0.0223 (6)	0.0225 (6)	0.0213 (6)	−0.0007 (5)	0.0154 (5)	−0.0007 (5)
C10	0.0361 (8)	0.0275 (7)	0.0312 (7)	−0.0034 (6)	0.0255 (7)	−0.0064 (6)
C11	0.0278 (7)	0.0386 (8)	0.0303 (7)	−0.0081 (6)	0.0218 (6)	−0.0078 (6)
C12	0.0361 (8)	0.0381 (8)	0.0308 (7)	0.0110 (6)	0.0258 (7)	0.0103 (6)
C13	0.0225 (6)	0.0208 (6)	0.0188 (6)	0.0018 (5)	0.0138 (5)	0.0002 (5)
C14	0.0208 (6)	0.0237 (6)	0.0245 (6)	0.0015 (5)	0.0151 (5)	0.0008 (5)
C15	0.0266 (7)	0.0237 (6)	0.0287 (7)	0.0010 (5)	0.0185 (6)	0.0036 (5)
C16	0.0274 (7)	0.0218 (6)	0.0230 (6)	0.0036 (5)	0.0143 (6)	0.0002 (5)
C17	0.0217 (6)	0.0290 (7)	0.0284 (7)	0.0048 (5)	0.0151 (6)	0.0016 (5)
C18	0.0243 (7)	0.0299 (7)	0.0293 (7)	0.0016 (5)	0.0189 (6)	0.0026 (6)
C19	0.0327 (8)	0.0305 (8)	0.0383 (8)	0.0102 (6)	0.0180 (7)	0.0111 (6)

Geometric parameters (Å, º)

Cl1—C2	1.7163 (13)	C10—H10B	0.9800
Cl2—C2	1.7229 (13)	C10—H10C	0.9800
N1—N2	1.2613 (16)	C11—H11A	0.9800

N1—C1	1.4202 (16)	C11—H11B	0.9800
N2—C13	1.4199 (17)	C11—H11C	0.9800
C1—C2	1.3415 (19)	C12—H12A	0.9800
C1—C3	1.4871 (17)	C12—H12B	0.9800
C3—C8	1.3887 (18)	C12—H12C	0.9800
C3—C4	1.3964 (18)	C13—C18	1.3921 (19)
C4—C5	1.3898 (19)	C13—C14	1.3944 (18)
C4—H4	0.9500	C14—C15	1.3844 (19)
C5—C6	1.3942 (18)	C14—H14	0.9500
C5—H5	0.9500	C15—C16	1.394 (2)
C6—C7	1.3995 (18)	C15—H15	0.9500
C6—C9	1.5348 (17)	C16—C17	1.391 (2)
C7—C8	1.3915 (18)	C16—C19	1.5089 (19)
C7—H7	0.9500	C17—C18	1.391 (2)
C8—H8	0.9500	C17—H17	0.9500
C9—C10	1.5303 (18)	C18—H18	0.9500
C9—C11	1.5349 (18)	C19—H19A	0.9800
C9—C12	1.5353 (19)	C19—H19B	0.9800
C10—H10A	0.9800	C19—H19C	0.9800

N2—N1—C1	112.90 (11)	H10B—C10—H10C	109.5
N1—N2—C13	113.32 (10)	C9—C11—H11A	109.5
C2—C1—N1	115.67 (11)	C9—C11—H11B	109.5
C2—C1—C3	123.67 (12)	H11A—C11—H11B	109.5
N1—C1—C3	120.60 (11)	C9—C11—H11C	109.5
C1—C2—Cl1	123.05 (10)	H11A—C11—H11C	109.5
C1—C2—Cl2	123.35 (10)	H11B—C11—H11C	109.5
Cl1—C2—Cl2	113.60 (7)	C9—C12—H12A	109.5
C8—C3—C4	118.82 (12)	C9—C12—H12B	109.5
C8—C3—C1	122.23 (12)	H12A—C12—H12B	109.5
C4—C3—C1	118.92 (11)	C9—C12—H12C	109.5
C5—C4—C3	120.59 (12)	H12A—C12—H12C	109.5
C5—C4—H4	119.7	H12B—C12—H12C	109.5
C3—C4—H4	119.7	C18—C13—C14	120.14 (12)
C4—C5—C6	121.38 (12)	C18—C13—N2	117.00 (12)
C4—C5—H5	119.3	C14—C13—N2	122.78 (12)
C6—C5—H5	119.3	C15—C14—C13	119.31 (12)
C5—C6—C7	117.26 (11)	C15—C14—H14	120.3
C5—C6—C9	122.75 (11)	C13—C14—H14	120.3
C7—C6—C9	119.96 (11)	C14—C15—C16	121.31 (13)
C8—C7—C6	121.85 (12)	C14—C15—H15	119.3
C8—C7—H7	119.1	C16—C15—H15	119.3
C6—C7—H7	119.1	C17—C16—C15	118.81 (12)
C3—C8—C7	120.09 (12)	C17—C16—C19	120.69 (13)
C3—C8—H8	120.0	C15—C16—C19	120.49 (13)
C7—C8—H8	120.0	C18—C17—C16	120.58 (13)
C10—C9—C6	112.52 (11)	C18—C17—H17	119.7
C10—C9—C11	107.56 (11)	C16—C17—H17	119.7

C6—C9—C11	109.98 (10)	C17—C18—C13	119.81 (13)
C10—C9—C12	108.35 (12)	C17—C18—H18	120.1
C6—C9—C12	108.31 (10)	C13—C18—H18	120.1
C11—C9—C12	110.09 (12)	C16—C19—H19A	109.5
C9—C10—H10A	109.5	C16—C19—H19B	109.5
C9—C10—H10B	109.5	H19A—C19—H19B	109.5
H10A—C10—H10B	109.5	C16—C19—H19C	109.5
C9—C10—H10C	109.5	H19A—C19—H19C	109.5
H10A—C10—H10C	109.5	H19B—C19—H19C	109.5

C1—N1—N2—C13	175.97 (11)	C6—C7—C8—C3	1.1 (2)
N2—N1—C1—C2	164.44 (12)	C5—C6—C9—C10	12.41 (17)
N2—N1—C1—C3	−18.16 (17)	C7—C6—C9—C10	−169.31 (12)
N1—C1—C2—Cl1	179.34 (9)	C5—C6—C9—C11	132.31 (13)
C3—C1—C2—Cl1	2.03 (19)	C7—C6—C9—C11	−49.41 (16)
N1—C1—C2—Cl2	−1.51 (18)	C5—C6—C9—C12	−107.35 (14)
C3—C1—C2—Cl2	−178.82 (10)	C7—C6—C9—C12	70.94 (15)
C2—C1—C3—C8	−65.16 (18)	N1—N2—C13—C18	157.20 (12)
N1—C1—C3—C8	117.65 (14)	N1—N2—C13—C14	−26.07 (18)
C2—C1—C3—C4	116.87 (15)	C18—C13—C14—C15	−0.7 (2)
N1—C1—C3—C4	−60.31 (17)	N2—C13—C14—C15	−177.35 (12)
C8—C3—C4—C5	−0.2 (2)	C13—C14—C15—C16	−0.8 (2)
C1—C3—C4—C5	177.83 (12)	C14—C15—C16—C17	0.7 (2)
C3—C4—C5—C6	0.0 (2)	C14—C15—C16—C19	−179.95 (14)
C4—C5—C6—C7	0.74 (19)	C15—C16—C17—C18	0.9 (2)
C4—C5—C6—C9	179.07 (12)	C19—C16—C17—C18	−178.43 (14)
C5—C6—C7—C8	−1.27 (19)	C16—C17—C18—C13	−2.4 (2)
C9—C6—C7—C8	−179.65 (12)	C14—C13—C18—C17	2.3 (2)
C4—C3—C8—C7	−0.30 (19)	N2—C13—C18—C17	179.13 (12)
C1—C3—C8—C7	−178.27 (12)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the 4-*tert*-butylphenyl ring (C3–C8).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···*Cg*1^{i}	0.95	2.88	3.675 (2)	142

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

(*E*)-1-[1-(4-*tert*-Butylphenyl)-2,2-dichloroethenyl]-2-(4-methoxyphenyl)diazene (III)

Crystal data

$C_{19}H_{20}Cl_2N_2O$
M_r = 363.27
Monoclinic, $P2_1/c$
a = 13.8738 (2) Å
b = 12.5946 (2) Å
c = 11.3013 (1) Å
β = 112.505 (1)°
V = 1824.35 (4) Å^3
Z = 4
$F(000)$ = 760
D_x = 1.323 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 17727 reflections
θ = 3.4–77.6°
μ = 3.26 mm^{-1}
T = 100 K
Prism, red
0.24 × 0.20 × 0.18 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (*CrysAlisPro*; Rigaku OD, 2021)
T_{min} = 0.431, T_{max} = 0.550
25894 measured reflections
3843 independent reflections
3603 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 77.9°, θ_{min} = 3.5°
h = −15→17
k = −15→15
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.118
S = 1.06
3843 reflections
221 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0831P)^2 + 0.4008P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 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	0.20324 (11)	0.34882 (11)	0.22693 (13)	0.0187 (3)
C2	0.14902 (11)	0.30352 (11)	0.11245 (13)	0.0202 (3)
C3	0.19934 (10)	0.46520 (11)	0.24859 (12)	0.0176 (3)
C4	0.13412 (10)	0.50501 (11)	0.30620 (13)	0.0189 (3)
H4	0.093607	0.457391	0.333412	0.023*
C5	0.12770 (10)	0.61349 (11)	0.32425 (13)	0.0188 (3)
H5	0.081387	0.638876	0.361713	0.023*
C6	0.18772 (10)	0.68598 (11)	0.28860 (12)	0.0170 (3)
C7	0.25514 (11)	0.64453 (12)	0.23454 (14)	0.0213 (3)
H7	0.298483	0.691647	0.211415	0.026*
C8	0.26040 (11)	0.53661 (12)	0.21381 (13)	0.0214 (3)
H8	0.306116	0.511166	0.175511	0.026*
C9	0.18118 (11)	0.80655 (11)	0.30498 (13)	0.0205 (3)
C10	0.09974 (13)	0.83569 (12)	0.35970 (16)	0.0268 (3)
H10A	0.030833	0.811599	0.301035	0.040*
H10B	0.098759	0.912885	0.370051	0.040*
H10C	0.117338	0.801296	0.443148	0.040*
C11	0.28773 (13)	0.84892 (13)	0.39614 (16)	0.0282 (3)
H11A	0.305696	0.817148	0.481074	0.042*
H11B	0.284263	0.926299	0.402705	0.042*
H11C	0.341121	0.830301	0.362727	0.042*
C12	0.15139 (14)	0.86056 (13)	0.17359 (15)	0.0298 (3)

H12A	0.205161	0.845923	0.139406	0.045*
H12B	0.145827	0.937393	0.183169	0.045*
H12C	0.084214	0.832769	0.114538	0.045*
C13	0.37438 (10)	0.24915 (11)	0.52562 (13)	0.0184 (3)
C14	0.39042 (11)	0.14261 (11)	0.50182 (13)	0.0193 (3)
H14	0.360543	0.115106	0.417218	0.023*
C15	0.44961 (11)	0.07799 (11)	0.60150 (13)	0.0198 (3)
H15	0.461097	0.006053	0.585247	0.024*
C16	0.49311 (10)	0.11785 (11)	0.72709 (13)	0.0186 (3)
C17	0.47838 (11)	0.22386 (11)	0.75109 (13)	0.0199 (3)
H17	0.508107	0.251380	0.835695	0.024*
C18	0.41964 (11)	0.28891 (11)	0.64970 (13)	0.0206 (3)
H18	0.410262	0.361533	0.665345	0.025*
C19	0.59249 (13)	0.08155 (13)	0.94780 (14)	0.0275 (3)
H19A	0.641917	0.139312	0.955751	0.041*
H19B	0.629032	0.022336	1.003028	0.041*
H19C	0.536817	0.107057	0.973833	0.041*
Cl1	0.07489 (3)	0.37510 (3)	−0.01999 (3)	0.02558 (13)
Cl2	0.14590 (3)	0.16875 (3)	0.08679 (3)	0.02464 (13)
N1	0.26151 (9)	0.27761 (9)	0.32441 (11)	0.0193 (2)
N2	0.31434 (9)	0.32201 (9)	0.42989 (11)	0.0195 (2)
O1	0.54829 (8)	0.04642 (8)	0.81760 (10)	0.0246 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0212 (6)	0.0180 (6)	0.0175 (6)	0.0014 (5)	0.0081 (5)	0.0008 (5)
C2	0.0227 (7)	0.0178 (6)	0.0191 (6)	−0.0003 (5)	0.0070 (5)	0.0001 (5)
C3	0.0202 (6)	0.0168 (6)	0.0139 (6)	0.0012 (5)	0.0042 (5)	0.0002 (5)
C4	0.0200 (6)	0.0193 (7)	0.0168 (6)	−0.0019 (5)	0.0064 (5)	0.0009 (5)
C5	0.0192 (6)	0.0207 (7)	0.0168 (6)	0.0004 (5)	0.0072 (5)	−0.0002 (5)
C6	0.0188 (6)	0.0167 (6)	0.0129 (6)	0.0002 (5)	0.0034 (5)	0.0002 (5)
C7	0.0237 (7)	0.0200 (7)	0.0227 (7)	−0.0028 (5)	0.0116 (6)	0.0008 (5)
C8	0.0240 (7)	0.0217 (7)	0.0219 (6)	0.0017 (5)	0.0126 (5)	0.0008 (5)
C9	0.0253 (7)	0.0156 (6)	0.0193 (6)	−0.0009 (5)	0.0071 (5)	−0.0007 (5)
C10	0.0318 (8)	0.0185 (7)	0.0316 (8)	0.0042 (6)	0.0137 (6)	−0.0015 (6)
C11	0.0293 (8)	0.0225 (7)	0.0301 (8)	−0.0055 (6)	0.0084 (6)	−0.0064 (6)
C12	0.0457 (9)	0.0192 (7)	0.0230 (7)	0.0005 (6)	0.0114 (7)	0.0031 (6)
C13	0.0204 (6)	0.0172 (6)	0.0171 (6)	−0.0002 (5)	0.0065 (5)	0.0010 (5)
C14	0.0219 (7)	0.0182 (6)	0.0179 (6)	−0.0018 (5)	0.0079 (5)	−0.0020 (5)
C15	0.0227 (6)	0.0157 (6)	0.0202 (6)	−0.0001 (5)	0.0073 (5)	−0.0005 (5)
C16	0.0181 (6)	0.0180 (7)	0.0185 (6)	0.0003 (5)	0.0056 (5)	0.0030 (5)
C17	0.0218 (6)	0.0193 (7)	0.0169 (6)	−0.0010 (5)	0.0054 (5)	−0.0012 (5)
C18	0.0242 (7)	0.0165 (6)	0.0198 (6)	−0.0001 (5)	0.0069 (5)	−0.0009 (5)
C19	0.0326 (8)	0.0238 (7)	0.0183 (7)	0.0041 (6)	0.0009 (6)	0.0018 (5)
Cl1	0.0307 (2)	0.0239 (2)	0.01655 (19)	0.00034 (12)	0.00291 (15)	0.00222 (11)
Cl2	0.0306 (2)	0.0173 (2)	0.0225 (2)	−0.00119 (12)	0.00626 (15)	−0.00440 (11)
N1	0.0219 (6)	0.0179 (6)	0.0168 (5)	0.0010 (4)	0.0059 (4)	0.0004 (4)

N2	0.0225 (6)	0.0178 (6)	0.0170 (5)	0.0010 (4)	0.0064 (5)	0.0004 (4)
O1	0.0301 (5)	0.0187 (5)	0.0190 (5)	0.0039 (4)	0.0027 (4)	0.0019 (4)

Geometric parameters (Å, º)

C1—C2	1.349 (2)	C11—H11B	0.9800
C1—N1	1.4106 (18)	C11—H11C	0.9800
C1—C3	1.4904 (19)	C12—H12A	0.9800
C2—Cl1	1.7125 (14)	C12—H12B	0.9800
C2—Cl2	1.7196 (15)	C12—H12C	0.9800
C3—C8	1.3913 (19)	C13—C18	1.3920 (19)
C3—C4	1.3947 (19)	C13—C14	1.4029 (19)
C4—C5	1.389 (2)	C13—N2	1.4200 (18)
C4—H4	0.9500	C14—C15	1.377 (2)
C5—C6	1.3951 (19)	C14—H14	0.9500
C5—H5	0.9500	C15—C16	1.405 (2)
C6—C7	1.3993 (19)	C15—H15	0.9500
C6—C9	1.5366 (19)	C16—O1	1.3573 (17)
C7—C8	1.386 (2)	C16—C17	1.393 (2)
C7—H7	0.9500	C17—C18	1.3905 (19)
C8—H8	0.9500	C17—H17	0.9500
C9—C10	1.526 (2)	C18—H18	0.9500
C9—C11	1.538 (2)	C19—O1	1.4305 (18)
C9—C12	1.539 (2)	C19—H19A	0.9800
C10—H10A	0.9800	C19—H19B	0.9800
C10—H10B	0.9800	C19—H19C	0.9800
C10—H10C	0.9800	N1—N2	1.2658 (17)
C11—H11A	0.9800		

C2—C1—N1	114.99 (12)	H11A—C11—H11B	109.5
C2—C1—C3	122.10 (13)	C9—C11—H11C	109.5
N1—C1—C3	122.89 (12)	H11A—C11—H11C	109.5
C1—C2—Cl1	122.91 (11)	H11B—C11—H11C	109.5
C1—C2—Cl2	123.23 (11)	C9—C12—H12A	109.5
Cl1—C2—Cl2	113.85 (8)	C9—C12—H12B	109.5
C8—C3—C4	118.26 (13)	H12A—C12—H12B	109.5
C8—C3—C1	121.67 (12)	C9—C12—H12C	109.5
C4—C3—C1	120.07 (12)	H12A—C12—H12C	109.5
C5—C4—C3	120.77 (12)	H12B—C12—H12C	109.5
C5—C4—H4	119.6	C18—C13—C14	119.59 (13)
C3—C4—H4	119.6	C18—C13—N2	116.23 (12)
C4—C5—C6	121.48 (12)	C14—C13—N2	124.19 (12)
C4—C5—H5	119.3	C15—C14—C13	119.80 (13)
C6—C5—H5	119.3	C15—C14—H14	120.1
C5—C6—C7	117.03 (13)	C13—C14—H14	120.1
C5—C6—C9	122.86 (12)	C14—C15—C16	120.40 (13)
C7—C6—C9	120.10 (12)	C14—C15—H15	119.8
C8—C7—C6	121.80 (13)	C16—C15—H15	119.8

C8—C7—H7	119.1	O1—C16—C17	124.82 (13)
C6—C7—H7	119.1	O1—C16—C15	115.13 (12)
C7—C8—C3	120.60 (13)	C17—C16—C15	120.05 (12)
C7—C8—H8	119.7	C18—C17—C16	119.19 (12)
C3—C8—H8	119.7	C18—C17—H17	120.4
C10—C9—C6	111.93 (12)	C16—C17—H17	120.4
C10—C9—C11	108.42 (12)	C17—C18—C13	120.95 (13)
C6—C9—C11	109.73 (12)	C17—C18—H18	119.5
C10—C9—C12	108.52 (13)	C13—C18—H18	119.5
C6—C9—C12	109.09 (11)	O1—C19—H19A	109.5
C11—C9—C12	109.10 (13)	O1—C19—H19B	109.5
C9—C10—H10A	109.5	H19A—C19—H19B	109.5
C9—C10—H10B	109.5	O1—C19—H19C	109.5
H10A—C10—H10B	109.5	H19A—C19—H19C	109.5
C9—C10—H10C	109.5	H19B—C19—H19C	109.5
H10A—C10—H10C	109.5	N2—N1—C1	114.00 (12)
H10B—C10—H10C	109.5	N1—N2—C13	113.04 (11)
C9—C11—H11A	109.5	C16—O1—C19	117.79 (11)
C9—C11—H11B	109.5		

N1—C1—C2—Cl1	−178.80 (10)	C7—C6—C9—C11	−62.26 (17)
C3—C1—C2—Cl1	2.57 (19)	C5—C6—C9—C12	−122.02 (15)
N1—C1—C2—Cl2	2.48 (18)	C7—C6—C9—C12	57.21 (17)
C3—C1—C2—Cl2	−176.14 (10)	C18—C13—C14—C15	0.8 (2)
C2—C1—C3—C8	−82.01 (18)	N2—C13—C14—C15	−179.66 (12)
N1—C1—C3—C8	99.47 (16)	C13—C14—C15—C16	0.7 (2)
C2—C1—C3—C4	98.64 (16)	C14—C15—C16—O1	178.87 (12)
N1—C1—C3—C4	−79.88 (17)	C14—C15—C16—C17	−1.4 (2)
C8—C3—C4—C5	2.2 (2)	O1—C16—C17—C18	−179.72 (13)
C1—C3—C4—C5	−178.43 (12)	C15—C16—C17—C18	0.5 (2)
C3—C4—C5—C6	−1.6 (2)	C16—C17—C18—C13	1.0 (2)
C4—C5—C6—C7	−0.37 (19)	C14—C13—C18—C17	−1.7 (2)
C4—C5—C6—C9	178.89 (12)	N2—C13—C18—C17	178.79 (12)
C5—C6—C7—C8	1.7 (2)	C2—C1—N1—N2	177.92 (12)
C9—C6—C7—C8	−177.56 (13)	C3—C1—N1—N2	−3.46 (18)
C6—C7—C8—C3	−1.1 (2)	C1—N1—N2—C13	−178.51 (11)
C4—C3—C8—C7	−0.9 (2)	C18—C13—N2—N1	−168.92 (12)
C1—C3—C8—C7	179.78 (13)	C14—C13—N2—N1	11.54 (18)
C5—C6—C9—C10	−1.92 (18)	C17—C16—O1—C19	1.7 (2)
C7—C6—C9—C10	177.32 (13)	C15—C16—O1—C19	−178.58 (13)
C5—C6—C9—C11	118.51 (14)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the 4-*tert*-butylphenyl ring (C3–C8).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···O1^{i}	0.95	2.39	3.2753 (17)	155

C19—H19*B*···*Cg*1^{ii}	0.98	2.87	3.4276 (17)	117

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) −*x*+1, *y*−1/2, −*z*+3/2.

(*E*)-1-[1-(4-*tert*-Butylphenyl)-2,2-dichloroethenyl]-2-\ (3-methylphenyl)δiazene (IV)

Crystal data

$C_{19}H_{20}Cl_2N_2$
M_r = 347.27
Triclinic, $P\overline{1}$
a = 9.8352 (2) Å
b = 11.8401 (2) Å
c = 16.3964 (2) Å
α = 98.397 (1)°
β = 96.189 (1)°
γ = 107.149 (1)°
V = 1781.77 (5) Å^3

Z = 4
F(000) = 728
D_x = 1.295 Mg m^{-3}
Cu *Kα* radiation, *λ* = 1.54184 Å
Cell parameters from 36250 reflections
θ = 2.7–77.7°
μ = 3.27 mm^{-1}
T = 100 K
Prism, red
0.25 × 0.22 × 0.18 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and *ω* scans
Absorption correction: multi-scan (*CrysAlisPro*; Rigaku OD, 2021)
T_{min} = 0.328, T_{max} = 0.550
53607 measured reflections

7515 independent reflections
6948 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 77.9°, θ_{min} = 2.8°
h = −12→12
k = −14→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.171
S = 1.04
7515 reflections
423 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1247P)^2 + 0.6991P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.61178 (18)	0.35073 (16)	0.16342 (12)	0.0249 (4)
C2	0.6208 (2)	0.27286 (17)	0.09726 (12)	0.0286 (4)
C3	0.58777 (18)	0.31800 (15)	0.24597 (11)	0.0230 (3)
C4	0.46666 (19)	0.32673 (16)	0.28085 (12)	0.0265 (4)
H4	0.393723	0.347551	0.249429	0.032*
C5	0.45226 (19)	0.30530 (16)	0.36066 (12)	0.0265 (4)
H5	0.369067	0.311600	0.383040	0.032*

C6	0.55770 (18)	0.27437 (15)	0.40967 (11)	0.0239 (3)
C7	0.67636 (19)	0.26365 (16)	0.37312 (12)	0.0255 (4)
H7	0.748785	0.241541	0.403958	0.031*
C8	0.69106 (18)	0.28451 (16)	0.29288 (12)	0.0255 (4)
H8	0.772654	0.275817	0.269671	0.031*
C9	0.5398 (2)	0.25476 (16)	0.49849 (12)	0.0272 (4)
C10	0.5205 (2)	0.36724 (18)	0.54994 (13)	0.0333 (4)
H10A	0.603703	0.437581	0.550108	0.050*
H10B	0.512989	0.355418	0.607413	0.050*
H10C	0.432478	0.380217	0.525009	0.050*
C11	0.4060 (2)	0.14560 (18)	0.49507 (13)	0.0344 (4)
H11A	0.320435	0.160683	0.468623	0.052*
H11B	0.394079	0.132610	0.551906	0.052*
H11C	0.418147	0.073943	0.462518	0.052*
C12	0.6708 (2)	0.2312 (2)	0.54356 (13)	0.0343 (4)
H12A	0.681949	0.157211	0.513836	0.051*
H12B	0.656545	0.222374	0.600823	0.051*
H12C	0.757630	0.298939	0.544841	0.051*
C13	0.67080 (18)	0.66543 (17)	0.20121 (12)	0.0267 (4)
C14	0.67993 (19)	0.69894 (17)	0.12348 (12)	0.0273 (4)
H14	0.659272	0.638881	0.074597	0.033*
C15	0.7192 (2)	0.81996 (18)	0.11699 (13)	0.0300 (4)
C16	0.7485 (2)	0.90601 (17)	0.18984 (13)	0.0313 (4)
H16	0.776188	0.988838	0.186220	0.038*
C17	0.7382 (2)	0.87368 (18)	0.26740 (13)	0.0313 (4)
H17	0.757830	0.933887	0.316095	0.038*
C18	0.69929 (19)	0.75318 (17)	0.27368 (13)	0.0284 (4)
H18	0.691972	0.730266	0.326601	0.034*
C19	0.7313 (3)	0.85617 (19)	0.03339 (14)	0.0372 (5)
H19A	0.681665	0.915895	0.027531	0.056*
H19B	0.686864	0.785258	−0.010902	0.056*
H19C	0.833165	0.891001	0.028971	0.056*
C20	0.91894 (19)	0.62019 (16)	0.82034 (12)	0.0257 (4)
C21	0.9535 (2)	0.69058 (16)	0.89645 (12)	0.0290 (4)
C22	0.87259 (19)	0.48653 (16)	0.80936 (11)	0.0237 (3)
C23	0.72883 (19)	0.41702 (17)	0.79251 (12)	0.0278 (4)
H23	0.656334	0.454890	0.787674	0.033*
C24	0.68937 (18)	0.29242 (16)	0.78259 (12)	0.0261 (4)
H24	0.589993	0.246660	0.771607	0.031*
C25	0.79213 (18)	0.23299 (15)	0.78837 (11)	0.0228 (3)
C26	0.93658 (19)	0.30439 (17)	0.80626 (12)	0.0286 (4)
H26	1.009196	0.266638	0.811020	0.034*
C27	0.97708 (19)	0.42862 (17)	0.81727 (13)	0.0292 (4)
H27	1.076283	0.474732	0.830261	0.035*
C28	0.75234 (19)	0.09595 (16)	0.77649 (11)	0.0253 (4)
C29	0.5908 (2)	0.03328 (16)	0.74827 (13)	0.0306 (4)
H29A	0.537672	0.059455	0.790546	0.046*
H29B	0.570431	−0.054050	0.741081	0.046*

H29C	0.560719	0.054255	0.695097	0.046*
C30	0.8320 (2)	0.05048 (18)	0.70974 (14)	0.0341 (4)
H30A	0.808999	0.077558	0.657793	0.051*
H30B	0.801615	−0.037641	0.699604	0.051*
H30C	0.936143	0.082550	0.729276	0.051*
C31	0.7981 (2)	0.06146 (18)	0.85985 (14)	0.0369 (5)
H31A	0.902082	0.099535	0.877774	0.055*
H31B	0.774929	−0.026150	0.852401	0.055*
H31C	0.746315	0.089054	0.902386	0.055*
C32	0.92807 (19)	0.68230 (17)	0.61640 (12)	0.0254 (4)
C33	0.90203 (19)	0.61415 (17)	0.53664 (12)	0.0279 (4)
H33	0.868253	0.528857	0.529137	0.034*
C34	0.9247 (2)	0.66907 (18)	0.46696 (12)	0.0293 (4)
C35	0.9724 (2)	0.79377 (18)	0.48010 (13)	0.0310 (4)
H35	0.988008	0.832852	0.433702	0.037*
C36	0.9977 (2)	0.86290 (18)	0.55985 (13)	0.0328 (4)
H36	1.029797	0.948185	0.567020	0.039*
C37	0.9767 (2)	0.80869 (17)	0.62886 (12)	0.0293 (4)
H37	0.994786	0.855806	0.683334	0.035*
C38	0.8987 (3)	0.5940 (2)	0.38145 (13)	0.0393 (5)
H38A	0.955999	0.538846	0.381276	0.059*
H38B	0.926960	0.646511	0.341058	0.059*
H38C	0.796204	0.547539	0.366089	0.059*
Cl1	0.58942 (6)	0.12256 (4)	0.09905 (3)	0.03558 (15)
Cl2	0.66274 (6)	0.31202 (5)	0.00425 (3)	0.03661 (15)
Cl3	0.93882 (6)	0.63467 (4)	0.98652 (3)	0.03543 (15)
Cl4	1.01859 (6)	0.84553 (4)	0.91208 (3)	0.03931 (16)
N1	0.63865 (16)	0.47049 (14)	0.15050 (10)	0.0266 (3)
N2	0.63619 (16)	0.54441 (14)	0.21407 (10)	0.0260 (3)
N3	0.93773 (17)	0.68198 (14)	0.75331 (10)	0.0269 (3)
N4	0.90357 (16)	0.61543 (14)	0.68230 (10)	0.0264 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0242 (8)	0.0224 (8)	0.0308 (9)	0.0099 (6)	0.0048 (6)	0.0082 (7)
C2	0.0314 (9)	0.0264 (9)	0.0314 (9)	0.0123 (7)	0.0071 (7)	0.0083 (7)
C3	0.0257 (8)	0.0165 (7)	0.0286 (9)	0.0091 (6)	0.0043 (6)	0.0050 (6)
C4	0.0261 (8)	0.0235 (9)	0.0346 (9)	0.0135 (7)	0.0045 (7)	0.0085 (7)
C5	0.0254 (8)	0.0246 (9)	0.0339 (10)	0.0126 (7)	0.0073 (7)	0.0075 (7)
C6	0.0260 (8)	0.0180 (8)	0.0289 (9)	0.0088 (6)	0.0043 (7)	0.0047 (6)
C7	0.0256 (8)	0.0229 (8)	0.0308 (9)	0.0113 (6)	0.0035 (7)	0.0075 (7)
C8	0.0232 (8)	0.0231 (8)	0.0339 (9)	0.0116 (6)	0.0058 (7)	0.0067 (7)
C9	0.0302 (9)	0.0251 (9)	0.0286 (9)	0.0109 (7)	0.0061 (7)	0.0065 (7)
C10	0.0399 (10)	0.0312 (10)	0.0331 (10)	0.0164 (8)	0.0101 (8)	0.0048 (8)
C11	0.0365 (10)	0.0300 (10)	0.0355 (10)	0.0056 (8)	0.0084 (8)	0.0102 (8)
C12	0.0386 (10)	0.0387 (11)	0.0311 (10)	0.0184 (8)	0.0056 (8)	0.0107 (8)
C13	0.0223 (8)	0.0256 (9)	0.0354 (10)	0.0103 (7)	0.0055 (7)	0.0093 (7)

C14	0.0268 (8)	0.0248 (9)	0.0329 (9)	0.0121 (7)	0.0042 (7)	0.0057 (7)
C15	0.0276 (8)	0.0309 (10)	0.0346 (10)	0.0117 (7)	0.0048 (7)	0.0109 (8)
C16	0.0284 (9)	0.0236 (9)	0.0430 (11)	0.0100 (7)	0.0040 (8)	0.0075 (8)
C17	0.0306 (9)	0.0262 (9)	0.0367 (10)	0.0113 (7)	0.0027 (7)	0.0013 (7)
C18	0.0267 (8)	0.0266 (9)	0.0344 (10)	0.0118 (7)	0.0044 (7)	0.0064 (7)
C19	0.0501 (12)	0.0270 (10)	0.0386 (11)	0.0146 (9)	0.0089 (9)	0.0129 (8)
C20	0.0255 (8)	0.0235 (9)	0.0303 (9)	0.0093 (7)	0.0070 (7)	0.0070 (7)
C21	0.0361 (9)	0.0206 (8)	0.0327 (10)	0.0097 (7)	0.0094 (7)	0.0082 (7)
C22	0.0280 (8)	0.0214 (8)	0.0237 (8)	0.0101 (7)	0.0059 (6)	0.0048 (6)
C23	0.0270 (8)	0.0233 (9)	0.0364 (10)	0.0137 (7)	0.0045 (7)	0.0048 (7)
C24	0.0214 (8)	0.0232 (9)	0.0344 (9)	0.0086 (6)	0.0033 (7)	0.0053 (7)
C25	0.0269 (8)	0.0221 (8)	0.0224 (8)	0.0117 (7)	0.0042 (6)	0.0048 (6)
C26	0.0254 (8)	0.0271 (9)	0.0371 (10)	0.0145 (7)	0.0039 (7)	0.0056 (7)
C27	0.0217 (8)	0.0260 (9)	0.0398 (10)	0.0076 (7)	0.0048 (7)	0.0059 (7)
C28	0.0287 (8)	0.0212 (8)	0.0287 (9)	0.0120 (7)	0.0035 (7)	0.0052 (6)
C29	0.0303 (9)	0.0197 (8)	0.0417 (11)	0.0071 (7)	0.0063 (8)	0.0059 (7)
C30	0.0329 (9)	0.0263 (9)	0.0426 (11)	0.0127 (7)	0.0069 (8)	−0.0026 (8)
C31	0.0492 (12)	0.0264 (10)	0.0375 (11)	0.0158 (8)	−0.0009 (9)	0.0112 (8)
C32	0.0246 (8)	0.0269 (9)	0.0293 (9)	0.0130 (7)	0.0054 (7)	0.0086 (7)
C33	0.0278 (8)	0.0237 (9)	0.0336 (10)	0.0113 (7)	0.0020 (7)	0.0050 (7)
C34	0.0298 (9)	0.0309 (10)	0.0300 (9)	0.0159 (7)	0.0008 (7)	0.0041 (7)
C35	0.0352 (9)	0.0308 (10)	0.0324 (10)	0.0168 (8)	0.0052 (7)	0.0100 (7)
C36	0.0411 (10)	0.0254 (9)	0.0351 (10)	0.0147 (8)	0.0052 (8)	0.0078 (8)
C37	0.0340 (9)	0.0263 (9)	0.0315 (9)	0.0154 (7)	0.0052 (7)	0.0053 (7)
C38	0.0563 (13)	0.0344 (11)	0.0305 (10)	0.0231 (10)	−0.0010 (9)	0.0040 (8)
Cl1	0.0505 (3)	0.0238 (3)	0.0367 (3)	0.0175 (2)	0.0099 (2)	0.00496 (19)
Cl2	0.0483 (3)	0.0372 (3)	0.0302 (3)	0.0181 (2)	0.0131 (2)	0.01026 (19)
Cl3	0.0526 (3)	0.0272 (3)	0.0286 (3)	0.0135 (2)	0.0108 (2)	0.00704 (18)
Cl4	0.0583 (3)	0.0196 (2)	0.0377 (3)	0.0078 (2)	0.0127 (2)	0.00383 (18)
N1	0.0252 (7)	0.0249 (8)	0.0330 (8)	0.0104 (6)	0.0055 (6)	0.0099 (6)
N2	0.0246 (7)	0.0228 (7)	0.0335 (8)	0.0108 (6)	0.0052 (6)	0.0072 (6)
N3	0.0290 (7)	0.0252 (8)	0.0299 (8)	0.0114 (6)	0.0074 (6)	0.0079 (6)
N4	0.0253 (7)	0.0259 (8)	0.0311 (8)	0.0116 (6)	0.0044 (6)	0.0079 (6)

Geometric parameters (Å, º)

C1—C2	1.346 (3)	C20—N3	1.406 (2)
C1—N1	1.416 (2)	C20—C22	1.489 (2)
C1—C3	1.485 (2)	C21—Cl3	1.7074 (19)
C2—Cl2	1.715 (2)	C21—Cl4	1.7252 (19)
C2—Cl1	1.7193 (19)	C22—C23	1.384 (3)
C3—C8	1.392 (2)	C22—C27	1.399 (2)
C3—C4	1.400 (2)	C23—C24	1.390 (3)
C4—C5	1.383 (3)	C23—H23	0.9500
C4—H4	0.9500	C24—C25	1.394 (2)
C5—C6	1.409 (2)	C24—H24	0.9500
C5—H5	0.9500	C25—C26	1.396 (3)
C6—C7	1.398 (2)	C25—C28	1.530 (2)

C6—C9	1.528 (2)	C26—C27	1.384 (3)
C7—C8	1.389 (3)	C26—H26	0.9500
C7—H7	0.9500	C27—H27	0.9500
C8—H8	0.9500	C28—C29	1.528 (2)
C9—C12	1.533 (3)	C28—C30	1.537 (3)
C9—C11	1.538 (3)	C28—C31	1.541 (3)
C9—C10	1.542 (3)	C29—H29A	0.9800
C10—H10A	0.9800	C29—H29B	0.9800
C10—H10B	0.9800	C29—H29C	0.9800
C10—H10C	0.9800	C30—H30A	0.9800
C11—H11A	0.9800	C30—H30B	0.9800
C11—H11B	0.9800	C30—H30C	0.9800
C11—H11C	0.9800	C31—H31A	0.9800
C12—H12A	0.9800	C31—H31B	0.9800
C12—H12B	0.9800	C31—H31C	0.9800
C12—H12C	0.9800	C32—C33	1.387 (3)
C13—C14	1.393 (3)	C32—C37	1.406 (3)
C13—C18	1.402 (3)	C32—N4	1.430 (2)
C13—N2	1.425 (2)	C33—C34	1.402 (3)
C14—C15	1.393 (3)	C33—H33	0.9500
C14—H14	0.9500	C34—C35	1.387 (3)
C15—C16	1.395 (3)	C34—C38	1.499 (3)
C15—C19	1.501 (3)	C35—C36	1.392 (3)
C16—C17	1.386 (3)	C35—H35	0.9500
C16—H16	0.9500	C36—C37	1.385 (3)
C17—C18	1.386 (3)	C36—H36	0.9500
C17—H17	0.9500	C37—H37	0.9500
C18—H18	0.9500	C38—H38A	0.9800
C19—H19A	0.9800	C38—H38B	0.9800
C19—H19B	0.9800	C38—H38C	0.9800
C19—H19C	0.9800	N1—N2	1.267 (2)
C20—C21	1.344 (3)	N3—N4	1.257 (2)

C2—C1—N1	114.51 (16)	N3—C20—C22	123.14 (16)
C2—C1—C3	123.57 (16)	C20—C21—Cl3	123.03 (15)
N1—C1—C3	121.73 (16)	C20—C21—Cl4	123.05 (15)
C1—C2—Cl2	124.11 (15)	Cl3—C21—Cl4	113.91 (11)
C1—C2—Cl1	122.10 (15)	C23—C22—C27	118.47 (16)
Cl2—C2—Cl1	113.79 (11)	C23—C22—C20	122.24 (16)
C8—C3—C4	118.29 (17)	C27—C22—C20	119.28 (16)
C8—C3—C1	120.08 (15)	C22—C23—C24	120.73 (16)
C4—C3—C1	121.52 (15)	C22—C23—H23	119.6
C5—C4—C3	120.57 (16)	C24—C23—H23	119.6
C5—C4—H4	119.7	C23—C24—C25	121.58 (16)
C3—C4—H4	119.7	C23—C24—H24	119.2
C4—C5—C6	121.76 (16)	C25—C24—H24	119.2
C4—C5—H5	119.1	C24—C25—C26	117.00 (16)
C6—C5—H5	119.1	C24—C25—C28	122.87 (15)

C7—C6—C5	116.83 (16)	C26—C25—C28	120.13 (15)
C7—C6—C9	123.00 (15)	C27—C26—C25	121.91 (16)
C5—C6—C9	120.17 (16)	C27—C26—H26	119.0
C8—C7—C6	121.65 (16)	C25—C26—H26	119.0
C8—C7—H7	119.2	C26—C27—C22	120.28 (16)
C6—C7—H7	119.2	C26—C27—H27	119.9
C7—C8—C3	120.87 (16)	C22—C27—H27	119.9
C7—C8—H8	119.6	C29—C28—C25	112.29 (14)
C3—C8—H8	119.6	C29—C28—C30	107.92 (15)
C6—C9—C12	112.17 (15)	C25—C28—C30	109.58 (15)
C6—C9—C11	109.16 (15)	C29—C28—C31	108.82 (16)
C12—C9—C11	108.39 (16)	C25—C28—C31	109.01 (15)
C6—C9—C10	109.85 (15)	C30—C28—C31	109.17 (16)
C12—C9—C10	107.88 (16)	C28—C29—H29A	109.5
C11—C9—C10	109.34 (16)	C28—C29—H29B	109.5
C9—C10—H10A	109.5	H29A—C29—H29B	109.5
C9—C10—H10B	109.5	C28—C29—H29C	109.5
H10A—C10—H10B	109.5	H29A—C29—H29C	109.5
C9—C10—H10C	109.5	H29B—C29—H29C	109.5
H10A—C10—H10C	109.5	C28—C30—H30A	109.5
H10B—C10—H10C	109.5	C28—C30—H30B	109.5
C9—C11—H11A	109.5	H30A—C30—H30B	109.5
C9—C11—H11B	109.5	C28—C30—H30C	109.5
H11A—C11—H11B	109.5	H30A—C30—H30C	109.5
C9—C11—H11C	109.5	H30B—C30—H30C	109.5
H11A—C11—H11C	109.5	C28—C31—H31A	109.5
H11B—C11—H11C	109.5	C28—C31—H31B	109.5
C9—C12—H12A	109.5	H31A—C31—H31B	109.5
C9—C12—H12B	109.5	C28—C31—H31C	109.5
H12A—C12—H12B	109.5	H31A—C31—H31C	109.5
C9—C12—H12C	109.5	H31B—C31—H31C	109.5
H12A—C12—H12C	109.5	C33—C32—C37	120.41 (17)
H12B—C12—H12C	109.5	C33—C32—N4	115.61 (16)
C14—C13—C18	120.31 (17)	C37—C32—N4	123.98 (17)
C14—C13—N2	124.27 (17)	C32—C33—C34	121.09 (17)
C18—C13—N2	115.41 (17)	C32—C33—H33	119.5
C15—C14—C13	120.41 (18)	C34—C33—H33	119.5
C15—C14—H14	119.8	C35—C34—C33	117.91 (18)
C13—C14—H14	119.8	C35—C34—C38	121.73 (18)
C14—C15—C16	118.46 (18)	C33—C34—C38	120.36 (18)
C14—C15—C19	120.42 (18)	C34—C35—C36	121.39 (18)
C16—C15—C19	121.12 (18)	C34—C35—H35	119.3
C17—C16—C15	121.63 (18)	C36—C35—H35	119.3
C17—C16—H16	119.2	C37—C36—C35	120.73 (18)
C15—C16—H16	119.2	C37—C36—H36	119.6
C16—C17—C18	119.78 (18)	C35—C36—H36	119.6
C16—C17—H17	120.1	C36—C37—C32	118.46 (18)
C18—C17—H17	120.1	C36—C37—H37	120.8

C17—C18—C13	119.40 (18)	C32—C37—H37	120.8
C17—C18—H18	120.3	C34—C38—H38A	109.5
C13—C18—H18	120.3	C34—C38—H38B	109.5
C15—C19—H19A	109.5	H38A—C38—H38B	109.5
C15—C19—H19B	109.5	C34—C38—H38C	109.5
H19A—C19—H19B	109.5	H38A—C38—H38C	109.5
C15—C19—H19C	109.5	H38B—C38—H38C	109.5
H19A—C19—H19C	109.5	N2—N1—C1	114.26 (15)
H19B—C19—H19C	109.5	N1—N2—C13	113.47 (16)
C21—C20—N3	115.13 (16)	N4—N3—C20	114.67 (16)
C21—C20—C22	121.64 (16)	N3—N4—C32	112.53 (15)

N1—C1—C2—Cl2	0.6 (2)	N3—C20—C22—C23	−86.1 (2)
C3—C1—C2—Cl2	−174.56 (13)	C21—C20—C22—C27	−81.6 (2)
N1—C1—C2—Cl1	−178.98 (13)	N3—C20—C22—C27	94.7 (2)
C3—C1—C2—Cl1	5.9 (3)	C27—C22—C23—C24	−0.8 (3)
C2—C1—C3—C8	64.6 (2)	C20—C22—C23—C24	179.97 (17)
N1—C1—C3—C8	−110.21 (19)	C22—C23—C24—C25	−0.6 (3)
C2—C1—C3—C4	−119.3 (2)	C23—C24—C25—C26	1.3 (3)
N1—C1—C3—C4	65.9 (2)	C23—C24—C25—C28	−179.07 (17)
C8—C3—C4—C5	1.5 (3)	C24—C25—C26—C27	−0.5 (3)
C1—C3—C4—C5	−174.67 (16)	C28—C25—C26—C27	179.86 (17)
C3—C4—C5—C6	0.1 (3)	C25—C26—C27—C22	−1.0 (3)
C4—C5—C6—C7	−1.4 (3)	C23—C22—C27—C26	1.6 (3)
C4—C5—C6—C9	178.32 (16)	C20—C22—C27—C26	−179.16 (17)
C5—C6—C7—C8	1.1 (3)	C24—C25—C28—C29	6.5 (2)
C9—C6—C7—C8	−178.62 (16)	C26—C25—C28—C29	−173.87 (17)
C6—C7—C8—C3	0.5 (3)	C24—C25—C28—C30	126.39 (19)
C4—C3—C8—C7	−1.8 (3)	C26—C25—C28—C30	−54.0 (2)
C1—C3—C8—C7	174.42 (16)	C24—C25—C28—C31	−114.2 (2)
C7—C6—C9—C12	4.0 (2)	C26—C25—C28—C31	65.5 (2)
C5—C6—C9—C12	−175.72 (17)	C37—C32—C33—C34	0.6 (3)
C7—C6—C9—C11	−116.16 (19)	N4—C32—C33—C34	−178.73 (16)
C5—C6—C9—C11	64.1 (2)	C32—C33—C34—C35	−0.8 (3)
C7—C6—C9—C10	123.96 (18)	C32—C33—C34—C38	178.83 (18)
C5—C6—C9—C10	−55.7 (2)	C33—C34—C35—C36	0.3 (3)
C18—C13—C14—C15	0.8 (3)	C38—C34—C35—C36	−179.32 (19)
N2—C13—C14—C15	−177.87 (16)	C34—C35—C36—C37	0.4 (3)
C13—C14—C15—C16	−0.2 (3)	C35—C36—C37—C32	−0.5 (3)
C13—C14—C15—C19	179.04 (17)	C33—C32—C37—C36	0.0 (3)
C14—C15—C16—C17	−0.6 (3)	N4—C32—C37—C36	179.35 (17)
C19—C15—C16—C17	−179.74 (18)	C2—C1—N1—N2	−177.09 (16)
C15—C16—C17—C18	0.6 (3)	C3—C1—N1—N2	−1.8 (2)
C16—C17—C18—C13	0.0 (3)	C1—N1—N2—C13	176.92 (14)
C14—C13—C18—C17	−0.7 (3)	C14—C13—N2—N1	11.6 (2)
N2—C13—C18—C17	178.04 (16)	C18—C13—N2—N1	−167.08 (15)
N3—C20—C21—Cl3	179.92 (13)	C21—C20—N3—N4	−179.22 (16)
C22—C20—C21—Cl3	−3.5 (3)	C22—C20—N3—N4	4.3 (2)

N3—C20—C21—Cl4	−0.8 (2)	C20—N3—N4—C32	−178.50 (14)
C22—C20—C21—Cl4	175.73 (13)	C33—C32—N4—N3	175.76 (15)
C21—C20—C22—C23	97.6 (2)	C37—C32—N4—N3	−3.6 (2)

Hydrogen-bond geometry (Å, º)

*Cg*1 and *Cg*2 are the centroids of the 4-*tert*-butylphenyl rings [(**IVA**: C3–C8 and (**IVB**): C22–C27, respectively]. *Cg*4 is the centroid of the 3-methylphenyl ring (C32–C37) of molecule (**IVB**).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···*Cg*4^{i}	0.95	2.91	3.768 (2)	151
C24—H24···*Cg*2^{ii}	0.95	2.97	3.824 (2)	150
C29—H29*B*···*Cg*1^{iii}	0.98	2.78	3.706 (2)	157

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