



Crystal structure and Hirshfeld surface analysis of (*E*)-1-[2,2-dichloro-1-(4-fluorophenyl)ethenyl]-2-(2,4-dichlorophenyl)diazene

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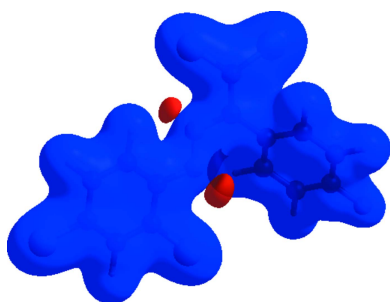
In the title compound, $C_{14}H_7Cl_4FN_2$, the dihedral angle between the 4-fluorophenyl ring and the 2,4-dichlorophenyl ring is $46.03(19)^\circ$. In the crystal, the molecules are linked by $C-H \cdots N$ interactions along the *a*-axis direction, forming a $C(6)$ chain. The molecules are further connected by $C-Cl \cdots \pi$ interactions and face-to-face $\pi-\pi$ stacking interactions, forming ribbons along the *a*-axis direction. Hirshfeld surface analysis indicates that the greatest contributions to the crystal packing are from $Cl \cdots H/H \cdots Cl$ (35.1%), $H \cdots H$ (10.6%), $C \cdots C$ (9.7%), $Cl \cdots Cl$ (9.4%) and $C \cdots H/H \cdots C$ (9.2%) interactions.

1. Chemical context

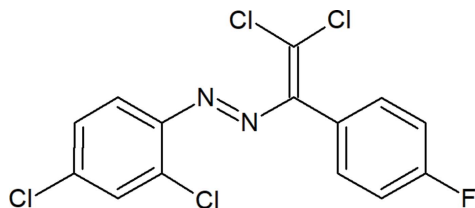
Azo dyes find numerous applications in a diversity of areas, including as antimicrobial agents, in molecular recognition, optical data storage, molecular switches, non-linear optics, liquid crystals, dye-sensitized solar cells, color-changing materials, *etc.*, mainly due to the possibility of the *cis-to-trans* isomerization and the chromophoric properties of the $-N=N-$ synthon (Maharramov *et al.*, 2018; Viswanathan *et al.*, 2019). Not only azo-hydrazone tautomerism, but also *E/Z* isomerization are important phenomena in the synthetic chemistry of azo dyes (Ma *et al.*, 2017*a,b*; Mahmoudi *et al.*, 2018*a,b*). The design of azo dyes with functional groups led to multifunctional ligands, the corresponding transition-metal complexes of which have been used effectively as catalysts in $C-C$ coupling and oxidation reactions (Ma *et al.*, 2020, 2021; Mahmudov *et al.*, 2013; Mizar *et al.*, 2012). Moreover, the functional properties of azo dyes can be improved by attaching substituents with non-covalent bond donor or acceptor site(s) to the $-N=N-$ synthon (Gurbanov *et al.*, 2020*a,b*; Kopylovich *et al.*, 2011; Mahmudov *et al.*, 2020; Shikhaliyev *et al.*, 2014). Thus, we have attached halogen-bond donor centres to the $-N=N-$ moiety, leading to a new azo dye, (*E*)-1-[2,2-dichloro-1-(4-fluorophenyl)ethenyl]-2-(2,4-dichlorophenyl)diazene, which provides multiple intermolecular non-covalent interactions.

2. Structural commentary

In the title compound, (Fig. 1), the dihedral angle between the 4-fluorophenyl ring C3–C8 and the 2,4-dichlorophenyl ring



C9–C14 is $46.0(2)^\circ$. The N2/N1/C1/C2/C11/C12 moiety is approximately planar, with a maximum deviation of $0.029(1)$ Å for C11, and makes dihedral angles of $50.53(18)$ and $11.75(18)^\circ$ with the C3–C8 and C9–C14 rings, respectively. In the molecule, the aromatic ring and olefin synthon adopt a *trans*-configuration with respect to the N=N double bond and are almost coplanar with a C1–N1=N2–C9 torsion angle of $179.1(4)^\circ$.



3. Supramolecular features

In the crystal, the molecules are linked by C–H···N interactions along the *a*-axis direction, forming a *C*(6) chain (Table 1; Fig. 2; Bernstein *et al.*, 1995). Furthermore, molecules are connected by C–Cl···Cg2 interactions (Table 1) and face-to-face π - π stacking interactions [$Cg1 \cdots Cg1^i = 3.873(3)$ Å, slippage = 1.831 Å; $Cg2 \cdots Cg2^i = 3.872(3)$ Å, slippage = 1.554 Å; symmetry codes: (i) $x - 1, y, z$; (ii) $x + 1, y, z$; where Cg1 and Cg2 are the centroids of the 4-fluorophenyl (C3–C8) and 2,4-dichlorophenyl ring (C9–C14) rings, respectively], forming ribbons along the *a*-axis direction (Figs. 2, 3 and 4).

4. Hirshfeld surface analysis

Crystal Explorer (Turner *et al.*, 2017) was used to perform a Hirshfeld surface analysis and generate the associated two-dimensional fingerprint plots, with a standard resolution of the three-dimensional d_{norm} surfaces plotted over a fixed colour scale of -0.1450 (red) to 1.1580 (blue) a.u (Fig. 5). In the Hirshfeld surface mapped over d_{norm} (Fig. 5), the bright-red spots near atoms Cl1, Cl3, H4, N2 and F1 indicate the short C–H···N, C–H···Cl and Cl···F contacts (Table 2). Other

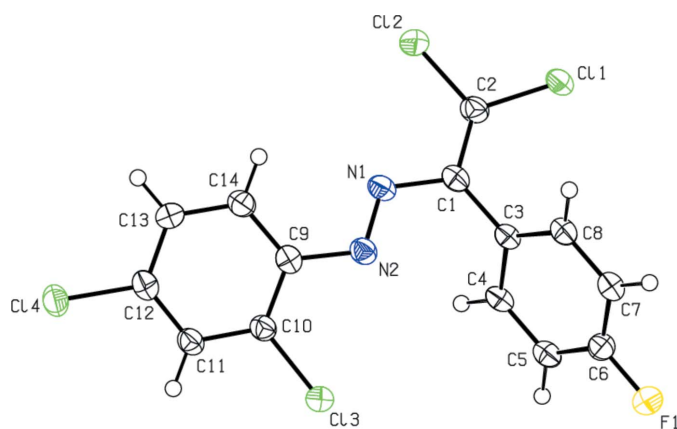


Figure 1

The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the 2,4-dichlorophenyl ring (C9–C14).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C4–H4···N2 ⁱ	0.95	2.53	3.265 (5)	134
C12–Cl4···Cg2 ⁱⁱ	1.735 (5)	3.920 (3)	3.569 (6)	66.51 (18)

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

contacts are equal to or longer than the sum of van der Waals radii. The Hirshfeld surface of the title compound mapped over the electrostatic potential (Spackman *et al.*, 2008) is

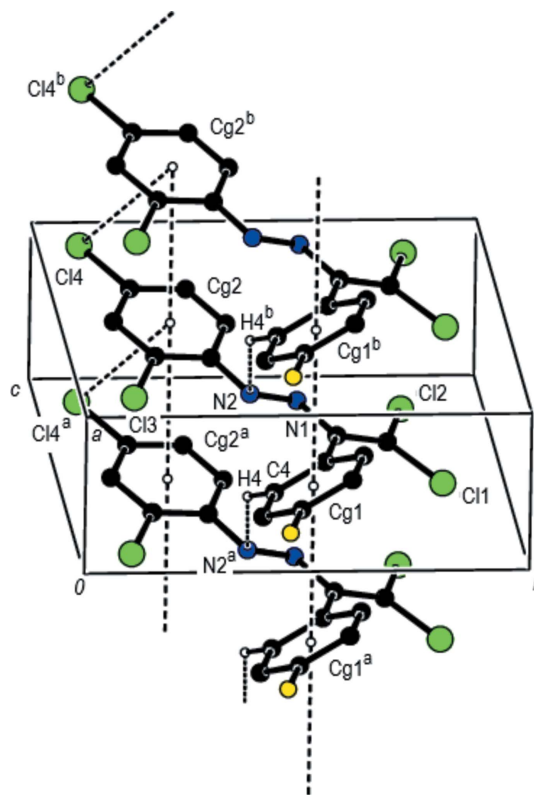


Figure 2

A general view of the intermolecular C–H···N and C–Cl··· π interactions and π - π stacking interactions, shown as dashed lines. Symmetry codes: (a) $-1 + x, y, z$; (b) $1 + x, y, z$.

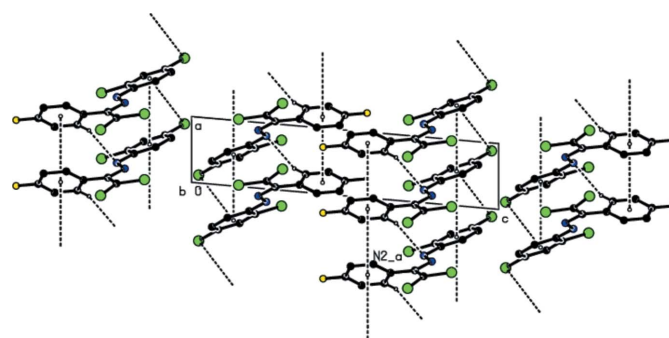


Figure 3

The crystal packing of the title compound viewed along the *b* axis with intermolecular C–H···N and C–Cl··· π interactions and π - π stacking interactions shown as dashed lines.

Table 2
Summary of short interatomic contacts (Å) in the title compound.

Contact	Distance	Symmetry operation
Cl1...H11	3.06	$-1 + x, 1 + y, z$
H4...N2	2.53	$-1 + x, y, z$
Cl1...F1	3.016 (3)	$-1 - x, \frac{1}{2} + y, 1 - z$
H5...H7	2.55	$-x, -\frac{1}{2} + y, 1 - z$
Cl4...H13	2.95	$2 - x, -\frac{1}{2} + y, 2 - z$
Cl4...H14	2.93	$1 - x, -\frac{1}{2} + y, 2 - z$
Cl3...F1	3.116 (3)	$-x, -\frac{1}{2} + y, 1 - z$

shown in Fig. 6. The positive electrostatic potential (blue regions) over the surface indicates hydrogen-donor potential, whereas the hydrogen-bond acceptors are represented by negative electrostatic potential (red regions).

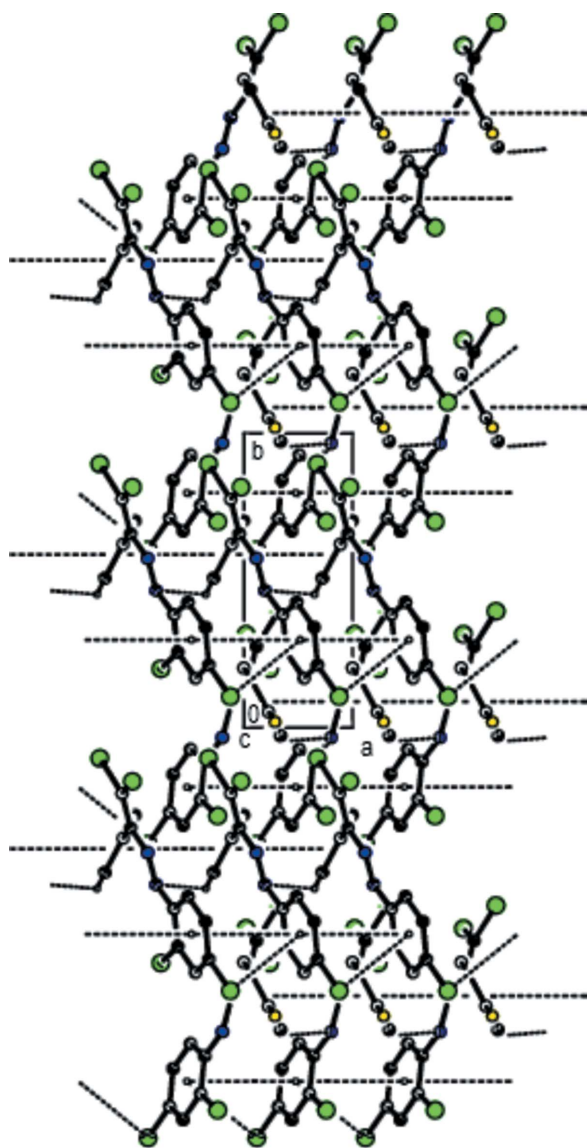


Figure 4
The crystal packing of the title compound viewed along the *c* axis with intermolecular C—H...N and C—Cl... π interactions and π - π stacking interactions shown as dashed lines.

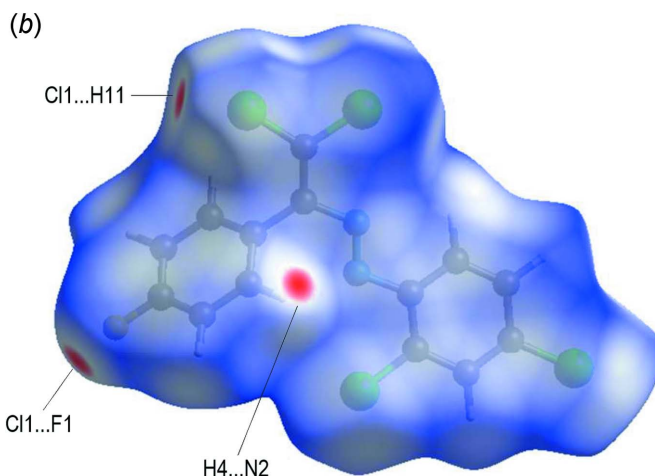
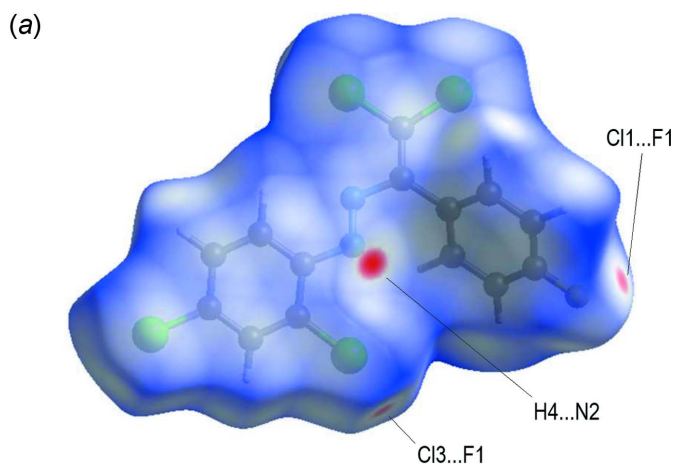


Figure 5
(*a*) Front and (*b*) back sides of the three-dimensional Hirshfeld surface of the title compound plotted over d_{norm} in the range -0.1450 to 1.1580 a.u.

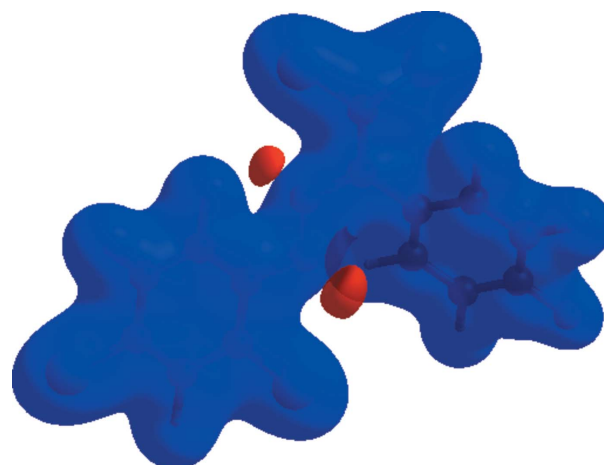


Figure 6
View of the three-dimensional Hirshfeld surface of the title compound plotted over electrostatic potential in the range -0.0500 to 0.0500 a.u. using the *STO-3G* basis set at the Hartree-Fock level of theory. Hydrogen-bond donors and acceptors are shown as blue and red regions around the atoms, corresponding to positive and negative potentials, respectively.

Table 3

Percentage contributions of interatomic contacts to the Hirshfeld surface for the title compound..

Contact	Percentage contribution
Cl···H/H···Cl	35.1
H···H	10.6
C···C	9.7
Cl···Cl	9.4
C···H/H···C	9.2
Cl···F/F···Cl	6.7
Cl···C/C···Cl	5.0
F···H/H···F	5.0
N···H/H···N	4.4
N···C/C···N	3.5
F···F	0.9
N···N	0.3
F···C/C···F	0.1

The overall two-dimensional fingerprint plot and those delineated into Cl···H/H···Cl, H···H, C···C, Cl···Cl and C···H/H···C contacts in the title molecule are illustrated in Fig. 7. The most important interaction is Cl···H/H···Cl, contributing 35.1% to the overall crystal packing (Fig. 7*b*). The secondary important H···H and C···C interactions contribute 10.6% (Fig. 7*c*) and 9.7% (Fig. 7*d*), respectively, to the Hirshfeld surface. The remaining contributions for the title compound are from Cl···Cl, C···H/H···C, Cl···F/F···Cl, Cl···C/C···Cl, F···H/H···F, N···H/H···N, N···N and F···C/C···F contacts, which are less than 9.7% and have a negligible effect on the packing. The percentage contributions of all interactions are listed in Table 3.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.41, update of November 2019; Groom *et al.*, 2016) for the (*E*)-1-(2,2-dichloro-1-phenylethenyl)-2-phenyldiazene unit resulted in 28 hits. Nine compounds are closely related to the title compound, *viz.* LEQXOX (**I**; Shikhaliyev *et al.*, 2018), LEQXIR (**II**; Shikhaliyev *et al.*, 2018), XIZREG (**III**; Atioğlu *et al.*, 2019), HODQAV (**IV**; Shikhaliyev *et al.*, 2019), HONBUK (**V**; Akkurt *et al.*, 2019), HONBOE (**VI**; Akkurt *et al.*, 2019), DULTAI (**VII**; Özkaraca *et al.*, 2020*b*), GUPHIL (**VIII**; Özkaraca *et al.*, 2020*a*) and EBUCUD (**IX**; Shikhaliyev *et al.*, 2021).

In the crystals of **I** and **II**, the dihedral angles between the aromatic rings are 56.18 (12) and 60.31 (14)°, respectively. In **I**, C—H···N and short Cl···Cl contacts are observed and in **II**, C—H···N and C—H···O hydrogen bonds and short C—Cl···O contacts occur. In **III**, the benzene rings form a dihedral angle of 63.29 (8)° and the molecules are linked by C—H···O hydrogen bonds into zigzag chains running along the *c*-axis direction. The crystal packing also features C—Cl··· π , C—F··· π and N—O··· π interactions. In **IV**, the benzene rings make a dihedral angle of 56.13 (13)°. Molecules are stacked in columns along the *a*-axis direction *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 **V** and **VI**, the aromatic rings form dihedral angles

of 60.9 (2) and 64.1 (2)°, respectively. In the crystals, molecules are linked through weak *X*···Cl contacts (*X* = Cl for **V** and Br for **VI**), C—H···Cl and C—Cl··· π interactions into sheets parallel to the *ab* plane. Additional van der Waals interactions consolidate the three-dimensional packing. In **VII**, the dihedral angle between the two aromatic rings is 64.12 (14)°. The crystal structure is stabilized by a short C—H···Cl contact, C—Cl··· π and van der Waals interactions. In **VIII**, the benzene rings subtend a dihedral angle of 77.07 (10)°. In the crystal, molecules are associated into inversion dimers *via* short Cl···Cl contacts [3.3763 (9) Å]. In **IX**, the asymmetric unit comprises two similar molecules, in which the dihedral angles between the two aromatic rings are 70.1 (3) and 73.2 (2)°. The crystal structure features short C—H···Cl and C—H···O contacts and C—H··· π and van der Waals interactions.

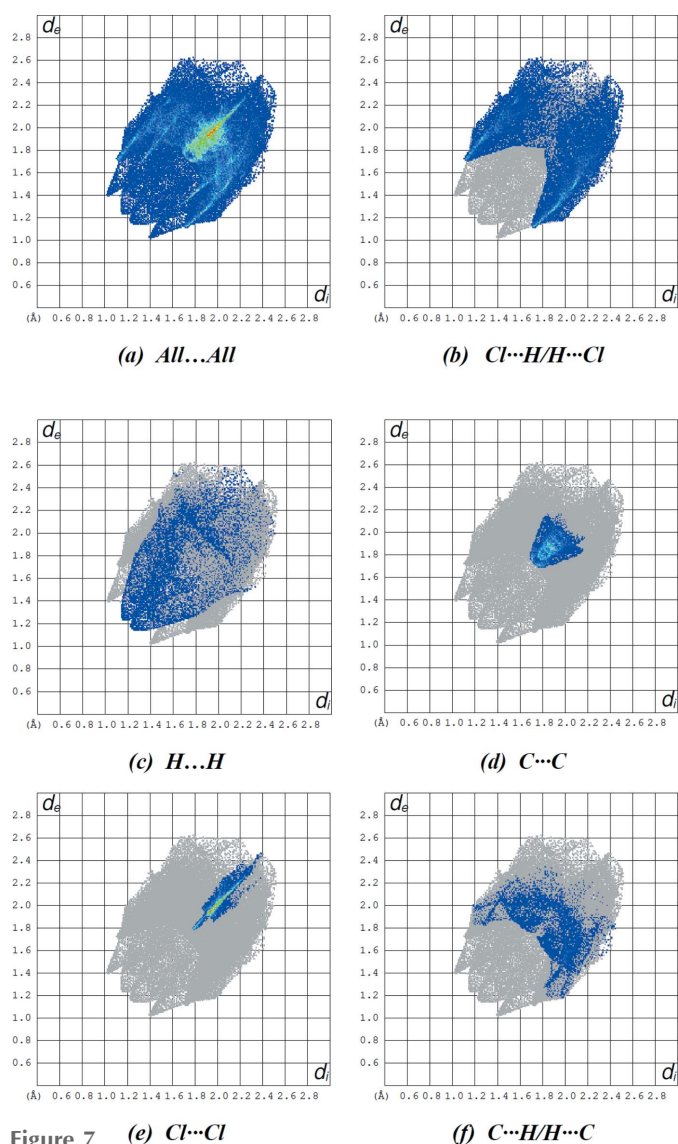


Figure 7 (e) Cl···Cl (9.4%) and (f) C···H/H···C (9.2%) interactions. The full two-dimensional fingerprint plot for the title compound and those delineated into (b) Cl···H/H···Cl (35.1%), (c) H···H (10.6%), (d) C···C (9.7%), (e) Cl···Cl (9.4%) and (f) C···H/H···C (9.2%) interactions.

6. Synthesis and crystallization

The title dye was synthesized according to the reported method (Shikhaliyev *et al.*, 2018, 2019). A 20 mL screw-neck vial was charged with DMSO (10 mL), (*E*)-1-(2,4-dichlorophenyl)-2-(4-fluorobenzylidene)hydrazine (283 mg, 1 mmol), tetramethylethylenediamine (TMEDA) (295 mg, 2.5 mmol), CuCl (2 mg, 0.02 mmol) and CCl₄ (20 mmol, 10 equiv.). After 1–3 h (until TLC analysis showed complete consumption of the corresponding Schiff base), the reaction mixture was poured into ~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) and brine (30 mL), dried over anhydrous Na₂SO₄ and concentrated using a vacuum rotary evaporator. The residue was purified by column chromatography on silica gel using appropriate mixtures of hexane and dichloromethane (3/1–1/1). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution. Colourless solid (44%); m.p. 345 K. Analysis calculated for C₁₄H₇Cl₄FN₂ (*M* = 364.02): C 46.19, H 1.94, N 7.70; found: C 46.11, H 1.98, N 7.67%. ¹H NMR (300 MHz, CDCl₃) δ 7.31–7.83 (7H, Ar). ¹³C NMR (75 MHz, CDCl₃) δ 114.89, 115.12, 115.41, 115.74, 115.97, 118.33, 127.73, 128.08, 128.67, 129.17, 130.48, 132.04, 132.15 and 136.83. ESI-MS: *m/z*: 365.11 [*M* + H]⁺.

7. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 4. The Moscow synchrotron radiation source was used for the data collection. H atoms were positioned geometrically and treated as riding atoms where C–H = 0.95 Å with *U*_{iso}(H) = 1.2*U*_{eq}(C). Five outliers $\bar{3} \ 2 \ 2$, $\bar{3} \ \bar{2} \ 2$, $\bar{2} \ 11 \ 3$, $\bar{2} \ 2 \ 1$ and $\bar{2} \ \bar{2} \ 1$ were omitted during the final refinement cycle because of large differences between observed and calculated intensities.

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The author's contributions are as follows. Conceptualization, NQS, MA and SM; synthesis, XNB, GTS and MSA; X-ray analysis, KÖ and MA; writing (review and editing of the manuscript), funding acquisition, NQS, XNB, GTS and MSA; supervision, NQS, MA and SM.

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Table 4
Experimental details.

Crystal data	
Chemical formula	C ₁₄ H ₇ Cl ₄ FN ₂
<i>M_r</i>	364.02
Crystal system, space group	Monoclinic, <i>P2</i> ₁
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	3.8720 (8), 10.434 (2), 18.138 (4)
β (°)	95.03 (3)
<i>V</i> (Å ³)	730.0 (3)
<i>Z</i>	2
Radiation type	Synchrotron, λ = 0.79475 Å
μ (mm ^{−1})	1.10
Crystal size (mm)	0.20 × 0.15 × 0.10
Data collection	
Diffractometer	Rayonix SX165 CCD
Absorption correction	Multi-scan (<i>SCALA</i> ; Evans, 2006)
<i>T</i> _{min} , <i>T</i> _{max}	0.800, 0.880
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	8595, 3120, 2972
<i>R</i> _{int}	0.027
(sin θ/λ) _{max} (Å ^{−1})	0.648
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.036, 0.106, 1.09
No. of reflections	3120
No. of parameters	191
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ^{−3})	0.61, −0.30
Absolute structure	Flack <i>x</i> determined using 1318 quotients [(<i>I</i> ⁺) − (<i>I</i> [−])]/[(<i>I</i> ⁺) + (<i>I</i> [−])] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.04 (2)

Computer programs: *Marccd* (Doyle, 2011), *iMosflm* (Battye *et al.*, 2011), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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Crystal structure and Hirshfeld surface analysis of (*E*)-1-[2,2-dichloro-1-(4-fluorophenyl)ethenyl]-2-(2,4-dichlorophenyl)diazene

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Computing details

Data collection: *Marccd* (Doyle, 2011); cell refinement: *iMosflm* (Battye *et al.*, 2011); data reduction: *iMosflm* (Battye *et al.*, 2011); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

(*E*)-1-[2,2-Dichloro-1-(4-fluorophenyl)ethenyl]-2-(2,4-dichlorophenyl)diazene

Crystal data

$C_{14}H_7Cl_4FN_2$

$M_r = 364.02$

Monoclinic, $P2_1$

$a = 3.8720$ (8) Å

$b = 10.434$ (2) Å

$c = 18.138$ (4) Å

$\beta = 95.03$ (3)°

$V = 730.0$ (3) Å³

$Z = 2$

$F(000) = 364$

$D_x = 1.656$ Mg m⁻³

Synchrotron radiation, $\lambda = 0.79475$ Å

Cell parameters from 600 reflections

$\theta = 2.8$ – 28.0 °

$\mu = 1.12$ mm⁻¹

$T = 100$ K

Prism, colourless

$0.20 \times 0.15 \times 0.10$ mm

Data collection

Rayonix SX165 CCD
diffractometer

/f scan

Absorption correction: multi-scan
(Scala; Evans, 2006)

$T_{\min} = 0.800$, $T_{\max} = 0.880$

8595 measured reflections

3120 independent reflections

2972 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 31.0$ °, $\theta_{\min} = 2.5$ °

$h = -5 \rightarrow 5$

$k = -12 \rightarrow 13$

$l = -23 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.106$

$S = 1.09$

3120 reflections

191 parameters

1 restraint

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.7552P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.61$ e Å⁻³

$\Delta\rho_{\min} = -0.30$ e Å⁻³

Extinction correction: SHELXL,
 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.044 (8)

Absolute structure: Flack x determined using
 1318 quotients $[(F^+) - (F^-)] / [(F^+) + (F^-)]$ (Parsons et
 al., 2013)
 Absolute structure parameter: 0.04 (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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	−0.3214 (3)	0.89506 (12)	0.70389 (6)	0.0309 (3)
Cl2	−0.0221 (4)	0.81658 (13)	0.84672 (7)	0.0392 (3)
Cl3	0.2392 (3)	0.19949 (12)	0.70702 (6)	0.0334 (3)
Cl4	0.8795 (3)	0.10530 (13)	0.97679 (6)	0.0340 (3)
F1	−0.2885 (9)	0.5192 (3)	0.42861 (16)	0.0383 (7)
N1	0.1181 (11)	0.5745 (4)	0.7820 (2)	0.0281 (9)
N2	0.1962 (11)	0.4658 (4)	0.7569 (2)	0.0273 (8)
C1	−0.0396 (12)	0.6583 (5)	0.7275 (3)	0.0274 (9)
C2	−0.1180 (12)	0.7756 (5)	0.7555 (3)	0.0293 (10)
C3	−0.1089 (12)	0.6232 (5)	0.6480 (2)	0.0255 (9)
C4	−0.2763 (12)	0.5073 (5)	0.6280 (3)	0.0267 (9)
H4	−0.347529	0.452035	0.665430	0.032*
C5	−0.3391 (13)	0.4726 (5)	0.5540 (3)	0.0288 (10)
H5	−0.455606	0.394787	0.540530	0.035*
C6	−0.2292 (13)	0.5531 (5)	0.5008 (3)	0.0295 (10)
C7	−0.0634 (12)	0.6678 (5)	0.5181 (3)	0.0289 (10)
H7	0.006934	0.722093	0.480114	0.035*
C8	−0.0016 (12)	0.7022 (5)	0.5920 (3)	0.0281 (9)
H8	0.114818	0.780287	0.604727	0.034*
C9	0.3594 (11)	0.3839 (5)	0.8125 (2)	0.0261 (9)
C10	0.3960 (12)	0.2556 (5)	0.7935 (3)	0.0265 (9)
C11	0.5577 (13)	0.1679 (5)	0.8440 (3)	0.0275 (9)
H11	0.581566	0.080365	0.830976	0.033*
C12	0.6813 (13)	0.2120 (5)	0.9131 (3)	0.0291 (10)
C13	0.6495 (12)	0.3405 (5)	0.9334 (3)	0.0289 (10)
H13	0.736480	0.368972	0.981195	0.035*
C14	0.4893 (13)	0.4255 (5)	0.8827 (3)	0.0300 (10)
H14	0.467401	0.513039	0.895888	0.036*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0349 (6)	0.0218 (6)	0.0353 (6)	0.0044 (5)	−0.0005 (4)	−0.0001 (4)
Cl2	0.0528 (8)	0.0325 (7)	0.0312 (6)	0.0116 (6)	−0.0029 (5)	−0.0065 (5)
Cl3	0.0426 (6)	0.0263 (6)	0.0301 (6)	0.0037 (5)	−0.0030 (4)	−0.0036 (4)

C14	0.0385 (6)	0.0315 (7)	0.0318 (5)	0.0058 (5)	0.0018 (4)	0.0071 (5)
F1	0.0507 (18)	0.0339 (18)	0.0296 (15)	0.0000 (14)	0.0002 (12)	-0.0029 (12)
N1	0.031 (2)	0.022 (2)	0.032 (2)	0.0034 (16)	0.0042 (15)	-0.0011 (15)
N2	0.028 (2)	0.025 (2)	0.0291 (19)	0.0041 (15)	0.0052 (15)	0.0005 (15)
C1	0.027 (2)	0.023 (2)	0.033 (2)	0.0038 (17)	0.0032 (17)	0.0004 (18)
C2	0.027 (2)	0.027 (3)	0.034 (2)	0.0060 (18)	0.0015 (18)	-0.0031 (19)
C3	0.027 (2)	0.020 (2)	0.029 (2)	0.0037 (17)	0.0026 (16)	0.0005 (17)
C4	0.028 (2)	0.019 (2)	0.034 (2)	0.0029 (17)	0.0062 (17)	0.0004 (17)
C5	0.029 (2)	0.022 (2)	0.036 (2)	0.0031 (17)	0.0024 (18)	0.0000 (18)
C6	0.030 (2)	0.030 (3)	0.028 (2)	0.0053 (18)	0.0009 (17)	-0.0018 (17)
C7	0.028 (2)	0.025 (3)	0.033 (2)	0.0024 (17)	0.0034 (17)	0.0035 (18)
C8	0.028 (2)	0.023 (2)	0.033 (2)	0.0029 (19)	0.0019 (16)	0.0018 (19)
C9	0.024 (2)	0.026 (2)	0.029 (2)	0.0012 (18)	0.0052 (15)	0.0031 (18)
C10	0.029 (2)	0.024 (2)	0.027 (2)	0.0040 (18)	0.0044 (17)	-0.0001 (17)
C11	0.029 (2)	0.024 (3)	0.030 (2)	0.0045 (17)	0.0046 (16)	0.0013 (17)
C12	0.029 (2)	0.027 (3)	0.032 (2)	0.0030 (19)	0.0055 (17)	0.0057 (19)
C13	0.031 (2)	0.029 (3)	0.026 (2)	-0.0010 (19)	0.0017 (17)	-0.0041 (18)
C14	0.035 (2)	0.024 (3)	0.031 (2)	0.0021 (18)	0.0043 (18)	0.0002 (18)

Geometric parameters (Å, °)

C11—C2	1.709 (5)	C5—H5	0.9500
C12—C2	1.718 (5)	C6—C7	1.381 (7)
C13—C10	1.733 (5)	C7—C8	1.388 (7)
C14—C12	1.735 (5)	C7—H7	0.9500
F1—C6	1.357 (6)	C8—H8	0.9500
N1—N2	1.269 (6)	C9—C10	1.393 (7)
N1—C1	1.416 (6)	C9—C14	1.398 (7)
N2—C9	1.426 (6)	C10—C11	1.403 (7)
C1—C2	1.369 (7)	C11—C12	1.380 (7)
C1—C3	1.490 (6)	C11—H11	0.9500
C3—C8	1.399 (7)	C12—C13	1.399 (7)
C3—C4	1.404 (7)	C13—C14	1.384 (7)
C4—C5	1.390 (7)	C13—H13	0.9500
C4—H4	0.9500	C14—H14	0.9500
C5—C6	1.375 (7)		
N2—N1—C1	113.8 (4)	C8—C7—H7	120.7
N1—N2—C9	112.8 (4)	C7—C8—C3	120.8 (5)
C2—C1—N1	112.9 (4)	C7—C8—H8	119.6
C2—C1—C3	123.4 (4)	C3—C8—H8	119.6
N1—C1—C3	123.6 (4)	C10—C9—C14	119.2 (4)
C1—C2—C11	123.8 (4)	C10—C9—N2	116.7 (4)
C1—C2—C12	122.9 (4)	C14—C9—N2	124.1 (5)
C11—C2—C12	113.3 (3)	C9—C10—C11	121.0 (4)
C8—C3—C4	118.7 (4)	C9—C10—C13	120.9 (4)
C8—C3—C1	121.2 (4)	C11—C10—C13	118.1 (4)
C4—C3—C1	120.1 (4)	C12—C11—C10	118.4 (5)

C5—C4—C3	120.8 (4)	C12—C11—H11	120.8
C5—C4—H4	119.6	C10—C11—H11	120.8
C3—C4—H4	119.6	C11—C12—C13	121.8 (5)
C6—C5—C4	118.6 (5)	C11—C12—C14	119.3 (4)
C6—C5—H5	120.7	C13—C12—C14	118.9 (4)
C4—C5—H5	120.7	C14—C13—C12	118.9 (4)
F1—C6—C5	118.8 (5)	C14—C13—H13	120.5
F1—C6—C7	118.7 (5)	C12—C13—H13	120.5
C5—C6—C7	122.5 (5)	C13—C14—C9	120.7 (5)
C6—C7—C8	118.7 (5)	C13—C14—H14	119.6
C6—C7—H7	120.7	C9—C14—H14	119.6
C1—N1—N2—C9	179.1 (4)	C6—C7—C8—C3	-0.8 (7)
N2—N1—C1—C2	-179.2 (4)	C4—C3—C8—C7	0.9 (7)
N2—N1—C1—C3	0.0 (7)	C1—C3—C8—C7	179.1 (4)
N1—C1—C2—C11	-178.0 (4)	N1—N2—C9—C10	168.4 (4)
C3—C1—C2—C11	2.8 (7)	N1—N2—C9—C14	-13.2 (7)
N1—C1—C2—C12	1.7 (6)	C14—C9—C10—C11	0.6 (7)
C3—C1—C2—C12	-177.6 (4)	N2—C9—C10—C11	179.1 (4)
C2—C1—C3—C8	50.4 (7)	C14—C9—C10—C13	180.0 (4)
N1—C1—C3—C8	-128.7 (5)	N2—C9—C10—C13	-1.6 (6)
C2—C1—C3—C4	-131.3 (5)	C9—C10—C11—C12	-0.2 (7)
N1—C1—C3—C4	49.5 (6)	C13—C10—C11—C12	-179.6 (4)
C8—C3—C4—C5	-0.9 (7)	C10—C11—C12—C13	-0.1 (7)
C1—C3—C4—C5	-179.2 (4)	C10—C11—C12—C14	179.5 (4)
C3—C4—C5—C6	1.0 (7)	C11—C12—C13—C14	0.1 (7)
C4—C5—C6—F1	179.7 (4)	C14—C12—C13—C14	-179.6 (4)
C4—C5—C6—C7	-0.9 (7)	C12—C13—C14—C9	0.3 (7)
F1—C6—C7—C8	-179.8 (4)	C10—C9—C14—C13	-0.7 (7)
C5—C6—C7—C8	0.9 (7)	N2—C9—C14—C13	-179.0 (4)

Hydrogen-bond geometry (\AA , $^\circ$)

Cg2 is the centroid of the C9—C14 2,4-dichlorophenyl ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C4—H4...N2 ⁱ	0.95	2.53	3.265 (6)	134
C12—C14...Cg2 ⁱⁱ	1.74 (1)	3.92 (1)	3.569 (6)	66 (1)

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