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, C14H7Cl4FN2, the dihedral angle between the 4-fluorophenyl ring and the 2,4-dichlorophenyl ring is 46.03 (19)°. In the crystal, the molecules are linked by C—H···Cl interactions along the a-axis direction, forming a C(6) chain. The molecules are further connected by C—Cl···π interactions and face-to-face π···π stacking interactions, forming ribbons along the a-axis direction. Hirshfeld surface analysis indicates that the greatest contributions to the crystal packing are from Cl···H···Cl (35.1%), H···H (10.6%), C···C (9.7%), Cl···Cl (9.4%) and C···H/H···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., 2017a,b; Mahmoudi et al., 2018a,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., 2020a,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)°. The N2/N1/C1/C2/C11/C12 moiety is approximately planar, with a maximum deviation of 0.029 (1) Å for Cl1, and makes dihedral angles of 50.53 (18)° and 11.75 (18)° 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)°.

### 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⋯Cg1′ = 3.873 (3) Å, slippage = 1.831 Å; Cg2⋯Cg2′ = 3.872 (3) Å, slippage = 1.554 Å; symmetry codes: (i) *x* − 1, *y*, *z*; (ii) *x* + 1, *y*, *z*] 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 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

|       | *D*—H⋯A | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
|-------|---------|-------|-------|---------|-----------|
| C4—H4⋯N2′ | 0.95    | 2.53  | 3.265 (5) | 134     |
| C12—Cl4⋯Cg2ii | 1.735 (5) | 3.920 (3) | 3.569 (6) | 66.51 (18) |

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

### Table 1

Hydrogen-bond geometry (Å, °).

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

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**Figure 1**

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

**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.
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).

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

| Contact  | Distance | Symmetry operation |
|----------|----------|--------------------|
| C1⋯H11  | 3.06     | –1 + x, 1 + y, z   |
| H4⋯N2   | 2.53     | –1 + x, y, z       |
| C1⋯F1   | 3.016 (3) | –1 – x, ½ + y, 1 – z |
| H5⋯H7   | 2.55     | –x, –½ + y, 1 – z  |
| C4⋯H13  | 2.95     | 2 – x, ½ + y, 2 – z |
| C4⋯H14  | 2.93     | 1 – x, ½ + y, 2 – z |
| C3⋯F1   | 3.116 (3) | –x, –½ + y, 1 – z  |

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 dnorm 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 energy in the range –0.0500 to 0.0500 a.u. using the STO-3 G 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.
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. 7b). The secondary important H···H and C···C interactions contribute 10.6% (Fig. 7c) and 9.7% (Fig. 7d), respectively, to the Hirshfeld surface. The remaining contributions for the title compound are from Cl···Cl, C···H/H···Cl, 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-dichloro-1-phenylethyl)-2-phenylidazene 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; Atioglu et al., 2019), HODQAV (IV; Shikhaliyev et al., 2019), HONBUK (V; Akkurt et al., 2019), HONBOE (VI; Akkurt et al., 2019), DULTAI (VII; Özkaraça et al., 2020b), GUPHIL (VIII; Özkaraça et al., 2020a) 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.

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                     |

Figure 7 (a) All···All  (b) Cl···H/H···Cl  (c) H···H  (d) C···C  (e) Cl···Cl  (f) C···H/H···C
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.

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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), \( (E)-1-(2,4\text{-dichlorophenyl})-2-(4\text{-fluorobenzylidene})\text{hydrazine} \) (283 mg, 1 mmol), tetramethylethlenediamine (TMEDA) (295 mg, 2.5 mmol), CuCl (2 mg, 0.02 mmol) and CCl\(_4\) (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 Na\(_2\)SO\(_4\) 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. Suitable crystals for X-ray analysis were obtained by slow evaporation of an ethanol solution. Colourless solid (44%); m.p. 345 K.

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 \( U_{iso}(H) = 1.2U_{eq}(C) \). Five outliers \( 2 2 2, 2 2 2 \), \( 1 1 3, 2 2 1 \) and \( 2 2 1 \) 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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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: Marcdd (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_{7}Cl_{4}FN_{2}  
M_r = 364.02
Monoclinic, P2_1
a = 3.8720 (8) Å
b = 10.434 (2) Å
c = 18.138 (4) Å
β = 95.03 (3)°
V = 730.0 (3) Å³
Z = 2

F(000) = 364  
D_x = 1.656 Mg m⁻³

Synchrotron radiation, λ = 0.79475 Å

Cell parameters from 600 reflections
θ = 2.8–28.0°
µ = 1.12 mm⁻¹
T = 100 K
Prism, colourless
0.20 × 0.15 × 0.10 mm

Data collection

Rayonix SX165 CCD
diffractometer

/i 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 > 2σ(I)

θ_max = 31.0°, θ_min = 2.5°
h = −5→5
k = −12→13
l = −23→23

Refinement

Refinement on F²
Least-squares matrix: full
R[F² > 2σ(F²)] = 0.036
wR(F²) = 0.106
S = 1.09

3120 reflections
191 parameters
1 restraint

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

w = 1/[σ(F²) + (0.0549P)² + 0.7552P]

where P = (F_c² + 2F_s²)/3

(Δ/σ)_{max} < 0.001
Δρ_{max} = 0.61 e Å⁻³
Δρ_{min} = −0.30 e Å⁻³
Extinction correction: SHELXL,
$F_c^o = k F_c [1 + 0.001 x F_c^2 / \sin(2 \theta)]^{1/4}$
Extinction coefficient: 0.044 (8)

Absolute structure: Flack $x$ determined using
1318 quotients $[I^+ - I^-] / [I^+ + I^-]$ (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 ($\text{Å}^2$)

| Atom | x     | y     | z     | $U_{eq}$/$U_{eq}$ |
|------|-------|-------|-------|-------------------|
| 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) |
| C5   | 0.3391 (13) | 0.4726 (5) | 0.5540 (3) | 0.0288 (10) |
| C6   | 0.455606 (10) | 0.394787 | 0.540530 | 0.035 (6) |
| C7   | -0.2292 (13) | 0.5531 (5) | 0.5008 (3) | 0.0295 (10) |
| C8   | -0.0634 (12) | 0.6678 (5) | 0.5181 (3) | 0.0289 (10) |
| H7   | 0.006934 | 0.722093 | 0.480114 | 0.035 (6) |
| C9   | -0.0016 (12) | 0.7022 (5) | 0.5920 (3) | 0.0281 (9) |
| H8   | 0.114818 | 0.780287 | 0.604727 | 0.034 (6) |
| C10  | 0.3594 (11) | 0.3835 (9) | 0.8125 (2) | 0.0261 (9) |
| C11  | 0.3960 (12) | 0.2556 (5) | 0.7935 (3) | 0.0265 (9) |
| H11  | 0.5577 (13) | 0.1679 (5) | 0.8440 (3) | 0.0275 (9) |
| C12  | 0.581566 | 0.080365 | 0.830976 | 0.033 (6) |
| C13  | 0.6813 (13) | 0.2120 (5) | 0.9131 (3) | 0.0291 (10) |
| C14  | 0.6495 (12) | 0.3405 (5) | 0.9334 (3) | 0.0289 (10) |
| C15  | 0.736480 | 0.368972 | 0.981195 | 0.035 (6) |
| C16  | 0.4893 (13) | 0.4255 (5) | 0.8827 (3) | 0.0300 (10) |
| H14  | 0.467401 | 0.513039 | 0.895888 | 0.036 (6) |

Atomic displacement parameters ($\text{Å}^2$)

|     | 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) |

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### Geometric parameters (Å, °)

|        |        |        |        |        |        |        |
|--------|--------|--------|--------|--------|--------|--------|
| C1     | C2     | C5     | H5     | 0.9500 |        |        |
| C12    | C2     | C6     | C7     | 1.381  | 7      |
| C13    | C10    | C7     | C8     | 1.388  | 7      |
| C14    | C12    | C7     | H7     | 0.9500 |        |        |
| F1     | C6     | C8     | H8     | 0.9500 |        |        |
| N1     | N2     | C9     | C10    | 1.393  | 7      |
| N1     | C1     | C9     | C14    | 1.398  | 7      |
| N2     | C9     | C1     | C10    | 1.403  | 7      |
| C1     | C2     | C11    | C12    | 1.380  | 7      |
| C1     | C3     | C11    | H11    | 0.9500 |        |        |
| C3     | C8     | C12    | C13    | 1.399  | 7      |
| C3     | C4     | C13    | C14    | 1.384  | 7      |
| C4     | C5     | C13    | H13    | 0.9500 |        |        |
| C4     | H4     | 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—C1| 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—Cl4 119.3 (4)
C6—C5—H5 120.7 C13—C12—Cl4 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 179.2 (4)
N1—C1—C2—Cl1 −178.0 (4) N1—N2—C9—C10 168.4 (4)
C3—C1—C2—Cl1 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—Cl3 180.0 (4)
N1—C1—C3—C8 −128.7 (5) N2—C9—C10—Cl3 −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—Cl4 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 (Å, °)
Cg2 is the centroid of the C9–C14 2,4-dichlorophenyl ring.

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| C4—H4···N2i | 0.95 | 2.53 | 3.265 (6) | 134 |
| C12—Cl4···Cg2ii | 1.74 (1) | 3.92 (1) | 3.569 (6) | 66 (1) |

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