Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS
ISSN 2056-9890

Crystal structure and Hirshfeld surface analysis of (*E*)-2,4-di-*tert*-butyl-6-[(3-chloro-4-methylphenylimino)methyl]phenol

Sevgi Kansiz,[a] Mustafa Macit,[b] Necmi Dege[a] and Vadim A. Pavlenko[c]*

[a]Ondokuz Mayıs University, Faculty of Arts and Sciences, Department of Physics, 55139, Kurupelit, Samsun, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs, University, 55139, Samsun, Turkey, and [c]Taras Shevchenko National University of Kyiv, Department of Chemistry, Volodymyrska Str., 64, 01601 Kiev, Ukraine. *Correspondence e-mail: pavlenko_vadim@univ.kiev.ua

Received 24 October 2018
Accepted 18 November 2018

Edited by D.-J. Xu, Zhejiang University (Yuquan Campus), China

Keywords: crystal structure; Schiff bases; 3-chloro-4-methylphenylimino; Hirshfeld surface.

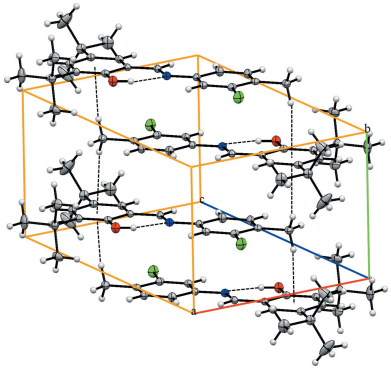
CCDC reference: 1873612

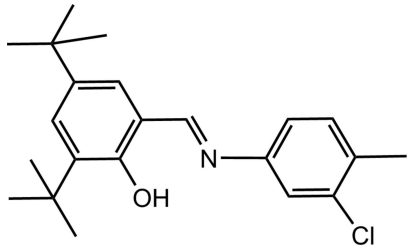
Supporting information: this article has supporting information at journals.iucr.org/e

The title Schiff base compound, $C_{22}H_{28}ClNO$, shows mirror symmetry with all its non-H atoms, except the *tert*-butyl groups, located on the mirror plane. There is an intramolecular O—H···N hydrogen bond present forming an *S*(6) ring motif. In the crystal, the molecules are connected by C—H···π interactions, generating a three-dimensional supramolecular structure. Hirshfeld surface analysis and two dimensional fingerprint plots were used to analyse the intermolecular interactions present in the crystal, indicating that the most important contributions for the crystal packing are from H···H (68.9%) and C···H/H···C (11.7%) interactions.

1. Chemical context

In coordination chemistry, Schiff bases have found wide use as ligands (Calligaris *et al.*, 1972; Hökelek *et al.*, 2004; Moroz *et al.*, 2012; Kansiz *et al.*, 2018). Schiff bases are important for various areas of chemistry and biochemistry because of their biological activity (El-masry *et al.*, 2000) and photochromic properties and have applications in various fields such as the measurement and control of radiation intensities in imaging systems and optical computers (Elmalı *et al.*, 1999), electronics, optoelectronics and photonics (Iwan *et al.*, 2007). They have been used as starting materials in the synthesis of many important medicinal substances. In the present study, a new Schiff base compound was synthesized and its crystal structure determined by X-ray diffraction. In addition, to understand the intermolecular interactions in the crystal structure, Hirshfeld surface analysis was performed.





2. Structural commentary

The molecular structure of the title compound is illustrated in Fig. 1. The title Schiff base compound shows mirror symmetry with all the non-H atoms, except the *tert*-butyl groups, located

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

Cg is the centroid of the C9–C14 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.84	2.582 (3)	149
C1—H1*B*···*Cg*1^{i}	0.96	2.77	3.5072 (4)	134

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

on the mirror plane. The C14—O1 bond distance is 1.349 (3) Å, the C8═N1 and C5—N1 bond lengths are 1.278 (4) and 1.412 (4) Å, respectively, and the C7—Cl1 bond distance is 1.744 (3) Å. There is an intramolecular O—H···N hydrogen bond present (Table 1), forming an S(6) ring motif.

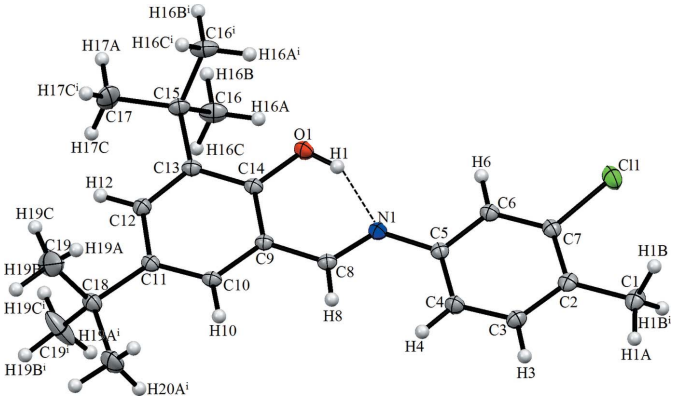


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 10% probability level. Symmetry code: (i) $x, -y+\frac{1}{2}, z$.

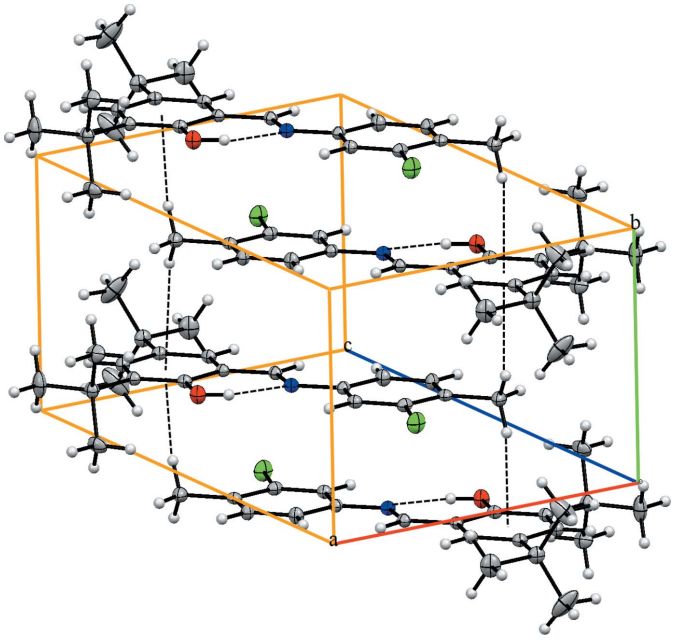


Figure 2
A view of the crystal packing of the title compound. Dashed lines denote the intramolecular and intermolecular hydrogen bonds.

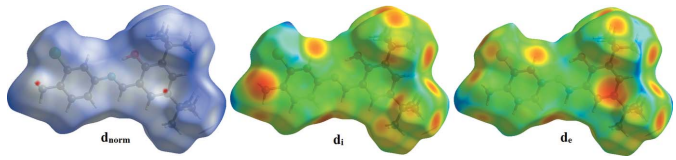


Figure 3
The Hirshfeld surface of the title compound mapped over d_{norm}, d_i and d_e.

3. Supramolecular features

In the crystal, the molecules are connected by C1—H1*B*···π interactions, generating a three-dimensional supramolecular structure (Table 1 and Fig. 2).

4. Database survey

There are no previous reports of the title structure. However, several related structure have been reported (CSD, version 5.39, update May 2018; Groom *et al.*, 2016), including bis{(*E*)-1-[(3-chloro-4-methylphenylimino)methyl]naphthalen-2-olate-*N*,*O*}copper(II) (SICXOU; Toprak *et al.*, 2018), 2-{(*E*)-[(3-chloro-4-methylphenyl)imino]methyl}-4-(trifluoromethoxy)-phenol (TERTUI; Atalay *et al.*, 2017), {2,2′-[4-chloro-5-methyl-*o*-phenylenebis(nitrilomethylidyne)]diphenolato}nickel(II) (WABDEK; Wang, 2010) and 4-[(*E*)-(3-chloro-4-methylphenyl)iminomethyl]-2-methoxy-3-nitrophenyl acetate (GAPPOE; Su *et al.*, 2012). In all four compounds, the C—Cl bond lengths vary from 1.724 to 1.743 Å. In the title compound, the C7—Cl1 bond length is 1.744 (3) Å.

5. Hirshfeld surface analysis

The Hirshfeld surface analysis was performed using *CrystalExplorer* (Turner *et al.*, 2017). The Hirshfeld surfaces and their associated two-dimensional fingerprint plots were used to quantify the various intermolecular interactions in the synthesized complex. The Hirshfeld surfaces mapped over d_{norm}, d_e and d_i are illustrated in Figs. 3 and 4. The red spots on

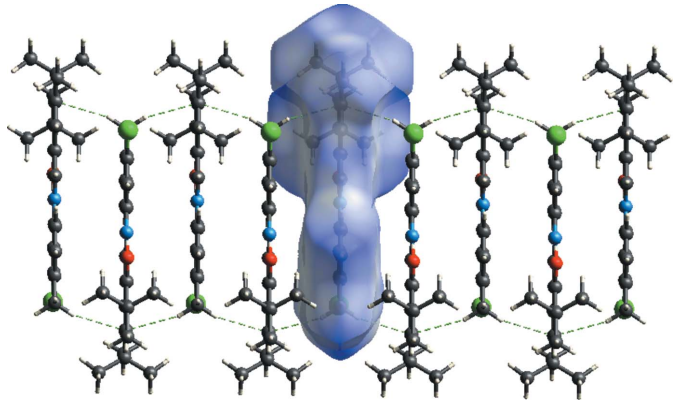


Figure 4
Hirshfeld surface mapped over d_{norm} for visualizing the intermolecular interactions of the title compound.

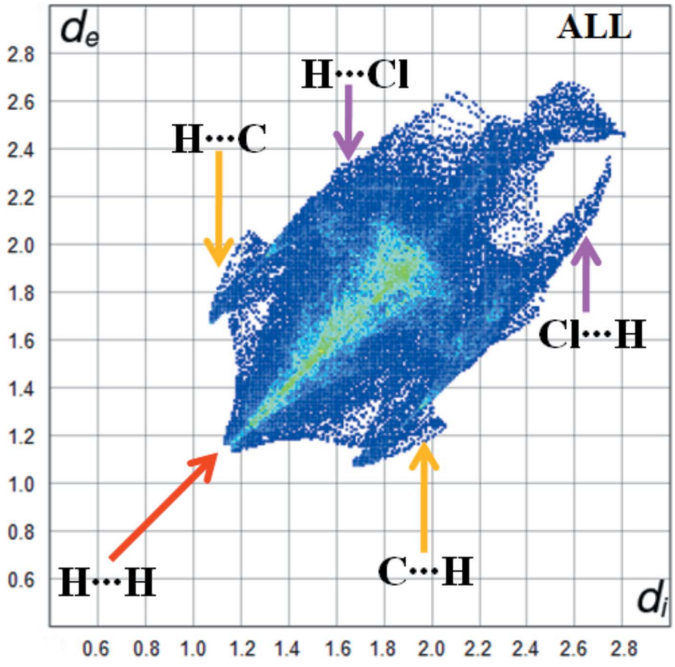


Figure 5
Overall fingerprint plot for the title compound.

the surfaces indicate the intermolecular contacts involved in strong hydrogen bonds and interatomic contacts (Şen *et al.*, 2017; Kansız & Dege, 2018; Sen *et al.*, 2018; Gumus *et al.*, 2018). The Hirshfeld surfaces were calculated using a standard (high) surface resolution with the three-dimensional d_{norm} surfaces mapped over a fixed colour scale of −0.031 (red) to 2.139 (blue) a.u. The red spots identified in Fig. 3 correspond to the near-type H···π contacts resulting from the C—H···π interactions (Table 1).

Fig. 5 shows the two-dimensional fingerprint of the sum of the contacts contributing to the Hirshfeld surface represented in normal mode. The graph shown in Fig. 6(*a*) (H···H) shows the two-dimensional fingerprint of the (d_i, d_e) points associated with hydrogen atoms. It is characterized by an end point that points to the origin and corresponds to $d_i = d_e = 1.08$ Å, which indicates the presence of the H···H contacts in this study (68.9%). The graph shown in Fig. 6(*b*) shows the (C···H/H···C) contacts between the carbon atoms inside the surface and the hydrogen atoms outside the Hirshfeld surface and *vice versa*, which contribute 11.7%. There are two symmetrical wings on the left and right sides. Furthermore, there are also Cl···H/H···Cl (11%), C···C (4.5%), C···N/N···C (2.2%), O···H/H···O (1.3%) and N···H/H···N (0.4%) contacts.

A view of the three-dimensional Hirshfeld surface of the title compound plotted over electrostatic potential energy in the range −0.030 to 0.044 a.u. using the STO-3G basis set at the Hartree–Fock level of theory is shown in Fig. 7 where the C—H···π donors and acceptors are shown as blue and red areas around the atoms related with positive (hydrogen-bond donors) and negative (hydrogen-bond acceptors) electrostatic potentials, respectively.

6. Synthesis and crystallization

The title compound was prepared by refluxing a mixture of a solution containing 3,5-di-*tert*-butyl-2-hydroxybenzaldehyde (46.8 mg, 0.2 mmol) in ethanol (30 mL) and a solution containing 3-chloro-4-methylaniline (28.32 mg, 0.2 mmol) in ethanol (20 mL). The reaction mixture was stirred for 4 h under reflux. Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (m.p. 417–419 K; yield 84%).

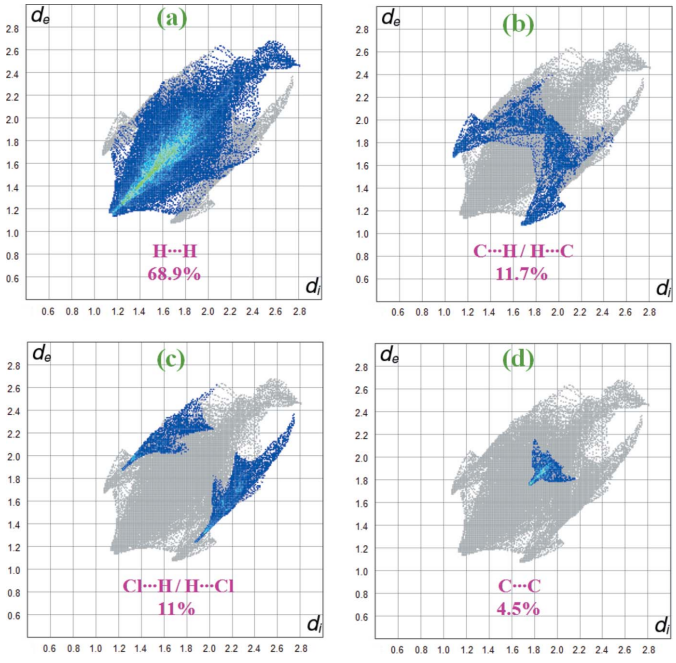


Figure 6
Two-dimensional fingerprint plots with a d_{norm} view of the (*a*) H···H (68.9%), (*b*) C···H/H···C (11.7%), (*c*) Cl···H/H···Cl (11%) and (*d*) C···C (4.5%) contacts in the title compound.

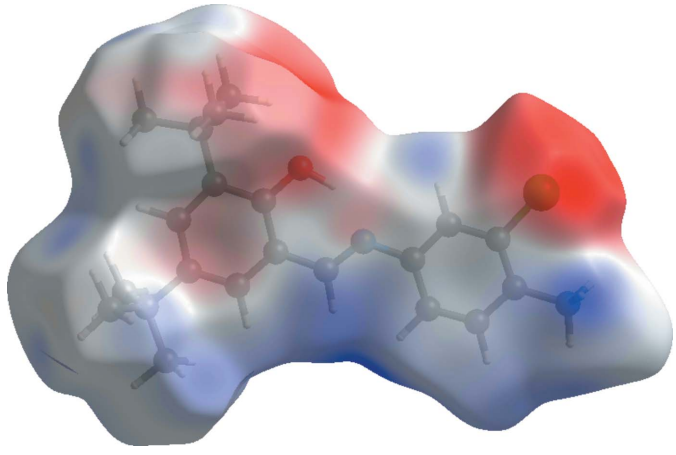


Figure 7
A view of the three-dimensional Hirshfeld surface of the title compound plotted over electrostatic potential energy.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{28}ClNO$
M_r	357.90
Crystal system, space group	Monoclinic, $P2_1/m$
Temperature (K)	296
a, b, c (Å)	9.6753 (10), 7.0072 (6), 15.3749 (13)
β (°)	93.425 (7)
V (Å^3)	1040.51 (17)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.19
Crystal size (mm)	0.74 × 0.65 × 0.48
Data collection	
Diffractometer	Stoe IPDS 2
Absorption correction	Integration (*X-RED32*; Stoe & Cie, 2002)
T_{min}, T_{max}	0.879, 0.940
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5895, 2300, 1298
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.628
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.168, 1.00
No. of reflections	2300
No. of parameters	145
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.22

Computer programs: *X-AREA* and *X-RED* (Stoe & Cie, 2002), *SHELXLXT* (Sheldrick, 2015*a*), *SHELXL2017/1* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were positioned geometrically with C—H distances of 0.93–0.97 Å and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Acknowledgements

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS 2 diffractometer (purchased under grant F.279 of the University Research Fund).

References

Atalay, Ş., Gerçeker, S., Meral, S. & Bülbül, H. (2017). *IUCrData*, **2**, x171725.
Calligaris, M., Nardin, G. M. J. & Randaccio, C. (1972). *Coord. Chem. Rev.* **7**, 385–403.
Elmalı, A., Kabak, M., Kavlakoğlu, E. & Elerman, Y. (1999). *J. Mol. Struct.* **510**, 207–214.
El-masry, A. H., Fahmy, H. H. & Ali Abdelwahed, S. (2000). *Molecules*, **5**, 1429–1438.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Gumus, M. K., Kansiz, S., Dege, N. & Kalibabchuk, V. A. (2018). *Acta Cryst.* E**74**, 1211–1214.
Hökelek, T., Bilge, S., Demiriz, Ş., Özgüç, B. & Kılıç, Z. (2004). *Acta Cryst.* C**60**, o803–o805.
Iwan, A., Kaczmarczyk, B., Janeczek, H., Sek, D. & Ostrowski, S. (2007). *Spectrochim. Acta A Mol. Biomol. Spectrosc.* **66**, 1030–1041.
Kansız, S. & Dege, N. (2018). *J. Mol. Struct.* **1173**, 42–51.
Kansiz, S., Macit, M., Dege, N. & Tsapyuk, G. G. (2018). *Acta Cryst.* E**74**, 1513–1516.
Moroz, Y. S., Demeshko, S., Haukka, M., Mokhir, A., Mitra, U., Stocker, M., Müller, P., Meyer, F. & Fritsky, I. O. (2012). *Inorg. Chem.* **51**, 7445–7447.
Sen, P., Kansiz, S., Golenya, I. A. & Dege, N. (2018). *Acta Cryst.* E**74**, 1147–1150.
Şen, F., Kansiz, S. & Uçar, İ. (2017). *Acta Cryst.* C**73**, 517–524.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Stoe & Cie (2002). *X-AREA* and *X-RED32*. Stoe & Cie GmbH, Darmstadt, Germany.
Su, D.-C., Wang, F.-T., Mao, C.-G. & Qian, S.-S. (2012). *Acta Cryst.* E**68**, o303.
Toprak, Ş., Tanak, H., Macit, M., Dege, N. & Orbay, M. (2018). *J. Mol. Struct.* **1174**, 184–191.
Turner, M. J., MacKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17.5*. University of Western Australia, Perth.
Wang, H. (2010). *Acta Cryst.* E**66**, m1571.

supporting information

Acta Cryst. (2018). E**74**, 1887-1890 [https://doi.org/10.1107/S2056989018016377]

Crystal structure and Hirshfeld surface analysis of (*E*)-2,4-di-*tert*-butyl-6-[(3-chloro-4-methylphenylimino)methyl]phenol

Sevgi Kansiz, Mustafa Macit, Necmi Dege and Vadim A. Pavlenko

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXLXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2017/1* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

(*E*)-2,4-di-*tert*-butyl-6-[(3-chloro-4-methylphenylimino)methyl]phenol

Crystal data

$C_{22}H_{28}ClNO$
$M_r = 357.90$
Monoclinic, $P2_1/m$
$a = 9.6753$ (10) Å
$b = 7.0072$ (6) Å
$c = 15.3749$ (13) Å
$\beta = 93.425$ (7)°
$V = 1040.51$ (17) Å^3
$Z = 2$
$F(000) = 384$
$D_x = 1.142$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5548 reflections
$\theta = 2.1$–30.7°
$\mu = 0.19$ mm^{-1}
$T = 296$ K
Prism, orange
0.74 × 0.65 × 0.48 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)
$T_{min} = 0.879$, $T_{max} = 0.940$
5895 measured reflections
2300 independent reflections
1298 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 26.5$°, $\theta_{min} = 2.1$°
$h = -12 \rightarrow 12$
$k = -8 \rightarrow 8$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.168$
$S = 1.00$
2300 reflections
145 parameters
0 restraints
Hydrogen site location: mixed
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0964P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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	0.2129 (4)	0.250000	0.2502 (2)	0.0799 (9)
H1A	0.122313	0.250000	0.272431	0.120*
H1B	0.223846	0.361862	0.215178	0.120*
C2	0.3181 (3)	0.250000	0.3253 (2)	0.0633 (8)
C3	0.2795 (3)	0.250000	0.4107 (2)	0.0703 (9)
H3	0.185649	0.250000	0.420637	0.084*
C4	0.3723 (3)	0.250000	0.4806 (2)	0.0700 (9)
H4	0.340566	0.250000	0.536544	0.084*
C5	0.5133 (3)	0.250000	0.46997 (18)	0.0556 (7)
C6	0.5560 (3)	0.250000	0.38600 (19)	0.0600 (7)
H6	0.649961	0.250000	0.376348	0.072*
C7	0.4596 (3)	0.250000	0.3165 (2)	0.0639 (8)
C8	0.5942 (3)	0.250000	0.61807 (19)	0.0568 (7)
H8	0.502444	0.250000	0.632881	0.068*
C9	0.7006 (3)	0.250000	0.68668 (18)	0.0521 (7)
C10	0.6637 (3)	0.250000	0.77307 (19)	0.0566 (7)
H10	0.570247	0.250000	0.784241	0.068*
C11	0.7595 (3)	0.250000	0.84146 (18)	0.0571 (7)
C12	0.8995 (3)	0.250000	0.82148 (19)	0.0620 (8)
H12	0.966318	0.250000	0.867572	0.074*
C13	0.9445 (3)	0.250000	0.7374 (2)	0.0590 (7)
C14	0.8423 (3)	0.250000	0.66939 (18)	0.0551 (7)
C15	1.0991 (3)	0.250000	0.7198 (2)	0.0722 (9)
C16	1.1330 (2)	0.0710 (4)	0.6677 (2)	0.0980 (10)
H16A	1.076649	0.068596	0.614163	0.147*
H16B	1.228999	0.073060	0.655013	0.147*
H16C	1.114737	−0.040681	0.701290	0.147*
C17	1.1899 (4)	0.250000	0.8041 (3)	0.1274 (18)
H17A	1.285592	0.250000	0.790824	0.191*
H17C	1.170713	0.138138	0.837395	0.191*
C18	0.7224 (3)	0.250000	0.9368 (2)	0.0753 (9)
C19	0.7730 (5)	0.4303 (8)	0.9793 (2)	0.176 (2)
H19A	0.734855	0.537623	0.947277	0.264*
H19B	0.744536	0.434730	1.037976	0.264*
H19C	0.872234	0.434730	0.979833	0.264*
C20	0.5646 (4)	0.250000	0.9437 (3)	0.1131 (15)
H20A	0.525969	0.136290	0.917256	0.170*
H20B	0.543785	0.250000	1.003968	0.170*
Cl1	0.52181 (11)	0.250000	0.21237 (6)	0.1032 (4)

N1	0.6191 (2)	0.250000	0.53735 (15)	0.0599 (6)
O1	0.8791 (2)	0.250000	0.58613 (13)	0.0748 (6)
H1	0.809294	0.250000	0.553116	0.112*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.088 (2)	0.066 (2)	0.083 (2)	0.000	−0.0157 (18)	0.000
C2	0.0734 (18)	0.0410 (17)	0.0749 (19)	0.000	−0.0011 (15)	0.000
C3	0.0559 (16)	0.077 (2)	0.077 (2)	0.000	0.0003 (16)	0.000
C4	0.0621 (17)	0.086 (2)	0.0633 (18)	0.000	0.0113 (15)	0.000
C5	0.0611 (16)	0.0480 (17)	0.0576 (16)	0.000	0.0032 (13)	0.000
C6	0.0630 (16)	0.0543 (18)	0.0631 (17)	0.000	0.0085 (14)	0.000
C7	0.0786 (19)	0.0547 (19)	0.0587 (16)	0.000	0.0068 (15)	0.000
C8	0.0531 (14)	0.0530 (18)	0.0649 (17)	0.000	0.0079 (13)	0.000
C9	0.0527 (14)	0.0458 (16)	0.0582 (15)	0.000	0.0074 (13)	0.000
C10	0.0546 (15)	0.0551 (18)	0.0616 (16)	0.000	0.0165 (14)	0.000
C11	0.0642 (16)	0.0530 (18)	0.0550 (15)	0.000	0.0112 (14)	0.000
C12	0.0595 (16)	0.065 (2)	0.0611 (17)	0.000	0.0016 (13)	0.000
C13	0.0554 (15)	0.0556 (18)	0.0669 (17)	0.000	0.0113 (14)	0.000
C14	0.0574 (15)	0.0524 (17)	0.0566 (16)	0.000	0.0128 (13)	0.000
C15	0.0519 (16)	0.082 (2)	0.083 (2)	0.000	0.0124 (15)	0.000
C16	0.0684 (14)	0.090 (2)	0.139 (2)	0.0156 (13)	0.0353 (16)	−0.0004 (17)
C17	0.0520 (18)	0.219 (6)	0.110 (3)	0.000	−0.002 (2)	0.000
C18	0.079 (2)	0.091 (3)	0.0563 (17)	0.000	0.0149 (16)	0.000
C19	0.204 (4)	0.235 (5)	0.095 (2)	−0.106 (4)	0.061 (3)	−0.087 (3)
C20	0.102 (3)	0.168 (4)	0.073 (2)	0.000	0.036 (2)	0.000
Cl1	0.1117 (8)	0.1390 (10)	0.0595 (5)	0.000	0.0104 (5)	0.000
N1	0.0608 (13)	0.0617 (16)	0.0578 (14)	0.000	0.0075 (11)	0.000
O1	0.0613 (11)	0.1072 (18)	0.0574 (12)	0.000	0.0166 (10)	0.000

Geometric parameters (Å, º)

C1—C2	1.494 (5)	C12—C13	1.389 (4)
C1—H1A	0.9600	C12—H12	0.9300
C1—H1B	0.9600	C13—C14	1.395 (4)
C1—H1B^{i}	0.9600	C13—C15	1.536 (4)
C2—C7	1.383 (4)	C14—O1	1.349 (3)
C2—C3	1.387 (4)	C15—C17	1.523 (5)
C3—C4	1.359 (4)	C15—C16	1.534 (3)
C3—H3	0.9300	C15—C16^{i}	1.534 (3)
C4—C5	1.383 (4)	C16—H16A	0.9600
C4—H4	0.9300	C16—H16B	0.9600
C5—C6	1.379 (4)	C16—H16C	0.9600
C5—N1	1.412 (4)	C17—H17A	0.9600
C6—C7	1.376 (4)	C17—H17C	0.9600
C6—H6	0.9300	C17—H17C^{i}	0.9600
C7—Cl1	1.744 (3)	C18—C19^{i}	1.491 (4)

C8—N1	1.278 (4)	C18—C19	1.491 (4)
C8—C9	1.429 (4)	C18—C20	1.537 (5)
C8—H8	0.9300	C19—H19A	0.9600
C9—C10	1.396 (4)	C19—H19B	0.9600
C9—C14	1.412 (3)	C19—H19C	0.9600
C10—C11	1.360 (4)	C20—H20A	0.9600
C10—H10	0.9300	C20—H20B	0.9595
C11—C12	1.407 (4)	C20—H20A^{i}	0.9600
C11—C18	1.530 (4)	O1—H1	0.8200

C2—C1—H1A	108.6	O1—C14—C13	119.7 (2)
C2—C1—H1B	109.9	O1—C14—C9	119.5 (3)
H1A—C1—H1B	109.5	C13—C14—C9	120.8 (2)
C2—C1—H1B^{i}	109.91 (9)	C17—C15—C16	108.31 (19)
H1A—C1—H1B^{i}	109.5	C17—C15—C16^{i}	108.3 (2)
H1B—C1—H1B^{i}	109.5	C16—C15—C16^{i}	109.7 (3)
C7—C2—C3	114.6 (3)	C17—C15—C13	111.6 (3)
C7—C2—C1	123.8 (3)	C16—C15—C13	109.45 (18)
C3—C2—C1	121.5 (3)	C16^{i}—C15—C13	109.45 (18)
C4—C3—C2	123.1 (3)	C15—C16—H16A	109.5
C4—C3—H3	118.4	C15—C16—H16B	109.5
C2—C3—H3	118.4	H16A—C16—H16B	109.5
C3—C4—C5	121.1 (3)	C15—C16—H16C	109.5
C3—C4—H4	119.5	H16A—C16—H16C	109.5
C5—C4—H4	119.5	H16B—C16—H16C	109.5
C6—C5—C4	117.6 (3)	C15—C17—H17A	109.4
C6—C5—N1	116.2 (2)	C15—C17—H17C	109.5
C4—C5—N1	126.1 (2)	H17A—C17—H17C	109.5
C7—C6—C5	120.0 (3)	C15—C17—H17C^{i}	109.48 (8)
C7—C6—H6	120.0	H17A—C17—H17C^{i}	109.5
C5—C6—H6	120.0	H17C—C17—H17C^{i}	109.5
C6—C7—C2	123.6 (3)	C19^{i}—C18—C19	115.8 (5)
C6—C7—Cl1	117.2 (2)	C19^{i}—C18—C11	109.23 (18)
C2—C7—Cl1	119.2 (3)	C19—C18—C11	109.23 (18)
N1—C8—C9	123.2 (2)	C19^{i}—C18—C20	105.8 (2)
N1—C8—H8	118.4	C19—C18—C20	105.8 (2)
C9—C8—H8	118.4	C11—C18—C20	110.9 (3)
C10—C9—C14	119.1 (3)	C18—C19—H19A	109.5
C10—C9—C8	119.2 (2)	C18—C19—H19B	109.5
C14—C9—C8	121.7 (2)	H19A—C19—H19B	109.5
C11—C10—C9	122.3 (2)	C18—C19—H19C	109.5
C11—C10—H10	118.9	H19A—C19—H19C	109.5
C9—C10—H10	118.9	H19B—C19—H19C	109.5
C10—C11—C12	116.9 (2)	C18—C20—H20A	109.5
C10—C11—C18	123.5 (2)	C18—C20—H20B	109.4
C12—C11—C18	119.6 (3)	H20A—C20—H20B	108.1
C13—C12—C11	124.2 (3)	C18—C20—H20A^{i}	109.49 (9)
C13—C12—H12	117.9	H20A—C20—H20A^{i}	112.2

C11—C12—H12	117.9	H20B—C20—H20A^{i}	108.1
C12—C13—C14	116.8 (2)	C8—N1—C5	122.8 (2)
C12—C13—C15	121.8 (3)	C14—O1—H1	109.5
C14—C13—C15	121.5 (3)		
C7—C2—C3—C4	0.000 (1)	C12—C13—C14—O1	180.000 (1)
C1—C2—C3—C4	180.000 (1)	C15—C13—C14—O1	0.000 (1)
C2—C3—C4—C5	0.000 (1)	C12—C13—C14—C9	0.000 (1)
C3—C4—C5—C6	0.000 (1)	C15—C13—C14—C9	180.000 (1)
C3—C4—C5—N1	180.000 (1)	C10—C9—C14—O1	180.000 (1)
C4—C5—C6—C7	0.000 (1)	C8—C9—C14—O1	0.000 (1)
N1—C5—C6—C7	180.000 (1)	C10—C9—C14—C13	0.000 (1)
C5—C6—C7—C2	0.000 (1)	C8—C9—C14—C13	180.000 (1)
C5—C6—C7—Cl1	180.000 (1)	C12—C13—C15—C17	0.000 (1)
C3—C2—C7—C6	0.000 (1)	C14—C13—C15—C17	180.000 (1)
C1—C2—C7—C6	180.000 (1)	C12—C13—C15—C16	119.9 (2)
C3—C2—C7—Cl1	180.000 (1)	C14—C13—C15—C16	−60.1 (2)
C1—C2—C7—Cl1	0.000 (1)	C12—C13—C15—C16^{i}	−119.9 (2)
N1—C8—C9—C10	180.000 (1)	C14—C13—C15—C16^{i}	60.1 (2)
N1—C8—C9—C14	0.000 (1)	C10—C11—C18—C19^{i}	116.2 (3)
C14—C9—C10—C11	0.000 (1)	C12—C11—C18—C19^{i}	−63.8 (3)
C8—C9—C10—C11	180.000 (1)	C10—C11—C18—C19	−116.2 (3)
C9—C10—C11—C12	0.000 (1)	C12—C11—C18—C19	63.8 (3)
C9—C10—C11—C18	180.000 (1)	C10—C11—C18—C20	0.000 (2)
C10—C11—C12—C13	0.000 (2)	C12—C11—C18—C20	180.000 (1)
C18—C11—C12—C13	180.000 (1)	C9—C8—N1—C5	180.000 (1)
C11—C12—C13—C14	0.000 (1)	C6—C5—N1—C8	180.000 (1)
C11—C12—C13—C15	180.000 (1)	C4—C5—N1—C8	0.000 (1)

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

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C9–C14 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.84	2.582 (3)	149
C1—H1*B*···*Cg*1^{ii}	0.96	2.77	3.5072 (4)	134

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