

2,6-Dichloro-*N*-phenylbenzamide

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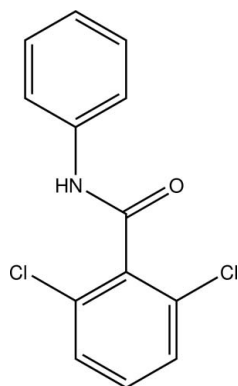
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.067; wR factor = 0.168; data-to-parameter ratio = 14.9.

There are two independent molecules in the asymmetric unit of the title compound, $\text{C}_{13}\text{H}_9\text{Cl}_2\text{NO}$, in which the dihedral angles between the phenyl and dichlorophenyl rings have significantly different values [48.5 (3) and 65.1 (3)°]. In the crystal, the molecules are linked *via* intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds into chains running parallel to the c axis.

Related literature

For the synthesis, see: Houlihan *et al.* (1981). For standard bond lengths, see: Allen *et al.* (1987). For related structures, see: Cockroft *et al.* (2007).



Experimental

Crystal data

$\text{C}_{13}\text{H}_9\text{Cl}_2\text{NO}$
 $M_r = 266.11$

Monoclinic, $P2_1/c$
 $a = 12.378$ (3) Å

$b = 11.657$ (2) Å
 $c = 17.525$ (4) Å
 $\beta = 91.43$ (3)°
 $V = 2527.9$ (9) Å³
 $Z = 8$

Mo $K\alpha$ radiation
 $\mu = 0.50$ mm⁻¹
 $T = 293$ K
 $0.30 \times 0.10 \times 0.10$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\text{min}} = 0.866$, $T_{\text{max}} = 0.952$
4807 measured reflections

4586 independent reflections
2154 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.168$
 $S = 1.00$
4586 reflections

307 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O2}^{\text{i}}$	0.86	2.09	2.927 (5)	163
$\text{N2}-\text{H2B}\cdots\text{O1}^{\text{ii}}$	0.86	1.99	2.830 (5)	165

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

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2414).

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supplementary materials

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Comment

In the title compound (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). There are two independent molecules in an asymmetric unit. The dihedral angle between phenyl (C1–C6) and dichlorophenyl (C8–C13) rings in one molecule is 48.5 (3)° compared to 65.1 (3)° in the other molecule. In the crystal structure, intermolecular N—H···O hydrogen bonds (Table 1) link the molecules into chains running parallel to the *c*-axis (Fig. 2). The structure is further stabilized by intramolecular interactions of the type C—H···O (Table 1).

Experimental

The title compound was prepared by following a reported procedure (Houlihan *et al.*, 1981). A mixture of aniline (2.8 g, 0.03 mol), 2,6-dichlorobenzoyl chloride (6.3 g, 0.03 mol), and 6 ml triethylamine in 50 ml anhydrous tetrahydrofuran was stirred and refluxed for 8 h and then allowed to stand at room temperature. The resulting solid was filtered off and washed with water (2 × 30 ml), dried over sodium sulfate (yield: 7.2 g, 90%). The title compound was purified by crystallizing from ethanol yielding crystals suitable for X-ray diffraction analysis.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and N—H = 0.86 Å and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C/N})$.

Figures

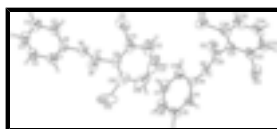


Fig. 1. The molecular structure of the title compound showing the atom-numbering scheme and displacement ellipsoids at the 30% probability level.

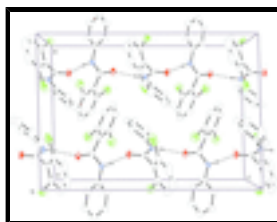


Fig. 2. A packing diagram of the title compound. The intermolecular hydrogen bonds are shown as dashed lines; H-atoms not involved in H-bonding have been excluded for clarity.

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Crystal data

C₁₃H₉Cl₂NO

$F(000) = 1088$

supplementary materials

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Hall symbol: -P 2ybc

$a = 12.378$ (3) Å

$b = 11.657$ (2) Å

$c = 17.525$ (4) Å

$\beta = 91.43$ (3)°

$V = 2527.9$ (9) Å³

$Z = 8$

$D_x = 1.398$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 9$ – 13 °

$\mu = 0.50$ mm⁻¹

$T = 293$ K

Block, colourless

$0.30 \times 0.10 \times 0.10$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

graphite

$\omega/2\theta$ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.866$, $T_{\max} = 0.952$

4807 measured reflections

4586 independent reflections

2154 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 25.3$ °, $\theta_{\min} = 1.7$ °

$h = 0$ → 14

$k = 0$ → 14

$l = -21$ → 21

3 standard reflections every 200 reflections

intensity decay: 1%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.067$

$wR(F^2) = 0.168$

$S = 1.00$

4586 reflections

307 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.070P)^2]$

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

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

$\Delta\rho_{\max} = 0.24$ e Å⁻³

$\Delta\rho_{\min} = -0.36$ e Å⁻³

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.97924 (12)	0.86429 (16)	-0.00070 (10)	0.1283 (6)
N1	1.2544 (2)	0.8856 (3)	0.00933 (17)	0.0602 (9)
H1A	1.2464	0.8846	0.0579	0.072*
O1	1.2151 (2)	0.7888 (3)	-0.10032 (14)	0.0815 (9)
C1	1.3839 (4)	0.9621 (4)	-0.0806 (3)	0.0815 (13)
H1B	1.3899	0.8905	-0.1035	0.098*
C12	1.31603 (18)	0.57910 (17)	0.01462 (10)	0.1680 (9)
C2	1.4429 (4)	1.0533 (5)	-0.1066 (3)	0.0895 (15)
H2A	1.4888	1.0421	-0.1471	0.107*
C3	1.4363 (4)	1.1573 (5)	-0.0756 (3)	0.0950 (16)
H3A	1.4769	1.2179	-0.0942	0.114*
C4	1.3676 (5)	1.1736 (4)	-0.0149 (3)	0.1019 (17)
H4A	1.3620	1.2457	0.0075	0.122*
C5	1.3076 (4)	1.0833 (4)	0.0123 (3)	0.0827 (13)
H5A	1.2615	1.0945	0.0528	0.099*
C6	1.3161 (3)	0.9770 (4)	-0.0205 (2)	0.0566 (10)
C7	1.2075 (3)	0.8004 (3)	-0.0308 (2)	0.0564 (10)
C8	1.1439 (4)	0.7168 (4)	0.0145 (2)	0.0638 (11)
C9	1.1858 (5)	0.6147 (5)	0.0379 (3)	0.1027 (19)
C10	1.1226 (9)	0.5356 (7)	0.0811 (4)	0.147 (3)
H10A	1.1506	0.4658	0.0981	0.177*
C11	1.0196 (9)	0.5681 (8)	0.0959 (5)	0.164 (5)
H11A	0.9770	0.5185	0.1238	0.197*
C12	0.9770 (6)	0.6660 (7)	0.0728 (3)	0.129 (2)
H12A	0.9061	0.6841	0.0843	0.155*
C13	1.0376 (5)	0.7408 (4)	0.0320 (2)	0.0881 (15)
C13	0.66623 (13)	0.16121 (13)	0.29111 (9)	0.1217 (6)
C14	0.69136 (12)	0.58215 (11)	0.17119 (8)	0.1060 (5)
O2	0.7863 (2)	0.4326 (3)	0.32969 (15)	0.0806 (9)
N2	0.8572 (2)	0.3470 (3)	0.22519 (16)	0.0549 (8)
H2B	0.8389	0.3164	0.1821	0.066*
C14	1.0337 (3)	0.2715 (4)	0.2072 (2)	0.0687 (11)
H14A	1.0021	0.2178	0.1743	0.082*
C15	1.1440 (4)	0.2708 (4)	0.2186 (3)	0.0863 (14)
H15A	1.1866	0.2176	0.1935	0.104*
C16	1.1907 (4)	0.3504 (5)	0.2678 (3)	0.0919 (15)
H16A	1.2651	0.3510	0.2762	0.110*
C17	1.1277 (4)	0.4273 (5)	0.3037 (3)	0.0875 (15)
H17A	1.1596	0.4807	0.3366	0.105*
C18	1.0159 (4)	0.4280 (4)	0.2922 (2)	0.0740 (12)
H18A	0.9735	0.4811	0.3174	0.089*
C19	0.9687 (3)	0.3490 (3)	0.2431 (2)	0.0562 (10)
C20	0.7758 (3)	0.3869 (3)	0.2669 (2)	0.0579 (10)
C21	0.6667 (3)	0.3711 (4)	0.2297 (2)	0.0549 (10)
C22	0.6084 (4)	0.2723 (4)	0.2402 (2)	0.0726 (12)

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C23	0.5063 (5)	0.2590 (5)	0.2082 (3)	0.0966 (17)
H23A	0.4684	0.1911	0.2154	0.116*
C24	0.4610 (4)	0.3457 (7)	0.1659 (3)	0.109 (2)
H24A	0.3915	0.3377	0.1452	0.131*
C25	0.5177 (4)	0.4442 (6)	0.1540 (3)	0.0988 (18)
H25A	0.4874	0.5027	0.1244	0.119*
C26	0.6198 (4)	0.4571 (4)	0.1857 (2)	0.0722 (12)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.1012 (11)	0.1715 (16)	0.1128 (12)	0.0422 (11)	0.0185 (9)	0.0025 (11)
N1	0.071 (2)	0.075 (2)	0.0347 (16)	-0.0089 (19)	0.0004 (15)	-0.0037 (16)
O1	0.096 (2)	0.110 (2)	0.0395 (16)	-0.0249 (19)	0.0091 (14)	-0.0131 (16)
C1	0.086 (3)	0.092 (4)	0.067 (3)	-0.003 (3)	0.011 (3)	-0.003 (3)
C12	0.227 (2)	0.1771 (17)	0.0973 (12)	0.1220 (17)	-0.0434 (12)	-0.0265 (11)
C2	0.082 (3)	0.112 (4)	0.076 (3)	-0.012 (3)	0.016 (3)	0.022 (3)
C3	0.103 (4)	0.099 (4)	0.082 (4)	-0.024 (4)	-0.009 (3)	0.028 (3)
C4	0.134 (5)	0.073 (4)	0.098 (4)	-0.017 (4)	-0.005 (4)	-0.008 (3)
C5	0.100 (4)	0.079 (3)	0.069 (3)	-0.011 (3)	0.005 (3)	-0.005 (3)
C6	0.058 (2)	0.069 (3)	0.043 (2)	-0.006 (2)	-0.0025 (19)	0.006 (2)
C7	0.065 (3)	0.064 (3)	0.041 (2)	0.000 (2)	-0.0014 (19)	-0.004 (2)
C8	0.094 (3)	0.058 (3)	0.039 (2)	-0.012 (3)	-0.001 (2)	0.000 (2)
C9	0.177 (6)	0.077 (4)	0.053 (3)	0.011 (4)	-0.020 (3)	0.000 (3)
C10	0.277 (11)	0.083 (5)	0.080 (5)	-0.002 (7)	-0.042 (6)	0.012 (4)
C11	0.269 (13)	0.133 (8)	0.091 (5)	-0.096 (9)	-0.009 (7)	0.028 (5)
C12	0.142 (6)	0.162 (7)	0.084 (4)	-0.058 (6)	0.031 (4)	-0.007 (4)
C13	0.108 (4)	0.109 (4)	0.048 (3)	-0.043 (3)	0.014 (3)	-0.002 (3)
C13	0.1448 (13)	0.1094 (11)	0.1111 (11)	-0.0318 (10)	0.0069 (9)	0.0454 (9)
C14	0.1334 (12)	0.0765 (9)	0.1080 (10)	0.0172 (8)	-0.0024 (9)	0.0099 (8)
O2	0.092 (2)	0.109 (2)	0.0412 (15)	-0.0032 (19)	0.0053 (14)	-0.0202 (16)
N2	0.056 (2)	0.067 (2)	0.0414 (17)	0.0034 (17)	-0.0032 (15)	-0.0082 (15)
C14	0.067 (3)	0.063 (3)	0.076 (3)	0.003 (2)	-0.005 (2)	-0.009 (2)
C15	0.061 (3)	0.103 (4)	0.095 (4)	0.014 (3)	0.000 (3)	-0.006 (3)
C16	0.067 (3)	0.113 (4)	0.095 (4)	0.000 (3)	-0.010 (3)	0.005 (3)
C17	0.079 (4)	0.103 (4)	0.080 (3)	-0.016 (3)	-0.023 (3)	-0.007 (3)
C18	0.072 (3)	0.081 (3)	0.069 (3)	-0.002 (3)	-0.010 (2)	-0.011 (2)
C19	0.063 (3)	0.060 (3)	0.045 (2)	-0.003 (2)	-0.0066 (19)	0.0000 (19)
C20	0.068 (3)	0.066 (3)	0.039 (2)	0.001 (2)	0.008 (2)	0.000 (2)
C21	0.055 (2)	0.068 (3)	0.042 (2)	0.007 (2)	0.0118 (18)	-0.006 (2)
C22	0.068 (3)	0.091 (4)	0.059 (3)	-0.005 (3)	0.015 (2)	-0.006 (3)
C23	0.074 (4)	0.130 (5)	0.088 (4)	-0.020 (4)	0.032 (3)	-0.027 (4)
C24	0.049 (3)	0.182 (7)	0.097 (4)	0.011 (4)	0.000 (3)	-0.047 (5)
C25	0.069 (4)	0.143 (6)	0.083 (4)	0.039 (4)	-0.008 (3)	-0.021 (4)
C26	0.066 (3)	0.088 (3)	0.062 (3)	0.021 (3)	0.006 (2)	-0.011 (3)

Geometric parameters (\AA , $^\circ$)

C11—C13	1.704 (6)	C13—C22	1.719 (5)
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N1—C7	1.341 (4)	C14—C26	1.728 (5)
N1—C6	1.418 (5)	O2—C20	1.226 (4)
N1—H1A	0.8600	N2—C20	1.343 (4)
O1—C7	1.232 (4)	N2—C19	1.409 (4)
C1—C2	1.374 (6)	N2—H2B	0.8600
C1—C6	1.374 (5)	C14—C19	1.373 (5)
C1—H1B	0.9300	C14—C15	1.375 (5)
C12—C9	1.723 (7)	C14—H14A	0.9300
C2—C3	1.331 (7)	C15—C16	1.384 (6)
C2—H2A	0.9300	C15—H15A	0.9300
C3—C4	1.393 (7)	C16—C17	1.354 (6)
C3—H3A	0.9300	C16—H16A	0.9300
C4—C5	1.380 (6)	C17—C18	1.393 (6)
C4—H4A	0.9300	C17—H17A	0.9300
C5—C6	1.371 (6)	C18—C19	1.380 (5)
C5—H5A	0.9300	C18—H18A	0.9300
C7—C8	1.494 (5)	C20—C21	1.496 (5)
C8—C9	1.358 (6)	C21—C22	1.374 (5)
C8—C13	1.387 (6)	C21—C26	1.383 (5)
C9—C10	1.437 (10)	C22—C23	1.378 (6)
C10—C11	1.361 (11)	C23—C24	1.367 (7)
C10—H10A	0.9300	C23—H23A	0.9300
C11—C12	1.317 (10)	C24—C25	1.365 (8)
C11—H11A	0.9300	C24—H24A	0.9300
C12—C13	1.365 (7)	C25—C26	1.375 (6)
C12—H12A	0.9300	C25—H25A	0.9300
C7—N1—C6	126.4 (3)	C20—N2—C19	128.2 (3)
C7—N1—H1A	116.8	C20—N2—H2B	115.9
C6—N1—H1A	116.8	C19—N2—H2B	115.9
C2—C1—C6	119.8 (5)	C19—C14—C15	121.9 (4)
C2—C1—H1B	120.1	C19—C14—H14A	119.0
C6—C1—H1B	120.1	C15—C14—H14A	119.0
C3—C2—C1	122.1 (5)	C14—C15—C16	118.9 (5)
C3—C2—H2A	119.0	C14—C15—H15A	120.5
C1—C2—H2A	119.0	C16—C15—H15A	120.5
C2—C3—C4	118.7 (5)	C17—C16—C15	119.9 (5)
C2—C3—H3A	120.6	C17—C16—H16A	120.1
C4—C3—H3A	120.6	C15—C16—H16A	120.1
C5—C4—C3	120.3 (5)	C16—C17—C18	121.2 (5)
C5—C4—H4A	119.9	C16—C17—H17A	119.4
C3—C4—H4A	119.9	C18—C17—H17A	119.4
C6—C5—C4	119.8 (5)	C19—C18—C17	119.3 (4)
C6—C5—H5A	120.1	C19—C18—H18A	120.4
C4—C5—H5A	120.1	C17—C18—H18A	120.4
C5—C6—C1	119.4 (4)	C14—C19—C18	118.8 (4)
C5—C6—N1	118.5 (4)	C14—C19—N2	118.0 (3)
C1—C6—N1	122.1 (4)	C18—C19—N2	123.2 (4)
O1—C7—N1	123.9 (4)	O2—C20—N2	125.1 (4)
O1—C7—C8	120.6 (4)	O2—C20—C21	121.3 (4)

supplementary materials

N1—C7—C8	115.6 (3)	N2—C20—C21	113.7 (3)
C9—C8—C13	117.9 (5)	C22—C21—C26	117.9 (4)
C9—C8—C7	122.0 (5)	C22—C21—C20	121.1 (4)
C13—C8—C7	120.1 (4)	C26—C21—C20	121.0 (4)
C8—C9—C10	120.8 (7)	C21—C22—C23	121.3 (5)
C8—C9—C12	119.5 (5)	C21—C22—C13	119.2 (4)
C10—C9—C12	119.7 (6)	C23—C22—C13	119.4 (5)
C11—C10—C9	116.5 (8)	C24—C23—C22	119.8 (5)
C11—C10—H10A	121.7	C24—C23—H23A	120.1
C9—C10—H10A	121.7	C22—C23—H23A	120.1
C12—C11—C10	123.6 (10)	C25—C24—C23	119.9 (5)
C12—C11—H11A	118.2	C25—C24—H24A	120.0
C10—C11—H11A	118.2	C23—C24—H24A	120.0
C11—C12—C13	119.6 (8)	C24—C25—C26	120.1 (6)
C11—C12—H12A	120.2	C24—C25—H25A	119.9
C13—C12—H12A	120.2	C26—C25—H25A	119.9
C12—C13—C8	121.6 (6)	C25—C26—C21	121.0 (5)
C12—C13—C11	118.8 (5)	C25—C26—C14	120.1 (4)
C8—C13—C11	119.5 (4)	C21—C26—C14	118.9 (4)
C6—C1—C2—C3	-0.3 (8)	C19—C14—C15—C16	0.2 (7)
C1—C2—C3—C4	0.1 (8)	C14—C15—C16—C17	-0.1 (8)
C2—C3—C4—C5	0.0 (8)	C15—C16—C17—C18	0.2 (8)
C3—C4—C5—C6	0.2 (8)	C16—C17—C18—C19	-0.3 (7)
C4—C5—C6—C1	-0.5 (7)	C15—C14—C19—C18	-0.4 (6)
C4—C5—C6—N1	179.2 (4)	C15—C14—C19—N2	176.9 (4)
C2—C1—C6—C5	0.5 (7)	C17—C18—C19—C14	0.4 (6)
C2—C1—C6—N1	-179.2 (4)	C17—C18—C19—N2	-176.8 (4)
C7—N1—C6—C5	143.6 (4)	C20—N2—C19—C14	158.0 (4)
C7—N1—C6—C1	-36.8 (6)	C20—N2—C19—C18	-24.8 (6)
C6—N1—C7—O1	2.4 (6)	C19—N2—C20—O2	-0.4 (6)
C6—N1—C7—C8	-178.1 (4)	C19—N2—C20—C21	179.5 (4)
O1—C7—C8—C9	81.7 (5)	O2—C20—C21—C22	-91.6 (5)
N1—C7—C8—C9	-97.9 (5)	N2—C20—C21—C22	88.5 (4)
O1—C7—C8—C13	-96.4 (5)	O2—C20—C21—C26	86.2 (5)
N1—C7—C8—C13	84.1 (5)	N2—C20—C21—C26	-93.7 (4)
C13—C8—C9—C10	-1.6 (7)	C26—C21—C22—C23	-0.2 (6)
C7—C8—C9—C10	-179.7 (5)	C20—C21—C22—C23	177.7 (4)
C13—C8—C9—C12	177.8 (3)	C26—C21—C22—C13	177.3 (3)
C7—C8—C9—C12	-0.3 (6)	C20—C21—C22—C13	-4.9 (5)
C8—C9—C10—C11	0.9 (10)	C21—C22—C23—C24	-0.8 (7)
C12—C9—C10—C11	-178.5 (6)	C13—C22—C23—C24	-178.2 (4)
C9—C10—C11—C12	0.0 (13)	C22—C23—C24—C25	1.4 (8)
C10—C11—C12—C13	-0.2 (13)	C23—C24—C25—C26	-1.2 (8)
C11—C12—C13—C8	-0.6 (9)	C24—C25—C26—C21	0.2 (7)
C11—C12—C13—C11	177.3 (6)	C24—C25—C26—C14	-179.6 (4)
C9—C8—C13—C12	1.5 (7)	C22—C21—C26—C25	0.5 (6)
C7—C8—C13—C12	179.6 (4)	C20—C21—C26—C25	-177.4 (4)
C9—C8—C13—C11	-176.4 (3)	C22—C21—C26—C14	-179.8 (3)
C7—C8—C13—C11	1.7 (5)	C20—C21—C26—C14	2.4 (5)

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A \cdots O2 ⁱ	0.86	2.09	2.927 (5)	163
N2—H2B \cdots O1 ⁱⁱ	0.86	1.99	2.830 (5)	165
C1—H1B \cdots O1	0.93	2.46	2.920 (7)	110
C18—H18A \cdots O2	0.93	2.41	2.937 (6)	116

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

Fig. 1

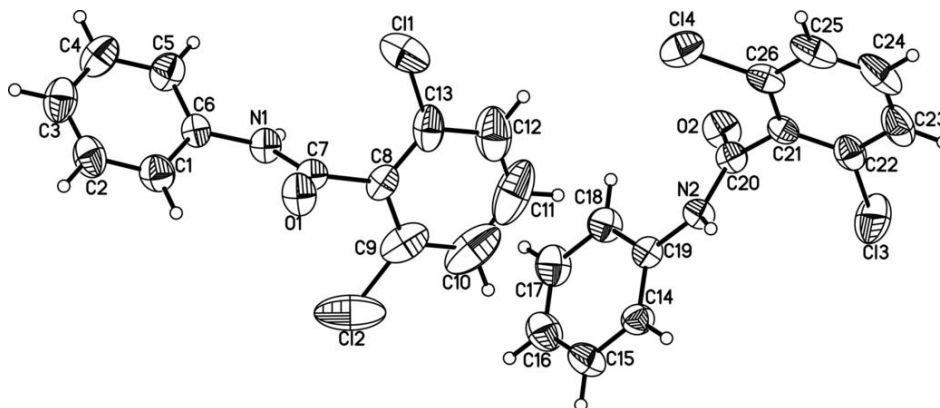


Fig. 2

