

2-Chloro-N-(2,3-dichlorophenyl)-benzamide

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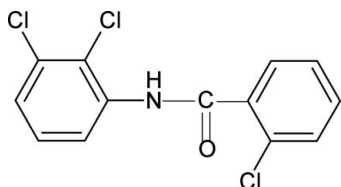
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Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.033; wR factor = 0.105; data-to-parameter ratio = 12.1.

Two independent molecules comprise the asymmetric unit in the title compound, $\text{C}_{13}\text{H}_8\text{Cl}_3\text{NO}$, each with the amide $\text{N}-\text{H}$ and $\text{C}=\text{O}$ bonds *trans* to each other. The molecules are linked into chains through intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2003, 2007, 2008).



Experimental

Crystal data

$\text{C}_{13}\text{H}_8\text{Cl}_3\text{NO}$
 $M_r = 300.55$
Monoclinic, Pc
 $a = 12.310$ (1) Å
 $b = 7.8307$ (6) Å
 $c = 14.407$ (2) Å
 $\beta = 111.52$ (1)°

$V = 1292.0$ (2) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.69$ mm⁻¹
 $T = 299$ (2) K
 $0.75 \times 0.75 \times 0.18$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford)

Diffraction, 2007)
 $T_{\min} = 0.624$, $T_{\max} = 0.885$
5882 measured reflections
3936 independent reflections
3430 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.014$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.104$
 $S = 1.14$
3936 reflections
326 parameters
2 restraints

H-atom parameters constrained
 $\Delta\rho_{\max} = 0.29$ e Å⁻³
 $\Delta\rho_{\min} = -0.28$ e Å⁻³
Absolute structure: (Flack, 1983),
365 Friedel pairs
Flack parameter: 0.12 (5)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O2}$	0.86	2.16	2.850 (3)	137
$\text{N1}-\text{H1N}\cdots\text{Cl3}$	0.86	2.64	3.114 (3)	116
$\text{N2}-\text{H2N}\cdots\text{O1}^{\dagger}$	0.86	2.05	2.896 (3)	167

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); 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: TK2277).

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supplementary materials

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2-Chloro-*N*-(2,3-dichlorophenyl)benzamide

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Comment

In the present work, the structure of 2-chloro-*N*-(2,3-dichlorophenyl)- benzamide (I, N23DCP2CBA) has been determined to explore the effect of substituents on the structures of benzanilides (Gowda *et al.*, 2003; 2007; 2008). The amide N—H and C=O bonds in each of the two molecules comprising the crystallographic asymmetric unit are *trans* to each other (Fig. 1), similar to that observed in 2-chloro-*N*-(phenyl)-benzamide (NP2CBA) (Gowda *et al.*, 2003), 2-chloro-*N*-(2-chlorophenyl)-benzamide (N2CP2CBA) (Gowda *et al.*, 2007), and 2-chloro-*N*-(3-chlorophenyl)-benzamide (N3CP2CBA) (Gowda *et al.*, 2008). In one of the molecules, the conformation of the N—H bond is *syn* to both the *ortho* and *meta*-chloro groups in the aniline ring and of the C=O bond group is also *syn* to the *ortho*-chloro group in the benzoyl ring. By contrast, the conformations of these bonds in the second independent molecule are intermediate between *syn* and *anti* to the respective groups. The above conformations are in contrast to the *syn* conformations of both the amide N—H and C=O bonds, with respect to the *ortho*-chloro groups in the benzoyl and aniline rings, respectively, observed in N2CP2CBA (Gowda *et al.*, 2007). Further, in N3CP2CBA, the conformation of the C=O bond is *syn* to the *ortho*-chloro group of the benzoyl ring, while the N—H bond is *anti* to the *meta*-chloro group of the aniline ring (Gowda *et al.*, 2008). The —NHCO— group makes the dihedral angles of 42.24 (14)° (molecule 1), 48.89 (12)° (molecule 2), and 35.31 (19)° (molecule 1), 41.88 (13)° (molecule 2) with the benzoyl and aniline rings, respectively. The benzoyl and aniline rings form the dihedral angles of 12.30 (10)° (molecule 1) and 7.25 (9)° (molecule 2). In the crystal structure of (I), the molecules are linked by intermolecular N—H···O and N—H···Cl hydrogen bonds (Table 1) forming chains running along the *a* axis, as shown in Fig. 2.

Experimental

Compound (I) was prepared according to the literature method (Gowda *et al.*, 2003). The purity of the compound was confirmed by melting point, and IR and NMR spectra. Single crystals were obtained from an ethanolic solution of (I)

Refinement

The H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å and N—H = 0.86 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N}, \text{C})$.

Figures

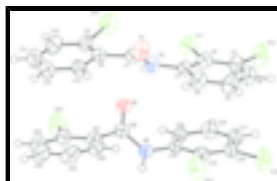


Fig. 1. Molecular structure of (I) showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level.

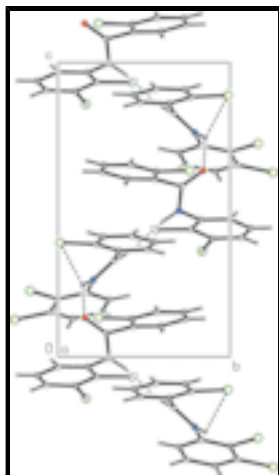


Fig. 2. Molecular packing of (I) with hydrogen bonding shown as dashed lines.

2-Chloro-*N*-(2,3-dichlorophenyl)benzamide

Crystal data

$C_{13}H_8Cl_3NO$

$M_r = 300.55$

Monoclinic, *Pc*

Hall symbol: *P* -2yc

$a = 12.310$ (1) Å

$b = 7.8307$ (6) Å

$c = 14.407$ (2) Å

$\beta = 111.52$ (1)°

$V = 1292.0$ (2) Å³

$Z = 4$

$F_{000} = 608$

$D_x = 1.545$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 3409 reflections

$\theta = 2.6$ – 27.5°

$\mu = 0.69$ mm⁻¹

$T = 299$ (2) K

Thick plate, colourless

$0.75 \times 0.75 \times 0.18$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 299$ (2) K

Rotation method data acquisition using ω and φ scans $\theta_{\min} = 2.6^\circ$

Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)

$T_{\min} = 0.624$, $T_{\max} = 0.885$

5882 measured reflections

3936 independent reflections

3430 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.014$

$\theta_{\max} = 26.4^\circ$

$\theta_{\min} = 2.6^\circ$

$h = -15 \rightarrow 13$

$k = -9 \rightarrow 9$

$l = -15 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0715P)^2 + 0.0104P]$
$wR(F^2) = 0.104$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{\max} = 0.003$
3936 reflections	$\Delta\rho_{\max} = 0.29 \text{ e } \text{\AA}^{-3}$
326 parameters	$\Delta\rho_{\min} = -0.28 \text{ e } \text{\AA}^{-3}$
2 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0118 (14)
Secondary atom site location: difference Fourier map	Absolute structure: (Flack, 1983), 365 Friedel pairs
	Flack parameter: 0.12 (5)

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.80355 (8)	-0.16289 (10)	0.22458 (7)	0.0542 (2)
C12	0.53668 (10)	-0.25096 (14)	0.12596 (9)	0.0739 (3)
C13	1.08381 (10)	0.01157 (12)	0.38808 (9)	0.0745 (3)
O1	0.8488 (2)	0.4258 (3)	0.36026 (18)	0.0537 (6)
N1	0.8566 (2)	0.2051 (3)	0.26179 (19)	0.0411 (6)
H1N	0.9028	0.1426	0.2437	0.049*
C1	0.7362 (3)	0.1682 (4)	0.2183 (2)	0.0359 (6)
C2	0.7006 (3)	-0.0018 (4)	0.1965 (2)	0.0420 (7)
C3	0.5819 (3)	-0.0414 (5)	0.1521 (3)	0.0493 (8)
C4	0.4996 (3)	0.0858 (5)	0.1303 (3)	0.0566 (9)
H4	0.4206	0.0589	0.1018	0.068*
C5	0.5342 (4)	0.2543 (5)	0.1510 (3)	0.0597 (10)
H5	0.4783	0.3403	0.1357	0.072*
C6	0.6515 (3)	0.2954 (5)	0.1941 (3)	0.0498 (8)
H6	0.6738	0.4091	0.2071	0.060*
C7	0.9063 (3)	0.3294 (4)	0.3292 (2)	0.0388 (7)
C8	1.0362 (3)	0.3540 (4)	0.3601 (2)	0.0379 (7)
C9	1.1208 (3)	0.2248 (5)	0.3829 (3)	0.0478 (8)
C10	1.2384 (4)	0.2639 (6)	0.4080 (3)	0.0613 (10)
H10	1.2936	0.1769	0.4226	0.074*
C11	1.2727 (3)	0.4310 (6)	0.4112 (3)	0.0629 (10)

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H11	1.3513	0.4569	0.4276	0.076*
C12	1.1924 (4)	0.5604 (5)	0.3904 (3)	0.0576 (9)
H12	1.2164	0.6735	0.3931	0.069*
C13	1.0746 (3)	0.5220 (4)	0.3654 (3)	0.0455 (7)
H13	1.0206	0.6104	0.3519	0.055*
C14	0.61868 (9)	0.43793 (11)	-0.06792 (10)	0.0700 (3)
C15	0.41892 (8)	0.16238 (16)	-0.14120 (9)	0.0747 (3)
C16	1.22481 (9)	0.23655 (14)	0.13296 (10)	0.0727 (3)
O2	0.9822 (2)	0.1549 (3)	0.13253 (16)	0.0436 (5)
N2	0.8590 (2)	0.2974 (3)	-0.00345 (19)	0.0400 (6)
H2N	0.8503	0.3882	-0.0390	0.048*
C14	0.7697 (3)	0.1737 (4)	-0.0342 (2)	0.0351 (6)
C15	0.6526 (3)	0.2227 (4)	-0.0670 (2)	0.0412 (7)
C16	0.5648 (3)	0.1028 (4)	-0.0983 (2)	0.0422 (7)
C17	0.5907 (3)	-0.0713 (5)	-0.0947 (3)	0.0485 (8)
H17	0.5314	-0.1525	-0.1133	0.058*
C18	0.7064 (3)	-0.1199 (4)	-0.0630 (3)	0.0471 (8)
H18	0.7250	-0.2351	-0.0618	0.056*
C19	0.7949 (3)	-0.0002 (4)	-0.0329 (2)	0.0413 (7)
H19	0.8723	-0.0359	-0.0115	0.050*
C20	0.9589 (3)	0.2819 (4)	0.0796 (2)	0.0347 (6)
C21	1.0337 (3)	0.4382 (4)	0.1036 (2)	0.0364 (6)
C22	1.1550 (3)	0.4300 (4)	0.1294 (2)	0.0432 (7)
C23	1.2224 (3)	0.5764 (6)	0.1521 (3)	0.0598 (9)
H23	1.3026	0.5697	0.1680	0.072*
C24	1.1699 (4)	0.7327 (5)	0.1510 (3)	0.0635 (11)
H24	1.2149	0.8316	0.1656	0.076*
C25	1.0513 (4)	0.7428 (5)	0.1285 (3)	0.0604 (10)
H25	1.0168	0.8479	0.1297	0.072*
C26	0.9839 (3)	0.5976 (4)	0.1043 (2)	0.0464 (8)
H26	0.9037	0.6060	0.0882	0.056*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0515 (5)	0.0378 (4)	0.0674 (5)	0.0092 (4)	0.0148 (4)	-0.0055 (4)
C12	0.0619 (7)	0.0521 (5)	0.0969 (8)	-0.0162 (5)	0.0164 (6)	-0.0149 (5)
C13	0.0614 (6)	0.0395 (5)	0.1037 (8)	0.0091 (5)	0.0080 (6)	0.0133 (5)
O1	0.0443 (14)	0.0479 (13)	0.0663 (14)	0.0016 (11)	0.0173 (11)	-0.0199 (12)
N1	0.0360 (14)	0.0392 (13)	0.0486 (14)	0.0038 (11)	0.0162 (11)	-0.0078 (11)
C1	0.0353 (15)	0.0343 (15)	0.0375 (15)	0.0061 (12)	0.0127 (12)	-0.0007 (12)
C2	0.0448 (17)	0.0418 (17)	0.0389 (16)	0.0093 (15)	0.0149 (13)	-0.0026 (13)
C3	0.0467 (19)	0.0471 (18)	0.0511 (19)	-0.0055 (16)	0.0147 (15)	-0.0106 (15)
C4	0.0379 (19)	0.060 (2)	0.064 (2)	-0.0022 (17)	0.0095 (15)	-0.0069 (18)
C5	0.043 (2)	0.053 (2)	0.074 (3)	0.0176 (17)	0.0104 (17)	-0.0041 (18)
C6	0.050 (2)	0.0376 (17)	0.055 (2)	0.0071 (15)	0.0115 (15)	-0.0063 (15)
C7	0.0414 (17)	0.0326 (15)	0.0438 (16)	0.0041 (13)	0.0172 (13)	0.0011 (13)
C8	0.0400 (17)	0.0393 (16)	0.0336 (14)	0.0029 (13)	0.0128 (12)	0.0023 (12)

C9	0.0426 (19)	0.0434 (18)	0.0506 (18)	0.0012 (15)	0.0090 (14)	0.0056 (14)
C10	0.044 (2)	0.068 (2)	0.064 (2)	0.0131 (18)	0.0096 (16)	0.0015 (19)
C11	0.042 (2)	0.073 (3)	0.071 (2)	-0.007 (2)	0.0159 (17)	0.003 (2)
C12	0.054 (2)	0.055 (2)	0.065 (2)	-0.0116 (18)	0.0231 (17)	0.0018 (18)
C13	0.0457 (19)	0.0384 (16)	0.0527 (19)	-0.0038 (15)	0.0185 (15)	0.0002 (14)
C14	0.0492 (5)	0.0352 (4)	0.1229 (9)	0.0110 (4)	0.0283 (5)	0.0141 (5)
C15	0.0330 (4)	0.0743 (7)	0.1059 (8)	0.0019 (5)	0.0126 (4)	0.0079 (6)
C16	0.0455 (5)	0.0593 (6)	0.1157 (9)	0.0121 (5)	0.0322 (5)	-0.0116 (6)
O2	0.0459 (13)	0.0357 (11)	0.0453 (11)	0.0033 (10)	0.0119 (9)	0.0058 (9)
N2	0.0359 (14)	0.0321 (12)	0.0449 (14)	0.0007 (11)	0.0065 (11)	0.0086 (10)
C14	0.0328 (15)	0.0351 (15)	0.0367 (14)	-0.0006 (12)	0.0119 (11)	0.0055 (12)
C15	0.0423 (18)	0.0341 (16)	0.0485 (17)	0.0067 (14)	0.0184 (14)	0.0075 (13)
C16	0.0329 (16)	0.0432 (17)	0.0510 (18)	-0.0021 (13)	0.0161 (14)	0.0028 (14)
C17	0.047 (2)	0.0457 (18)	0.0525 (19)	-0.0114 (16)	0.0185 (15)	-0.0047 (15)
C18	0.054 (2)	0.0301 (15)	0.0572 (19)	0.0024 (14)	0.0201 (16)	-0.0038 (14)
C19	0.0352 (16)	0.0394 (16)	0.0454 (17)	0.0053 (14)	0.0101 (13)	0.0010 (13)
C20	0.0359 (16)	0.0339 (14)	0.0383 (15)	0.0072 (13)	0.0184 (12)	0.0006 (12)
C21	0.0363 (16)	0.0335 (15)	0.0374 (15)	0.0019 (13)	0.0111 (12)	-0.0031 (12)
C22	0.0395 (18)	0.0407 (17)	0.0472 (17)	0.0038 (14)	0.0133 (13)	-0.0028 (14)
C23	0.043 (2)	0.067 (2)	0.060 (2)	-0.0104 (19)	0.0078 (16)	-0.0007 (19)
C24	0.077 (3)	0.0399 (19)	0.054 (2)	-0.0137 (19)	-0.0003 (19)	0.0006 (15)
C25	0.074 (3)	0.0357 (17)	0.0509 (19)	0.0061 (18)	-0.0013 (17)	-0.0010 (14)
C26	0.0487 (19)	0.0397 (16)	0.0413 (17)	0.0060 (15)	0.0052 (14)	0.0001 (14)

Geometric parameters (Å, °)

C11—C2	1.728 (3)	C14—C15	1.735 (3)
C12—C3	1.730 (4)	C15—C16	1.735 (3)
C13—C9	1.739 (4)	C16—C22	1.733 (3)
O1—C7	1.226 (4)	O2—C20	1.222 (4)
N1—C7	1.353 (4)	N2—C20	1.371 (4)
N1—C1	1.411 (4)	N2—C14	1.409 (4)
N1—H1N	0.8600	N2—H2N	0.8600
C1—C6	1.391 (5)	C14—C19	1.395 (4)
C1—C2	1.401 (4)	C14—C15	1.396 (4)
C2—C3	1.397 (5)	C15—C16	1.377 (5)
C3—C4	1.373 (5)	C16—C17	1.397 (5)
C4—C5	1.384 (6)	C17—C18	1.380 (5)
C4—H4	0.9300	C17—H17	0.9300
C5—C6	1.384 (6)	C18—C19	1.381 (5)
C5—H5	0.9300	C18—H18	0.9300
C6—H6	0.9300	C19—H19	0.9300
C7—C8	1.507 (5)	C20—C21	1.493 (4)
C8—C13	1.390 (5)	C21—C26	1.393 (4)
C8—C9	1.402 (5)	C21—C22	1.402 (4)
C9—C10	1.392 (6)	C22—C23	1.382 (5)
C10—C11	1.371 (6)	C23—C24	1.382 (6)
C10—H10	0.9300	C23—H23	0.9300
C11—C12	1.370 (6)	C24—C25	1.376 (7)

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C11—H11	0.9300	C24—H24	0.9300
C12—C13	1.392 (5)	C25—C26	1.375 (5)
C12—H12	0.9300	C25—H25	0.9300
C13—H13	0.9300	C26—H26	0.9300
C7—N1—C1	126.2 (3)	C20—N2—C14	124.1 (3)
C7—N1—H1N	116.9	C20—N2—H2N	118.0
C1—N1—H1N	116.9	C14—N2—H2N	118.0
C6—C1—C2	118.7 (3)	C19—C14—C15	118.0 (3)
C6—C1—N1	122.2 (3)	C19—C14—N2	121.5 (3)
C2—C1—N1	119.1 (3)	C15—C14—N2	120.5 (3)
C3—C2—C1	120.2 (3)	C16—C15—C14	120.8 (3)
C3—C2—C11	119.9 (3)	C16—C15—C14	120.1 (3)
C1—C2—C11	119.9 (3)	C14—C15—C14	119.0 (3)
C4—C3—C2	120.3 (3)	C15—C16—C17	120.8 (3)
C4—C3—C12	119.1 (3)	C15—C16—C15	121.3 (3)
C2—C3—C12	120.6 (3)	C17—C16—C15	117.9 (3)
C3—C4—C5	119.9 (3)	C18—C17—C16	118.4 (3)
C3—C4—H4	120.0	C18—C17—H17	120.8
C5—C4—H4	120.0	C16—C17—H17	120.8
C6—C5—C4	120.4 (4)	C17—C18—C19	121.1 (3)
C6—C5—H5	119.8	C17—C18—H18	119.4
C4—C5—H5	119.8	C19—C18—H18	119.4
C5—C6—C1	120.6 (4)	C18—C19—C14	120.8 (3)
C5—C6—H6	119.7	C18—C19—H19	119.6
C1—C6—H6	119.7	C14—C19—H19	119.6
O1—C7—N1	122.3 (3)	O2—C20—N2	123.1 (3)
O1—C7—C8	120.4 (3)	O2—C20—C21	122.6 (3)
N1—C7—C8	117.1 (3)	N2—C20—C21	114.2 (2)
C13—C8—C9	117.5 (3)	C26—C21—C22	117.9 (3)
C13—C8—C7	116.1 (3)	C26—C21—C20	120.0 (3)
C9—C8—C7	126.4 (3)	C22—C21—C20	122.0 (3)
C10—C9—C8	121.0 (3)	C23—C22—C21	120.9 (3)
C10—C9—C13	117.6 (3)	C23—C22—C16	118.0 (3)
C8—C9—C13	121.3 (3)	C21—C22—C16	121.1 (3)
C11—C10—C9	119.8 (4)	C22—C23—C24	119.7 (4)
C11—C10—H10	120.1	C22—C23—H23	120.2
C9—C10—H10	120.1	C24—C23—H23	120.2
C12—C11—C10	120.7 (4)	C25—C24—C23	120.3 (4)
C12—C11—H11	119.6	C25—C24—H24	119.9
C10—C11—H11	119.6	C23—C24—H24	119.9
C11—C12—C13	119.7 (4)	C26—C25—C24	120.1 (4)
C11—C12—H12	120.1	C26—C25—H25	119.9
C13—C12—H12	120.1	C24—C25—H25	119.9
C8—C13—C12	121.3 (3)	C25—C26—C21	121.1 (3)
C8—C13—H13	119.4	C25—C26—H26	119.5
C12—C13—H13	119.4	C21—C26—H26	119.5
C7—N1—C1—C6	36.2 (5)	C20—N2—C14—C19	-43.2 (4)
C7—N1—C1—C2	-145.3 (3)	C20—N2—C14—C15	136.7 (3)

C6—C1—C2—C3	-0.5 (5)	C19—C14—C15—C16	-0.8 (4)
N1—C1—C2—C3	-179.1 (3)	N2—C14—C15—C16	179.2 (3)
C6—C1—C2—C11	179.5 (3)	C19—C14—C15—C14	179.2 (2)
N1—C1—C2—C11	0.8 (4)	N2—C14—C15—C14	-0.7 (4)
C1—C2—C3—C4	-0.6 (5)	C14—C15—C16—C17	2.3 (5)
C11—C2—C3—C4	179.5 (3)	C14—C15—C16—C17	-177.8 (3)
C1—C2—C3—C12	-179.4 (3)	C14—C15—C16—C15	-178.9 (2)
C11—C2—C3—C12	0.7 (4)	C14—C15—C16—C15	1.1 (4)
C2—C3—C4—C5	1.0 (6)	C15—C16—C17—C18	-2.6 (5)
C12—C3—C4—C5	179.9 (3)	C15—C16—C17—C18	178.5 (3)
C3—C4—C5—C6	-0.5 (6)	C16—C17—C18—C19	1.6 (5)
C4—C5—C6—C1	-0.6 (6)	C17—C18—C19—C14	-0.3 (5)
C2—C1—C6—C5	1.0 (5)	C15—C14—C19—C18	-0.1 (5)
N1—C1—C6—C5	179.6 (3)	N2—C14—C19—C18	179.8 (3)
C1—N1—C7—O1	0.1 (5)	C14—N2—C20—O2	3.4 (5)
C1—N1—C7—C8	-175.7 (3)	C14—N2—C20—C21	-173.0 (3)
O1—C7—C8—C13	-39.9 (4)	O2—C20—C21—C26	-128.9 (3)
N1—C7—C8—C13	135.9 (3)	N2—C20—C21—C26	47.5 (4)
O1—C7—C8—C9	140.8 (3)	O2—C20—C21—C22	48.7 (4)
N1—C7—C8—C9	-43.4 (4)	N2—C20—C21—C22	-134.9 (3)
C13—C8—C9—C10	-1.1 (5)	C26—C21—C22—C23	-1.8 (5)
C7—C8—C9—C10	178.2 (3)	C20—C21—C22—C23	-179.4 (3)
C13—C8—C9—C13	175.0 (2)	C26—C21—C22—C16	178.6 (2)
C7—C8—C9—C13	-5.7 (5)	C20—C21—C22—C16	1.0 (4)
C8—C9—C10—C11	0.3 (6)	C21—C22—C23—C24	1.1 (5)
C13—C9—C10—C11	-175.8 (3)	C16—C22—C23—C24	-179.3 (3)
C9—C10—C11—C12	0.4 (6)	C22—C23—C24—C25	0.6 (6)
C10—C11—C12—C13	-0.3 (6)	C23—C24—C25—C26	-1.7 (6)
C9—C8—C13—C12	1.2 (5)	C24—C25—C26—C21	1.0 (6)
C7—C8—C13—C12	-178.2 (3)	C22—C21—C26—C25	0.7 (5)
C11—C12—C13—C8	-0.5 (6)	C20—C21—C26—C25	178.4 (3)

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

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1N \cdots O2	0.86	2.16	2.850 (3)	137
N1—H1N \cdots C13	0.86	2.64	3.114 (3)	116
N2—H2N \cdots O1 ⁱ	0.86	2.05	2.896 (3)	167

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

Fig. 1

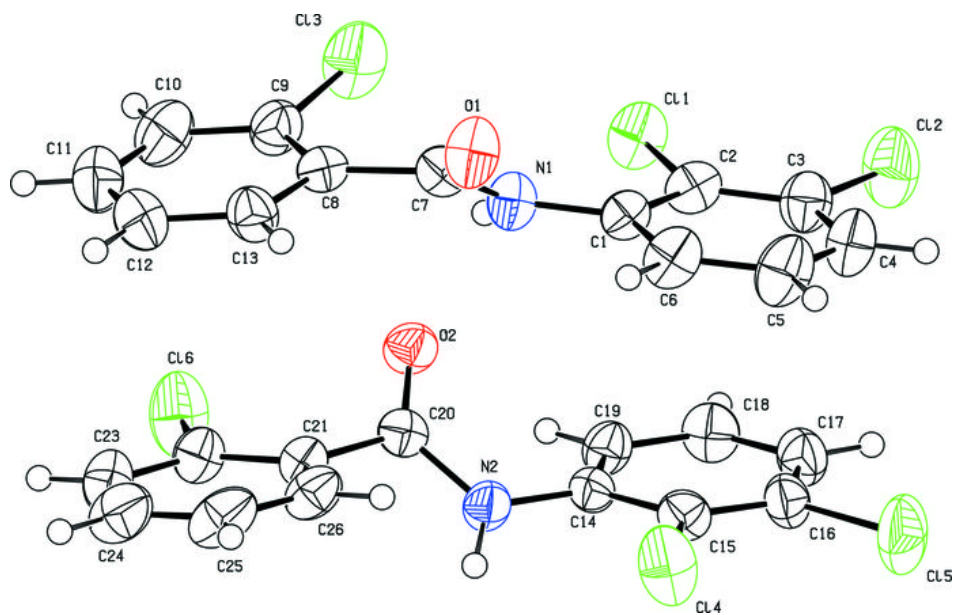


Fig. 2

