Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(2-Chloroanilino)-3-phenylfuran-2(5*H*)-one

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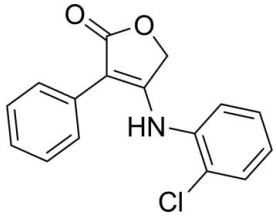
Received 23 October 2011; accepted 24 October 2011

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.144; data-to-parameter ratio = 17.8.

The title compound, $C_{16}H_{12}ClNO_2$, featuring a furan-2(5*H*)-one (γ-butyrolactone) core, contains two molecules (*A* and *B*) in the asymmetric unit, with different dihedral angles between the central ring and the pendant phenyl and chlorobenzene rings [43.33 (8) and 20.16 (8)°, respectively, for *A*, and 47.79 (8) and 13.87 (8)°, respectively, for *B*]. In the crystal, the *A* molecules are linked into [001] chains by single C—H···O interactions. The *B* molecules also form [001] chains, but their relative orientations in the chains are quite different to those of the *A* molecules so that adjacent *B* molecules are linked by two C—H···O hydrogen bonds. Finally, C—H···O interactions and aromatic π–π stacking contacts [centroid–centroid separations = 3.754 (1) and 3.817 (1) Å] link the chains into a two-dimensional array parallel to (010).

Related literature

For a related structure and background references, see: Xiao *et al.* (2011).



Experimental

Crystal data

$C_{16}H_{12}ClNO_2$
M_r = 285.72
Monoclinic, $P2_1/c$
a = 7.7305 (5) Å
b = 27.4374 (18) Å
c = 12.6242 (9) Å
β = 92.145 (1)°
V = 2675.8 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 298 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.919, T_{max} = 0.945
32744 measured reflections
6603 independent reflections
5086 reflections with $I > 2\sigma(I)$
R_{int} = 0.096

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.144
S = 1.06
6603 reflections
370 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

*Cg*2 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O1^{i}	0.93	2.47	3.305 (2)	149
C31—H31···O4^{ii}	0.93	2.58	3.422 (2)	151
C32—H32···O3^{ii}	0.93	2.48	3.305 (2)	148
C19—H19···*Cg*2^{iii}	0.93	2.84	3.553 (2)	134

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x, y+\frac{3}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The work was financed by a project supported by the Hunan Provincial Natural Science Foundation of China (grant No. 11 J J3113), by the Key Laboratory of Hunan Forest Products and Chemical Industry Engineering of Hunan Province (grant No. JDZ201102) and by an aid program for the Science and Technology Innovative Research Team (Chemicals of Forestry Resources and Development of Forest Products) in Higher Educational Institutions of Hunan Province.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6469).

References

Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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Xiao, Z.-P., Yi, L.-C., Li, J.-L., Zhang, B. & Liao, M.-L. (2011). *Acta Cryst.* E**57**, o3086.

supplementary materials

Acta Cryst. (2011). E**67**, o3091 [**doi:10.1107/S1600536811044308**]

4-(2-Chloroanilino)-3-phenylfuran-2(5*H*)-one

Z.-P. Xiao, Z.-J. Huang, X.-Y. Liu, K.-S. Xiang and S.-R. Yu

Comment

As part of our ongoing studies of compounds with a γ-butyrolactone (furanone) core (Xiao *et al.*, 2011), we now report the structure of the title compound, (I).

The crystal structure of the title compound, 4-(2-chlorophenylamino)-3-phenylfuran-2(5*H*)-one, contains two crystallographically independent molecules (Fig. 1) in an asymmetric unit with difference of bond length lower than 0.009 Å. In molecule **A** (from C1 to C16, O1, O2, N1 and Cl1), the central furan-2(5*H*)-one ring make a dihedral angles of 43.33 (8) and 20.16 (8) ° with the benzene ring and the *o*-chloroaniline ring, repectively. While in the molecule **B** (from C17 to C32, O3, O4, N2 and Cl2), they are 47.79 (8) and 13.87 (8) °, respectively. For the convenience of description, molecular structure was discussed based on **A**. Bond distance C7—C10 (1.3490 (19) Å) is indicative of a double bond, and the title compound was therefore identified as a furan-2(5*H*)-one.

Interestingly, molecule **A** and molecule **B** show different interemolecular hydrogen bonding patterns. For molecule **A**, an infinite one-dimensional line is formed by C—H···O hydrogen bondings (Fig 2a). While molecules **B** are linked into a line by $R^2_2(7)$ rings, which built from C31—H31···O4 and C32—H32···O3 hydrogen bonds centred at (0, 0, n) and (0, 0.0695, n) respectively, where n represents an integer (Fig. 2 b). Between the resulted lines, three kinds of intermolecular interactions were found and link molecules to further generate an infinite two-dimensional sheet. Of them, C—H···π occurs between C19 (in molecule **B**) and 3-benzene ring with "H···centroid" length of 2.840 Å, while π–π contacts occur between furanone rings and aniline rings with "centroid···centroid" lengths of 3.754 (1) and 3.817 (1) Å, respectively (Fig. 3a and Fig. 3 b).

Experimental

To a methanol solution (20 ml) of 2-methoxy-1-naphthaldehyde (0.1 mmol, 17.4 mg) and 4-methylbenzohydrazide (0.1 mmol, 15.0 mg), a few drops of acetic acid were added. The mixture was refluxed for 1 h and then cooled to room temperature. The white crystalline solid was collected by filtration, washed with cold methanol and dried in air. Single crystals, suitable for X-ray diffraction, were obtained by slow evaporation of a methanol solution of the product in air.

Refinement

The NH H-atom was located in a difference Fourier map and was refined with a distance restraint, N—H = 0.90 (1) \%A. The C-bound H atoms were positioned geometrically and refined using a riding model: C—H = 0.93 and 0.96 \%A, for CH and CH_3 H-atoms, respectively, with $U_{iso}(H) = k \times U_{eq}(C)$ where k = 1.5 for CH_3 H-atoms and k = 1.2 for all other H-atoms.

Figures

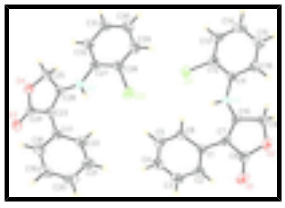

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

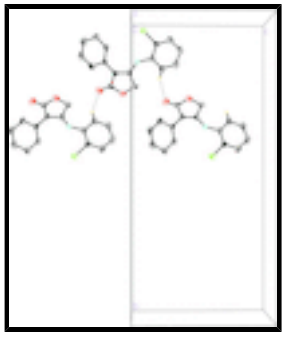

Fig. 2. a. Molecules (**A**) form a one-dimensional line through intermolecular C—H···O hydrogen bonds. For the sake of clarity, the H atoms have been omitted except that involving in hydrogen bonds.

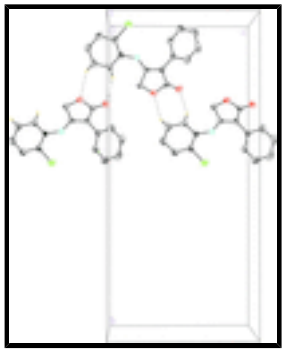

Fig. 3. b. Molecules (**B**) form a one-dimensional line through intermolecular C—H···O hydrogen bonds. For the sake of clarity, the H atoms have been omitted except that involving in hydrogen bonds.

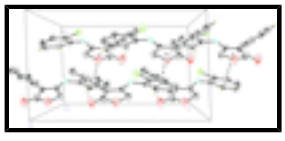

Fig. 4. a. A two-dimensional sheet is formed by intermolecular C—H···π interactions and π–π contacts.

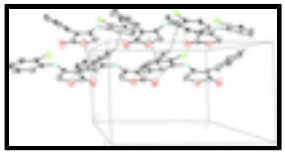

Fig. 5. b. A two-dimensional sheet is formed by intermolecular C—H···π interactions and π–π contacts.

4-(2-Chloroanilino)-3-phenylfuran-2(5*H*)-one

Crystal data

$C_{16}H_{12}ClNO_2$	$Z = 8$
$M_r = 285.72$	$F(000) = 1184$
Monoclinic, $P2_1/c$	$D_x = 1.418$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.7305$ (5) Å	$\theta = 2.6$–$27.8°$
$b = 27.4374$ (18) Å	$\mu = 0.29$ mm^{-1}

c = 12.6242 (9) Å	T = 298 K
β = 92.145 (1)°	Block, colorless
V = 2675.8 (3) Å^3	0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer	6603 independent reflections
Radiation source: fine-focus sealed tube	5086 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.096
φ and ω scan	θ_{max} = 28.3°, θ_{min} = 2.2°
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	h = −10→10
T_{min} = 0.919, T_{max} = 0.945	k = −36→36
32744 measured reflections	l = −16→16

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.144	$w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 0.1033P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
6603 reflections	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
370 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0084 (10)

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}

C1	0.27814 (18)	0.35945 (5)	0.29763 (10)	0.0461 (3)
C2	0.3577 (2)	0.34203 (6)	0.20759 (12)	0.0583 (4)
H2	0.3631	0.3086	0.1954	0.070*
C3	0.4284 (2)	0.37386 (8)	0.13655 (13)	0.0682 (5)
H3	0.4800	0.3618	0.0766	0.082*
C4	0.4231 (2)	0.42301 (7)	0.15360 (13)	0.0684 (5)
H4	0.4722	0.4442	0.1058	0.082*
C5	0.3450 (2)	0.44111 (6)	0.24147 (13)	0.0609 (4)
H5	0.3413	0.4746	0.2529	0.073*
C6	0.27233 (19)	0.40972 (5)	0.31272 (11)	0.0504 (3)
H6	0.2188	0.4223	0.3715	0.060*
C7	0.20474 (18)	0.32524 (5)	0.37337 (11)	0.0475 (3)
C8	0.1029 (2)	0.28279 (5)	0.34135 (13)	0.0608 (4)
C9	0.1273 (2)	0.28158 (5)	0.52194 (13)	0.0578 (4)
H9A	0.2096	0.2607	0.5599	0.069*
H9B	0.0365	0.2906	0.5691	0.069*
C10	0.21487 (17)	0.32582 (5)	0.48027 (11)	0.0454 (3)
C11	0.28478 (17)	0.37210 (5)	0.64825 (10)	0.0457 (3)
C12	0.33208 (18)	0.41894 (5)	0.68118 (11)	0.0500 (3)
C13	0.3164 (2)	0.43397 (7)	0.78420 (13)	0.0656 (4)
H13	0.3484	0.4655	0.8038	0.079*
C14	0.2536 (2)	0.40257 (8)	0.85839 (13)	0.0729 (5)
H14	0.2403	0.4129	0.9278	0.088*
C15	0.2108 (2)	0.35592 (7)	0.82878 (13)	0.0681 (5)
H15	0.1711	0.3343	0.8791	0.082*
C16	0.2257 (2)	0.34051 (6)	0.72529 (12)	0.0561 (4)
H16	0.1959	0.3087	0.7069	0.067*
C17	0.22903 (18)	0.63216 (5)	0.06184 (11)	0.0487 (3)
C18	0.1337 (2)	0.64534 (7)	−0.02958 (12)	0.0626 (4)
H18	0.1155	0.6781	−0.0452	0.075*
C19	0.0664 (2)	0.61005 (9)	−0.09697 (13)	0.0758 (6)
H19	0.0023	0.6193	−0.1575	0.091*
C20	0.0925 (2)	0.56142 (9)	−0.07617 (15)	0.0782 (6)
H20	0.0468	0.5379	−0.1223	0.094*
C21	0.1860 (2)	0.54794 (7)	0.01279 (15)	0.0692 (5)
H21	0.2038	0.5150	0.0273	0.083*
C22	0.2544 (2)	0.58261 (5)	0.08146 (12)	0.0554 (4)
H22	0.3183	0.5728	0.1416	0.066*
C23	0.29904 (19)	0.66934 (5)	0.13540 (11)	0.0490 (3)
C24	0.3918 (2)	0.71252 (6)	0.10214 (13)	0.0621 (4)
C25	0.3729 (2)	0.71710 (5)	0.28216 (12)	0.0559 (4)
H25A	0.2888	0.7379	0.3150	0.067*
H25B	0.4661	0.7101	0.3335	0.067*
C26	0.29004 (18)	0.67104 (5)	0.24190 (11)	0.0458 (3)
C27	0.21703 (17)	0.62944 (5)	0.41166 (11)	0.0451 (3)
C28	0.16217 (18)	0.58432 (5)	0.44911 (12)	0.0499 (3)
C29	0.1665 (2)	0.57327 (6)	0.55559 (14)	0.0648 (4)
H29	0.1286	0.5430	0.5783	0.078*
C30	0.2268 (2)	0.60706 (7)	0.62796 (13)	0.0708 (5)

H30	0.2321	0.5996	0.6999	0.085*
C31	0.2794 (2)	0.65192 (7)	0.59359 (13)	0.0640 (4)
H31	0.3190	0.6750	0.6428	0.077*
C32	0.2744 (2)	0.66332 (6)	0.48734 (12)	0.0548 (4)
H32	0.3098	0.6940	0.4658	0.066*
Cl1	0.40795 (6)	0.460028 (15)	0.58859 (4)	0.06829 (15)
Cl2	0.09240 (6)	0.540051 (15)	0.35831 (4)	0.06933 (16)
N1	0.30072 (17)	0.35959 (5)	0.54159 (10)	0.0512 (3)
N2	0.21099 (18)	0.63755 (5)	0.30234 (10)	0.0553 (3)
O1	0.05550 (19)	0.26896 (4)	0.25415 (10)	0.0813 (4)
O2	0.05665 (17)	0.25763 (4)	0.42950 (10)	0.0711 (3)
O3	0.4329 (2)	0.72534 (4)	0.01522 (10)	0.0833 (4)
O4	0.43819 (18)	0.73964 (4)	0.18943 (10)	0.0716 (3)
H1	0.354 (2)	0.3800 (6)	0.5078 (13)	0.054 (4)*
H2A	0.164 (2)	0.6156 (6)	0.2687 (14)	0.061 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0511 (7)	0.0492 (7)	0.0377 (6)	0.0074 (6)	−0.0023 (5)	−0.0037 (5)
C2	0.0671 (9)	0.0633 (9)	0.0442 (8)	0.0156 (7)	0.0002 (7)	−0.0096 (7)
C3	0.0691 (10)	0.0927 (13)	0.0437 (8)	0.0134 (9)	0.0127 (7)	−0.0060 (8)
C4	0.0713 (10)	0.0840 (13)	0.0506 (9)	−0.0060 (9)	0.0108 (8)	0.0071 (8)
C5	0.0717 (10)	0.0574 (9)	0.0538 (8)	−0.0063 (7)	0.0037 (7)	0.0001 (7)
C6	0.0591 (8)	0.0521 (8)	0.0401 (7)	0.0035 (6)	0.0037 (6)	−0.0043 (6)
C7	0.0551 (8)	0.0409 (7)	0.0464 (7)	0.0075 (5)	0.0001 (6)	−0.0039 (5)
C8	0.0805 (11)	0.0430 (8)	0.0585 (9)	0.0052 (7)	−0.0026 (8)	−0.0088 (7)
C9	0.0736 (10)	0.0434 (8)	0.0565 (9)	−0.0004 (7)	0.0014 (7)	0.0026 (6)
C10	0.0498 (7)	0.0411 (7)	0.0455 (7)	0.0071 (5)	0.0028 (6)	−0.0014 (5)
C11	0.0437 (7)	0.0534 (8)	0.0399 (7)	0.0039 (5)	0.0008 (5)	−0.0001 (6)
C12	0.0482 (7)	0.0535 (8)	0.0481 (7)	0.0027 (6)	−0.0014 (6)	−0.0021 (6)
C13	0.0693 (10)	0.0725 (11)	0.0545 (9)	0.0040 (8)	−0.0057 (7)	−0.0160 (8)
C14	0.0790 (11)	0.0965 (14)	0.0434 (8)	0.0055 (10)	0.0022 (8)	−0.0121 (9)
C15	0.0726 (10)	0.0881 (13)	0.0440 (8)	0.0045 (9)	0.0078 (7)	0.0088 (8)
C16	0.0619 (9)	0.0595 (9)	0.0472 (8)	0.0006 (7)	0.0053 (6)	0.0040 (7)
C17	0.0500 (7)	0.0552 (8)	0.0411 (7)	0.0031 (6)	0.0045 (6)	0.0018 (6)
C18	0.0627 (9)	0.0801 (11)	0.0451 (8)	0.0156 (8)	0.0036 (7)	0.0056 (8)
C19	0.0630 (10)	0.1212 (18)	0.0428 (8)	0.0052 (10)	−0.0054 (7)	−0.0056 (10)
C20	0.0736 (11)	0.1020 (16)	0.0588 (10)	−0.0176 (10)	0.0018 (9)	−0.0241 (10)
C21	0.0794 (11)	0.0623 (10)	0.0662 (11)	−0.0134 (8)	0.0068 (9)	−0.0119 (8)
C22	0.0615 (9)	0.0550 (9)	0.0493 (8)	−0.0023 (7)	−0.0016 (7)	−0.0003 (6)
C23	0.0588 (8)	0.0424 (7)	0.0458 (7)	0.0057 (6)	0.0017 (6)	0.0049 (6)
C24	0.0901 (12)	0.0408 (8)	0.0559 (9)	0.0046 (7)	0.0109 (8)	0.0076 (7)
C25	0.0767 (10)	0.0398 (7)	0.0513 (8)	−0.0004 (6)	0.0055 (7)	0.0003 (6)
C26	0.0509 (7)	0.0409 (7)	0.0454 (7)	0.0032 (5)	−0.0005 (6)	0.0032 (5)
C27	0.0447 (7)	0.0465 (7)	0.0442 (7)	0.0031 (5)	0.0024 (5)	0.0026 (5)
C28	0.0472 (7)	0.0479 (8)	0.0550 (8)	0.0042 (6)	0.0071 (6)	0.0025 (6)
C29	0.0677 (10)	0.0620 (10)	0.0655 (10)	0.0057 (8)	0.0139 (8)	0.0197 (8)

C30	0.0814 (11)	0.0846 (12)	0.0469 (9)	0.0096 (10)	0.0076 (8)	0.0123 (8)
C31	0.0689 (10)	0.0760 (11)	0.0469 (8)	0.0049 (8)	−0.0009 (7)	−0.0058 (8)
C32	0.0633 (9)	0.0528 (8)	0.0482 (8)	0.0000 (6)	−0.0008 (6)	0.0000 (6)
Cl1	0.0816 (3)	0.0550 (3)	0.0685 (3)	−0.01316 (18)	0.0057 (2)	0.00081 (18)
Cl2	0.0762 (3)	0.0517 (2)	0.0803 (3)	−0.01332 (18)	0.0058 (2)	−0.00368 (19)
N1	0.0619 (7)	0.0526 (7)	0.0397 (6)	−0.0100 (6)	0.0081 (5)	−0.0016 (5)
N2	0.0683 (8)	0.0554 (7)	0.0419 (6)	−0.0165 (6)	−0.0028 (6)	0.0001 (5)
O1	0.1134 (10)	0.0628 (7)	0.0665 (8)	−0.0094 (7)	−0.0115 (7)	−0.0203 (6)
O2	0.0986 (9)	0.0456 (6)	0.0688 (7)	−0.0136 (6)	−0.0024 (7)	−0.0031 (5)
O3	0.1370 (12)	0.0537 (7)	0.0611 (7)	−0.0046 (7)	0.0279 (8)	0.0119 (6)
O4	0.1118 (10)	0.0415 (6)	0.0624 (7)	−0.0131 (6)	0.0159 (7)	0.0007 (5)

Geometric parameters (Å, °)

C1—C6	1.393 (2)	C17—C22	1.395 (2)
C1—C2	1.3968 (19)	C17—C23	1.469 (2)
C1—C7	1.469 (2)	C18—C19	1.378 (3)
C2—C3	1.379 (3)	C18—H18	0.9300
C2—H2	0.9300	C19—C20	1.373 (3)
C3—C4	1.367 (3)	C19—H19	0.9300
C3—H3	0.9300	C20—C21	1.364 (3)
C4—C5	1.375 (2)	C20—H20	0.9300
C4—H4	0.9300	C21—C22	1.379 (2)
C5—C6	1.380 (2)	C21—H21	0.9300
C5—H5	0.9300	C22—H22	0.9300
C6—H6	0.9300	C23—C26	1.3497 (19)
C7—C10	1.3490 (19)	C23—C24	1.455 (2)
C7—C8	1.455 (2)	C24—O3	1.2063 (19)
C8—O1	1.208 (2)	C24—O4	1.367 (2)
C8—O2	1.368 (2)	C25—O4	1.4323 (19)
C9—O2	1.4296 (19)	C25—C26	1.4972 (19)
C9—C10	1.495 (2)	C25—H25A	0.9700
C9—H9A	0.9700	C25—H25B	0.9700
C9—H9B	0.9700	C26—N2	1.3547 (18)
C10—N1	1.3637 (18)	C27—C32	1.394 (2)
C11—C16	1.393 (2)	C27—C28	1.3966 (19)
C11—C12	1.395 (2)	C27—N2	1.3969 (18)
C11—N1	1.3995 (18)	C28—C29	1.377 (2)
C12—C13	1.374 (2)	C28—Cl2	1.7419 (16)
C12—Cl1	1.7415 (15)	C29—C30	1.371 (3)
C13—C14	1.374 (3)	C29—H29	0.9300
C13—H13	0.9300	C30—C31	1.372 (3)
C14—C15	1.371 (3)	C30—H30	0.9300
C14—H14	0.9300	C31—C32	1.377 (2)
C15—C16	1.382 (2)	C31—H31	0.9300
C15—H15	0.9300	C32—H32	0.9300
C16—H16	0.9300	N1—H1	0.824 (16)
C17—C18	1.393 (2)	N2—H2A	0.815 (17)
C6—C1—C2	117.86 (14)	C19—C18—H18	119.8

C6—C1—C7	121.89 (12)	C17—C18—H18	119.8
C2—C1—C7	120.25 (13)	C20—C19—C18	121.00 (16)
C3—C2—C1	120.65 (16)	C20—C19—H19	119.5
C3—C2—H2	119.7	C18—C19—H19	119.5
C1—C2—H2	119.7	C21—C20—C19	119.37 (17)
C4—C3—C2	120.50 (15)	C21—C20—H20	120.3
C4—C3—H3	119.7	C19—C20—H20	120.3
C2—C3—H3	119.7	C20—C21—C22	120.64 (18)
C3—C4—C5	120.00 (16)	C20—C21—H21	119.7
C3—C4—H4	120.0	C22—C21—H21	119.7
C5—C4—H4	120.0	C21—C22—C17	120.84 (15)
C4—C5—C6	120.14 (16)	C21—C22—H22	119.6
C4—C5—H5	119.9	C17—C22—H22	119.6
C6—C5—H5	119.9	C26—C23—C24	107.68 (13)
C5—C6—C1	120.84 (14)	C26—C23—C17	128.47 (13)
C5—C6—H6	119.6	C24—C23—C17	123.84 (13)
C1—C6—H6	119.6	O3—C24—O4	120.29 (15)
C10—C7—C8	107.34 (13)	O3—C24—C23	130.52 (16)
C10—C7—C1	129.37 (13)	O4—C24—C23	109.15 (13)
C8—C7—C1	123.29 (13)	O4—C25—C26	104.26 (12)
O1—C8—O2	120.20 (15)	O4—C25—H25A	110.9
O1—C8—C7	130.33 (17)	C26—C25—H25A	110.9
O2—C8—C7	109.45 (13)	O4—C25—H25B	110.9
O2—C9—C10	104.48 (12)	C26—C25—H25B	110.9
O2—C9—H9A	110.9	H25A—C25—H25B	108.9
C10—C9—H9A	110.9	C23—C26—N2	125.37 (13)
O2—C9—H9B	110.9	C23—C26—C25	109.27 (12)
C10—C9—H9B	110.9	N2—C26—C25	125.29 (13)
H9A—C9—H9B	108.9	C32—C27—C28	116.88 (13)
C7—C10—N1	125.78 (13)	C32—C27—N2	124.67 (13)
C7—C10—C9	109.41 (12)	C28—C27—N2	118.45 (13)
N1—C10—C9	124.69 (12)	C29—C28—C27	121.94 (15)
C16—C11—C12	117.02 (13)	C29—C28—Cl2	118.97 (12)
C16—C11—N1	124.21 (14)	C27—C28—Cl2	119.06 (11)
C12—C11—N1	118.76 (13)	C30—C29—C28	119.78 (15)
C13—C12—C11	121.81 (15)	C30—C29—H29	120.1
C13—C12—Cl1	119.00 (13)	C28—C29—H29	120.1
C11—C12—Cl1	119.17 (11)	C29—C30—C31	119.56 (16)
C12—C13—C14	120.18 (17)	C29—C30—H30	120.2
C12—C13—H13	119.9	C31—C30—H30	120.2
C14—C13—H13	119.9	C30—C31—C32	120.96 (17)
C15—C14—C13	119.17 (16)	C30—C31—H31	119.5
C15—C14—H14	120.4	C32—C31—H31	119.5
C13—C14—H14	120.4	C31—C32—C27	120.86 (15)
C14—C15—C16	121.04 (17)	C31—C32—H32	119.6
C14—C15—H15	119.5	C27—C32—H32	119.6
C16—C15—H15	119.5	C10—N1—C11	130.87 (13)
C15—C16—C11	120.73 (16)	C10—N1—H1	114.2 (12)
C15—C16—H16	119.6	C11—N1—H1	113.3 (12)

C11—C16—H16	119.6	C26—N2—C27	131.72 (13)
C18—C17—C22	117.82 (14)	C26—N2—H2A	114.2 (13)
C18—C17—C23	120.94 (14)	C27—N2—H2A	113.2 (13)
C22—C17—C23	121.24 (13)	C8—O2—C9	109.19 (12)
C19—C18—C17	120.33 (17)	C24—O4—C25	109.52 (12)
C6—C1—C2—C3	0.2 (2)	C23—C17—C22—C21	179.00 (14)
C7—C1—C2—C3	−179.41 (14)	C18—C17—C23—C26	132.18 (16)
C1—C2—C3—C4	0.6 (2)	C22—C17—C23—C26	−47.3 (2)
C2—C3—C4—C5	−0.8 (3)	C18—C17—C23—C24	−47.0 (2)
C3—C4—C5—C6	0.1 (3)	C22—C17—C23—C24	133.49 (16)
C4—C5—C6—C1	0.7 (2)	C26—C23—C24—O3	178.08 (19)
C2—C1—C6—C5	−0.8 (2)	C17—C23—C24—O3	−2.6 (3)
C7—C1—C6—C5	178.78 (13)	C26—C23—C24—O4	0.26 (18)
C6—C1—C7—C10	−42.7 (2)	C17—C23—C24—O4	179.59 (13)
C2—C1—C7—C10	136.91 (16)	C24—C23—C26—N2	178.94 (14)
C6—C1—C7—C8	137.21 (15)	C17—C23—C26—N2	−0.3 (2)
C2—C1—C7—C8	−43.2 (2)	C24—C23—C26—C25	1.93 (17)
C10—C7—C8—O1	176.81 (18)	C17—C23—C26—C25	−177.36 (14)
C1—C7—C8—O1	−3.1 (3)	O4—C25—C26—C23	−3.30 (17)
C10—C7—C8—O2	−1.51 (17)	O4—C25—C26—N2	179.68 (13)
C1—C7—C8—O2	178.58 (13)	C32—C27—C28—C29	−0.9 (2)
C8—C7—C10—N1	179.36 (13)	N2—C27—C28—C29	179.05 (14)
C1—C7—C10—N1	−0.7 (2)	C32—C27—C28—Cl2	−178.93 (11)
C8—C7—C10—C9	3.25 (16)	N2—C27—C28—Cl2	1.05 (18)
C1—C7—C10—C9	−176.85 (13)	C27—C28—C29—C30	−0.3 (2)
O2—C9—C10—C7	−3.77 (16)	Cl2—C28—C29—C30	177.69 (13)
O2—C9—C10—N1	−179.94 (13)	C28—C29—C30—C31	1.2 (3)
C16—C11—C12—C13	−2.0 (2)	C29—C30—C31—C32	−0.8 (3)
N1—C11—C12—C13	178.63 (14)	C30—C31—C32—C27	−0.5 (3)
C16—C11—C12—Cl1	179.71 (10)	C28—C27—C32—C31	1.3 (2)
N1—C11—C12—Cl1	0.30 (18)	N2—C27—C32—C31	−178.65 (15)
C11—C12—C13—C14	0.4 (2)	C7—C10—N1—C11	160.68 (15)
Cl1—C12—C13—C14	178.70 (13)	C9—C10—N1—C11	−23.8 (2)
C12—C13—C14—C15	1.5 (3)	C16—C11—N1—C10	26.5 (2)
C13—C14—C15—C16	−1.7 (3)	C12—C11—N1—C10	−154.17 (14)
C14—C15—C16—C11	0.0 (3)	C23—C26—N2—C27	166.70 (15)
C12—C11—C16—C15	1.8 (2)	C25—C26—N2—C27	−16.8 (3)
N1—C11—C16—C15	−178.88 (15)	C32—C27—N2—C26	18.0 (3)
C22—C17—C18—C19	0.6 (2)	C28—C27—N2—C26	−161.96 (15)
C23—C17—C18—C19	−178.91 (14)	O1—C8—O2—C9	−179.46 (16)
C17—C18—C19—C20	−0.5 (3)	C7—C8—O2—C9	−0.95 (18)
C18—C19—C20—C21	0.2 (3)	C10—C9—O2—C8	2.77 (17)
C19—C20—C21—C22	−0.1 (3)	O3—C24—O4—C25	179.48 (17)
C20—C21—C22—C17	0.3 (3)	C23—C24—O4—C25	−2.43 (19)
C18—C17—C22—C21	−0.5 (2)	C26—C25—O4—C24	3.44 (17)

Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C16—H16···O1^{i}	0.93	2.47	3.305 (2)	149
C31—H31···O4^{ii}	0.93	2.58	3.422 (2)	151
C32—H32···O3^{ii}	0.93	2.48	3.305 (2)	148
C19—H19···Cg2^{iii}	0.93	2.84	3.553 (2)	134

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2; (ii) *x*, −*y*+3/2, *z*+1/2; (iii) −*x*, *y*+3/2, −*z*+1/2.

Fig. 1

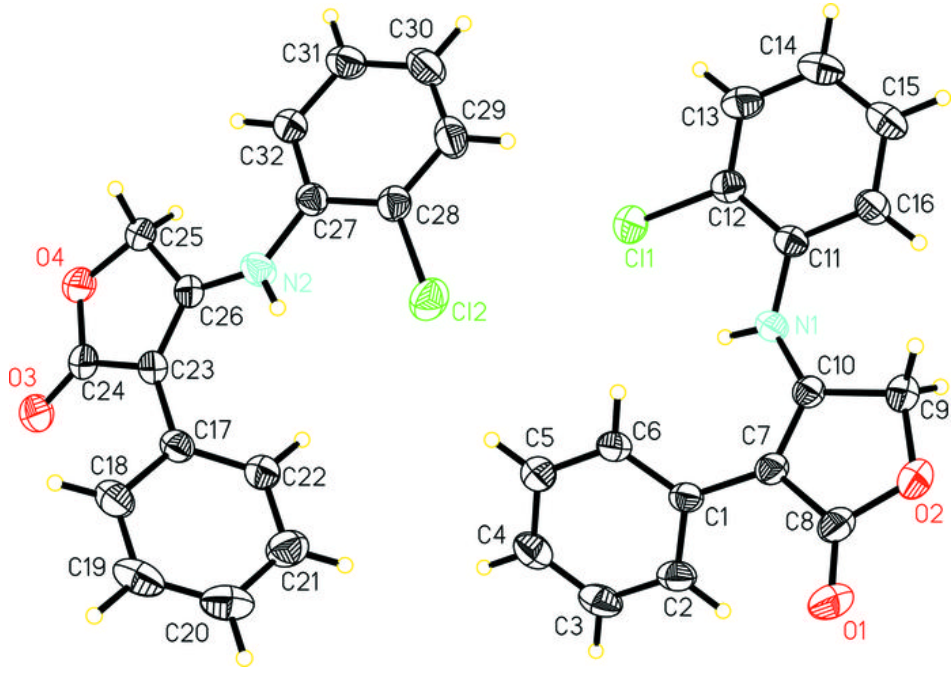
C31
C30
C29
C32
C27
C28
C25
O4
N2
C26
Cl2
O3
C24
C23
C17
C18
C22
C19
C21
C20
C14
C15
C13
C16
C12
Cl1
C11
N1
C10
C9
C5
C6
C7
C1
C8
O2
C4
C2
C3
O1

Fig. 2

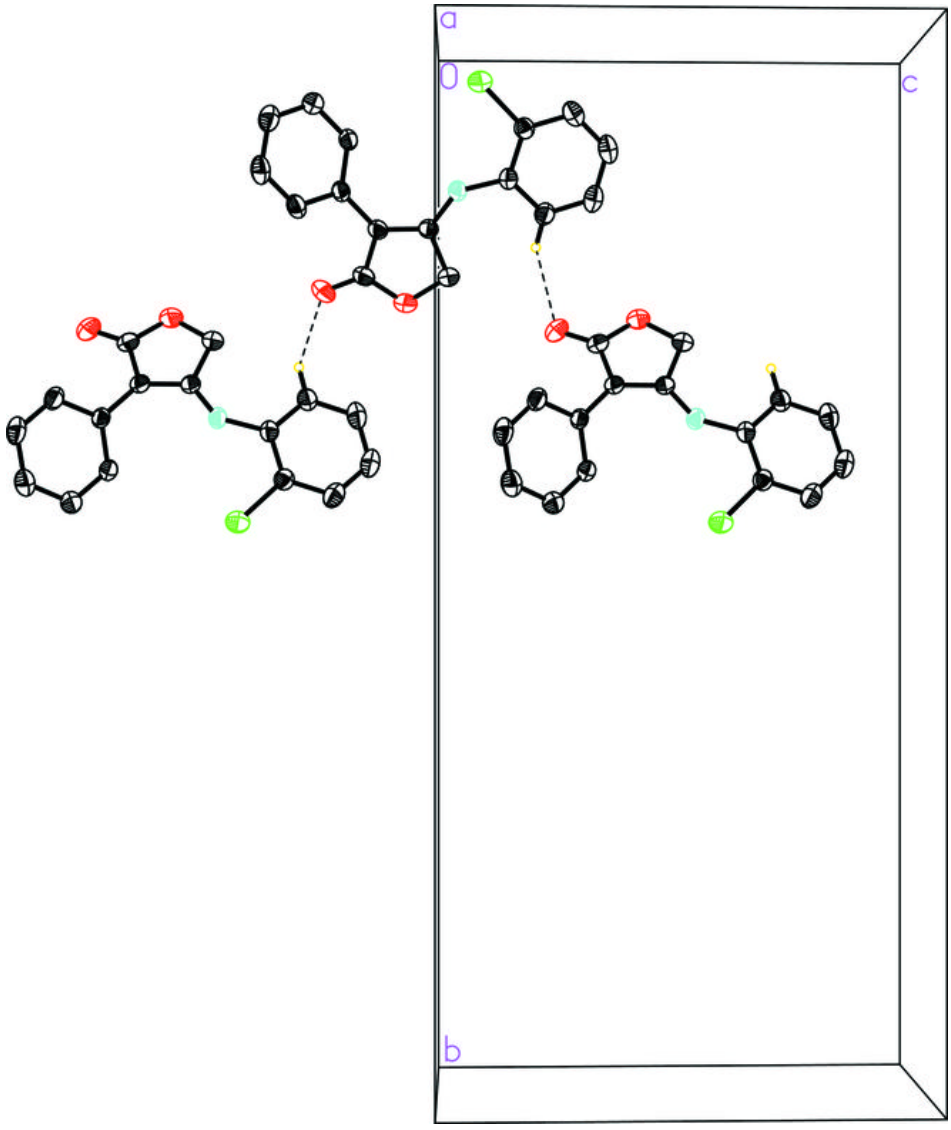

Fig. 3

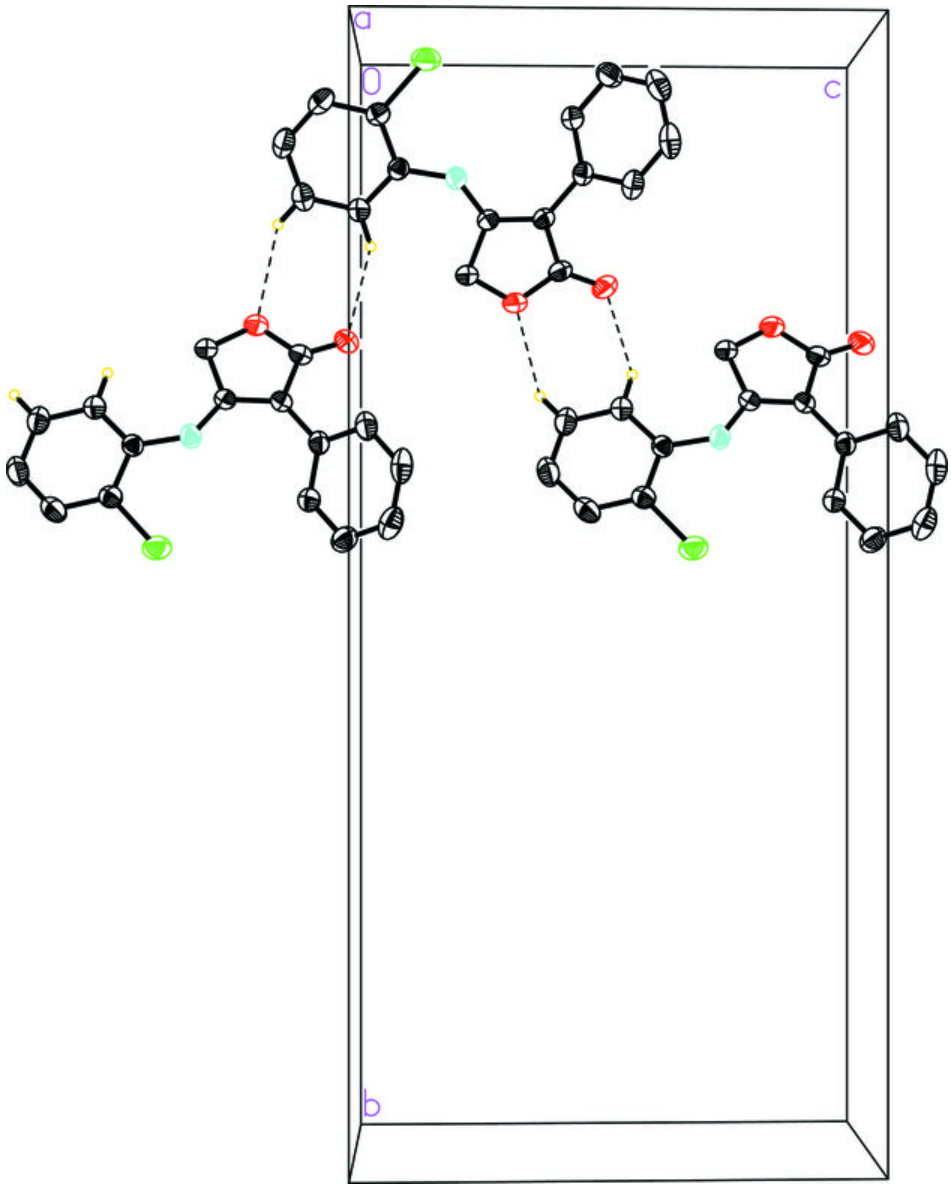

Fig. 4

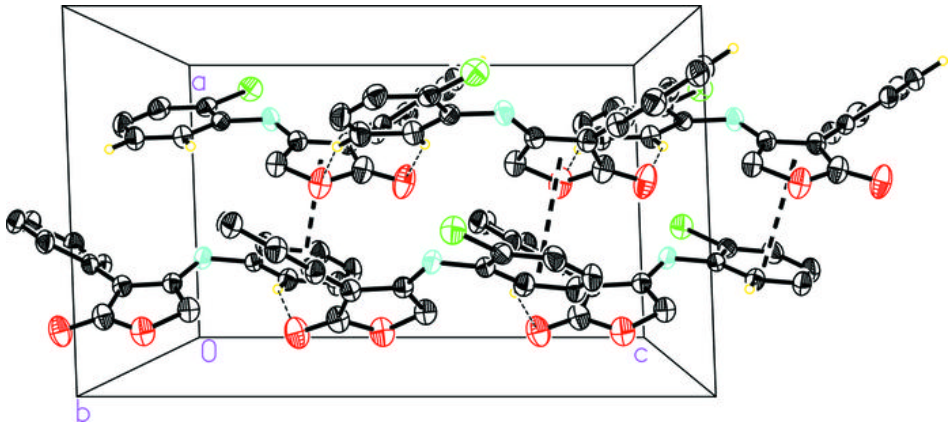

Fig. 5