Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[(4-Chlorophenyl)aminomethyl]-6-methoxyphenol

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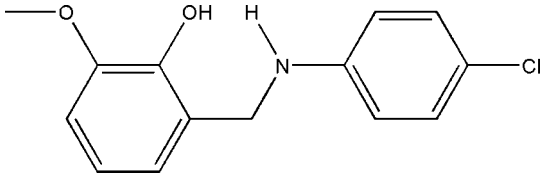
Received 4 June 2007; accepted 6 June 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.053; wR factor = 0.158; data-to-parameter ratio = 13.8.

In the title compound, $C_{14}H_{14}ClNO_2$, molecules are linked by a pair of O—H···O hydrogen bonds, generating dimers involving $R_2^2(10)$ rings. Neighbouring dimers are linked by C—H···π hydrogen bonds into sheets parallel to the (010) plane, and neighbouring sheets are linked into a three-dimensional network structure through N—H···π hydrogen bonds between the dimers.

Related literature

For related literature, see: Allen *et al.* (1987); Bernstein *et al.* (1995); Xia *et al.* (2006, 2007*a*,*b*,*c*).



Experimental

Crystal data

$C_{14}H_{14}ClNO_2$
M_r = 263.71
Monoclinic, $C2/c$
a = 24.346 (2) Å
b = 5.4437 (12) Å
c = 20.478 (2) Å
β = 109.496 (2)°
V = 2558.5 (7) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 298 (2) K
0.59 × 0.42 × 0.30 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.847, T_{max} = 0.918
6143 measured reflections
2264 independent reflections
1305 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.158
S = 1.05
2264 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroid of rings C2–C7 and C9–C14, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*A*···O2	0.82	2.21	2.667 (3)	115
O1—H1*A*···O2^{i}	0.82	2.18	2.965 (3)	161
C7—H7···N1	0.93	2.59	2.917 (5)	101
C6—H6···*Cg*2^{ii}	0.93	3.18	3.906 (2)	136
C1—H1*B*···*Cg*2^{iii}	0.97	3.08	3.996 (2)	159
N1—H1···*Cg*1^{iv}	0.86	2.63	3.437 (6)	157

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the financial support of the Huaihai Institute of Technology Science Foundation.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2320).

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 doi:10.1107/S1600536807027766

supplementary materials

Acta Cryst. (2007). E**63**, o3561 [**doi:10.1107/S1600536807027766**]

2-[(4-Chlorophenyl)aminomethyl]-6-methoxyphenol

Y.-F. Liu, H.-T. Xia, S.-P. Yang and D.-Q. Wang

Comment

We have recently reported the crystal structure of *o*-vanillin diamine derivatives (Xia *et al.*, 2006, 2007*a*, *b*, *c*). We report here the crystal structure of *o*-vanillin 4-chlorobenzen amine derivative(I).

The molecular structure of (I) is illustrated in Fig. 1. In (I), the dihedral angle between the two benzene rings is 88.47 (10)°, the bond lengths and angles are normal (Allen *et al.*, 1987). The molecules are linked into the dimer by a pair of O—H···O hydrogen bonds, atom O1 in the molecule (*x*, *y*, *z*) and O2 in the molecule (1 − *x*, *y*, 1/2 − *z*) act as hydrogen-bond donor to atom O2 in the molecule (1 − *x*, *y*, 1/2 − *z*) and O1 in the molecule (*x*, *y*, *z*), respectively, generating a dimer involving $R_2^2(10)$ rings (Bernstein *et al.*, 1995) (Fig. 2 and Table 1). A neighboring dimers are linked by C—H···π hydrogen bonds into sheets parallel to the [010] plane (Fig. 3), and neighboring sheets are linked into three-dimensional network structure through N—H···π hydrogen bonds between the dimers (Fig. 4).

Experimental

A solution of 2-[(4-chlorophenylimino)methyl]-6-methoxy phenol (10 mmol) in methanol–chloroform (*v*/*v* = 1/1) (20 ml) and $NaBH_4$ (20 mmol) were mixed, the mixture solution was stirred under room temperature for 48 h and then mixtures was filtered, and then solution was left to produce crystals of (I) slowly.

Refinement

All H atoms were located in difference Fourier maps. H atoms were treated as riding atoms, with C—H distances of 0.93 Å (aryl), 0.96 Å (methyl), 0.97 Å (methylene), N—H distances of 0.86 Å (amino) and O—H distances of 0.82 Å and with U_{iso}(H) = 1.2 ($C_{aryl,\ methylene}$ or N_{amino}) or 1.5 U_{eq}(C_{methyl} or $O_{hydroxy}$).

Figures

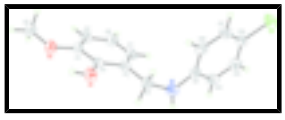

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are at the 30% probability level.

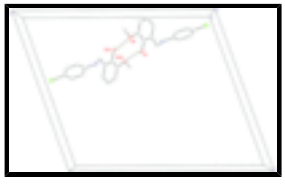

Fig. 2. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded sheet built from O—H···O. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry code: (A) 1 − *x*, *y*, 1/2 − *z*].

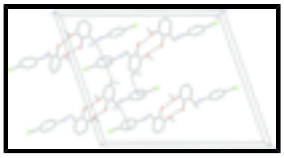

Fig. 3. A larger portion of the crystal structure of (I), showing the formation of a hydrogen-bonded sheet built from C—H···π. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry code: (A) 1 − *x*, *y*, 1/2 − *z*; (F) 1/2 + *x*, 1/2 + *y*, *z*; (I) 1 − *x*, 1 − *y*, 1 − *z*; (J) 1/2 + *x*, 1/2 − *y*, 1/2 + *z*].

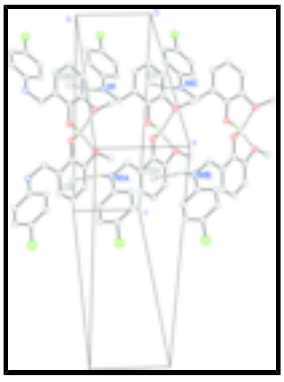

Fig. 4. A different view of the crystal struture of (I), showing the formation of a three-dimensional network struture built from N—H···π hydrogen-bonded. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry code: (A) 1 − *x*, *y*, 1/2 − *z*; (B) 1 − *x*, −1 + *y*, 1/2 − *z*; (C) *x*, −1 + *y*, *z*; (D) *x*, 1 + *y*, *z*; (E) 1 − *x*, 1 + *y*, 1/2 − *z*].

2-[(4-Chlorophenyl)aminomethyl]-6-methoxyphenol

Crystal data

$C_{14}H_{14}ClNO_2$	F_{000} = 1104
M_r = 263.71	D_x = 1.369 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1485 reflections
a = 24.346 (2) Å	θ = 3.2–22.5º
b = 5.4437 (12) Å	μ = 0.29 mm^{-1}
c = 20.478 (2) Å	*T* = 298 (2) K
β = 109.496 (2)º	Block, colourless
V = 2558.5 (7) Å^3	0.59 × 0.42 × 0.30 mm
Z = 8	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2264 independent reflections
Radiation source: fine-focus sealed tube	1305 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.068
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −28→20
T_{min} = 0.847, T_{max} = 0.918	*k* = −6→6
6143 measured reflections	*l* = −24→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.158$	$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 2.5185P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
2264 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
164 parameters	$\Delta\rho_{min} = -0.36$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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}
Cl1	0.04664 (4)	0.6829 (2)	0.07190 (5)	0.0730 (4)
N1	0.30405 (13)	0.7025 (6)	0.17647 (17)	0.0618 (9)
H1	0.3194	0.8409	0.1719	0.074*
O1	0.43176 (9)	0.1644 (5)	0.25625 (10)	0.0528 (7)
H1A	0.4576	0.0604	0.2658	0.079*
O2	0.46516 (10)	−0.1488 (4)	0.17665 (11)	0.0522 (7)
C1	0.34326 (15)	0.5057 (7)	0.20886 (18)	0.0559 (10)
H1B	0.3266	0.4155	0.2386	0.067*
H1C	0.3796	0.5772	0.2382	0.067*
C2	0.35693 (13)	0.3247 (6)	0.15996 (16)	0.0410 (8)
C3	0.40223 (13)	0.1606 (6)	0.18656 (15)	0.0371 (8)
C4	0.41828 (13)	−0.0012 (6)	0.14358 (16)	0.0401 (8)
C5	0.38754 (15)	−0.0042 (7)	0.07349 (16)	0.0492 (9)
H5	0.3976	−0.1139	0.0445	0.059*
C6	0.34193 (15)	0.1566 (7)	0.04686 (17)	0.0530 (10)
H6	0.3210	0.1543	−0.0003	0.064*
C7	0.32685 (15)	0.3204 (7)	0.08898 (17)	0.0492 (9)
H7	0.2963	0.4294	0.0699	0.059*
C8	0.48033 (15)	−0.3420 (7)	0.13784 (19)	0.0556 (10)
H8A	0.4469	−0.4441	0.1170	0.083*
H8B	0.5112	−0.4393	0.1683	0.083*
H8C	0.4930	−0.2716	0.1023	0.083*

C9	0.24382 (14)	0.6881 (7)	0.15203 (18)	0.0457 (9)
C10	0.21322 (16)	0.5003 (7)	0.17032 (18)	0.0528 (9)
H10	0.2333	0.3736	0.1989	0.063*
C11	0.15244 (16)	0.5013 (7)	0.14589 (19)	0.0538 (10)
H11	0.1322	0.3748	0.1582	0.065*
C12	0.12270 (14)	0.6849 (7)	0.10439 (16)	0.0457 (9)
C13	0.15200 (16)	0.8713 (7)	0.08636 (19)	0.0572 (10)
H13	0.1316	0.9980	0.0582	0.069*
C14	0.21174 (17)	0.8717 (7)	0.1099 (2)	0.0567 (10)
H14	0.2313	0.9998	0.0970	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0505 (6)	0.1044 (9)	0.0590 (6)	−0.0045 (6)	0.0117 (5)	−0.0064 (6)
N1	0.0519 (19)	0.0502 (19)	0.083 (2)	−0.0038 (17)	0.0220 (17)	−0.0036 (18)
O1	0.0489 (13)	0.0746 (17)	0.0284 (12)	0.0063 (14)	0.0040 (10)	−0.0055 (13)
O2	0.0528 (14)	0.0581 (16)	0.0402 (13)	0.0090 (13)	0.0081 (11)	−0.0035 (13)
C1	0.045 (2)	0.067 (3)	0.050 (2)	0.005 (2)	0.0076 (17)	−0.009 (2)
C2	0.0374 (17)	0.046 (2)	0.0382 (18)	−0.0056 (17)	0.0108 (15)	−0.0015 (17)
C3	0.0385 (17)	0.0428 (19)	0.0282 (16)	−0.0087 (16)	0.0087 (14)	−0.0015 (16)
C4	0.0407 (18)	0.044 (2)	0.0340 (18)	−0.0035 (17)	0.0110 (15)	0.0001 (17)
C5	0.058 (2)	0.055 (2)	0.0333 (18)	0.000 (2)	0.0135 (17)	−0.0085 (18)
C6	0.058 (2)	0.065 (3)	0.0287 (17)	−0.002 (2)	0.0048 (16)	0.0006 (19)
C7	0.0440 (19)	0.055 (2)	0.044 (2)	−0.0001 (19)	0.0085 (16)	0.0052 (19)
C8	0.060 (2)	0.046 (2)	0.062 (2)	0.002 (2)	0.0216 (19)	−0.004 (2)
C9	0.046 (2)	0.046 (2)	0.047 (2)	−0.0067 (19)	0.0193 (16)	−0.0142 (19)
C10	0.061 (2)	0.046 (2)	0.050 (2)	0.005 (2)	0.0163 (18)	0.0047 (19)
C11	0.060 (2)	0.054 (2)	0.055 (2)	−0.013 (2)	0.0289 (19)	0.000 (2)
C12	0.048 (2)	0.053 (2)	0.0360 (18)	−0.0043 (19)	0.0146 (16)	−0.0067 (18)
C13	0.060 (2)	0.051 (2)	0.054 (2)	0.000 (2)	0.0097 (19)	0.003 (2)
C14	0.061 (2)	0.040 (2)	0.071 (3)	−0.011 (2)	0.025 (2)	0.003 (2)

Geometric parameters (Å, °)

Cl1—C12	1.746 (3)	C6—C7	1.373 (5)
N1—C9	1.384 (4)	C6—H6	0.9300
N1—C1	1.441 (4)	C7—H7	0.9300
N1—H1	0.8600	C8—H8A	0.9600
O1—C3	1.367 (3)	C8—H8B	0.9600
O1—H1A	0.8200	C8—H8C	0.9600
O2—C4	1.375 (4)	C9—C14	1.380 (5)
O2—C8	1.439 (4)	C9—C10	1.388 (5)
C1—C2	1.519 (5)	C10—C11	1.395 (5)
C1—H1B	0.9700	C10—H10	0.9300
C1—H1C	0.9700	C11—C12	1.355 (5)
C2—C3	1.382 (4)	C11—H11	0.9300
C2—C7	1.393 (4)	C12—C13	1.360 (5)
C3—C4	1.390 (4)	C13—C14	1.371 (5)

C4—C5	1.380 (4)	C13—H13	0.9300
C5—C6	1.376 (5)	C14—H14	0.9300
C5—H5	0.9300		
C9—N1—C1	125.7 (3)	C6—C7—H7	119.7
C9—N1—H1	117.1	C2—C7—H7	119.7
C1—N1—H1	117.1	O2—C8—H8A	109.5
C3—O1—H1A	109.5	O2—C8—H8B	109.5
C4—O2—C8	118.6 (3)	H8A—C8—H8B	109.5
N1—C1—C2	115.9 (3)	O2—C8—H8C	109.5
N1—C1—H1B	108.3	H8A—C8—H8C	109.5
C2—C1—H1B	108.3	H8B—C8—H8C	109.5
N1—C1—H1C	108.3	C14—C9—N1	119.7 (3)
C2—C1—H1C	108.3	C14—C9—C10	117.4 (3)
H1B—C1—H1C	107.4	N1—C9—C10	122.9 (3)
C3—C2—C7	118.3 (3)	C9—C10—C11	120.1 (3)
C3—C2—C1	118.8 (3)	C9—C10—H10	120.0
C7—C2—C1	123.0 (3)	C11—C10—H10	120.0
O1—C3—C2	118.3 (3)	C12—C11—C10	120.6 (3)
O1—C3—C4	120.6 (3)	C12—C11—H11	119.7
C2—C3—C4	121.1 (3)	C10—C11—H11	119.7
O2—C4—C5	125.3 (3)	C11—C12—C13	120.1 (3)
O2—C4—C3	114.9 (3)	C11—C12—Cl1	120.7 (3)
C5—C4—C3	119.8 (3)	C13—C12—Cl1	119.1 (3)
C6—C5—C4	119.4 (3)	C12—C13—C14	119.8 (4)
C6—C5—H5	120.3	C12—C13—H13	120.1
C4—C5—H5	120.3	C14—C13—H13	120.1
C7—C6—C5	120.9 (3)	C13—C14—C9	122.1 (3)
C7—C6—H6	119.5	C13—C14—H14	119.0
C5—C6—H6	119.5	C9—C14—H14	119.0
C6—C7—C2	120.6 (3)		
C9—N1—C1—C2	82.9 (4)	C5—C6—C7—C2	−1.0 (5)
N1—C1—C2—C3	167.8 (3)	C3—C2—C7—C6	0.2 (5)
N1—C1—C2—C7	−10.4 (5)	C1—C2—C7—C6	178.4 (3)
C7—C2—C3—O1	−179.9 (3)	C1—N1—C9—C14	−166.9 (3)
C1—C2—C3—O1	1.8 (4)	C1—N1—C9—C10	15.9 (5)
C7—C2—C3—C4	1.3 (5)	C14—C9—C10—C11	0.4 (5)
C1—C2—C3—C4	−177.0 (3)	N1—C9—C10—C11	177.7 (3)
C8—O2—C4—C5	−7.4 (5)	C9—C10—C11—C12	−0.2 (5)
C8—O2—C4—C3	172.5 (3)	C10—C11—C12—C13	−0.3 (5)
O1—C3—C4—O2	−0.6 (4)	C10—C11—C12—Cl1	178.4 (3)
C2—C3—C4—O2	178.1 (3)	C11—C12—C13—C14	0.5 (5)
O1—C3—C4—C5	179.3 (3)	Cl1—C12—C13—C14	−178.1 (3)
C2—C3—C4—C5	−2.0 (5)	C12—C13—C14—C9	−0.3 (6)
O2—C4—C5—C6	−179.0 (3)	N1—C9—C14—C13	−177.5 (3)
C3—C4—C5—C6	1.1 (5)	C10—C9—C14—C13	−0.1 (5)
C4—C5—C6—C7	0.3 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O2	0.82	2.21	2.667 (3)	115
O1—H1A···O2^{i}	0.82	2.18	2.965 (3)	161
C7—H7···N1	0.93	2.59	2.917 (5)	101

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

Fig. 1

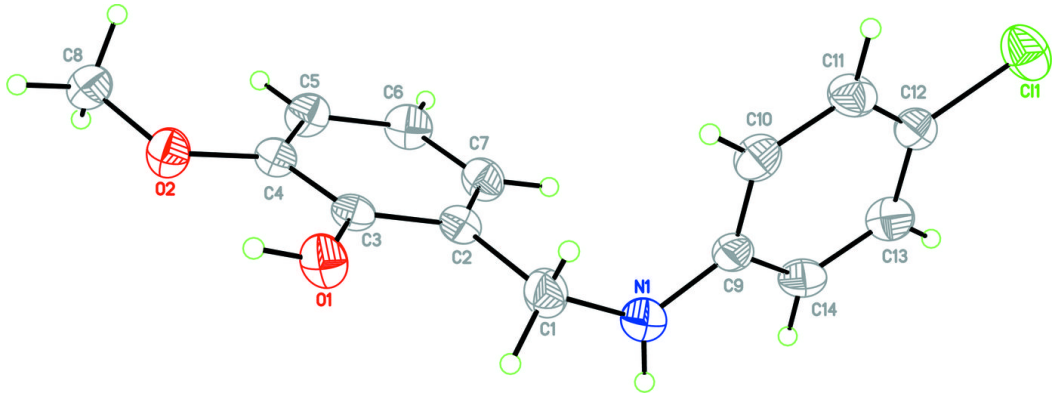

Fig. 2

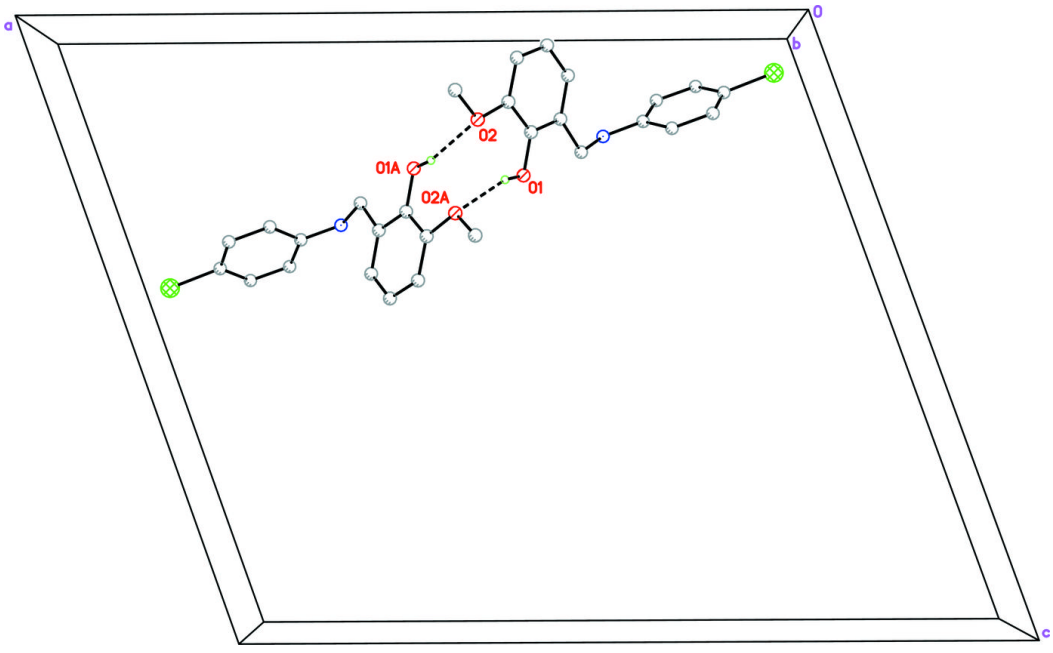

Fig. 3

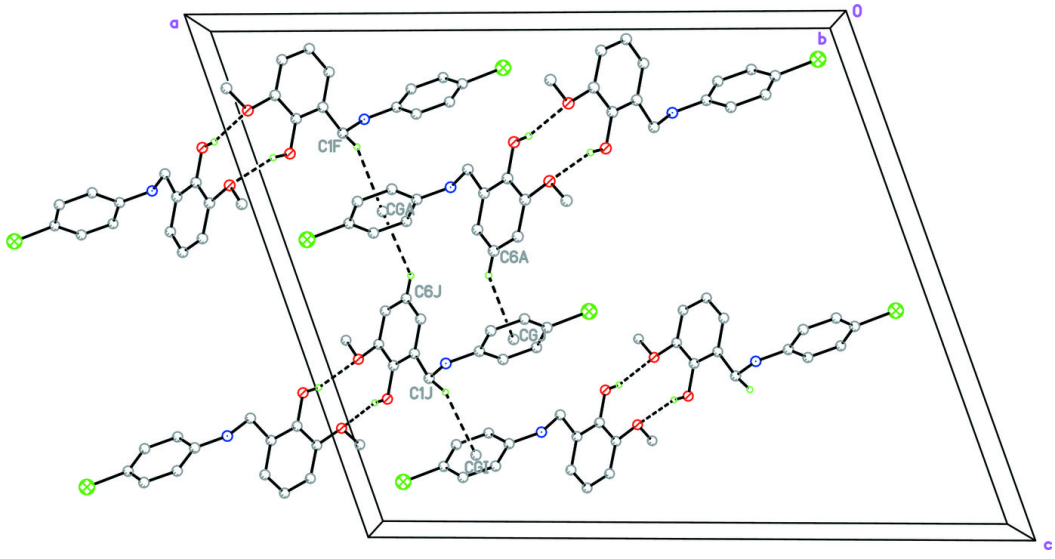

Fig. 4