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(2*Z*)-2-Bromo-3-[3,5-dibromo-4-(ethylamino)phenyl]-1-(2,4-dichlorophenyl)prop-2-en-1-one

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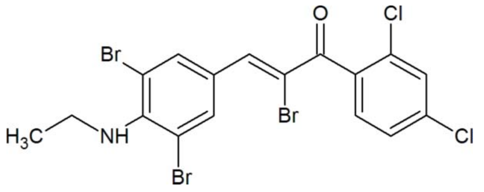
Key indicators: single-crystal X-ray study; *T* = 296 K; mean σ(C–C) = 0.012 Å; *R* factor = 0.067; *wR* factor = 0.275; data-to-parameter ratio = 25.5.

In the title compound, $C_{17}H_{12}Br_3Cl_2NO$, the mean planes of the 3,5-dibromo-4-phenyl and 2,4-dichlorophenyl groups make a dihedral angle of 72.4 (2)°. The dihedral angles between the 2-bromoprop-2-en-1-one group and the two phenyl ring groups (3,5-dibromo-4-phenyl and 2,4-dichlorophenyl) are 71.1 (1) and 10.9 (4)°, respectively. The crystal packing is stabilized by intermolecular N—H···O hydrogen-bond interactions between the ethylamino H atom and the propyl ketone O atom, with the 3,5-dibromo-4-phenyl rings linked in chains in an alternate inverted pattern parallel and oblique to the *ac* face and diagonally along the *a* axis of the unit cell. An intramolecular hydrogen bond between the ethyl amino H atom and the 5-Br atom from the 3,5-dibromo-4-phenyl group helps stabilize the molecular conformation.

Related literature

For related structures see: Butcher *et al.* (2006*a*,*b*); Harrison *et al.* (2006). For related literature see: Fichou *et al.* (1988); Tam *et al.* (1989); Goto *et al.* (1991); Cho *et al.* (1996); Uchida *et al.* (1998); Holla *et al.* (2001, 2006); Indira *et al.* (2002); Zhao *et al.* (2002); Sarojini *et al.* (2006); Shivarama Holla *et al.* (2001).



Experimental

Crystal data

$C_{17}H_{12}Br_3Cl_2NO$
M_r = 556.91
Monoclinic, $P2_1/n$
a = 9.7939 (4) Å
b = 9.7333 (4) Å
c = 19.4436 (6) Å
β = 91.635 (3)°
V = 1852.74 (12) Å^3
Z = 4
Mo *K*α radiation
μ = 6.83 mm^{-1}
T = 296 K
0.51 × 0.43 × 0.29 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.550, T_{max} = 1.000 (expected range = 0.076–0.138)
18303 measured reflections
5670 independent reflections
1957 reflections with *I* > 2σ(*I*)
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.275
S = 1.04
5670 reflections
222 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −1.22 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^i	0.89 (10)	2.37 (10)	3.207 (10)	158 (9)
N1—H1···Br3	0.89 (10)	2.63 (10)	3.070 (8)	112 (8)

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2025).

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supplementary materials

Acta Cryst. (2007). E**63**, o4308-o4309 [**doi:10.1107/S160053680704946X**]

(2*Z*)-2-Bromo-3-[3,5-dibromo-4-(ethylamino)phenyl]-1-(2,4-dichlorophenyl)prop-2-en-1-one

R. J. Butcher, **J. P. Jasinski**, **A. N. Mayekar**, **B. Narayana** and **H. S. Yathirajan**

Comment

The important goal of crystal growth is the improvement of microscopic and macroscopic homogeneity, which is a necessity for any application. Different types of crystals being used are semiconductor crystals, oxide crystals, alkali halide crystals and non-linear optical (NLO) crystals. The NLO effect in the organic molecules originates from a strong donor-acceptor intermolecular interaction, delocalized π-electron system, and also due to the ability to crystallize in a non-centrosymmetric space group. Among several organic compounds reported for NLO property, chalcone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability. They provide a necessary configuration to show NLO property with two planar rings connected through a conjugated double bond (Goto *et al.* 1991; Uchida *et al.* 1998; Tam *et al.* 1989; Indira *et al.* 2002, Sarojini *et al.* 2006). Substitution on either of the phenyl rings greatly influences non-centrosymmetric crystal packing. It is speculated that in order to improve the activity, more bulky substituents should be introduced to increase the spontaneous polarization of an noncentrosymmetric crystal (Fichou *et al.* 1988). The molecular hyperpolarizability β are strongly influenced not only by the electronic effect but also by the steric effect of the substituent (Cho *et al.* 1996). A bromo group, therefore, can obviously improve the molecular first order hyperpolarizabilities and can effectively reduce the dipole-dipole interactions between the molecules (Zhao *et al.* 2002). Alpha-bromochalcones are used to synthesize triazolothiadiazines which showed promising antiproliferative activity (Holla *et al.* 2001, 2006). The structures of a few alpha-bromochalcones *viz*., 2-bromo-1-(4-methylphenyl)-3-[4-(methylsulfanyl)phenyl] prop-2-en-1-one (Butcher *et al.* 2006*a*); 2-bromo-3-hydroxy-1-(4-methylphenyl)-3-[4-(methylsulfanyl)phenyl] propan-1-one (Butcher *et al.* 2006*b*) and 2-Bromo-1-chlorophenyl-3-(4-methoxyphenyl)prop-2-en-1-one (Harrison *et al.* 2006) have been published. Prompted by this and in continuation of our quest to synthesize newer materials which can find use in Photonics industries, we have synthesized a new a-bromochalcone, (I), $C_{17}H_{12}Br_3Cl_2NO$ and its crystal structure is reported here.

The mean planes of the 3,5-dibromo-4-phenyl and 2,4-dichlorophenyl groups are separated by a dihedral angle of 72.4 (2)° (Fig. 1). The dihedral angles between the 2-bromo-prop-2-en-1-one group and the two phenyl ring groups (3,5-dibromo-4-phenyl and 2,4-dichlorophenyl) are 71.1 (1) and 10.9 (4)°, respectively.

Crystal packing is stabilized by intermolecular N1—H1···O1 hydrogen bond interactions between the ethyl amino hydrogen atom (H1) and the propyl ketone oxygen atom (O1) with the 3,5-dibromo-4-phenyl rings linked in chains in an alternate inverted pattern parallel and oblique to the *ac* face and diagonal along the *a* axis of the unit cell (Fig. 2). Intramolecular hydrogen bonds between the ethyl amino hydrogen atom and the 5-bromo atom from the 3,5-dibromo-4-phenyl group [N1—H1···Br3 (H1···Br3 = 2.63 (0))] Å] provide additonal strength to the molecule within the asymmetric unit.

Experimental

2,3-Dibromo-3-[3,5-dibromo-4-(ethylamino)phenyl]-1- (2,4-dichlorophenyl)propan-1-one (6.37 g, 0.01 mol) is mixed with triethylamine (5 ml, 0.05 mol) in toluene (80 ml) (Fig. 3). This mixture was stirred well for 24 hrs. and the precipitated triethyamine hydrobromide was filtered. [Triethylene hydrobromide is produced during the dehydrobrominaton of the corresponding 2,3 dibromopropanone. The HBr produced forms a salt with triethyl amine which is added to dehydrobominate the chalcone dibromide and the reaction produces 2-bromopropenone (Shivarama Holla *et al.*, 2001)]. The solvent was then removed under reduced pressure. The resulting solid mass obtained on cooling was collected by filtration. The compound was dried and recrystallized from a 1: 1 mixture of acetone: toluene (m.p.: 393–395 K). Analysis found: C 36.58, H 2.14, N 2.47%; $C_{17}H_{12}Br_3Cl_2NO$ requires: C 36.66, H 2.17, N 2.52%.

Refinement

H1 was refined isotropically [N1—H1 = 0.89 (1) Å] and all other H atoms were then refined using a riding model with and C—H = 0.93–0.97 Å, and with $U_{iso}(H) = 1.19–1.49U_{eq}(C,N)$. The maximum residual electron density peaks of 0.91 and −1.22 e Å^3, were located at 0.08 and 0.65Å from Br3 and Br2, respectively.

Figures

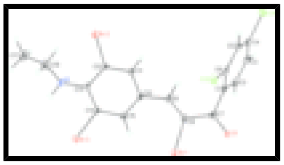

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids.

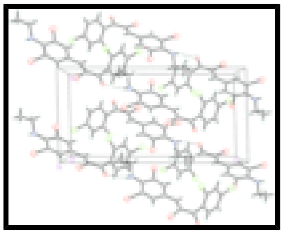

Fig. 2. Packing diagram of the title compound, viewed down the *b* axis. Dashed lines indicate intermolecular N—H···O hydrogen bonds.

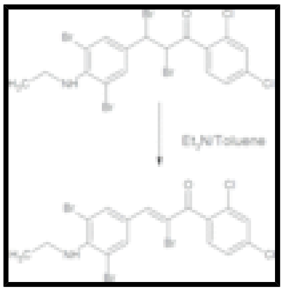

Fig. 3. Synthesis scheme for $C_{17}H_{12}Br_3Cl_2NO$.

(2*Z*)-2-Bromo-3-[3,5-dibromo-4-(ethylamino)phenyl]-1- (2,4-dichlorophenyl)prop-2-en-1-one

Crystal data

$C_{17}H_{12}Br_3Cl_2NO$

$M_r = 556.91$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 9.7939\ (4)$ Å

$b = 9.7333\ (4)$ Å

$c = 19.4436\ (6)$ Å

$F_{000} = 1072$

$D_x = 1.997$ Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 4393 reflections

θ = 4.7–32.4°

μ = 6.83 mm^{-1}

$T = 296$ K

$\beta = 91.635\ (3)°$

$V = 1852.74\ (12)$ Å^3

$Z = 4$

Chunk, pale yellow

$0.51 \times 0.43 \times 0.29$ mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 10.5081 pixels mm^{-1}

$T = 296$ K

φ and ω scans

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

$T_{\text{min}} = 0.550$, $T_{\text{max}} = 1.000$

18303 measured reflections

5670 independent reflections

1957 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\text{max}} = 32.5°$

$\theta_{\text{min}} = 4.7°$

$h = -13 \rightarrow 14$

$k = -10 \rightarrow 14$

$l = -28 \rightarrow 27$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2) = 0.275$

$S = 1.04$

5670 reflections

222 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.1284P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\text{max}} = 0.91$ e Å^{-3}

$\Delta\rho_{\text{min}} = -1.22$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0063 (12)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	1.08392 (12)	0.40693 (12)	−0.08410 (5)	0.0801 (4)
Br2	0.61985 (14)	−0.18958 (12)	−0.00324 (6)	0.0859 (5)
Br3	0.91770 (10)	0.21197 (11)	0.15167 (4)	0.0642 (4)
Cl1	0.8346 (3)	−0.0762 (3)	−0.44044 (14)	0.0842 (8)
Cl2	0.7686 (2)	0.3262 (3)	−0.25570 (12)	0.0642 (6)
O1	1.1575 (7)	0.3537 (7)	−0.2283 (3)	0.0708 (19)
N1	0.6938 (7)	−0.0046 (9)	0.1267 (4)	0.062 (2)
H1	0.704 (10)	0.051 (10)	0.163 (5)	0.075*
C1	1.0030 (8)	0.1851 (8)	−0.2672 (4)	0.0458 (19)
C2	1.0855 (8)	0.0894 (10)	−0.2993 (4)	0.053 (2)
H2A	1.1759	0.0792	−0.2842	0.064*
C3	1.0360 (9)	0.0096 (10)	−0.3528 (5)	0.062 (2)
H3A	1.0923	−0.0533	−0.3741	0.075*
C4	0.9006 (11)	0.0247 (10)	−0.3744 (5)	0.064 (2)
C5	0.8164 (9)	0.1187 (9)	−0.3441 (4)	0.055 (2)
H5A	0.7260	0.1287	−0.3592	0.066*
C6	0.8700 (9)	0.1993 (9)	−0.2898 (4)	0.053 (2)
C7	1.0664 (8)	0.2737 (9)	−0.2120 (4)	0.054 (2)
C8	1.0235 (8)	0.2615 (9)	−0.1405 (4)	0.050 (2)
C9	0.9444 (8)	0.1596 (8)	−0.1201 (4)	0.0458 (18)
H9A	0.9182	0.1008	−0.1558	0.055*
C10	0.8895 (7)	0.1190 (8)	−0.0547 (3)	0.0434 (18)
C11	0.7920 (8)	0.0112 (7)	−0.0549 (4)	0.0407 (16)
H11A	0.7680	−0.0309	−0.0965	0.049*
C12	0.7322 (7)	−0.0329 (9)	0.0036 (4)	0.0477 (19)
C13	0.7570 (8)	0.0320 (8)	0.0678 (4)	0.0440 (18)
C14	0.8579 (8)	0.1315 (8)	0.0674 (3)	0.0429 (17)
C15	0.9201 (8)	0.1790 (8)	0.0082 (4)	0.0439 (18)
H15A	0.9823	0.2511	0.0112	0.053*
C16	0.5512 (11)	−0.0216 (13)	0.1337 (5)	0.083 (3)
H16A	0.5113	−0.0515	0.0900	0.099*
H16B	0.5111	0.0665	0.1448	0.099*
C17	0.5162 (16)	−0.1207 (15)	0.1867 (8)	0.121 (5)
H17A	0.4215	−0.1451	0.1814	0.181*
H17B	0.5326	−0.0808	0.2313	0.181*
H17C	0.5714	−0.2015	0.1822	0.181*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.1079 (9)	0.0730 (8)	0.0607 (6)	−0.0378 (6)	0.0233 (5)	−0.0105 (5)
Br2	0.1158 (10)	0.0712 (8)	0.0718 (7)	−0.0343 (6)	0.0229 (6)	−0.0091 (5)
Br3	0.0769 (7)	0.0760 (7)	0.0400 (5)	−0.0135 (5)	0.0057 (4)	−0.0073 (4)
Cl1	0.094 (2)	0.0786 (18)	0.0798 (18)	−0.0087 (15)	−0.0026 (14)	−0.0277 (14)

Cl2	0.0594 (14)	0.0731 (16)	0.0606 (13)	0.0116 (11)	0.0109 (10)	−0.0024 (11)
O1	0.090 (5)	0.073 (4)	0.050 (3)	−0.034 (4)	0.019 (3)	−0.006 (3)
N1	0.047 (4)	0.096 (7)	0.044 (4)	−0.017 (4)	0.009 (3)	0.010 (4)
C1	0.055 (5)	0.042 (5)	0.040 (4)	−0.001 (4)	0.000 (3)	0.020 (3)
C2	0.038 (4)	0.062 (6)	0.061 (5)	0.017 (4)	0.017 (3)	0.013 (4)
C3	0.044 (5)	0.060 (6)	0.084 (6)	0.009 (4)	0.027 (4)	0.009 (5)
C4	0.080 (7)	0.063 (6)	0.050 (5)	−0.017 (5)	0.017 (4)	0.005 (4)
C5	0.057 (5)	0.059 (5)	0.047 (5)	−0.020 (4)	−0.011 (4)	0.002 (4)
C6	0.059 (5)	0.052 (5)	0.049 (4)	0.010 (4)	0.015 (4)	0.016 (4)
C7	0.045 (5)	0.062 (6)	0.054 (5)	−0.009 (4)	0.003 (4)	0.009 (4)
C8	0.042 (4)	0.064 (6)	0.043 (4)	0.012 (4)	0.002 (3)	0.012 (4)
C9	0.053 (5)	0.045 (4)	0.041 (4)	0.001 (4)	0.011 (3)	0.013 (3)
C10	0.037 (4)	0.059 (5)	0.034 (3)	0.002 (3)	−0.001 (3)	0.019 (3)
C11	0.040 (4)	0.035 (4)	0.047 (4)	0.006 (3)	0.000 (3)	−0.006 (3)
C12	0.029 (4)	0.063 (5)	0.051 (4)	−0.018 (3)	0.006 (3)	−0.001 (4)
C13	0.049 (4)	0.045 (4)	0.038 (4)	0.006 (4)	0.006 (3)	0.003 (3)
C14	0.052 (5)	0.045 (4)	0.033 (3)	−0.005 (4)	0.018 (3)	0.005 (3)
C15	0.051 (4)	0.044 (5)	0.037 (4)	−0.005 (4)	−0.005 (3)	0.005 (3)
C16	0.073 (8)	0.105 (9)	0.071 (7)	0.012 (6)	−0.001 (5)	−0.005 (6)
C17	0.140 (13)	0.093 (10)	0.131 (11)	−0.042 (9)	0.048 (9)	0.023 (9)

Geometric parameters (Å, °)

Br1—C8	1.877 (9)	C7—C8	1.468 (11)
Br2—C12	1.882 (8)	C8—C9	1.327 (11)
Br3—C14	1.894 (7)	C9—C10	1.449 (9)
Cl1—C4	1.728 (10)	C9—H9A	0.9300
Cl2—C6	1.729 (9)	C10—C15	1.380 (10)
O1—C7	1.232 (10)	C10—C11	1.419 (11)
N1—C13	1.366 (10)	C11—C12	1.364 (11)
N1—C16	1.418 (13)	C11—H11A	0.9300
N1—H1	0.89 (10)	C12—C13	1.414 (10)
C1—C6	1.369 (11)	C13—C14	1.383 (11)
C1—C2	1.393 (11)	C14—C15	1.396 (10)
C1—C7	1.497 (12)	C15—H15A	0.9300
C2—C3	1.375 (13)	C16—C17	1.459 (16)
C2—H2A	0.9300	C16—H16A	0.9700
C3—C4	1.388 (13)	C16—H16B	0.9700
C3—H3A	0.9300	C17—H17A	0.9600
C4—C5	1.375 (14)	C17—H17B	0.9600
C5—C6	1.405 (12)	C17—H17C	0.9600
C5—H5A	0.9300		
C13—N1—C16	125.6 (8)	C15—C10—C11	116.4 (6)
C13—N1—H1	118 (7)	C15—C10—C9	125.9 (7)
C16—N1—H1	95 (7)	C11—C10—C9	117.7 (7)
C6—C1—C2	118.8 (8)	C12—C11—C10	122.4 (7)
C6—C1—C7	122.9 (8)	C12—C11—H11A	118.8
C2—C1—C7	118.2 (7)	C10—C11—H11A	118.8
C3—C2—C1	121.4 (8)	C11—C12—C13	121.9 (7)

C3—C2—H2A	119.3	C11—C12—Br2	117.4 (6)
C1—C2—H2A	119.3	C13—C12—Br2	120.7 (6)
C2—C3—C4	118.8 (8)	N1—C13—C14	121.9 (7)
C2—C3—H3A	120.6	N1—C13—C12	123.6 (8)
C4—C3—H3A	120.6	C14—C13—C12	114.4 (7)
C5—C4—C3	121.4 (9)	C13—C14—C15	124.4 (7)
C5—C4—Cl1	118.7 (8)	C13—C14—Br3	119.2 (5)
C3—C4—Cl1	119.9 (8)	C15—C14—Br3	116.4 (6)
C4—C5—C6	118.5 (8)	C10—C15—C14	120.1 (7)
C4—C5—H5A	120.8	C10—C15—H15A	120.0
C6—C5—H5A	120.8	C14—C15—H15A	120.0
C1—C6—C5	121.2 (8)	N1—C16—C17	113.4 (10)
C1—C6—Cl2	120.0 (7)	N1—C16—H16A	108.9
C5—C6—Cl2	118.7 (7)	C17—C16—H16A	108.9
O1—C7—C8	121.6 (8)	N1—C16—H16B	108.9
O1—C7—C1	117.9 (8)	C17—C16—H16B	108.9
C8—C7—C1	120.5 (7)	H16A—C16—H16B	107.7
C9—C8—C7	122.0 (8)	C16—C17—H17A	109.5
C9—C8—Br1	124.5 (6)	C16—C17—H17B	109.5
C7—C8—Br1	113.4 (6)	H17A—C17—H17B	109.5
C8—C9—C10	134.5 (8)	C16—C17—H17C	109.5
C8—C9—H9A	112.8	H17A—C17—H17C	109.5
C10—C9—H9A	112.8	H17B—C17—H17C	109.5

C6—C1—C2—C3	0.0 (12)	Br1—C8—C9—C10	−5.1 (14)
C7—C1—C2—C3	−176.5 (7)	C8—C9—C10—C15	−5.9 (14)
C1—C2—C3—C4	−0.7 (13)	C8—C9—C10—C11	171.8 (9)
C2—C3—C4—C5	1.0 (13)	C15—C10—C11—C12	−0.7 (11)
C2—C3—C4—Cl1	−178.8 (7)	C9—C10—C11—C12	−178.7 (7)
C3—C4—C5—C6	−0.6 (13)	C10—C11—C12—C13	4.1 (12)
Cl1—C4—C5—C6	179.2 (6)	C10—C11—C12—Br2	−173.3 (6)
C2—C1—C6—C5	0.4 (11)	C16—N1—C13—C14	134.1 (10)
C7—C1—C6—C5	176.7 (7)	C16—N1—C13—C12	−50.0 (14)
C2—C1—C6—Cl2	−175.0 (6)	C11—C12—C13—N1	176.5 (8)
C7—C1—C6—Cl2	1.4 (10)	Br2—C12—C13—N1	−6.1 (11)
C4—C5—C6—C1	−0.1 (12)	C11—C12—C13—C14	−7.3 (11)
C4—C5—C6—Cl2	175.4 (6)	Br2—C12—C13—C14	170.1 (6)
C6—C1—C7—O1	−112.8 (10)	N1—C13—C14—C15	−176.0 (8)
C2—C1—C7—O1	63.6 (11)	C12—C13—C14—C15	7.8 (12)
C6—C1—C7—C8	69.0 (11)	N1—C13—C14—Br3	3.7 (11)
C2—C1—C7—C8	−114.6 (9)	C12—C13—C14—Br3	−172.6 (6)
O1—C7—C8—C9	−167.5 (9)	C11—C10—C15—C14	1.0 (11)
C1—C7—C8—C9	10.6 (12)	C9—C10—C15—C14	178.8 (7)
O1—C7—C8—Br1	15.4 (11)	C13—C14—C15—C10	−4.9 (12)
C1—C7—C8—Br1	−166.6 (6)	Br3—C14—C15—C10	175.4 (6)
C7—C8—C9—C10	178.1 (8)	C13—N1—C16—C17	151.4 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N1—H1···O1^{i}	0.89 (10)	2.37 (10)	3.207 (10)	158 (9)
N1—H1···Br3	0.89 (10)	2.63 (10)	3.070 (8)	112 (8)

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

Fig. 1

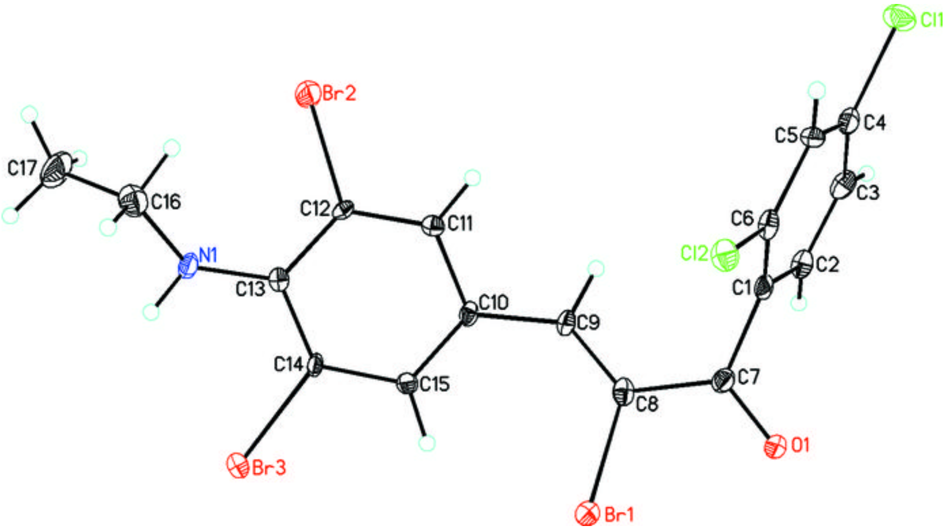
Cl1
Br2
C5
C4
C17
C16
C12
C11
C3
C6
N1
Cl2
C2
C13
C1
C10
C9
C14
C15
C7
C8
O1
Br3
Br1

Fig. 2

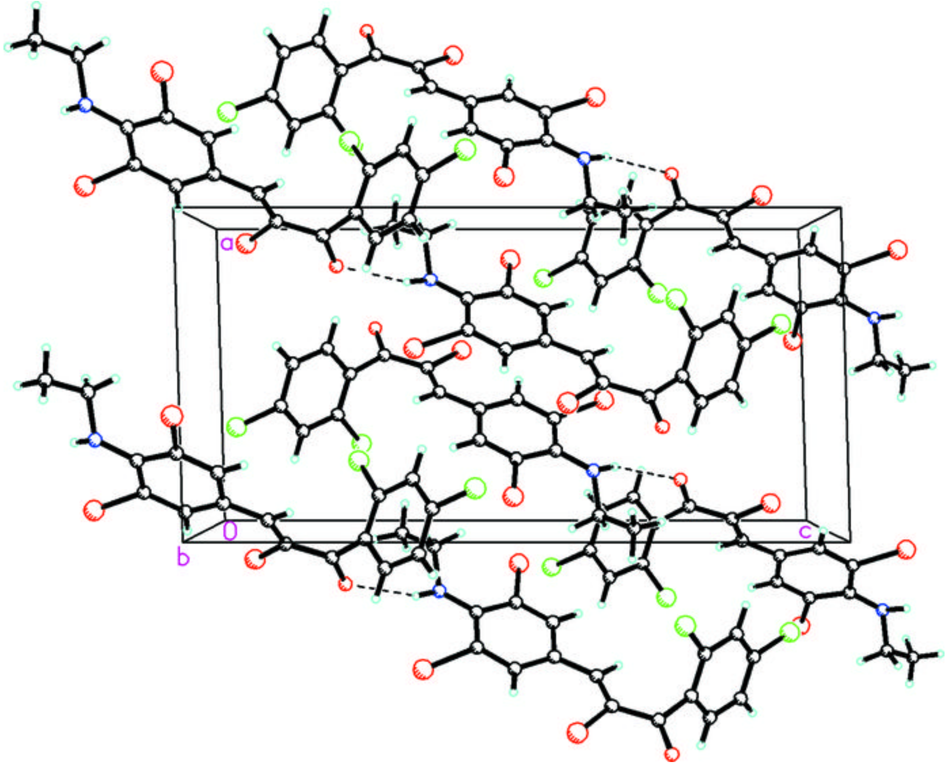

Fig. 3