organic compounds

1-(2,4-Dichlorophenyl)-3-[4-(dimethyl-amino)phenyl]prop-2-enone

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In the title compound, $C_{17}H_{15}Cl_2NO$, the dimethylaminophenyl group is close to coplanar with the central propenone group [dihedral angle = 13.1 (1)° between the mean planes], while the dichlorophenyl group is twisted from the plane [dihedral angle = 64.0 (1)°]. In the crystal, $C-H\cdots O$ and weak $C-H\cdots\pi$ interactions are formed between molecules.

Related literature

For related structures, see: Murafuji *et al.* (1999); Liu *et al.* (2002); Patil *et al.* (2007a,b); Rosli *et al.* (2007).
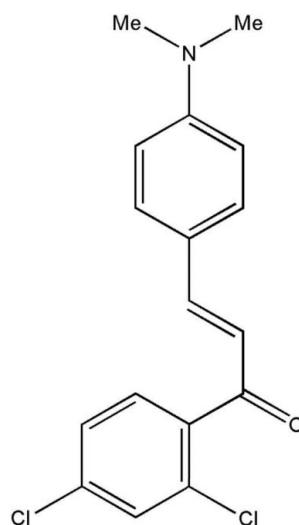
Experimental

Crystal data

$C_{17}H_{15}Cl_2NO$	Monoclinic, $P2_1/c$
M_r = 320.20	a = 8.5741 (19) Å
b = 12.706 (3) Å	Mo $K\alpha$ radiation
c = 14.671 (3) Å	μ = 0.41 mm^{-1}
β = 102.645 (4)°	T = 290 K
V = 1559.5 (6) Å^3	$0.25 \times 0.15 \times 0.07$ mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	11540 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2908 independent reflections
T_{min} = 0.923, T_{max} = 0.972	2039 reflections with $I > 2\sigma(I)$
	R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042	192 parameters
$wR(F^2)$ = 0.106	H-atom parameters constrained
S = 1.03	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
2908 reflections	$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12$\cdots$O1^i	0.93	2.55	3.252 (3)	132
C4—H4$\cdots$Cg1^{ii}	0.93	2.95	3.784 (3)	150

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$. Cg1 is the centroid of the C10–C15 ring.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2009).

References

Bruker (2004). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Liu, Z.-Q., Fang, Q., Yu, W.-T., Xue, G., Cao, D.-X. & Jiang, M.-H. (2002). *Acta Cryst.* C**58**, o445–o446.
Murafuji, T., Sugihara, Y., Moriya, T., Mikata, Y. & Yan, S. (1999). *New J. Chem.* **23**, 683–685.
Patil, P. S., Chantrapromma, S., Fun, H.-K. & Dharmaprakash, S. M. (2007a). *Acta Cryst.* E**63**, o1738–o1740.
Patil, P. S., Chantrapromma, S., Fun, H.-K. & Dharmaprakash, S. M. (2007b). *Acta Cryst.* E**63**, o3253–o3254.
Rosli, M. M., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2007). *Acta Cryst.* E**63**, o2692.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Watkin, D. J., Pearce, L. & Prout, C. K. (1993). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.

supporting information

1-(2,4-Dichlorophenyl)-3-[4-(dimethylamino)phenyl]prop-2-enone

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S1. Experimental

A solution of potassium hydroxide (6.25 g, 0.11 mol) in ethanol (25 ml) was added slowly to a mixture of dichloroaceto-phenone (18.8 g, 0.01 mol) and *N*-dimethyl benzaldehyde (14.9 g, 0.01 mol) in a conical flask. After stirring for two hours, the precipitate was filtered and recrystallized from ethanol to give pale orange crystals.

S2. Refinement

H atoms were positioned geometrically with C—H bond lengths of 0.93–0.96 Å and refined using a riding model with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.
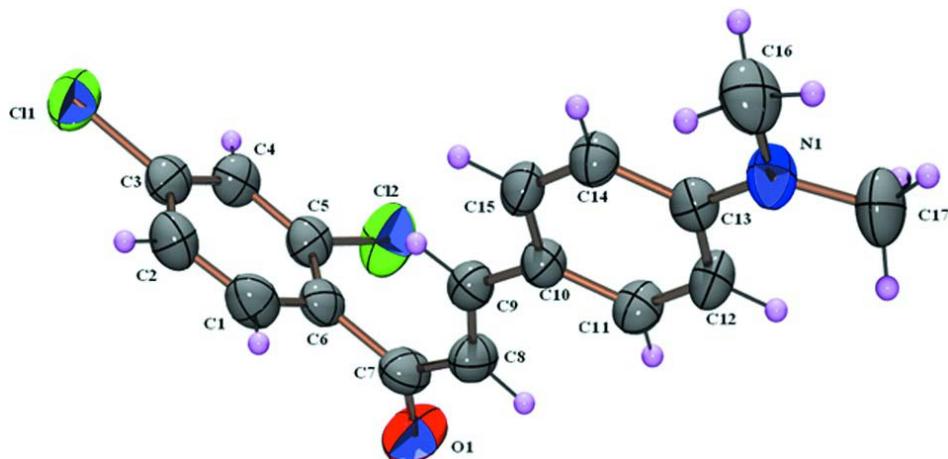
Figure 1

The molecular structure with displacement ellipsoids drawn at the 50% probability level for non-H atoms. H atoms are shown as small spheres of arbitrary radius.
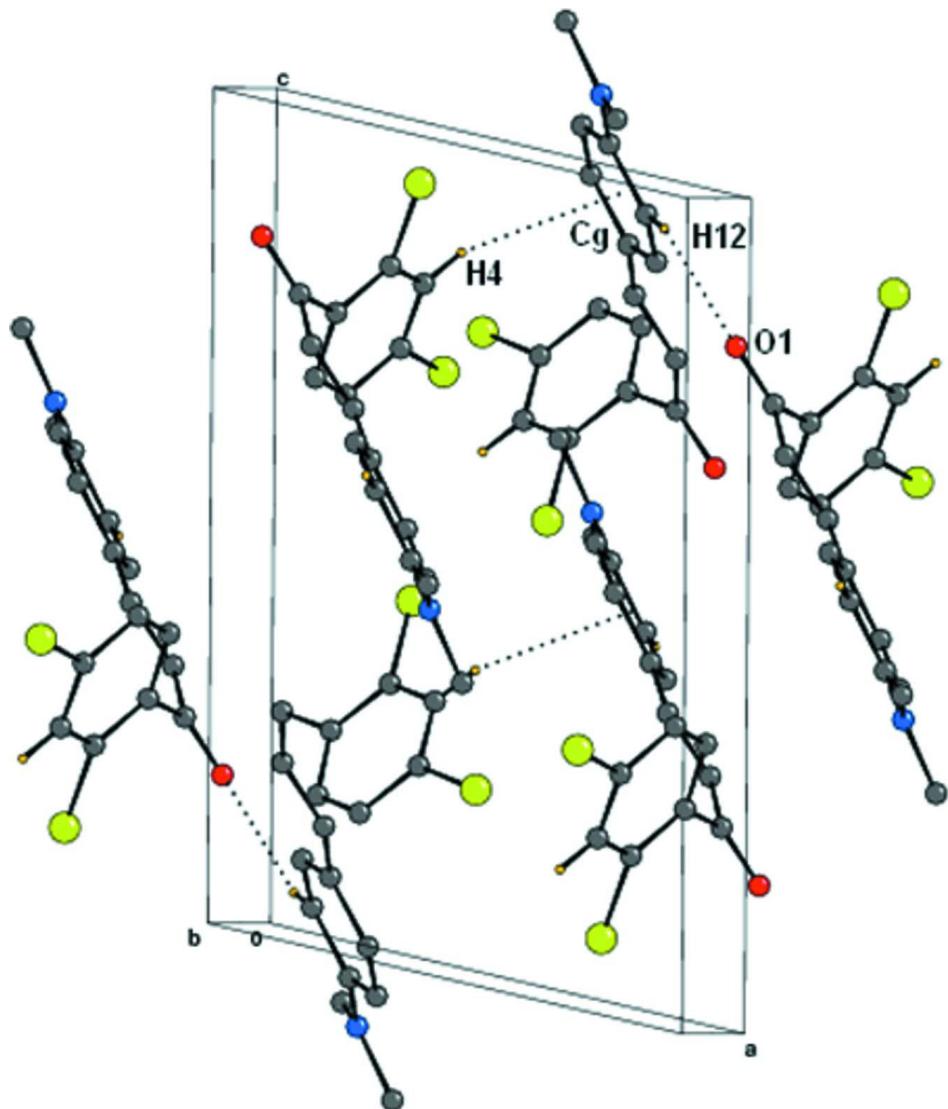
Figure 2

Packing diagram. The dotted lines indicate intermolecular C—H···O and C—H···π interactions.

1-(2,4-Dichlorophenyl)-3-[4-(dimethylamino)phenyl]prop-2-enone

Crystal data

$C_{17}H_{15}Cl_2NO$	$F(000) = 664$
$M_r = 320.20$	$D_x = 1.364$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3980 reflections
$a = 8.5741$ (19) Å	$\theta = 2.0–26.0°$
$b = 12.706$ (3) Å	$\mu = 0.41$ mm^{-1}
$c = 14.671$ (3) Å	$T = 290$ K
$\beta = 102.645$ (4)°	Block, orange
$V = 1559.5$ (6) Å^3	$0.25 \times 0.15 \times 0.07$ mm
$Z = 4$	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	11540 measured reflections
Radiation source: fine-focus sealed tube	2908 independent reflections
Graphite monochromator	2039 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.031$
Absorption correction: multi-scan ($SADABS$; Sheldrick, 1996)	$\theta_{max} = 25.5°$, $\theta_{min} = 2.1°$
$T_{min} = 0.923$, $T_{max} = 0.972$	$h = -10\rightarrow10$
	$k = -15\rightarrow15$
	$l = -16\rightarrow17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.106$	
$S = 1.03$	H-atom parameters constrained
2908 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 0.1972P]$
192 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.20$ e Å^{-3}
	$\Delta\rho_{min} = -0.17$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.42606 (8)	−0.03118 (5)	0.21634 (5)	0.0704 (2)
Cl2	0.33039 (10)	0.29372 (6)	0.42942 (5)	0.0851 (3)
C13	0.2618 (2)	0.71607 (15)	−0.03057 (14)	0.0421 (5)
C10	0.1972 (2)	0.54646 (15)	0.08139 (14)	0.0414 (5)
C9	0.1721 (2)	0.45849 (17)	0.13874 (15)	0.0461 (5)
H9	0.2244	0.3964	0.1299	0.055*
C15	0.2754 (2)	0.53119 (16)	0.00809 (15)	0.0459 (5)
H15	0.3078	0.4636	−0.0037	0.055*
C8	0.0829 (3)	0.45512 (17)	0.20297 (16)	0.0508 (6)
H8	0.0247	0.5151	0.2101	0.061*
N1	0.2898 (2)	0.79802 (13)	−0.08543 (13)	0.0518 (5)
C12	0.1844 (3)	0.73163 (16)	0.04341 (14)	0.0481 (5)
H12	0.1548	0.7993	0.0568	0.058*
C6	0.1595 (2)	0.26655 (16)	0.25224 (16)	0.0469 (5)
C3	0.3204 (3)	0.08209 (17)	0.23089 (17)	0.0509 (6)
C14	0.3057 (2)	0.61262 (16)	−0.04685 (14)	0.0456 (5)

H14	0.3561	0.599	−0.0957	0.055*
C4	0.3608 (3)	0.13662 (17)	0.31339 (16)	0.0519 (6)
H4	0.4425	0.1129	0.3616	0.062*
C11	0.1517 (2)	0.64926 (17)	0.09597 (15)	0.0476 (5)
H11	0.0972	0.6622	0.1431	0.057*
C7	0.0693 (3)	0.36611 (18)	0.26236 (17)	0.0547 (6)
O1	−0.0115 (2)	0.37083 (15)	0.32101 (14)	0.0849 (6)
C5	0.2780 (3)	0.22710 (17)	0.32357 (15)	0.0501 (5)
C2	0.2015 (3)	0.11710 (19)	0.15886 (17)	0.0576 (6)
H2	0.1737	0.079	0.1036	0.069*
C17	0.2722 (3)	0.90604 (18)	−0.05879 (18)	0.0685 (7)
H17A	0.1625	0.9193	−0.0574	0.103*
H17B	0.304	0.9521	−0.1033	0.103*
H17C	0.3383	0.9185	0.0021	0.103*
C16	0.3630 (3)	0.77905 (19)	−0.16414 (17)	0.0665 (7)
H16A	0.4725	0.7587	−0.1417	0.1*
H16B	0.3584	0.8422	−0.2006	0.1*
H16C	0.3064	0.7238	−0.2022	0.1*
C1	0.1244 (3)	0.20911 (18)	0.16968 (17)	0.0577 (6)
H1	0.046	0.2339	0.1202	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0823 (5)	0.0539 (4)	0.0800 (5)	0.0084 (3)	0.0288 (4)	0.0038 (3)
Cl2	0.1090 (6)	0.0798 (5)	0.0577 (4)	0.0164 (4)	−0.0008 (4)	−0.0118 (3)
C13	0.0447 (12)	0.0425 (12)	0.0377 (11)	−0.0018 (9)	0.0062 (9)	0.0013 (9)
C10	0.0437 (11)	0.0407 (12)	0.0406 (12)	0.0008 (9)	0.0110 (10)	0.0024 (9)
C9	0.0442 (12)	0.0439 (12)	0.0499 (13)	0.0026 (9)	0.0098 (10)	0.0023 (10)
C15	0.0531 (13)	0.0363 (11)	0.0508 (13)	0.0034 (10)	0.0166 (11)	−0.0031 (10)
C8	0.0476 (12)	0.0472 (13)	0.0604 (15)	0.0057 (10)	0.0178 (11)	0.0116 (11)
N1	0.0671 (12)	0.0415 (10)	0.0496 (11)	−0.0017 (9)	0.0187 (9)	0.0063 (8)
C12	0.0629 (14)	0.0365 (11)	0.0466 (13)	0.0078 (10)	0.0158 (11)	0.0002 (9)
C6	0.0451 (12)	0.0426 (12)	0.0546 (14)	−0.0054 (10)	0.0142 (11)	0.0104 (10)
C3	0.0543 (14)	0.0443 (13)	0.0585 (15)	−0.0036 (10)	0.0219 (12)	0.0083 (11)
C14	0.0524 (13)	0.0448 (12)	0.0430 (12)	0.0010 (10)	0.0176 (10)	−0.0010 (10)
C4	0.0545 (13)	0.0502 (13)	0.0496 (14)	0.0017 (11)	0.0081 (11)	0.0124 (11)
C11	0.0556 (13)	0.0496 (13)	0.0413 (12)	0.0050 (10)	0.0189 (10)	0.0009 (10)
C7	0.0451 (12)	0.0573 (14)	0.0645 (15)	−0.0020 (11)	0.0181 (12)	0.0118 (12)
O1	0.0906 (13)	0.0778 (13)	0.1068 (15)	0.0194 (10)	0.0665 (12)	0.0326 (11)
C5	0.0550 (13)	0.0484 (13)	0.0480 (13)	−0.0035 (11)	0.0135 (11)	0.0069 (10)
C2	0.0610 (15)	0.0550 (15)	0.0539 (14)	−0.0095 (12)	0.0061 (12)	−0.0027 (11)
C17	0.0926 (19)	0.0432 (14)	0.0702 (17)	−0.0039 (13)	0.0186 (15)	0.0076 (12)
C16	0.0852 (18)	0.0624 (16)	0.0571 (15)	−0.0086 (13)	0.0268 (14)	0.0111 (12)
C1	0.0508 (13)	0.0598 (15)	0.0562 (15)	−0.0032 (12)	−0.0019 (11)	0.0079 (12)

Geometric parameters (Å, º)

Cl1—C3	1.738 (2)	C6—C1	1.389 (3)
Cl2—C5	1.739 (2)	C6—C7	1.507 (3)
C13—N1	1.369 (2)	C3—C4	1.372 (3)
C13—C14	1.402 (3)	C3—C2	1.372 (3)
C13—C12	1.405 (3)	C14—H14	0.930
C10—C11	1.393 (3)	C4—C5	1.376 (3)
C10—C15	1.400 (3)	C4—H4	0.9300
C10—C9	1.443 (3)	C11—H11	0.930
C9—C8	1.338 (3)	C7—O1	1.218 (3)
C9—H9	0.930	C2—C1	1.369 (3)
C15—C14	1.371 (3)	C2—H2	0.930
C15—H15	0.930	C17—H17A	0.960
C8—C7	1.448 (3)	C17—H17B	0.960
C8—H8	0.930	C17—H17C	0.960
N1—C17	1.444 (3)	C16—H16A	0.960
N1—C16	1.450 (3)	C16—H16B	0.960
C12—C11	1.365 (3)	C16—H16C	0.960
C12—H12	0.930	C1—H1	0.930
C6—C5	1.383 (3)		
N1—C13—C14	121.63 (18)	C3—C4—C5	118.8 (2)
N1—C13—C12	121.38 (18)	C3—C4—H4	120.6
C14—C13—C12	116.97 (18)	C5—C4—H4	120.6
C11—C10—C15	116.45 (18)	C12—C11—C10	122.21 (19)
C11—C10—C9	123.63 (19)	C12—C11—H11	118.9
C15—C10—C9	119.89 (18)	C10—C11—H11	118.9
C8—C9—C10	128.1 (2)	O1—C7—C8	121.3 (2)
C8—C9—H9	116.0	O1—C7—C6	119.6 (2)
C10—C9—H9	116.0	C8—C7—C6	119.03 (19)
C14—C15—C10	122.09 (19)	C4—C5—C6	122.1 (2)
C14—C15—H15	119.0	C4—C5—Cl2	117.72 (18)
C10—C15—H15	119.0	C6—C5—Cl2	120.17 (18)
C9—C8—C7	125.7 (2)	C1—C2—C3	118.9 (2)
C9—C8—H8	117.2	C1—C2—H2	120.5
C7—C8—H8	117.2	C3—C2—H2	120.5
C13—N1—C17	121.42 (18)	N1—C17—H17A	109.5
C13—N1—C16	120.27 (18)	N1—C17—H17B	109.5
C17—N1—C16	117.56 (18)	H17A—C17—H17B	109.5
C11—C12—C13	121.25 (19)	N1—C17—H17C	109.5
C11—C12—H12	119.4	H17A—C17—H17C	109.5
C13—C12—H12	119.4	H17B—C17—H17C	109.5
C5—C6—C1	116.9 (2)	N1—C16—H16A	109.5
C5—C6—C7	122.5 (2)	N1—C16—H16B	109.5
C1—C6—C7	120.6 (2)	H16A—C16—H16B	109.5
C4—C3—C2	121.1 (2)	N1—C16—H16C	109.5
C4—C3—Cl1	119.27 (18)	H16A—C16—H16C	109.5

C2—C3—Cl1	119.55 (19)	H16B—C16—H16C	109.5
C15—C14—C13	120.99 (19)	C2—C1—C6	122.1 (2)
C15—C14—H14	119.5	C2—C1—H1	118.9
C13—C14—H14	119.5	C6—C1—H1	118.9
C11—C10—C9—C8	11.4 (4)	C9—C10—C11—C12	176.6 (2)
C15—C10—C9—C8	−170.5 (2)	C9—C8—C7—O1	177.9 (2)
C11—C10—C15—C14	−0.1 (3)	C9—C8—C7—C6	−0.9 (3)
C9—C10—C15—C14	−178.3 (2)	C5—C6—C7—O1	−61.9 (3)
C10—C9—C8—C7	−176.3 (2)	C1—C6—C7—O1	117.2 (3)
C14—C13—N1—C17	−168.4 (2)	C5—C6—C7—C8	117.0 (2)
C12—C13—N1—C17	13.1 (3)	C1—C6—C7—C8	−64.0 (3)
C14—C13—N1—C16	1.6 (3)	C3—C4—C5—C6	−2.3 (3)
C12—C13—N1—C16	−177.0 (2)	C3—C4—C5—Cl2	179.29 (16)
N1—C13—C12—C11	177.7 (2)	C1—C6—C5—C4	1.5 (3)
C14—C13—C12—C11	−0.9 (3)	C7—C6—C5—C4	−179.42 (19)
C10—C15—C14—C13	1.2 (3)	C1—C6—C5—Cl2	179.91 (16)
N1—C13—C14—C15	−179.3 (2)	C7—C6—C5—Cl2	−1.0 (3)
C12—C13—C14—C15	−0.7 (3)	C4—C3—C2—C1	1.1 (3)
C2—C3—C4—C5	0.9 (3)	Cl1—C3—C2—C1	−176.93 (17)
Cl1—C3—C4—C5	178.95 (16)	C3—C2—C1—C6	−1.9 (3)
C13—C12—C11—C10	2.1 (3)	C5—C6—C1—C2	0.6 (3)
C15—C10—C11—C12	−1.5 (3)	C7—C6—C1—C2	−178.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1[i]	0.93	2.55	3.252 (3)	132
C4—H4···*Cg*1[ii]	0.93	2.95	3.784 (3)	150

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