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# An orthorhombic polymorph of (*E*)-1-(benzo[*d*]-[1,3]dioxol-5-yl)-3-(2,3-dichlorophenyl)prop-2-en-1-one

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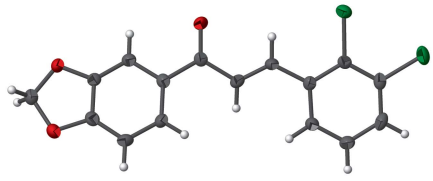
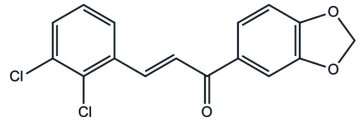
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $C_{16}H_{10}Cl_2O_3$, is almost planar with a dihedral angle of 0.14 (16)° between the benzodioxole ring system and the dichlorobenzene ring that are bridged by the olefinic double bond. The corresponding value reported for the monoclinic polymorph is [5.57 (9)° (Lokeshwari *et al.* (2017). *IUCrData*, **2**, x170103). The carbonyl group lies almost in the plane of the olefinic double bond and is twisted slightly from the benzodioxole ring plane. In the crystal, the molecules are linked by weak C—H···O and C—H···Cl hydrogen bonds, forming a chain propagating along the *b*-axis direction.

**3D view**



**Chemical scheme**




## Structure description

Chalcones and their derivatives exhibit a plethora of biological applications that include use as antioxidants, or antifungal, antibacterial and cardioprotective agents. As part of our ongoing work on such molecules (Rajendraprasad *et al.*, 2017; Naveen *et al.*, 2016*a*,*b*), we report here the synthesis and crystal structure of the title compound.

The structure of the title molecule is shown in Fig. 1. It is a polymorph having been reported previously in the monoclinic space-group $P2_1/c$ (Lokeshwari *et al.*, 2017). The molecule is nearly planar as seen by the dihedral angle of 0.14 (16)° between the benzodioxole ring system and the dichlorobenzene ring; these are bridged by an olefinic double bond that adopts an *E* conformation. The corresponding dihedral angle reported for the monoclinic polymorph is 5.57 (9)° (Lokeshwari *et al.*, 2017). The *trans* conformation of the C=C double bond in the central enone group is confirmed by the C—

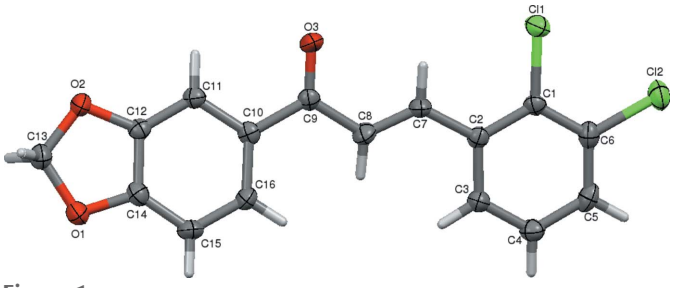



**Figure 1**
The molecular structure of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

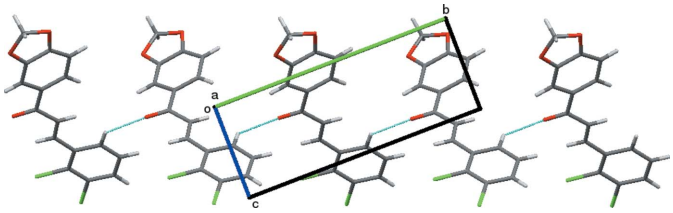



**Figure 2**
Packing of the molecules, viewed along the *b* axis, with hydrogen bonds shown as blue lines.

C═C—C torsion angle of −174.9 (4)°. The carbonyl group at C9 lies almost in the plane of the olefinic double bond and is twisted slightly from the benzodioxole ring as indicated by the C11—C10—C9—O3 and C7—C8—C9—O3 torsion angles of 13.7 (5) and 5.0 (6)° respectively.

In the crystal, the molecules are linked by weak C—H···O and C—H···Cl hydrogen bonds (Table 1), forming a chain propagating along the *b*-axis direction, Fig. 2.

## Synthesis and crystallization

A mixture of 2,3-dichlorobenzaldehyde (5 mmol), 1-(benzo[*d*][1,3]dioxol-5-yl)ethanone (5 mmol) and sodium hydroxide (5 mmol) in methanol (25 ml) was stirred at room temperature for 3 h. The progress of the reaction was monitored by TLC. After completion, the mixture was poured into ice-cold water and kept in the refrigerator for 18 h. The solid formed was filtered, and washed with cold 5% hydrochloric acid. Pale-green crystals were obtained from methanol solution by using the slow solvent evaporation technique, yield 88%, m.p. 401–402 K.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

## Acknowledgements

The authors are grateful to the Institution of Excellence, Vijnana Bhavana, University of Mysore, India, for providing the single-crystal X-ray diffractometer facility.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3···O3$^{i}$ | 0.93 | 2.46 | 3.185 (5) | 135 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{16}H_{10}Cl_2O_3$ |
| $M_r$ | 321.14 |
| Crystal system, space group | Orthorhombic, $Pna2_1$ |
| Temperature (K) | 296 |
| *a*, *b*, *c* (Å) | 21.9756 (11), 12.7354 (6), 4.9889 (3) |
| *V* (Å$^3$) | 1396.23 (13) |
| *Z* | 4 |
| Radiation type | Cu *Kα* |
| $\mu$ (mm$^{-1}$) | 4.25 |
| Crystal size (mm) | 0.27 × 0.26 × 0.22 |
| Data collection | |
| Diffractometer | Bruker X8 Proteum |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2013) |
| $T_{min}$, $T_{max}$ | 0.393, 0.455 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 6212, 1801, 1639 |
| $R_{int}$ | 0.061 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.585 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.044, 0.120, 1.06 |
| No. of reflections | 1801 |
| No. of parameters | 190 |
| No. of restraints | 1 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.29, −0.37 |
| Absolute structure | Flack (1983) |
| Absolute structure parameter | 0.02 (2) |

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

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# full crystallographic data

*IUCrData* (2017). **2**, x171590 [https://doi.org/10.1107/S2414314617015905]

## An orthorhombic polymorph of (*E*)-1-(benzo[*d*][1,3]dioxol-5-yl)-3-(2,3-dichlorophenyl)prop-2-en-1-one

**S. Naveen, A. Dileep Kumar, M. V. Deepa Urs, K. Ajay Kumar, N. K. Lokanath and Ismail Warad**

**(*E*)-1-(Benzo[*d*][1,3]dioxol-5-yl)-3-(2,3-dichlorophenyl)prop-2-en-1-one**

*Crystal data*

$C_{16}H_{10}Cl_2O_3$
$M_r$ = 321.14
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a$ = 21.9756 (11) Å
$b$ = 12.7354 (6) Å
$c$ = 4.9889 (3) Å
$V$ = 1396.23 (13) Å$^3$
$Z$ = 4
$F(000)$ = 656
$D_x$ = 1.528 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54178 Å
Cell parameters from 1639 reflections
$\theta$ = 4.0–64.5°
$\mu$ = 4.25 mm$^{-1}$
$T$ = 296 K
Prism, green
0.27 × 0.26 × 0.22 mm

*Data collection*

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
$T_{min}$ = 0.393, $T_{max}$ = 0.455
6212 measured reflections
1801 independent reflections
1639 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061
$\theta_{max}$ = 64.5°, $\theta_{min}$ = 4.0°
$h$ = −25→24
$k$ = −13→14
$l$ = −4→5

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
$S$ = 1.06
1801 reflections
190 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.29 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$
Absolute structure: Flack (1983)
Absolute structure parameter: 0.02 (2)

*Special details*

**Geometry**. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.40504 (4) | 0.22650 (8) | 1.0103 (2) | 0.0306 (3) |
| Cl2 | 0.48016 (5) | 0.35770 (9) | 1.4215 (3) | 0.0386 (3) |
| O1 | 0.05572 (13) | 0.4848 (2) | −0.3392 (7) | 0.0333 (10) |
| O2 | 0.05823 (13) | 0.3043 (2) | −0.2738 (7) | 0.0335 (10) |
| O3 | 0.23955 (15) | 0.2272 (2) | 0.3436 (7) | 0.0399 (11) |
| C1 | 0.38991 (17) | 0.3592 (3) | 1.0505 (8) | 0.0229 (11) |
| C2 | 0.34376 (17) | 0.4072 (3) | 0.8997 (9) | 0.0227 (11) |
| C3 | 0.33324 (17) | 0.5145 (3) | 0.9436 (9) | 0.0260 (11) |
| C4 | 0.36566 (19) | 0.5703 (3) | 1.1311 (9) | 0.0283 (12) |
| C5 | 0.41077 (18) | 0.5219 (4) | 1.2808 (9) | 0.0300 (14) |
| C6 | 0.42298 (18) | 0.4164 (4) | 1.2366 (8) | 0.0268 (13) |
| C7 | 0.30817 (18) | 0.3496 (3) | 0.7011 (9) | 0.0263 (12) |
| C8 | 0.26308 (18) | 0.3868 (3) | 0.5549 (8) | 0.0283 (12) |
| C9 | 0.22949 (17) | 0.3220 (3) | 0.3630 (7) | 0.0232 (11) |
| C10 | 0.18281 (17) | 0.3718 (3) | 0.1898 (8) | 0.0220 (11) |
| C11 | 0.14240 (17) | 0.3059 (3) | 0.0514 (8) | 0.0242 (11) |
| C12 | 0.10171 (17) | 0.3520 (3) | −0.1190 (9) | 0.0224 (11) |
| C13 | 0.02917 (19) | 0.3861 (3) | −0.4182 (9) | 0.0307 (14) |
| C14 | 0.10051 (17) | 0.4598 (3) | −0.1576 (8) | 0.0270 (14) |
| C15 | 0.13913 (18) | 0.5262 (3) | −0.0252 (9) | 0.0307 (14) |
| C16 | 0.17994 (18) | 0.4807 (3) | 0.1541 (9) | 0.0270 (12) |
| H3 | 0.30360 | 0.54870 | 0.84320 | 0.0310* |
| H4 | 0.35730 | 0.64110 | 1.15780 | 0.0340* |
| H5 | 0.43250 | 0.55950 | 1.40880 | 0.0360* |
| H7 | 0.31840 | 0.27940 | 0.67500 | 0.0320* |
| H8 | 0.25220 | 0.45690 | 0.57450 | 0.0340* |
| H11 | 0.14330 | 0.23350 | 0.07480 | 0.0290* |
| H13A | −0.01410 | 0.38620 | −0.37970 | 0.0370* |
| H13B | 0.03460 | 0.37540 | −0.60930 | 0.0370* |
| H15 | 0.13820 | 0.59830 | −0.05360 | 0.0370* |
| H16 | 0.20590 | 0.52370 | 0.25230 | 0.0320* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0342 (5) | 0.0241 (6) | 0.0335 (6) | 0.0047 (4) | −0.0025 (4) | 0.0021 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| Cl2 | 0.0333 (5) | 0.0449 (7) | 0.0375 (6) | 0.0001 (5) | −0.0139 (5) | 0.0056 (5) |
| O1 | 0.0329 (16) | 0.0280 (17) | 0.0389 (18) | 0.0053 (13) | −0.0114 (13) | −0.0013 (15) |
| O2 | 0.0322 (15) | 0.0252 (17) | 0.0431 (19) | 0.0008 (13) | −0.0158 (14) | −0.0055 (15) |
| O3 | 0.0466 (18) | 0.0182 (18) | 0.055 (2) | −0.0044 (14) | −0.0244 (17) | 0.0006 (14) |
| C1 | 0.0237 (19) | 0.021 (2) | 0.024 (2) | −0.0026 (16) | 0.0011 (18) | 0.0057 (17) |
| C2 | 0.0239 (19) | 0.024 (2) | 0.0203 (19) | −0.0035 (15) | −0.0004 (16) | 0.0030 (18) |
| C3 | 0.0259 (18) | 0.022 (2) | 0.030 (2) | 0.0005 (16) | −0.0036 (17) | 0.0009 (19) |
| C4 | 0.034 (2) | 0.023 (2) | 0.028 (2) | 0.0007 (18) | −0.0004 (19) | −0.001 (2) |
| C5 | 0.028 (2) | 0.039 (3) | 0.023 (2) | −0.0089 (18) | −0.0015 (16) | −0.006 (2) |
| C6 | 0.0214 (18) | 0.036 (3) | 0.023 (2) | −0.0028 (17) | −0.0016 (17) | 0.002 (2) |
| C7 | 0.029 (2) | 0.018 (2) | 0.032 (2) | 0.0014 (16) | −0.0055 (19) | −0.0016 (19) |
| C8 | 0.031 (2) | 0.024 (2) | 0.030 (2) | 0.0005 (17) | −0.0033 (19) | −0.0078 (19) |
| C9 | 0.0225 (18) | 0.025 (2) | 0.022 (2) | −0.0022 (17) | 0.0014 (16) | 0.0039 (18) |
| C10 | 0.0230 (19) | 0.026 (2) | 0.017 (2) | 0.0003 (16) | 0.0024 (16) | 0.0018 (18) |
| C11 | 0.0275 (19) | 0.021 (2) | 0.024 (2) | −0.0002 (17) | 0.0006 (16) | −0.0002 (18) |
| C12 | 0.0231 (18) | 0.022 (2) | 0.022 (2) | 0.0002 (16) | 0.0018 (17) | −0.0020 (18) |
| C13 | 0.029 (2) | 0.032 (3) | 0.031 (2) | 0.0012 (18) | −0.0066 (18) | −0.001 (2) |
| C14 | 0.0249 (19) | 0.028 (3) | 0.028 (2) | 0.0035 (18) | −0.0004 (16) | 0.0006 (19) |
| C15 | 0.037 (2) | 0.018 (2) | 0.037 (3) | −0.0012 (18) | −0.0029 (19) | 0.0009 (19) |
| C16 | 0.027 (2) | 0.024 (2) | 0.030 (2) | −0.0023 (17) | −0.0055 (17) | −0.004 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C1 | 1.734 (4) | C10—C11 | 1.404 (5) |
| Cl2—C6 | 1.729 (4) | C10—C16 | 1.400 (5) |
| O1—C13 | 1.441 (5) | C11—C12 | 1.366 (6) |
| O1—C14 | 1.375 (5) | C12—C14 | 1.387 (5) |
| O2—C12 | 1.371 (5) | C14—C15 | 1.368 (6) |
| O2—C13 | 1.419 (5) | C15—C16 | 1.393 (6) |
| O3—C9 | 1.231 (5) | C3—H3 | 0.9300 |
| C1—C2 | 1.403 (6) | C4—H4 | 0.9300 |
| C1—C6 | 1.386 (6) | C5—H5 | 0.9300 |
| C2—C3 | 1.403 (5) | C7—H7 | 0.9300 |
| C2—C7 | 1.460 (6) | C8—H8 | 0.9300 |
| C3—C4 | 1.374 (6) | C11—H11 | 0.9300 |
| C4—C5 | 1.386 (6) | C13—H13A | 0.9700 |
| C5—C6 | 1.388 (7) | C13—H13B | 0.9700 |
| C7—C8 | 1.318 (6) | C15—H15 | 0.9300 |
| C8—C9 | 1.464 (5) | C16—H16 | 0.9300 |
| C9—C10 | 1.484 (5) | | |
| | | | |
| C13—O1—C14 | 105.6 (3) | O1—C14—C12 | 109.5 (3) |
| C12—O2—C13 | 105.9 (3) | O1—C14—C15 | 128.2 (3) |
| Cl1—C1—C2 | 120.1 (3) | C12—C14—C15 | 122.2 (4) |
| Cl1—C1—C6 | 119.3 (3) | C14—C15—C16 | 116.9 (4) |
| C2—C1—C6 | 120.6 (4) | C10—C16—C15 | 121.5 (4) |
| C1—C2—C3 | 117.4 (4) | C2—C3—H3 | 119.00 |
| C1—C2—C7 | 122.2 (3) | C4—C3—H3 | 119.00 |

| | | | |
|---|---|---|---|
| C3—C2—C7 | 120.5 (4) | C3—C4—H4 | 120.00 |
| C2—C3—C4 | 121.6 (4) | C5—C4—H4 | 120.00 |
| C3—C4—C5 | 120.5 (4) | C4—C5—H5 | 121.00 |
| C4—C5—C6 | 118.9 (4) | C6—C5—H5 | 121.00 |
| Cl2—C6—C1 | 120.8 (4) | C2—C7—H7 | 117.00 |
| Cl2—C6—C5 | 118.3 (3) | C8—C7—H7 | 117.00 |
| C1—C6—C5 | 120.9 (4) | C7—C8—H8 | 119.00 |
| C2—C7—C8 | 126.7 (4) | C9—C8—H8 | 119.00 |
| C7—C8—C9 | 122.6 (4) | C10—C11—H11 | 121.00 |
| O3—C9—C8 | 120.9 (3) | C12—C11—H11 | 121.00 |
| O3—C9—C10 | 119.8 (3) | O1—C13—H13A | 110.00 |
| C8—C9—C10 | 119.3 (3) | O1—C13—H13B | 110.00 |
| C9—C10—C11 | 117.9 (3) | O2—C13—H13A | 110.00 |
| C9—C10—C16 | 121.9 (3) | O2—C13—H13B | 110.00 |
| C11—C10—C16 | 120.1 (4) | H13A—C13—H13B | 108.00 |
| C10—C11—C12 | 117.6 (4) | C14—C15—H15 | 122.00 |
| O2—C12—C11 | 128.1 (3) | C16—C15—H15 | 122.00 |
| O2—C12—C14 | 110.3 (3) | C10—C16—H16 | 119.00 |
| C11—C12—C14 | 121.6 (4) | C15—C16—H16 | 119.00 |
| O1—C13—O2 | 108.6 (3) | | |

| | | | |
|---|---|---|---|
| C14—O1—C13—O2 | 1.6 (4) | C4—C5—C6—C1 | −1.4 (6) |
| C13—O1—C14—C12 | −1.1 (4) | C2—C7—C8—C9 | −179.1 (4) |
| C13—O1—C14—C15 | 179.6 (4) | C7—C8—C9—O3 | 5.0 (6) |
| C13—O2—C12—C11 | −178.6 (4) | C7—C8—C9—C10 | −174.9 (4) |
| C13—O2—C12—C14 | 0.8 (4) | O3—C9—C10—C11 | 13.7 (5) |
| C12—O2—C13—O1 | −1.5 (4) | O3—C9—C10—C16 | −163.7 (4) |
| Cl1—C1—C2—C3 | 179.3 (3) | C8—C9—C10—C11 | −166.4 (4) |
| Cl1—C1—C2—C7 | −1.6 (6) | C8—C9—C10—C16 | 16.2 (6) |
| C6—C1—C2—C3 | 0.6 (6) | C9—C10—C11—C12 | −176.5 (4) |
| C6—C1—C2—C7 | 179.7 (4) | C16—C10—C11—C12 | 1.0 (6) |
| Cl1—C1—C6—Cl2 | 1.7 (5) | C9—C10—C16—C15 | 174.8 (4) |
| Cl1—C1—C6—C5 | −177.8 (3) | C11—C10—C16—C15 | −2.6 (6) |
| C2—C1—C6—Cl2 | −179.7 (3) | C10—C11—C12—O2 | −179.9 (4) |
| C2—C1—C6—C5 | 0.9 (6) | C10—C11—C12—C14 | 0.8 (6) |
| C1—C2—C3—C4 | −1.5 (6) | O2—C12—C14—O1 | 0.2 (5) |
| C7—C2—C3—C4 | 179.3 (4) | O2—C12—C14—C15 | 179.6 (4) |
| C1—C2—C7—C8 | 178.2 (4) | C11—C12—C14—O1 | 179.6 (4) |
| C3—C2—C7—C8 | −2.8 (7) | C11—C12—C14—C15 | −1.0 (6) |
| C2—C3—C4—C5 | 1.0 (7) | O1—C14—C15—C16 | 178.7 (4) |
| C3—C4—C5—C6 | 0.5 (6) | C12—C14—C15—C16 | −0.5 (6) |
| C4—C5—C6—Cl2 | 179.1 (3) | C14—C15—C16—C10 | 2.3 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3···O3$^{i}$ | 0.93 | 2.46 | 3.185 (5) | 135 |

| | | | | |
|---|---|---|---|---|
| C7—H7···Cl1 | 0.93 | 2.62 | 3.061 (4) | 109 |
| C7—H7···O3 | 0.93 | 2.49 | 2.808 (5) | 100 |

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