# (E)-3-(4-Chlorophenyl)-1-(1-naphthyl)-prop-2-en-1-one

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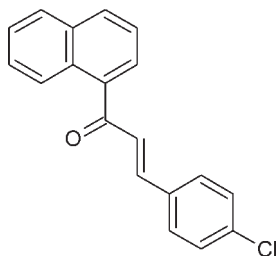Correspondence e-mail: mkubicki@amu.edu.pl

In the title compound, $C_{19}H_{13}ClO$, the benzene ring and the naphthalene system, are twisted by 12.3 (3) and 36.1 (2)°, respectively, and in opposite directions with respect to the central propenone bridge. The bond-angle pattern within the benzene ring is influence by both substituents; these influences are almost additive. In the crystal, the molecules are linked by C—H···O and C—H···Cl interactions.

## Related literature

For chalcones, see: Dhar (1981); Di Carlo et al. (1999); Dimmock et al. (1999); Goto et al. (1991); Indira et al. (2002); Sarojini et al. (2006); Satyanarayana et al. (2004); Uchida et al. (1998); Yarishkin (2008). For the 1-naphtyl analogue, see: Eswaramoorthy et al. (1994). For the influence of substituents on the geometry of the phenyl ring, see: Domenicano (1988). For a description of the Cambridge Crystallographic Database, see: Allen (2002).



## Experimental

### Crystal data

| | |
|---|---|
| $C_{19}H_{13}ClO$ | $b$ = 8.0544 (5) Å |
| $M_r$ = 292.74 | $c$ = 7.8472 (6) Å |
| Monoclinic, $Pc$ | $\beta$ = 98.091 (10)° |
| $a$ = 12.0392 (14) Å | $V$ = 753.36 (11) Å$^3$ |

| | |
|---|---|
| $Z$ = 2 | $T$ = 295 K |
| Mo $K\alpha$ radiation | $0.30 \times 0.20 \times 0.15$ mm |
| $\mu$ = 0.25 mm$^{-1}$ | |

### Data collection

| | |
|---|---|
| Oxford Diffraction Xcalibur (Sapphire2, large Be window) diffractometer | Diffraction, 2009) |
| | $T_{min}$ = 0.666, $T_{max}$ = 1.000 |
| | 2481 measured reflections |
| Absorption correction: multi-scan (CrysAlis PRO; Oxford | 1866 independent reflections |
| | 1440 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.014 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.035 | H-atom parameters constrained |
| $wR(F^2)$ = 0.083 | $\Delta\rho_{max}$ = 0.12 e Å$^{-3}$ |
| $S$ = 0.96 | $\Delta\rho_{min}$ = −0.13 e Å$^{-3}$ |
| 1866 reflections | Absolute structure: Flack (1983), |
| 190 parameters | 423 Friedel pairs |
| 2 restraints | Flack parameter: 0.08 (7) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C17—H17···O12$^i$ | 0.93 | 2.42 | 3.180 (4) | 139 |
| C3—H3···Cl21$^{ii}$ | 0.93 | 2.92 | 3.703 (3) | 143 |
| C8—H8···O12$^{iii}$ | 0.93 | 2.64 | 3.546 (4) | 163 |

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

Data collection: CrysAlis PRO (Oxford Diffraction, 2009); cell refinement: CrysAlis PRO; data reduction: CrysAlis PRO; program(s) used to solve structure: SIR92 (Altomare et al., 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Stereochemical Workstation Operation Manual (Siemens, 1989); software used to prepare material for publication: SHELXL97.

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**supplementary materials**

## (*E*)-3-(4-Chlorophenyl)-1-(1-naphthyl)prop-2-en-1-one

### G. Dutkiewicz, S. Samshuddin, B. Narayana, H. S. Yathirajan and M. Kubicki

### Comment

Chalcones constitute an important family of flavonoids. They have been reported to possess many interesting pharmacological activities (Dhar, 1981) including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, antitumor and anticancer activities (Dimmock *et al.*, 1999; Satyanarayana *et al.*, 2004). Some chalcones demonstrated the ability to block voltage-dependent potassium channels (Yarishkin *et al.*, 2008). Chalcones are also finding application as organic nonlinear optical materials (NLO) for their SHG conversion efficiency (Sarojini *et al.*, 2006). Chalcone derivatives are recognized material in the NLO applications because of their excellent blue light transmittance and good crystallization ability (Goto *et al.*,1991; Uchida *et al.*,1998; Indira *et al.*, 2002). Chemically chalcones consists of open-chain flavonoids in which the two aromatic rings are joined by α,\&s-unsaturated carbonyl system. The radical quenching properties of the phenolic groups present in many chalcones have raised interest in using these compounds or chalcone rich plant extracts as drugs or food preservatives (Di Carlo *et al.*, 1999). As a part of our efforts on the synthesis of naphthyl chalcones, this paper describes the crystal structure of a new naphthyl chalcone, (2*E*)-3-(4-Chlorophenyl)-1-(naphthalen-1-yl)prop-2-en-1-one (**I**, Scheme 1). There are 298 structures in the Cambridge Crystallographic Database (Allen, 2002: Ver. 5.30, Nov. 2008, last update Sep. 2009) that posses two aromatic moieties connected *via* CH=CH—CO– fragment, but only 10 of them are naphthyl chalcones, and the single one example with 1-naphthalene substituent (1-(1-Naphthalenyl)-3-(4-nitrophenyl)-2-propenone, Eswaramoorthy *et al.*, 1994). It might be noted, that this structure apparently has errors: one of the torsion angles in the aromatic ring is as large as 5°.

The molecule of **I** is built of three approximately planar fragments (Fig. 1): the phenyl ring (A, maximum deviation form the least-squares plane is 0.006 (3) Å), propenone fragment C=C—C=O (B, 0.014 (2) Å), and the naphtalene ring system (C). This last fragment however is significantly folded, even though both individual rings are almost planar, the dihedral angle between these planes is as high as 5.05 (13)°. The overall conformation of **I** can be described in terms of dihedral angles between these fragments: A/B 36.1 (2)°, B/C 12.3 (3)°, and A/C 25.51 (9)°. These values show that the terminal planes are twisted in opposite sense with respect to the central bridging fragment. This situation is relatively rare, the majority of chalcones found in the CDB shows the same sense of rotation with respect to the central bridge.

The bond lengths within the conjugated linear fragment suggest the large degree of localization: C—C bond length of 1.480 (4) Å, C=C of 1.329 (4)Å and C=O 1.232 (3) Å. The bond angles within the phenyl ring are influenced by both Cl and C=C– substituents, and these influences are almost additive, as suggested *e.g.*, by Domenicano (1988). The distribution is almost symmetrical with respect to the C15···C18 line, and the values are close to those calculated by summing the effects of both substituents.

In the crystal structure there is one relatively short C—H···O potential hydrogen bond, C17—H17···O12(*x*,1 + *y*,*z*), that link molecules into infinite chains along *y* direction, and few weak C—H···O and C—H···π contacts, which can stabilize the packing otherwise determined by the van der Waals interactions and close packing requirements (Fig. 2).

# supplementary materials

**Experimental**

To a mixture of 1-acetonaphthone (1.7 g, 0.01 mol) and *p*-chlorobenzaldehyde (1.4 g, 0.01 mol) in 30 ml e thanol, 10 ml of 10% sodium hydroxide solution was added and stirred at 5–10 $^{o}$C for 3 h. The precipitate formed was collected by filtration and purified by recrystallization from ethanol. The single-crystal was grown from DMF by slow evaporation method and yield of the compound was 82%. (m.p. 360–362 K). Analytical data: Found (Calculated): C %: 76.89 (77.95); H %: 4.23 (4.48).

**Refinement**

Hydrogen atoms were located geometrically and refined as a riding model; their $U_{iso}$ values were set at 1.2 times $U_{eq}$ of their carrier carbon atom.

**Figures**
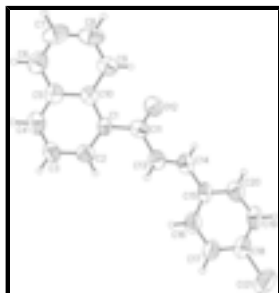


Fig. 1. Anisotropic ellipsoid representation of the compound **I** together with atom labelling scheme. The ellipsoids are drawn at 50% probability level, hydrogen atoms are depicted as spheres with arbitrary radii.
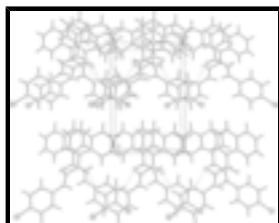


Fig. 2. The crystal packing of **I** as seen along *z* direction; weak C—H···O bonds are shown as dashed lines.



Fig. 3. The formation of the title compound.

**(*E*)-3-(4-Chlorophenyl)-1-(1-naphthyl)prop-2-en-1-one**

*Crystal data*

| | |
|---|---|
| $C_{19}H_{13}ClO$ | $F(000) = 304$ |
| $M_r = 292.74$ | $D_x = 1.291$ Mg m$^{-3}$ |
| Monoclinic, *Pc* | Mo *Kα* radiation, λ = 0.71073 Å |
| Hall symbol: P -2yc | Cell parameters from 1288 reflections |
| $a = 12.0392$ (14) Å | θ = 2.5–26.6° |
| $b = 8.0544$ (5) Å | μ = 0.25 mm$^{-1}$ |
| $c = 7.8472$ (6) Å | $T = 295$ K |

$\beta = 98.091\ (10)°$

$V = 753.36\ (11)\ \text{Å}^3$

$Z = 2$

Block, colourless

$0.30 \times 0.20 \times 0.15$ mm

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur (Sapphire2, large Be window) diffractometer | 1866 independent reflections |
| Radiation source: Enhance (Mo) X-ray Source | 1440 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.014$ |
| Detector resolution: 8.1929 pixels mm$^{-1}$ | $\theta_{max} = 26.6°$, $\theta_{min} = 2.5°$ |
| ω scan | $h = -14 \rightarrow 11$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009) | $k = -9 \rightarrow 4$ |
| $T_{min} = 0.667$, $T_{max} = 1.000$ | $l = -9 \rightarrow 6$ |
| 2481 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.035$ | H-atom parameters constrained |
| $wR(F^2) = 0.083$ | $w = 1/[\sigma^2(F_o^2) + (0.050P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.96$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 1866 reflections | $\Delta\rho_{max} = 0.12$ e Å$^{-3}$ |
| 190 parameters | $\Delta\rho_{min} = -0.13$ e Å$^{-3}$ |
| 2 restraints | Absolute structure: Flack (1983), 423 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.08 (7) |

*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 | 0.0117 (2) | 0.4299 (3) | 0.5052 (3) | 0.0451 (6) |
| C2 | −0.0556 (2) | 0.5690 (3) | 0.4967 (3) | 0.0543 (7) |
| H2 | −0.0256 | 0.6681 | 0.5435 | 0.065* |
| C3 | −0.1681 (2) | 0.5651 (4) | 0.4195 (4) | 0.0618 (7) |
| H3 | −0.2119 | 0.6605 | 0.4154 | 0.074* |
| C4 | −0.2124 (2) | 0.4207 (4) | 0.3508 (4) | 0.0617 (7) |
| H4 | −0.2879 | 0.4175 | 0.3048 | 0.074* |
| C5 | −0.1473 (2) | 0.2754 (3) | 0.3471 (3) | 0.0521 (6) |
| C6 | −0.1908 (2) | 0.1292 (4) | 0.2642 (4) | 0.0657 (7) |
| H6 | −0.2661 | 0.1256 | 0.2173 | 0.079* |
| C7 | −0.1260 (3) | −0.0057 (4) | 0.2513 (4) | 0.0753 (9) |
| H7 | −0.1567 | −0.1010 | 0.1967 | 0.090* |
| C8 | −0.0125 (3) | −0.0015 (4) | 0.3204 (4) | 0.0697 (8) |
| H8 | 0.0325 | −0.0934 | 0.3084 | 0.084* |
| C9 | 0.0335 (2) | 0.1362 (3) | 0.4058 (4) | 0.0563 (7) |
| H9 | 0.1088 | 0.1355 | 0.4528 | 0.068* |
| C10 | −0.0321 (2) | 0.2793 (3) | 0.4233 (3) | 0.0469 (6) |
| C11 | 0.1246 (2) | 0.4368 (3) | 0.6114 (3) | 0.0526 (6) |
| O12 | 0.16532 (16) | 0.3125 (2) | 0.6876 (3) | 0.0740 (6) |
| C13 | 0.1853 (2) | 0.5973 (3) | 0.6331 (3) | 0.0562 (7) |
| H13 | 0.1563 | 0.6890 | 0.5698 | 0.067* |
| C14 | 0.2804 (2) | 0.6132 (3) | 0.7411 (4) | 0.0581 (7) |
| H14 | 0.3076 | 0.5175 | 0.7989 | 0.070* |
| C15 | 0.3469 (2) | 0.7639 (4) | 0.7790 (4) | 0.0543 (7) |
| C16 | 0.3072 (2) | 0.9202 (3) | 0.7270 (4) | 0.0637 (8) |
| H16 | 0.2357 | 0.9297 | 0.6651 | 0.076* |
| C17 | 0.3705 (2) | 1.0620 (4) | 0.7642 (4) | 0.0682 (9) |
| H17 | 0.3421 | 1.1656 | 0.7282 | 0.082* |
| C18 | 0.4770 (2) | 1.0472 (4) | 0.8560 (4) | 0.0674 (9) |
| C19 | 0.5195 (2) | 0.8945 (4) | 0.9109 (4) | 0.0711 (8) |
| H19 | 0.5912 | 0.8856 | 0.9723 | 0.085* |
| C20 | 0.4540 (2) | 0.7544 (4) | 0.8731 (4) | 0.0674 (8) |
| H20 | 0.4821 | 0.6514 | 0.9115 | 0.081* |
| Cl21 | 0.55687 (8) | 1.22525 (11) | 0.90310 (13) | 0.1042 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0455 (14) | 0.0522 (15) | 0.0381 (14) | 0.0023 (11) | 0.0074 (11) | 0.0011 (12) |
| C2 | 0.0602 (17) | 0.0538 (15) | 0.0500 (16) | 0.0043 (12) | 0.0113 (13) | −0.0061 (13) |
| C3 | 0.0541 (17) | 0.0693 (18) | 0.0619 (18) | 0.0165 (13) | 0.0081 (14) | −0.0018 (16) |
| C4 | 0.0477 (15) | 0.085 (2) | 0.0521 (16) | 0.0047 (14) | 0.0058 (12) | 0.0001 (16) |
| C5 | 0.0527 (15) | 0.0656 (17) | 0.0384 (15) | −0.0037 (13) | 0.0074 (12) | 0.0013 (14) |
| C6 | 0.0662 (18) | 0.077 (2) | 0.0528 (17) | −0.0111 (17) | 0.0052 (14) | −0.0025 (17) |
| C7 | 0.102 (3) | 0.066 (2) | 0.057 (2) | −0.0178 (18) | 0.0114 (18) | −0.0110 (16) |
| C8 | 0.104 (3) | 0.0555 (17) | 0.0522 (17) | 0.0068 (16) | 0.0217 (17) | −0.0032 (15) |
| C9 | 0.0653 (18) | 0.0581 (15) | 0.0469 (16) | 0.0059 (13) | 0.0126 (13) | 0.0024 (14) |
| C10 | 0.0550 (16) | 0.0516 (14) | 0.0364 (14) | 0.0008 (12) | 0.0144 (12) | 0.0049 (12) |

| C11 | 0.0533 (16) | 0.0559 (16) | 0.0491 (16) | 0.0055 (12) | 0.0090 (12) | 0.0026 (13) |
| O12 | 0.0674 (13) | 0.0677 (12) | 0.0812 (15) | 0.0034 (10) | −0.0100 (11) | 0.0117 (12) |
| C13 | 0.0557 (17) | 0.0613 (16) | 0.0510 (16) | 0.0029 (12) | 0.0059 (14) | 0.0043 (13) |
| C14 | 0.0491 (15) | 0.0708 (17) | 0.0544 (17) | 0.0051 (13) | 0.0071 (13) | 0.0069 (15) |
| C15 | 0.0413 (15) | 0.073 (2) | 0.0478 (16) | −0.0009 (13) | 0.0049 (12) | 0.0011 (13) |
| C16 | 0.0448 (16) | 0.079 (2) | 0.065 (2) | −0.0034 (14) | −0.0015 (13) | 0.0077 (16) |
| C17 | 0.0483 (17) | 0.077 (2) | 0.078 (2) | −0.0085 (13) | 0.0042 (15) | 0.0113 (16) |
| C18 | 0.0488 (18) | 0.089 (2) | 0.065 (2) | −0.0120 (15) | 0.0101 (15) | −0.0020 (17) |
| C19 | 0.0420 (16) | 0.096 (2) | 0.073 (2) | 0.0000 (15) | −0.0023 (14) | −0.0061 (19) |
| C20 | 0.0532 (17) | 0.080 (2) | 0.066 (2) | 0.0088 (14) | −0.0019 (14) | 0.0034 (16) |
| Cl21 | 0.0772 (5) | 0.1122 (7) | 0.1174 (8) | −0.0353 (5) | −0.0068 (5) | −0.0004 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.379 (3) | C9—H9 | 0.9300 |
| C1—C10 | 1.438 (3) | C11—O12 | 1.232 (3) |
| C1—C11 | 1.491 (3) | C11—C13 | 1.483 (4) |
| C2—C3 | 1.404 (4) | C13—C14 | 1.331 (3) |
| C2—H2 | 0.9300 | C13—H13 | 0.9300 |
| C3—C4 | 1.359 (4) | C14—C15 | 1.462 (4) |
| C3—H3 | 0.9300 | C14—H14 | 0.9300 |
| C4—C5 | 1.410 (4) | C15—C16 | 1.387 (4) |
| C4—H4 | 0.9300 | C15—C20 | 1.395 (4) |
| C5—C6 | 1.410 (4) | C16—C17 | 1.382 (4) |
| C5—C10 | 1.431 (3) | C16—H16 | 0.9300 |
| C6—C7 | 1.350 (4) | C17—C18 | 1.385 (4) |
| C6—H6 | 0.9300 | C17—H17 | 0.9300 |
| C7—C8 | 1.398 (4) | C18—C19 | 1.378 (4) |
| C7—H7 | 0.9300 | C18—Cl21 | 1.737 (3) |
| C8—C9 | 1.371 (4) | C19—C20 | 1.385 (4) |
| C8—H8 | 0.9300 | C19—H19 | 0.9300 |
| C9—C10 | 1.415 (3) | C20—H20 | 0.9300 |
| | | | |
| C2—C1—C10 | 119.2 (2) | C5—C10—C1 | 118.6 (2) |
| C2—C1—C11 | 118.7 (2) | O12—C11—C13 | 119.8 (3) |
| C10—C1—C11 | 122.0 (2) | O12—C11—C1 | 120.6 (2) |
| C1—C2—C3 | 121.9 (3) | C13—C11—C1 | 119.5 (2) |
| C1—C2—H2 | 119.1 | C14—C13—C11 | 121.5 (3) |
| C3—C2—H2 | 119.1 | C14—C13—H13 | 119.2 |
| C4—C3—C2 | 119.4 (3) | C11—C13—H13 | 119.2 |
| C4—C3—H3 | 120.3 | C13—C14—C15 | 127.3 (3) |
| C2—C3—H3 | 120.3 | C13—C14—H14 | 116.3 |
| C3—C4—C5 | 122.0 (2) | C15—C14—H14 | 116.3 |
| C3—C4—H4 | 119.0 | C16—C15—C20 | 117.4 (3) |
| C5—C4—H4 | 119.0 | C16—C15—C14 | 122.5 (2) |
| C4—C5—C6 | 122.1 (2) | C20—C15—C14 | 120.1 (3) |
| C4—C5—C10 | 118.8 (2) | C17—C16—C15 | 122.1 (3) |
| C6—C5—C10 | 119.1 (2) | C17—C16—H16 | 119.0 |
| C7—C6—C5 | 121.7 (3) | C15—C16—H16 | 119.0 |
| C7—C6—H6 | 119.1 | C16—C17—C18 | 118.8 (3) |

| | | | |
|---|---|---|---|
| C5—C6—H6 | 119.1 | C16—C17—H17 | 120.6 |
| C6—C7—C8 | 119.7 (3) | C18—C17—H17 | 120.6 |
| C6—C7—H7 | 120.1 | C19—C18—C17 | 121.0 (3) |
| C8—C7—H7 | 120.1 | C19—C18—Cl21 | 120.0 (2) |
| C9—C8—C7 | 121.0 (3) | C17—C18—Cl21 | 118.9 (3) |
| C9—C8—H8 | 119.5 | C18—C19—C20 | 119.0 (3) |
| C7—C8—H8 | 119.5 | C18—C19—H19 | 120.5 |
| C8—C9—C10 | 120.9 (3) | C20—C19—H19 | 120.5 |
| C8—C9—H9 | 119.5 | C19—C20—C15 | 121.6 (3) |
| C10—C9—H9 | 119.5 | C19—C20—H20 | 119.2 |
| C9—C10—C5 | 117.6 (2) | C15—C20—H20 | 119.2 |
| C9—C10—C1 | 123.7 (2) | | |
| C10—C1—C2—C3 | 4.0 (4) | C11—C1—C10—C5 | 170.1 (2) |
| C11—C1—C2—C3 | −171.1 (2) | C2—C1—C11—O12 | 146.6 (3) |
| C1—C2—C3—C4 | −0.1 (4) | C10—C1—C11—O12 | −28.3 (4) |
| C2—C3—C4—C5 | −3.1 (4) | C2—C1—C11—C13 | −29.9 (3) |
| C3—C4—C5—C6 | −175.0 (3) | C10—C1—C11—C13 | 155.1 (2) |
| C3—C4—C5—C10 | 2.1 (4) | O12—C11—C13—C14 | −3.9 (4) |
| C4—C5—C6—C7 | 175.5 (3) | C1—C11—C13—C14 | 172.7 (2) |
| C10—C5—C6—C7 | −1.6 (4) | C11—C13—C14—C15 | −178.0 (3) |
| C5—C6—C7—C8 | −0.4 (4) | C13—C14—C15—C16 | 11.7 (4) |
| C6—C7—C8—C9 | 1.9 (4) | C13—C14—C15—C20 | −169.2 (3) |
| C7—C8—C9—C10 | −1.3 (4) | C20—C15—C16—C17 | 0.6 (4) |
| C8—C9—C10—C5 | −0.7 (3) | C14—C15—C16—C17 | 179.7 (3) |
| C8—C9—C10—C1 | −177.5 (2) | C15—C16—C17—C18 | 0.2 (4) |
| C4—C5—C10—C9 | −175.1 (2) | C16—C17—C18—C19 | −0.4 (4) |
| C6—C5—C10—C9 | 2.1 (3) | C16—C17—C18—Cl21 | −180.0 (2) |
| C4—C5—C10—C1 | 1.9 (3) | C17—C18—C19—C20 | −0.1 (4) |
| C6—C5—C10—C1 | 179.1 (2) | Cl21—C18—C19—C20 | 179.4 (2) |
| C2—C1—C10—C9 | 171.9 (2) | C18—C19—C20—C15 | 0.9 (4) |
| C11—C1—C10—C9 | −13.2 (4) | C16—C15—C20—C19 | −1.2 (4) |
| C2—C1—C10—C5 | −4.8 (3) | C14—C15—C20—C19 | 179.7 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H⋯*A* | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
|---|---|---|---|---|
| C17—H17⋯O12[i] | 0.93 | 2.42 | 3.180 (4) | 139. |
| C3—H3⋯Cl21[ii] | 0.93 | 2.92 | 3.703 (3) | 143. |
| C8—H8⋯O12[iii] | 0.93 | 2.64 | 3.546 (4) | 163. |

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

**Fig. 1**

**Fig. 2**

**Fig. 3**