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# (*E*,*Z*)-1-(4-Chlorophenyl)-5-phenyl-5-(phenylsulfanyl)penta-2,4-dien-1-one

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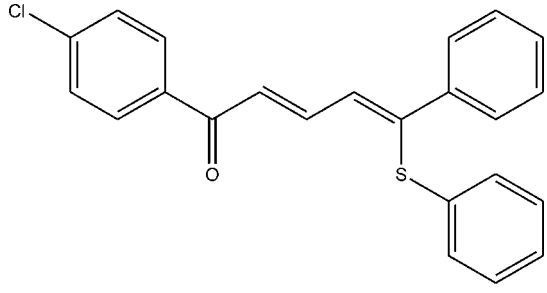
Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.049; $wR$ factor = 0.100; data-to-parameter ratio = 22.6.

The penta-2,4-dien-1-one fragment of the title compound, $C_{23}H_{17}ClOS$, is twisted by 20.0 (3)°, as measured by the dihedral angle between the planes of the carbonyl group and its attached C atom and the distant C=C double bond and its attached C atom. The 4-chlorophenyl group forms a dihedral angle of 4.0 (3)° with the adjacent carbonyl group. Conjugation between the phenyl ring and the C=C double bond is absent; the dihedral angle between the phenyl ring and the C—C=C fragment is 34.3 (2)°. In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming chains parallel to the *b*-axis direction.

## Related literature

For the biological activity of chalcones, and their arylthio-containing derivatives, see: Chate *et al.* (2012); Nielsen *et al.* (2005); Wu *et al.* (2011), Karaman *et al.* (2012). For the synthesis and crystal structures of precursor 1,5-diarylpent-2-en-4-yn-1-ones, see: Golovanov *et al.* (2013). For standard bond lengths, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{23}H_{17}ClOS$
$M_r$ = 376.88
Orthorhombic, *Pbca*
$a$ = 8.2663 (11) Å
$b$ = 11.1661 (13) Å
$c$ = 39.478 (6) Å
$V$ = 3643.9 (8) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.33 mm$^{-1}$
$T$ = 120 K
0.38 × 0.08 × 0.07 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min}$ = 0.903, $T_{max}$ = 0.967
20709 measured reflections
5311 independent reflections
3104 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.088

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.100
$S$ = 1.00
5311 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C7—H7$A$···O1$^{i}$ | 0.95 | 2.57 | 3.515 (3) | 178 |

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2112).

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# supplementary materials

*Acta Cryst.* (2013). E**69**, o1479 [doi:10.1107/S160053681302312X]

## (*E*,*Z*)-1-(4-Chlorophenyl)-5-phenyl-5-(phenylsulfanyl)penta-2,4-dien-1-one

**Anna V. Vologzhanina, Dmitry M. Gusev, Alexander A. Golovanov and Valentina S. Pisareva**

### 1. Comment

The family of chalcones exhibit antibiotic (Nielsen *et al.*, 2005) and anti-inflammatory (Wu *et al.*, 2011) activity. Arylthio-containing ketones are also active against some human pathogenic microorganisms (Chate *et al.*, 2012; Karaman *et al.*, 2012). Thus, a molecule which contains both fragments may have a high biological effect. Herein, we present the structure of (E, *Z*)-1-(4-chlorophenyl)-5-phenyl-5-phenylthio-penta-2,4-dien-1-one prepared by Michael-type addition reaction between thiophenol and 1-(4-chlorophenyl)-5-phenyl-2-penten-4-yn-1-one.

All bond lengths have characteristic values (Allen *et al.*, 1987), although the length of the C3—C4 bond (1.429 (3) Å) indicates some electron delocalization along polyene C═C—C═C chain. The S—C distances of 1.769 (2) and 1.774 (2) Å, are slightly shortened due to mesomeric effect of sulfur electron pairs. The penta-2,4-dien-1-one fragment is twisted, the angle between two meanplanes (O1═C1—C2 and C3—C4═C5) is equal to 20.0 (3) °. The 4-chlorophenyl ring makes with the carbonyl group a dihedral angle of 4.0 (3) °. A dihedral angle between the phenyl ring and C3—C4═C5 fragment is 34.3 (2)°.

The molecules are linked in the crystal *via* C7—H7A···O bonds into chains parallel to the crystallographic *b* axis. It is worth mentioning that the C—H···O bonds which involve the hydrogen atom at *o* position of phenyl ring are typical for 1,5-diarylsubstituted penten-yn-ones (Golovanov, *et al.*, 2013).

### 2. Experimental

Three drops of triethylamine were added to a solution of 1-(4-chlorophenyl)-5-phenylpent-2-en-4-yn-1-one (322 mg, 1.21 mmol) and thiophenol (133 mg, 1.21 mmol) in 3 ml 95% ethanol. After 12 h, the precipitated yellow crystals were filtered and washed with 2 ml of cold 40% alcohol. Yield 82%. The single crystal was obtained from mixture of acetone and water. M.p. 366–367K.

### 3. Refinement

All non-H atoms were refined anisotropically. Hydrogen atoms were positioned geometrically and refined isotropically being constrained to ride on their adjacent carbon atoms with $U_{iso}$(H) = 1.2$U_{eq}$(C).

### Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

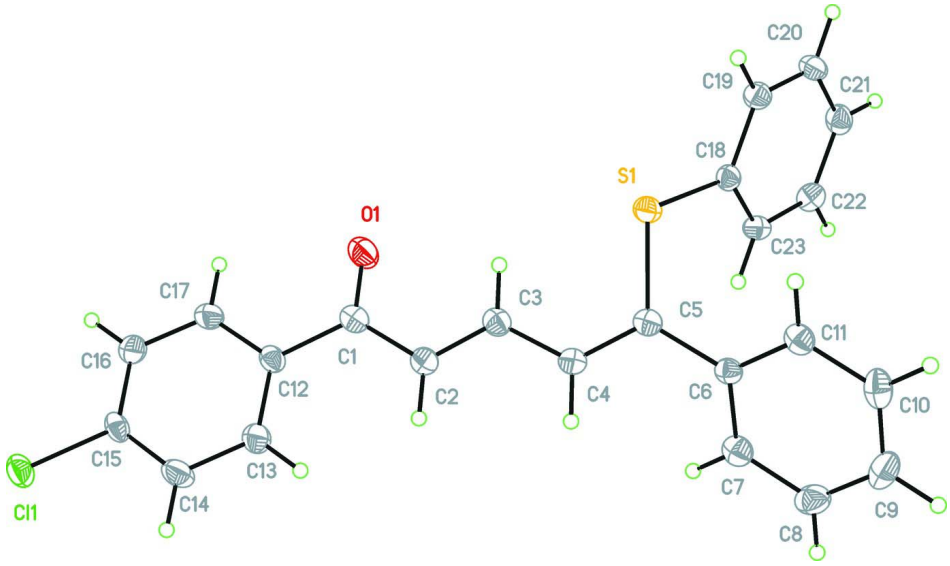


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at 50% probability level.

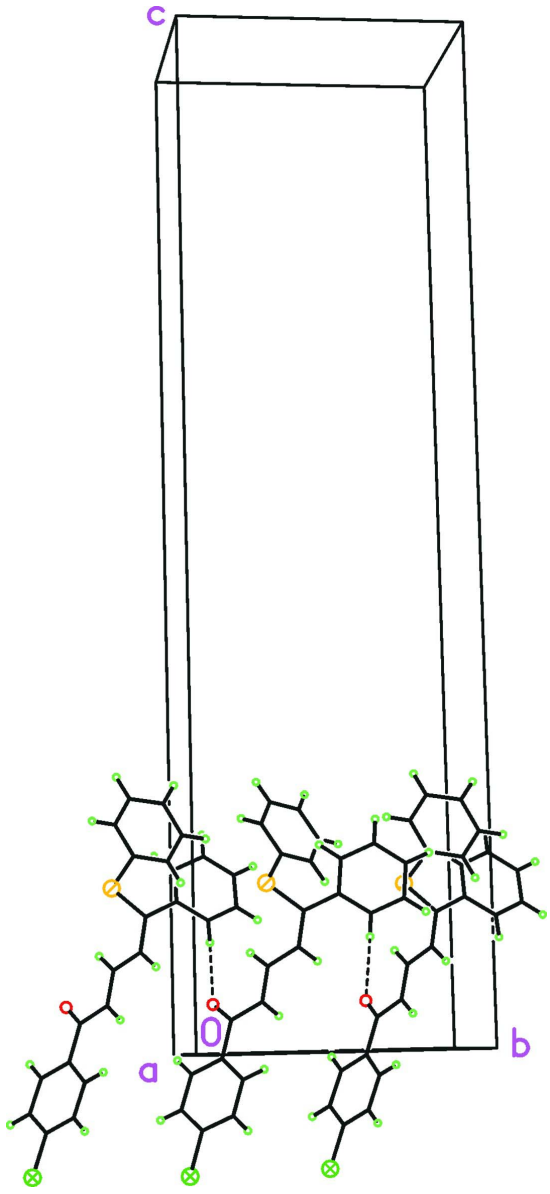


**Figure 2**

The C—H···O bonded chain viewed down the *a* axis. Dashed lines indicate hydrogen bonds.

### (*E*,*Z*)-1-(4-Chlorophenyl)-5-phenyl-5-(phenylsulfanyl)penta-2,4-dien-1-one

*Crystal data*

$C_{23}H_{17}ClOS$
$M_r = 376.88$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 8.2663\ (11)$ Å
$b = 11.1661\ (13)$ Å
$c = 39.478\ (6)$ Å
$V = 3643.9\ (8)$ Å$^3$
$Z = 8$
$F(000) = 1568$
$D_x = 1.374$ Mg m$^{-3}$
Melting point = 366–280 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1957 reflections
$\theta = 2.7$–$27.8°$
$\mu = 0.33$ mm$^{-1}$
$T = 120$ K
Needle, yellow
0.38 × 0.08 × 0.07 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min}$ = 0.903, $T_{max}$ = 0.967
20709 measured reflections
5311 independent reflections
3104 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.088
$\theta_{max}$ = 30.0°, $\theta_{min}$ = 2.1°
$h$ = −11→11
$k$ = −11→15
$l$ = −55→38

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.100
$S$ = 1.00
5311 reflections
235 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.019P)^2 + 2.8P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

*Special details*

**Experimental**. IR (KBr), $\nu$/cm$^{-1}$: 3051, 1648, 1589, 1573, 1559, 1481, 1441, 1397, 1356, 1333, 1272, 1225, 1176, 1091, 1025, 1009, 939. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.02 (d, 1H, J = 11.2 Hz), 7.12 (d, 1H, J = 14.9 Hz), 7.20–8.00 (m, 14H), 8.27 (dd, 1H, J = 11.2 Hz, J = 15.0 Hz). $^{13}$C NMR (100 MHz, CDCl3): 77.5, 123.2, 127.3, 129.0, 130.1, 132.3, 134.7, 136.6, 139.2, 141.5, 153.9, 189.5. Anal. Calcd. for $C_{23}H_{17}ClSO$: C, 73.29; H, 4.67. Found: C, 73.33; H, 4.56.

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.88212 (7) | 0.25480 (5) | 0.159299 (14) | 0.02170 (13) |
| Cl1 | 0.91964 (8) | −0.02110 (5) | −0.110391 (14) | 0.02792 (15) |
| O1 | 0.6697 (2) | 0.08592 (16) | 0.04724 (4) | 0.0328 (4) |
| C1 | 0.7800 (3) | 0.1369 (2) | 0.03200 (6) | 0.0222 (5) |
| C2 | 0.8736 (3) | 0.2331 (2) | 0.04818 (6) | 0.0220 (5) |
| H2A | 0.9446 | 0.2803 | 0.0348 | 0.026* |
| C3 | 0.8611 (3) | 0.2558 (2) | 0.08142 (5) | 0.0210 (5) |
| H3A | 0.7946 | 0.2043 | 0.0946 | 0.025* |
| C4 | 0.9409 (3) | 0.35209 (19) | 0.09840 (6) | 0.0207 (5) |
| H4A | 0.9973 | 0.4078 | 0.0845 | 0.025* |
| C5 | 0.9444 (3) | 0.37216 (19) | 0.13219 (6) | 0.0188 (5) |
| C6 | 1.0132 (3) | 0.48280 (19) | 0.14683 (6) | 0.0173 (5) |
| C7 | 1.0076 (3) | 0.5896 (2) | 0.12817 (6) | 0.0233 (5) |

| | | | | |
|---|---|---|---|---|
| H7A | 0.9575 | 0.5906 | 0.1065 | 0.028* |
| C8 | 1.0748 (3) | 0.6937 (2) | 0.14119 (7) | 0.0294 (6) |
| H8A | 1.0716 | 0.7655 | 0.1283 | 0.035* |
| C9 | 1.1464 (3) | 0.6935 (2) | 0.17291 (7) | 0.0293 (6) |
| H9A | 1.1925 | 0.7648 | 0.1817 | 0.035* |
| C10 | 1.1504 (3) | 0.5892 (2) | 0.19162 (6) | 0.0266 (6) |
| H10A | 1.1986 | 0.5890 | 0.2135 | 0.032* |
| C11 | 1.0847 (3) | 0.4850 (2) | 0.17873 (6) | 0.0213 (5) |
| H11A | 1.0884 | 0.4137 | 0.1918 | 0.026* |
| C12 | 0.8177 (3) | 0.1007 (2) | −0.00365 (6) | 0.0199 (5) |
| C13 | 0.9341 (3) | 0.1579 (2) | −0.02328 (6) | 0.0275 (6) |
| H13A | 0.9929 | 0.2234 | −0.0141 | 0.033* |
| C14 | 0.9652 (3) | 0.1205 (2) | −0.05610 (6) | 0.0292 (6) |
| H14A | 1.0441 | 0.1605 | −0.0695 | 0.035* |
| C15 | 0.8809 (3) | 0.0248 (2) | −0.06919 (5) | 0.0206 (5) |
| C16 | 0.7655 (3) | −0.0342 (2) | −0.05040 (6) | 0.0262 (6) |
| H16A | 0.7082 | −0.1002 | −0.0597 | 0.031* |
| C17 | 0.7343 (3) | 0.0043 (2) | −0.01770 (6) | 0.0261 (5) |
| H17A | 0.6546 | −0.0358 | −0.0046 | 0.031* |
| C18 | 0.7446 (3) | 0.32191 (19) | 0.18812 (6) | 0.0176 (5) |
| C19 | 0.7105 (3) | 0.2586 (2) | 0.21755 (6) | 0.0209 (5) |
| H19A | 0.7657 | 0.1857 | 0.2222 | 0.025* |
| C20 | 0.5960 (3) | 0.3016 (2) | 0.24015 (6) | 0.0229 (5) |
| H20A | 0.5721 | 0.2575 | 0.2601 | 0.028* |
| C21 | 0.5163 (3) | 0.4082 (2) | 0.23384 (6) | 0.0243 (5) |
| H21A | 0.4386 | 0.4380 | 0.2495 | 0.029* |
| C22 | 0.5510 (3) | 0.4712 (2) | 0.20447 (6) | 0.0232 (5) |
| H22A | 0.4961 | 0.5442 | 0.2000 | 0.028* |
| C23 | 0.6647 (3) | 0.4293 (2) | 0.18159 (6) | 0.0204 (5) |
| H23A | 0.6879 | 0.4735 | 0.1616 | 0.024* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0278 (3) | 0.0179 (3) | 0.0194 (3) | 0.0019 (3) | 0.0046 (3) | 0.0014 (2) |
| Cl1 | 0.0348 (3) | 0.0317 (3) | 0.0173 (3) | 0.0022 (3) | 0.0017 (3) | −0.0028 (2) |
| O1 | 0.0357 (11) | 0.0387 (10) | 0.0240 (9) | −0.0100 (9) | 0.0075 (8) | −0.0041 (8) |
| C1 | 0.0218 (13) | 0.0246 (13) | 0.0202 (13) | 0.0011 (10) | 0.0013 (10) | 0.0018 (10) |
| C2 | 0.0254 (12) | 0.0218 (12) | 0.0188 (11) | −0.0005 (10) | −0.0001 (10) | 0.0009 (9) |
| C3 | 0.0217 (12) | 0.0217 (11) | 0.0197 (11) | 0.0028 (10) | 0.0003 (9) | 0.0012 (10) |
| C4 | 0.0218 (12) | 0.0204 (12) | 0.0198 (12) | −0.0018 (10) | 0.0022 (10) | 0.0011 (9) |
| C5 | 0.0176 (11) | 0.0188 (11) | 0.0200 (11) | 0.0027 (9) | 0.0012 (10) | 0.0020 (9) |
| C6 | 0.0152 (11) | 0.0184 (11) | 0.0183 (11) | 0.0014 (9) | 0.0032 (9) | 0.0004 (9) |
| C7 | 0.0226 (13) | 0.0239 (12) | 0.0233 (13) | 0.0047 (10) | 0.0025 (10) | 0.0005 (10) |
| C8 | 0.0338 (15) | 0.0199 (13) | 0.0344 (15) | 0.0018 (11) | 0.0083 (12) | 0.0022 (11) |
| C9 | 0.0247 (14) | 0.0253 (13) | 0.0381 (15) | −0.0041 (11) | 0.0018 (12) | −0.0099 (12) |
| C10 | 0.0208 (13) | 0.0343 (14) | 0.0247 (13) | 0.0020 (11) | −0.0023 (11) | −0.0093 (11) |
| C11 | 0.0204 (12) | 0.0230 (12) | 0.0205 (11) | 0.0041 (10) | 0.0020 (10) | −0.0001 (10) |
| C12 | 0.0230 (12) | 0.0217 (12) | 0.0149 (11) | 0.0028 (10) | −0.0004 (10) | 0.0012 (9) |
| C13 | 0.0326 (15) | 0.0299 (14) | 0.0199 (12) | −0.0100 (12) | 0.0000 (11) | −0.0037 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C14 | 0.0281 (14) | 0.0381 (15) | 0.0213 (13) | −0.0121 (12) | 0.0055 (11) | −0.0006 (11) |
| C15 | 0.0244 (12) | 0.0252 (12) | 0.0122 (10) | 0.0059 (11) | −0.0013 (9) | −0.0003 (9) |
| C16 | 0.0330 (14) | 0.0240 (13) | 0.0216 (13) | −0.0065 (11) | −0.0009 (11) | −0.0022 (10) |
| C17 | 0.0297 (14) | 0.0263 (13) | 0.0223 (12) | −0.0086 (11) | 0.0043 (11) | 0.0000 (11) |
| C18 | 0.0171 (11) | 0.0189 (11) | 0.0168 (11) | −0.0018 (9) | −0.0001 (9) | −0.0013 (9) |
| C19 | 0.0228 (12) | 0.0198 (12) | 0.0203 (12) | 0.0004 (10) | −0.0027 (9) | 0.0016 (10) |
| C20 | 0.0266 (13) | 0.0259 (12) | 0.0164 (11) | −0.0048 (11) | 0.0009 (10) | 0.0033 (9) |
| C21 | 0.0222 (13) | 0.0273 (13) | 0.0232 (13) | −0.0016 (10) | 0.0045 (10) | −0.0045 (10) |
| C22 | 0.0215 (13) | 0.0212 (12) | 0.0271 (13) | 0.0000 (10) | 0.0003 (10) | −0.0003 (10) |
| C23 | 0.0211 (12) | 0.0198 (11) | 0.0202 (12) | −0.0018 (10) | 0.0012 (10) | 0.0030 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C5 | 1.769 (2) | C11—H11A | 0.9500 |
| S1—C18 | 1.774 (2) | C12—C13 | 1.391 (3) |
| Cl1—C15 | 1.735 (2) | C12—C17 | 1.393 (3) |
| O1—C1 | 1.231 (3) | C13—C14 | 1.386 (3) |
| C1—C2 | 1.470 (3) | C13—H13A | 0.9500 |
| C1—C12 | 1.497 (3) | C14—C15 | 1.377 (3) |
| C2—C3 | 1.340 (3) | C14—H14A | 0.9500 |
| C2—H2A | 0.9500 | C15—C16 | 1.376 (3) |
| C3—C4 | 1.429 (3) | C16—C17 | 1.385 (3) |
| C3—H3A | 0.9500 | C16—H16A | 0.9500 |
| C4—C5 | 1.353 (3) | C17—H17A | 0.9500 |
| C4—H4A | 0.9500 | C18—C19 | 1.389 (3) |
| C5—C6 | 1.478 (3) | C18—C23 | 1.394 (3) |
| C6—C11 | 1.391 (3) | C19—C20 | 1.387 (3) |
| C6—C7 | 1.402 (3) | C19—H19A | 0.9500 |
| C7—C8 | 1.388 (3) | C20—C21 | 1.384 (3) |
| C7—H7A | 0.9500 | C20—H20A | 0.9500 |
| C8—C9 | 1.385 (3) | C21—C22 | 1.386 (3) |
| C8—H8A | 0.9500 | C21—H21A | 0.9500 |
| C9—C10 | 1.379 (3) | C22—C23 | 1.384 (3) |
| C9—H9A | 0.9500 | C22—H22A | 0.9500 |
| C10—C11 | 1.381 (3) | C23—H23A | 0.9500 |
| C10—H10A | 0.9500 | | |

| | | | |
|---|---|---|---|
| C5—S1—C18 | 105.17 (10) | C13—C12—C1 | 122.9 (2) |
| O1—C1—C2 | 121.0 (2) | C17—C12—C1 | 118.7 (2) |
| O1—C1—C12 | 119.2 (2) | C14—C13—C12 | 120.7 (2) |
| C2—C1—C12 | 119.8 (2) | C14—C13—H13A | 119.6 |
| C3—C2—C1 | 121.5 (2) | C12—C13—H13A | 119.6 |
| C3—C2—H2A | 119.2 | C15—C14—C13 | 119.4 (2) |
| C1—C2—H2A | 119.2 | C15—C14—H14A | 120.3 |
| C2—C3—C4 | 124.5 (2) | C13—C14—H14A | 120.3 |
| C2—C3—H3A | 117.8 | C16—C15—C14 | 121.3 (2) |
| C4—C3—H3A | 117.8 | C16—C15—Cl1 | 119.48 (18) |
| C5—C4—C3 | 126.7 (2) | C14—C15—Cl1 | 119.17 (18) |
| C5—C4—H4A | 116.7 | C15—C16—C17 | 118.9 (2) |
| C3—C4—H4A | 116.7 | C15—C16—H16A | 120.6 |

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| C4—C5—C6 | 122.2 (2) | C17—C16—H16A | 120.6 |
| C4—C5—S1 | 117.89 (17) | C16—C17—C12 | 121.3 (2) |
| C6—C5—S1 | 119.65 (17) | C16—C17—H17A | 119.4 |
| C11—C6—C7 | 118.3 (2) | C12—C17—H17A | 119.4 |
| C11—C6—C5 | 122.2 (2) | C19—C18—C23 | 119.8 (2) |
| C7—C6—C5 | 119.5 (2) | C19—C18—S1 | 116.83 (17) |
| C8—C7—C6 | 120.3 (2) | C23—C18—S1 | 123.27 (17) |
| C8—C7—H7A | 119.8 | C20—C19—C18 | 120.0 (2) |
| C6—C7—H7A | 119.8 | C20—C19—H19A | 120.0 |
| C9—C8—C7 | 120.3 (2) | C18—C19—H19A | 120.0 |
| C9—C8—H8A | 119.9 | C21—C20—C19 | 120.5 (2) |
| C7—C8—H8A | 119.9 | C21—C20—H20A | 119.8 |
| C10—C9—C8 | 119.8 (2) | C19—C20—H20A | 119.8 |
| C10—C9—H9A | 120.1 | C20—C21—C22 | 119.2 (2) |
| C8—C9—H9A | 120.1 | C20—C21—H21A | 120.4 |
| C9—C10—C11 | 120.3 (2) | C22—C21—H21A | 120.4 |
| C9—C10—H10A | 119.9 | C23—C22—C21 | 121.0 (2) |
| C11—C10—H10A | 119.9 | C23—C22—H22A | 119.5 |
| C10—C11—C6 | 121.1 (2) | C21—C22—H22A | 119.5 |
| C10—C11—H11A | 119.5 | C22—C23—C18 | 119.5 (2) |
| C6—C11—H11A | 119.5 | C22—C23—H23A | 120.3 |
| C13—C12—C17 | 118.4 (2) | C18—C23—H23A | 120.3 |

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| O1—C1—C2—C3 | 11.0 (4) | O1—C1—C12—C17 | −4.6 (3) |
| C12—C1—C2—C3 | −169.6 (2) | C2—C1—C12—C17 | 176.0 (2) |
| C1—C2—C3—C4 | −176.1 (2) | C17—C12—C13—C14 | 0.6 (4) |
| C2—C3—C4—C5 | −173.4 (2) | C1—C12—C13—C14 | 179.6 (2) |
| C3—C4—C5—C6 | −172.1 (2) | C12—C13—C14—C15 | −0.7 (4) |
| C3—C4—C5—S1 | 14.1 (3) | C13—C14—C15—C16 | 0.4 (4) |
| C18—S1—C5—C4 | −131.58 (19) | C13—C14—C15—Cl1 | 179.6 (2) |
| C18—S1—C5—C6 | 54.5 (2) | C14—C15—C16—C17 | 0.0 (4) |
| C4—C5—C6—C11 | −150.1 (2) | Cl1—C15—C16—C17 | −179.20 (19) |
| S1—C5—C6—C11 | 23.6 (3) | C15—C16—C17—C12 | −0.2 (4) |
| C4—C5—C6—C7 | 29.7 (3) | C13—C12—C17—C16 | −0.1 (4) |
| S1—C5—C6—C7 | −156.70 (18) | C1—C12—C17—C16 | −179.2 (2) |
| C11—C6—C7—C8 | 1.2 (3) | C5—S1—C18—C19 | −163.19 (18) |
| C5—C6—C7—C8 | −178.6 (2) | C5—S1—C18—C23 | 20.6 (2) |
| C6—C7—C8—C9 | −0.7 (4) | C23—C18—C19—C20 | 0.7 (3) |
| C7—C8—C9—C10 | −0.1 (4) | S1—C18—C19—C20 | −175.65 (18) |
| C8—C9—C10—C11 | 0.6 (4) | C18—C19—C20—C21 | −0.8 (3) |
| C9—C10—C11—C6 | −0.1 (4) | C19—C20—C21—C22 | 0.6 (4) |
| C7—C6—C11—C10 | −0.8 (3) | C20—C21—C22—C23 | −0.4 (4) |
| C5—C6—C11—C10 | 179.0 (2) | C21—C22—C23—C18 | 0.3 (4) |
| O1—C1—C12—C13 | 176.4 (2) | C19—C18—C23—C22 | −0.5 (3) |
| C2—C1—C12—C13 | −3.0 (3) | S1—C18—C23—C22 | 175.62 (18) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7*A*···O1$^{i}$ | 0.95 | 2.57 | 3.515 (3) | 178 |

Symmetry code: (i) −*x*+3/2, *y*+1/2, *z*.