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# (2*E*)-1-(5-Bromothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one

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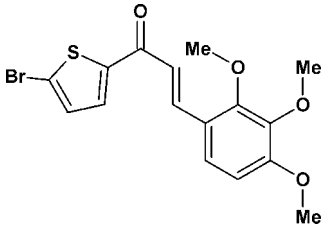
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.033; $wR$ factor = 0.082; data-to-parameter ratio = 14.0.

In the title compound, $C_{16}H_{15}BrO_4S$, the thiophene ring is not coplanar with the benzene ring; the dihedral angle between the two planes is 11.08 (12)°. The crystal structure is characterized by C—H···O interactions. Weak intramolecular C—H···O hydrogen bonds also occur.

## Related literature

For general background to chalcones, see: Chun *et al.* (2001); Horng *et al.* (2003); Lopez *et al.* (2001); Zubieta *et al.* (2001); Howard *et al.* (2004); Petrash (2004); Lu *et al.* (2010). Mei *et al.* (2003). For related structures, see: Liang *et al.* (2011); Alex *et al.* (1993); Li & Su (1993).




## Experimental

### Crystal data

$C_{16}H_{15}BrO_4S$
$M_r$ = 383.25
Monoclinic, $P2_1/c$
$a$ = 8.114 (5) Å
$b$ = 12.775 (5) Å
$c$ = 15.404 (5) Å
$\beta$ = 98.813 (5)°
$V$ = 1577.9 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.75 mm$^{-1}$
$T$ = 293 K
0.22 × 0.15 × 0.12 mm

### Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2010)
$T_{min}$ = 0.228, $T_{max}$ = 1.000
16471 measured reflections
2784 independent reflections
2343 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.082
$S$ = 1.06
2784 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8*B*···O5 | 0.96 | 2.23 | 2.861 (4) | 122 |
| C9—H9*B*···O4 | 0.96 | 2.38 | 2.985 (4) | 120 |
| C21—H21···O6$^{i}$ | 0.93 | 2.41 | 3.322 (4) | 165 |

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

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2039).

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# supporting information

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## (2*E*)-1-(5-Bromothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one

**K. Sunitha, H. C. Devarajegowda, Waleed Fadl Ali Al-eryani, Y. Rajendra Prasad and A. Uma Mahesh Kumar**

### S1. Comment

Chalcones are alpha, beta unsaturated ketones, widely distributed in nature and are extensively studied for their biological activity (Chun *et al.*, 2001; Horng *et al.*, 2003; Lopez *et al.*, 2001; Mei *et al.*, 2003). Chalcones readily crystallize because of their intermolecular hydrogen bonding (Liang *et al.*, 2011; Alex *et al.*, 1993; Li *et al.*, 1993). The same property has been shown to be responsible for its biological activity (Zubieta *et al.*, 2001). However, halogen containing chalcones are of special interest in drug design process because of the raising importance of hlogen bond contribution in target recognition process (Howard *et al.*, 2004; Petrash, 2004; Lu *et al.*, 2010). Crystal structure conformation of small molecule has always been the choice for binding energy calculations in docking studies. In this paper we report the crystal structure of (2E)-1-(5-bromothiophen-2-yl)- 3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one which is a part of insilico lead identification studies.

The asymmetric unit of (2E)-1-(5-bromothiophen-2-yl)-3-(2,3,4- trimethoxyphenyl)prop-2-en-1-one, $C_{16}H_{15}Br_{O}4_{S}$, contains just one molecule (Fig. 1). The five-membered thiophene ring (S2\C19\···C22) is not coplanar with the phenyl ring (C10\C11\···C15) system; the dihedral angle between the two planes is 11.08 (12)°. The crystal structure displays intermolecular C21—H21···O6 and weak intramolecular C8—H8B···O5 and C9—H9B···O4 hydrogen bonds (Table 1). The packing of molecules in the crystal structure is depicted in Fig. 2.

### S2. Experimental

A mixture of 2-acetyl-5-BromoThiophene (0.01 mole) and 2,3,4- trimethoxybenzaldehyde (0.01 mole) were stirred in ethanol (30 ml) and then an aqueous solution of potassium hydroxide (40%,15 ml)was added to it. The mixture was kept over night at room temperature and then it was poured into crushed ice and acidified with dilute hydrochloric acid. The precipiteted chalcone was filtered and crystallized from ethanol.

### S3. Refinement

All H atoms were positioned at calculated positions C—H = 0.93Å for aromatic H and C—H = 0.96Å for methyl H and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C)for aromatic and $U_{iso}$(H) = 1.2$U_{eq}$(C)for for methyl H.

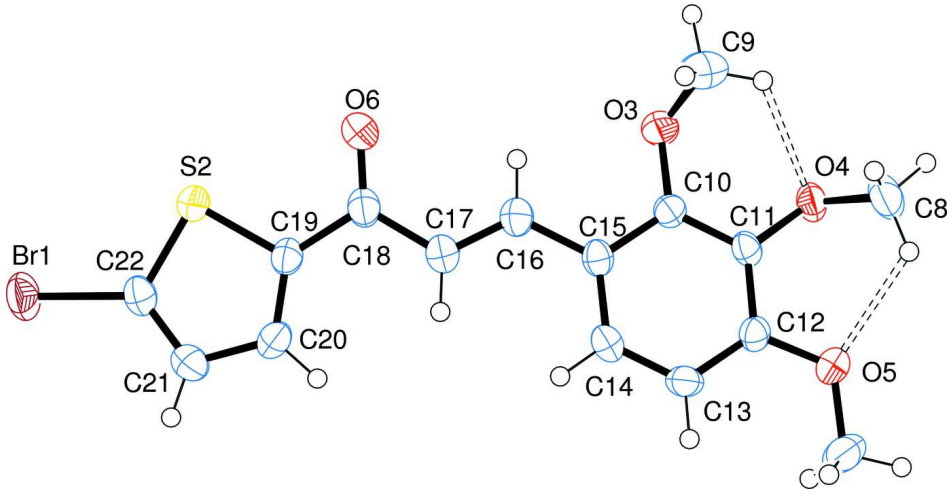


**Figure 1**

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. The H atoms are shown as spheres of arbitrary radii. The dashed line indicates the intramolecular hydrogen bond.

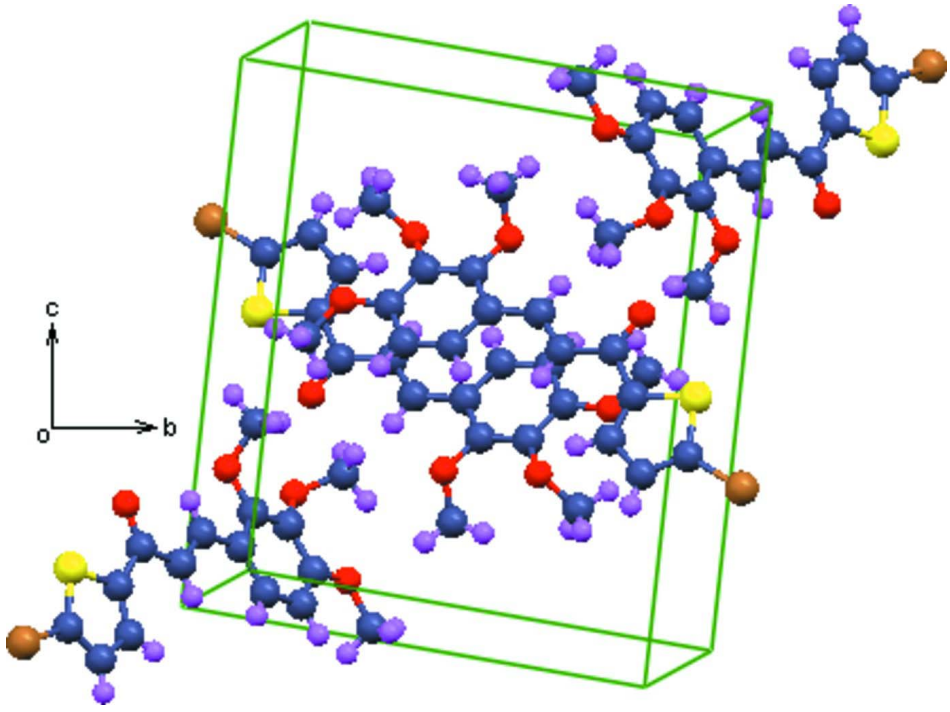


**Figure 2**

Packing of the molecules.

**(2*E*)-1-(5-Bromothiophen-2-yl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one**

*Crystal data*

| | |
|---|---|
| $C_{16}H_{15}BrO_4S$ | $a$ = 8.114 (5) Å |
| $M_r$ = 383.25 | $b$ = 12.775 (5) Å |
| Monoclinic, $P2_1/c$ | $c$ = 15.404 (5) Å |
| Hall symbol: -P 2ybc | $\beta$ = 98.813 (5)° |

$V$ = 1577.9 (13) Å$^3$
$Z$ = 4
$F$(000) = 776
$D_x$ = 1.613 Mg m$^{-3}$
Melting point: 400 K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å

Cell parameters from 2784 reflections
$\theta$ = 2.5–25.0°
$\mu$ = 2.75 mm$^{-1}$
$T$ = 293 K
Prism, colourless
0.22 × 0.15 × 0.12 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0839 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2010)
$T_{min}$ = 0.228, $T_{max}$ = 1.000

16471 measured reflections
2784 independent reflections
2343 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.5°
$h$ = −9→9
$k$ = −15→15
$l$ = −18→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.082
$S$ = 1.06
2784 reflections
199 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
$w = 1/[\sigma^2(F_o^2) + (0.0349P)^2 + 0.9331P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.59 e Å$^{-3}$

*Special details*

**Experimental**. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.33.55 (release 05–01–2010 CrysAlis171. NET) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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 | −0.24507 (4) | 0.00703 (2) | 0.22076 (2) | 0.05109 (14) |
| S2 | −0.11145 (9) | 0.10763 (6) | 0.06120 (5) | 0.03737 (19) |
| O3 | 0.3504 (3) | 0.47747 (15) | −0.20529 (13) | 0.0450 (5) |
| O4 | 0.5493 (2) | 0.65241 (14) | −0.19864 (12) | 0.0378 (5) |
| O5 | 0.5662 (2) | 0.78703 (15) | −0.06147 (13) | 0.0429 (5) |
| O6 | 0.0059 (3) | 0.22557 (18) | −0.08036 (14) | 0.0561 (6) |
| C7 | 0.5915 (4) | 0.8532 (3) | 0.0134 (2) | 0.0527 (8) |
| H7A | 0.6611 | 0.9111 | 0.0026 | 0.079* |

| | | | | |
|---|---|---|---|---|
| H7B | 0.6446 | 0.8143 | 0.0633 | 0.079* |
| H7C | 0.4859 | 0.8790 | 0.0250 | 0.079* |
| C8 | 0.5199 (4) | 0.7480 (2) | −0.2465 (2) | 0.0566 (9) |
| H8A | 0.5915 | 0.7515 | −0.2906 | 0.085* |
| H8B | 0.5428 | 0.8062 | −0.2070 | 0.085* |
| H8C | 0.4056 | 0.7507 | −0.2742 | 0.085* |
| C9 | 0.2743 (4) | 0.5175 (3) | −0.2882 (2) | 0.0592 (10) |
| H9A | 0.2735 | 0.4642 | −0.3322 | 0.089* |
| H9B | 0.3363 | 0.5769 | −0.3036 | 0.089* |
| H9C | 0.1619 | 0.5383 | −0.2847 | 0.089* |
| C10 | 0.3613 (3) | 0.5446 (2) | −0.13548 (17) | 0.0301 (6) |
| C11 | 0.4561 (3) | 0.6350 (2) | −0.13228 (17) | 0.0294 (6) |
| C12 | 0.4695 (3) | 0.6998 (2) | −0.05918 (17) | 0.0305 (6) |
| C13 | 0.3899 (3) | 0.6724 (2) | 0.01106 (17) | 0.0351 (6) |
| H13 | 0.3962 | 0.7162 | 0.0597 | 0.042* |
| C14 | 0.3017 (3) | 0.5805 (2) | 0.00854 (18) | 0.0340 (6) |
| H14 | 0.2531 | 0.5616 | 0.0571 | 0.041* |
| C15 | 0.2827 (3) | 0.5150 (2) | −0.06390 (18) | 0.0305 (6) |
| C16 | 0.1893 (3) | 0.4176 (2) | −0.06729 (19) | 0.0358 (6) |
| H16 | 0.1706 | 0.3834 | −0.1212 | 0.043* |
| C17 | 0.1279 (3) | 0.3722 (2) | −0.00165 (19) | 0.0387 (7) |
| H17 | 0.1416 | 0.4057 | 0.0526 | 0.046* |
| C18 | 0.0399 (3) | 0.2720 (2) | −0.01058 (19) | 0.0368 (7) |
| C19 | −0.0079 (3) | 0.2265 (2) | 0.06962 (18) | 0.0331 (6) |
| C20 | 0.0083 (3) | 0.2636 (2) | 0.15283 (19) | 0.0401 (7) |
| H20 | 0.0614 | 0.3264 | 0.1700 | 0.048* |
| C21 | −0.0624 (4) | 0.1988 (2) | 0.21091 (19) | 0.0419 (7) |
| H21 | −0.0613 | 0.2134 | 0.2702 | 0.050* |
| C22 | −0.1317 (3) | 0.1132 (2) | 0.16997 (18) | 0.0363 (7) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0619 (2) | 0.0412 (2) | 0.0540 (2) | −0.00626 (15) | 0.02110 (16) | 0.01379 (15) |
| S2 | 0.0458 (4) | 0.0314 (4) | 0.0354 (4) | −0.0079 (3) | 0.0077 (3) | 0.0008 (3) |
| O3 | 0.0683 (14) | 0.0315 (11) | 0.0382 (12) | −0.0042 (10) | 0.0176 (10) | −0.0070 (9) |
| O4 | 0.0486 (11) | 0.0292 (11) | 0.0407 (11) | −0.0010 (9) | 0.0227 (9) | 0.0033 (9) |
| O5 | 0.0549 (12) | 0.0330 (12) | 0.0421 (12) | −0.0122 (9) | 0.0114 (9) | −0.0037 (9) |
| O6 | 0.0809 (16) | 0.0551 (15) | 0.0335 (12) | −0.0242 (12) | 0.0124 (11) | 0.0002 (11) |
| C7 | 0.059 (2) | 0.0403 (19) | 0.060 (2) | −0.0117 (16) | 0.0121 (16) | −0.0162 (16) |
| C8 | 0.087 (3) | 0.043 (2) | 0.0442 (19) | −0.0002 (18) | 0.0262 (18) | 0.0127 (16) |
| C9 | 0.065 (2) | 0.065 (2) | 0.044 (2) | −0.0103 (18) | 0.0000 (17) | −0.0121 (17) |
| C10 | 0.0364 (14) | 0.0231 (14) | 0.0320 (15) | 0.0040 (11) | 0.0093 (11) | 0.0001 (11) |
| C11 | 0.0346 (14) | 0.0260 (14) | 0.0292 (14) | 0.0040 (11) | 0.0103 (11) | 0.0053 (11) |
| C12 | 0.0336 (14) | 0.0247 (14) | 0.0333 (15) | 0.0009 (11) | 0.0058 (11) | 0.0031 (12) |
| C13 | 0.0430 (16) | 0.0350 (16) | 0.0272 (14) | 0.0009 (13) | 0.0056 (12) | −0.0046 (12) |
| C14 | 0.0360 (15) | 0.0367 (16) | 0.0310 (15) | 0.0009 (12) | 0.0109 (11) | 0.0057 (12) |
| C15 | 0.0296 (14) | 0.0287 (15) | 0.0340 (15) | 0.0026 (11) | 0.0073 (11) | 0.0053 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16 | 0.0370 (15) | 0.0327 (16) | 0.0377 (16) | −0.0007 (12) | 0.0061 (12) | 0.0048 (13) |
| C17 | 0.0424 (16) | 0.0383 (17) | 0.0364 (16) | −0.0056 (13) | 0.0093 (13) | 0.0036 (13) |
| C18 | 0.0367 (15) | 0.0373 (17) | 0.0369 (17) | −0.0042 (12) | 0.0070 (12) | 0.0062 (13) |
| C19 | 0.0331 (14) | 0.0303 (15) | 0.0355 (16) | −0.0037 (11) | 0.0036 (11) | 0.0041 (12) |
| C20 | 0.0444 (16) | 0.0334 (16) | 0.0419 (18) | −0.0105 (13) | 0.0043 (13) | −0.0023 (13) |
| C21 | 0.0514 (18) | 0.0434 (18) | 0.0319 (16) | −0.0024 (14) | 0.0094 (13) | 0.0016 (14) |
| C22 | 0.0383 (15) | 0.0337 (16) | 0.0386 (16) | 0.0015 (12) | 0.0113 (12) | 0.0071 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C22 | 1.876 (3) | C10—C11 | 1.384 (4) |
| S2—C22 | 1.710 (3) | C10—C15 | 1.407 (4) |
| S2—C19 | 1.730 (3) | C11—C12 | 1.388 (4) |
| O3—C10 | 1.368 (3) | C12—C13 | 1.387 (4) |
| O3—C9 | 1.426 (4) | C13—C14 | 1.372 (4) |
| O4—C11 | 1.379 (3) | C13—H13 | 0.9300 |
| O4—C8 | 1.428 (3) | C14—C15 | 1.384 (4) |
| O5—C12 | 1.366 (3) | C14—H14 | 0.9300 |
| O5—C7 | 1.419 (3) | C15—C16 | 1.454 (4) |
| O6—C18 | 1.222 (3) | C16—C17 | 1.327 (4) |
| C7—H7A | 0.9600 | C16—H16 | 0.9300 |
| C7—H7B | 0.9600 | C17—C18 | 1.462 (4) |
| C7—H7C | 0.9600 | C17—H17 | 0.9300 |
| C8—H8A | 0.9600 | C18—C19 | 1.470 (4) |
| C8—H8B | 0.9600 | C19—C20 | 1.354 (4) |
| C8—H8C | 0.9600 | C20—C21 | 1.404 (4) |
| C9—H9A | 0.9600 | C20—H20 | 0.9300 |
| C9—H9B | 0.9600 | C21—C22 | 1.342 (4) |
| C9—H9C | 0.9600 | C21—H21 | 0.9300 |
| | | | |
| C22—S2—C19 | 90.49 (13) | C14—C13—C12 | 119.8 (3) |
| C10—O3—C9 | 116.5 (2) | C14—C13—H13 | 120.1 |
| C11—O4—C8 | 117.0 (2) | C12—C13—H13 | 120.1 |
| C12—O5—C7 | 118.5 (2) | C13—C14—C15 | 122.2 (2) |
| O5—C7—H7A | 109.5 | C13—C14—H14 | 118.9 |
| O5—C7—H7B | 109.5 | C15—C14—H14 | 118.9 |
| H7A—C7—H7B | 109.5 | C14—C15—C10 | 117.5 (2) |
| O5—C7—H7C | 109.5 | C14—C15—C16 | 122.6 (2) |
| H7A—C7—H7C | 109.5 | C10—C15—C16 | 119.9 (2) |
| H7B—C7—H7C | 109.5 | C17—C16—C15 | 126.9 (3) |
| O4—C8—H8A | 109.5 | C17—C16—H16 | 116.5 |
| O4—C8—H8B | 109.5 | C15—C16—H16 | 116.5 |
| H8A—C8—H8B | 109.5 | C16—C17—C18 | 123.1 (3) |
| O4—C8—H8C | 109.5 | C16—C17—H17 | 118.5 |
| H8A—C8—H8C | 109.5 | C18—C17—H17 | 118.5 |
| H8B—C8—H8C | 109.5 | O6—C18—C17 | 123.3 (3) |
| O3—C9—H9A | 109.5 | O6—C18—C19 | 119.6 (3) |
| O3—C9—H9B | 109.5 | C17—C18—C19 | 117.1 (3) |

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|---|---|---|---|
| H9A—C9—H9B | 109.5 | C20—C19—C18 | 131.0 (3) |
| O3—C9—H9C | 109.5 | C20—C19—S2 | 110.7 (2) |
| H9A—C9—H9C | 109.5 | C18—C19—S2 | 118.2 (2) |
| H9B—C9—H9C | 109.5 | C19—C20—C21 | 114.0 (3) |
| O3—C10—C11 | 121.3 (2) | C19—C20—H20 | 123.0 |
| O3—C10—C15 | 117.7 (2) | C21—C20—H20 | 123.0 |
| C11—C10—C15 | 120.8 (2) | C22—C21—C20 | 111.3 (3) |
| O4—C11—C10 | 118.2 (2) | C22—C21—H21 | 124.3 |
| O4—C11—C12 | 121.4 (2) | C20—C21—H21 | 124.3 |
| C10—C11—C12 | 120.0 (2) | C21—C22—S2 | 113.4 (2) |
| O5—C12—C13 | 124.3 (2) | C21—C22—Br1 | 126.2 (2) |
| O5—C12—C11 | 116.1 (2) | S2—C22—Br1 | 120.36 (16) |
| C13—C12—C11 | 119.6 (2) | | |

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|---|---|---|---|
| C9—O3—C10—C11 | −63.9 (3) | O3—C10—C15—C16 | −2.1 (4) |
| C9—O3—C10—C15 | 120.7 (3) | C11—C10—C15—C16 | −177.5 (2) |
| C8—O4—C11—C10 | 123.4 (3) | C14—C15—C16—C17 | −8.3 (4) |
| C8—O4—C11—C12 | −63.4 (3) | C10—C15—C16—C17 | 170.2 (3) |
| O3—C10—C11—O4 | −4.4 (4) | C15—C16—C17—C18 | −178.0 (3) |
| C15—C10—C11—O4 | 170.9 (2) | C16—C17—C18—O6 | −5.1 (5) |
| O3—C10—C11—C12 | −177.7 (2) | C16—C17—C18—C19 | 174.6 (3) |
| C15—C10—C11—C12 | −2.5 (4) | O6—C18—C19—C20 | −176.7 (3) |
| C7—O5—C12—C13 | 1.7 (4) | C17—C18—C19—C20 | 3.6 (4) |
| C7—O5—C12—C11 | −176.7 (2) | O6—C18—C19—S2 | −0.1 (4) |
| O4—C11—C12—O5 | 6.6 (4) | C17—C18—C19—S2 | −179.73 (19) |
| C10—C11—C12—O5 | 179.7 (2) | C22—S2—C19—C20 | 0.8 (2) |
| O4—C11—C12—C13 | −172.0 (2) | C22—S2—C19—C18 | −176.6 (2) |
| C10—C11—C12—C13 | 1.2 (4) | C18—C19—C20—C21 | 176.4 (3) |
| O5—C12—C13—C14 | −177.0 (2) | S2—C19—C20—C21 | −0.5 (3) |
| C11—C12—C13—C14 | 1.4 (4) | C19—C20—C21—C22 | −0.2 (4) |
| C12—C13—C14—C15 | −2.8 (4) | C20—C21—C22—S2 | 0.8 (3) |
| C13—C14—C15—C10 | 1.5 (4) | C20—C21—C22—Br1 | −178.3 (2) |
| C13—C14—C15—C16 | −179.9 (2) | C19—S2—C22—C21 | −0.9 (2) |
| O3—C10—C15—C14 | 176.5 (2) | C19—S2—C22—Br1 | 178.24 (17) |
| C11—C10—C15—C14 | 1.1 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8*B*···O5 | 0.96 | 2.23 | 2.861 (4) | 122 |
| C9—H9*B*···O4 | 0.96 | 2.38 | 2.985 (4) | 120 |
| C21—H21···O6$^{i}$ | 0.93 | 2.41 | 3.322 (4) | 165 |

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