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(*Z*)-5-(3,4,5-Trimethoxystyryl)-2,3-dihydrothieno[3,4-*b*][1,4]dioxine

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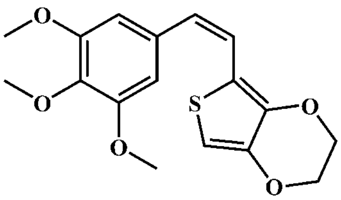
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.066; wR factor = 0.179; data-to-parameter ratio = 14.4.

In the title compound, $C_{17}H_{18}O_5S$, an analogue of the potent anticancer agent combretastatin A-4, the alkene C═C bond has a *cis* conformation and the C—C═C—C torsion angle is 9.0 (3)°. The dihedral angle between the benzene and thiophene rings is 54.07 (4)°. The dioxene ring adopts a half-chair conformation, with the C atoms of the methylene groups displaced by −0.325 (2) and 0.341 (3) Å from the plane of the other atoms. The C atoms of the two *meta*-methoxy groups are close to being coplanar with their attached benzene ring [displacements = −0.025 (2) and −0.196 (2) Å], whereas the C atom of the *para*-methoxy group is significantly displaced [by −1.107 (2) Å]. In the crystal, C—H⋯O hydrogen bonds link the molecules into $[0\bar{1}1]$ chains, which feature two different types of $R_2^2(6)$ loops.

Related literature

For background to combretastatin [systematic name: (*Z*)-2-methoxy-5-(3,4,5-trimethoxystyryl)phenol], see Pettit *et al.* (1987, 1995); Dark *et al.* (1997); Thorpe *et al.* (2003); Tozer *et al.* (2005). For further synthesis details, see Mohannkrishnan *et al.* (1999).



Experimental

Crystal data

$C_{17}H_{18}O_5S$
M_r = 334.37
Triclinic, $P\bar{1}$
a = 8.197 (2) Å
b = 8.4527 (15) Å
c = 11.835 (3) Å
α = 88.774 (1)°
β = 85.484 (3)°
γ = 76.422 (2)°
V = 794.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 296 K
0.30 × 0.28 × 0.26 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.963, T_{max} = 0.985
4342 measured reflections
3059 independent reflections
2766 reflections with $I > 2\sigma(I)$
R_{int} = 0.159

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.179
S = 0.99
3059 reflections
212 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C15—H15B⋯O1^{i}	0.96	2.57	3.477 (3)	157
C17—H17B⋯O3^{ii}	0.96	2.57	3.266 (3)	129

Symmetry codes: (i) $-x+2, -y+2, -z$; (ii) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7200).

References

Bruker (2008). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dark, G. G., Hill, S. A., Prise, V. E., Tozer, G. M., Pettit, G. R. & Chaplin, D. J. (1997). *Cancer Res.* **57**, 1829–1834.
Mohannkrishnan, A. K., Hucke, A., Lyon, M. A., Lakshmikantham, M. V. & Cava, M. P. (1999). *Tetrahedron*, **55**, 11745–11754.
Pettit, G. R., Singh, S. B., Niven, M. L., Hamel, E. & Schmidt, J. M. (1987). *J. Nat. Prod.* **50**, 119–131.
Pettit, G. R., Temple, C. Jr, Narayanan, V. L., Varma, R., Simpson, M. J., Boyd, M. R. & Bansal, N. (1995). *Anticancer Drug Res.* **10**, 299–309.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Thorpe, P. E., Chaplin, D. J. & Blakey, D. C. (2003). *Cancer Res.* **63**, 1144–1147.
Tozer, G. M., Kanthou, C. & Baguley, B. C. (2005). *Nat. Rev. Cancer*, **5**, 423–425.

supporting information

Acta Cryst. (2014). E**70**, o384 [doi:10.1107/S1600536814004437]

(*Z*)-5-(3,4,5-Trimethoxystyryl)-2,3-dihydrothieno[3,4-*b*][1,4]dioxine

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S1. Comment

Combretastatins are natural products with extraordinary anticancer activity, which were isolated from tree *Combretum caffrum* (Pettit *et al.*1987). Among these compounds, combretastatin A-4 ((*Z*)-2-methoxy-5-(3,4,5-trimethoxy-styryl)phenol, CA-4) possesses the most potent antitumor activity as a result of specifically targeting the vasculature of tumors. (Pettit *et al.* 1995; Dark *et al.* 1997). Its disodium phosphate prodrug has already developed and entered clinical trials (Thorpe *et al.*2003; Tozer *et al.* 2005). Therefore, CA-4 is a very attractive leading compound because of the relatively simple structure and the strong potency against a broad spectrum of human cancer cell lines. The title compound is a new CA-4 analogue, which was prepared by the Wittig reaction (Mohannkrishnan *et al.* 1999). The antitumor activities of the title compound against HL-60, SMMC-7721 and A549 cancer cell lines in vitro are closely to the natural CA-4. We now report the structure of the title compound (Fig. 1). The C=C bond length is 1.335 (2) Å and two aryl units are on the same sides of the double bond plane. Therefore, it exists as *Z* configuration. The planes of the two aryl units, benzene ring and thiophene ring, in the molecule make a dihedral angle of 54.07 (4)°. Therefore, the structure of the title compound is very similar as that of the natural combretastatin A-4 (CA-4). In the crystal structure of the title compound, the C—H···O interactions extend the molecules into a zigzag supramolecular array with dangling thiophene rings (Fig. 2).

S2. Experimental

To the bromotriphenyl(3,4,5-trimethoxybenzyl)phosphonium salt (5.2 g,10.0 mmol) in dry THF (60 ml) at -78 °C, was added 2.5 Mn-BuLi in hexane (4.0 ml,10.0 mmol) with stirring. After 20 min., a solution of 2,3-dihydrothieno[3,4-*b*][1,4]dioxine-5-carbaldehyde (1.7 g,10.0 mmol) in dry THF (20 ml) was added and resulting mixture stirred at room temperature for 2 h. Then, the mixture was poured into crushed ice, extracted with ethyl acetate (3*30 ml), dried with $MgSO_4$, and concentrated *in vacuo*. The resulting solid was purified by column chromatography (petroleum ether/ ethyl acetate, V:V = 5:1) to give white product (1.38 g). Yield: 41.9%. mp. 122–123 °C. The ^{1}H NMR, ^{13}CNMR, MS spectra and elemental analysis are in accord with the assigned structures. Colourless blocks of the title compound were obtained by the slow evaporation of a petroleum ether/ ethyl acetate solution.

S3. Refinement

(type here to add refinement details)

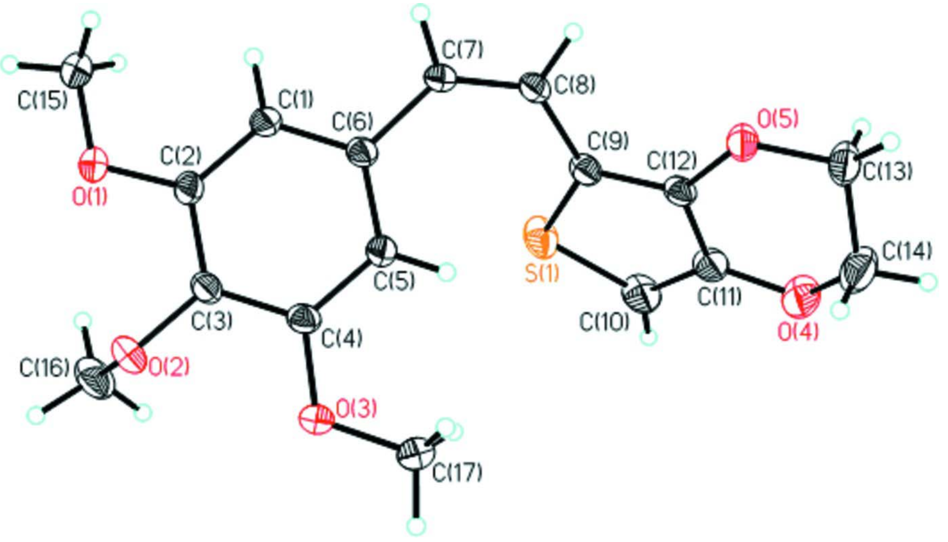

Figure 1

View of the title compound, showing 50% probability ellipsoids.

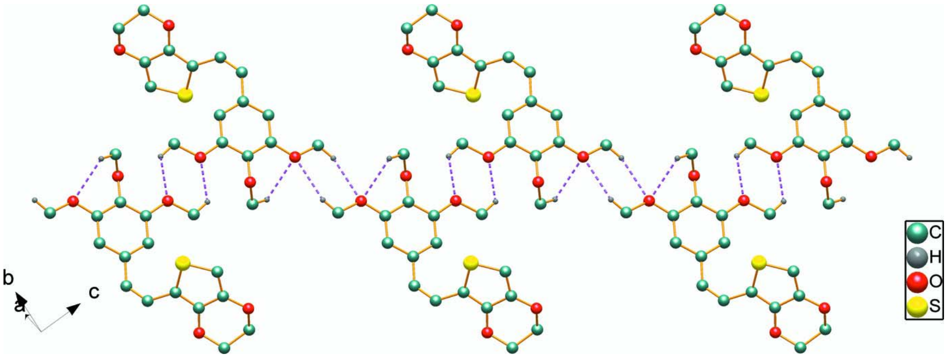

Figure 2

A hydrogen-bonded chain in the title compound.

(*Z*)-5-(3,4,5-Trimethoxystyryl)-2,3-dihydrothieno[3,4-*b*][1,4]dioxine

Crystal data

$C_{17}H_{18}O_5S$
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c = 11.835 (3) Å
α = 88.774 (1)°
β = 85.484 (3)°
γ = 76.422 (2)°
V = 794.6 (3) Å^3

Z = 2
F(000) = 352
D_x = 1.397 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3471 reflections
θ = 2.5–28.3°
μ = 0.23 mm^{-1}
T = 296 K
Block, colorless
0.30 × 0.28 × 0.26 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{\min} = 0.963$, $T_{\max} = 0.985$

4342 measured reflections
3059 independent reflections
2766 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.159$
$\theta_{\max} = 26.0°$, $\theta_{\min} = 2.5°$
$h = -10 \rightarrow 5$
$k = -10 \rightarrow 10$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.179$
$S = 0.99$
3059 reflections
212 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
$w = 1/[\sigma^2(F_o^2) + (0.1373P)^2 + 0.0901P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.57$ e Å^{-3}
$\Delta\rho_{\min} = -0.69$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.75 (5)

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 (Å²)

	x	*y*	*z*	$U_{\text{iso}}*/U_{\text{eq}}$
C1	0.7976 (2)	0.5843 (2)	0.05341 (13)	0.0332 (4)
H1	0.7750	0.6054	−0.0219	0.040*
C2	0.8766 (2)	0.6846 (2)	0.10955 (14)	0.0341 (4)
C3	0.9126 (2)	0.6527 (2)	0.22295 (14)	0.0346 (4)
C4	0.8656 (2)	0.5213 (2)	0.27815 (13)	0.0339 (4)
C5	0.7875 (2)	0.4201 (2)	0.22159 (13)	0.0339 (4)
H5	0.7591	0.3311	0.2588	0.041*
C6	0.75215 (19)	0.4526 (2)	0.10883 (13)	0.0319 (4)
C7	0.6789 (2)	0.3434 (2)	0.04398 (13)	0.0358 (4)
H7	0.7074	0.3418	−0.0337	0.043*
C8	0.5779 (2)	0.2464 (2)	0.07919 (14)	0.0362 (4)
H8	0.5606	0.1761	0.0243	0.043*
C9	0.4900 (2)	0.2326 (2)	0.19020 (14)	0.0354 (4)
C10	0.3068 (3)	0.2738 (3)	0.37088 (18)	0.0544 (6)
H10	0.2395	0.3115	0.4362	0.065*

C11	0.3539 (2)	0.1146 (3)	0.33906 (15)	0.0439 (5)
C12	0.4559 (2)	0.0932 (2)	0.23456 (13)	0.0340 (4)
C13	0.4314 (3)	−0.1752 (2)	0.23211 (18)	0.0548 (6)
H13A	0.4955	−0.2826	0.2088	0.066*
H13B	0.3206	−0.1585	0.2040	0.066*
C14	0.4144 (4)	−0.1663 (3)	0.3584 (2)	0.0671 (7)
H14A	0.3653	−0.2536	0.3888	0.081*
H14B	0.5250	−0.1809	0.3865	0.081*
C15	0.8706 (3)	0.8662 (2)	−0.04727 (16)	0.0465 (5)
H15A	0.9172	0.7818	−0.1016	0.070*
H15B	0.9068	0.9631	−0.0697	0.070*
H15C	0.7500	0.8883	−0.0437	0.070*
C16	0.9071 (3)	0.9017 (3)	0.3128 (2)	0.0597 (6)
H16A	0.8508	0.9574	0.2502	0.090*
H16B	0.9818	0.9629	0.3387	0.090*
H16C	0.8253	0.8909	0.3734	0.090*
C17	0.8570 (3)	0.3659 (3)	0.44741 (16)	0.0570 (6)
H17A	0.7378	0.3771	0.4470	0.085*
H17B	0.8873	0.3637	0.5243	0.085*
H17C	0.9152	0.2664	0.4103	0.085*
O1	0.92692 (17)	0.81485 (16)	0.06163 (10)	0.0434 (4)
O2	1.00158 (17)	0.74368 (16)	0.27742 (11)	0.0449 (4)
O3	0.90251 (18)	0.49911 (17)	0.38942 (10)	0.0426 (4)
O4	0.3099 (2)	−0.0118 (2)	0.39693 (13)	0.0637 (5)
O5	0.51392 (17)	−0.05526 (15)	0.18353 (10)	0.0418 (4)
S1	0.38731 (7)	0.39573 (6)	0.27505 (5)	0.0536 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0339 (8)	0.0410 (9)	0.0268 (7)	−0.0138 (7)	0.0016 (6)	−0.0030 (6)
C2	0.0317 (8)	0.0386 (9)	0.0341 (8)	−0.0145 (7)	0.0038 (6)	−0.0020 (7)
C3	0.0356 (8)	0.0388 (9)	0.0329 (8)	−0.0154 (7)	−0.0012 (6)	−0.0075 (7)
C4	0.0352 (8)	0.0407 (9)	0.0268 (8)	−0.0111 (7)	0.0003 (6)	−0.0067 (6)
C5	0.0393 (9)	0.0349 (8)	0.0301 (8)	−0.0149 (7)	0.0010 (6)	−0.0021 (6)
C6	0.0315 (8)	0.0367 (8)	0.0289 (7)	−0.0119 (6)	0.0029 (6)	−0.0069 (6)
C7	0.0449 (9)	0.0405 (9)	0.0253 (7)	−0.0174 (7)	0.0006 (6)	−0.0057 (6)
C8	0.0430 (9)	0.0380 (9)	0.0314 (8)	−0.0172 (7)	0.0007 (6)	−0.0084 (6)
C9	0.0344 (8)	0.0391 (9)	0.0347 (8)	−0.0130 (7)	0.0016 (6)	−0.0094 (7)
C10	0.0538 (11)	0.0611 (13)	0.0480 (11)	−0.0191 (10)	0.0214 (9)	−0.0226 (9)
C11	0.0442 (10)	0.0529 (11)	0.0366 (9)	−0.0185 (8)	0.0090 (7)	−0.0094 (8)
C12	0.0341 (8)	0.0391 (9)	0.0300 (8)	−0.0121 (7)	0.0030 (6)	−0.0093 (6)
C13	0.0737 (14)	0.0382 (10)	0.0539 (12)	−0.0231 (10)	0.0185 (10)	−0.0036 (8)
C14	0.0922 (18)	0.0546 (13)	0.0543 (13)	−0.0253 (13)	0.0184 (12)	0.0081 (10)
C15	0.0553 (11)	0.0502 (11)	0.0403 (9)	−0.0253 (9)	−0.0041 (8)	0.0072 (8)
C16	0.0674 (14)	0.0547 (12)	0.0625 (13)	−0.0240 (11)	−0.0031 (10)	−0.0239 (10)
C17	0.0788 (15)	0.0702 (14)	0.0343 (9)	−0.0404 (12)	−0.0135 (9)	0.0104 (9)
O1	0.0514 (8)	0.0488 (8)	0.0388 (7)	−0.0296 (6)	−0.0044 (5)	0.0062 (6)

O2	0.0485 (8)	0.0448 (8)	0.0480 (7)	−0.0216 (6)	−0.0104 (6)	−0.0074 (6)
O3	0.0574 (8)	0.0486 (7)	0.0284 (6)	−0.0242 (6)	−0.0078 (5)	−0.0003 (5)
O4	0.0793 (11)	0.0662 (10)	0.0479 (8)	−0.0317 (9)	0.0283 (7)	−0.0076 (7)
O5	0.0534 (8)	0.0344 (7)	0.0382 (7)	−0.0164 (6)	0.0142 (5)	−0.0073 (5)
S1	0.0570 (4)	0.0406 (4)	0.0624 (4)	−0.0154 (3)	0.0180 (3)	−0.0209 (2)

Geometric parameters (Å, º)

C1—C2	1.389 (2)	C11—C12	1.427 (2)
C1—C6	1.391 (2)	C12—O5	1.368 (2)
C1—H1	0.9300	C13—O5	1.432 (2)
C2—O1	1.3611 (19)	C13—C14	1.492 (3)
C2—C3	1.404 (2)	C13—H13A	0.9700
C3—O2	1.3778 (18)	C13—H13B	0.9700
C3—C4	1.392 (2)	C14—O4	1.444 (3)
C4—O3	1.3734 (19)	C14—H14A	0.9700
C4—C5	1.393 (2)	C14—H14B	0.9700
C5—C6	1.396 (2)	C15—O1	1.428 (2)
C5—H5	0.9300	C15—H15A	0.9600
C6—C7	1.471 (2)	C15—H15B	0.9600
C7—C8	1.335 (2)	C15—H15C	0.9600
C7—H7	0.9300	C16—O2	1.431 (3)
C8—C9	1.464 (2)	C16—H16A	0.9600
C8—H8	0.9300	C16—H16B	0.9600
C9—C12	1.359 (2)	C16—H16C	0.9600
C9—S1	1.7322 (17)	C17—O3	1.415 (2)
C10—C11	1.363 (3)	C17—H17A	0.9600
C10—S1	1.713 (2)	C17—H17B	0.9600
C10—H10	0.9300	C17—H17C	0.9600
C11—O4	1.360 (2)		
C2—C1—C6	120.60 (14)	O5—C13—C14	111.46 (17)
C2—C1—H1	119.7	O5—C13—H13A	109.3
C6—C1—H1	119.7	C14—C13—H13A	109.3
O1—C2—C1	124.50 (15)	O5—C13—H13B	109.3
O1—C2—C3	115.47 (14)	C14—C13—H13B	109.3
C1—C2—C3	120.02 (15)	H13A—C13—H13B	108.0
O2—C3—C4	120.04 (14)	O4—C14—C13	111.1 (2)
O2—C3—C2	120.78 (15)	O4—C14—H14A	109.4
C4—C3—C2	119.08 (14)	C13—C14—H14A	109.4
O3—C4—C3	115.81 (14)	O4—C14—H14B	109.4
O3—C4—C5	123.31 (15)	C13—C14—H14B	109.4
C3—C4—C5	120.88 (14)	H14A—C14—H14B	108.0
C4—C5—C6	119.71 (15)	O1—C15—H15A	109.5
C4—C5—H5	120.1	O1—C15—H15B	109.5
C6—C5—H5	120.1	H15A—C15—H15B	109.5
C1—C6—C5	119.70 (14)	O1—C15—H15C	109.5
C1—C6—C7	118.70 (14)	H15A—C15—H15C	109.5

C5—C6—C7	121.44 (14)	H15B—C15—H15C	109.5
C8—C7—C6	130.10 (14)	O2—C16—H16A	109.5
C8—C7—H7	115.0	O2—C16—H16B	109.5
C6—C7—H7	115.0	H16A—C16—H16B	109.5
C7—C8—C9	130.45 (14)	O2—C16—H16C	109.5
C7—C8—H8	114.8	H16A—C16—H16C	109.5
C9—C8—H8	114.8	H16B—C16—H16C	109.5
C12—C9—C8	125.05 (15)	O3—C17—H17A	109.5
C12—C9—S1	109.52 (12)	O3—C17—H17B	109.5
C8—C9—S1	124.81 (13)	H17A—C17—H17B	109.5
C11—C10—S1	111.34 (14)	O3—C17—H17C	109.5
C11—C10—H10	124.3	H17A—C17—H17C	109.5
S1—C10—H10	124.3	H17B—C17—H17C	109.5
O4—C11—C10	125.54 (17)	C2—O1—C15	117.07 (13)
O4—C11—C12	122.54 (17)	C3—O2—C16	114.95 (14)
C10—C11—C12	111.91 (18)	C4—O3—C17	117.00 (13)
C9—C12—O5	123.02 (14)	C11—O4—C14	111.51 (15)
C9—C12—C11	114.32 (16)	C12—O5—C13	112.21 (13)
O5—C12—C11	122.66 (16)	C10—S1—C9	92.85 (9)

C6—C1—C2—O1	179.31 (15)	S1—C9—C12—O5	177.21 (13)
C6—C1—C2—C3	0.5 (2)	C8—C9—C12—C11	−173.91 (17)
O1—C2—C3—O2	−3.6 (2)	S1—C9—C12—C11	−2.66 (19)
C1—C2—C3—O2	175.28 (15)	O4—C11—C12—C9	−178.64 (16)
O1—C2—C3—C4	−179.85 (14)	C10—C11—C12—C9	2.1 (2)
C1—C2—C3—C4	−1.0 (3)	O4—C11—C12—O5	1.5 (3)
O2—C3—C4—O3	4.7 (2)	C10—C11—C12—O5	−177.77 (17)
C2—C3—C4—O3	−179.03 (15)	O5—C13—C14—O4	63.0 (3)
O2—C3—C4—C5	−174.82 (15)	C1—C2—O1—C15	10.4 (3)
C2—C3—C4—C5	1.5 (3)	C3—C2—O1—C15	−170.77 (16)
O3—C4—C5—C6	179.03 (15)	C4—C3—O2—C16	−106.9 (2)
C3—C4—C5—C6	−1.5 (3)	C2—C3—O2—C16	76.9 (2)
C2—C1—C6—C5	−0.6 (2)	C3—C4—O3—C17	−179.64 (17)
C2—C1—C6—C7	−176.03 (15)	C5—C4—O3—C17	−0.2 (3)
C4—C5—C6—C1	1.0 (2)	C10—C11—O4—C14	−164.6 (2)
C4—C5—C6—C7	176.38 (15)	C12—C11—O4—C14	16.3 (3)
C1—C6—C7—C8	−155.46 (19)	C13—C14—O4—C11	−46.7 (3)
C5—C6—C7—C8	29.2 (3)	C9—C12—O5—C13	−166.87 (17)
C6—C7—C8—C9	9.0 (3)	C11—C12—O5—C13	13.0 (2)
C7—C8—C9—C12	−148.21 (19)	C14—C13—O5—C12	−43.6 (2)
C7—C8—C9—S1	41.8 (3)	C11—C10—S1—C9	−0.85 (18)
S1—C10—C11—O4	−179.73 (16)	C12—C9—S1—C10	2.00 (14)
S1—C10—C11—C12	−0.5 (2)	C8—C9—S1—C10	173.28 (16)
C8—C9—C12—O5	5.9 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*B*···O1^{i}	0.96	2.57	3.477 (3)	157
C17—H17*B*···O3^{ii}	0.96	2.57	3.266 (3)	129

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