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(2*E*,6*E*)-2,6-Bis(3-bromo-4-hydroxy-5-methoxybenzylidene)cyclohexanone

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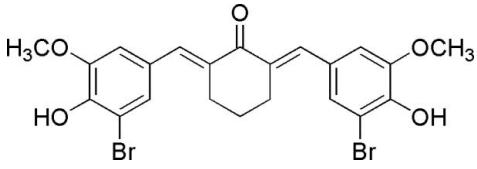
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.110; data-to-parameter ratio = 16.3.

In the title compound, $C_{22}H_{20}Br_2O_5$, the dihedral angle between the two benzene rings is 12.0 (3)°. The cyclohexanone ring has an envelope conformation with the flap atom displaced by 0.675 (6) Å from the plane of the other five atoms. The crystal structure has intra- and intermolecular hydrogen bonds between the hydroxy and methoxy groups.

Related literature

For related literature, see: Du, Bao *et al.* (2006); Du, Liu *et al.* (2006); Sardjiman *et al.* (1997); Youssef *et al.* (2004).



Experimental

Crystal data

$C_{22}H_{20}Br_2O_5$
M_r = 524.20
Monoclinic, $P2_1/c$
a = 7.5550 (11) Å
b = 14.938 (2) Å
c = 17.763 (3) Å
β = 95.201 (3)°
V = 1996.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.09 mm^{-1}
T = 173 (2) K
0.32 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.354, T_{max} = 0.685
10131 measured reflections
4349 independent reflections
2760 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.110
S = 1.02
4349 reflections
266 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.84	2.15	2.613 (5)	115
O5—H5A···O1^{i}	0.84	1.98	2.796 (5)	163
O1—H1···O4^{ii}	0.84	2.30	2.809 (4)	120
O5—H5A···O4	0.84	2.27	2.706 (5)	113

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2146).

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supplementary materials

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(2*E*,6*E*)-2,6-Bis(3-bromo-4-hydroxy-5-methoxybenzylidene)cyclohexanone

Z.-Y. Du, B.-H. Huang, K. Zhang and Y.-X. Fang

Comment

Curcumin analogs exhibit potential antioxidative properties (Sardjiman *et al.*, 1997, Youssef *et al.*, 2004) and inhibitory activities on α-glucosidase (Du, Liu *et al.*, 2006) and on aldose reductase (Du, Bao *et al.*, 2006). The title compound, $C_{22}H_{20}Br_2O_5$, is a synthesized curcumin analog and we report here its crystal structure.

The X-ray crystallographic study of the title compound confirms the previously proposed molecular structure based on spectroscopic data (Fig. 1). The C—C, C═C, C—O and C═O distances show no remarkable features.

A structural feature is the presence of intermolecular O—H···O hydrogen bonds between the hydroxy groups and the methoxy groups O of neighboring molecules (Table 2), resulting in infinite chains along the *c* axis (Fig. 2). Furthermore, there is a short intermolecular contact between the carbonyl O atom and a Br atom; Br2···O3 = 3.051 (3) Å.

Experimental

The title compound was synthesized as previously described (Du, Liu *et al.*, 2006). A mixture of 3-bromo-4-hydroxy-5-methoxybenzaldehyde (0.01 mol) and cyclohexanone (0.005 mol) was dissolved in glacial acetic acid (10 ml) saturated with anhydrous hydrogen chloride and heated in a water bath at 25–30 °C for 2 h. After standing for 2 days, the mixture was treated with cold water and filtered to obtain a yellow solid. Crystals were obtained by recrystallization from acetic acid and water (1:1) The compound identity was confirmed by the ^{1}H NMR spectra and ESI-MS. ^{1}H NMR (DMSO-d_6, 300 MHz) δ, 9.94 (br, 2H, –OH), 7.50 (s, 2H, –CH=), 7.27 (2*H*, aromatic), 7.13 (2*H*, aromatic), 3.86 (s, 6H, OCH_3), 2.88 (t, J = 6.7 Hz, 4H, $–CH_2—C—CH_2–$), 1.73 (q, J = 6.7 Hz, 2H, $–C—CH_2—C–$). ESI-MS (m/*z*):523$[M]^-$.

Refinement

All H atoms were positioned geometrically and refined in a riding model, with C—H = 0.98 Å for methyl, C—H = 0.99 Å for methylene, Csp^2—H = 0.95 Å and O—H = 0.84 Å. U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl and 1.2 for other C; U_{iso}(H) = 1.5U_{eq}(O).

Figures

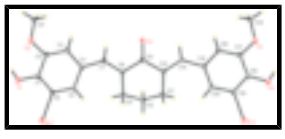

Fig. 1. The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

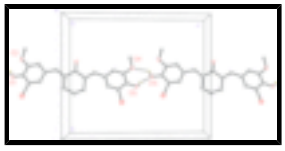

Fig. 2. The packing of the title compound, viewed down the *a* axis, showing one chain of molecules connected by O—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted. [Symmetry code: (I) *x*,*y*,1 + *z*].

(2E,6E)-2,6-Bis(3-bromo-4-hydroxy-5-methoxybenzylidene)cyclohexanone

Crystal data

$C_{22}H_{20}Br_2O_5$	F_{000} = 1048
M_r = 524.20	D_x = 1.744 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2576 reflections
a = 7.5550 (11) Å	θ = 2.3–26.7º
b = 14.938 (2) Å	μ = 4.09 mm^{-1}
c = 17.763 (3) Å	T = 173 (2) K
β = 95.201 (3)º	Needle, colorless
V = 1996.4 (5) Å^3	0.32 × 0.12 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	4349 independent reflections
Radiation source: fine-focus sealed tube	2760 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.052
T = 173(2) K	θ_{max} = 27.1º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→9
T_{min} = 0.354, T_{max} = 0.685	k = −19→11
10131 measured reflections	l = −21→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.110	$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
4349 reflections	$\Delta\rho_{max}$ = 0.78 e Å^{-3}
266 parameters	$\Delta\rho_{min}$ = −0.54 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.34530 (7)	0.66581 (3)	−0.31408 (3)	0.03229 (16)
Br2	0.52599 (7)	0.71802 (3)	0.39084 (3)	0.02742 (15)
C1	0.1939 (6)	0.4930 (3)	−0.3194 (2)	0.0212 (10)
C2	0.1366 (6)	0.4134 (3)	−0.2891 (2)	0.0223 (11)
C3	0.1561 (6)	0.3987 (3)	−0.2116 (2)	0.0213 (10)
H3	0.1203	0.3434	−0.1915	0.026*
C4	0.2296 (6)	0.4667 (3)	−0.1626 (2)	0.0190 (10)
C5	0.2868 (6)	0.5456 (3)	−0.1942 (2)	0.0209 (10)
H5	0.3390	0.5915	−0.1624	0.025*
C6	0.2681 (6)	0.5576 (3)	−0.2718 (2)	0.0196 (10)
C7	0.2418 (6)	0.4468 (3)	−0.0817 (2)	0.0203 (10)
H7	0.2416	0.3849	−0.0695	0.024*
C8	0.2534 (6)	0.5023 (3)	−0.0219 (2)	0.0174 (10)
C9	0.2528 (6)	0.4578 (3)	0.0543 (2)	0.0219 (10)
C10	0.2709 (6)	0.5150 (3)	0.1238 (2)	0.0196 (10)
C11	0.2874 (6)	0.6152 (3)	0.1154 (2)	0.0214 (10)
H11A	0.4147	0.6314	0.1168	0.026*
H11B	0.2375	0.6451	0.1585	0.026*
C12	0.1907 (6)	0.6488 (3)	0.0415 (2)	0.0222 (11)
H12A	0.0618	0.6367	0.0415	0.027*
H12B	0.2070	0.7143	0.0375	0.027*
C13	0.2619 (6)	0.6028 (3)	−0.0258 (2)	0.0209 (10)
H13A	0.1927	0.6232	−0.0726	0.025*
H13B	0.3870	0.6211	−0.0287	0.025*
C14	0.2704 (6)	0.4718 (3)	0.1901 (2)	0.0213 (10)
H14	0.2517	0.4090	0.1859	0.026*
C15	0.2938 (6)	0.5054 (3)	0.2679 (2)	0.0189 (10)
C16	0.2337 (6)	0.4519 (3)	0.3252 (2)	0.0214 (10)
H16	0.1781	0.3962	0.3123	0.026*
C17	0.2540 (6)	0.4787 (3)	0.4005 (2)	0.0212 (10)
C18	0.3355 (6)	0.5595 (3)	0.4206 (2)	0.0230 (11)
C19	0.4016 (6)	0.6104 (3)	0.3643 (2)	0.0205 (10)
C20	0.3827 (6)	0.5844 (3)	0.2892 (2)	0.0207 (10)

H20	0.4304	0.6206	0.2520	0.025*
C21	0.0191 (6)	0.2687 (3)	−0.3221 (3)	0.0253 (11)
H21A	0.1239	0.2395	−0.2965	0.038*
H21B	−0.0219	0.2347	−0.3676	0.038*
H21C	−0.0757	0.2710	−0.2880	0.038*
C22	0.1460 (7)	0.3418 (3)	0.4464 (3)	0.0317 (13)
H22A	0.0396	0.3405	0.4105	0.048*
H22B	0.1194	0.3140	0.4940	0.048*
H22C	0.2420	0.3086	0.4252	0.048*
O1	0.1786 (5)	0.5049 (2)	−0.39617 (16)	0.0311 (8)
H1	0.1417	0.4573	−0.4174	0.047*
O2	0.0631 (5)	0.3551 (2)	−0.34238 (17)	0.0318 (8)
O3	0.2381 (5)	0.3768 (2)	0.05909 (16)	0.0324 (9)
O4	0.1989 (5)	0.4304 (2)	0.45967 (17)	0.0320 (8)
O5	0.3565 (5)	0.5901 (2)	0.49255 (16)	0.0345 (9)
H5A	0.3062	0.5550	0.5208	0.052*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0472 (4)	0.0255 (3)	0.0249 (3)	−0.0022 (2)	0.0072 (2)	0.0048 (2)
Br2	0.0337 (3)	0.0243 (3)	0.0237 (3)	−0.0030 (2)	−0.0007 (2)	−0.0040 (2)
C1	0.019 (2)	0.030 (3)	0.014 (2)	0.008 (2)	0.0015 (18)	0.003 (2)
C2	0.019 (3)	0.026 (3)	0.023 (2)	0.002 (2)	0.003 (2)	−0.008 (2)
C3	0.020 (2)	0.023 (3)	0.021 (2)	0.003 (2)	0.0027 (19)	−0.004 (2)
C4	0.016 (2)	0.026 (3)	0.015 (2)	0.006 (2)	0.0057 (18)	−0.0016 (19)
C5	0.024 (3)	0.026 (3)	0.012 (2)	0.003 (2)	0.0013 (18)	−0.0012 (19)
C6	0.024 (3)	0.015 (2)	0.021 (2)	0.0020 (19)	0.0035 (19)	0.0045 (19)
C7	0.022 (3)	0.020 (2)	0.019 (2)	0.001 (2)	0.0006 (19)	0.003 (2)
C8	0.017 (2)	0.019 (2)	0.016 (2)	0.0032 (19)	0.0024 (18)	0.0001 (19)
C9	0.026 (3)	0.020 (3)	0.019 (2)	0.004 (2)	−0.002 (2)	0.003 (2)
C10	0.024 (3)	0.019 (2)	0.016 (2)	0.001 (2)	−0.0020 (19)	−0.0012 (19)
C11	0.030 (3)	0.020 (2)	0.014 (2)	0.002 (2)	0.0021 (19)	−0.0030 (19)
C12	0.032 (3)	0.013 (2)	0.022 (2)	0.004 (2)	−0.001 (2)	0.0020 (19)
C13	0.026 (3)	0.020 (2)	0.016 (2)	0.000 (2)	−0.0001 (19)	0.002 (2)
C14	0.026 (3)	0.019 (2)	0.018 (2)	−0.001 (2)	0.001 (2)	0.0001 (19)
C15	0.024 (3)	0.020 (2)	0.012 (2)	0.004 (2)	0.0005 (18)	0.0012 (19)
C16	0.023 (3)	0.019 (2)	0.023 (2)	0.001 (2)	0.002 (2)	−0.002 (2)
C17	0.016 (2)	0.026 (3)	0.020 (2)	0.002 (2)	−0.0009 (19)	0.005 (2)
C18	0.025 (3)	0.031 (3)	0.014 (2)	0.006 (2)	0.0031 (19)	0.003 (2)
C19	0.019 (2)	0.023 (3)	0.019 (2)	0.005 (2)	−0.0009 (19)	−0.001 (2)
C20	0.021 (3)	0.025 (3)	0.017 (2)	0.001 (2)	0.0029 (19)	0.001 (2)
C21	0.027 (3)	0.017 (3)	0.033 (3)	−0.009 (2)	0.005 (2)	−0.014 (2)
C22	0.045 (3)	0.034 (3)	0.015 (2)	−0.011 (3)	−0.003 (2)	0.010 (2)
O1	0.041 (2)	0.036 (2)	0.0162 (16)	0.0011 (18)	0.0039 (15)	−0.0011 (15)
O2	0.043 (2)	0.030 (2)	0.0216 (17)	−0.0027 (16)	−0.0006 (16)	−0.0059 (15)
O3	0.064 (3)	0.0154 (18)	0.0175 (16)	0.0019 (17)	−0.0005 (16)	0.0017 (14)
O4	0.043 (2)	0.034 (2)	0.0186 (17)	−0.0100 (17)	0.0035 (15)	0.0032 (15)

O5	0.053 (2)	0.036 (2)	0.0152 (17)	−0.0095 (18)	0.0047 (16)	−0.0047 (15)

Geometric parameters (Å, °)

Br1—C6	1.896 (4)	C12—H12B	0.9900
Br2—C19	1.899 (5)	C13—H13A	0.9900
C1—C6	1.369 (6)	C13—H13B	0.9900
C1—O1	1.369 (5)	C14—C15	1.465 (6)
C1—C2	1.390 (6)	C14—H14	0.9500
C2—O2	1.365 (5)	C15—C20	1.393 (6)
C2—C3	1.390 (6)	C15—C16	1.401 (6)
C3—C4	1.417 (6)	C16—C17	1.392 (6)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.391 (6)	C17—O4	1.370 (5)
C4—C7	1.462 (6)	C17—C18	1.387 (6)
C5—C6	1.385 (6)	C18—O5	1.353 (5)
C5—H5	0.9500	C18—C19	1.385 (6)
C7—C8	1.344 (6)	C19—C20	1.385 (6)
C7—H7	0.9500	C20—H20	0.9500
C8—C13	1.505 (6)	C21—O2	1.388 (5)
C8—C9	1.508 (6)	C21—H21A	0.9800
C9—O3	1.219 (5)	C21—H21B	0.9800
C9—C10	1.498 (6)	C21—H21C	0.9800
C10—C14	1.343 (6)	C22—O4	1.397 (5)
C10—C11	1.511 (6)	C22—H22A	0.9800
C11—C12	1.527 (6)	C22—H22B	0.9800
C11—H11A	0.9900	C22—H22C	0.9800
C11—H11B	0.9900	O1—H1	0.8400
C12—C13	1.520 (6)	O5—H5A	0.8400
C12—H12A	0.9900		
C6—C1—O1	121.1 (4)	C8—C13—H13A	108.9
C6—C1—C2	119.2 (4)	C12—C13—H13A	108.9
O1—C1—C2	119.6 (4)	C8—C13—H13B	108.9
O2—C2—C3	125.9 (4)	C12—C13—H13B	108.9
O2—C2—C1	113.5 (4)	H13A—C13—H13B	107.7
C3—C2—C1	120.6 (4)	C10—C14—C15	130.8 (4)
C2—C3—C4	119.8 (4)	C10—C14—H14	114.6
C2—C3—H3	120.1	C15—C14—H14	114.6
C4—C3—H3	120.1	C20—C15—C16	117.8 (4)
C5—C4—C3	118.6 (4)	C20—C15—C14	124.1 (4)
C5—C4—C7	125.1 (4)	C16—C15—C14	118.0 (4)
C3—C4—C7	116.4 (4)	C17—C16—C15	121.3 (4)
C6—C5—C4	120.3 (4)	C17—C16—H16	119.4
C6—C5—H5	119.9	C15—C16—H16	119.4
C4—C5—H5	119.9	O4—C17—C18	114.8 (4)
C1—C6—C5	121.5 (4)	O4—C17—C16	124.8 (4)
C1—C6—Br1	118.7 (3)	C18—C17—C16	120.4 (4)
C5—C6—Br1	119.8 (3)	O5—C18—C19	118.5 (4)
C8—C7—C4	130.2 (4)	O5—C18—C17	123.3 (4)

C8—C7—H7	114.9	C19—C18—C17	118.3 (4)
C4—C7—H7	114.9	C18—C19—C20	121.9 (4)
C7—C8—C13	125.4 (4)	C18—C19—Br2	119.3 (3)
C7—C8—C9	115.6 (4)	C20—C19—Br2	118.8 (3)
C13—C8—C9	119.0 (4)	C19—C20—C15	120.3 (4)
O3—C9—C10	120.7 (4)	C19—C20—H20	119.8
O3—C9—C8	120.6 (4)	C15—C20—H20	119.8
C10—C9—C8	118.7 (4)	O2—C21—H21A	109.5
C14—C10—C9	116.2 (4)	O2—C21—H21B	109.5
C14—C10—C11	124.7 (4)	H21A—C21—H21B	109.5
C9—C10—C11	119.1 (4)	O2—C21—H21C	109.5
C10—C11—C12	111.9 (3)	H21A—C21—H21C	109.5
C10—C11—H11A	109.2	H21B—C21—H21C	109.5
C12—C11—H11A	109.2	O4—C22—H22A	109.5
C10—C11—H11B	109.2	O4—C22—H22B	109.5
C12—C11—H11B	109.2	H22A—C22—H22B	109.5
H11A—C11—H11B	107.9	O4—C22—H22C	109.5
C13—C12—C11	110.5 (4)	H22A—C22—H22C	109.5
C13—C12—H12A	109.5	H22B—C22—H22C	109.5
C11—C12—H12A	109.5	C1—O1—H1	109.5
C13—C12—H12B	109.5	C2—O2—C21	120.3 (4)
C11—C12—H12B	109.5	C17—O4—C22	118.1 (4)
H12A—C12—H12B	108.1	C18—O5—H5A	109.5
C8—C13—C12	113.3 (4)		

C6—C1—C2—O2	179.2 (4)	C9—C10—C11—C12	29.9 (6)
O1—C1—C2—O2	−2.1 (6)	C10—C11—C12—C13	−57.8 (5)
C6—C1—C2—C3	−0.8 (7)	C7—C8—C13—C12	153.4 (4)
O1—C1—C2—C3	177.9 (4)	C9—C8—C13—C12	−24.9 (6)
O2—C2—C3—C4	−177.8 (4)	C11—C12—C13—C8	55.5 (5)
C1—C2—C3—C4	2.1 (7)	C9—C10—C14—C15	176.6 (5)
C2—C3—C4—C5	−2.4 (6)	C11—C10—C14—C15	−3.7 (8)
C2—C3—C4—C7	178.6 (4)	C10—C14—C15—C20	−23.8 (8)
C3—C4—C5—C6	1.4 (7)	C10—C14—C15—C16	160.6 (5)
C7—C4—C5—C6	−179.8 (4)	C20—C15—C16—C17	3.1 (7)
O1—C1—C6—C5	−178.9 (4)	C14—C15—C16—C17	179.0 (4)
C2—C1—C6—C5	−0.3 (7)	C15—C16—C17—O4	180.0 (4)
O1—C1—C6—Br1	1.4 (6)	C15—C16—C17—C18	−0.3 (7)
C2—C1—C6—Br1	−179.9 (3)	O4—C17—C18—O5	−1.5 (7)
C4—C5—C6—C1	−0.1 (7)	C16—C17—C18—O5	178.8 (4)
C4—C5—C6—Br1	179.6 (3)	O4—C17—C18—C19	177.3 (4)
C5—C4—C7—C8	23.3 (8)	C16—C17—C18—C19	−2.4 (7)
C3—C4—C7—C8	−157.9 (5)	O5—C18—C19—C20	−178.8 (4)
C4—C7—C8—C13	−2.0 (8)	C17—C18—C19—C20	2.3 (7)
C4—C7—C8—C9	176.4 (5)	O5—C18—C19—Br2	2.4 (6)
C7—C8—C9—O3	−1.7 (7)	C17—C18—C19—Br2	−176.4 (3)
C13—C8—C9—O3	176.8 (4)	C18—C19—C20—C15	0.6 (7)
C7—C8—C9—C10	178.1 (4)	Br2—C19—C20—C15	179.3 (3)
C13—C8—C9—C10	−3.3 (6)	C16—C15—C20—C19	−3.2 (6)
O3—C9—C10—C14	0.2 (7)	C14—C15—C20—C19	−178.8 (4)

C8—C9—C10—C14	−179.7 (4)	C3—C2—O2—C21	−7.8 (7)
O3—C9—C10—C11	−179.6 (4)	C1—C2—O2—C21	172.3 (4)
C8—C9—C10—C11	0.6 (6)	C18—C17—O4—C22	−168.4 (4)
C14—C10—C11—C12	−149.8 (5)	C16—C17—O4—C22	11.4 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.84	2.15	2.613 (5)	115
O5—H5A···O1^{i}	0.84	1.98	2.796 (5)	163
O1—H1···O4^{ii}	0.84	2.30	2.809 (4)	120
O5—H5A···O4	0.84	2.27	2.706 (5)	113

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

Fig. 1

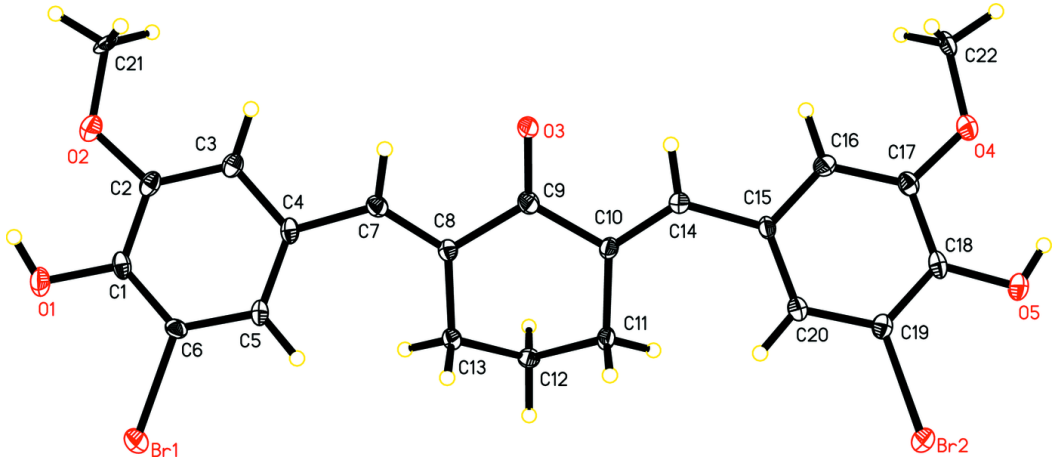
C21
O2
C3
C2
C4
C7
C8
O3
C9
C10
C14
C15
C16
C17
O4
C22
C18
O5
O1
C1
C6
C5
C13
C12
C11
C20
C19
Br1
Br2

Fig. 2