3,4-Dibromo-2,2,5,5-tetraphenyl-2,5-dihydrofuran

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The crystal structure of the title compound, $C_{28}H_{20}Br_2O$, was solved in the orthorhombic space group $P2_12_12_1$ with one molecule in the asymmetric unit. The phenyl rings are nearly planar and inclined at angles of 67.7 (1), 68.8 (1), 79.3 (1) and 62.3 (1)° to the plane of the 2,5-dihydrofuran ring. The crystal structure features C—H···π and Br···Br interactions, which connect the molecules to a three-dimensional supramolecular network.

3D view

Chemical scheme
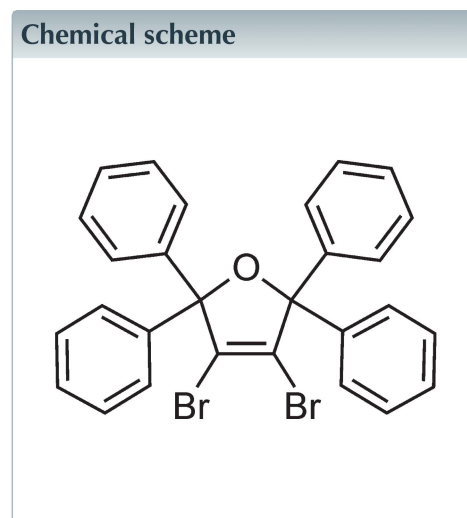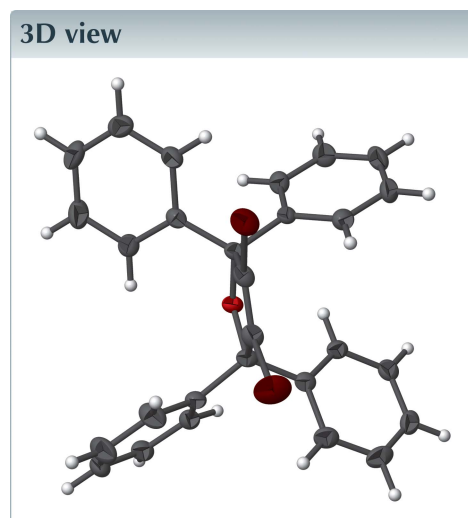
Structure description

The title compound was obtained as an unexpected product in a bromination reaction of 1,1-diphenylprop-2-yne-1-ol in order to obtain 1,1-diphenyl-3-bromo-2-propyne-1-ol. Performance of this transformation using potassium hydroxide dissolved in water, bromine and 1,1-diphenyl-2-propyne-1-ol (Maraval *et al.*, 2008) added as a solution in *n*-pentane at 273 K following conditions of a described procedure (Saalfrank *et al.*, 1996) yielded the intended product. However, when applying the same synthesis but heating the reaction mixture to reflux for 12 h instead of stirring for 60 h at room temperature, the modified reaction condition surprisingly led to the formation of the title compound as the main product. Nevertheless, upon closer inspection of the circumstances, a potential course of the reaction may be assumed in a first step by base-induced abstraction of a proton from the starting compound (1,1-diphenylprop-2-yne-1-ol) to yield an equilibrium mixture of both corresponding alkoxide and acetylide species. Deprotonation of the acetylide species following a *retro* Favorskii-type reaction (Wuts & Greene, 2007) gives rise to the formation of diphenyl ketone as an intermediate, which on nucleophilic attack by the acetylide species may produce a mono-deprotonated acetylenic diol (1,1,4,4-tetraphenylbut-2-yne-1,4-diol) (Kostikov *et al.*, 1996). Subsequent hydrolysis and addition of bromine may then give a dibromo-substituted secondary product (2,3-dibromo-1,1,4,4-tetraphenylbut-2-ene-1,4-diol), which finally *via* dehydration and ring closure
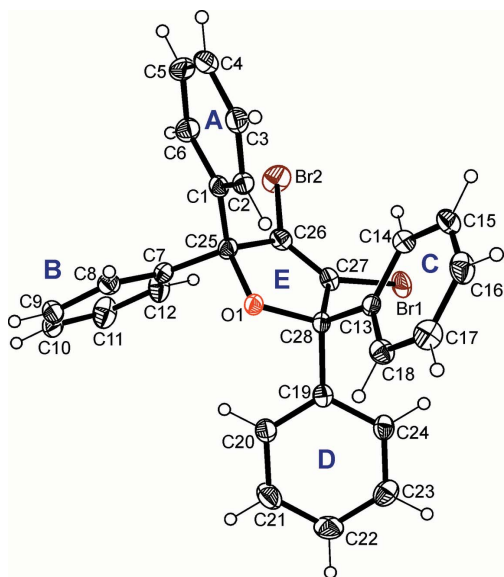
Figure 1
Perspective view of the title compound including atom labelling and ring specification. Non-hydrogen atoms are shown with 50% probability displacement ellipsoids.

reactions (Salkind & Teterin, 1929) ends up with the formation of the title compound. Crystals of this latter compound were used for X-ray crystal structure analysis.

The asymmetric unit contains one molecule (Fig. 1). The furan ring deviates slightly from planarity with maximum atomic distances from the the least-squares plane being -0.044 (2) Å for O1 and 0.042 (1) Å for C28. In addition, the aromatic rings are not perfectly planar. The maximum distances from the least-squares plane are 0.012 (2) and
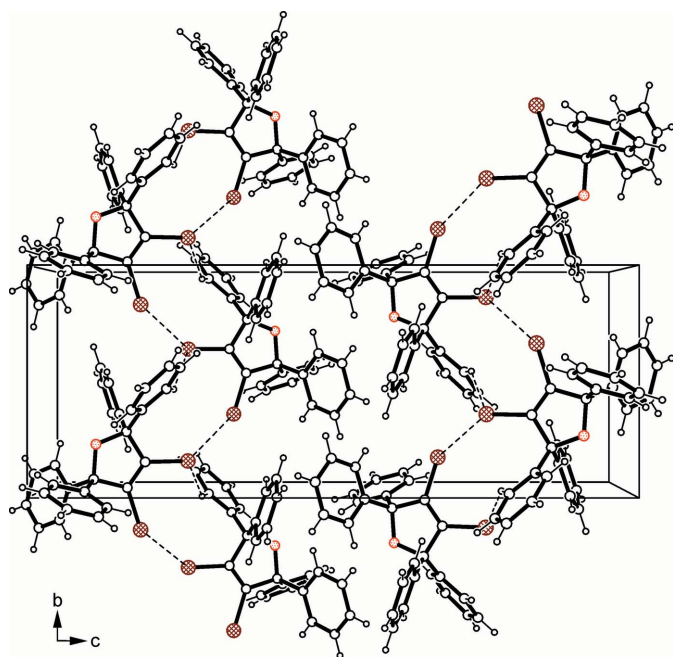

Figure 2
Part of the packing of the title compound viewed along the *a*-axis. Oxygen atoms are displayed as dotted circles (red) and bromine atoms as cross-hatched circles. The intermolecular contacts are shown as dashed lines.

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

*Cg*2 and *Cg*3 are the centroids of the C1–C6 and C7–C12 rings, respectively.

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
C5—H5$\cdots Cg2^i$	0.95	2.82	3.701 (3)	155
C10—H10$\cdots Cg1^{ii}$	0.95	2.96	3.835 (3)	154
C16—H16$\cdots Cg1^{iii}$	0.95	2.75	3.508 (3)	137

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

0.015 (2) for atoms C1 and C6 of ring *A*. The phenyl rings *A*, *B*, *C* and *D* are inclined at angles of 67.7 (1), 68.8 (1), 79.3 (1) and 62.3 (1)°, respectively, to the plane of the 2,5-dihydrofuran ring.

In the crystal structure, molecules are connected by C—H$\cdots\pi$ interactions (Nishio *et al.* 2009) with the aromatic rings *A* and *B* acting as acceptors (Table 1, Fig. 2). Moreover, type I Br$\cdots$Br contacts (Awwadi *et al.*, 2006) [d(Br$\cdots$Br) 3.814 (4) Å; θ_1 = 136.0°, θ_2 = 135.1°] connect the molecules into a three-dimensional supramolecular network.

Synthesis and crystallization

To a solution of potassium hydroxide (5.46 g, 140 mmol) in water (26 ml), bromine (2.3 g, 13.91 mmol) was added at

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{20}Br_2O$
M_r	532.26
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	153
a, b, c (Å)	9.4301 (5), 9.4561 (5), 24.8572 (12)
V (Å³)	2216.6 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm⁻¹)	3.68
Crystal size (mm)	$0.43 \times 0.24 \times 0.09$
Data collection	
Diffractometer	Bruker Kappa goniometer with an APEXII CCD area detector
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2008*a*)
T_{min}, T_{max}	0.301, 0.733
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	39405, 4867, 4510
R_{int}	0.031
$(\sin\theta/\lambda)_{max}$ (Å⁻¹)	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.047, 1.06
No. of reflections	4867
No. of parameters	280
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å⁻³)	0.50, -0.36
Absolute structure	Flack x determined using 1813 quotients [$(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.014 (3)

Computer programs: *APEX2* and *SAINT-NT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *SHELXTL* (Sheldrick, 2008*b*).

277 K. 1,1-Diphenylprop-2-yne-1-ol (3.90 g, 18.72 mmol) dissolved in *n*-pentane (35 ml) was added dropwise at 273 K and the mixture was then heated to reflux for 12 h. After cooling and extraction with dichloromethane, the combined organic layers were washed with water, dried over sodium sulfate and evaporated. Crystallization from *n*-hexane yielded 6.9 g (70%) red crystals with m.p. 371 K. ^{1}H NMR (500.1 MHz, CDCl$_3$): δ = 7.21–7.35 (*m*, 20H, ArH) p.p.m.; ^{13}C NMR (125.8 MHz, CDCl$_3$): δ = 83.8 (C—O), 113.4 (C—Br), 127.5, 128.1, 129.3, 142.2 (Ar) p.p.m. Yellow scaly crystals were grown by slow evaporation of the solvent from a 1:1 solvent mixture of ethanol and THF.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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Crystal data

$C_{28}H_{20}Br_2O$	$D_x = 1.595$ Mg m^{-3}
$M_r = 532.26$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 9991 reflections
$a = 9.4301$ (5) Å	$\theta = 2.3$–$25.3°$
$b = 9.4561$ (5) Å	$\mu = 3.68$ mm^{-1}
$c = 24.8572$ (12) Å	$T = 153$ K
$V = 2216.6$ (2) Å^3	Column, yellow
$Z = 4$	$0.43 \times 0.24 \times 0.09$ mm
$F(000) = 1064$	

Data collection

Bruker Kappa goniometer with an APEXII CCD area detector diffractometer	4867 independent reflections
	4510 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.031$
φ and ω scans	$\theta_{max} = 27.1°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (SADABS; Sheldrick, 2008a)	$h = -12 \rightarrow 12$
	$k = -12 \rightarrow 12$
$T_{min} = 0.301$, $T_{max} = 0.733$	$l = -31 \rightarrow 31$
39405 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0208P)^2 + 0.686P]$
$R[F^2 > 2\sigma(F^2)] = 0.022$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.047$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.06$	$\Delta\rho_{max} = 0.50$ e Å^{-3}
4867 reflections	$\Delta\rho_{min} = -0.36$ e Å^{-3}
280 parameters	Absolute structure: Flack x determined using
0 restraints	1813 quotients $[(I^+)\text{-}(I^-)]/[(I^+)\text{+}(I^-)]$ (Parsons *et al.*, 2013)
Hydrogen site location: inferred from neighbouring sites	Absolute structure parameter: 0.014 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.89406 (3)	0.13600 (3)	0.75235 (2)	0.03301 (8)
Br2	0.81193 (4)	−0.16441 (3)	0.67457 (2)	0.04367 (10)
O1	0.72096 (19)	0.21958 (19)	0.60295 (8)	0.0221 (4)
C1	0.8180 (3)	0.0195 (3)	0.55259 (11)	0.0227 (5)
C2	0.9027 (3)	0.1164 (3)	0.52542 (11)	0.0249 (6)
H2	0.8987	0.2137	0.5348	0.030*
C3	0.9935 (3)	0.0718 (3)	0.48454 (12)	0.0287 (6)
H3	1.0505	0.1390	0.4661	0.034*
C4	1.0009 (3)	−0.0690 (4)	0.47076 (13)	0.0309 (7)
H4	1.0639	−0.0994	0.4432	0.037*
C5	0.9164 (3)	−0.1659 (3)	0.49715 (12)	0.0350 (7)
H5	0.9220	−0.2632	0.4879	0.042*
C6	0.8235 (3)	−0.1225 (3)	0.53706 (11)	0.0306 (6)
H6	0.7632	−0.1897	0.5540	0.037*
C7	0.5668 (3)	0.0223 (3)	0.59101 (11)	0.0242 (6)
C8	0.5012 (3)	0.0558 (3)	0.54270 (12)	0.0256 (6)
H8	0.5553	0.0954	0.5142	0.031*
C9	0.3571 (3)	0.0319 (3)	0.53566 (13)	0.0299 (7)
H9	0.3126	0.0586	0.5029	0.036*
C10	0.2784 (3)	−0.0302 (3)	0.57589 (13)	0.0334 (7)
H10	0.1800	−0.0473	0.5709	0.040*
C11	0.3431 (4)	−0.0672 (4)	0.62314 (14)	0.0426 (9)
H11	0.2896	−0.1114	0.6508	0.051*
C12	0.4873 (3)	−0.0405 (4)	0.63092 (13)	0.0367 (8)
H12	0.5309	−0.0658	0.6640	0.044*
C13	0.9269 (3)	0.3462 (3)	0.63427 (10)	0.0222 (5)
C14	1.0550 (3)	0.2743 (3)	0.63200 (12)	0.0298 (7)
H14	1.0605	0.1793	0.6442	0.036*
C15	1.1751 (3)	0.3406 (4)	0.61195 (12)	0.0347 (7)
H15	1.2620	0.2900	0.6098	0.042*
C16	1.1693 (3)	0.4786 (4)	0.59515 (12)	0.0356 (7)
H16	1.2524	0.5241	0.5821	0.043*
C17	1.0433 (3)	0.5508 (4)	0.59718 (12)	0.0336 (7)
H17	1.0391	0.6464	0.5855	0.040*
C18	0.9221 (3)	0.4851 (3)	0.61623 (11)	0.0277 (6)
H18	0.8349	0.5354	0.6170	0.033*
C19	0.6891 (3)	0.3723 (3)	0.68066 (10)	0.0228 (5)
C20	0.5465 (3)	0.3771 (3)	0.66836 (12)	0.0305 (6)
H20	0.5084	0.3145	0.6422	0.037*
C21	0.4587 (3)	0.4733 (4)	0.69428 (13)	0.0411 (8)
H21	0.3604	0.4754	0.6860	0.049*
C22	0.5128 (4)	0.5661 (4)	0.73193 (13)	0.0390 (8)
H22	0.4530	0.6346	0.7483	0.047*
C23	0.6546 (3)	0.5585 (3)	0.74557 (13)	0.0343 (7)
H23	0.6917	0.6194	0.7725	0.041*

C24	0.7425 (3)	0.4628 (3)	0.72030 (11)	0.0275 (6)
H24	0.8399	0.4582	0.7299	0.033*
C25	0.7222 (3)	0.0655 (3)	0.59914 (11)	0.0226 (6)
C26	0.7833 (3)	0.0246 (3)	0.65326 (12)	0.0252 (6)
C27	0.8166 (3)	0.1362 (3)	0.68208 (10)	0.0246 (5)
C28	0.7898 (3)	0.2722 (3)	0.65141 (11)	0.0213 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02996 (13)	0.03975 (17)	0.02930 (14)	0.00078 (13)	−0.01210 (13)	0.00297 (15)
Br2	0.0640 (2)	0.02275 (15)	0.04424 (18)	0.00568 (16)	−0.01158 (17)	0.00825 (14)
O1	0.0226 (10)	0.0183 (9)	0.0254 (10)	−0.0006 (7)	−0.0052 (8)	−0.0013 (8)
C1	0.0222 (13)	0.0213 (13)	0.0246 (14)	0.0017 (12)	−0.0060 (11)	0.0013 (11)
C2	0.0244 (13)	0.0213 (14)	0.0289 (14)	0.0016 (12)	−0.0047 (12)	−0.0024 (11)
C3	0.0237 (15)	0.0326 (16)	0.0297 (16)	−0.0018 (12)	−0.0023 (12)	−0.0014 (12)
C4	0.0233 (16)	0.0391 (18)	0.0303 (17)	0.0071 (14)	−0.0012 (12)	−0.0045 (13)
C5	0.0416 (17)	0.0240 (15)	0.0394 (17)	0.0099 (14)	−0.0092 (14)	−0.0064 (13)
C6	0.0338 (15)	0.0228 (14)	0.0352 (16)	−0.0004 (13)	−0.0035 (13)	−0.0002 (12)
C7	0.0239 (14)	0.0201 (14)	0.0285 (15)	−0.0018 (11)	−0.0025 (11)	−0.0039 (11)
C8	0.0256 (15)	0.0211 (15)	0.0301 (16)	−0.0004 (12)	0.0000 (12)	0.0002 (12)
C9	0.0265 (15)	0.0269 (16)	0.0364 (17)	0.0018 (12)	−0.0075 (12)	−0.0015 (13)
C10	0.0216 (15)	0.0390 (19)	0.0397 (18)	−0.0056 (13)	0.0001 (13)	−0.0111 (14)
C11	0.0357 (18)	0.058 (2)	0.0344 (18)	−0.0193 (16)	0.0068 (14)	−0.0028 (16)
C12	0.0346 (17)	0.049 (2)	0.0266 (17)	−0.0114 (15)	−0.0028 (13)	0.0017 (14)
C13	0.0195 (12)	0.0250 (14)	0.0222 (13)	−0.0029 (11)	−0.0006 (9)	−0.0058 (12)
C14	0.0253 (15)	0.0289 (16)	0.0351 (17)	0.0013 (12)	−0.0022 (12)	−0.0059 (13)
C15	0.0189 (13)	0.0455 (19)	0.0398 (17)	0.0019 (15)	0.0009 (12)	−0.0100 (15)
C16	0.0250 (15)	0.051 (2)	0.0309 (17)	−0.0106 (15)	0.0055 (13)	−0.0035 (14)
C17	0.0367 (17)	0.0339 (18)	0.0303 (17)	−0.0051 (14)	0.0049 (14)	0.0048 (13)
C18	0.0253 (15)	0.0320 (16)	0.0258 (15)	0.0004 (12)	0.0019 (11)	0.0013 (12)
C19	0.0222 (12)	0.0238 (13)	0.0222 (12)	−0.0036 (12)	−0.0002 (11)	0.0028 (11)
C20	0.0252 (13)	0.0380 (17)	0.0283 (15)	0.0018 (12)	−0.0022 (12)	−0.0062 (14)
C21	0.0248 (15)	0.060 (2)	0.0387 (18)	0.0095 (16)	−0.0014 (13)	−0.0068 (16)
C22	0.0375 (18)	0.046 (2)	0.0339 (18)	0.0114 (15)	0.0093 (14)	−0.0067 (14)
C23	0.0403 (16)	0.0347 (16)	0.0280 (16)	−0.0054 (13)	0.0053 (14)	−0.0054 (14)
C24	0.0240 (14)	0.0319 (17)	0.0266 (15)	−0.0056 (12)	0.0003 (12)	−0.0007 (13)
C25	0.0246 (14)	0.0178 (13)	0.0255 (15)	−0.0018 (11)	−0.0035 (12)	−0.0004 (11)
C26	0.0239 (14)	0.0208 (14)	0.0310 (15)	0.0001 (11)	−0.0008 (12)	0.0057 (11)
C27	0.0202 (12)	0.0279 (14)	0.0257 (13)	−0.0011 (12)	−0.0036 (11)	0.0032 (12)
C28	0.0199 (13)	0.0219 (13)	0.0222 (13)	−0.0021 (11)	−0.0036 (11)	−0.0020 (11)

Geometric parameters (Å, °)

Br1—C27	1.894 (3)	C13—C14	1.387 (4)
Br2—C26	1.884 (3)	C13—C18	1.389 (4)
O1—C28	1.456 (3)	C13—C28	1.530 (4)
O1—C25	1.460 (3)	C14—C15	1.387 (4)

C1—C2	1.390 (4)	C14—H14	0.9500
C1—C6	1.399 (4)	C15—C16	1.372 (5)
C1—C25	1.531 (4)	C15—H15	0.9500
C2—C3	1.394 (4)	C16—C17	1.371 (5)
C2—H2	0.9500	C16—H16	0.9500
C3—C4	1.377 (5)	C17—C18	1.385 (4)
C3—H3	0.9500	C17—H17	0.9500
C4—C5	1.380 (5)	C18—H18	0.9500
C4—H4	0.9500	C19—C20	1.379 (4)
C5—C6	1.386 (4)	C19—C24	1.399 (4)
C5—H5	0.9500	C19—C28	1.526 (4)
C6—H6	0.9500	C20—C21	1.389 (4)
C7—C12	1.378 (4)	C20—H20	0.9500
C7—C8	1.388 (4)	C21—C22	1.380 (5)
C7—C25	1.535 (4)	C21—H21	0.9500
C8—C9	1.388 (4)	C22—C23	1.381 (4)
C8—H8	0.9500	C22—H22	0.9500
C9—C10	1.377 (4)	C23—C24	1.379 (4)
C9—H9	0.9500	C23—H23	0.9500
C10—C11	1.369 (5)	C24—H24	0.9500
C10—H10	0.9500	C25—C26	1.514 (4)
C11—C12	1.396 (4)	C26—C27	1.313 (4)
C11—H11	0.9500	C27—C28	1.517 (4)
C12—H12	0.9500		
C28—O1—C25	113.0 (2)	C17—C16—C15	119.8 (3)
C2—C1—C6	118.5 (3)	C17—C16—H16	120.1
C2—C1—C25	121.3 (2)	C15—C16—H16	120.1
C6—C1—C25	120.2 (3)	C16—C17—C18	120.3 (3)
C1—C2—C3	120.5 (3)	C16—C17—H17	119.9
C1—C2—H2	119.7	C18—C17—H17	119.9
C3—C2—H2	119.7	C17—C18—C13	120.5 (3)
C4—C3—C2	120.3 (3)	C17—C18—H18	119.7
C4—C3—H3	119.8	C13—C18—H18	119.7
C2—C3—H3	119.8	C20—C19—C24	119.1 (3)
C3—C4—C5	119.6 (3)	C20—C19—C28	121.5 (2)
C3—C4—H4	120.2	C24—C19—C28	119.4 (2)
C5—C4—H4	120.2	C19—C20—C21	120.0 (3)
C4—C5—C6	120.6 (3)	C19—C20—H20	120.0
C4—C5—H5	119.7	C21—C20—H20	120.0
C6—C5—H5	119.7	C22—C21—C20	120.7 (3)
C5—C6—C1	120.3 (3)	C22—C21—H21	119.6
C5—C6—H6	119.8	C20—C21—H21	119.6
C1—C6—H6	119.8	C21—C22—C23	119.4 (3)
C12—C7—C8	118.6 (3)	C21—C22—H22	120.3
C12—C7—C25	122.6 (3)	C23—C22—H22	120.3
C8—C7—C25	118.6 (3)	C24—C23—C22	120.3 (3)
C7—C8—C9	120.5 (3)	C24—C23—H23	119.9

C7—C8—H8	119.7	C22—C23—H23	119.9
C9—C8—H8	119.7	C23—C24—C19	120.4 (3)
C10—C9—C8	120.4 (3)	C23—C24—H24	119.8
C10—C9—H9	119.8	C19—C24—H24	119.8
C8—C9—H9	119.8	O1—C25—C26	101.5 (2)
C11—C10—C9	119.4 (3)	O1—C25—C1	109.7 (2)
C11—C10—H10	120.3	C26—C25—C1	112.0 (2)
C9—C10—H10	120.3	O1—C25—C7	105.5 (2)
C10—C11—C12	120.5 (3)	C26—C25—C7	114.3 (2)
C10—C11—H11	119.8	C1—C25—C7	112.9 (2)
C12—C11—H11	119.8	C27—C26—C25	111.8 (2)
C7—C12—C11	120.5 (3)	C27—C26—Br2	125.1 (2)
C7—C12—H12	119.7	C25—C26—Br2	123.1 (2)
C11—C12—H12	119.7	C26—C27—C28	111.6 (2)
C14—C13—C18	118.6 (3)	C26—C27—Br1	126.5 (2)
C14—C13—C28	121.5 (3)	C28—C27—Br1	121.91 (19)
C18—C13—C28	119.6 (2)	O1—C28—C27	101.5 (2)
C13—C14—C15	120.3 (3)	O1—C28—C19	109.2 (2)
C13—C14—H14	119.9	C27—C28—C19	113.0 (2)
C15—C14—H14	119.9	O1—C28—C13	107.6 (2)
C16—C15—C14	120.4 (3)	C27—C28—C13	112.8 (2)
C16—C15—H15	119.8	C19—C28—C13	112.1 (2)
C14—C15—H15	119.8		
C6—C1—C2—C3	−1.5 (4)	C2—C1—C25—C7	125.6 (3)
C25—C1—C2—C3	177.5 (2)	C6—C1—C25—C7	−55.4 (3)
C1—C2—C3—C4	−0.4 (4)	C12—C7—C25—O1	−106.8 (3)
C2—C3—C4—C5	0.9 (4)	C8—C7—C25—O1	69.0 (3)
C3—C4—C5—C6	0.5 (5)	C12—C7—C25—C26	3.9 (4)
C4—C5—C6—C1	−2.5 (5)	C8—C7—C25—C26	179.7 (2)
C2—C1—C6—C5	2.9 (4)	C12—C7—C25—C1	133.5 (3)
C25—C1—C6—C5	−176.1 (3)	C8—C7—C25—C1	−50.7 (3)
C12—C7—C8—C9	2.6 (4)	O1—C25—C26—C27	−2.3 (3)
C25—C7—C8—C9	−173.3 (3)	C1—C25—C26—C27	114.7 (3)
C7—C8—C9—C10	−2.4 (5)	C7—C25—C26—C27	−115.3 (3)
C8—C9—C10—C11	0.6 (5)	O1—C25—C26—Br2	179.54 (18)
C9—C10—C11—C12	0.9 (5)	C1—C25—C26—Br2	−63.5 (3)
C8—C7—C12—C11	−1.2 (5)	C7—C25—C26—Br2	66.5 (3)
C25—C7—C12—C11	174.7 (3)	C25—C26—C27—C28	−2.5 (3)
C10—C11—C12—C7	−0.6 (5)	Br2—C26—C27—C28	175.6 (2)
C18—C13—C14—C15	−0.1 (4)	C25—C26—C27—Br1	179.32 (19)
C28—C13—C14—C15	174.5 (3)	Br2—C26—C27—Br1	−2.5 (4)
C13—C14—C15—C16	1.3 (5)	C25—O1—C28—C27	−7.8 (3)
C14—C15—C16—C17	−1.3 (5)	C25—O1—C28—C19	−127.3 (2)
C15—C16—C17—C18	0.2 (5)	C25—O1—C28—C13	110.9 (2)
C16—C17—C18—C13	1.0 (5)	C26—C27—C28—O1	6.2 (3)
C14—C13—C18—C17	−1.0 (4)	Br1—C27—C28—O1	−175.57 (17)
C28—C13—C18—C17	−175.7 (3)	C26—C27—C28—C19	123.0 (3)

C24—C19—C20—C21	1.6 (4)	Br1—C27—C28—C19	−58.8 (3)
C28—C19—C20—C21	−177.5 (3)	C26—C27—C28—C13	−108.7 (3)
C19—C20—C21—C22	0.8 (5)	Br1—C27—C28—C13	69.5 (3)
C20—C21—C22—C23	−2.9 (5)	C20—C19—C28—O1	15.0 (3)
C21—C22—C23—C24	2.5 (5)	C24—C19—C28—O1	−164.0 (2)
C22—C23—C24—C19	−0.1 (5)	C20—C19—C28—C27	−97.1 (3)
C20—C19—C24—C23	−2.0 (4)	C24—C19—C28—C27	83.8 (3)
C28—C19—C24—C23	177.1 (3)	C20—C19—C28—C13	134.2 (3)
C28—O1—C25—C26	6.5 (3)	C24—C19—C28—C13	−44.9 (3)
C28—O1—C25—C1	−112.2 (2)	C14—C13—C28—O1	−92.0 (3)
C28—O1—C25—C7	126.0 (2)	C18—C13—C28—O1	82.5 (3)
C2—C1—C25—O1	8.3 (4)	C14—C13—C28—C27	19.1 (4)
C6—C1—C25—O1	−172.7 (2)	C18—C13—C28—C27	−166.3 (2)
C2—C1—C25—C26	−103.6 (3)	C14—C13—C28—C19	147.9 (2)
C6—C1—C25—C26	75.4 (3)	C18—C13—C28—C19	−37.5 (3)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of the C1–C6 and C7–C12 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···Cg2[i]	0.95	2.82	3.701 (3)	155
C10—H10···Cg1[ii]	0.95	2.96	3.835 (3)	154
C16—H16···Cg1[iii]	0.95	2.75	3.508 (3)	137

Symmetry codes: (i) −x, y−1/2, −z+3/2; (ii) x−1, y, z; (iii) −x, y+1/2, −z+3/2.