(3aS,4S,6S,7aR)-Hexahydro-3a,5,5-trimethyl-2-phenyl-4,6-methano-1,3,2-benzodioxaborole

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The molecule of the title compound, $C_{16}H_{21}BO_2$, comprises a chiral fused tricyclic system containing five-membered (1,3,2-dioxaborolane), six-membered (cyclohexane) and four-membered (cyclobutane) rings. The 1,3,2-dioxaborolane ring is almost planar (r.m.s. deviation = 0.035 Å), and the *syn* H and Me substituents at this ring are in an eclipsed conformation. The cyclohexane and cyclobutane rings adopt sofa and butterfly conformations, respectively. The B atom has a trigonal–planar configuration (sum of the bond angles = 360.0°). The phenyl ring is practically coplanar with the 1,3,2-dioxaborolane ring [dihedral angle between the ring planes = 1.96 (8)°]. The absolute structure was determined from the known configuration of (+)-pinanediol which was used in the synthesis. In the crystal, weak C—H···π(Ph) interactions occur.

Related literature

For the Matteson homologation reaction, see: Matteson *et al.* (1983); Matteson (1989). For 2-substituted (+)-pinane-diolboronates, see: Carmès *et al.* (2000); Caselli *et al.* (2003); Morandi *et al.* (2003, 2005).
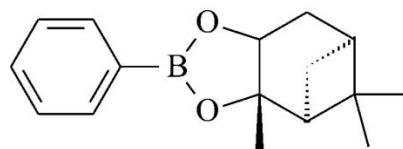
Experimental

Crystal data

$C_{16}H_{21}BO_2$	$V = 1406.27$ (8) Å^3
$M_r = 256.14$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.4974$ (3) Å	$\mu = 0.08$ mm^{-1}
$b = 11.8566$ (4) Å	$T = 100$ K
$c = 13.9580$ (4) Å	$0.25 \times 0.22 \times 0.18$ mm

Data collection

Bruker APEXII CCD diffractometer	21778 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	2905 independent reflections
	2717 reflections with $I > 2\sigma(I)$
$T_{min} = 0.981$, $T_{max} = 0.986$	$R_{int} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$	176 parameters
$wR(F^2) = 0.092$	H-atom parameters constrained
$S = 1.05$	$\Delta\rho_{max} = 0.30$ e Å^{-3}
2905 reflections	$\Delta\rho_{min} = -0.20$ e Å^{-3}

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

Cg is the centroid of the C12–C17 phenyl ring

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···Cg^i	0.99	2.94	3.7532 (13)	140
C11—H11A···Cg^{ii}	0.98	2.97	3.9481 (13)	174

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; 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*.

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(3a*S*,4*S*,6*S*,7a*R*)-Hexahydro-3a,5,5-trimethyl-2-phenyl-4,6-methano-1,3,2-benzodioxaborole

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Comment

2-Substituted (+)-pinanediolboronates are well known compounds (Carmès *et al.*, 2000; Caselli *et al.*, 2003; Morandi *et al.*, 2003; Morandi *et al.*, 2005). In the present work, the (+)-pinanediol phenylboronate (CAS Registry Number: 76110-78-6) has been synthesized by the reaction of phenylboronic acid with (+)-pinanediol in diethyl ether (Fig. 1) as a starting material for the Matteson homologation reaction (Matteson *et al.*, 1983; Matteson, 1989).

The molecule of the title compound, $C_{16}H_{21}BO_2$, comprises a chiral fused tricyclic system containing five-membered (1,3,2-dioxaborolane), six-membered (cyclohexane) and four-membered (cyclobutane) rings (Fig. 2). The 1,3,2-dioxaborolane ring is almost planar (s.u. = 0.035 Å), and *syn* hydrogen and methyl substituents at this ring are in an eclipsed conformation. The cyclohexane (C8/C4/C3a/C7a/C7/C6 and C5/C4/C3a/C7a/C7/C6) and cyclobutane rings adopt *sofa* and *butterfly* conformations, respectively. The boron atom has a trigonal-planar configuration (sum of the bond angles is 360.0 (3)°). The phenyl ring is practically coplanar to the 1,3,2-dioxaborolane ring (the interplanar angle between the ring planes is 1.96 (8)°).

The absolute structure was determined from the known configuration of (+)-pinanediol that has been used in the synthesis. The title molecule possesses four asymmetric centres at C3a, C4, C6 and C7a carbon atoms. The configurations at these asymmetric centres are *S*, *S*, *S*, *R*, respectively.

The crystal packing of the title molecules is stabilized by the weak intermolecular C8—H8A···π(Ph) [the H···Cg^i distance is 2.94 Å; Cg means the centroid of the phenyl ring composed of C12/C13–C17] and C11—H11A···π(Ph) [the H···Cg^{ii} distance is 2.97 Å] interactions. Symmetry codes: (i) -1 + *x*, *y*, *z*; (ii) 1/2 - *x*, 1 - *y*, 1/2 + *z*.

Experimental

(+)-Pinanediol (10 g, 0.059 mol) was added to a solution of phenylboronic acid (7.16 g, 0.059 mol) in ether (80 ml). The reaction mixture was stirred for 4 h at room temperature. Then the solvent was evaporated under reduced pressure to give the title compound as colourless prismatic crystals. Yield is 15 g (99%). ¹H NMR (400 MHz, CDCl₃): δ = 8.25 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.83–7.80 (m, 1H), 7.63–7.35 (m, 3H), 4.46 (dd, *J* = 8.8, 1.9 Hz, 1H), 2.41 (ddd, *J* = 8.6, 8.0, 5.6 Hz,1*H*), 2.23 (ddd, *J* = 10.8, 6.1, 2.3 Hz, 1H), 2.15 (d, *J* = 5.9 Hz, 1H), 1.96 (ddd, *J* = 12.2, 5.5, 3.0 Hz, 2H), 1.49 (s, 3H), 1.32 (s, 3H), 1.23 (d, *J* = 10.8 Hz, 1H), 0.90 (s, 3H). ¹³C NMR (101 MHz, CDCl₃): δ = 135.62, 134.76, 132.68, 131.15, 127.97, 127.72, 86.22, 78.24, 51.42, 39.54, 38.19, 35.57, 28.71, 27.10, 26.49, 24.04.

Refinement

All the H atoms were discernible in the difference electron density map. Nevertheless, all the H atoms were fully constrained. The values of the used constraints were following: C_{aryl}—H = 0.95, C_{methyl}—H = 0.98, $C_{methylene}$—H = 0.99, $C_{methine}$—H = 1.00 Å; $U_{iso}(H) = 1.2U_{eq}(C_{aryl/methylene/methine})$; $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$. After the refinement converged the

extremal residual density peaks equalled to -0.197 and 0.302 e A^{-3}. All the highest positive peaks in the range of 0.170–0.302 e A^{-3}) were situated between the covalently bonded atoms. 2225 Friedel pairs were merged in the refinement process. The absolute structure was determined from the known configuration of (+)-pinanediol that had been used in the synthesis.

Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus* (Bruker, 2001); 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).
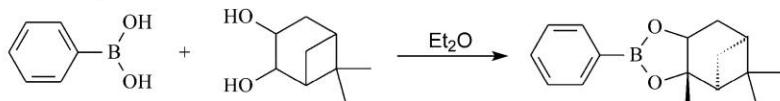
Figure 1

Reaction of phenylboronic acid with (+)-pinanediol.
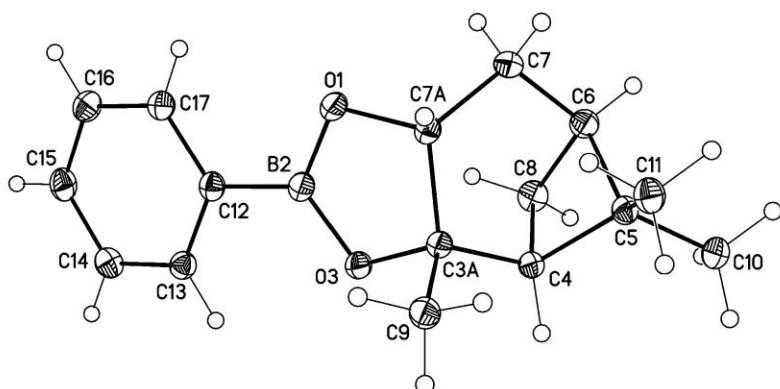
Figure 2

The title molecule with the atom numbering scheme. The displacement ellipsoids are shown at the 50% probability level. H atoms are presented as small spheres of arbitrary radius.

(3a*S*,4*S*,6*S*,7a*R*)-Hexahydro-3a,5,5-trimethyl-2- phenyl-4,6-methano-1,3,2-benzodioxaborole

Crystal data

C$_{16}$H$_{21}$BO$_2$	F(000) = 552
M_r = 256.14	D_x = 1.210 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo Kα radiation, λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 7519 reflections
a = 8.4974 (3) Å	θ = 2.3–32.2°
b = 11.8566 (4) Å	μ = 0.08 mm^{-1}
c = 13.9580 (4) Å	T = 100 K
V = 1406.27 (8) Å^3	Prism, colourless
Z = 4	0.25 × 0.22 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer	21778 measured reflections
Radiation source: fine-focus sealed tube	2905 independent reflections
Graphite monochromator	2717 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.037$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$\theta_{max} = 32.7°$, $\theta_{min} = 2.3°$
$T_{min} = 0.981$, $T_{max} = 0.986$	$h = -12 \rightarrow 12$
	$k = -17 \rightarrow 18$
	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.0967P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
2905 reflections	$(\Delta/\sigma)_{max} < 0.001$
176 parameters	$\Delta\rho_{max} = 0.30$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc²λ³/sin(2θ)]$^{-1/4}$
	Extinction coefficient: 0.015 (3)

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	$U_{iso}*/U_{eq}$
O1	0.47304 (10)	0.46977 (7)	0.16126 (6)	0.01697 (16)
B2	0.51357 (15)	0.50773 (11)	0.07183 (9)	0.0155 (2)
O3	0.43471 (10)	0.60223 (7)	0.04344 (6)	0.01612 (16)
C3A	0.33535 (12)	0.64035 (9)	0.12251 (7)	0.01379 (18)
C4	0.16707 (12)	0.65105 (9)	0.08556 (7)	0.01398 (18)
H4	0.1503	0.7117	0.0368	0.017*
C5	0.04178 (12)	0.64743 (9)	0.16843 (8)	0.01482 (18)
C6	0.05741 (14)	0.51655 (9)	0.16181 (8)	0.0170 (2)
H6	−0.0424	0.4734	0.1719	0.020*
C7	0.19909 (14)	0.47449 (10)	0.21897 (8)	0.0181 (2)
H7A	0.2184	0.3944	0.2029	0.022*
H7B	0.1743	0.4788	0.2882	0.022*
C7A	0.35083 (13)	0.54313 (9)	0.19900 (7)	0.01454 (19)
H7C	0.3886	0.5765	0.2606	0.017*
C8	0.10773 (14)	0.53195 (10)	0.05572 (8)	0.0182 (2)

H8A	0.0190	0.5329	0.0097	0.022*
H8B	0.1920	0.4800	0.0346	0.022*
C9	0.40689 (14)	0.75145 (9)	0.15593 (8)	0.0180 (2)
H9A	0.4052	0.8059	0.1031	0.027*
H9B	0.5158	0.7388	0.1763	0.027*
H9C	0.3457	0.7811	0.2098	0.027*
C10	−0.11904 (13)	0.68839 (11)	0.13230 (9)	0.0195 (2)
H10A	−0.1992	0.6736	0.1812	0.029*
H10B	−0.1464	0.6482	0.0733	0.029*
H10C	−0.1142	0.7696	0.1194	0.029*
C11	0.07336 (14)	0.70381 (10)	0.26519 (8)	0.0189 (2)
H11A	−0.0121	0.6856	0.3097	0.028*
H11B	0.0791	0.7857	0.2566	0.028*
H11C	0.1733	0.6762	0.2912	0.028*
C12	0.63777 (13)	0.44754 (9)	0.00804 (8)	0.01522 (19)
C13	0.68207 (13)	0.49218 (10)	−0.08098 (8)	0.0167 (2)
H13	0.6353	0.5602	−0.1029	0.020*
C14	0.79409 (15)	0.43795 (10)	−0.13785 (8)	0.0191 (2)
H14	0.8243	0.4695	−0.1976	0.023*
C15	0.86127 (14)	0.33749 (10)	−0.10656 (9)	0.0202 (2)
H15	0.9356	0.2995	−0.1459	0.024*
C16	0.82009 (15)	0.29237 (10)	−0.01792 (9)	0.0219 (2)
H16	0.8673	0.2243	0.0037	0.026*
C17	0.70942 (14)	0.34746 (10)	0.03884 (8)	0.0186 (2)
H17	0.6820	0.3167	0.0994	0.022*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0158 (4)	0.0176 (4)	0.0175 (3)	0.0048 (3)	0.0017 (3)	0.0028 (3)
B2	0.0141 (5)	0.0152 (5)	0.0171 (5)	0.0012 (4)	0.0001 (4)	−0.0003 (4)
O3	0.0159 (4)	0.0166 (3)	0.0159 (3)	0.0034 (3)	0.0031 (3)	0.0019 (3)
C3A	0.0135 (4)	0.0135 (4)	0.0144 (4)	0.0010 (4)	0.0011 (3)	0.0007 (3)
C4	0.0129 (4)	0.0138 (4)	0.0152 (4)	−0.0002 (3)	0.0001 (3)	0.0006 (3)
C5	0.0127 (4)	0.0146 (4)	0.0172 (4)	−0.0005 (4)	0.0003 (4)	−0.0001 (4)
C6	0.0153 (4)	0.0139 (4)	0.0217 (5)	−0.0018 (4)	−0.0006 (4)	0.0010 (4)
C7	0.0167 (5)	0.0157 (4)	0.0218 (5)	−0.0006 (4)	0.0016 (4)	0.0047 (4)
C7A	0.0140 (4)	0.0145 (4)	0.0151 (4)	0.0020 (4)	0.0010 (3)	0.0008 (4)
C8	0.0187 (5)	0.0169 (5)	0.0191 (5)	−0.0017 (4)	−0.0019 (4)	−0.0036 (4)
C9	0.0157 (5)	0.0151 (4)	0.0231 (5)	−0.0019 (4)	0.0004 (4)	−0.0004 (4)
C10	0.0143 (5)	0.0214 (5)	0.0228 (5)	0.0020 (4)	−0.0003 (4)	0.0026 (4)
C11	0.0182 (5)	0.0203 (5)	0.0182 (5)	0.0007 (4)	0.0022 (4)	−0.0024 (4)
C12	0.0138 (4)	0.0151 (4)	0.0167 (4)	−0.0001 (4)	−0.0001 (4)	−0.0014 (4)
C13	0.0158 (5)	0.0170 (5)	0.0173 (4)	0.0002 (4)	−0.0008 (4)	−0.0004 (4)
C14	0.0191 (5)	0.0213 (5)	0.0169 (5)	−0.0010 (4)	0.0014 (4)	−0.0021 (4)
C15	0.0179 (5)	0.0207 (5)	0.0220 (5)	0.0013 (4)	0.0040 (4)	−0.0043 (4)
C16	0.0205 (5)	0.0180 (5)	0.0272 (5)	0.0054 (4)	0.0036 (4)	0.0004 (4)
C17	0.0175 (5)	0.0180 (5)	0.0204 (5)	0.0031 (4)	0.0034 (4)	0.0015 (4)

Geometric parameters (Å, °)

O1—B2	1.3709 (15)	C8—H8B	0.9900
O1—C7A	1.4535 (13)	C9—H9A	0.9800
B2—O3	1.3644 (15)	C9—H9B	0.9800
B2—C12	1.5544 (16)	C9—H9C	0.9800
O3—C3A	1.4612 (13)	C10—H10A	0.9800
C3A—C9	1.5239 (15)	C10—H10B	0.9800
C3A—C4	1.5254 (15)	C10—H10C	0.9800
C3A—C7A	1.5767 (15)	C11—H11A	0.9800
C4—C8	1.5563 (16)	C11—H11B	0.9800
C4—C5	1.5727 (15)	C11—H11C	0.9800
C4—H4	1.0000	C12—C17	1.4012 (15)
C5—C11	1.5307 (15)	C12—C13	1.4020 (15)
C5—C10	1.5355 (15)	C13—C14	1.3963 (16)
C5—C6	1.5602 (15)	C13—H13	0.9500
C6—C7	1.5280 (16)	C14—C15	1.3911 (17)
C6—C8	1.5520 (17)	C14—H14	0.9500
C6—H6	1.0000	C15—C16	1.3927 (17)
C7—C7A	1.5500 (16)	C15—H15	0.9500
C7—H7A	0.9900	C16—C17	1.3924 (16)
C7—H7B	0.9900	C16—H16	0.9500
C7A—H7C	1.0000	C17—H17	0.9500
C8—H8A	0.9900		
B2—O1—C7A	108.24 (9)	C6—C8—H8A	114.2
O3—B2—O1	114.25 (10)	C4—C8—H8A	114.2
O3—B2—C12	122.96 (10)	C6—C8—H8B	114.2
O1—B2—C12	122.78 (10)	C4—C8—H8B	114.2
B2—O3—C3A	108.56 (8)	H8A—C8—H8B	111.4
O3—C3A—C9	105.55 (8)	C3A—C9—H9A	109.5
O3—C3A—C4	108.18 (8)	C3A—C9—H9B	109.5
C9—C3A—C4	113.93 (9)	H9A—C9—H9B	109.5
O3—C3A—C7A	103.72 (8)	C3A—C9—H9C	109.5
C9—C3A—C7A	113.04 (9)	H9A—C9—H9C	109.5
C4—C3A—C7A	111.59 (9)	H9B—C9—H9C	109.5
C3A—C4—C8	108.59 (9)	C5—C10—H10A	109.5
C3A—C4—C5	112.56 (8)	C5—C10—H10B	109.5
C8—C4—C5	87.29 (8)	H10A—C10—H10B	109.5
C3A—C4—H4	115.1	C5—C10—H10C	109.5
C8—C4—H4	115.1	H10A—C10—H10C	109.5
C5—C4—H4	115.1	H10B—C10—H10C	109.5
C11—C5—C10	107.92 (9)	C5—C11—H11A	109.5
C11—C5—C6	118.15 (9)	C5—C11—H11B	109.5
C10—C5—C6	111.77 (9)	H11A—C11—H11B	109.5
C11—C5—C4	121.22 (9)	C5—C11—H11C	109.5
C10—C5—C4	110.62 (9)	H11A—C11—H11C	109.5
C6—C5—C4	85.75 (8)	H11B—C11—H11C	109.5
C7—C6—C8	108.63 (10)	C17—C12—C13	118.35 (10)
C7—C6—C5	111.14 (9)	C17—C12—B2	120.53 (10)

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C8—C6—C5	87.88 (8)	C13—C12—B2	121.11 (10)
C7—C6—H6	115.3	C14—C13—C12	120.87 (11)
C8—C6—H6	115.3	C14—C13—H13	119.6
C5—C6—H6	115.3	C12—C13—H13	119.6
C6—C7—C7A	112.97 (9)	C15—C14—C13	119.71 (11)
C6—C7—H7A	109.0	C15—C14—H14	120.1
C7A—C7—H7A	109.0	C13—C14—H14	120.1
C6—C7—H7B	109.0	C14—C15—C16	120.31 (11)
C7A—C7—H7B	109.0	C14—C15—H15	119.8
H7A—C7—H7B	107.8	C16—C15—H15	119.8
O1—C7A—C7	110.20 (9)	C17—C16—C15	119.67 (11)
O1—C7A—C3A	104.58 (8)	C17—C16—H16	120.2
C7—C7A—C3A	115.87 (9)	C15—C16—H16	120.2
O1—C7A—H7C	108.7	C16—C17—C12	121.07 (11)
C7—C7A—H7C	108.7	C16—C17—H17	119.5
C3A—C7A—H7C	108.7	C12—C17—H17	119.5
C6—C8—C4	86.60 (8)		
C7A—O1—B2—O3	1.42 (13)	B2—O1—C7A—C7	119.37 (10)
C7A—O1—B2—C12	−178.09 (10)	B2—O1—C7A—C3A	−5.80 (11)
O1—B2—O3—C3A	4.09 (13)	C6—C7—C7A—O1	−120.17 (10)
C12—B2—O3—C3A	−176.40 (10)	C6—C7—C7A—C3A	−1.72 (14)
B2—O3—C3A—C9	111.83 (10)	O3—C3A—C7A—O1	7.86 (10)
B2—O3—C3A—C4	−125.86 (10)	C9—C3A—C7A—O1	−105.95 (10)
B2—O3—C3A—C7A	−7.25 (11)	C4—C3A—C7A—O1	124.09 (9)
O3—C3A—C4—C8	63.98 (10)	O3—C3A—C7A—C7	−113.64 (10)
C9—C3A—C4—C8	−178.99 (9)	C9—C3A—C7A—C7	132.54 (10)
C7A—C3A—C4—C8	−49.50 (11)	C4—C3A—C7A—C7	2.59 (13)
O3—C3A—C4—C5	158.89 (8)	C7—C6—C8—C4	−85.15 (9)
C9—C3A—C4—C5	−84.08 (11)	C5—C6—C8—C4	26.47 (8)
C7A—C3A—C4—C5	45.42 (12)	C3A—C4—C8—C6	86.66 (9)
C3A—C4—C5—C11	37.66 (14)	C5—C4—C8—C6	−26.25 (8)
C8—C4—C5—C11	146.68 (10)	O3—B2—C12—C17	−176.74 (11)
C3A—C4—C5—C10	165.43 (9)	O1—B2—C12—C17	2.72 (17)
C8—C4—C5—C10	−85.55 (10)	O3—B2—C12—C13	3.88 (17)
C3A—C4—C5—C6	−82.88 (10)	O1—B2—C12—C13	−176.66 (11)
C8—C4—C5—C6	26.13 (8)	C17—C12—C13—C14	0.39 (17)
C11—C5—C6—C7	−40.37 (13)	B2—C12—C13—C14	179.78 (11)
C10—C5—C6—C7	−166.49 (9)	C12—C13—C14—C15	0.88 (17)
C4—C5—C6—C7	82.98 (10)	C13—C14—C15—C16	−1.55 (18)
C11—C5—C6—C8	−149.55 (10)	C14—C15—C16—C17	0.94 (19)
C10—C5—C6—C8	84.33 (10)	C15—C16—C17—C12	0.36 (19)
C4—C5—C6—C8	−26.20 (8)	C13—C12—C17—C16	−1.01 (17)
C8—C6—C7—C7A	47.70 (12)	B2—C12—C17—C16	179.59 (11)
C5—C6—C7—C7A	−47.38 (13)		

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C12–C17 phenyl ring

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···Cg[i]	0.99	2.94	3.7532 (13)	140
C11—H11A···Cg[ii]	0.98	2.97	3.9481 (13)	174

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

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