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1,4-Anhydro-2-*C*-benzyloxymethyl-2,3:5,6-di-*O*-isopropylidene-D-tallitol

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Key indicators

Single-crystal X-ray study
T = 170 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.047
wR factor = 0.075
Data-to-parameter ratio = 9.4

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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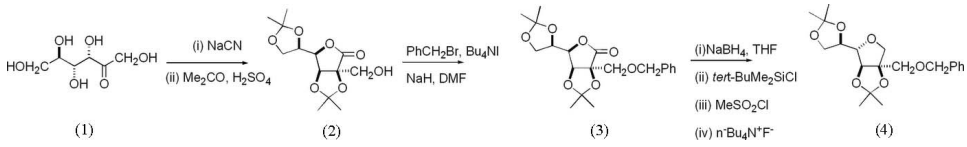
The crystal structure of the title compound, $C_{20}H_{28}O_6$, allows a firm assignment of the stereochemistry at C-4 of formation of the tetrahydrofuran (THF) ring.

Comment

Hitherto, most carbohydrate building blocks have linear carbon chains (Lichtenthaler & Peters, 2004). However, the Kiliani reaction on each of the four ketohexoses provides branched sugar lactones which are readily crystallized as a new family of chiral carbohydrate building blocks (Soengas *et al.*, 2005). Such materials have been used to make novel sugar amino acids as potential dipeptide isosteres (Simone *et al.*, 2005). In further studies on the potential of such intermediates to form complex chiral targets, further investigations into the synthesis of branched THF rings have been carried out. Thus reaction of D-fructose (1) with sodium cyanide, followed by acetonation of the crude mixture of the resulting lactones, gave the crystalline diacetonide (2) (Hotchkiss *et al.*, 2004). Reaction of (2) with benzyl bromide and sodium hydride in the presence of tetra-*n*-butyl ammonium iodide in dimethylformamide afforded the corresponding benzyl ether (3). The lactone (3) was subjected to a sequence of reactions to construct the THF ring: reduction of (3) to the corresponding diol, followed by protection of one of the hydroxy groups as a silyl ether, activation of the remaining hydroxy group by mesyl chloride and ring closure of the resulting silyl ether by treatment with tetrabutylammonium fluoride gave a crystalline ether (4). As silyl ethers are particularly prone to migrate under basic conditions, there were a number of stages in the sequence that could have given rise to alternative stereochemistry at C-4; the crystal structure of the title compound (Fig. 1) firmly establishes that the closure of the THF ring proceeded by nucleophilic displacement of a C-4 mesylate by the C-1 hydroxy function of the polyol (Soengas & Fleet, 2005).



The crystal structure of (4) (Fig. 2) contains a close contact, H231···O70 = 2.49 Å, which, if it were a weak C—H···O interaction, would link molecules along 2_1 screw axes to form extended chains in the *b* axis direction. However, this interaction is too weak to prevent the O70/O71 disorder.

Experimental

The benzyl ether (4) was crystallized from 60–80′ petroleum spirit (m.p. 317–318 K, $[\alpha]_D^{23}$ −13.2, c 1.0 in chloroform) (Soengas & Fleet, 2005).

Crystal data

$C_{20}H_{28}O_6$
M_r = 364.44
Orthorhombic, $P2_12_12_1$
a = 5.9504 (2) Å
b = 14.5676 (4) Å
c = 22.0403 (8) Å
V = 1910.52 (11) Å^3
Z = 4
D_x = 1.267 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2296 reflections
θ = 5–27°
μ = 0.09 mm^{-1}
T = 170 K
Lath, colourless
0.90 × 0.15 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*DENZO/SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.84, T_{max} = 0.99
10188 measured reflections
2486 independent reflections
2305 reflections with $I > -3\sigma(I)$
R_{int} = 0.037
θ_{max} = 27.5°
$h = -7 \rightarrow 7$
$k = -18 \rightarrow 18$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.075
S = 0.99
2305 reflections
245 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.03P)^2 + 0.2P]$ where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: Larson (1970), equation 22
Extinction coefficient: 7.9 (11) × 10^2

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

D—H···A	D—H	H···A	D···A	D—H···A
C23—H231···O70^{i}	0.95	2.49	3.372 (2)	155

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

In the absence of significant anomalous scattering, Friedel pairs were merged, and the absolute configuration was arbitrarily assigned. Changes in illuminated volume were kept to a minimum, and were taken into account (Görbitz, 1999) by multi-scan inter-frame scaling (*DENZO/SCALEPACK*; Otwinowski & Minor, 1997). H atoms were all located in a difference map, but those attached to C atoms were repositioned geometrically. H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.98 Å) and displacement parameters [U_{iso}(H) in the range 1.2–1.5 times U_{eq} of the parent atom], after which they were refined with riding constraints. The crystal structure shows disorder in the C4–C8 ring. One of the O atoms was modelled as split (O70 and O71, with site-occupancy factors of 0.44 and 0.56, respectively). The consequential alternative sites for C9 and C10 were adequately accommodated by their anisotropic displacement parameters. No attempt was made to model disordered H atoms on C8, C9 and C10; stable positions were found for 'average' atoms during the restrained least-squares refinement.

Data collection: *COLLECT* (Nonius, 2001).; cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997; data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

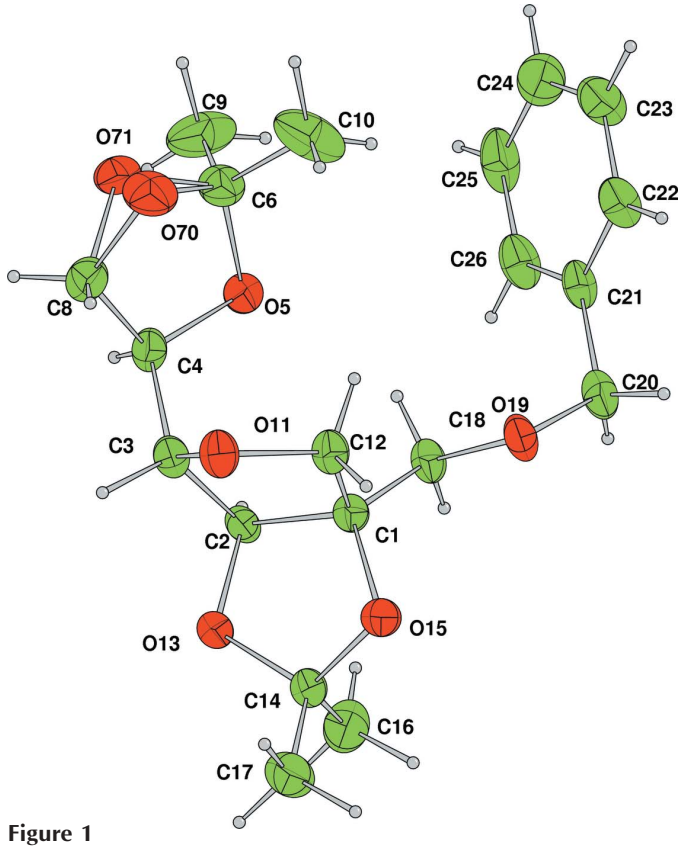


Figure 1
The title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. Both disorder components are shown.

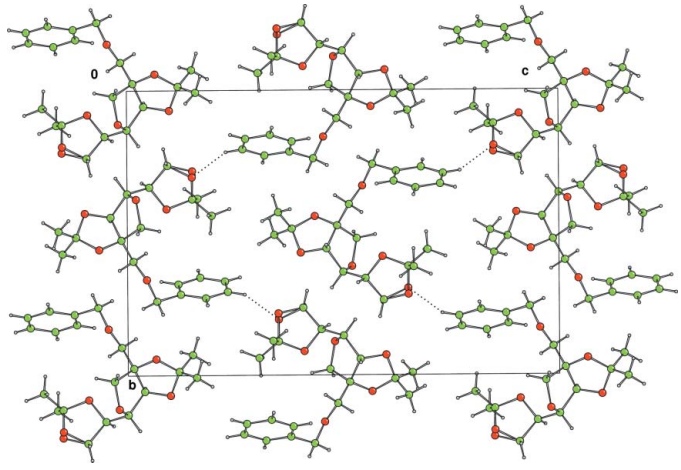


Figure 2
A projection of the crystal structure of the title compound along the *a* axis. Putative hydrogen bonding is shown by dotted lines.

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supporting information

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$\theta_{max} = 27.5°$, $\theta_{min} = 5.2°$
$h = -7\rightarrow7$
$k = -18\rightarrow18$
$l = -28\rightarrow28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.075$
$S = 0.99$
2305 reflections
245 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.03P)^2 + 0.2P]$ where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.000389$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: Larson 1970 Crystallographic Computing eq 22
Extinction coefficient: 790 (110)

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.4054 (3)	0.02469 (12)	0.51386 (8)	0.0259	
C2	0.5454 (3)	−0.05597 (12)	0.53868 (7)	0.0255	
C3	0.4794 (3)	−0.13805 (13)	0.50008 (8)	0.0286	

C4	0.6390 (4)	−0.16062 (12)	0.44865 (8)	0.0303	
O5	0.6652 (2)	−0.08412 (8)	0.40887 (6)	0.0347	
C6	0.7076 (4)	−0.11835 (14)	0.34932 (9)	0.0360	
O70	0.5562 (9)	−0.1956 (4)	0.3499 (2)	0.0447	0.4412
O71	0.6677 (8)	−0.2170 (3)	0.34900 (19)	0.0443	0.5588
C8	0.5589 (4)	−0.23673 (13)	0.40643 (9)	0.0372	
C9	0.9553 (4)	−0.1208 (2)	0.33683 (11)	0.0621	
C10	0.5849 (4)	−0.0607 (2)	0.30437 (10)	0.0626	
O11	0.2561 (2)	−0.11806 (9)	0.47960 (6)	0.0314	
C12	0.2451 (3)	−0.02028 (12)	0.46856 (8)	0.0289	
O13	0.4616 (2)	−0.07040 (8)	0.59844 (5)	0.0315	
C14	0.3653 (4)	0.01380 (13)	0.61898 (8)	0.0313	
O15	0.2823 (2)	0.05770 (8)	0.56549 (5)	0.0321	
C16	0.5412 (4)	0.07157 (15)	0.65028 (10)	0.0461	
C17	0.1677 (4)	−0.00759 (17)	0.65927 (10)	0.0477	
C18	0.5505 (3)	0.09920 (12)	0.48604 (8)	0.0282	
O19	0.4125 (2)	0.16380 (8)	0.45525 (6)	0.0332	
C20	0.5411 (4)	0.23965 (13)	0.43153 (10)	0.0384	
C21	0.6787 (3)	0.21552 (13)	0.37669 (9)	0.0316	
C22	0.5918 (4)	0.22880 (14)	0.31876 (9)	0.0383	
C23	0.7158 (4)	0.20694 (15)	0.26792 (10)	0.0489	
C24	0.9296 (5)	0.17026 (16)	0.27436 (13)	0.0548	
C25	1.0174 (4)	0.15653 (15)	0.33164 (12)	0.0502	
C26	0.8945 (4)	0.17985 (14)	0.38224 (11)	0.0383	
H21	0.7063	−0.0438	0.5393	0.0296*	
H31	0.4738	−0.1937	0.5267	0.0323*	
H41	0.7890	−0.1757	0.4658	0.0372*	
H81	0.6308	−0.2954	0.4155	0.0441*	
H82	0.3979	−0.2456	0.4097	0.0449*	
H91	0.9799	−0.1477	0.2973	0.0922*	
H92	1.0089	−0.0577	0.3371	0.0946*	
H93	1.0326	−0.1552	0.3671	0.0935*	
H101	0.6131	−0.0840	0.2633	0.0941*	
H102	0.6400	0.0011	0.3075	0.0942*	
H103	0.4280	−0.0617	0.3117	0.0947*	
H121	0.2908	−0.0072	0.4259	0.0322*	
H122	0.0887	0.0020	0.4757	0.0342*	
H161	0.4723	0.1306	0.6619	0.0699*	
H162	0.6694	0.0821	0.6232	0.0694*	
H163	0.5921	0.0407	0.6873	0.0696*	
H171	0.0929	0.0501	0.6709	0.0725*	
H172	0.0666	−0.0453	0.6364	0.0734*	
H173	0.2151	−0.0395	0.6949	0.0729*	
H181	0.6585	0.0704	0.4571	0.0336*	
H182	0.6364	0.1299	0.5183	0.0345*	
H201	0.4305	0.2854	0.4184	0.0471*	
H202	0.6392	0.2639	0.4635	0.0461*	
H221	0.4429	0.2538	0.3148	0.0456*	

H231	0.6533	0.2167	0.2289	0.0584*
H241	1.0137	0.1563	0.2396	0.0668*
H251	1.1637	0.1315	0.3364	0.0600*
H261	0.9562	0.1700	0.4217	0.0465*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0272 (10)	0.0244 (9)	0.0260 (9)	0.0029 (9)	0.0009 (8)	0.0019 (8)
C2	0.0280 (9)	0.0251 (9)	0.0232 (9)	0.0014 (9)	0.0011 (8)	0.0061 (8)
C3	0.0311 (10)	0.0246 (10)	0.0303 (10)	0.0009 (9)	−0.0001 (9)	0.0049 (8)
C4	0.0351 (11)	0.0231 (9)	0.0329 (10)	0.0050 (9)	−0.0019 (9)	0.0012 (8)
O5	0.0442 (8)	0.0279 (7)	0.0321 (7)	0.0018 (7)	0.0084 (7)	0.0016 (6)
C6	0.0432 (13)	0.0364 (11)	0.0284 (10)	−0.0045 (11)	−0.0029 (10)	−0.0022 (9)
O70	0.054 (3)	0.051 (3)	0.029 (2)	−0.008 (3)	−0.010 (3)	−0.004 (2)
O71	0.069 (3)	0.033 (2)	0.0308 (17)	−0.003 (2)	0.011 (2)	−0.0067 (14)
C8	0.0459 (12)	0.0309 (10)	0.0347 (11)	0.0038 (11)	−0.0032 (11)	−0.0047 (9)
C9	0.0492 (14)	0.095 (2)	0.0419 (13)	0.0311 (16)	−0.0001 (12)	−0.0151 (14)
C10	0.0398 (13)	0.105 (2)	0.0428 (13)	0.0065 (16)	0.0005 (11)	0.0263 (14)
O11	0.0280 (7)	0.0266 (7)	0.0397 (8)	−0.0043 (6)	−0.0026 (6)	0.0026 (6)
C12	0.0263 (10)	0.0260 (10)	0.0343 (10)	0.0014 (9)	−0.0009 (9)	0.0031 (8)
O13	0.0426 (8)	0.0272 (7)	0.0246 (6)	0.0078 (7)	0.0045 (6)	0.0045 (5)
C14	0.0405 (12)	0.0282 (10)	0.0250 (9)	0.0096 (10)	−0.0014 (9)	0.0030 (8)
O15	0.0374 (7)	0.0329 (7)	0.0261 (6)	0.0102 (7)	0.0026 (6)	0.0024 (6)
C16	0.0563 (14)	0.0388 (12)	0.0432 (12)	0.0079 (12)	−0.0150 (11)	−0.0051 (10)
C17	0.0523 (14)	0.0517 (14)	0.0392 (12)	0.0146 (13)	0.0116 (12)	0.0115 (11)
C18	0.0292 (9)	0.0245 (9)	0.0310 (10)	0.0020 (9)	−0.0061 (9)	0.0050 (8)
O19	0.0350 (7)	0.0258 (6)	0.0386 (7)	0.0044 (7)	0.0033 (6)	0.0126 (6)
C20	0.0475 (13)	0.0256 (10)	0.0420 (12)	0.0006 (10)	0.0039 (11)	0.0103 (9)
C21	0.0329 (11)	0.0218 (10)	0.0400 (11)	−0.0047 (9)	0.0001 (10)	0.0089 (9)
C22	0.0362 (12)	0.0363 (11)	0.0425 (12)	−0.0007 (11)	0.0001 (11)	0.0122 (10)
C23	0.0635 (16)	0.0440 (13)	0.0391 (12)	−0.0048 (13)	0.0026 (12)	0.0109 (11)
C24	0.0622 (16)	0.0403 (13)	0.0619 (16)	0.0025 (14)	0.0294 (14)	0.0071 (12)
C25	0.0347 (12)	0.0342 (12)	0.0816 (18)	0.0046 (10)	0.0144 (13)	0.0215 (12)
C26	0.0310 (12)	0.0335 (12)	0.0504 (13)	−0.0049 (10)	−0.0028 (10)	0.0134 (10)

Geometric parameters (Å, º)

C1—C2	1.541 (2)	O11—C12	1.447 (2)
C1—C12	1.528 (3)	C12—H121	0.998
C1—O15	1.436 (2)	C12—H122	0.998
C1—C18	1.516 (2)	O13—C14	1.428 (2)
C2—C3	1.519 (3)	C14—O15	1.429 (2)
C2—O13	1.424 (2)	C14—C16	1.510 (3)
C2—H21	0.974	C14—C17	1.506 (3)
C3—C4	1.515 (3)	C16—H161	0.986
C3—O11	1.433 (2)	C16—H162	0.982
C3—H31	1.002	C16—H163	0.979

C4—O5	1.426 (2)	C17—H171	0.985
C4—C8	1.524 (3)	C17—H172	0.958
C4—H41	0.994	C17—H173	0.955
O5—C6	1.427 (2)	C18—O19	1.421 (2)
C6—O70	1.441 (6)	C18—H181	0.998
C6—C9	1.500 (4)	C18—H182	0.984
C6—C10	1.490 (3)	O19—C20	1.442 (2)
C6—O71	1.457 (5)	C20—C21	1.501 (3)
C6—C9	1.500 (4)	C20—H201	0.980
C6—C10	1.490 (3)	C20—H202	0.982
O70—C8	1.384 (6)	C21—C22	1.391 (3)
O71—C8	1.450 (5)	C21—C26	1.391 (3)
C8—H81	0.976	C22—C23	1.379 (3)
C8—H82	0.970	C22—H221	0.962
C8—H81	0.976	C23—C24	1.387 (4)
C8—H82	0.970	C23—H231	0.948
C9—H91	0.966	C24—C25	1.381 (4)
C9—H92	0.972	C24—H241	0.937
C9—H93	0.953	C25—C26	1.376 (3)
C10—H101	0.982	C25—H251	0.949
C10—H102	0.961	C26—H261	0.955
C10—H103	0.947		

C2—C1—C12	104.03 (14)	H101—C10—H103	108.7
C2—C1—O15	104.47 (13)	H102—C10—H103	109.8
C12—C1—O15	110.03 (15)	C3—O11—C12	107.15 (14)
C2—C1—C18	112.45 (15)	C1—C12—O11	106.49 (14)
C12—C1—C18	113.44 (15)	C1—C12—H121	111.4
O15—C1—C18	111.79 (14)	O11—C12—H121	109.5
C1—C2—C3	105.17 (14)	C1—C12—H122	109.8
C1—C2—O13	104.58 (14)	O11—C12—H122	109.6
C3—C2—O13	108.14 (14)	H121—C12—H122	109.9
C1—C2—H21	113.5	C2—O13—C14	107.88 (13)
C3—C2—H21	113.9	O13—C14—O15	105.17 (13)
O13—C2—H21	110.9	O13—C14—C16	110.22 (17)
C2—C3—C4	115.33 (16)	O15—C14—C16	111.54 (16)
C2—C3—O11	104.84 (15)	O13—C14—C17	108.82 (16)
C4—C3—O11	112.94 (15)	O15—C14—C17	107.99 (16)
C2—C3—H31	108.5	C16—C14—C17	112.77 (17)
C4—C3—H31	106.5	C1—O15—C14	109.10 (12)
O11—C3—H31	108.5	C14—C16—H161	108.5
C3—C4—O5	111.02 (15)	C14—C16—H162	110.3
C3—C4—C8	114.75 (17)	H161—C16—H162	110.2
O5—C4—C8	103.14 (14)	C14—C16—H163	109.8
C3—C4—H41	109.0	H161—C16—H163	108.2
O5—C4—H41	108.0	H162—C16—H163	109.8
C8—C4—H41	110.7	C14—C17—H171	109.3
C4—O5—C6	108.16 (13)	C14—C17—H172	107.4

O5—C6—O70	98.9 (3)	H171—C17—H172	110.0
O5—C6—C9	110.54 (19)	C14—C17—H173	110.8
O70—C6—C9	126.7 (3)	H171—C17—H173	109.6
O5—C6—C10	109.16 (18)	H172—C17—H173	109.7
O70—C6—C10	98.0 (3)	C1—C18—O19	109.76 (15)
C9—C6—C10	111.9 (2)	C1—C18—H181	108.9
O5—C6—O71	108.7 (2)	O19—C18—H181	110.2
O5—C6—C9	110.54 (19)	C1—C18—H182	109.2
O71—C6—C9	97.8 (3)	O19—C18—H182	110.1
O5—C6—C10	109.16 (18)	H181—C18—H182	108.6
O71—C6—C10	118.2 (3)	C18—O19—C20	111.94 (14)
C9—C6—C10	111.9 (2)	O19—C20—C21	113.68 (16)
C6—O70—C8	109.8 (3)	O19—C20—H201	105.7
C6—O71—C8	105.3 (3)	C21—C20—H201	106.8
C4—C8—O70	103.8 (3)	O19—C20—H202	109.3
C4—C8—H81	112.0	C21—C20—H202	109.8
O70—C8—H81	124.7	H201—C20—H202	111.5
C4—C8—H82	111.2	C20—C21—C22	120.25 (19)
O70—C8—H82	96.4	C20—C21—C26	121.3 (2)
H81—C8—H82	107.5	C22—C21—C26	118.4 (2)
C4—C8—O71	104.4 (2)	C21—C22—C23	121.0 (2)
C4—C8—H81	112.0	C21—C22—H221	118.6
O71—C8—H81	99.0	C23—C22—H221	120.4
C4—C8—H82	111.2	C22—C23—C24	119.8 (2)
O71—C8—H82	122.1	C22—C23—H231	119.5
H81—C8—H82	107.5	C24—C23—H231	120.7
C6—C9—H91	108.9	C23—C24—C25	119.8 (2)
C6—C9—H92	107.4	C23—C24—H241	119.4
H91—C9—H92	109.8	C25—C24—H241	120.9
C6—C9—H93	111.0	C24—C25—C26	120.3 (2)
H91—C9—H93	110.1	C24—C25—H251	120.2
H92—C9—H93	109.5	C26—C25—H251	119.5
C6—C10—H101	109.5	C21—C26—C25	120.8 (2)
C6—C10—H102	108.2	C21—C26—H261	119.4
H101—C10—H102	109.4	C25—C26—H261	119.8
C6—C10—H103	111.2		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H231···O70^{i}	0.95	2.49	3.372 (2)	155

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*+1/2.