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2,3:6,7-Di-*O*-diethylidene-D-*glycero*-L-*talo*-heptono-1,4-lactone

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.006 Å
R factor = 0.052
wR factor = 0.113
Data-to-parameter ratio = 7.4

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

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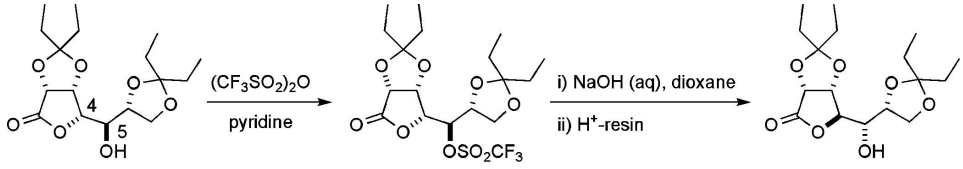
The title compound, $C_{17}H_{28}O_7$, was prepared from protected D-*glycero*-D-*gulo*-heptono-1,4-lactone by tandem S_N2 displacements. The relative configuration of the crystal structure establishes that two stereocentres have been inverted; the absolute configuration was determined by the use of D-glucose as the starting material. There are three independent molecules in the asymmetric unit (*Z*′=3).

Comment

Although carbohydrates are the most widely used chiral scaffolds (Lichtenthaler & Peters, 2004; Bols, 1996), D-*glycero*-D-*gulo*-heptono-1,4-lactone – prepared industrially from D-glucose – is the only seven-carbon sugar that is cheaply available. The value of this carbohydrate lactone as a starting material has been illustrated by the syntheses of the antibiotic gonifurfuranone (Shing *et al.*, 1992; Shing & Tsui, 1992) and a number of imino sugars (Watson *et al.*, 2001; Asano *et al.*, 2000; Fairbanks *et al.*, 1991; Myerscough *et al.*, 1992). Otherwise the use of protected seven-carbon sugars is rare (Choi *et al.*, 1991; Beacham *et al.*, 1991).



(1) (2) (3)

This paper reports the structure of the protected D-*glycero*-L-*talo*-heptono-1,4-lactone (3) which is likely to be another easily available and valuable seven-carbon sugar chiron for the enantiospecific synthesis of complex bioactive compounds. D-*glycero*-D-*gulo*-Heptono-1,4-lactone was treated with 3-pentanone to give the diketal (1) in which only the hydroxyl atom C5 is unprotected (Burke *et al.*, 1994; Burke *et al.*, 2000). Esterification of the alcohol group in (1) with triflic anhydride in the presence of pyridine gave the trifluoromethanesulfonate ester (2), which on treatment with hydroxide gives an open chain epoxide, which upon neutralization gives the title lactone (3). The X-ray crystal analysis of (3) shows that there has been an overall inversion of configuration at atoms C4 and C5 from the starting lactone (1); the absolute configuration of (3) arises from the use of D-glucose as the starting material for the synthesis of the protected lactone (1). The technique of double inversion of the stereochemistry at atoms C4 and C5 of sugar lactones used in this paper appears to be general (Hotchkiss *et al.*, 2004; van Ameijde *et al.*, 2004) and may allow

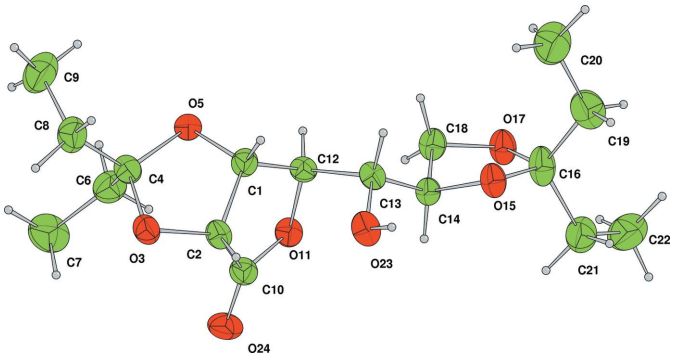


Figure 1
Molecule *A* of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius.

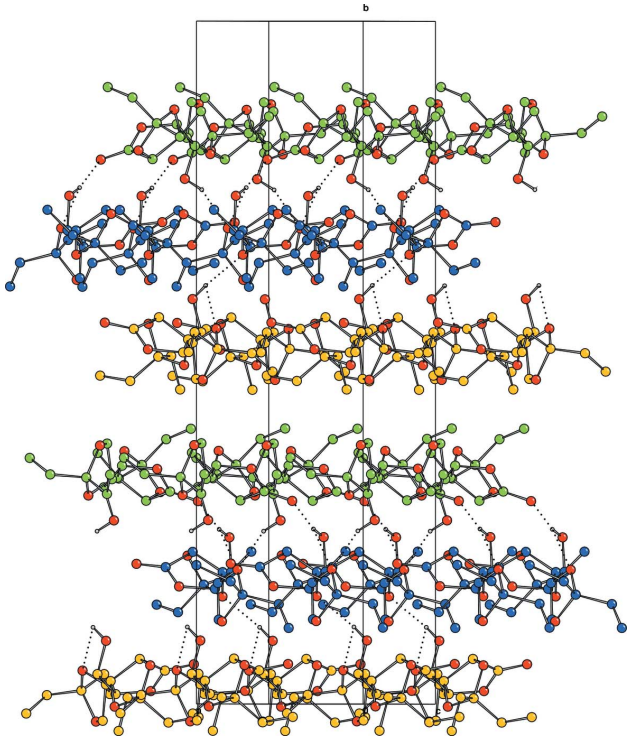


Figure 2
Layers of molecules perpendicular to the *b*-axis direction. The layers are linked by hydrogen bonds in the order molecule *B* (green C atoms) to molecule *C* (blue C atoms) to molecule *A* (orange C atoms). Layers of molecules *A* are not hydrogen-bonded to layers of molecules *B*. Hydrogen bonds are shown as dotted lines.

a considerable increase in the number of carbohydrate lactones available as synthetic intermediates.

There are three independent molecules in the asymmetric unit. The molecules C1–O24 (molecule *A*) and C201–O224 (molecule *B*) are related by an approximately pseudo twofold axis, with a pseudo-symmetry operator of form: 0.17 + *x*, 0.36 − *y*, 1.76 − *z*. On molecular superposition, the r.m.s. positional deviation is 0.90 Å, the r.m.s. bond-length deviation is 0.019 Å, and the r.m.s. torsion-angle deviation is 48.06°. Molecule C101–O124 (molecule *C*) has no rational relationship with the other molecules. The crystal structure consists of

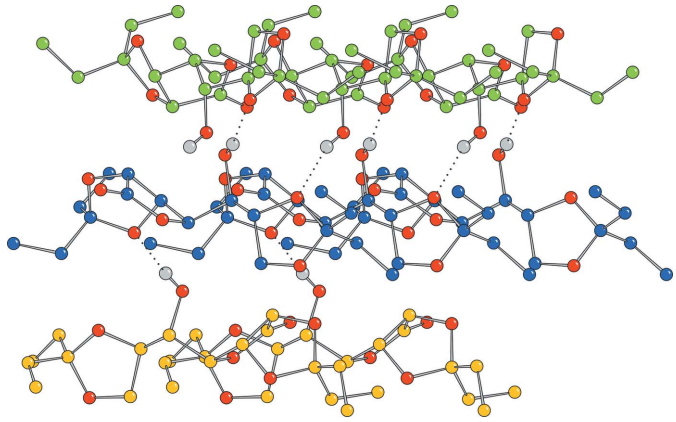


Figure 3
The asymmetric hydrogen-bonding network. Layers of molecules *B* and *C* are bonded by one donor and one acceptor hydrogen bond; layers of molecules *C* and *A* are only linked by one type of bond. H atoms not involved in hydrogen bonding have been omitted. Blue, green and yellow C atoms are as in Fig. 2 and hydrogen bonds are shown as dotted lines.

layers perpendicular to the *b* axis, with each layer composed solely of one type of molecule (Fig. 2). The layers form a type of sandwich, with the filling (molecule *C*) hydrogen-bonded to molecules *A* and *B* below and above it (Fig. 3). There is no hydrogen bonding between the layers *A* and *B*.

Experimental

Diketal (1)(Burke *et al.*, 2000) was converted into (2) by treatment with trifluoromethanesulfonic anhydride (1.3 eq) in the presence of pyridine (2.5 eq). Crude (2) was stirred under basic conditions (KOH, 3 eq) followed by a careful acidic work-up (Amberlyst 15) to produce (3) (Håkansson *et al.*, 2006). The title material was crystallized from heptane to yield fine colourless lath-like crystals with m.p. 366–367 K and $[\alpha]_D^{21} = -28.4$ (c=1.93, $CHCl_3$).

Crystal data

$C_{17}H_{28}O_7$
$M_r = 344.41$
Monoclinic, $P2_1$
$a = 6.7757\ (2)$ Å
$b = 27.7655\ (6)$ Å
$c = 14.8433\ (3)$ Å
$\beta = 101.4341\ (8)^\circ$
$V = 2737.06\ (11)$ Å^3
$Z = 6$
$D_x = 1.254$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 150$ K
Lath, colourless
0.40 × 0.20 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan *DENZO/SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.37$, $T_{max} = 0.99$
16244 measured reflections
4828 independent reflections
4828 reflections with $I > -3\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.113$
$S = 0.97$
4828 reflections
649 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F^2) + (0.05P)^2 + 1.81P]$, where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O223—H2225···O115^{i}	0.82	1.92	2.696 (2)	157
O123—H123···O224	0.83	1.90	2.719 (2)	166
O23—H23···O105^{i}	0.80	1.96	2.738 (2)	162

Symmetry code: (i) $x+1, y, z$.

In the absence of significant anomalous scattering, Friedel pairs were merged and the absolute configuration was assigned from the known configuration of the starting materials.

The H atoms were all located in a difference map, but those attached to C atoms were repositioned geometrically. The 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, O—H = 0.82 Å) and U_{iso}(H) in the range 1.2–1.5 times U_{eq} of the parent atom], after which the positions were refined with riding constraints.

Data collection: *COLLECT* (Nonius, 1997-2001).; 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*.

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Crystal data

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$c = 14.8433\ (3)$ Å
$\beta = 101.4341\ (8)°$
$V = 2737.06\ (11)$ Å^3
$Z = 6$
$F(000) = 1116$
$D_x = 1.254$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4289 reflections
$\theta = 5–25°$
$\mu = 0.10$ mm^{-1}
$T = 150$ K
Lath, colourless
0.40 × 0.20 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
Graphite monochromator
ω scans
Absorption correction: multi-scan DENZO/SCALEPACK; Otwinowski & Minor, 1997)
$T_{min} = 0.37$, $T_{max} = 0.99$
16244 measured reflections
4828 independent reflections
4828 reflections with $I > -3.0\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 25.0°$, $\theta_{min} = 5.1°$
$h = -8\rightarrow8$
$k = -33\rightarrow30$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.113$
$S = 0.97$
4828 reflections
649 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.05P)^2 + 1.81P]$, where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C201	0.8313 (5)	0.33181 (14)	0.8217 (2)	0.0294
C202	0.6660 (5)	0.29794 (14)	0.8383 (2)	0.0302

O203	0.6188 (4)	0.31060 (10)	0.92324 (17)	0.0350
C204	0.7446 (6)	0.35047 (15)	0.9604 (3)	0.0335
O205	0.8167 (4)	0.37046 (10)	0.88458 (17)	0.0323
C206	0.6132 (7)	0.38806 (17)	0.9944 (3)	0.0450
C207	0.4344 (8)	0.4034 (2)	0.9231 (4)	0.0602
C208	0.9150 (6)	0.33053 (17)	1.0332 (3)	0.0426
C209	1.0627 (8)	0.3679 (2)	1.0820 (4)	0.0602
C210	0.4894 (6)	0.31130 (15)	0.7613 (3)	0.0340
O211	0.5422 (4)	0.34438 (10)	0.70516 (17)	0.0310
C212	0.7613 (5)	0.34914 (14)	0.7236 (2)	0.0284
C213	0.8409 (6)	0.31737 (14)	0.6556 (3)	0.0308
C214	0.7491 (6)	0.32936 (14)	0.5568 (2)	0.0318
O215	0.8654 (4)	0.30547 (10)	0.49849 (17)	0.0358
C216	0.8417 (6)	0.33184 (15)	0.4152 (3)	0.0375
O217	0.7673 (4)	0.37868 (10)	0.43336 (17)	0.0374
C218	0.7664 (6)	0.38150 (15)	0.5293 (3)	0.0372
C221	0.6860 (7)	0.30765 (17)	0.3417 (3)	0.0463
C222	0.6278 (9)	0.3360 (2)	0.2527 (3)	0.0620
C219	1.0474 (7)	0.33632 (19)	0.3901 (3)	0.0519
C220	1.2024 (7)	0.3604 (2)	0.4641 (4)	0.0703
O223	0.7884 (4)	0.26900 (10)	0.67432 (19)	0.0383
O224	0.3175 (4)	0.29725 (13)	0.7512 (2)	0.0507
H2011	0.9621	0.3169	0.8323	0.0349*
H2021	0.7016	0.2643	0.8376	0.0348*
H2061	0.6950	0.4159	1.0170	0.0541*
H2062	0.5650	0.3743	1.0458	0.0538*
H2071	0.3674	0.4301	0.9447	0.0896*
H2072	0.4748	0.4118	0.8663	0.0897*
H2073	0.3412	0.3771	0.9115	0.0900*
H2081	0.8508	0.3143	1.0793	0.0496*
H2082	0.9897	0.3077	1.0033	0.0504*
H2091	1.1717	0.3526	1.1235	0.0858*
H2092	0.9968	0.3905	1.1144	0.0860*
H2093	1.1173	0.3851	1.0370	0.0858*
H2121	0.7969	0.3824	0.7175	0.0336*
H2131	0.9869	0.3201	0.6661	0.0358*
H2141	0.6071	0.3189	0.5421	0.0379*
H2181	0.8897	0.3958	0.5626	0.0429*
H2182	0.6521	0.4003	0.5408	0.0430*
H2211	0.5643	0.3026	0.3658	0.0537*
H2212	0.7430	0.2766	0.3296	0.0541*
H2221	0.5210	0.3196	0.2128	0.0891*
H2222	0.5859	0.3682	0.2655	0.0890*
H2223	0.7414	0.3379	0.2231	0.0893*
H2191	1.0321	0.3558	0.3341	0.0640*
H2192	1.0920	0.3041	0.3794	0.0643*
H2201	1.3292	0.3639	0.4438	0.1036*
H2202	1.1556	0.3916	0.4783	0.1038*

H2203	1.2239	0.3413	0.5198	0.1038*
H2225	0.8930	0.2532	0.6815	0.0562*
C1	0.9236 (6)	0.03387 (14)	0.9400 (2)	0.0315
C2	0.7418 (5)	0.06629 (14)	0.9237 (2)	0.0306
O3	0.6392 (4)	0.05689 (10)	0.83259 (17)	0.0352
C4	0.6881 (6)	0.00855 (15)	0.8104 (3)	0.0346
O5	0.8709 (4)	−0.00365 (11)	0.87419 (18)	0.0410
C6	0.5276 (6)	−0.02698 (17)	0.8276 (3)	0.0436
C7	0.3217 (7)	−0.0191 (2)	0.7693 (4)	0.0616
C8	0.7241 (7)	0.00972 (18)	0.7138 (3)	0.0466
C9	0.7602 (9)	−0.0394 (2)	0.6740 (4)	0.0635
C10	0.6215 (5)	0.04923 (14)	0.9944 (3)	0.0314
O11	0.7324 (3)	0.01923 (10)	1.05519 (17)	0.0306
C12	0.9365 (5)	0.01475 (14)	1.0386 (2)	0.0274
C13	1.0763 (5)	0.04417 (14)	1.1096 (2)	0.0280
C14	1.0668 (5)	0.02896 (13)	1.2060 (2)	0.0275
O15	1.2350 (4)	0.04941 (10)	1.26846 (17)	0.0358
C16	1.2767 (7)	0.02018 (16)	1.3488 (3)	0.0428
O17	1.1777 (4)	−0.02533 (10)	1.32302 (18)	0.0371
C18	1.0959 (6)	−0.02409 (14)	1.2270 (3)	0.0338
C19	1.4973 (7)	0.0134 (2)	1.3797 (4)	0.0563
C20	1.5924 (8)	−0.0135 (2)	1.3131 (4)	0.0672
C21	1.1724 (8)	0.04427 (18)	1.4238 (3)	0.0504
C22	1.1742 (9)	0.0151 (2)	1.5077 (4)	0.0714
O23	1.0175 (4)	0.09288 (10)	1.09325 (19)	0.0363
O24	0.4486 (4)	0.05844 (11)	0.9968 (2)	0.0419
C101	0.2944 (6)	0.19339 (15)	1.0398 (3)	0.0338
C102	0.4841 (5)	0.22309 (14)	1.0624 (3)	0.0333
O103	0.5567 (4)	0.21757 (10)	1.15862 (18)	0.0372
C104	0.4728 (7)	0.17508 (17)	1.1889 (3)	0.0447
O105	0.3271 (4)	0.15780 (10)	1.11168 (19)	0.0384
C106	0.6363 (7)	0.13477 (19)	1.2105 (3)	0.0506
C107	0.8008 (9)	0.1459 (2)	1.2925 (4)	0.0720
C108	0.3736 (8)	0.1864 (2)	1.2668 (4)	0.0634
C109	0.2113 (10)	0.2236 (2)	1.2437 (5)	0.0802
C110	0.6212 (6)	0.20074 (15)	1.0046 (3)	0.0337
O111	0.5123 (4)	0.17239 (11)	0.93880 (19)	0.0399
C112	0.3011 (5)	0.16896 (14)	0.9488 (3)	0.0341
C113	0.1680 (6)	0.19372 (14)	0.8680 (3)	0.0368
C114	0.2094 (6)	0.17741 (16)	0.7771 (3)	0.0414
O115	0.0596 (5)	0.19682 (11)	0.7036 (2)	0.0491
C116	−0.0007 (7)	0.16029 (18)	0.6343 (3)	0.0516
O117	0.1341 (6)	0.12115 (13)	0.6613 (2)	0.0625
C118	0.1961 (8)	0.12378 (18)	0.7596 (3)	0.0592
C121	0.0305 (8)	0.1797 (2)	0.5418 (3)	0.0569
C122	0.2377 (10)	0.2034 (3)	0.5465 (5)	0.0895
C119	−0.2182 (8)	0.14645 (19)	0.6341 (4)	0.0584
C120	−0.3106 (10)	0.1115 (2)	0.5590 (4)	0.0741

O123	0.1852 (4)	0.24423 (10)	0.88144 (19)	0.0404
O124	0.7996 (4)	0.20554 (12)	1.0113 (2)	0.0458
H2224	1.0505	0.0497	0.9337	0.0371*
H21	0.7743	0.1005	0.9321	0.0359*
H61	0.5151	−0.0250	0.8917	0.0511*
H62	0.5692	−0.0591	0.8139	0.0509*
H71	0.2286	−0.0416	0.7867	0.0911*
H72	0.2784	0.0137	0.7777	0.0910*
H73	0.3294	−0.0237	0.7048	0.0909*
H81	0.6047	0.0237	0.6745	0.0552*
H82	0.8425	0.0308	0.7125	0.0549*
H91	0.8147	−0.0344	0.6195	0.0951*
H92	0.6361	−0.0574	0.6603	0.0950*
H93	0.8573	−0.0567	0.7197	0.0950*
H121	0.9757	−0.0192	1.0420	0.0315*
H131	1.2146	0.0403	1.0997	0.0313*
H141	0.9404	0.0398	1.2214	0.0315*
H181	1.1920	−0.0374	1.1927	0.0384*
H182	0.9708	−0.0415	1.2149	0.0397*
H191	1.5621	0.0457	1.3905	0.0665*
H192	1.5172	−0.0050	1.4389	0.0665*
H201	1.7343	−0.0161	1.3375	0.1020*
H202	1.5688	0.0031	1.2544	0.1018*
H203	1.5382	−0.0459	1.3054	0.1019*
H211	1.2508	0.0735	1.4422	0.0582*
H212	1.0316	0.0516	1.3933	0.0578*
H1011	0.1701	0.2124	1.0377	0.0390*
H1021	0.4586	0.2571	1.0456	0.0390*
H1061	0.6996	0.1316	1.1568	0.0577*
H1062	0.5706	0.1050	1.2215	0.0581*
H1071	0.9123	0.1231	1.2960	0.1063*
H1072	0.8499	0.1793	1.2892	0.1062*
H1073	0.7430	0.1429	1.3478	0.1061*
H1081	0.4783	0.1984	1.3169	0.0790*
H1082	0.3174	0.1557	1.2850	0.0792*
H1121	0.2646	0.1344	0.9482	0.0401*
H1131	0.0286	0.1846	0.8707	0.0422*
H1141	0.3421	0.1899	0.7719	0.0465*
H1181	0.0891	0.1094	0.7886	0.0643*
H1182	0.3240	0.1070	0.7814	0.0642*
H1211	−0.0724	0.2034	0.5219	0.0650*
H1212	0.0088	0.1529	0.4982	0.0647*
H1221	0.2674	0.2097	0.4845	0.1369*
H1222	0.2487	0.2332	0.5819	0.1372*
H1223	0.3369	0.1804	0.5795	0.1371*
H1191	−0.2980	0.1761	0.6278	0.0659*
H1192	−0.2229	0.1317	0.6952	0.0665*
H1201	−0.4386	0.0973	0.5685	0.1061*

H1202	−0.3348	0.1291	0.5005	0.1063*
H1203	−0.2131	0.0857	0.5559	0.1065*
H221	1.1057	0.0332	1.5492	0.1090*
H222	1.3162	0.0088	1.5368	0.1093*
H223	1.1045	−0.0159	1.4894	0.1089*
H1091	0.1555	0.2304	1.2975	0.1249*
H1092	0.2636	0.2532	1.2221	0.1249*
H1093	0.1037	0.2102	1.1965	0.1249*
H123	0.2275	0.2561	0.8372	0.0610*
H23	1.1028	0.1127	1.1096	0.0520*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C201	0.0293 (18)	0.030 (2)	0.0286 (18)	0.0002 (15)	0.0043 (14)	−0.0047 (16)
C202	0.0317 (19)	0.0247 (19)	0.033 (2)	0.0011 (15)	0.0030 (15)	0.0036 (15)
O203	0.0356 (14)	0.0363 (15)	0.0333 (14)	−0.0021 (12)	0.0071 (11)	0.0028 (12)
C204	0.036 (2)	0.033 (2)	0.033 (2)	−0.0014 (17)	0.0100 (16)	0.0029 (16)
O205	0.0391 (14)	0.0312 (14)	0.0282 (13)	−0.0038 (12)	0.0102 (11)	−0.0029 (11)
C206	0.054 (3)	0.041 (3)	0.044 (2)	0.008 (2)	0.020 (2)	0.002 (2)
C207	0.068 (3)	0.058 (3)	0.058 (3)	0.028 (3)	0.023 (2)	0.008 (3)
C208	0.042 (2)	0.048 (3)	0.036 (2)	−0.001 (2)	0.0034 (17)	0.0014 (19)
C209	0.059 (3)	0.065 (3)	0.053 (3)	−0.015 (3)	0.000 (2)	0.004 (3)
C210	0.032 (2)	0.034 (2)	0.034 (2)	0.0013 (17)	0.0032 (16)	0.0034 (17)
O211	0.0279 (13)	0.0328 (14)	0.0322 (13)	0.0048 (11)	0.0054 (10)	0.0069 (12)
C212	0.0282 (18)	0.0278 (19)	0.0289 (19)	−0.0024 (15)	0.0044 (14)	0.0002 (15)
C213	0.0292 (18)	0.030 (2)	0.0320 (19)	0.0053 (16)	0.0038 (15)	−0.0004 (16)
C214	0.0317 (19)	0.029 (2)	0.033 (2)	0.0042 (16)	0.0039 (15)	−0.0053 (16)
O215	0.0460 (16)	0.0326 (15)	0.0292 (14)	0.0095 (12)	0.0087 (12)	−0.0001 (11)
C216	0.046 (2)	0.031 (2)	0.036 (2)	0.0066 (18)	0.0121 (17)	0.0013 (18)
O217	0.0514 (16)	0.0310 (15)	0.0295 (14)	0.0048 (12)	0.0072 (12)	−0.0002 (11)
C218	0.043 (2)	0.034 (2)	0.034 (2)	0.0019 (17)	0.0056 (17)	−0.0041 (17)
C221	0.063 (3)	0.039 (2)	0.034 (2)	−0.001 (2)	0.0047 (19)	−0.0027 (19)
C222	0.090 (4)	0.051 (3)	0.037 (2)	−0.003 (3)	−0.007 (2)	−0.001 (2)
C219	0.057 (3)	0.053 (3)	0.050 (3)	0.009 (2)	0.022 (2)	0.006 (2)
C220	0.041 (3)	0.095 (5)	0.073 (4)	0.000 (3)	0.006 (2)	0.027 (3)
O223	0.0421 (15)	0.0266 (14)	0.0451 (16)	0.0086 (12)	0.0057 (12)	−0.0004 (12)
O224	0.0279 (15)	0.071 (2)	0.0491 (18)	−0.0086 (14)	−0.0014 (12)	0.0145 (16)
C1	0.0299 (19)	0.037 (2)	0.0280 (19)	−0.0014 (16)	0.0065 (14)	−0.0017 (16)
C2	0.0303 (19)	0.030 (2)	0.0296 (19)	−0.0003 (16)	0.0014 (15)	0.0040 (16)
O3	0.0353 (14)	0.0342 (15)	0.0329 (14)	0.0037 (12)	−0.0010 (11)	0.0020 (12)
C4	0.0313 (19)	0.036 (2)	0.034 (2)	0.0029 (17)	0.0015 (15)	−0.0002 (17)
O5	0.0395 (15)	0.0459 (18)	0.0346 (15)	0.0144 (13)	−0.0002 (12)	−0.0088 (13)
C6	0.044 (2)	0.041 (3)	0.046 (2)	−0.0026 (19)	0.0118 (19)	−0.005 (2)
C7	0.043 (3)	0.058 (3)	0.082 (4)	−0.010 (2)	0.008 (2)	−0.006 (3)
C8	0.046 (2)	0.060 (3)	0.033 (2)	−0.002 (2)	0.0059 (18)	0.000 (2)
C9	0.072 (3)	0.077 (4)	0.044 (3)	−0.005 (3)	0.017 (2)	−0.014 (3)
C10	0.029 (2)	0.031 (2)	0.034 (2)	−0.0007 (16)	0.0053 (15)	−0.0002 (16)

O11	0.0270 (13)	0.0341 (15)	0.0316 (13)	−0.0063 (11)	0.0076 (10)	0.0004 (11)
C12	0.0246 (17)	0.030 (2)	0.0289 (18)	−0.0001 (15)	0.0078 (14)	0.0023 (16)
C13	0.0249 (17)	0.030 (2)	0.0287 (18)	−0.0017 (15)	0.0038 (14)	0.0045 (15)
C14	0.0288 (18)	0.027 (2)	0.0261 (18)	−0.0018 (15)	0.0032 (14)	0.0003 (15)
O15	0.0382 (14)	0.0335 (15)	0.0321 (14)	−0.0073 (12)	−0.0020 (11)	0.0023 (11)
C16	0.055 (3)	0.032 (2)	0.034 (2)	−0.009 (2)	−0.0071 (18)	0.0038 (18)
O17	0.0467 (16)	0.0307 (15)	0.0303 (14)	−0.0035 (12)	−0.0015 (12)	0.0058 (12)
C18	0.040 (2)	0.031 (2)	0.0293 (19)	−0.0039 (17)	0.0046 (16)	0.0021 (16)
C19	0.051 (3)	0.055 (3)	0.058 (3)	−0.002 (2)	−0.001 (2)	0.001 (2)
C20	0.049 (3)	0.094 (4)	0.061 (3)	−0.018 (3)	0.016 (2)	−0.014 (3)
C21	0.057 (3)	0.046 (3)	0.044 (2)	0.003 (2)	0.000 (2)	−0.006 (2)
C22	0.083 (4)	0.082 (4)	0.052 (3)	0.020 (3)	0.021 (3)	−0.006 (3)
O23	0.0392 (15)	0.0247 (14)	0.0413 (15)	−0.0084 (11)	−0.0011 (11)	0.0051 (12)
O24	0.0273 (15)	0.0465 (18)	0.0538 (17)	0.0033 (12)	0.0128 (12)	−0.0025 (14)
C101	0.0287 (19)	0.031 (2)	0.040 (2)	−0.0030 (16)	0.0022 (15)	0.0059 (17)
C102	0.0310 (19)	0.027 (2)	0.040 (2)	−0.0020 (16)	0.0033 (16)	0.0025 (17)
O103	0.0363 (14)	0.0357 (15)	0.0384 (15)	−0.0095 (12)	0.0046 (11)	0.0010 (12)
C104	0.051 (2)	0.042 (2)	0.039 (2)	−0.023 (2)	0.0038 (18)	0.000 (2)
O105	0.0344 (15)	0.0326 (15)	0.0455 (16)	−0.0093 (12)	0.0010 (12)	0.0094 (13)
C106	0.047 (3)	0.053 (3)	0.049 (3)	−0.006 (2)	0.004 (2)	0.000 (2)
C107	0.073 (4)	0.075 (4)	0.058 (3)	0.000 (3)	−0.014 (3)	0.007 (3)
C108	0.066 (3)	0.066 (4)	0.063 (3)	−0.016 (3)	0.026 (3)	−0.014 (3)
C109	0.092 (4)	0.072 (4)	0.087 (4)	−0.005 (3)	0.045 (4)	−0.020 (3)
C110	0.031 (2)	0.034 (2)	0.035 (2)	−0.0019 (17)	0.0029 (16)	0.0065 (17)
O111	0.0297 (14)	0.0423 (17)	0.0453 (16)	0.0046 (12)	0.0019 (12)	−0.0014 (13)
C112	0.0286 (19)	0.025 (2)	0.048 (2)	0.0015 (16)	0.0058 (16)	0.0034 (17)
C113	0.0298 (19)	0.028 (2)	0.049 (2)	−0.0003 (16)	−0.0017 (16)	−0.0012 (18)
C114	0.038 (2)	0.038 (2)	0.043 (2)	0.0120 (19)	−0.0044 (17)	0.0038 (19)
O115	0.0556 (18)	0.0358 (17)	0.0445 (17)	0.0155 (14)	−0.0175 (13)	−0.0094 (13)
C116	0.057 (3)	0.043 (3)	0.048 (3)	0.017 (2)	−0.007 (2)	−0.011 (2)
O117	0.075 (2)	0.052 (2)	0.0487 (19)	0.0295 (18)	−0.0171 (16)	−0.0162 (16)
C118	0.065 (3)	0.044 (3)	0.056 (3)	0.019 (2)	−0.017 (2)	−0.014 (2)
C121	0.058 (3)	0.057 (3)	0.050 (3)	0.014 (2)	−0.003 (2)	−0.011 (2)
C122	0.074 (4)	0.118 (6)	0.078 (4)	0.017 (4)	0.020 (3)	0.006 (4)
C119	0.055 (3)	0.048 (3)	0.063 (3)	0.003 (2)	−0.011 (2)	−0.004 (2)
C120	0.087 (4)	0.062 (4)	0.061 (3)	−0.013 (3)	−0.017 (3)	−0.001 (3)
O123	0.0478 (16)	0.0291 (15)	0.0450 (16)	0.0030 (13)	0.0109 (13)	0.0023 (12)
O124	0.0264 (15)	0.0537 (19)	0.0572 (19)	−0.0043 (13)	0.0080 (12)	0.0059 (15)

Geometric parameters (Å, º)

C201—C202	1.519 (5)	C12—H121	0.978
C201—O205	1.439 (4)	C13—C14	1.506 (5)
C201—C212	1.517 (5)	C13—O23	1.417 (5)
C201—H2011	0.963	C13—H131	0.982
C202—O203	1.406 (5)	C14—O15	1.436 (4)
C202—C210	1.527 (5)	C14—C18	1.510 (5)
C202—H2021	0.965	C14—H141	0.977

O203—C204	1.439 (5)	O15—C16	1.424 (5)
C204—O205	1.425 (5)	C16—O17	1.446 (5)
C204—C206	1.521 (6)	C16—C19	1.485 (6)
C204—C208	1.521 (6)	C16—C21	1.581 (7)
C206—C207	1.503 (7)	O17—C18	1.424 (4)
C206—H2061	0.971	C18—H181	0.975
C206—H2062	0.966	C18—H182	0.961
C207—H2071	0.957	C19—C20	1.484 (8)
C207—H2072	0.966	C19—H191	0.997
C207—H2073	0.957	C19—H192	1.003
C208—C209	1.522 (6)	C20—H201	0.960
C208—H2081	0.990	C20—H202	0.970
C208—H2082	0.971	C20—H203	0.971
C209—H2091	0.962	C21—C22	1.483 (8)
C209—H2092	0.952	C21—H211	0.979
C209—H2093	0.954	C21—H212	0.992
C210—O211	1.336 (5)	C22—H221	0.980
C210—O224	1.209 (5)	C22—H222	0.989
O211—C212	1.461 (4)	C22—H223	0.993
C212—C213	1.518 (5)	O23—H23	0.801
C212—H2121	0.964	C101—C102	1.508 (5)
C213—C214	1.513 (5)	C101—O105	1.439 (5)
C213—O223	1.431 (5)	C101—C112	1.520 (6)
C213—H2131	0.974	C101—H1011	0.989
C214—O215	1.443 (4)	C102—O103	1.424 (5)
C214—C218	1.515 (6)	C102—C110	1.517 (6)
C214—H2141	0.988	C102—H1021	0.984
O215—C216	1.419 (5)	O103—C104	1.420 (5)
C216—O217	1.440 (5)	C104—O105	1.439 (5)
C216—C221	1.515 (6)	C104—C106	1.563 (7)
C216—C219	1.518 (6)	C104—C108	1.482 (7)
O217—C218	1.427 (5)	C106—C107	1.510 (7)
C218—H2181	0.968	C106—H1061	0.981
C218—H2182	0.977	C106—H1062	0.968
C221—C222	1.521 (6)	C107—H1071	0.979
C221—H2211	0.972	C107—H1072	0.991
C221—H2212	0.976	C107—H1073	0.981
C222—H2221	0.955	C108—C109	1.498 (9)
C222—H2222	0.969	C108—H1081	0.978
C222—H2223	0.961	C108—H1082	0.992
C219—C220	1.517 (8)	C109—H1091	0.967
C219—H2191	0.980	C109—H1092	0.974
C219—H2192	0.967	C109—H1093	0.979
C220—H2201	0.970	C110—O111	1.353 (5)
C220—H2202	0.960	C110—O124	1.200 (5)
C220—H2203	0.970	O111—C112	1.471 (5)
O223—H2225	0.823	C112—C113	1.515 (5)
C1—C2	1.506 (5)	C112—H1121	0.990

C1—O5	1.425 (5)	C113—C114	1.500 (6)
C1—C12	1.542 (5)	C113—O123	1.418 (5)
C1—H2224	0.986	C113—H1131	0.987
C2—O3	1.417 (4)	C114—O115	1.440 (5)
C2—C10	1.526 (5)	C114—C118	1.511 (7)
C2—H21	0.978	C114—H1141	0.982
O3—C4	1.436 (5)	O115—C116	1.445 (5)
C4—O5	1.442 (4)	C116—O117	1.425 (5)
C4—C6	1.527 (6)	C116—C121	1.528 (7)
C4—C8	1.502 (6)	C116—C119	1.522 (7)
C6—C7	1.505 (7)	O117—C118	1.438 (6)
C6—H61	0.973	C118—H1181	0.997
C6—H62	0.969	C118—H1182	0.980
C7—H71	0.958	C121—C122	1.540 (9)
C7—H72	0.973	C121—H1211	0.963
C7—H73	0.976	C121—H1212	0.977
C8—C9	1.525 (7)	C122—H1221	0.995
C8—H81	0.980	C122—H1222	0.976
C8—H82	0.996	C122—H1223	0.985
C9—H91	0.964	C119—C120	1.516 (7)
C9—H92	0.964	C119—H1191	0.980
C9—H93	0.974	C119—H1192	1.002
C10—O11	1.343 (5)	C120—H1201	0.989
C10—O24	1.206 (4)	C120—H1202	0.981
O11—C12	1.457 (4)	C120—H1203	0.983
C12—C13	1.510 (5)	O123—H123	0.835

C202—C201—O205	102.0 (3)	C13—C12—H121	111.0
C202—C201—C212	104.6 (3)	C12—C13—C14	111.9 (3)
O205—C201—C212	109.7 (3)	C12—C13—O23	106.3 (3)
C202—C201—H2011	113.0	C14—C13—O23	111.5 (3)
O205—C201—H2011	113.3	C12—C13—H131	108.8
C212—C201—H2011	113.4	C14—C13—H131	109.4
C201—C202—O203	107.3 (3)	O23—C13—H131	108.9
C201—C202—C210	102.8 (3)	C13—C14—O15	108.9 (3)
O203—C202—C210	109.0 (3)	C13—C14—C18	116.2 (3)
C201—C202—H2021	113.8	O15—C14—C18	101.4 (3)
O203—C202—H2021	110.7	C13—C14—H141	109.9
C210—C202—H2021	112.8	O15—C14—H141	110.3
C202—O203—C204	108.3 (3)	C18—C14—H141	109.7
O203—C204—O205	105.5 (3)	C14—O15—C16	108.4 (3)
O203—C204—C206	108.3 (3)	O15—C16—O17	105.8 (3)
O205—C204—C206	108.0 (3)	O15—C16—C19	110.5 (4)
O203—C204—C208	107.5 (3)	O17—C16—C19	110.9 (4)
O205—C204—C208	111.8 (3)	O15—C16—C21	107.8 (3)
C206—C204—C208	115.2 (3)	O17—C16—C21	107.9 (4)
C201—O205—C204	107.5 (3)	C19—C16—C21	113.5 (4)
C204—C206—C207	113.8 (4)	C16—O17—C18	108.2 (3)

C204—C206—H2061	109.2	C14—C18—O17	103.8 (3)
C207—C206—H2061	110.1	C14—C18—H181	109.6
C204—C206—H2062	107.7	O17—C18—H181	110.2
C207—C206—H2062	108.3	C14—C18—H182	112.3
H2061—C206—H2062	107.4	O17—C18—H182	109.2
C206—C207—H2071	110.7	H181—C18—H182	111.5
C206—C207—H2072	110.7	C16—C19—C20	113.7 (4)
H2071—C207—H2072	109.8	C16—C19—H191	108.7
C206—C207—H2073	108.9	C20—C19—H191	108.9
H2071—C207—H2073	108.1	C16—C19—H192	106.7
H2072—C207—H2073	108.5	C20—C19—H192	109.1
C204—C208—C209	115.1 (4)	H191—C19—H192	109.7
C204—C208—H2081	106.4	C19—C20—H201	108.7
C209—C208—H2081	108.6	C19—C20—H202	110.0
C204—C208—H2082	107.7	H201—C20—H202	110.4
C209—C208—H2082	108.1	C19—C20—H203	110.0
H2081—C208—H2082	111.0	H201—C20—H203	107.5
C208—C209—H2091	110.6	H202—C20—H203	110.1
C208—C209—H2092	111.1	C16—C21—C22	115.4 (4)
H2091—C209—H2092	110.2	C16—C21—H211	104.7
C208—C209—H2093	108.5	C22—C21—H211	107.7
H2091—C209—H2093	108.3	C16—C21—H212	106.8
H2092—C209—H2093	108.2	C22—C21—H212	110.0
C202—C210—O211	111.5 (3)	H211—C21—H212	112.2
C202—C210—O224	127.4 (4)	C21—C22—H221	108.8
O211—C210—O224	121.0 (3)	C21—C22—H222	108.0
C210—O211—C212	109.5 (3)	H221—C22—H222	111.0
C201—C212—O211	105.3 (3)	C21—C22—H223	108.6
C201—C212—C213	111.6 (3)	H221—C22—H223	110.9
O211—C212—C213	107.7 (3)	H222—C22—H223	109.5
C201—C212—H2121	111.0	C13—O23—H23	116.3
O211—C212—H2121	109.5	C102—C101—O105	102.2 (3)
C213—C212—H2121	111.4	C102—C101—C112	105.5 (3)
C212—C213—C214	112.6 (3)	O105—C101—C112	109.0 (3)
C212—C213—O223	106.4 (3)	C102—C101—H1011	113.5
C214—C213—O223	108.9 (3)	O105—C101—H1011	113.2
C212—C213—H2131	109.4	C112—C101—H1011	112.7
C214—C213—H2131	110.3	C101—C102—O103	105.9 (3)
O223—C213—H2131	109.0	C101—C102—C110	104.0 (3)
C213—C214—O215	108.2 (3)	O103—C102—C110	113.2 (3)
C213—C214—C218	115.7 (3)	C101—C102—H1021	111.7
O215—C214—C218	101.3 (3)	O103—C102—H1021	111.4
C213—C214—H2141	110.2	C110—C102—H1021	110.3
O215—C214—H2141	110.8	C102—O103—C104	109.0 (3)
C218—C214—H2141	110.3	O103—C104—O105	106.2 (3)
C214—O215—C216	107.7 (3)	O103—C104—C106	110.4 (4)
O215—C216—O217	106.6 (3)	O105—C104—C106	105.7 (4)
O215—C216—C221	109.9 (3)	O103—C104—C108	110.0 (4)

O217—C216—C221	108.4 (3)	O105—C104—C108	110.3 (4)
O215—C216—C219	107.8 (3)	C106—C104—C108	113.9 (4)
O217—C216—C219	110.2 (4)	C101—O105—C104	110.0 (3)
C221—C216—C219	113.7 (4)	C104—C106—C107	113.5 (4)
C216—O217—C218	107.9 (3)	C104—C106—H1061	107.7
C214—C218—O217	103.5 (3)	C107—C106—H1061	107.6
C214—C218—H2181	111.1	C104—C106—H1062	108.4
O217—C218—H2181	111.0	C107—C106—H1062	109.2
C214—C218—H2182	110.9	H1061—C106—H1062	110.5
O217—C218—H2182	111.4	C106—C107—H1071	110.4
H2181—C218—H2182	108.9	C106—C107—H1072	110.7
C216—C221—C222	114.8 (4)	H1071—C107—H1072	110.2
C216—C221—H2211	108.6	C106—C107—H1073	107.7
C222—C221—H2211	107.5	H1071—C107—H1073	109.5
C216—C221—H2212	106.3	H1072—C107—H1073	108.2
C222—C221—H2212	109.9	C104—C108—C109	113.1 (5)
H2211—C221—H2212	109.8	C104—C108—H1081	107.0
C221—C222—H2221	109.1	C109—C108—H1081	109.2
C221—C222—H2222	110.1	C104—C108—H1082	106.8
H2221—C222—H2222	110.2	C109—C108—H1082	110.5
C221—C222—H2223	109.5	H1081—C108—H1082	110.1
H2221—C222—H2223	108.7	C108—C109—H1091	109.6
H2222—C222—H2223	109.2	C108—C109—H1092	111.0
C216—C219—C220	113.3 (4)	H1091—C109—H1092	109.4
C216—C219—H2191	107.8	C108—C109—H1093	108.1
C220—C219—H2191	108.2	H1091—C109—H1093	107.9
C216—C219—H2192	107.2	H1092—C109—H1093	110.7
C220—C219—H2192	109.5	C102—C110—O111	109.8 (3)
H2191—C219—H2192	110.9	C102—C110—O124	128.8 (4)
C219—C220—H2201	110.3	O111—C110—O124	121.4 (4)
C219—C220—H2202	110.2	C110—O111—C112	111.5 (3)
H2201—C220—H2202	109.4	C101—C112—O111	105.2 (3)
C219—C220—H2203	110.0	C101—C112—C113	112.5 (3)
H2201—C220—H2203	109.0	O111—C112—C113	109.2 (3)
H2202—C220—H2203	107.9	C101—C112—H1121	112.8
C213—O223—H2225	106.5	O111—C112—H1121	108.0
C2—C1—O5	103.9 (3)	C113—C112—H1121	108.9
C2—C1—C12	104.4 (3)	C112—C113—C114	112.7 (3)
O5—C1—C12	111.0 (3)	C112—C113—O123	108.5 (3)
C2—C1—H2224	114.8	C114—C113—O123	113.6 (4)
O5—C1—H2224	111.4	C112—C113—H1131	106.0
C12—C1—H2224	110.9	C114—C113—H1131	108.1
C1—C2—O3	105.9 (3)	O123—C113—H1131	107.5
C1—C2—C10	103.6 (3)	C113—C114—O115	109.8 (3)
O3—C2—C10	111.8 (3)	C113—C114—C118	115.9 (4)
C1—C2—H21	113.8	O115—C114—C118	103.3 (3)
O3—C2—H21	110.9	C113—C114—H1141	107.6
C10—C2—H21	110.6	O115—C114—H1141	109.1

C2—O3—C4	107.4 (3)	C118—C114—H1141	111.0
O3—C4—O5	106.0 (3)	C114—O115—C116	109.5 (3)
O3—C4—C6	111.2 (3)	O115—C116—O117	105.1 (3)
O5—C4—C6	106.6 (3)	O115—C116—C121	108.8 (4)
O3—C4—C8	106.7 (3)	O117—C116—C121	109.0 (4)
O5—C4—C8	110.5 (3)	O115—C116—C119	108.4 (4)
C6—C4—C8	115.4 (4)	O117—C116—C119	112.0 (4)
C4—O5—C1	110.2 (3)	C121—C116—C119	113.2 (4)
C4—C6—C7	114.8 (4)	C116—O117—C118	106.8 (3)
C4—C6—H61	109.3	C114—C118—O117	102.7 (4)
C7—C6—H61	107.7	C114—C118—H1181	110.2
C4—C6—H62	108.2	O117—C118—H1181	109.1
C7—C6—H62	106.7	C114—C118—H1182	113.2
H61—C6—H62	110.0	O117—C118—H1182	111.8
C6—C7—H71	109.5	H1181—C118—H1182	109.7
C6—C7—H72	109.3	C116—C121—C122	113.4 (4)
H71—C7—H72	110.1	C116—C121—H1211	107.3
C6—C7—H73	108.7	C122—C121—H1211	108.6
H71—C7—H73	110.2	C116—C121—H1212	107.3
H72—C7—H73	108.9	C122—C121—H1212	111.8
C4—C8—C9	114.8 (4)	H1211—C121—H1212	108.2
C4—C8—H81	107.9	C121—C122—H1221	112.6
C9—C8—H81	107.5	C121—C122—H1222	111.0
C4—C8—H82	108.4	H1221—C122—H1222	109.9
C9—C8—H82	109.0	C121—C122—H1223	105.7
H81—C8—H82	109.1	H1221—C122—H1223	109.4
C8—C9—H91	108.4	H1222—C122—H1223	108.1
C8—C9—H92	110.2	C116—C119—C120	114.9 (5)
H91—C9—H92	111.1	C116—C119—H1191	107.7
C8—C9—H93	108.1	C120—C119—H1191	109.2
H91—C9—H93	109.7	C116—C119—H1192	107.8
H92—C9—H93	109.4	C120—C119—H1192	108.8
C2—C10—O11	110.5 (3)	H1191—C119—H1192	108.3
C2—C10—O24	127.5 (3)	C119—C120—H1201	113.4
O11—C10—O24	121.9 (3)	C119—C120—H1202	107.7
C10—O11—C12	111.2 (3)	H1201—C120—H1202	109.2
C1—C12—O11	104.7 (3)	C119—C120—H1203	108.6
C1—C12—C13	112.7 (3)	H1201—C120—H1203	109.3
O11—C12—C13	108.7 (3)	H1202—C120—H1203	108.5
C1—C12—H121	110.2	C113—O123—H123	108.1
O11—C12—H121	109.3		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O223—H2225···O115^{i}	0.82	1.92	2.696 (2)	157

O123—H123···O224	0.83	1.90	2.719 (2)	166
O23—H23···O105^{i}	0.80	1.96	2.738 (2)	162

Symmetry code: (i) $x+1, y, z$.