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Crystal and molecular structures of datiscetin and its monohydrate isolated from *Datisca cannabina* L.

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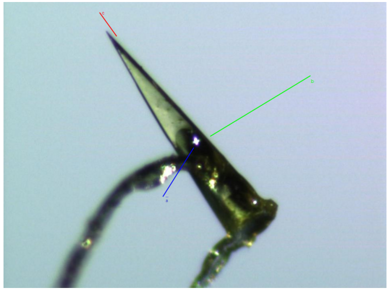
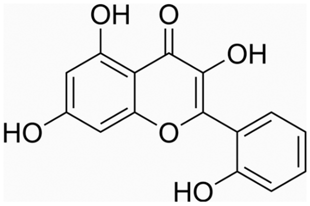
The crystal structures of the flavonoid datiscetin [3,5,7-trihydroxy-2-(2-hydroxyphenyl)chromen-4-one], $C_{15}H_{10}O_6$, and its monohydrate, $C_{15}H_{10}O_6{\cdot}H_2O$, were determined by single-crystal X-ray diffraction analysis. The flavonoid was isolated from the ethyl acetate fraction of *Datisca cannabina* L. collected in Tashkent region, Uzbekistan. In both structures, the chromenone ring system and the phenyl ring form nearly the same dihedral angles (38.3 and 38.7° for the anhydrate and monohydrate, respectively). In addition, in both structures, the molecules stack through π–π interactions along the shortest translation axis of the unit cell [3.7601 (1) and 3.9274 (5) Å, respectively], resulting in the formation of needle-shaped single crystals.

1. Chemical context

Datisca cannabina L. (commonly known as false hemp) is a shrub of the family Datiscaceae that resembles hemp (*Cannabis sativa* L.) in many aspects, including its general morphology and the arrangement of its leaves. It is a robust single genus of perennial plant that reaches up to 1–2 m in height and is predominantly found in riparian environments (Holmes & Blizzard, 2010; Bohmer *et al.*, 2002). The family Datiscaceae includes three genera and four species, the genus Datisca consists of two species: *D. glomerata* (Presl) Baill., found in California, and *D. cannabina* L., which grows in the area from southwest Asia to Crete (Christopher, 1973). The aerial parts of the plant are rich in biologically active compounds, including flavonoids (17%), tannins (2.9%), coumarins (0.9–1.5%) and alkaloids (0.31%). *Datisca cannabina* L. is used as a medicinal raw material in the production of Datiscan, a preparation containing a complex of flavonoids. This formulation is recommended as part of combination therapy for digestive disorders, including gastric ailments, scrofulous conditions and gastrointestinal diseases accompanied by smooth muscle spasms. In traditional medicine, infusions and decoctions prepared from the aerial parts of the plant are employed as diuretics, expectorants and laxatives. Moreover, the plant has been reported to exhibit a range of biological activities, such as antioxidant, anti-inflammatory, antibacterial and anticarcinogenic properties (Ahmad *et al.*, 2008). Additionally, the roots are used for obtaining a yellow dye for colouring wool and silk, while the stems provide bast fiber suitable for netting (Muhammed *et al.*, 2012). In this work, we report the crystal structures of datiscetin (**I**) and its monohydrate (**II**) isolated from *Datisca cannabina* L.



https://doi.org/10.1107/S2056989026004056



I

II = **I**·H_2O

2. Structural commentary

Solvent (hydrate)-free crystals (**I**) of datiscetin were obtained from a chloroform–methanol (7:3 *v*/*v*) mixture. The molecular structure of datiscetin is shown in Fig. 1. The chromenone ring system and the phenyl ring are planar, with r.m.s. deviations of 0.008 and 0.005 Å, respectively, and the dihedral angle between them is 38.3°. The torsion angle between these two rings is stabilized by an intramolecular O6—H6⋯O2 hydrogen bond formed between the hydroxyl group of the phenyl ring and the hydroxyl group located at position 3 [2.625 (2) Å and 155 (3)°]. The hydroxyl group at position 5 in the molecule also forms an intramolecular O4—H4⋯O3 hydrogen bond with the carbonyl group [2.631 (2) Å and 155 (3)°] Table 1.

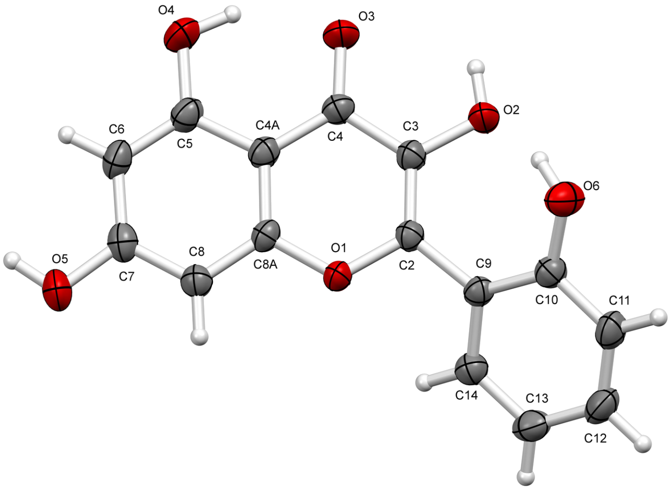


Figure 1
The molecular structure of **I**. Displacement ellipsoids are drawn at the 50% probability level.

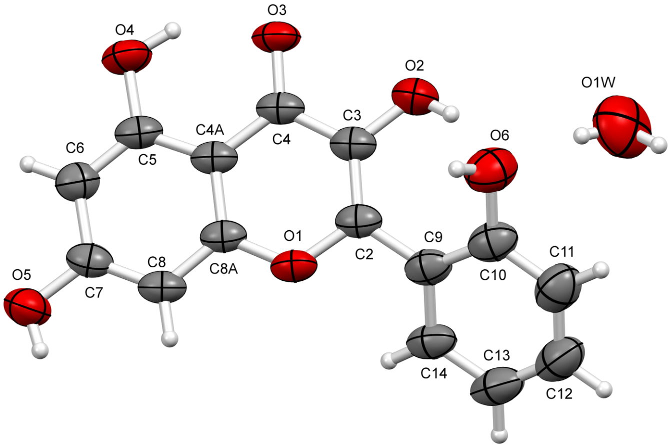


Figure 2
The molecular structure of **II**. Displacement ellipsoids are drawn at the 50% probability level

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O2—H2⋯O3^{i}	0.85 (3)	1.85 (3)	2.6094 (18)	147 (3)
O4—H4⋯O3	0.91 (3)	1.78 (3)	2.631 (2)	155 (3)
O5—H5⋯O6^{ii}	0.91 (4)	1.98 (4)	2.7778 (19)	146 (3)
O6—H6⋯O2	0.89 (3)	1.79 (3)	2.6253 (19)	155 (3)

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

Table 2
Hydrogen-bond geometry (Å, °) for **II**.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O2—H2⋯O6	0.82	1.85	2.609 (3)	153
O4—H4⋯O3	0.82	1.91	2.639 (3)	147
O5—H5⋯O3^{i}	0.82	2.00	2.803 (3)	166
O1*W*—H1*WB*⋯O5^{ii}	0.85	2.76	3.281 (5)	121
O1*W*—H1*WB*⋯O5^{iii}	0.85	2.28	2.934 (4)	134

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

Datiscetin monohydrate crystals (**II**) were obtained from methanol at room temperature and crystallize in the orthorhombic space group *Pna*2_1. The asymmetric unit consists of one flavonoid molecule and one water molecule (Fig. 2). The chromenone ring system and the phenyl ring are planar, with r.m.s. deviations of 0.015 and 0.004 Å, respectively, and the dihedral angle between them is 38.7°, which is the same as that observed in crystal form **I**, and is stabilized by an intramolecular O2—H2⋯O6 hydrogen bond formed between the hydroxyl group of the phenyl ring and the hydroxyl group located at position 3 [2.609 (3) Å and 153°; Table 2].

3. Supramolecular features

The crystal of **I** possesses an inversion centre, therefore, the crystals contain 'left' and 'right' molecules with respect to the orientation of the chromenone and phenyl rings. In crystal

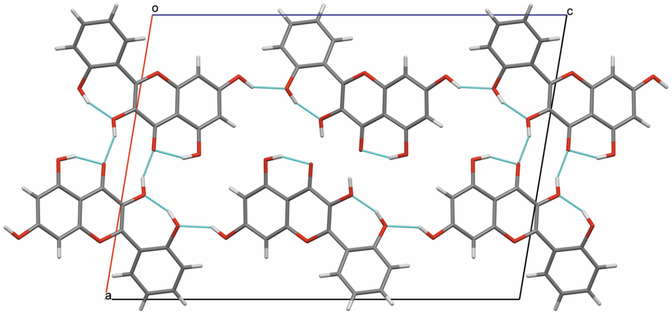


Figure 3
Packing of molecules of **I**, viewed along the *b* axis, showing the formation of a hydrogen-bonded macrocycle consisting of six molecules.

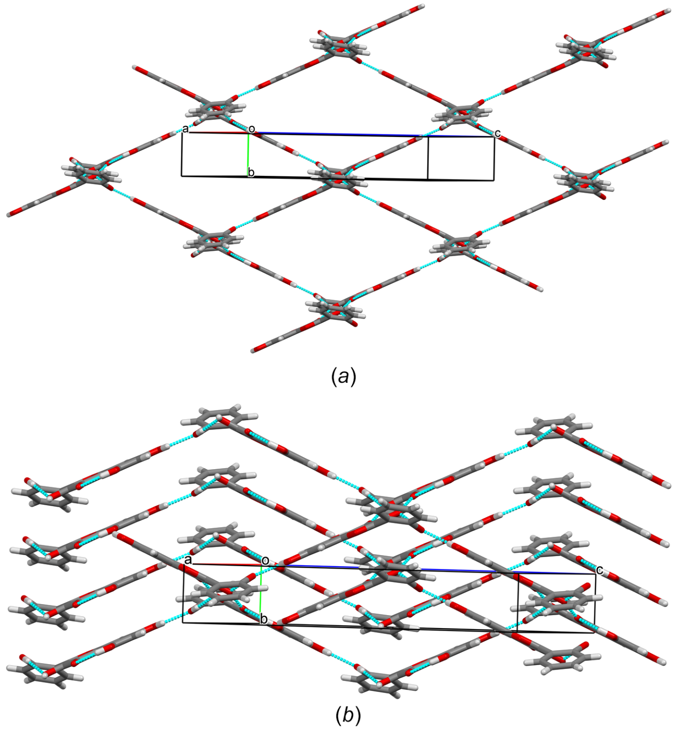


Figure 4
(*a*) Formation of a hydrogen-bonded network, where the hydrogen-bonded rings consist of six molecules of datiscetin. (*b*) Translation (stacking) of the network along the *b* axis. In both cases, the packing is shown along the [40$\overline{1}$] direction.

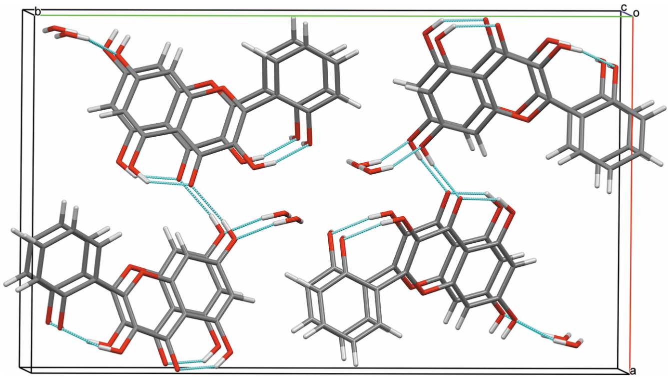


Figure 6
Packing of molecules and hydrogen bonding in **II**.

form **I**, the 'left' and 'right' molecules related by the inversion centre form hydrogen-bonded dimers through the hydroxyl at position 3 and carbonyl groups [0.85 (3), 1.86 (3), 2.6094 (19) Å and 147 (3)°]. The dimers are connected by hydrogen bonds *via* the hydroxyl groups at position 7 and on the phenyl ring, leading to the formation of a two-dimensional supramolecular network in the crystal (Table 1, Fig. 3). The supramolecules formed from 'supercells' [Fig. 4(*a*)] are further packed along the *b* axis through π–π stacking interactions, with centroid-to-centroid distances equal to the unit-cell translation along the *b* axis [3.7601 (1) Å], with a slippage of 1.59 Å [Fig. 4(*b*)]. This particular stacking corresponds to the preferential growth direction during crystallization, leading to the formation of needle-shaped single crystals (Fig. 5).

Packing analysis of the crystal structure of **II** shows that flavonoid molecules related by glide-plane symmetry are connected through an O5—H5$\cdots$O3^{i} hydrogen bond [O5$\cdots$O3^{i} = 2.803 (3) Å and 166°; symmetry code: (i) $x - \frac{1}{2}$, $-y + \frac{3}{2}$, $z + 1$]. Water molecules bridge flavonoid molecules stacked along the *c* axis [O1*W*$\cdots$ O5^{ii} = 3.281 (5) Å and O1*W*$\cdots$ O5^{iii} = 2.934 (4) Å; symmetry codes: (ii) $-x + \frac{1}{2}$, $y - \frac{1}{2}$, $z - \frac{3}{2}$; (iii) $-x + \frac{1}{2}$, $y - \frac{1}{2}$, $z - \frac{1}{2}$] (Table 2, Fig. 6). It should be noted that, due to the difficulty of experimentally determining the coordinates of hydrogen atoms in water molecules, the observed other short Ow$\cdots$O distances may indicate the possible presence of alternative hydrogen bonds, not taken into account in the table

The stacking of molecules along the *c* axis corresponds to the preferential growth direction during crystallization, resulting in the formation of conical-needle-shaped single crystals along this axis (Fig. 7).

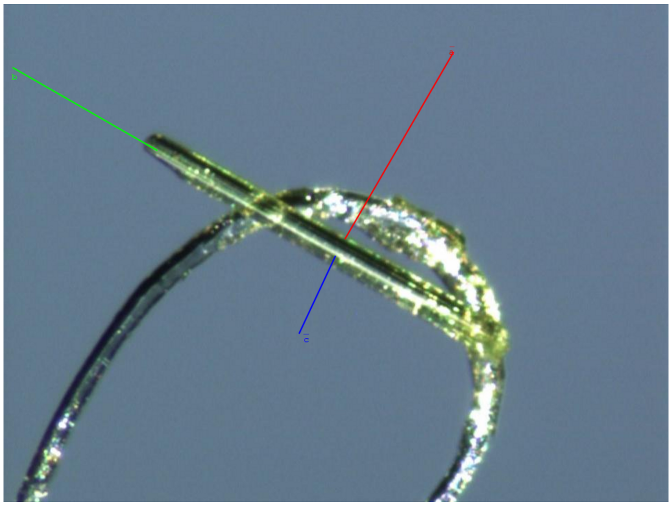


Figure 5
Single crystal of **I** exhibiting a needle-like morphology.

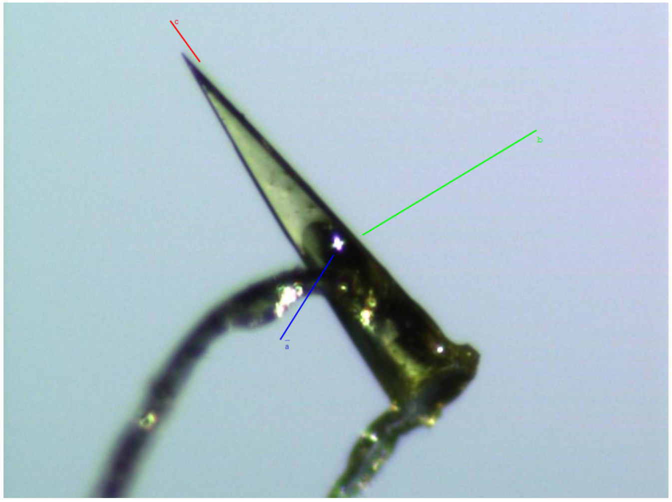


Figure 7
Single crystal of **II** exhibiting a conical-needle-shaped morphology.

Table 3
Experimental details.

For all structures: $Z = 4$. Experiments were carried out with Cu $K\alpha$ radiation using a Bruker D8 VENTURE dual wavelength Mo/Cu diffractometer. Absorption was corrected for by multi-scan methods, (*SADABS2016*; Krause *et al.*, 2015). H atoms were treated by a mixture of independent and constrained refinement.

	I	**II**
Crystal data		
Chemical formula	$C_{15}H_{10}O_6$	$C_{15}H_{10}O_6 \cdot H_2O$
M_r	286.23	304.25
Crystal system, space group	Monoclinic, $P2_1/c$	Orthorhombic, $Pna2_1$
Temperature (K)	293	291
a, b, c (Å)	15.0296 (5), 3.7601 (1), 21.6148 (7)	14.0628 (15), 23.714 (3), 3.9274 (5)
α, β, γ (°)	90, 99.453 (2), 90	90, 90, 90
V (Å^3)	1204.93 (6)	1309.7 (3)
μ (mm^{-1})	1.06	1.06
Crystal size (mm)	0.50 × 0.08 × 0.05	0.65 × 0.14 × 0.07
Data collection		
$T_{\min}, T_{\max}$	0.592, 0.753	0.66, 0.93
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26195, 2220, 2026	8711, 2305, 2142
R_{int}	0.052	0.038
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.603	0.602
Refinement		
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.046, 0.141, 1.17	0.043, 0.116, 0.93
No. of reflections	2220	2305
No. of parameters	199	207
No. of restraints	0	1
$\Delta\rho_{\max}, \Delta\rho_{\min}$ (e Å^{-3})	0.39, −0.37	0.25, −0.21
Absolute structure	–	Flack x determined using 811 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	–	0.25 (10)

Computer programs: *APEX5* (Bruker, 2023), *SAINT* (Bruker, 2019), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *Mercury* (Macrae *et al.*, 2020) and *publCIF* (Westrip, 2010).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.41, including the update of January 2020; Groom *et al.*, 2016) for flavonoids with a 2-phenyl substituent yields more than 1400 hits.

5. Isolation and crystallization

5.1. Plant material

The above-ground parts (leaves, flowers and stems) of *Datisca cannabina* L. were collected in the Tashkent region, Uzbekistan, in October 2024, during the seed-bearing period. The species identification was confirmed by comparing the collected specimen with herbarium material of *Datisca cannabina* L. preserved at the Central Herbarium of Uzbekistan. The taxonomic identification was carried out by A. M. Nigmatullaev, Senior Researcher at the Laboratory of Biology of Medicinal and Technical Plants, S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan.

5.2. Extraction and isolation

The freshly collected air-dried powdered plant material (3.0 kg) was extracted ten times by percolation with 75% ethanol. The combined concentrated viscous extract was consecutively partitioned with solvents of increasing polarity between chloroform, ethyl acetate and *n*-butanol. The ethyl acetate fraction was adsorbed onto silica gel (1:1 *v*/*v*, 99 g) and subjected to column chromatography (165 × 4.5 cm) with stepwise elution using chloroform and chloroform–methanol mixtures (9:1, 8:2 and 7:3 *v*/*v*). The obtained mixture of flavonoids was further separated into individual compounds by molecular weight using a Sephadex LH-20 column with methanol as the eluent, yielding 14.3 g of datiscetin.

5.3. NMR spectroscopy

NMR spectra were recorded on a JNM-ECZ600R spectrometer (JEOL, Japan) operating at 600 MHz for ^{1}H and 150 MHz for ^{13}C, using DMSO-d_6 (Cambridge Isotope Laboratories, Inc., USA) as solvent. Tetramethylsilane (TMS, 0 ppm) served as the internal standard for ^{1}H NMR and ^{13}C NMR, the residual solvent signal of DMSO-d_6 (39.52 ppm relative to TMS) was used. Spectral data were processed with *MestReNova* software (Version 14.2.0; Mestrelab Research S.L., Santiago de Compostela, Spain).

^{1}H NMR (600 MHz, CD_3OD, ppm δ, J/Hz): 7.55 (1H, *dd*, J = 7.8, 1.7, H-6′), 7.37 (1H, *ddd*, J = 8.3, 7.3, 1.7, H-4′), 7.00 (1H, *ddd*, J = 7.8, 7.3, 1.0, H-5′), 6.98 (1H, *dd*, J = 8.3, 1.0, H-3′), 6.34 (1H, *d*, J = 2.1, H-8), 6.19 (1H, *d*, J = 2.1, H-6).

^{13}C NMR (150 MHz, CD_3OD, ppm. δ): 149.09 (C-2), 137.76 (C-3), 177.98 (C-4), 162.88 (C-5), 99.34 (C-6), 165.74 (C-7), 94.62 (C-8), 159.16 (C-9), 105.22 (C-10), 119.89 (C-1′), 156.37 (C-2′), 118.13 (C-3′), 132.93 (C-4′), 120.90 (C-5′), 131.35 (C-6′).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. For **I** and **II**, the H atoms bonded to C atoms were placed in calculated positions and refined to ride on their parent atoms: C—H = 0.93 Å with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic H atoms. Hydroxyl H atoms in **I** were located using electron-density difference maps, and were refined freely. For **II**, H atoms of the hydroxyl groups and water molecule were placed in calculated positions.

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supporting information

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Crystal and molecular structures of datiscetin and its monohydrate isolated from *Datisca cannabina* L.

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Computing details

3,5,7-Trihydroxy-2-(2-hydroxyphenyl)chromen-4-one (h200)

Crystal data

$C_{15}H_{10}O_6$
$M_r = 286.23$
Monoclinic, $P2_1/c$
$a = 15.0296\ (5)$ Å
$b = 3.7601\ (1)$ Å
$c = 21.6148\ (7)$ Å
$\beta = 99.453\ (2)°$
$V = 1204.93\ (6)$ Å^3
$Z = 4$

$F(000) = 592$
$D_x = 1.578$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 8258 reflections
$\theta = 4.2–68.2°$
$\mu = 1.06$ mm^{-1}
$T = 293$ K
Needle, colourless
0.50 × 0.08 × 0.05 mm

Data collection

Bruker D8 VENTURE dual wavelength Mo/Cu diffractometer
Radiation source: microfocus X-ray source, Incoatec IμS 3.0 Microfocus Source
Mirror monochromator
Detector resolution: 7.3910 pixels mm^{-1}
ω–φ scans
Absorption correction: multi-scan (SADABS2016; Krause *et al.*, 2015)

$T_{min} = 0.592$, $T_{max} = 0.753$
26195 measured reflections
2220 independent reflections
2026 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 68.3°$, $\theta_{min} = 3.0°$
$h = -18 \rightarrow 17$
$k = -4 \rightarrow 4$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.141$
$S = 1.17$
2220 reflections
199 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.079P)^2 + 0.4321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0098 (12)

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 (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
O1	0.20372 (8)	0.6063 (3)	0.53557 (5)	0.0305 (3)
O2	0.36717 (9)	0.9638 (4)	0.44792 (6)	0.0398 (4)
H2	0.424 (2)	0.986 (7)	0.4589 (6)	0.060*
O3	0.47468 (8)	0.7623 (4)	0.55722 (6)	0.0463 (4)
O4	0.49049 (9)	0.4646 (5)	0.66865 (7)	0.0526 (5)
H4	0.5088 (7)	0.561 (9)	0.6349 (13)	0.079*
O5	0.21619 (10)	0.1003 (4)	0.73305 (7)	0.0474 (4)
H5	0.2541 (14)	0.037 (8)	0.7676 (14)	0.071*
O6	0.25875 (9)	0.6804 (4)	0.35317 (6)	0.0451 (4)
H6	0.3070 (16)	0.742 (7)	0.3810 (12)	0.068*
C2	0.24158 (11)	0.7541 (5)	0.48810 (7)	0.0271 (4)
C3	0.33153 (11)	0.8063 (5)	0.49504 (8)	0.0298 (4)
C4	0.39130 (11)	0.7049 (5)	0.55145 (8)	0.0310 (4)
C4A	0.35007 (12)	0.5439 (5)	0.59939 (8)	0.0299 (4)
C5	0.40008 (12)	0.4289 (5)	0.65774 (8)	0.0349 (4)
C6	0.35701 (13)	0.2818 (5)	0.70293 (8)	0.0376 (5)
H6A	0.3899	0.2079	0.7410	0.045*
C7	0.26335 (13)	0.2443 (5)	0.69115 (8)	0.0351 (4)
C8	0.21210 (12)	0.3543 (5)	0.63513 (8)	0.0329 (4)
H8	0.1497	0.3289	0.6280	0.039*
C8A	0.25639 (12)	0.5021 (5)	0.59043 (8)	0.0284 (4)
C9	0.17216 (11)	0.8532 (4)	0.43451 (8)	0.0276 (4)
C10	0.18276 (12)	0.8150 (5)	0.37161 (8)	0.0317 (4)
C11	0.11160 (13)	0.9013 (6)	0.32428 (8)	0.0393 (5)
H11	0.1185	0.8731	0.2826	0.047*
C12	0.03171 (14)	1.0270 (6)	0.33804 (10)	0.0430 (5)
H12	−0.0152	1.0817	0.3058	0.052*
C13	0.02049 (13)	1.0730 (5)	0.40003 (10)	0.0396 (5)
H13	−0.0334	1.1620	0.4095	0.047*
C14	0.09014 (12)	0.9853 (5)	0.44718 (9)	0.0334 (4)
H14	0.0824	1.0148	0.4887	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0263 (6)	0.0411 (7)	0.0231 (6)	−0.0033 (5)	0.0007 (5)	0.0043 (5)
O2	0.0265 (7)	0.0625 (9)	0.0292 (7)	−0.0102 (6)	0.0007 (5)	0.0095 (6)
O3	0.0252 (7)	0.0706 (10)	0.0408 (8)	−0.0103 (6)	−0.0010 (5)	0.0121 (7)
O4	0.0321 (8)	0.0806 (12)	0.0405 (8)	−0.0066 (7)	−0.0078 (6)	0.0149 (8)

O5	0.0500 (8)	0.0630 (10)	0.0304 (7)	−0.0006 (7)	0.0099 (6)	0.0147 (7)
O6	0.0338 (7)	0.0715 (10)	0.0293 (7)	0.0027 (7)	0.0029 (5)	−0.0133 (7)
C2	0.0277 (8)	0.0308 (8)	0.0227 (8)	−0.0026 (7)	0.0034 (6)	−0.0005 (6)
C3	0.0287 (9)	0.0361 (9)	0.0241 (8)	−0.0040 (7)	0.0028 (7)	0.0001 (7)
C4	0.0262 (8)	0.0358 (9)	0.0296 (9)	−0.0039 (7)	0.0007 (7)	−0.0010 (7)
C4A	0.0293 (9)	0.0330 (9)	0.0259 (8)	−0.0020 (7)	0.0002 (7)	−0.0011 (7)
C5	0.0327 (9)	0.0394 (10)	0.0296 (9)	−0.0018 (7)	−0.0037 (7)	−0.0003 (8)
C6	0.0425 (11)	0.0416 (10)	0.0258 (9)	0.0011 (8)	−0.0031 (7)	0.0045 (8)
C7	0.0445 (11)	0.0343 (9)	0.0269 (9)	−0.0004 (8)	0.0073 (7)	0.0010 (7)
C8	0.0322 (9)	0.0375 (10)	0.0288 (9)	−0.0028 (7)	0.0045 (7)	0.0020 (7)
C8A	0.0297 (9)	0.0309 (9)	0.0228 (8)	0.0000 (7)	−0.0010 (6)	−0.0011 (7)
C9	0.0258 (8)	0.0298 (8)	0.0258 (8)	−0.0045 (6)	0.0003 (6)	0.0012 (7)
C10	0.0296 (9)	0.0364 (10)	0.0282 (9)	−0.0036 (7)	0.0022 (7)	−0.0022 (7)
C11	0.0409 (10)	0.0493 (11)	0.0250 (9)	−0.0048 (9)	−0.0026 (7)	0.0019 (8)
C12	0.0354 (10)	0.0483 (12)	0.0402 (11)	−0.0013 (8)	−0.0092 (8)	0.0105 (9)
C13	0.0280 (9)	0.0418 (11)	0.0475 (11)	0.0032 (8)	0.0020 (8)	0.0040 (9)
C14	0.0298 (9)	0.0388 (10)	0.0313 (9)	−0.0019 (7)	0.0042 (7)	0.0004 (7)

Geometric parameters (Å, º)

O1—C2	1.370 (2)	C5—C6	1.374 (3)
O1—C8A	1.370 (2)	C6—C7	1.396 (3)
O2—C3	1.361 (2)	C6—H6A	0.9300
O2—H2	0.85 (3)	C7—C8	1.387 (3)
O3—C4	1.257 (2)	C8—C8A	1.377 (2)
O4—C5	1.347 (2)	C8—H8	0.9300
O4—H4	0.90 (3)	C9—C14	1.397 (3)
O5—C7	1.352 (2)	C9—C10	1.402 (2)
O5—H5	0.89 (3)	C10—C11	1.392 (3)
O6—C10	1.367 (2)	C11—C12	1.368 (3)
O6—H6	0.89 (3)	C11—H11	0.9300
C2—C3	1.350 (2)	C12—C13	1.389 (3)
C2—C9	1.474 (2)	C12—H12	0.9300
C3—C4	1.442 (2)	C13—C14	1.376 (3)
C4—C4A	1.427 (2)	C13—H13	0.9300
C4A—C8A	1.398 (2)	C14—H14	0.9300
C4A—C5	1.425 (2)		
C2—O1—C8A	120.81 (13)	C8—C7—C6	121.86 (17)
C3—O2—H2	109.5	C8A—C8—C7	118.02 (17)
C5—O4—H4	109.5	C8A—C8—H8	121.0
C7—O5—H5	109.5	C7—C8—H8	121.0
C10—O6—H6	109.5	O1—C8A—C8	116.45 (15)
C3—C2—O1	120.48 (15)	O1—C8A—C4A	120.87 (15)
C3—C2—C9	128.12 (15)	C8—C8A—C4A	122.67 (16)
O1—C2—C9	111.33 (14)	C14—C9—C10	118.09 (16)
C2—C3—O2	119.34 (15)	C14—C9—C2	117.99 (15)
C2—C3—C4	121.93 (16)	C10—C9—C2	123.90 (16)

O2—C3—C4	118.72 (15)	O6—C10—C11	116.75 (16)
O3—C4—C4A	123.05 (16)	O6—C10—C9	123.65 (16)
O3—C4—C3	120.72 (16)	C11—C10—C9	119.54 (17)
C4A—C4—C3	116.22 (15)	C12—C11—C10	121.12 (18)
C8A—C4A—C5	117.47 (16)	C12—C11—H11	119.4
C8A—C4A—C4	119.65 (16)	C10—C11—H11	119.4
C5—C4A—C4	122.87 (16)	C11—C12—C13	120.20 (17)
O4—C5—C6	119.70 (17)	C11—C12—H12	119.9
O4—C5—C4A	119.65 (17)	C13—C12—H12	119.9
C6—C5—C4A	120.65 (17)	C14—C13—C12	119.12 (18)
C5—C6—C7	119.34 (16)	C14—C13—H13	120.4
C5—C6—H6A	120.3	C12—C13—H13	120.4
C7—C6—H6A	120.3	C13—C14—C9	121.90 (17)
O5—C7—C8	115.30 (17)	C13—C14—H14	119.0
O5—C7—C6	122.84 (17)	C9—C14—H14	119.0

C8A—O1—C2—C3	−1.3 (3)	C2—O1—C8A—C8	−179.56 (15)
C8A—O1—C2—C9	−178.60 (14)	C2—O1—C8A—C4A	0.0 (2)
O1—C2—C3—O2	−177.97 (15)	C7—C8—C8A—O1	179.72 (16)
C9—C2—C3—O2	−1.2 (3)	C7—C8—C8A—C4A	0.2 (3)
O1—C2—C3—C4	1.1 (3)	C5—C4A—C8A—O1	−179.98 (15)
C9—C2—C3—C4	177.86 (17)	C4—C4A—C8A—O1	1.5 (3)
C2—C3—C4—O3	−178.72 (18)	C5—C4A—C8A—C8	−0.5 (3)
O2—C3—C4—O3	0.4 (3)	C4—C4A—C8A—C8	−178.93 (17)
C2—C3—C4—C4A	0.4 (3)	C3—C2—C9—C14	−140.56 (19)
O2—C3—C4—C4A	179.49 (16)	O1—C2—C9—C14	36.4 (2)
O3—C4—C4A—C8A	177.41 (18)	C3—C2—C9—C10	41.0 (3)
C3—C4—C4A—C8A	−1.7 (3)	O1—C2—C9—C10	−141.99 (17)
O3—C4—C4A—C5	−1.0 (3)	C14—C9—C10—O6	−178.23 (17)
C3—C4—C4A—C5	179.91 (16)	C2—C9—C10—O6	0.2 (3)
C8A—C4A—C5—O4	−179.79 (17)	C14—C9—C10—C11	−1.4 (3)
C4—C4A—C5—O4	−1.4 (3)	C2—C9—C10—C11	177.08 (17)
C8A—C4A—C5—C6	0.2 (3)	O6—C10—C11—C12	177.87 (18)
C4—C4A—C5—C6	178.67 (18)	C9—C10—C11—C12	0.8 (3)
O4—C5—C6—C7	−179.73 (18)	C10—C11—C12—C13	0.4 (3)
C4A—C5—C6—C7	0.2 (3)	C11—C12—C13—C14	−1.0 (3)
C5—C6—C7—O5	179.59 (18)	C12—C13—C14—C9	0.4 (3)
C5—C6—C7—C8	−0.5 (3)	C10—C9—C14—C13	0.8 (3)
O5—C7—C8—C8A	−179.78 (16)	C2—C9—C14—C13	−177.76 (17)
C6—C7—C8—C8A	0.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3^{i}	0.85 (3)	1.85 (3)	2.6094 (18)	147 (3)
O4—H4···O3	0.91 (3)	1.78 (3)	2.631 (2)	155 (3)

O5—H5···O6^{ii}	0.91 (4)	1.98 (4)	2.7778 (19)	146 (3)
O6—H6···O2	0.89 (3)	1.79 (3)	2.6253 (19)	155 (3)

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

3,5,7-Trihydroxy-2-(2-hydroxyphenyl)chromen-4-one monohydrate (h149)

Crystal data

$C_{15}H_{10}O_6 \cdot H_2O$	D_x = 1.543 Mg m^{-3}
M_r = 304.25	Cu *Kα* radiation, λ = 1.54178 Å
Orthorhombic, *Pna*2$_1$	Cell parameters from 4404 reflections
a = 14.0628 (15) Å	θ = 7.3–68.1°
b = 23.714 (3) Å	μ = 1.06 mm^{-1}
c = 3.9274 (5) Å	*T* = 291 K
V = 1309.7 (3) Å^3	Needle, colourless
Z = 4	0.65 × 0.14 × 0.07 mm
F(000) = 632	

Data collection

Bruker D8 VENTURE dual wavelength Mo/Cu diffractometer	T_{min} = 0.66, T_{max} = 0.93
Radiation source: microfocus X-ray source, Incoatec IµS 3.0 Microfocus Source	8711 measured reflections
	2305 independent reflections
Mirror monochromator	2142 reflections with $I > 2\sigma(I)$
Detector resolution: 7.3910 pixels mm^{-1}	R_{int} = 0.038
ω–φ scans	θ_{max} = 68.3°, θ_{min} = 7.3°
Absorption correction: multi-scan (SADABS2016; Krause *et al.*, 2015)	*h* = −16→16
	k = −25→28
	l = −4→4

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0954P)^2 + 0.0942P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	
$wR(F^2)$ = 0.116	$(\Delta/\sigma)_{max}$ = 0.002
S = 0.93	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
2305 reflections	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
207 parameters	Absolute structure: Flack *x* determined using 811 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
1 restraint	
Hydrogen site location: mixed	Absolute structure parameter: 0.25 (10)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.21017 (12)	0.67355 (8)	0.4950 (5)	0.0496 (5)
O2	0.42512 (15)	0.62983 (10)	0.0550 (7)	0.0659 (6)
H2	0.4119	0.5962	0.0606	0.099*

O3	0.47772 (13)	0.73003 (8)	0.2957 (6)	0.0594 (5)
O4	0.43416 (14)	0.82483 (10)	0.6100 (7)	0.0670 (6)
H4	0.472 (3)	0.7990 (17)	0.501 (15)	0.101*
O5	0.12647 (14)	0.83978 (9)	1.0763 (7)	0.0663 (6)
H5	0.0782	0.8212	1.1113	0.099*
O6	0.36173 (17)	0.53262 (11)	0.2674 (9)	0.0776 (7)
H6	0.3647	0.5392	0.4721	0.116*
C2	0.27162 (18)	0.64084 (11)	0.3106 (7)	0.0474 (6)
C3	0.36183 (17)	0.65904 (12)	0.2473 (7)	0.0492 (6)
C4	0.39466 (18)	0.71322 (12)	0.3617 (7)	0.0488 (6)
C4A	0.32752 (17)	0.74680 (12)	0.5469 (7)	0.0465 (6)
C5	0.34735 (17)	0.80153 (11)	0.6692 (7)	0.0501 (6)
C6	0.2810 (2)	0.83166 (11)	0.8462 (8)	0.0542 (7)
H6A	0.2953	0.8675	0.9271	0.065*
C7	0.19053 (19)	0.80783 (12)	0.9051 (7)	0.0511 (6)
C8	0.16834 (17)	0.75469 (12)	0.7910 (7)	0.0501 (6)
H8	0.1090	0.7390	0.8345	0.060*
C8A	0.23623 (16)	0.72515 (10)	0.6101 (7)	0.0454 (6)
C9	0.22479 (19)	0.58975 (12)	0.1862 (7)	0.0527 (7)
C10	0.2694 (2)	0.53740 (13)	0.1606 (8)	0.0611 (8)
C11	0.2213 (3)	0.49107 (15)	0.0292 (10)	0.0738 (10)
H11	0.2522	0.4565	0.0125	0.089*
C12	0.1298 (3)	0.49590 (18)	−0.0747 (11)	0.0772 (10)
H12	0.0983	0.4646	−0.1618	0.093*
C13	0.0833 (2)	0.54674 (18)	−0.0524 (9)	0.0729 (9)
H13	0.0207	0.5498	−0.1264	0.087*
C14	0.1295 (2)	0.59331 (14)	0.0801 (8)	0.0586 (7)
H14	0.0972	0.6274	0.0993	0.070*
O1W	0.4385 (3)	0.43331 (13)	0.1462 (13)	0.1119 (12)
H1WA	0.4279	0.4453	0.3467	0.168*
H1WB	0.4247	0.3984	0.1542	0.168*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0353 (9)	0.0610 (10)	0.0525 (11)	−0.0084 (7)	0.0025 (8)	0.0096 (9)
O2	0.0449 (11)	0.0735 (12)	0.0795 (15)	−0.0039 (9)	0.0108 (10)	−0.0067 (12)
O3	0.0327 (9)	0.0747 (11)	0.0708 (13)	−0.0106 (8)	0.0067 (8)	0.0018 (10)
O4	0.0434 (10)	0.0699 (12)	0.0878 (17)	−0.0176 (8)	0.0086 (11)	0.0024 (12)
O5	0.0467 (11)	0.0675 (11)	0.0846 (16)	0.0038 (9)	0.0102 (11)	0.0011 (12)
O6	0.0639 (13)	0.0716 (13)	0.0973 (19)	−0.0017 (10)	−0.0159 (14)	0.0092 (15)
C2	0.0370 (12)	0.0619 (14)	0.0435 (13)	−0.0044 (10)	−0.0025 (10)	0.0124 (12)
C3	0.0367 (12)	0.0630 (14)	0.0480 (14)	−0.0027 (10)	−0.0001 (11)	0.0094 (13)
C4	0.0323 (12)	0.0667 (15)	0.0475 (14)	−0.0048 (11)	−0.0005 (10)	0.0129 (13)
C4A	0.0334 (12)	0.0607 (14)	0.0455 (13)	−0.0044 (10)	−0.0014 (10)	0.0134 (12)
C5	0.0341 (11)	0.0607 (14)	0.0555 (15)	−0.0064 (10)	−0.0040 (11)	0.0125 (13)
C6	0.0470 (15)	0.0543 (14)	0.0612 (18)	−0.0028 (11)	−0.0028 (13)	0.0071 (13)
C7	0.0369 (13)	0.0630 (15)	0.0532 (14)	0.0042 (11)	−0.0008 (11)	0.0108 (13)

C8	0.0326 (12)	0.0636 (15)	0.0540 (15)	−0.0034 (10)	−0.0006 (11)	0.0133 (13)
C8A	0.0340 (12)	0.0580 (13)	0.0442 (13)	−0.0046 (9)	−0.0035 (11)	0.0141 (12)
C9	0.0458 (14)	0.0670 (16)	0.0454 (14)	−0.0118 (11)	0.0028 (11)	0.0090 (12)
C10	0.0553 (17)	0.0714 (17)	0.0565 (17)	−0.0116 (13)	−0.0028 (14)	0.0107 (15)
C11	0.081 (2)	0.0707 (18)	0.070 (2)	−0.0196 (16)	0.0053 (18)	−0.0015 (17)
C12	0.074 (2)	0.091 (2)	0.0660 (19)	−0.032 (2)	0.0016 (18)	−0.0084 (18)
C13	0.0527 (17)	0.107 (3)	0.0587 (18)	−0.0280 (19)	−0.0013 (14)	0.0002 (18)
C14	0.0426 (14)	0.0837 (19)	0.0497 (15)	−0.0141 (13)	0.0021 (12)	0.0066 (15)
O1W	0.119 (3)	0.0767 (16)	0.140 (3)	0.0237 (16)	0.004 (2)	0.015 (2)

Geometric parameters (Å, º)

O1—C8A	1.355 (3)	C6—C7	1.411 (4)
O1—C2	1.369 (3)	C6—H6A	0.9300
O2—C3	1.357 (4)	C7—C8	1.373 (4)
O2—H2	0.8200	C8—C8A	1.381 (4)
O3—C4	1.261 (3)	C8—H8	0.9300
O4—C5	1.360 (3)	C9—C10	1.395 (4)
O4—H4	0.92 (6)	C9—C14	1.405 (4)
O5—C7	1.356 (4)	C10—C11	1.390 (5)
O5—H5	0.8200	C11—C12	1.355 (6)
O6—C10	1.369 (4)	C11—H11	0.9300
O6—H6	0.8200	C12—C13	1.375 (6)
C2—C3	1.363 (3)	C12—H12	0.9300
C2—C9	1.463 (4)	C13—C14	1.383 (5)
C3—C4	1.437 (4)	C13—H13	0.9300
C4—C4A	1.433 (4)	C14—H14	0.9300
C4A—C8A	1.405 (3)	O1W—H1WA	0.8500
C4A—C5	1.412 (4)	O1W—H1WB	0.8499
C5—C6	1.365 (4)		
C8A—O1—C2	121.18 (19)	C7—C8—C8A	118.4 (2)
C3—O2—H2	109.5	C7—C8—H8	120.8
C5—O4—H4	109.5	C8A—C8—H8	120.8
C7—O5—H5	109.5	O1—C8A—C8	116.3 (2)
C10—O6—H6	109.5	O1—C8A—C4A	121.2 (2)
O1—C2—C3	120.3 (2)	C8—C8A—C4A	122.5 (3)
O1—C2—C9	111.2 (2)	C10—C9—C14	117.5 (3)
C3—C2—C9	128.4 (3)	C10—C9—C2	124.0 (2)
O2—C3—C2	123.4 (3)	C14—C9—C2	118.6 (3)
O2—C3—C4	114.8 (2)	O6—C10—C11	120.7 (3)
C2—C3—C4	121.7 (3)	O6—C10—C9	118.6 (3)
O3—C4—C4A	122.6 (3)	C11—C10—C9	120.7 (3)
O3—C4—C3	121.0 (3)	C12—C11—C10	120.5 (4)
C4A—C4—C3	116.3 (2)	C12—C11—H11	119.8
C8A—C4A—C5	117.2 (2)	C10—C11—H11	119.8
C8A—C4A—C4	119.2 (3)	C13—C12—C11	120.5 (3)
C5—C4A—C4	123.6 (2)	C13—C12—H12	119.8

O4—C5—C6	119.2 (3)	C11—C12—H12	119.8
O4—C5—C4A	119.5 (3)	C12—C13—C14	120.0 (3)
C6—C5—C4A	121.3 (2)	C12—C13—H13	120.0
C5—C6—C7	119.3 (3)	C14—C13—H13	120.0
C5—C6—H6A	120.3	C13—C14—C9	120.8 (3)
C7—C6—H6A	120.3	C13—C14—H14	119.6
O5—C7—C8	121.6 (2)	C9—C14—H14	119.6
O5—C7—C6	117.2 (3)	H1WA—O1W—H1WB	104.5
C8—C7—C6	121.2 (3)		

C8A—O1—C2—C3	1.9 (3)	C2—O1—C8A—C8	179.5 (2)
C8A—O1—C2—C9	−174.3 (2)	C2—O1—C8A—C4A	−0.5 (3)
O1—C2—C3—O2	−177.3 (2)	C7—C8—C8A—O1	−178.3 (2)
C9—C2—C3—O2	−1.7 (5)	C7—C8—C8A—C4A	1.7 (4)
O1—C2—C3—C4	−1.8 (4)	C5—C4A—C8A—O1	178.4 (2)
C9—C2—C3—C4	173.8 (2)	C4—C4A—C8A—O1	−1.0 (4)
O2—C3—C4—O3	−2.7 (4)	C5—C4A—C8A—C8	−1.6 (4)
C2—C3—C4—O3	−178.6 (3)	C4—C4A—C8A—C8	179.0 (2)
O2—C3—C4—C4A	176.1 (2)	O1—C2—C9—C10	−143.9 (3)
C2—C3—C4—C4A	0.3 (4)	C3—C2—C9—C10	40.2 (4)
O3—C4—C4A—C8A	179.9 (3)	O1—C2—C9—C14	37.2 (3)
C3—C4—C4A—C8A	1.1 (4)	C3—C2—C9—C14	−138.7 (3)
O3—C4—C4A—C5	0.6 (4)	C14—C9—C10—O6	−179.0 (3)
C3—C4—C4A—C5	−178.3 (2)	C2—C9—C10—O6	2.1 (5)
C8A—C4A—C5—O4	−178.9 (3)	C14—C9—C10—C11	1.1 (4)
C4—C4A—C5—O4	0.4 (4)	C2—C9—C10—C11	−177.8 (3)
C8A—C4A—C5—C6	1.0 (4)	O6—C10—C11—C12	179.7 (4)
C4—C4A—C5—C6	−179.6 (3)	C9—C10—C11—C12	−0.4 (5)
O4—C5—C6—C7	179.4 (3)	C10—C11—C12—C13	0.1 (6)
C4A—C5—C6—C7	−0.6 (4)	C11—C12—C13—C14	−0.7 (6)
C5—C6—C7—O5	−178.8 (3)	C12—C13—C14—C9	1.4 (5)
C5—C6—C7—C8	0.7 (4)	C10—C9—C14—C13	−1.6 (4)
O5—C7—C8—C8A	178.2 (3)	C2—C9—C14—C13	177.3 (3)
C6—C7—C8—C8A	−1.3 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O6	0.82	1.85	2.609 (3)	153
O4—H4···O3	0.82	1.91	2.639 (3)	147
O5—H5···O3^{i}	0.82	2.00	2.803 (3)	166
O1*W*—H1*WB*···O5^{ii}	0.85	2.76	3.281 (5)	121
O1*W*—H1*WB*···O5^{iii}	0.85	2.28	2.934 (4)	134

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