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Synthesis, crystal structure and Hirshfeld surface analysis of 4-(3-hydroxy-6-methoxy-4-oxo-4*H*-chromen-2-yl)benzaldehyde

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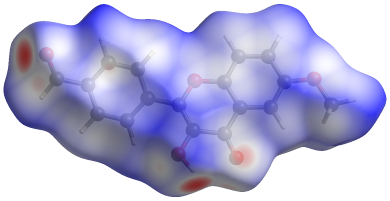
The asymmetric unit of the title compound, $C_{17}H_{12}O_5$, contains one crystallographically independent molecule featuring a chromenone fragment with hydroxy and methoxy substituents and a benzaldehyde group. Intramolecular O—H⋯O, C—H⋯O hydrogen bonds are observed. In the crystal, molecules are linked by O—H⋯O intermolecular bonds, forming chains along [201]. The Hirshfeld surface analysis shows that the H⋯H and O⋯H/H⋯O contacts dominate the crystal packing with contributions of 34.2% and 27.6%, respectively.

1. Chemical context

Compounds bearing a 3-hydroxy-2-phenyl-chromen-4-one core belong to the family specifically categorized as flavonol derivatives (common name: 3-hydroxyflavones). They feature a chromone (1-benzopyran-4-one) core, which is a privileged scaffold in medicinal chemistry due to its diverse biological activities (Borsari *et al.*, 2016). These derivatives, also referred to as 3-hydroxyflavones, can scavenge free radicals and chelate metal ions (Roshal, 2024; Mihajlović *et al.*, 2025), which is vital in preventing oxidative stress-related diseases.

In 3-hydroxyflavone derivatives, a crucial intramolecular hydrogen bond forms between the 3-hydroxyl group and the 4-oxo (carbonyl, C═O) oxygen. This bond forms a five-membered ring stabilized by a resonance-assisted hydrogen bond and is responsible for excited-state intramolecular proton transfer (ESIPT) (Zhao *et al.*, 2021; Pivovarenko, 2023; Pivovarenko & Klymchenko, 2024). The molecule absorbs light in its enol form but, after the proton jumps, it emits light as a keto form. This keto form has a much lower energy, shifting the emission to much longer wavelengths. ESIPT features can be tuned by C4′ substitutions making it possible to use 3-hydroxyflavones as environment-sensitive fluorescence probes (Pivovarenko, 2023; Snizhko *et al.*, 2025; Chepeleva *et al.*, 2023; Demidov *et al.*, 2022; Kyrychenko & Ladokhin, 2024).

The X-ray structures were vital for showing how various electron-donating and electron-withdrawing groups, especially at the C6, C7, and C4′ positions, and steric factors affect the planarity of 3-hydroxyflavones (Etter *et al.*, 1986; Shoja *et al.*, 1998; Shoja & Sullivan, 1999; Wera *et al.*, 2011*a*,*b*; Narita *et al.*, 2015; Koh, 2020). Recently, we have demonstrated that the nature and position of substituent groups can significantly influence crystal packing in the solid state, thereby tuning the



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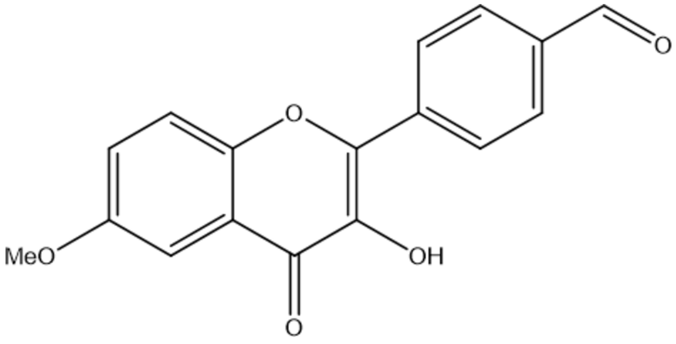
contributions of intra- and intermolecular hydrogen bonding and the ESIPT behavior (Demidov *et al.*, 2025). The investigation of the crystal structure of 3-hydroxyflavones bearing a C6-electron-donating group on the *A* ring and a C4′-electron-withdrawing group on the *B* ring provides insights into the role of electron conjugation and push–pull effects (Pivovarenko & Klymchenko, 2024; Doroshenko *et al.*, 2019, 2026) on the structure, optical properties and supramolecular interactions.



2. Structural commentary

The molecular structure of the title compound, **1**, is shown in Fig. 1. The asymmetric unit contains one crystallographically independent molecule. The molecule comprises a chromenone fragment bearing hydroxy and methoxy substituents and a benzaldehyde group. The methoxy substituent at atom C15 is almost coplanar with the chromenone fragment, as indicated by the C17—O5—C15—C16 torsion angle of 3.4 (3)°.

The benzaldehyde ring is rotated relative to the chromenone fragment. The interfragment torsion angle C6—C5—C8—C9 is −12.8 (3)°, indicating a slight twist between the two fragments. This orientation enables an intramolecular C6—H6···O3 hydrogen bond (Table 1) involving a phenyl C—H group and an oxygen atom of the chromenone moiety. The oxygen atom O3, which participates in the intramolecular C—H···O interaction also participates in the intramolecular resonant O3—H3···O4 hydrogen bond in the chromenone group (Table 1). This hydrogen bond is important as it is responsible for ESIPT in compounds of this type, as mentioned earlier in the *Chemical context*. Thus, the O3 atom participates in two intramolecular hydrogen bonds of different types.

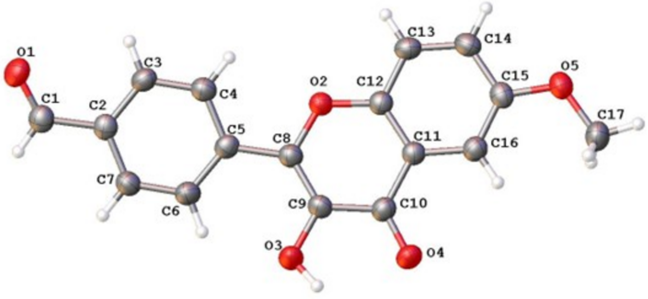


Figure 1
The molecular structure of **1**, showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1^{i}	0.89 (2)	2.02 (2)	2.8304 (18)	151 (2)
O3—H3···O4	0.89 (2)	2.20 (2)	2.6853 (18)	113.6 (19)
C6—H6···O3	0.93	2.20	2.834 (2)	12

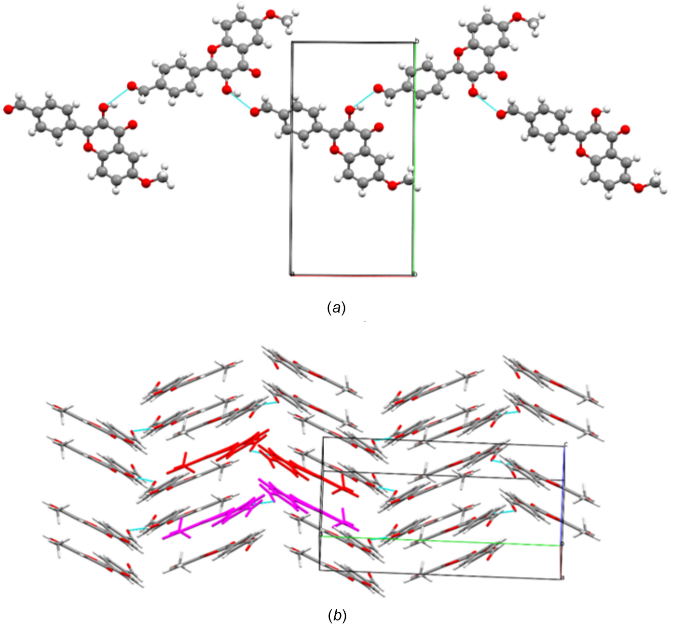
Symmetry code: (i) $x - 1, -y + \frac{3}{2}, z - \frac{1}{2}$.

3. Supramolecular features

In the crystal, molecules of **1** are linked by O3—H3···O1^{i} hydrogen bonds (Table 1, Fig. 2*a*), forming zigzag chains along [201] (Fig. 2*b*). The crystal packing is further consolidated by π–π stacking interactions between chromenone rings of molecules belonging to adjacent chains [*Cg*1···*Cg*3$(1 - x, 1 - y, 1 - z)$ = 3.575 (3) Å; *Cg*1 and *Cg*3 are the centroids of the O2/C8–C12 and C11 –C16 rings, respectively]. In addition, weak C7—H7···C3$(x, \frac{3}{2} - y, -\frac{1}{2} + z)(\pi)$ contacts are observed between molecules from neighboring chains [H···C = 2.86 (3) Å, C—H···C = 170.4 (2)°], which also contribute to the cohesion of the crystal packing.

4. Hirshfeld surface analysis and fingerprint plots

The intermolecular interactions were visualized using the *CrystalExplorer21* program (Spackman *et al.*, 2021). The Hirshfeld surface mapped over $d_{\rm norm}$ (Spackman & Jayatilaka, 2009) is shown in Fig. 3. The strongest contacts, which are visualized on the Hirshfeld surface as the dark-red spots,


(*a*)

(*b*)

Figure 2
(*a*) The hydrogen-bonded chains of **1**. (*b*) The crystal packing of **1**. Some hydrogen-bonded chains are highlighted in different colors.

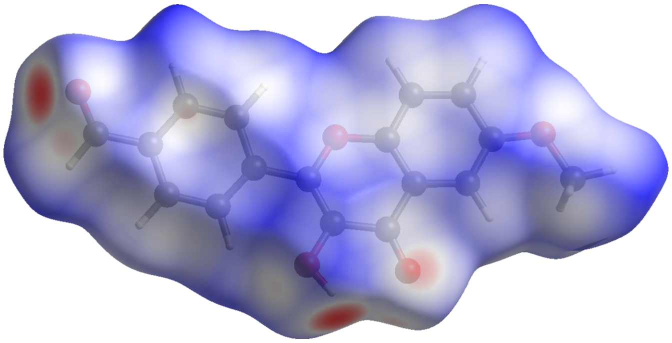


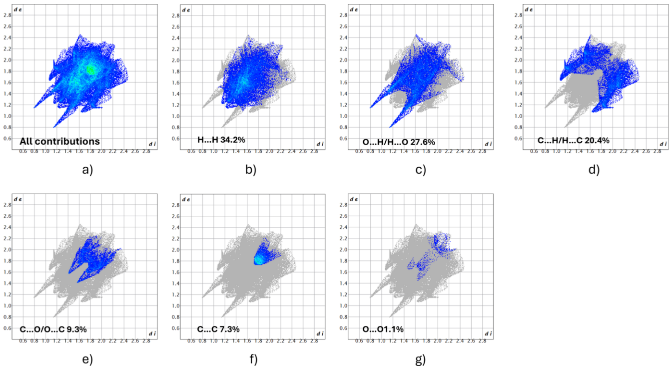
Figure 3
Three-dimensional Hirshfeld surface of title compound mapped over $d_{\rm norm}$.

correspond to the intermolecular O—H⋯O hydrogen bond between molecules. Lighter red spots correspond to weaker O⋯H/H⋯O interactions, such as C—H⋯O. The majority of the intermolecular interactions of **1** are weak, which results in the blue color of the Hirshfeld surface.

For further exploration of the intermolecular interactions, two-dimensional fingerprint plots (McKinnon *et al.*, 2007) were generated as shown in Fig. 4. The H⋯H and O⋯H/H⋯O interactions, with contributions of 34.2% and 27.6%, respectively, have the greatest impact on the crystal packing in the solid state. The C⋯H/H⋯C interactions with 20.4%, C⋯O/O⋯C with 9.3%, C⋯C with 7.3% or O⋯O with 1.1% are less impactful in comparison.

5. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.00, updated March 2025; Groom *et al.*, 2016) found 74 structures containing 3-hydroxyflavone. Of these, we would like to highlight 13 hits that are similar to title compound. These hits include the parent 3-hydroxyflavone itself and its derivatives (refcodes DUMFAS, DUMFEW, DUMFIA; Etter *et al.*, 1986). The C4′-fluoro (WACTUR; Wera *et al.*, 2010), C4′-hydroxy (IJUCAS; Wera *et al.*, 2011*a*), and C4′-methoxy (IKAHIM; Wera *et al.*, 2011*b*; IKAHIM01; Demidov *et al.*, 2025) derivatives have been reported. The C4′-*tert*-butyl 3-hydroxyflavone has been reported (OHELE; Narita *et al.*, 2015). Polymorphs of C4′-(dimethylamino) and C4′-(diethylamino) 3-hydroxyflavone has been found (BANJEN, BANJEN01, CEZDOC, CEZDOC; Hino *et al.*, 2011, 2013). 3-Hydroxyflavones with C2′-methoxy (LIGZIK01,; Shoja & Sullivan, 1999), C2′,C3-dimethoxy (PUWCUI; Koh, 2020), C3′-benzoxy (AMEBAZ, AMORUT; Demidov *et al.*, 2025), and C7-methoxy (NUZPUT; Shoja *et al.*, 1998) groups have been reported.



a) b) c) d)

e) f) g)

Figure 4
Two-dimensional fingerprint plots for the title compound showing (*a*) all interactions, and (*b*)–(*g*) delineated into contributions from other contacts [$d_{\rm e}$ and $d_{\rm i}$ represent the distances from a point on the Hirshfeld surface to the nearest atoms outside (external) and inside (internal) the surface, respectively].

6. Synthesis and crystallization

The compound was synthesized by a modified procedure reported earlier (Demidov *et al.*, 2025). All chemicals were purchased from commercial suppliers and used without further purification (Sigma-Aldrich, Enamine Ltd).

Hydroxy-5-methoxy-acetophenone (1.66 g, 10 mmol) and terephthalaldehyde diethyl-acetal (2.08 g, 10 mmol) were dissolved in ethanol (40 mL). Potassium hydroxide (3.36 g, 60 mmol) was added to the solution under stirring at room temperature. The reaction mixture was stirred for 24 h and conversion was monitored by TLC. After completion of the reaction hydrogen peroxide (30% H_2O_2, 3.4 mL, 30 mmol) was added dropwise to the reaction mixture, which was then placed in the ultrasound bath at room temperature for 10 minutes. After that the mixture was cooled to 273 K and acidified with 10% hydrochloric acid to reach a pH of 3 and stirred for additional 10 minutes. The resulting precipitate was filtered off and washed thoroughly with water and hexane. The crude product was recrystallized twice from *i*-PrOH–DMF (45:1) mixture. Yield 1.35 g (46%), yellow crystalline material, m.p. 472.5–473 K. Elemental analysis calculated for $C_{17}H_{12}O_{5}$: C, 68.92; H, 4.08. Found: C, 68.78; H, 4.15.

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker Avance DRX 500 spectrometer at a resonance frequency of 500 and 126 MHz in DMSO-d_6. Chemical shifts are reported in the δ scale (ppm). Mass spectra were recorded on an Agilent 1100 high-performance liquid chromatograph (HPLC) equipped with a diode matrix and an Agilent LC/MSD SL mass-selective detector, a SUPELCO Ascentis Express C18 chromatographic column 2.7 µm 4.6 mm x 15 cm.

^{1}H NMR spectrum, δ, ppm: 10.03 (*s*, 1H), 9.91 (*br. s*, 1H), 8.36 (*d*, J = 8.0 Hz, 2H), 8.01 (*d*, J = 8.1 Hz, 2H), 7.67 (*d*, J = 9.7 Hz, 1H), 7.40–7.24 (*m*, 2H), 3.84 (*s*, 3H) (see Fig. S1 top).

^{13}C NMR spectrum, δ, ppm: 193.1, 173.2, 156.5, 150.1, 143.7, 140.4, 137.3, 136.6, 129.9, 128.4, 124.4, 122.2, 120.6, 104.3, 56.2 (see Figure S1 bottom).

Mass spectrum, m/z ($I_{\rm rel}$, %): 297.0 [M + H]+(100) (see Fig. S2).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed in calculated positions and refined by riding model with $U_{\rm iso}(\rm H) = nU_{\rm eq}$ of the carrier atom (n = 1.5 for methyl groups and n = 1.2 for other hydrogen atoms).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{12}O_5$
M_r	296.27
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	9.9231 (10), 18.3524 (18), 7.5479 (8)
β (°)	103.118 (3)
V (Å^3)	1338.7 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.3 × 0.2 × 0.1
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{\rm min}$, $T_{\rm max}$	0.652, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23026, 3062, 2019
$R_{\rm int}$	0.063
(sin $\theta/\lambda)_{\rm max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.125, 1.04
No. of reflections	3062
No. of parameters	203
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.23, −0.21

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

References

Borsari, C., Luciani, R., Pozzi, C., Poehner, I., Henrich, S., Trande, M., Cordeiro-da-Silva, A., Santarem, N., Baptista, C., Tait, A., Di Pisa, F., Dello Iacono, L., Landi, G., Gul, S., Wolf, M., Kuzikov, M., Ellinger, B., Reinshagen, J., Witt, G., Gribbon, P., Kohler, M., Keminer, O., Behrens, B., Costantino, L., Tejera Nevado, P., Bifeld, E., Eick, J., Clos, J., Torrado, J., Jiménez-Antón, M. D., Corral, M. J., Alunda, J. M., Pellati, F., Wade, R. C., Ferrari, S., Mangani, S. & Costi, M. P. (2016). *J. Med. Chem.* **59**, 7598–7616.

Bruker (2014). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Chepeleva, L. V., Demidov, O. O., Snizhko, A. D., Tarasenko, D. O., Chumak, A. Y., Kolomoitsev, O. O., Kotliar, V. M., Gladkov, E. S., Kyrychenko, A. & Roshal, A. D. (2023). *RSC Adv.* **13**, 34107–34121.

Demidov, O. O., Chepeleva, L. V., Shishkina, S. V., Gladkov, E. S., Kyrychenko, A., Linnik, R. P. & Roshal, A. D. (2025). *RSC Adv.* **15**, 36300–36318.

Demidov, O. O., Gladkov, E. S., Kyrychenko, A. V. & Roshal, A. D. (2022). *Funct. Mater* **29**, 252–262.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Doroshenko, A. O., Chumak, A. Y., Kolomoitsev, O. O. & Kotlyar, V. M. (2026). *J. Photochem. Photobiol. A* **472**, 116817.

Doroshenko, A. O., Kyrychenko, A. V., Valyashko, O. M., Kotlyar, V. N. & Svechkarev, D. A. (2019). *J. Photochem. Photobiol. A* **383**, 111964.

Etter, M. C., Urbańczyk-Lipkowska, Z., Baer, S. & Barbara, P. F. (1986). *J. Mol. Struct.* **144**, 155–167.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Hino, K., Nakajima, K., Kawahara, M., Furukawa, K. & Sekiya, H. (2013). *Bull. Chem. Soc. Jpn* **86**, 721–723.

Hino, K., Nakajima, K., Kawahara, M., Kiyota, I. & Sekiya, H. (2011). *Bull. Chem. Soc. Jpn* **84**, 1234–1236.

Koh, D. (2020). *Z. Kristallogr. New Cryst. Struct.* **235**, 913–914.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Kyrychenko, A. & Ladokhin, A. S. (2024). *Chem. Rec.* **24**, e202300232.

McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2007). *Chem. Commun.* pp. 3814–3816.

Mihajlović, L., Trif, M. & Živković, M. B. (2025). *Inorganics* **13**, 250.

Narita, F., Takura, A. & Fujihara, T. (2015). *Acta Cryst.* E**71**, 824–826.

Pivovarenko, V. G. (2023). *BBA Adv.* **3**, 100094.

Pivovarenko, V. G. & Klymchenko, A. S. (2024). *Chem. Rec.* **24**, e202300321.

Roshal, A. D. (2024). *Chem. Rec.* **24**, e202300249.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Shoja, M. & Sullivan, P. (1999). *Z. Kristallogr. New Cryst. Struct.* **214**, 237–238.

Shoja, M., Sullivan, P., Athanasopoulos, D. & Kabbani, R. (1998). *Z. Kristallogr. New Cryst. Struct.* **213**, 607-608.

Snizhko, A. D., Chepeleva, L. V., Gladkov, E. S. & Kyrychenko, A. (2025). *J. Photochem. Photobiol. A* **469**, 116524.

Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm* **11**, 19–32.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

Wera, M., Pivovarenko, V. G. & Błażejowski, J. (2011*a*). *Acta Cryst.* E**67**, o264–o265.

Wera, M., Serdiuk, I. E., Roshal, A. D. & Błażejowski, J. (2010). *Acta Cryst.* E**66**, o3122.

Wera, M., Serdiuk, I. E., Roshal, A. D. & Błażejowski, J. (2011*b*). *Acta Cryst.* E**67**, o440.

Zhao, X., Li, X., Liang, S., Dong, X. & Zhang, Z. (2021). *RSC Adv.* **11**, 28851–28862.

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Synthesis, crystal structure and Hirshfeld surface analysis of 4-(3-hydroxy-6-methoxy-4-oxo-4*H*-chromen-2-yl)benzaldehyde

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Computing details

4-(3-Hydroxy-6-methoxy-4-oxo-4*H*-chromen-2-yl)benzaldehyde

Crystal data

$C_{17}H_{12}O_5$
$M_r = 296.27$
Monoclinic, $P2_1/c$
$a = 9.9231$ (10) Å
$b = 18.3524$ (18) Å
$c = 7.5479$ (8) Å
$\beta = 103.118$ (3)°
$V = 1338.7$ (2) Å^3
$Z = 4$

$F(000) = 616$
$D_x = 1.470$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3272 reflections
$\theta = 2.2$–24.7°
$\mu = 0.11$ mm^{-1}
$T = 296$ K
Block, yellow
0.3 × 0.2 × 0.1 mm

Data collection

Bruker APEXII CCD diffractometer
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.652$, $T_{max} = 0.746$
23026 measured reflections

3062 independent reflections
2019 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.1°$
$h = -12 \rightarrow 12$
$k = -23 \rightarrow 23$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.125$
$S = 1.04$
3062 reflections
203 parameters
0 restraints
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.2246P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

Special details

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

Refinement. Using Olex2 (Dolomanov *et al.*, 2009), the structure was solved with the SHELXT (Sheldrick, 2018) structure solution program using Intrinsic Phasing and refined with the SHELXL (Sheldrick, 2015) refinement package. Full-matrix least-squares refinement against F^2 in anisotropic approximation was used for non-hydrogen atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
O1	1.29775 (13)	0.69700 (7)	0.9257 (2)	0.0517 (4)
O2	0.64574 (11)	0.53802 (6)	0.76175 (16)	0.0363 (3)
O3	0.52689 (14)	0.70937 (7)	0.5462 (2)	0.0507 (4)
H3	0.440 (3)	0.7237 (13)	0.506 (3)	0.076*
O4	0.28735 (13)	0.63680 (7)	0.5116 (2)	0.0481 (4)
O5	0.17061 (13)	0.38516 (7)	0.75935 (19)	0.0459 (4)
C1	1.20045 (19)	0.71828 (10)	0.8100 (3)	0.0397 (5)
H1	1.215242	0.757103	0.737517	0.048*
C2	1.06098 (18)	0.68715 (9)	0.7761 (2)	0.0338 (4)
C3	1.03239 (18)	0.62416 (10)	0.8636 (3)	0.0374 (4)
H3A	1.103690	0.599247	0.941261	0.045*
C4	0.89871 (18)	0.59871 (10)	0.8353 (2)	0.0375 (4)
H4	0.880862	0.556435	0.893953	0.045*
C5	0.78883 (17)	0.63530 (9)	0.7197 (2)	0.0327 (4)
C6	0.81938 (19)	0.69798 (10)	0.6320 (3)	0.0402 (5)
H6	0.748651	0.723149	0.553968	0.048*
C7	0.95327 (18)	0.72287 (10)	0.6599 (3)	0.0380 (4)
H7	0.971821	0.764552	0.599509	0.046*
C8	0.64731 (17)	0.60722 (9)	0.6925 (2)	0.0331 (4)
C9	0.52761 (18)	0.64075 (9)	0.6130 (2)	0.0353 (4)
C10	0.39395 (18)	0.60553 (10)	0.5922 (2)	0.0352 (4)
C11	0.39709 (17)	0.53381 (9)	0.6732 (2)	0.0312 (4)
C12	0.52311 (17)	0.50293 (10)	0.7537 (2)	0.0326 (4)
C13	0.53046 (19)	0.43401 (10)	0.8322 (2)	0.0392 (4)
H13	0.615784	0.413493	0.885235	0.047*
C14	0.41102 (19)	0.39688 (10)	0.8306 (3)	0.0404 (5)
H14	0.415206	0.350797	0.882787	0.048*
C15	0.28218 (18)	0.42748 (10)	0.7510 (2)	0.0354 (4)
C16	0.27491 (18)	0.49510 (10)	0.6721 (2)	0.0361 (4)
H16	0.189425	0.515213	0.618100	0.043*
C17	0.03785 (19)	0.41217 (11)	0.6707 (3)	0.0479 (5)
H17A	0.035499	0.420573	0.544548	0.072*
H17B	0.020241	0.457065	0.726766	0.072*
H17C	−0.031685	0.377089	0.681216	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0366 (8)	0.0462 (9)	0.0653 (10)	−0.0042 (6)	−0.0031 (7)	0.0009 (7)
O2	0.0305 (7)	0.0323 (7)	0.0453 (8)	0.0010 (5)	0.0071 (5)	0.0060 (6)
O3	0.0325 (7)	0.0322 (8)	0.0835 (11)	0.0029 (6)	0.0051 (7)	0.0152 (7)
O4	0.0315 (7)	0.0401 (8)	0.0685 (10)	0.0041 (6)	0.0027 (6)	0.0121 (7)
O5	0.0385 (8)	0.0413 (8)	0.0565 (9)	−0.0074 (6)	0.0077 (6)	0.0086 (6)
C1	0.0383 (10)	0.0371 (11)	0.0443 (12)	−0.0015 (8)	0.0103 (8)	−0.0043 (8)
C2	0.0337 (10)	0.0303 (10)	0.0380 (10)	−0.0001 (8)	0.0097 (7)	−0.0062 (8)
C3	0.0322 (10)	0.0352 (10)	0.0418 (11)	0.0037 (8)	0.0024 (8)	0.0009 (8)
C4	0.0376 (10)	0.0316 (10)	0.0430 (11)	0.0017 (8)	0.0087 (8)	0.0025 (8)
C5	0.0305 (9)	0.0316 (10)	0.0359 (10)	0.0038 (7)	0.0073 (7)	−0.0033 (7)
C6	0.0339 (10)	0.0374 (11)	0.0486 (12)	0.0040 (8)	0.0081 (8)	0.0085 (9)
C7	0.0370 (10)	0.0331 (10)	0.0443 (11)	−0.0001 (8)	0.0105 (8)	0.0046 (8)
C8	0.0335 (10)	0.0289 (10)	0.0372 (10)	0.0016 (7)	0.0087 (7)	0.0007 (7)
C9	0.0354 (10)	0.0270 (10)	0.0431 (11)	0.0010 (8)	0.0082 (8)	0.0018 (8)
C10	0.0310 (10)	0.0341 (10)	0.0399 (11)	0.0024 (8)	0.0066 (8)	−0.0005 (8)
C11	0.0307 (9)	0.0294 (9)	0.0338 (10)	0.0011 (7)	0.0081 (7)	−0.0009 (7)
C12	0.0323 (9)	0.0313 (10)	0.0342 (10)	0.0004 (7)	0.0075 (7)	−0.0009 (7)
C13	0.0379 (10)	0.0360 (11)	0.0415 (11)	0.0049 (8)	0.0044 (8)	0.0062 (8)
C14	0.0436 (11)	0.0333 (10)	0.0427 (11)	−0.0001 (8)	0.0066 (8)	0.0068 (8)
C15	0.0372 (10)	0.0345 (10)	0.0352 (10)	−0.0051 (8)	0.0096 (8)	−0.0023 (8)
C16	0.0329 (10)	0.0352 (10)	0.0398 (11)	0.0012 (8)	0.0071 (7)	−0.0003 (8)
C17	0.0358 (11)	0.0466 (12)	0.0604 (14)	−0.0061 (9)	0.0093 (9)	0.0029 (10)

Geometric parameters (Å, º)

O1—C1	1.210 (2)	C6—H6	0.9300
O2—C8	1.375 (2)	C6—C7	1.375 (2)
O2—C12	1.366 (2)	C7—H7	0.9300
O3—H3	0.89 (2)	C8—C9	1.351 (2)
O3—C9	1.356 (2)	C9—C10	1.451 (2)
O4—C10	1.2354 (19)	C10—C11	1.449 (2)
O5—C15	1.366 (2)	C11—C12	1.382 (2)
O5—C17	1.424 (2)	C11—C16	1.404 (2)
C1—H1	0.9300	C12—C13	1.392 (2)
C1—C2	1.465 (2)	C13—H13	0.9300
C2—C3	1.392 (2)	C13—C14	1.365 (2)
C2—C7	1.384 (2)	C14—H14	0.9300
C3—H3A	0.9300	C14—C15	1.401 (2)
C3—C4	1.377 (2)	C15—C16	1.371 (3)
C4—H4	0.9300	C16—H16	0.9300
C4—C5	1.403 (2)	C17—H17A	0.9600
C5—C6	1.395 (3)	C17—H17B	0.9600
C5—C8	1.466 (2)	C17—H17C	0.9600
C12—O2—C8	120.37 (13)	C8—C9—C10	122.34 (16)

C9—O3—H3	108.8 (16)	O4—C10—C9	120.39 (16)
C15—O5—C17	116.97 (14)	O4—C10—C11	124.31 (16)
O1—C1—H1	117.7	C11—C10—C9	115.29 (15)
O1—C1—C2	124.56 (18)	C12—C11—C10	119.27 (15)
C2—C1—H1	117.7	C12—C11—C16	119.29 (16)
C3—C2—C1	121.82 (17)	C16—C11—C10	121.44 (15)
C7—C2—C1	119.26 (17)	O2—C12—C11	122.29 (15)
C7—C2—C3	118.86 (16)	O2—C12—C13	116.72 (15)
C2—C3—H3A	120.0	C11—C12—C13	120.99 (16)
C4—C3—C2	120.07 (17)	C12—C13—H13	120.4
C4—C3—H3A	120.0	C14—C13—C12	119.23 (17)
C3—C4—H4	119.3	C14—C13—H13	120.4
C3—C4—C5	121.30 (17)	C13—C14—H14	119.7
C5—C4—H4	119.3	C13—C14—C15	120.67 (17)
C4—C5—C8	120.21 (16)	C15—C14—H14	119.7
C6—C5—C4	117.91 (16)	O5—C15—C14	115.02 (16)
C6—C5—C8	121.88 (16)	O5—C15—C16	124.85 (16)
C5—C6—H6	119.7	C16—C15—C14	120.13 (17)
C7—C6—C5	120.51 (17)	C11—C16—H16	120.2
C7—C6—H6	119.7	C15—C16—C11	119.69 (17)
C2—C7—H7	119.3	C15—C16—H16	120.2
C6—C7—C2	121.33 (17)	O5—C17—H17A	109.5
C6—C7—H7	119.3	O5—C17—H17B	109.5
O2—C8—C5	111.39 (14)	O5—C17—H17C	109.5
C9—C8—O2	120.31 (15)	H17A—C17—H17B	109.5
C9—C8—C5	128.29 (16)	H17A—C17—H17C	109.5
O3—C9—C10	116.47 (15)	H17B—C17—H17C	109.5
C8—C9—O3	121.19 (16)		

O1—C1—C2—C3	−7.2 (3)	C7—C2—C3—C4	−0.6 (3)
O1—C1—C2—C7	170.05 (18)	C8—O2—C12—C11	1.6 (2)
O2—C8—C9—O3	179.08 (16)	C8—O2—C12—C13	−177.93 (16)
O2—C8—C9—C10	−1.7 (3)	C8—C5—C6—C7	−179.85 (17)
O2—C12—C13—C14	179.03 (16)	C8—C9—C10—O4	−176.81 (18)
O3—C9—C10—O4	2.4 (3)	C8—C9—C10—C11	3.9 (3)
O3—C9—C10—C11	−176.89 (16)	C9—C10—C11—C12	−3.3 (2)
O4—C10—C11—C12	177.41 (18)	C9—C10—C11—C16	176.49 (16)
O4—C10—C11—C16	−2.8 (3)	C10—C11—C12—O2	0.7 (3)
O5—C15—C16—C11	179.50 (15)	C10—C11—C12—C13	−179.71 (17)
C1—C2—C3—C4	176.63 (16)	C10—C11—C16—C15	−179.66 (17)
C1—C2—C7—C6	−176.28 (17)	C11—C12—C13—C14	−0.5 (3)
C2—C3—C4—C5	−0.3 (3)	C12—O2—C8—C5	178.44 (14)
C3—C2—C7—C6	1.0 (3)	C12—O2—C8—C9	−1.1 (2)
C3—C4—C5—C6	0.8 (3)	C12—C11—C16—C15	0.1 (3)
C3—C4—C5—C8	−179.71 (16)	C12—C13—C14—C15	0.0 (3)
C4—C5—C6—C7	−0.4 (3)	C13—C14—C15—O5	−179.54 (16)
C4—C5—C8—O2	−11.8 (2)	C13—C14—C15—C16	0.6 (3)
C4—C5—C8—C9	167.75 (18)	C14—C15—C16—C11	−0.7 (3)

C5—C6—C7—C2	−0.5 (3)	C16—C11—C12—O2	−179.07 (15)
C5—C8—C9—O3	−0.4 (3)	C16—C11—C12—C13	0.5 (3)
C5—C8—C9—C10	178.76 (16)	C17—O5—C15—C14	−176.38 (16)
C6—C5—C8—O2	167.64 (16)	C17—O5—C15—C16	3.4 (3)
C6—C5—C8—C9	−12.8 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1^{i}	0.89 (2)	2.02 (2)	2.8304 (18)	151 (2)
O3—H3···O4	0.89 (2)	2.20 (2)	2.6853 (18)	113.6 (19)
C6—H6···O3	0.93	2.20	2.834 (2)	12

Symmetry code: (i) *x*−1, −*y*+3/2, *z*−1/2.