

Crystal structure and Hirshfeld surface analysis of luteolin dimethyl sulfoxide monosolvate

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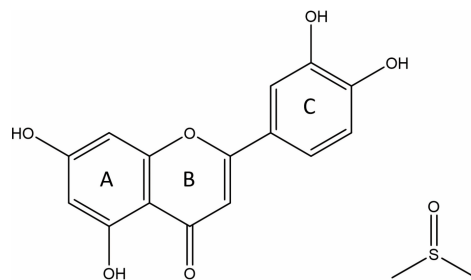
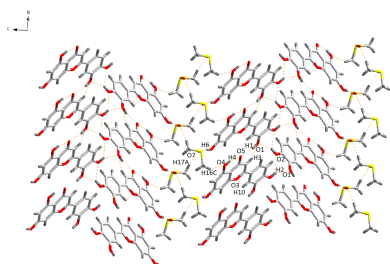
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Keywords: luteolin; dimethyl sulfoxide; Hirshfeld surface analysis; crystal structure.**CCDC reference:** 2537224**Supporting information:** this article has supporting information at journals.iucr.org/e

The title compound, 3',4',5,7-tetrahydroxyflavone dimethyl sulfoxide monosolvate (LUT-DMSO), $C_{21}H_{16}O_6 \cdot C_2H_6OS$, crystallizes in the monoclinic space group $P2_1$. The LUT molecule adopts a planar conformation, and the crystal structure is consolidated by extensive hydrogen-bonding interactions. Hirshfeld surface analysis indicates that the predominant intermolecular interactions are $O \cdots H/H \cdots O$, $C \cdots H/H \cdots C$, and $H \cdots H$, with these contacts contributing significantly to the overall cohesion of the crystal.

1. Chemical context

Luteolin (3',4',5-tetrahydroxyflavone) is a naturally occurring flavonoid found in multiple flora such as honeysuckle, scutellaria (Lamiaceae), dandelion (Asteraceae), as well as peanut shells and corn whiskers (Mahwish *et al.*, 2025). This compound has received worldwide research interest due to its wide variety of biological activities, particularly antioxidant, anti-inflammatory, anticancer, and neuroprotective properties (Zhang & Ma, 2024). Luteolin is a potent antioxidant which promotes the expression of antioxidant enzymes (*e.g.* SOD, heme oxygenase-1, HO-1) and scavenges reactive oxygen species (ROS) therefore reducing oxidative stress. Luteolin's anti-inflammatory activity results from the inhibition of numerous pro-inflammatory cytokines and enzymes (TNF- α , IL-6, COX-2, iNOS) and the modulation of cellular signalling pathways (NF- κ B, MAPK/AP-1) (Pandey *et al.*, 2025). With regards to cancer, luteolin has been shown to induce apoptosis, inhibit cell proliferation, and reduce angiogenesis in various cancer models from breast, colon, and pancreatic cancer (Prasher *et al.*, 2022). Research has shown that luteolin exerts neuroprotection in models of Alzheimer's and Parkinson's disease by decreasing neuro-inflammation, oxidative damage, and neuronal apoptosis (Zhu *et al.*, 2024).



In this study, we report the crystal structure and Hirshfeld surface analysis of luteolin dimethyl sulfoxide solvate, which has not previously been reported in the literature.

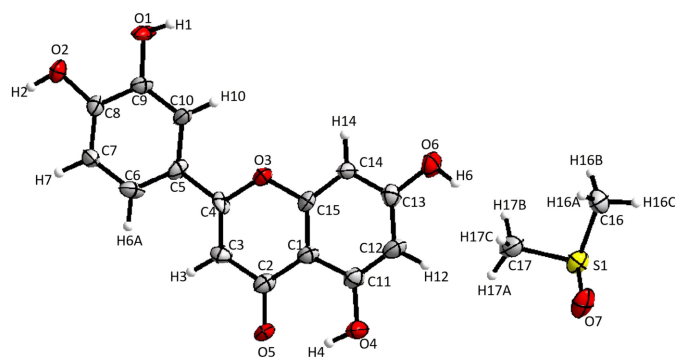


Figure 1
The molecular structure of LUT-DMSO, with atomic displacement ellipsoids drawn at the 30% probability level, showing the atom labeling. Hydrogen atoms are represented as small spheres with arbitrary radii.

2. Structural commentary

LUT-DMSO crystallizes in the monoclinic space group $P2_1$. The asymmetric unit consists of one LUT molecule and one DMSO molecule, as depicted in Fig. 1. The luteolin molecules adopt a planar configuration due to conjugation in the flavonoid backbone. The dihedral angle between the fused rings is $2.2 (5)^\circ$ and that between the phenyl ring and the fused ring system is $3.1 (4)^\circ$. The torsion angles for $O3-C4-C5-C6$, $O3-C4-C5-C10$, $C3-C4-C5-C6$, and $C3-C4-C5-C10$ are $177.7 (9)$, $-1.9 (14)$, $-1.8 (16)$, and $178.6 (10)^\circ$, respectively. Several intramolecular hydrogen bonds are also observed within the LUT molecules ($O4-H4 \cdots O5$, $O6-H6 \cdots O7$, and $C10-H10 \cdots O3$; Table 1).

3. Supramolecular features

In the crystal, each LUT and DMSO molecule is involved in extensive hydrogen-bonding interactions, contributing to crystal cohesion (Fig. 2, Table 1). DMSO molecules are connected to neighboring DMSO molecules through $C17-H17A \cdots O7$ interactions, forming a chain-like structure.

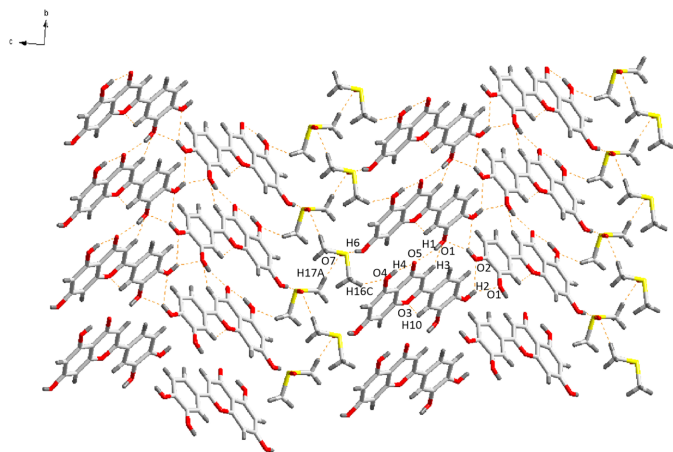


Figure 2
Hydrogen-bond networks in LUT-DMSO, showing the two-dimensional network parallel to the (100) plane (hydrogen bonding is indicated by orange dashed lines).

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1-H1 \cdots O5^i$	0.84	1.83	2.649 (11)	163
$O2-H2 \cdots O1^{ii}$	0.84	2.14	2.846 (11)	142
$O2-H2 \cdots O2^{ii}$	0.84	2.35	2.989 (11)	133
$O4-H4 \cdots O5$	0.84	1.79	2.626 (10)	170
$O6-H6 \cdots O7^{iii}$	0.84	1.79	2.626 (10)	170
$C3-H3 \cdots O1^{iv}$	0.95	2.54	3.220 (13)	129
$C10-H10 \cdots O3$	0.95	2.35	2.682 (11)	100
$C16-H16C \cdots O4^{iii}$	0.98	2.44	3.293 (15)	145
$C17-H17A \cdots O7^v$	0.98	2.39	3.308 (18)	156

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

The DMSO molecules also interact with LUT molecules through $C16-H16C \cdots O4$ and $O6-H6 \cdots O7$ hydrogen bonds. The LUT molecules are connected to each other through $O1-H1 \cdots O5$, $C3-H3 \cdots O1$, $O2-H2 \cdots O1$, and $O2-H2 \cdots O2$ hydrogen bonds. Collectively, these interactions give rise to a two-dimensional network that lies parallel to the (100) plane, as illustrated in Fig. 2.

To validate the hydrogen-bonding interactions observed in LUT-DMSO, we have compared the observed donor-acceptor distances with those found in other luteolin-containing crystal structures, such as ZIKPUG01 and ZIKPUG02 (cocrystals with isonicotinamide; Sowa *et al.*, 2013) and VOHKIO (a dapsone-luteolin-ethanol solvate; Jiang *et al.*, 2014). In our structure, the intramolecular $O \cdots O$ distances are $2.626 (10) \text{\AA}$ ($O4-H4 \cdots O5$) and the $C \cdots O$ distance is $2.682 (11) \text{\AA}$ ($C10-H10 \cdots O3$). The intermolecular $O \cdots O$ distances range from $2.649 (11)$ to $2.989 (11) \text{\AA}$, and the intermolecular $C \cdots O$ distances range from $3.220 (13)$ to $3.308 (18) \text{\AA}$. When compared with other luteolin-containing crystal structures, all $D \cdots A$ distances in the title structure fall within typical ranges for $O-H \cdots O$ and $C-H \cdots O$ hydrogen bonds, except for the intramolecular $C \cdots O$ contact ($C10-H10 \cdots O3$), which appears slightly shorter. However, this short distance is likely due to the rigidity of the luteolin backbone, which forces the $O3$ and $C10$ atoms into close proximity, rather than an artefact of the riding model. The $H \cdots A$ distance of 2.35\AA for this interaction is well within the range of normal $C-H \cdots O$ hydrogen bonds. No similar intramolecular $C-H \cdots O$ hydrogen bond has been reported in other LUT structures, possibly because of differences in molecular conformation or crystal packing. Therefore, we conclude that the hydrogen-bonding geometry in the title structure is reasonable and consistent with known LUT-containing crystals.

4. Hirshfeld surface analysis

The Hirshfeld surface analysis of LUT-DMSO was conducted to evaluate the intermolecular interactions within the crystal structure. Hirshfeld surfaces and fingerprint plots (Spackman & McKinnon, 2002; Spackman & Jayatilaka, 2009) were generated using *CrystalExplorer* software (Spackman *et al.*, 2021). Fig. 3 shows the Hirshfeld surfaces and the corresponding two-dimensional fingerprint plots for the LUT

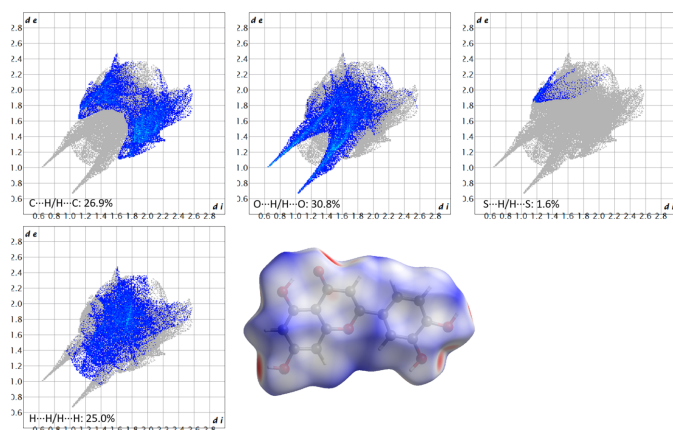


Figure 3
Hirshfeld surfaces and the corresponding two-dimensional fingerprint plots of various hydrogen-bonding and van der Waals interactions for the LUT molecule of LUT-DMSO. The d_i and d_e values represent the closest internal and external distances (in Å), respectively, from given points on the Hirshfeld surface.

molecule, while Fig. 4 illustrates the same for the DMSO molecule.

For the LUT molecule, the predominant intermolecular interactions are $O\cdots H/H\cdots O$, $C\cdots H/H\cdots C$, $H\cdots H$, and $S\cdots H/H\cdots S$, which account for 84.3% of the total interactions, indicating their significant role in consolidating the structure. Among these, $O\cdots H/H\cdots O$ interactions are the most prevalent, contributing 30.8% of the Hirshfeld surface, followed by $C\cdots H/H\cdots C$ (26.9%) and $H\cdots H$ (25.0%) interactions. The $S\cdots H/H\cdots S$ interaction is relatively weak, contributing only 1.6% of the Hirshfeld surface.

For the DMSO molecule (Fig. 4), the most significant contacts are $H\cdots H$, $O\cdots H/H\cdots O$, $S\cdots H/H\cdots S$ and $C\cdots H/H\cdots C$. The $H\cdots H$ interaction is the dominant contributor, accounting for 46.4%, followed by $O\cdots H/H\cdots O$ (35.9%), $S\cdots H/H\cdots S$ (9.3%) and $C\cdots H/H\cdots C$ (7.0%) interactions.

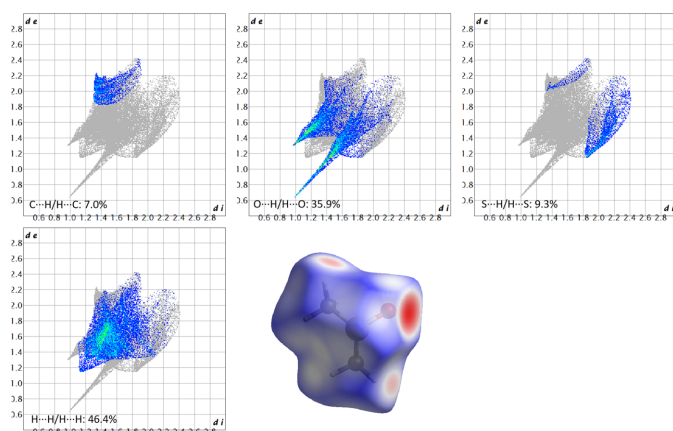


Figure 4
Hirshfeld surfaces and the corresponding two-dimensional fingerprint plots of various hydrogen-bonding and van der Waals interactions for the DMSO molecule of LUT-DMSO. The d_i and d_e values represent the closest internal and external distances (in Å), respectively, from given points on the Hirshfeld surface.

The total contribution of these interactions is 98.6%, emphasizing their dominant role in the structural cohesion.

In both molecules, the Hirshfeld surface offers a clear depiction of molecular interactions, with the majority of red spots on the surface corresponding to $O\cdots H$ interactions, which are also reflected in the 2D fingerprint plots as prominent spikes. These findings emphasize the crucial role of hydrogen bonding and van der Waals interactions in determining the packing and cohesion of the LUT-DMSO crystal.

5. Database survey

A survey of the Cambridge Structural Database WebCSD, May 2025; Groom *et al.*, 2016) did not reveal any structures of LUT-DMSO. The survey revealed seven crystal structures that related to LUT compounds, *viz.* OJEQUP, EJEPUG, EJEQIV, VOHKIO, ZIKPUG, ZIKPUG01 and ZIKPUG02. OJEQUP (Cox *et al.*, 2003) is a hemihydrate of luteolin, although the water molecules were disordered and not located, which crystallize in the monoclinic $C2$ space group. EJEPUG and EJEQIV (He *et al.*, 2016) are cocrystals of LUT with proline. Luteolin is a poorly soluble compound and the cocrystallization of LUT with L-proline and D-proline is useful for solubility enhancement. Additionally, the structures VOHKIO (a dapsone-luteolin ethanol solvate; Jiang *et al.*, 2014) and ZIKPUG, ZIKPUG01, ZIKPUG02 (cocrystals of luteolin with isonicotinamide, with ZIKPUG and ZIKPUG01 representing one polymorph and ZIKPUG02 a second polymorph; Sowa *et al.*, 2013) have also been reported, further illustrating the versatility of luteolin in forming multi-component crystals and its polymorphic behavior.

6. Synthesis and crystallization

The commercially available form of luteolin (98%) was purchased from Aladdin. LUT (50 mg, 0.18 mmol) was dissolved in 15 mL of DMSO by heating. Colorless plate-like single crystals were obtained by slowly evaporating the filtrated solution at room temperature for 30 days.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Due to the limited data quality, the hydrogen atoms attached to oxygen atoms could not be located in the difference-Fourier map. Therefore, all H atoms were placed in geometrically calculated positions and refined using a riding model.

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References

Bruker (2019). *APEX5* and *SAINT*. Bruker AXS Inc. Madison, Wisconsin, USA.

Cox, P. J., Kumarasamy, Y., Nahar, L., Sarker, S. D. & Shoeb, M. (2003). *Acta Cryst.* **E59**, o975–o977.

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

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.

He, H., Huang, Y., Zhang, Q., Wang, J.-R. & Mei, X. (2016). *Cryst. Growth Des.* **16**, 2348–2356.

Jiang, L., Huang, Y., Zhang, Q., He, H., Xu, Y. & Mei, X. (2014). *Cryst. Growth Des.* **14**, 4562–4573.

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

Mahwish, Imran, M., Naeem, H., Hussain, M., Alsagaby, S. A., Al Abdulmonem, W., Mujtaba, A., Abdelgawad, M. A., Ghoneim, M. M., El-Ghorab, A. H., Selim, S., Al Jaouni, S. K., Mostafa, E. M. & Yehuala, T. F. (2025). *Food. Sci. & Nutr.* **13**, e4682.

Pandey, P., Lakhanpal, S., Mahmood, D., Kang, H. N., Kim, B., Kang, S., Choi, J., Choi, M., Pandey, S., Bhat, M., Sharma, S., Khan, F., Park, M. N. & Kim, B. (2025). *Front. Pharmacol.* **15**, 1513422.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* **B69**, 249–259.

Pennington, W. T. (1999). *J. Appl. Cryst.* **32**, 1028–1029.

Prasher, P., Sharma, M., Singh, S. K., Gulati, M., Chellappan, D. K., Zaccaroni, F., De Rubis, G., Gupta, G., Sharifi-Rad, J., Cho, W. C. & Dua, K. (2022). *Cancer Cell Int.* **22**, 386.

Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.

Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.

Sowa, M., Ślepokura, K. & Matczak-Jon, E. (2013). *CrystEngComm* **15**, 7696–7708.

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

Spackman, M. A. & McKinnon, J. J. (2002). *CrystEngComm* **4**, 378–392.

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.

Spek, A. L. (2020). *Acta Cryst.* **E76**, 1–11.

Table 2

Experimental details.

Crystal data	
Chemical formula	C ₂ H ₆ OS·C ₁₅ H ₁₀ O ₆
<i>M_r</i>	364.36
Crystal system, space group	Monoclinic, <i>P2</i> ₁
Temperature (K)	170
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.676 (2), 5.6991 (17), 20.724 (6)
β (°)	90.749 (11)
<i>V</i> (Å ³)	788.4 (4)
<i>Z</i>	2
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.25
Crystal size (mm)	0.12 × 0.06 × 0.04
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.479, 0.745
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	5797, 3000, 1894
<i>R</i> _{int}	0.083
(sin θ/λ) _{max} (Å ⁻¹)	0.628
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.095, 0.284, 1.04
No. of reflections	3000
No. of parameters	232
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	1.08, -0.56
Absolute structure	Flack <i>x</i> determined using 528 quotients [(<i>I</i> ⁺) - (<i>I</i> ⁻)] / [(<i>I</i> ⁺) + (<i>I</i> ⁻)] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.3 (2)

Computer programs: *APEX5* (Bruker, 2019) and *SAINT* (Bruker, 2019), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL2025/1* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009), *DIAMOND* (Pennington, 1999) and *PLATON* (Spek, 2020).

Zhang, J. & Ma, Y. (2024). *Biomed. Pharmacother.* **176**, 116909.

Zhu, M., Sun, Y., Su, Y., Guan, W., Wang, Y., Han, J., Wang, S., Yang, B., Wang, Q. & Kuang, H. (2024). *Phytother. Res.* **38**, 3417–3443.

supporting information

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Crystal structure and Hirshfeld surface analysis of luteolin dimethyl sulfoxide monosolvate

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Computing details

3',4',5,7-Tetrahydroxyflavone dimethyl sulfoxide monosolvate

Crystal data

$C_2H_6OS \cdot C_{15}H_{10}O_6$

$M_r = 364.36$

Monoclinic, $P2_1$

$a = 6.676$ (2) Å

$b = 5.6991$ (17) Å

$c = 20.724$ (6) Å

$\beta = 90.749$ (11)°

$V = 788.4$ (4) Å³

$Z = 2$

$F(000) = 380$

$D_x = 1.535$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1758 reflections

$\theta = 3.0$ – 25.4 °

$\mu = 0.25$ mm⁻¹

$T = 170$ K

Plate, colourless

$0.12 \times 0.06 \times 0.04$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.479$, $T_{\max} = 0.745$

5797 measured reflections

3000 independent reflections

1894 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.083$

$\theta_{\max} = 26.5$ °, $\theta_{\min} = 2.0$ °

$h = -7 \rightarrow 8$

$k = -7 \rightarrow 7$

$l = -25 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.095$

$wR(F^2) = 0.284$

$S = 1.04$

3000 reflections

232 parameters

1 restraint

Primary atom site location: dual

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1706P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.08$ e Å⁻³

$\Delta\rho_{\min} = -0.56$ e Å⁻³

Absolute structure: Flack x determined using

528 quotients $[(I^-)-(I)]/[(I^+)+(I)]$ (Parsons *et al.*, 2013)

Absolute structure parameter: 0.3 (2)

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.1500 (4)	0.6686 (6)	0.42114 (13)	0.0341 (7)
O3	0.7284 (9)	0.6422 (15)	0.7946 (3)	0.0290 (17)
O5	0.2840 (9)	1.1285 (14)	0.8075 (3)	0.0307 (18)
O2	1.4443 (10)	0.7383 (14)	0.9875 (4)	0.0338 (19)
H2	1.455877	0.842373	1.015966	0.051*
O1	1.3744 (10)	0.4339 (13)	0.8997 (4)	0.0344 (18)
H1	1.328777	0.326151	0.876010	0.052*
O6	0.3923 (11)	0.2151 (16)	0.6316 (4)	0.040 (2)
H6	0.281819	0.208826	0.611833	0.060*
O7	-0.0686 (9)	0.6616 (19)	0.4402 (3)	0.044 (2)
O4	0.0868 (11)	0.9060 (15)	0.7183 (4)	0.039 (2)
H4	0.110142	1.006989	0.746933	0.059*
C8	1.2725 (15)	0.7742 (18)	0.9529 (5)	0.026 (2)
C2	0.4218 (15)	0.9746 (19)	0.8028 (5)	0.029 (2)
C3	0.5968 (16)	0.9797 (19)	0.8422 (5)	0.028 (2)
H3	0.613272	1.103081	0.872606	0.034*
C15	0.5642 (14)	0.6218 (19)	0.7539 (5)	0.028 (2)
C1	0.4081 (15)	0.7865 (19)	0.7581 (5)	0.027 (2)
C5	0.9248 (14)	0.8020 (18)	0.8774 (5)	0.026 (2)
C6	0.9677 (15)	0.9718 (19)	0.9236 (5)	0.031 (2)
H6A	0.877755	1.098973	0.929489	0.038*
C9	1.2322 (14)	0.6052 (18)	0.9063 (5)	0.028 (2)
C7	1.1419 (15)	0.957 (2)	0.9614 (5)	0.028 (2)
H7	1.170055	1.074020	0.992951	0.033*
C4	0.7407 (16)	0.8147 (17)	0.8377 (5)	0.027 (2)
C10	1.0600 (14)	0.618 (2)	0.8688 (5)	0.032 (3)
H10	1.033488	0.501847	0.836968	0.039*
C14	0.5649 (15)	0.436 (2)	0.7119 (5)	0.030 (2)
H14	0.676190	0.332721	0.709358	0.036*
C11	0.2402 (15)	0.750 (2)	0.7166 (6)	0.033 (3)
C13	0.3934 (16)	0.406 (2)	0.6728 (5)	0.032 (2)
C17	0.2812 (16)	0.694 (3)	0.4955 (6)	0.043 (3)
H17A	0.258720	0.850210	0.513707	0.065*
H17B	0.424791	0.671107	0.488408	0.065*
H17C	0.232927	0.574415	0.525507	0.065*
C12	0.2344 (17)	0.565 (2)	0.6751 (6)	0.040 (3)
H12	0.121274	0.543977	0.647397	0.048*
C16	0.2299 (19)	0.368 (2)	0.4044 (6)	0.042 (3)
H16A	0.194864	0.266227	0.440778	0.063*

H16B	0.375277	0.364226	0.398410	0.063*
H16C	0.162438	0.310979	0.365127	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0286 (13)	0.0364 (15)	0.0373 (14)	-0.0047 (13)	-0.0010 (9)	0.0028 (14)
O3	0.020 (3)	0.037 (4)	0.030 (3)	0.004 (4)	-0.005 (2)	-0.005 (4)
O5	0.022 (3)	0.037 (5)	0.033 (4)	0.010 (3)	-0.008 (3)	-0.003 (4)
O2	0.026 (4)	0.040 (5)	0.035 (4)	-0.001 (3)	-0.012 (3)	-0.007 (3)
O1	0.029 (4)	0.018 (4)	0.055 (5)	0.009 (3)	-0.010 (3)	-0.008 (4)
O6	0.030 (4)	0.051 (6)	0.039 (4)	-0.006 (4)	-0.008 (3)	-0.009 (4)
O7	0.022 (4)	0.069 (6)	0.040 (4)	-0.015 (5)	-0.002 (3)	0.006 (5)
O4	0.032 (4)	0.036 (5)	0.051 (5)	0.013 (4)	-0.009 (3)	-0.011 (4)
C8	0.029 (5)	0.023 (5)	0.025 (5)	-0.002 (4)	-0.006 (4)	0.002 (5)
C2	0.024 (5)	0.024 (6)	0.037 (6)	-0.001 (4)	-0.005 (4)	0.004 (5)
C3	0.033 (6)	0.019 (5)	0.034 (6)	0.004 (4)	-0.001 (4)	0.000 (5)
C15	0.027 (5)	0.032 (6)	0.023 (5)	0.004 (5)	-0.007 (3)	0.002 (5)
C1	0.021 (5)	0.029 (6)	0.033 (6)	0.002 (4)	-0.002 (4)	0.001 (5)
C5	0.017 (5)	0.026 (6)	0.036 (6)	-0.005 (4)	-0.007 (4)	0.001 (5)
C6	0.021 (5)	0.024 (6)	0.049 (7)	0.003 (4)	0.005 (4)	-0.006 (5)
C9	0.021 (5)	0.028 (6)	0.036 (6)	0.003 (4)	0.000 (4)	0.000 (5)
C7	0.035 (6)	0.027 (6)	0.022 (5)	0.007 (5)	0.001 (4)	-0.003 (5)
C4	0.042 (6)	0.013 (5)	0.025 (6)	-0.004 (4)	-0.004 (4)	-0.005 (4)
C10	0.024 (5)	0.047 (7)	0.026 (5)	0.012 (5)	-0.004 (4)	0.001 (5)
C14	0.024 (5)	0.027 (6)	0.040 (6)	0.007 (4)	-0.006 (4)	-0.009 (5)
C11	0.025 (6)	0.034 (6)	0.038 (6)	0.001 (4)	-0.003 (4)	-0.003 (5)
C13	0.030 (6)	0.031 (6)	0.034 (6)	-0.004 (5)	-0.003 (4)	-0.006 (5)
C17	0.038 (6)	0.049 (8)	0.043 (6)	0.009 (6)	-0.002 (5)	0.006 (7)
C12	0.027 (6)	0.049 (7)	0.043 (7)	0.010 (5)	-0.007 (5)	0.002 (6)
C16	0.047 (7)	0.035 (7)	0.045 (7)	0.001 (6)	-0.009 (5)	-0.011 (6)

Geometric parameters (Å, °)

S1—O7	1.518 (7)	C15—C14	1.370 (15)
S1—C17	1.768 (12)	C1—C11	1.419 (15)
S1—C16	1.831 (13)	C5—C6	1.388 (15)
O3—C15	1.380 (11)	C5—C4	1.472 (14)
O3—C4	1.330 (12)	C5—C10	1.395 (14)
O5—C2	1.276 (12)	C6—H6A	0.9500
O2—H2	0.8400	C6—C7	1.397 (14)
O2—C8	1.359 (12)	C9—C10	1.382 (14)
O1—H1	0.8400	C7—H7	0.9500
O1—C9	1.370 (12)	C10—H10	0.9500
O6—H6	0.8400	C14—H14	0.9500
O6—C13	1.382 (14)	C14—C13	1.405 (14)
O4—H4	0.8400	C11—C12	1.362 (17)
O4—C11	1.356 (13)	C13—C12	1.398 (15)

C8—C9	1.389 (15)	C17—H17A	0.9800
C8—C7	1.372 (14)	C17—H17B	0.9800
C2—C3	1.416 (14)	C17—H17C	0.9800
C2—C1	1.420 (15)	C12—H12	0.9500
C3—H3	0.9500	C16—H16A	0.9800
C3—C4	1.348 (14)	C16—H16B	0.9800
C15—C1	1.406 (14)	C16—H16C	0.9800
O7—S1—C17	104.0 (5)	C8—C7—H7	120.0
O7—S1—C16	107.9 (6)	C6—C7—H7	120.0
C17—S1—C16	95.7 (6)	O3—C4—C3	121.6 (9)
C4—O3—C15	121.0 (8)	O3—C4—C5	112.5 (9)
C8—O2—H2	109.5	C3—C4—C5	125.9 (9)
C9—O1—H1	109.5	C5—C10—H10	119.9
C13—O6—H6	109.5	C9—C10—C5	120.2 (10)
C11—O4—H4	109.5	C9—C10—H10	119.9
O2—C8—C9	114.6 (9)	C15—C14—H14	121.6
O2—C8—C7	125.5 (9)	C15—C14—C13	116.8 (9)
C7—C8—C9	119.9 (9)	C13—C14—H14	121.6
O5—C2—C3	122.2 (9)	O4—C11—C1	118.7 (10)
O5—C2—C1	121.9 (9)	O4—C11—C12	120.6 (10)
C3—C2—C1	115.9 (9)	C12—C11—C1	120.7 (10)
C2—C3—H3	119.0	O6—C13—C14	116.8 (9)
C4—C3—C2	122.0 (10)	O6—C13—C12	122.2 (10)
C4—C3—H3	119.0	C12—C13—C14	121.0 (11)
O3—C15—C1	119.3 (9)	S1—C17—H17A	109.5
C14—C15—O3	116.4 (9)	S1—C17—H17B	109.5
C14—C15—C1	124.3 (9)	S1—C17—H17C	109.5
C15—C1—C2	120.2 (9)	H17A—C17—H17B	109.5
C15—C1—C11	116.5 (10)	H17A—C17—H17C	109.5
C11—C1—C2	123.3 (9)	H17B—C17—H17C	109.5
C6—C5—C4	120.9 (9)	C11—C12—C13	120.6 (11)
C6—C5—C10	119.0 (9)	C11—C12—H12	119.7
C10—C5—C4	120.1 (9)	C13—C12—H12	119.7
C5—C6—H6A	119.7	S1—C16—H16A	109.5
C5—C6—C7	120.5 (9)	S1—C16—H16B	109.5
C7—C6—H6A	119.7	S1—C16—H16C	109.5
O1—C9—C8	115.9 (9)	H16A—C16—H16B	109.5
O1—C9—C10	123.7 (10)	H16A—C16—H16C	109.5
C10—C9—C8	120.4 (10)	H16B—C16—H16C	109.5
C8—C7—C6	120.0 (10)		
O3—C15—C1—C2	1.4 (15)	C15—C14—C13—O6	-178.5 (9)
O3—C15—C1—C11	-177.7 (9)	C15—C14—C13—C12	2.8 (17)
O3—C15—C14—C13	176.4 (10)	C1—C2—C3—C4	-0.6 (15)
O5—C2—C3—C4	179.0 (9)	C1—C15—C14—C13	-2.8 (16)
O5—C2—C1—C15	179.3 (10)	C1—C11—C12—C13	0.4 (17)
O5—C2—C1—C11	-1.8 (16)	C5—C6—C7—C8	0.1 (15)

O2—C8—C9—O1	-2.9 (13)	C6—C5—C4—O3	177.7 (9)
O2—C8—C9—C10	178.6 (10)	C6—C5—C4—C3	-1.8 (16)
O2—C8—C7—C6	-178.6 (10)	C6—C5—C10—C9	0.8 (15)
O1—C9—C10—C5	-178.3 (9)	C9—C8—C7—C6	0.7 (15)
O6—C13—C12—C11	179.6 (10)	C7—C8—C9—O1	177.7 (9)
O4—C11—C12—C13	179.4 (11)	C7—C8—C9—C10	-0.8 (15)
C8—C9—C10—C5	0.0 (15)	C4—O3—C15—C1	0.1 (14)
C2—C3—C4—O3	2.1 (16)	C4—O3—C15—C14	-179.1 (9)
C2—C3—C4—C5	-178.4 (10)	C4—C5—C6—C7	179.5 (10)
C2—C1—C11—O4	1.7 (16)	C4—C5—C10—C9	-179.6 (10)
C2—C1—C11—C12	-179.2 (10)	C10—C5—C6—C7	-0.9 (15)
C3—C2—C1—C15	-1.1 (14)	C10—C5—C4—O3	-1.9 (14)
C3—C2—C1—C11	177.8 (10)	C10—C5—C4—C3	178.6 (10)
C15—O3—C4—C3	-1.9 (14)	C14—C15—C1—C2	-179.5 (10)
C15—O3—C4—C5	178.6 (8)	C14—C15—C1—C11	1.5 (16)
C15—C1—C11—O4	-179.3 (9)	C14—C13—C12—C11	-1.7 (18)
C15—C1—C11—C12	-0.2 (16)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...O5 ⁱ	0.84	1.83	2.649 (11)	163
O2—H2...O1 ⁱⁱ	0.84	2.14	2.846 (11)	142
O2—H2...O2 ⁱⁱ	0.84	2.35	2.989 (11)	133
O4—H4...O5	0.84	1.79	2.626 (10)	170
O6—H6...O7 ⁱⁱⁱ	0.84	1.79	2.626 (10)	170
C3—H3...O1 ^{iv}	0.95	2.54	3.220 (13)	129
C10—H10...O3	0.95	2.35	2.682 (11)	100
C16—H16C...O4 ⁱⁱⁱ	0.98	2.44	3.293 (15)	145
C17—H17A...O7 ^v	0.98	2.39	3.308 (18)	156

Symmetry codes: (i) $x+1, y-1, z$; (ii) $-x+3, y+1/2, -z+2$; (iii) $-x, y-1/2, -z+1$; (iv) $x-1, y+1, z$; (v) $-x, y+1/2, -z+1$.