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2,3,4,6-Tetra-*O*-acetyl-1-[(dimethylcarbamothioyl)-sulfanyl]-*β*-D-galactopyranose

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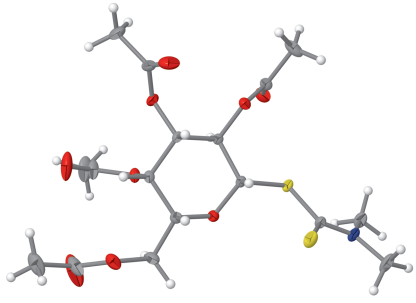
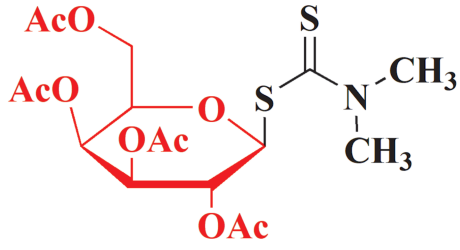
Structural data: full structural data are available from iucrdata.iucr.org

In the structure of the title compound, $C_{17}H_{25}NO_9S_2$, the bond lengths in the C—S—C moiety are almost equal at 1.7959 (8) and 1.7877 (9) Å, with a shorter formally double C—S bond of 1.6698 (9) Å at the other sulfur atom. The eight-atom sequence O3—C3—C2—C1—S—C—N—C (using standard sugar numbering) shows an extended conformation. The packing involves 'weak' hydrogen bonds, whereby the three shortest C—H···O contacts combine to form layers of molecules parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

Thioglycosides have been the focus of much attention because of their role as glycosyl donors in a variety of chemical processes. They can be subjected to most common manipulations of carbohydrate-protecting groups (Toshima *et al.*, 2007), and can be activated for glycosidation under a variety of conditions. An associated advantage is their stability in such processes (Lian *et al.*, 2015). Oligosaccharides and glycoconjugates have a wide range of biological roles because of the extensive variety of their molecular structures. They are particularly desirable synthetic targets in terms both of their biological significance and of the synthetic challenges they offer, and synthetic carbohydrate chemistry has long been a major area of interest in organic chemistry (Codée *et al.*, 2005). Additionally, some thioglycoside derivatives have been reported to be inhibitors of protein glycosylation (Scala *et al.*, 1997).

We have reported the structures of several thioglycosides, the most recent being four structures involving carbamimidothioate groups (Abu-Zaied *et al.*, 2024; see also references therein). Here, we report the structure of *N*,*N*-dimethylcarbamodithio(2,3,4,6-tetra-*O*-acetyl-*β*-D-galactopyranose), made by reacting potassium cyanocarbonimidodithioate with the protected *α*-D-galactopyranosyl bromide in dimethyl formamide in the

Table 1
Selected geometric parameters (Å, °).

C1—S1	1.7959 (8)	S2—C15	1.6698 (9)
S1—C15	1.7877 (9)	C15—N1	1.3327 (12)
C15—S1—C1	101.77 (4)	C15—N1—C17	119.92 (9)
N1—C15—S2	124.18 (7)	C15—N1—C16	123.38 (8)
N1—C15—S1	112.09 (7)	C17—N1—C16	116.62 (8)
S2—C15—S1	123.71 (5)		
S1—C1—C2—C3	−179.78 (5)	C1—S1—C15—N1	170.41 (7)
C1—C2—C3—O3	−173.98 (6)	C1—S1—C15—S2	−11.04 (7)
C2—C1—S1—C15	155.53 (6)	S1—C15—N1—C17	175.46 (10)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O7^{i}	1.00	2.45	3.2096 (11)	132
C8—H8*B*···O8^{ii}	0.98	2.41	3.3157 (15)	154
C16—H16*C*···O10^{iii}	0.98	2.44	3.1795 (18)	132
C17—H17*B*···O1^{iv}	0.98	2.55	3.3558 (13)	139
C1—H1···S2	1.00	2.56	3.1175 (8)	115
C8—H8*A*···O8^{v}	0.98	2.66	3.3384 (15)	127

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

presence of sodium ethoxide at room temperature for 24 h. The compound has been previously reported by Li *et al.* (2016), Pluigers *et al.* (1969), Ferrier & Furneaux (1977) and Tejima & Ishiguro (1967).

The molecule of the title compound is shown in Fig. 1, with selected molecular dimensions in Table 1. Bond lengths and angles may be considered normal, *e.g.* the two almost equal C—S1 bond lengths and the shorter S2—C15, corresponding to its formal double bond nature. The atom sequence O3—C3—C2—C1—S1—C15—N1—C17 shows an extended conformation, with absolute torsion angles 155.53 (6)° for C2—C1—S1—C15 (confirming the β position of the substituent at C1) and > 170° for all others. The geometry at the nitrogen atom is planar (angle sum 359.9°).

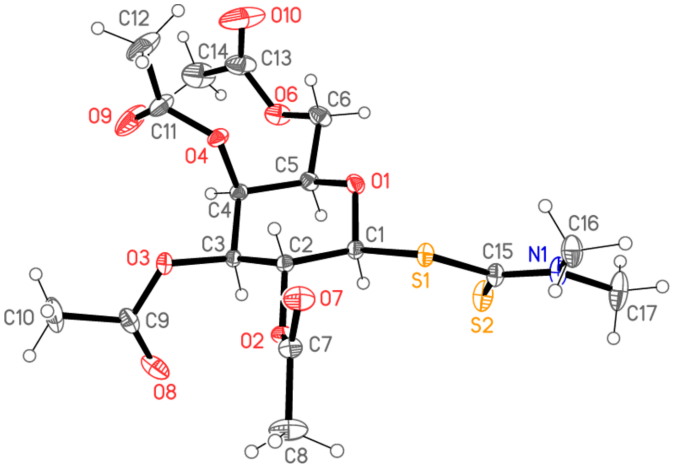


Figure 1
The molecule of the title compound in the crystal. Ellipsoids indicate 50% probability levels.

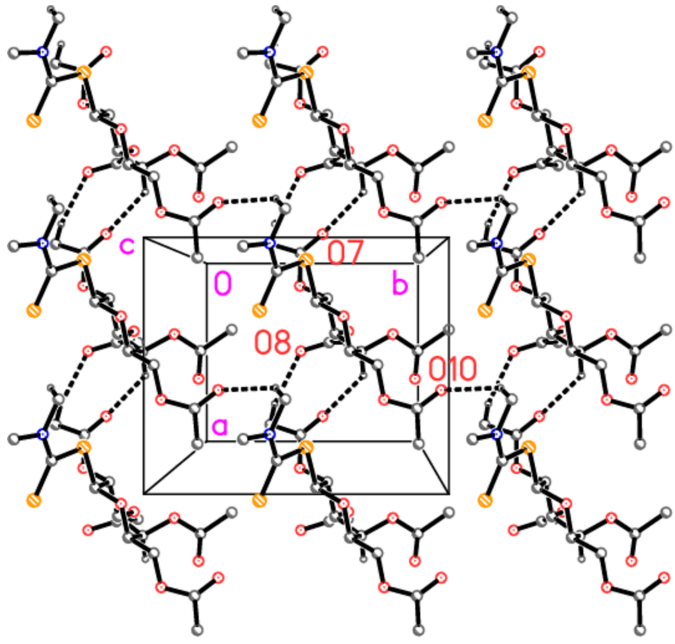


Figure 2
Packing diagram of the title compound, viewed parallel to the *c* axis, showing the layer at $z \simeq 0.25$. Dashed lines indicate C—H···O hydrogen bonds. Hydrogen atoms not involved in the hydrogen bonds are omitted for clarity. Atoms labels correspond to the asymmetric unit.

In the absence of classical hydrogen bond donors, the packing involves 'weak' hydrogen bonds. The three shortest C—H···O contacts (Table 2) combine to form layers of molecules parallel to the *ab* plane at z = 1/4, 1/2, 3/4, *etc*. (Fig. 2). Layers are linked by the other two C—H···O contacts (Fig. 3).

A search employing the routine CONQUEST (Bruno *et al.*, 2002), part of Version 2024.3.0 of the Cambridge Database (Groom *et al.*, 2016), found only one other pyranose sugar

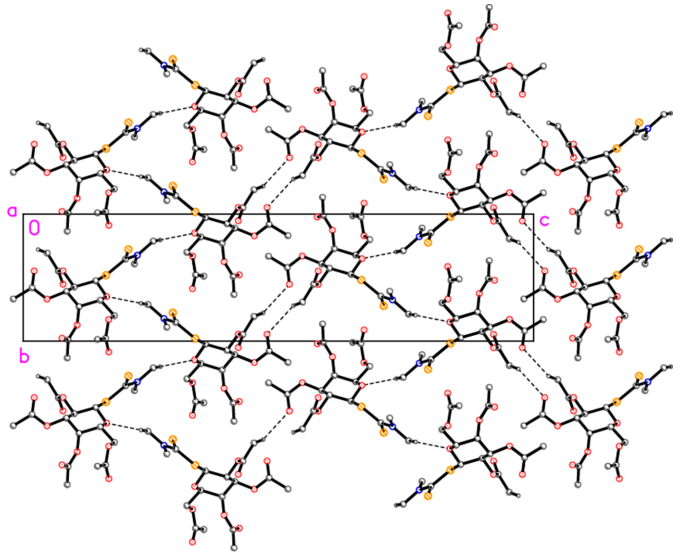


Figure 3
Packing diagram of the title compound, projected parallel to the *a* axis, showing the links between the layers of Fig. 2. Dashed lines indicate C—H···O hydrogen bonds. Hydrogen atoms not involved in the hydrogen bonds are omitted for clarity.

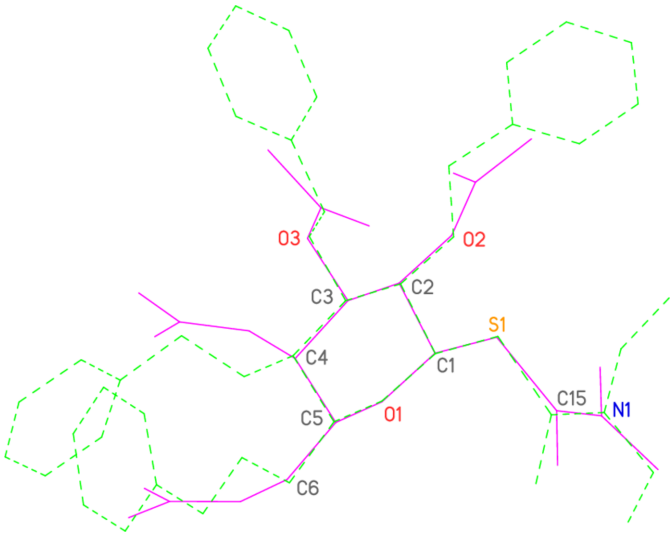


Figure 4
Least-squares fit of the title compound (purple) to YIYKEY (Padungros *et al.*, 2014) (green; coordinates taken from the CCDC). Fitted atoms are labelled.

with a dithiocarbamate substituent at the 1-position, namely 1-(*N*,*N*-diethyldithiocarbamato)-2,3,4,6-tetra-*O*-benzyl-β-D-glucopyranose (refcode YIYKEY; Padungros *et al.*, 2014). A least-squares fit of 13 selected atoms in or near the sugar rings of both molecules (Fig. 4) was performed. In view of the markedly different protecting groups of the sugar rings, together with the opposite configurations of glucose and galactose at C4, no great similarity should be expected, but the the r.m.s. deviation of the fitted atoms is still quite low at 0.08 Å. The deviation for S2, the terminal sulfur atom of the dithiocarbamate, is appreciably higher at 0.69 Å, reflecting the slightly larger torsion angles C2—C1—S1—C15 and C1—S1—C15—S2 (162.1 and 3.0°, respectively) for YIYKEY.

Synthesis and crystallization

A mixture of potassium cyanocarbonimidodithioate (0.01 mol, 1.94 g m) and 2,3,4,6-tetra-*O*-acetyl-β-D-galactopyranosyl bromide (0.01 mol, 4.11 g m) was reacted in dimethyl formamide (10 ml) in the presence of sodium ethoxide (0.01 mole, 0.68 g m) at room temperature for 24 h. Ice–water (10 ml) was then added and the solid product thus furnished was filtered off and recrystallized from dimethyl sulfoxide.

The title compound was obtained as a pale-yellow crystalline solid; m.p. 458–459 K; ^{1}H NMR (500 MHz, DMSO-d_6): δ 1.90, 1.94, 1.98, 2.09 (4 s, 12H, 4OAc), 3.29 (*s*, 3H, CH_3), 3.42 (*s*, 3H, CH_3), 3.93–3.96 (*m*, 2H, H-6), 4.25 (*t*, 1H, H-5), 5.22 (*t*, 1H, H-4), 5.28 (*t*, 1H, H-3), 5.36 (*t*, 1H, H-2), 5.79 (*d*, *J* = 10 Hz, 1H, H-1). Analysis calculated for $C_{17}H_{25}NO_9S_2$ (451.51): C 45.22, H 5.58, N 3.10; S 14.20. Found: C 45.20, H 5.56, N 3.10, S 14.18%. One large prism was cut to an irregular block for intensity measurements.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{25}NO_9S_2$
M_r	451.50
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, *b*, *c* (Å)	7.28265 (10), 8.64720 (15), 34.8789 (3)
V (Å^3)	2196.48 (5)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.29
Crystal size (mm)	0.22 × 0.20 × 0.15
Data collection	
Diffractometer	XtaLAB Synergy
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.818, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	225004, 14433, 13593
R_{int}	0.045
θ values (°)	θ_{max} = 41.4, θ_{min} = 2.3
(sin θ/λ)$_{max}$ (Å^{-1})	0.930
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.031, 0.083, 1.12
No. of reflections	14433
No. of parameters	268
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.27
Absolute structure	Flack *x* determined using 5769 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.001 (8)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*), *XP* (Bruker, 1998) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Methyl groups were refined as idealized rigid groups allowed to rotate but not tip (AFIX 137), with C—H 0.98, H—C—H 109.5°. Other hydrogen atoms were included using a riding model starting from calculated positions (C—H$_{methine}$ 1.00, *C*—H$_{methylene}$ 0.99 Å). The *U*(H) values were fixed for methyl groups at 1.5 × U_{eq}, and for other H atoms at 1.2 × U_{eq} of the parent carbon atoms. Three badly-fitting reflections (deviations > 8σ) were omitted from the refinement. The absolute configuration was confirmed by the Flack *x* value of 0.001 (8).

Acknowledgements

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References

Abu-Zaied, M. A., Nawwar, G. A., Elgemeie, G. H. & Jones, P. G. (2024). *Acta Cryst.* E**80**, 829–839.
Bruker (1998). *XP*. Bruker Analytical X–Ray Instruments, Madison, Wisconsin, USA.

Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Codée, J. D., Litjens, R. E., van den Bos, L. J., Overkleeft, H. S. & van der Marel, G. A. (2005). *Chem. Soc. Rev.* **34**, 769–782.
Ferrier, R. J. & Furneaux, R. H. (1977). *Carbohydr. Res.* **57**, 73–83.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Li, G., Noguchi, M., Kashiwagura, H., Tanaka, Y., Serizawa, K. & Shoda, S. (2016). *Tetrahedron Lett.* **57**, 3529–3531.
Lian, G., Zhang, X. & Yu, B. (2015). *Carbohydr. Res.* **403**, 13–22.
Padungros, P., Alberch, L. & Wei, A. (2014). *J. Org. Chem.* **79**, 2611–2624.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Pluijgers, C. W., Berg, J. & Thorn, G. D. (1969). *Recl Trav. Chim. Pays Bas* **88**, 241–253.
Rigaku OD (2022). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Scala, S., Akhmed, K., Rao, U. S., Paull, K., Lan, L., Dickstein, B., Lee, J., Elgemeie, G. H., Stein, W. D. & Bates, S. E. (1997). *Mol. Pharmacol.* **51**, 1024–1033.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Tejima, S. & Ishiguro, S. (1967). *Chem. Pharm. Bull.* **15**, 255–263.
Toshima, K. & Sasaki, K. (2007). *O-Glycosidation Methods* in *Comprehensive Glycoscience*, edited by J. Kamerling, pp. 261–311. Amsterdam: Elsevier, ISBN 9780444519672.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2025). **10**, x250544 [https://doi.org/10.1107/S2414314625005449]

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Crystal data

$C_{17}H_{25}NO_9S_2$
M_r = 451.50
Orthorhombic, $P2_12_12_1$
a = 7.28265 (10) Å
b = 8.64720 (15) Å
c = 34.8789 (3) Å
V = 2196.48 (5) Å^3
Z = 4
$F(000)$ = 952
D_x = 1.365 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 126110 reflections
θ = 2.3–41.3°
μ = 0.29 mm^{-1}
T = 100 K
Block, colourless
0.22 × 0.20 × 0.15 mm

Data collection

XtaLAB Synergy diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.818, T_{max} = 1.000
225004 measured reflections
14433 independent reflections
13593 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 41.4°, θ_{min} = 2.3°
h = −13→13
k = −15→15
l = −63→63

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
S = 1.12
14433 reflections
268 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.1937P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack x determined using 5769 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.001 (8)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.22016 (11)	0.52540 (10)	0.14258 (2)	0.01348 (11)
H1	0.301124	0.432274	0.144357	0.016*
C2	0.20058 (11)	0.57372 (9)	0.10035 (2)	0.01244 (11)

H2	0.119080	0.666256	0.097869	0.015*
C3	0.39260 (11)	0.60872 (9)	0.08518 (2)	0.01229 (11)
H3	0.466514	0.511270	0.084781	0.015*
C4	0.48993 (11)	0.72864 (9)	0.10985 (2)	0.01316 (10)
H4	0.620302	0.739994	0.101305	0.016*
C5	0.48404 (12)	0.67805 (10)	0.15167 (2)	0.01507 (12)
H5	0.557771	0.581254	0.154690	0.018*
C6	0.55721 (13)	0.80002 (13)	0.17912 (3)	0.02065 (15)
H6A	0.482407	0.895388	0.177473	0.025*
H6B	0.553206	0.761446	0.205830	0.025*
C7	−0.05084 (12)	0.44818 (10)	0.06923 (3)	0.01588 (12)
C8	−0.10298 (17)	0.30603 (14)	0.04748 (4)	0.0290 (2)
H8A	−0.004042	0.278698	0.029677	0.044*
H8B	−0.216034	0.325520	0.033023	0.044*
H8C	−0.123073	0.220596	0.065454	0.044*
C9	0.44387 (13)	0.57971 (13)	0.01780 (3)	0.02005 (15)
C10	0.4443 (2)	0.6688 (2)	−0.01898 (3)	0.0349 (3)
H10A	0.318449	0.699657	−0.025372	0.052*
H10B	0.493721	0.603806	−0.039557	0.052*
H10C	0.520872	0.761240	−0.016113	0.052*
C11	0.48662 (15)	0.99031 (11)	0.08844 (4)	0.02412 (18)
C12	0.3713 (2)	1.13341 (14)	0.08674 (6)	0.0395 (4)
H12A	0.250639	1.108055	0.075993	0.059*
H12B	0.431714	1.210509	0.070465	0.059*
H12C	0.355954	1.175358	0.112643	0.059*
C13	0.79252 (16)	0.97920 (15)	0.16185 (5)	0.0314 (2)
C14	0.98327 (19)	0.9884 (2)	0.14586 (6)	0.0408 (3)
H14A	1.061908	0.913046	0.158930	0.061*
H14B	1.032239	1.092733	0.149860	0.061*
H14C	0.980359	0.965477	0.118356	0.061*
O1	0.29972 (9)	0.64895 (8)	0.16373 (2)	0.01595 (10)
O2	0.13054 (9)	0.44673 (7)	0.07833 (2)	0.01412 (9)
O3	0.38060 (11)	0.67005 (8)	0.04701 (2)	0.01719 (11)
O4	0.39544 (9)	0.87439 (7)	0.10612 (2)	0.01611 (10)
O6	0.74333 (11)	0.83094 (10)	0.16784 (3)	0.02342 (14)
O7	−0.15325 (10)	0.55175 (9)	0.07833 (3)	0.02197 (13)
O8	0.49188 (14)	0.44747 (11)	0.02195 (2)	0.02792 (16)
O9	0.64113 (15)	0.97836 (12)	0.07640 (4)	0.0420 (3)
O10	0.69249 (18)	1.08682 (14)	0.16806 (6)	0.0599 (5)
S1	−0.00073 (3)	0.48124 (3)	0.16268 (2)	0.01509 (4)
S2	0.26816 (3)	0.27711 (4)	0.20661 (2)	0.02352 (5)
C15	0.05929 (12)	0.35345 (11)	0.20097 (2)	0.01559 (12)
N1	−0.08300 (11)	0.32376 (11)	0.22384 (2)	0.01961 (13)
C16	−0.26558 (14)	0.39147 (15)	0.21834 (3)	0.02370 (18)
H16A	−0.254152	0.503647	0.215141	0.036*
H16B	−0.342140	0.369253	0.240783	0.036*
H16C	−0.322539	0.346774	0.195424	0.036*
C17	−0.06368 (18)	0.2123 (2)	0.25515 (4)	0.0335 (3)

H17A	−0.028969	0.111306	0.244663	0.050*
H17B	−0.180709	0.203067	0.268826	0.050*
H17C	0.031589	0.247892	0.272924	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0139 (3)	0.0139 (3)	0.0126 (2)	−0.0006 (2)	0.0018 (2)	0.0012 (2)
C2	0.0134 (3)	0.0111 (3)	0.0128 (3)	0.0005 (2)	0.0010 (2)	0.0000 (2)
C3	0.0142 (3)	0.0114 (3)	0.0112 (2)	0.0007 (2)	0.0021 (2)	0.00144 (19)
C4	0.0124 (2)	0.0112 (2)	0.0159 (3)	0.0009 (2)	0.0020 (2)	−0.0005 (2)
C5	0.0137 (3)	0.0170 (3)	0.0146 (3)	0.0001 (2)	0.0002 (2)	−0.0010 (2)
C6	0.0169 (3)	0.0255 (4)	0.0195 (3)	−0.0028 (3)	−0.0002 (3)	−0.0068 (3)
C7	0.0145 (3)	0.0150 (3)	0.0181 (3)	0.0008 (2)	−0.0015 (2)	−0.0009 (2)
C8	0.0228 (4)	0.0222 (4)	0.0421 (6)	0.0004 (3)	−0.0091 (4)	−0.0124 (4)
C9	0.0173 (3)	0.0306 (4)	0.0123 (3)	−0.0039 (3)	0.0002 (2)	−0.0016 (3)
C10	0.0389 (6)	0.0525 (8)	0.0134 (3)	−0.0133 (6)	−0.0001 (4)	0.0069 (4)
C11	0.0218 (4)	0.0125 (3)	0.0380 (5)	0.0005 (3)	0.0094 (4)	0.0044 (3)
C12	0.0348 (6)	0.0154 (4)	0.0684 (10)	0.0063 (4)	0.0162 (7)	0.0115 (5)
C13	0.0208 (4)	0.0259 (5)	0.0474 (7)	−0.0059 (3)	0.0048 (4)	−0.0147 (5)
C14	0.0215 (5)	0.0388 (7)	0.0620 (10)	−0.0095 (5)	0.0094 (5)	−0.0147 (6)
O1	0.0155 (2)	0.0186 (3)	0.0138 (2)	−0.00277 (19)	0.00266 (18)	−0.0023 (2)
O2	0.0133 (2)	0.0123 (2)	0.0167 (2)	0.00077 (17)	−0.00018 (18)	−0.00223 (18)
O3	0.0224 (3)	0.0169 (2)	0.0123 (2)	−0.0007 (2)	0.00171 (19)	0.00366 (19)
O4	0.0152 (2)	0.0107 (2)	0.0225 (3)	0.00143 (18)	0.0041 (2)	0.00108 (19)
O6	0.0152 (3)	0.0243 (3)	0.0308 (4)	−0.0012 (2)	−0.0009 (2)	−0.0068 (3)
O7	0.0162 (3)	0.0204 (3)	0.0294 (3)	0.0049 (2)	−0.0024 (2)	−0.0041 (3)
O8	0.0306 (4)	0.0338 (4)	0.0194 (3)	0.0082 (3)	−0.0021 (3)	−0.0102 (3)
O9	0.0289 (4)	0.0214 (3)	0.0756 (8)	0.0018 (3)	0.0261 (5)	0.0143 (5)
O10	0.0344 (5)	0.0249 (5)	0.1202 (15)	−0.0055 (4)	0.0250 (7)	−0.0233 (7)
S1	0.01293 (7)	0.01785 (8)	0.01451 (7)	0.00059 (6)	0.00218 (6)	0.00388 (6)
S2	0.01376 (8)	0.03284 (13)	0.02396 (10)	0.00211 (8)	−0.00070 (7)	0.01238 (9)
C15	0.0137 (3)	0.0196 (3)	0.0136 (3)	−0.0015 (2)	−0.0003 (2)	0.0036 (2)
N1	0.0150 (3)	0.0284 (4)	0.0154 (3)	−0.0016 (3)	0.0019 (2)	0.0076 (3)
C16	0.0145 (3)	0.0331 (5)	0.0235 (4)	0.0011 (3)	0.0047 (3)	0.0061 (3)
C17	0.0257 (5)	0.0479 (7)	0.0270 (5)	−0.0008 (5)	0.0029 (4)	0.0226 (5)

Geometric parameters (Å, º)

C1—O1	1.4216 (11)	N1—C17	1.4631 (14)
C1—C2	1.5378 (11)	N1—C16	1.4655 (13)
C1—S1	1.7959 (8)	C1—H1	1.0000
C2—O2	1.4339 (10)	C2—H2	1.0000
C2—C3	1.5255 (11)	C3—H3	1.0000
C3—O3	1.4358 (10)	C4—H4	1.0000
C3—C4	1.5226 (11)	C5—H5	1.0000
C4—O4	1.4419 (10)	C6—H6A	0.9900
C4—C5	1.5234 (11)	C6—H6B	0.9900

C5—O1	1.4290 (11)	C8—H8A	0.9800
C5—C6	1.5209 (12)	C8—H8B	0.9800
C6—O6	1.4365 (13)	C8—H8C	0.9800
C7—O7	1.2079 (11)	C10—H10A	0.9800
C7—O2	1.3585 (11)	C10—H10B	0.9800
C7—C8	1.4936 (14)	C10—H10C	0.9800
C9—O8	1.2045 (15)	C12—H12A	0.9800
C9—O3	1.3639 (12)	C12—H12B	0.9800
C9—C10	1.4966 (15)	C12—H12C	0.9800
C11—O9	1.2055 (14)	C14—H14A	0.9800
C11—O4	1.3513 (12)	C14—H14B	0.9800
C11—C12	1.4968 (16)	C14—H14C	0.9800
C13—O10	1.2015 (18)	C16—H16A	0.9800
C13—O6	1.3475 (16)	C16—H16B	0.9800
C13—C14	1.4989 (18)	C16—H16C	0.9800
S1—C15	1.7877 (9)	C17—H17A	0.9800
S2—C15	1.6698 (9)	C17—H17B	0.9800
C15—N1	1.3327 (12)	C17—H17C	0.9800

O1—C1—C2	109.30 (7)	C2—C3—H3	109.3
O1—C1—S1	108.81 (5)	O4—C4—H4	109.9
C2—C1—S1	110.40 (6)	C3—C4—H4	109.9
O2—C2—C3	106.99 (6)	C5—C4—H4	109.9
O2—C2—C1	109.76 (6)	O1—C5—H5	109.0
C3—C2—C1	107.53 (6)	C6—C5—H5	109.0
O3—C3—C4	107.51 (6)	C4—C5—H5	109.0
O3—C3—C2	109.82 (7)	O6—C6—H6A	110.4
C4—C3—C2	111.46 (6)	C5—C6—H6A	110.4
O4—C4—C3	108.79 (7)	O6—C6—H6B	110.4
O4—C4—C5	108.90 (6)	C5—C6—H6B	110.4
C3—C4—C5	109.42 (6)	H6A—C6—H6B	108.6
O1—C5—C6	105.43 (7)	C7—C8—H8A	109.5
O1—C5—C4	111.03 (7)	C7—C8—H8B	109.5
C6—C5—C4	113.18 (7)	H8A—C8—H8B	109.5
O6—C6—C5	106.69 (8)	C7—C8—H8C	109.5
O7—C7—O2	123.08 (8)	H8A—C8—H8C	109.5
O7—C7—C8	125.92 (9)	H8B—C8—H8C	109.5
O2—C7—C8	110.99 (8)	C9—C10—H10A	109.5
O8—C9—O3	123.52 (9)	C9—C10—H10B	109.5
O8—C9—C10	126.22 (11)	H10A—C10—H10B	109.5
O3—C9—C10	110.25 (11)	C9—C10—H10C	109.5
O9—C11—O4	123.65 (10)	H10A—C10—H10C	109.5
O9—C11—C12	125.51 (10)	H10B—C10—H10C	109.5
O4—C11—C12	110.83 (9)	C11—C12—H12A	109.5
O10—C13—O6	123.22 (12)	C11—C12—H12B	109.5
O10—C13—C14	126.00 (14)	H12A—C12—H12B	109.5
O6—C13—C14	110.77 (11)	C11—C12—H12C	109.5
C1—O1—C5	111.25 (6)	H12A—C12—H12C	109.5

C7—O2—C2	117.64 (7)	H12B—C12—H12C	109.5
C9—O3—C3	117.41 (7)	C13—C14—H14A	109.5
C11—O4—C4	117.07 (7)	C13—C14—H14B	109.5
C13—O6—C6	118.06 (9)	H14A—C14—H14B	109.5
C15—S1—C1	101.77 (4)	C13—C14—H14C	109.5
N1—C15—S2	124.18 (7)	H14A—C14—H14C	109.5
N1—C15—S1	112.09 (7)	H14B—C14—H14C	109.5
S2—C15—S1	123.71 (5)	N1—C16—H16A	109.5
C15—N1—C17	119.92 (9)	N1—C16—H16B	109.5
C15—N1—C16	123.38 (8)	H16A—C16—H16B	109.5
C17—N1—C16	116.62 (8)	N1—C16—H16C	109.5
O1—C1—H1	109.4	H16A—C16—H16C	109.5
C2—C1—H1	109.4	H16B—C16—H16C	109.5
S1—C1—H1	109.4	N1—C17—H17A	109.5
O2—C2—H2	110.8	N1—C17—H17B	109.5
C3—C2—H2	110.8	H17A—C17—H17B	109.5
C1—C2—H2	110.8	N1—C17—H17C	109.5
O3—C3—H3	109.3	H17A—C17—H17C	109.5
C4—C3—H3	109.3	H17B—C17—H17C	109.5

O1—C1—C2—O2	176.61 (6)	C8—C7—O2—C2	−178.12 (9)
S1—C1—C2—O2	−63.74 (7)	C3—C2—O2—C7	−142.58 (7)
O1—C1—C2—C3	60.57 (8)	C1—C2—O2—C7	101.04 (8)
S1—C1—C2—C3	−179.78 (5)	O8—C9—O3—C3	7.42 (14)
O2—C2—C3—O3	68.17 (8)	C10—C9—O3—C3	−172.48 (9)
C1—C2—C3—O3	−173.98 (6)	C4—C3—O3—C9	127.59 (8)
O2—C2—C3—C4	−172.80 (6)	C2—C3—O3—C9	−110.98 (8)
C1—C2—C3—C4	−54.95 (8)	O9—C11—O4—C4	−1.10 (18)
O3—C3—C4—O4	53.85 (8)	C12—C11—O4—C4	179.96 (11)
C2—C3—C4—O4	−66.55 (8)	C3—C4—O4—C11	−113.01 (9)
O3—C3—C4—C5	172.72 (7)	C5—C4—O4—C11	127.80 (9)
C2—C3—C4—C5	52.32 (8)	O10—C13—O6—C6	5.4 (2)
O4—C4—C5—O1	64.22 (9)	C14—C13—O6—C6	−173.27 (11)
C3—C4—C5—O1	−54.58 (9)	C5—C6—O6—C13	127.99 (11)
O4—C4—C5—C6	−54.12 (9)	O1—C1—S1—C15	−84.52 (6)
C3—C4—C5—C6	−172.92 (7)	C2—C1—S1—C15	155.53 (6)
O1—C5—C6—O6	179.61 (8)	C1—S1—C15—N1	170.41 (7)
C4—C5—C6—O6	−58.86 (10)	C1—S1—C15—S2	−11.04 (7)
C2—C1—O1—C5	−65.67 (8)	S2—C15—N1—C17	−3.08 (15)
S1—C1—O1—C5	173.70 (6)	S1—C15—N1—C17	175.46 (10)
C6—C5—O1—C1	−174.41 (7)	S2—C15—N1—C16	−179.75 (9)
C4—C5—O1—C1	62.66 (9)	S1—C15—N1—C16	−1.21 (13)
O7—C7—O2—C2	1.12 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O7^{i}	1.00	2.45	3.2096 (11)	132

C8—H8*B*···O8^{ii}	0.98	2.41	3.3157 (15)	154
C16—H16*C*···O10^{iii}	0.98	2.44	3.1795 (18)	132
C17—H17*B*···O1^{iv}	0.98	2.55	3.3558 (13)	139
C1—H1···S2	1.00	2.56	3.1175 (8)	115
C8—H8*A*···O8^{v}	0.98	2.66	3.3384 (15)	127

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