Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Synthesis and crystal structure of ethyl 2-{[4-amino-5-cyano-6-(3,4-dimethoxyphenyl)pyrimidin-2-yl]-sulfanyl}acetate

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Received 7 September 2026
Accepted 6 October 2026

Edited by C. Schulzke, Universität Greifswald, Germany

Keywords: crystal structure; pyrimidine; hydrogen bond; ester; acetate.

CCDC reference: 2593312

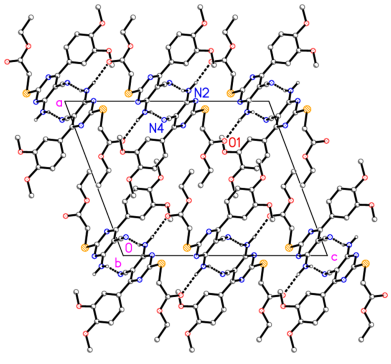
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In the title compound, $C_{17}H_{18}N_4O_4S$, the pyrimidine and phenyl rings subtend an interplanar angle of 30.05 (5)°. The ring angle at the C atom between the N atoms is very wide at 129.32 (11)° and the angles at the ring N atoms are narrow [115.58 (10) and 115.98 (10)°]. The molecules are linked by two classical hydrogen bonds with the amine group as donor, namely N—H···N≡C and N—H···O=C, *via* an inversion centre and a 2_1 screw axis, respectively. There are also short contacts of 3.6006 (7) Å between the centroids of pairs of pyrimidine rings across inversion centres.

1. Chemical context

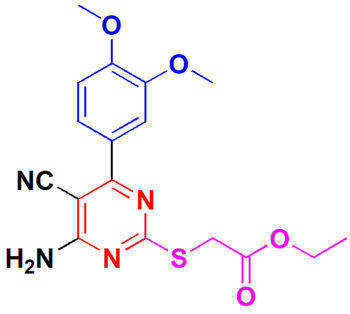
In medicinal chemistry, pyrimidines are an important class of nitrogen-containing heterocycles. As components of nucleic acids, they are necessarily constituents of every cell, and thus of all biological living matter. They are also present in many other naturally occurring molecules, such as vitamins, coenzymes and uric acids. Various pyrimidine scaffolds have been designed and used by chemists to produce innovative medicaments with a range of pharmacological activities (Luo *et al.*, 2026). There are many clinically approved drugs containing pyrimidine in their structures; some examples are 5-fluorouracil and Gemcitabine as anticancer, Zidovudine and Stavudine as anti-HIV, Buspirone as anti-anxiety, and Trimethoprim, Sulfadiazine and Sulfadoxine as antimicrobial agents (Sahu *et al.*, 2016; Stolarczyk *et al.*, 2018). One significant family of pyrimidines consists of 2-thiopyrimidine (2-TP) and its derivatives, also well known as 2-mercaptopyrimidine compounds, in which the S atom replaces the O atom of uridine-based systems. 2-TP derivatives have found a wide range of applications in the preparation of cardiotonic drugs and anticancer, antitubercular, anti-inflammatory and antibacterial agents (Lamie *et al.*, 2020; El-serwy *et al.*, 2019). They have attracted the attention of chemists and biochemists who wish to develop the range of potentially therapeutic compounds bearing thiopyrimidine scaffolds (Sondhi *et al.*, 2005; Rabeh *et al.*, 2026).

We have recently described various synthetic approaches to the synthesis of purine and pyrimidine analogs (Abu-Zaied *et al.*, 2020; Abu-Zaied *et al.*, 2021). In the majority of biochemical reactions, several derivatives of these ring structures are regarded as crucial antimetabolites (Khedr *et al.*, 2022; Khedr *et al.*, 2023). As a continuation of these studies of



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the synthesis of biologically active antimetabolic agents (Elgemeie *et al.*, 2019; Elgemeie *et al.*, 2022), the current study reports the synthesis of ethyl 2-{[4-amino-5-cyano-6-(3,4-dimethoxyphenyl)pyrimidin-2-yl]sulfanyl}acetate, **4**, by reacting the pyrimidine-2-thiol derivative **3** with ethyl chloroacetate (Fig. 1). The crystal structure was determined to confirm the nature of **4**, and is reported here.



2. Structural commentary

The molecule of compound **4** in the crystal is shown in Fig. 2, with selected molecular dimensions in Table 1. Both rings are essentially planar, with r.m.s. deviations of 0.010 and 0.013 Å for the pyrimidine and phenyl ring, respectively. The only substituent lying significantly out-of-plane is C7 [by 0.221 (2) Å]. The interplanar angle is 30.05 (5)°. The ring angle at C2 is the widest at 129.32 (11)°, associated with a narrow angle N3—C2—S1 of 112.01 (8)° at the planar centre C2. The narrowest ring angles are those at the N atoms [115.58 (10) and 115.98 (10)°]. The bond length S1—C2 is significantly shorter than S1—C8, consistent with the different hybridizations of the C atoms; similar considerations apply to C5—C7 being shorter than C6—C21. The NH_2 group is planar, with the N atom lying an insignificant 0.003 (9) Å out of the plane of its substituents. The atom sequence C8—C9—O2—C10—C11 of the side chain displays an extended conformation.

Table 1
Selected geometric parameters (Å, °).

S1—C2	1.7619 (12)	N3—C4	1.3473 (15)
S1—C8	1.7987 (12)	C4—C5	1.4335 (15)
N1—C2	1.3348 (14)	C5—C6	1.3980 (16)
N1—C6	1.3508 (15)	C5—C7	1.4250 (16)
C2—N3	1.3323 (15)	C6—C21	1.4801 (15)
C2—S1—C8	101.07 (6)	N3—C4—C5	119.76 (10)
C2—N1—C6	115.58 (10)	C6—C5—C4	118.35 (10)
N3—C2—N1	129.32 (11)	N1—C6—C5	120.76 (10)
C2—N3—C4	115.98 (10)		
C8—S1—C2—N1	−13.64 (10)	C8—C9—O2—C10	−179.59 (9)
C2—S1—C8—C9	−69.51 (9)	C11—C10—O2—C9	−174.39 (10)
S1—C8—C9—O2	144.75 (8)		

3. Supramolecular features

The main intermolecular contacts are the classical hydrogen bonds from the H atoms of the amino group, H021 and H022, to the acceptors N4 and O1 of adjacent molecules, *via* an inversion centre and the 2_1 screw axis, respectively (Table 2, which also includes some borderline weak hydrogen bonds). Fig. 3 shows the infinite chains of molecules parallel to the *b* axis formed by the contact H022···O1. It also shows (implicitly) the short contacts between pairs of pyrimidine rings connected by inversion, with a centroid-to-centroid distance of 3.6006 (7) Å and an offset of 1.2 Å (symmetry operator:

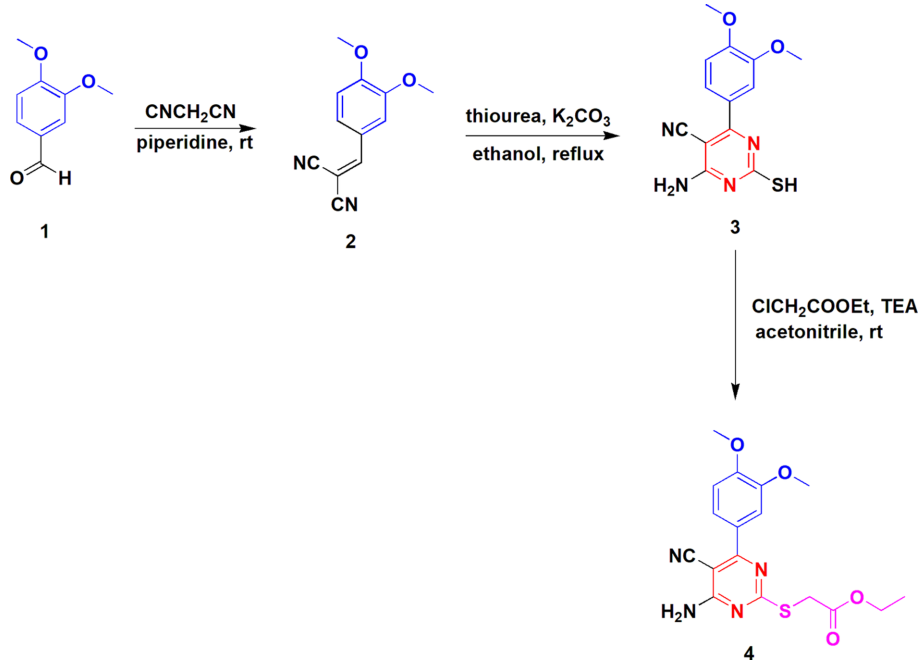


Figure 1
The synthesis of compound **4**.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H021···N4^{i}	0.862 (19)	2.201 (19)	3.0368 (15)	163.4 (16)
N2—H022···O1^{ii}	0.879 (19)	2.139 (19)	2.9942 (13)	164.0 (16)
C8—H8A···N4^{iii}	0.99	2.67	3.4693 (16)	138
C11—H11A···O3^{iv}	0.98	2.52	3.1459 (15)	122
C27—H27B···S1^{v}	0.98	2.95	3.6836 (12)	133

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

$-x + 2, -y + 1, -z + 1$) for the pair involving the reference molecule.

The combination of inversion and 2_1 symmetry for the two hydrogen bonds means that the overall packing is three-dimensional rather than a ribbon or layer structure. The second packing diagram (Fig. 4) is therefore a projection showing the combination of both hydrogen bonds.

4. Database survey

Searches were conducted using the Cambridge Structural Database (CSD, Version 6.01, update November 2025; Groom *et al.*, 2016) and the *ConQuest* routine (Version 2025.3.1; Bruno *et al.*, 2002), and were restricted to non-disordered 'organic' structures.

A general search for pyrimidine systems with no further annelation gave 2950 hits. The angle at C2 was consistently and significantly larger than 120°, with a mean angle of 126.9 (17)° for 3782 values. A search restricted to the substitution pattern of compound **4** (S at C2, N at C4, CN at C5 and C at C6) gave just two hits: 4-[4-(7-chloroquinolin-4-yl)piperazin-1-yl]-2-(methylsulfanyl)-6-phenylpyrimidine-5-carbonitrile (refcode HUKRUC; Kaur *et al.*, 2015) and 2-[(4-chlorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-[3-(trifluoromethyl)anilino]pyrimidine-5-carbonitrile (XAZLUH; El-Emam *et al.*, 2012). However, neither of these can be regarded as closely similar to **4**, thus underlining its novel nature.

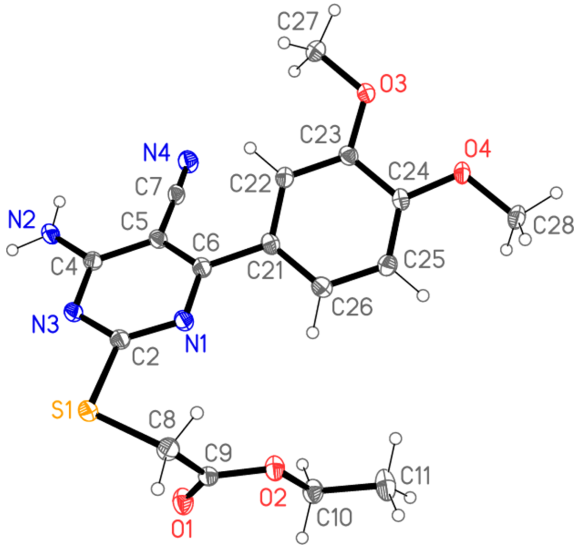


Figure 2
The molecule of compound **4** in the crystal. Displacement ellipsoids represent 50% probability levels.

5. Synthesis and crystallization

A mixture of compound **3** (1 mmol) and ethyl chloroacetate (1.2 mmol) in acetonitrile containing a few drops of triethylamine was stirred at room temperature for 48 h. The precipitate thus formed was filtered off and washed with ethanol to give the desired compound **4**, as a buff powder, which was recrystallized from acetonitrile to give pale-yellow crystals (isolated single crystals are effectively colourless) in 65% yield.

M.p. 453–455 K; IR (KBr, ν cm^{-1}): 3470, 3347 (NH_2) 2206 (CN), 1736, (C═O); ^{1}H NMR (DMSO-d_6, 500 MHz): δ (ppm) 1.11 (*t*, J = 7.0 Hz, 3H, CH_2CH_3), 3.84 (*s*, 3H, OCH_3), 3.85 (*s*, 3H, OCH_3), 4.03 (*s*, 2H, S-CH_2), 4.07 (*q*, J = 7.0 Hz, 2H, CH_2CH_3), 7.12 (*d*, J = 8.5 Hz, 1H, Ar-H), 7.54 (*d*, J = 2.0 Hz, 1H, Ar-H), 7.57 (*d*, J = 8.5 Hz, 1H, Ar-H), 8.03 (*br s*, 2H, NH_2, D_2O-exchangeable); ^{13}C NMR (DMSO-d_6, 150 MHz): δ (ppm) 14.4 (CH_2CH_3), 33.5 (S—CH_2), 56.2 (2OCH_3), 61.6 (CH_2CH_3), 82.3, 111.6, 112.4, 117.1, 122.6, 128.2, 148.8, 152.0, 164.1, 166.7, 169.4 (C═O ester), 172.4. Analysis calculated (%) for $C_{17}H_{18}N_4O_4S$: C 54.53, H 4.85, N 14.96, S 8.56; found: C 54.54, H 5.13, N 14.85, S 8.74.

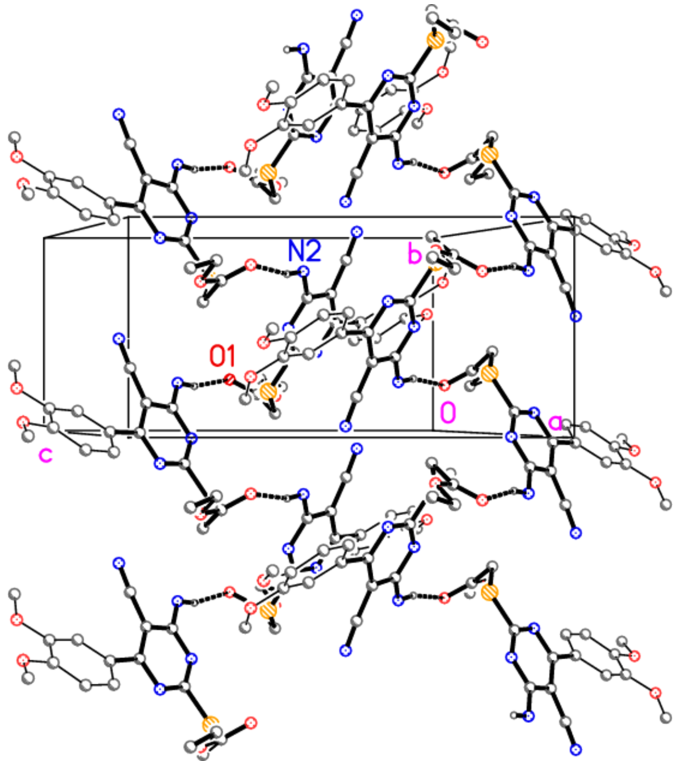


Figure 3
Two chains of molecules of compound **4**, running vertically, linked by the hydrogen bonds N2···H022—O1 (thick dashed lines). The view direction is perpendicular to the *bc* plane, in the region $a \simeq 0.75$. Atom names indicate the asymmetric unit. H atoms not involved in these interactions are omitted for clarity.

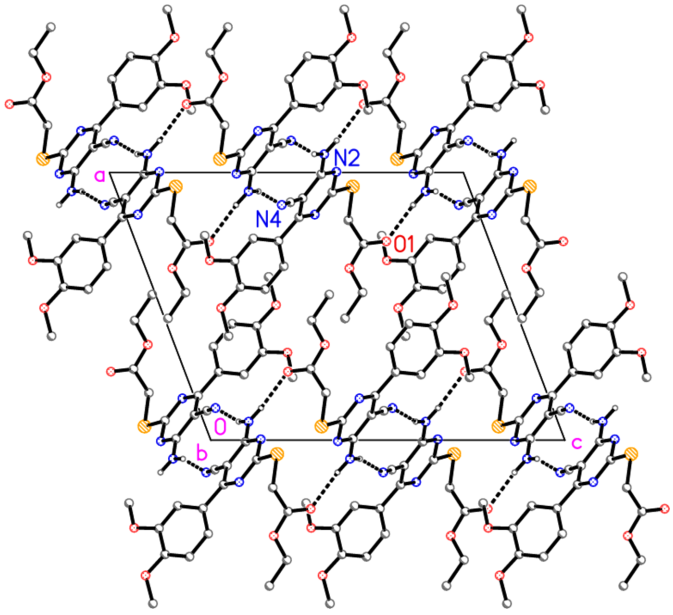


Figure 4
A projection of the three-dimensional packing of compound **4** parallel to the *b* axis, showing linkages *via* both classical hydrogen bonds (thick dashed lines). Atom names indicate the asymmetric unit. H atoms not involved in these interactions are omitted for clarity.

6. Refinement

Details of data collection and structure refinement are summarized in Table 3. H atoms of the NH_2 group were refined freely. Methyl groups were refined as idealized rigid groups allowed to rotate but not tip, with C—H = 0.98 Å and H—C—H = 109.5°. Other H atoms were refined using a riding model, with aromatic C—H = 0.95 Å and methylene C—H = 0.99 Å. The U_{iso}(H) values were fixed at 1.5U_{eq} of the parent C atoms for the methyl groups and 1.2U_{eq} for the other H atoms. Two badly fitting reflections ($\Delta/\sigma > 8$) were omitted from the refinement.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{18}N_4O_4S$
M_r	374.41
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.4276 (5), 8.2128 (3), 16.6201 (7)
β (°)	110.762 (5)
V (Å^3)	1713.80 (13)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.97
Crystal size (mm)	0.14 × 0.05 × 0.03
Data collection	
Diffractometer	Rigaku XtaLAB Synergy
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2026)
T_{min}, T_{max}	0.763, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	78100, 3747, 3512
R_{int}	0.044
θ values (°)	θ_{max} = 81.6, θ_{min} = 3.5
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.642
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.079, 1.09
No. of reflections	3747
No. of parameters	246
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.27

Computer programs: *CrysAlis PRO* (Rigaku OD, 2026), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019* (Sheldrick, 2015*b*), *XP* (Bruker, 1998) and *publCIF* (Westrip, 2010).

Acknowledgements

The authors acknowledge support by the Open Access Publication Funds of the Technical University of Braunschweig.

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supporting information

Acta Cryst. (2026). E**82**, 1313-1316 [https://doi.org/10.1107/S2056989026010352]

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Manar M. Abuzahra, Wafaa A. Zaghary, Nesreen S. Ahmed, Mohammed A. Khedr, Hesham R. S. Haffez, Galal H. Elgemeie and Peter G. Jones

Computing details

Ethyl 2-{[4-amino-5-cyano-6-(3,4-dimethoxyphenyl)pyrimidin-2-yl]sulfanyl}acetate

Crystal data

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$a = 13.4276$ (5) Å
$b = 8.2128$ (3) Å
$c = 16.6201$ (7) Å
$\beta = 110.762$ (5)°
$V = 1713.80$ (13) Å^3
$Z = 4$
$F(000) = 784$
$D_x = 1.451$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 44633 reflections
$\theta = 3.5$–$80.1°$
$\mu = 1.97$ mm^{-1}
$T = 100$ K
Prism, colourless
0.14 × 0.05 × 0.03 mm

Data collection

Rigaku XtaLAB Synergy diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2026)
$T_{min} = 0.763$, $T_{max} = 1.000$
78100 measured reflections
3747 independent reflections
3512 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 81.6°$, $\theta_{min} = 3.5°$
$h = -16 \rightarrow 17$
$k = -10 \rightarrow 10$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.079$
$S = 1.09$
3747 reflections
246 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.7704P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.94829 (2)	0.20843 (4)	0.67241 (2)	0.01892 (9)
N1	0.84359 (8)	0.39055 (12)	0.53524 (6)	0.0170 (2)
C2	0.92716 (9)	0.38561 (14)	0.60876 (7)	0.0165 (2)
N3	1.00361 (7)	0.49571 (12)	0.64206 (6)	0.0171 (2)
C4	0.99444 (9)	0.63454 (14)	0.59681 (7)	0.0167 (2)
C5	0.90500 (9)	0.65719 (14)	0.51876 (7)	0.0162 (2)
C6	0.83380 (9)	0.52791 (14)	0.48834 (7)	0.0160 (2)
C7	0.88980 (9)	0.81410 (14)	0.47967 (7)	0.0172 (2)
C8	0.82267 (9)	0.10613 (14)	0.62413 (8)	0.0194 (2)
H8A	0.805412	0.098954	0.561170	0.023*
H8B	0.828418	−0.006128	0.647040	0.023*
C9	0.73379 (9)	0.19453 (14)	0.64200 (7)	0.0167 (2)
C10	0.55229 (9)	0.26761 (15)	0.58683 (8)	0.0209 (2)
H10A	0.564619	0.386653	0.591305	0.025*
H10B	0.542433	0.229385	0.640011	0.025*
C11	0.45556 (10)	0.22845 (19)	0.50957 (8)	0.0292 (3)
H11A	0.467709	0.261922	0.457205	0.044*
H11B	0.393828	0.286890	0.513533	0.044*
H11C	0.442029	0.110989	0.507580	0.044*
C21	0.74471 (9)	0.53373 (14)	0.40457 (7)	0.0161 (2)
C22	0.75448 (9)	0.62478 (14)	0.33607 (7)	0.0159 (2)
H22	0.819795	0.677987	0.342878	0.019*
C23	0.67021 (9)	0.63755 (14)	0.25914 (7)	0.0160 (2)
C24	0.57304 (9)	0.55837 (13)	0.24843 (7)	0.0156 (2)
C25	0.56457 (9)	0.46370 (14)	0.31507 (7)	0.0177 (2)
H25	0.500013	0.407833	0.307827	0.021*
C26	0.65032 (9)	0.45039 (14)	0.39242 (7)	0.0179 (2)
H26	0.644264	0.383860	0.437216	0.021*
C27	0.76480 (10)	0.82281 (16)	0.20173 (8)	0.0217 (2)
H27A	0.755218	0.884562	0.149059	0.033*
H27B	0.827392	0.752223	0.214699	0.033*
H27C	0.775101	0.898458	0.249615	0.033*
C28	0.38928 (9)	0.52854 (16)	0.16163 (8)	0.0225 (2)
H28A	0.338779	0.564480	0.105858	0.034*
H28B	0.368932	0.574936	0.207907	0.034*
H28C	0.388298	0.409430	0.164783	0.034*
O1	0.74353 (7)	0.26372 (12)	0.70858 (5)	0.02394 (19)
O2	0.64265 (6)	0.18454 (11)	0.57556 (5)	0.02001 (18)
O3	0.67237 (6)	0.72523 (11)	0.18981 (5)	0.02081 (19)
O4	0.49428 (6)	0.58233 (10)	0.17089 (5)	0.01874 (18)
N2	1.06917 (8)	0.74770 (14)	0.62655 (7)	0.0207 (2)
H021	1.0695 (14)	0.837 (2)	0.5990 (11)	0.033 (4)*
H022	1.1204 (14)	0.733 (2)	0.6765 (12)	0.030 (4)*
N4	0.87969 (8)	0.94458 (13)	0.45245 (6)	0.0220 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01518 (14)	0.02360 (15)	0.01707 (14)	0.00250 (10)	0.00460 (11)	0.00545 (10)
N1	0.0160 (4)	0.0198 (5)	0.0144 (4)	0.0012 (4)	0.0043 (4)	0.0008 (4)
C2	0.0156 (5)	0.0214 (6)	0.0139 (5)	0.0034 (4)	0.0068 (4)	0.0004 (4)
N3	0.0150 (4)	0.0231 (5)	0.0133 (4)	0.0014 (4)	0.0052 (3)	0.0012 (4)
C4	0.0159 (5)	0.0226 (6)	0.0124 (5)	0.0005 (4)	0.0062 (4)	−0.0016 (4)
C5	0.0152 (5)	0.0202 (5)	0.0130 (5)	0.0020 (4)	0.0049 (4)	0.0000 (4)
C6	0.0150 (5)	0.0191 (5)	0.0139 (5)	0.0030 (4)	0.0052 (4)	−0.0009 (4)
C7	0.0138 (5)	0.0232 (6)	0.0133 (5)	−0.0011 (4)	0.0032 (4)	−0.0037 (4)
C8	0.0190 (5)	0.0182 (5)	0.0208 (5)	0.0002 (4)	0.0069 (4)	0.0003 (4)
C9	0.0165 (5)	0.0165 (5)	0.0162 (5)	−0.0019 (4)	0.0046 (4)	0.0021 (4)
C10	0.0173 (6)	0.0254 (6)	0.0194 (5)	0.0023 (5)	0.0058 (5)	−0.0026 (5)
C11	0.0200 (6)	0.0403 (8)	0.0224 (6)	0.0054 (5)	0.0014 (5)	−0.0069 (5)
C21	0.0159 (5)	0.0162 (5)	0.0147 (5)	0.0024 (4)	0.0036 (4)	−0.0011 (4)
C22	0.0137 (5)	0.0175 (5)	0.0156 (5)	0.0004 (4)	0.0040 (4)	−0.0017 (4)
C23	0.0164 (5)	0.0172 (5)	0.0141 (5)	0.0010 (4)	0.0049 (4)	−0.0007 (4)
C24	0.0142 (5)	0.0157 (5)	0.0145 (5)	0.0012 (4)	0.0020 (4)	−0.0020 (4)
C25	0.0165 (5)	0.0165 (5)	0.0193 (5)	−0.0018 (4)	0.0052 (4)	−0.0013 (4)
C26	0.0199 (5)	0.0173 (5)	0.0157 (5)	0.0000 (4)	0.0052 (4)	0.0005 (4)
C27	0.0175 (5)	0.0256 (6)	0.0211 (6)	−0.0054 (5)	0.0056 (4)	0.0014 (5)
C28	0.0131 (5)	0.0272 (6)	0.0232 (6)	−0.0034 (5)	0.0015 (4)	0.0016 (5)
O1	0.0190 (4)	0.0330 (5)	0.0179 (4)	0.0016 (4)	0.0042 (3)	−0.0049 (4)
O2	0.0161 (4)	0.0250 (4)	0.0172 (4)	0.0013 (3)	0.0038 (3)	−0.0031 (3)
O3	0.0166 (4)	0.0282 (5)	0.0146 (4)	−0.0054 (3)	0.0019 (3)	0.0041 (3)
O4	0.0131 (4)	0.0228 (4)	0.0162 (4)	−0.0025 (3)	0.0002 (3)	0.0016 (3)
N2	0.0183 (5)	0.0260 (5)	0.0139 (5)	−0.0042 (4)	0.0011 (4)	0.0019 (4)
N4	0.0216 (5)	0.0219 (5)	0.0198 (5)	−0.0010 (4)	0.0040 (4)	0.0001 (4)

Geometric parameters (Å, º)

S1—C2	1.7619 (12)	C11—H11C	0.9800
S1—C8	1.7987 (12)	C21—C26	1.3908 (16)
N1—C2	1.3348 (14)	C21—C22	1.4066 (16)
N1—C6	1.3508 (15)	C22—C23	1.3786 (15)
C2—N3	1.3323 (15)	C22—H22	0.9500
N3—C4	1.3473 (15)	C23—O3	1.3677 (13)
C4—N2	1.3279 (16)	C23—C24	1.4115 (16)
C4—C5	1.4335 (15)	C24—O4	1.3609 (13)
C5—C6	1.3980 (16)	C24—C25	1.3905 (16)
C5—C7	1.4250 (16)	C25—C26	1.3930 (16)
C6—C21	1.4801 (15)	C25—H25	0.9500
C7—N4	1.1522 (16)	C26—H26	0.9500
C8—C9	1.5136 (16)	C27—O3	1.4309 (14)
C8—H8A	0.9900	C27—H27A	0.9800
C8—H8B	0.9900	C27—H27B	0.9800
C9—O1	1.2091 (15)	C27—H27C	0.9800

C9—O2	1.3288 (14)	C28—O4	1.4328 (14)
C10—O2	1.4608 (14)	C28—H28A	0.9800
C10—C11	1.5023 (17)	C28—H28B	0.9800
C10—H10A	0.9900	C28—H28C	0.9800
C10—H10B	0.9900	N2—H021	0.862 (19)
C11—H11A	0.9800	N2—H022	0.879 (19)
C11—H11B	0.9800		

C2—S1—C8	101.07 (6)	C26—C21—C22	119.06 (10)
C2—N1—C6	115.58 (10)	C26—C21—C6	120.78 (10)
N3—C2—N1	129.32 (11)	C22—C21—C6	120.16 (10)
N3—C2—S1	112.01 (8)	C23—C22—C21	120.65 (10)
N1—C2—S1	118.62 (9)	C23—C22—H22	119.7
C2—N3—C4	115.98 (10)	C21—C22—H22	119.7
N2—C4—N3	118.49 (10)	O3—C23—C22	124.46 (10)
N2—C4—C5	121.75 (11)	O3—C23—C24	115.54 (10)
N3—C4—C5	119.76 (10)	C22—C23—C24	120.00 (10)
C6—C5—C7	123.56 (10)	O4—C24—C25	125.43 (10)
C6—C5—C4	118.35 (10)	O4—C24—C23	115.22 (10)
C7—C5—C4	117.94 (10)	C25—C24—C23	119.35 (10)
N1—C6—C5	120.76 (10)	C24—C25—C26	120.31 (10)
N1—C6—C21	116.78 (10)	C24—C25—H25	119.8
C5—C6—C21	122.46 (10)	C26—C25—H25	119.8
N4—C7—C5	176.29 (12)	C21—C26—C25	120.53 (10)
C9—C8—S1	111.62 (8)	C21—C26—H26	119.7
C9—C8—H8A	109.3	C25—C26—H26	119.7
S1—C8—H8A	109.3	O3—C27—H27A	109.5
C9—C8—H8B	109.3	O3—C27—H27B	109.5
S1—C8—H8B	109.3	H27A—C27—H27B	109.5
H8A—C8—H8B	108.0	O3—C27—H27C	109.5
O1—C9—O2	123.95 (11)	H27A—C27—H27C	109.5
O1—C9—C8	124.61 (10)	H27B—C27—H27C	109.5
O2—C9—C8	111.43 (10)	O4—C28—H28A	109.5
O2—C10—C11	107.23 (10)	O4—C28—H28B	109.5
O2—C10—H10A	110.3	H28A—C28—H28B	109.5
C11—C10—H10A	110.3	O4—C28—H28C	109.5
O2—C10—H10B	110.3	H28A—C28—H28C	109.5
C11—C10—H10B	110.3	H28B—C28—H28C	109.5
H10A—C10—H10B	108.5	C9—O2—C10	115.26 (9)
C10—C11—H11A	109.5	C23—O3—C27	117.04 (9)
C10—C11—H11B	109.5	C24—O4—C28	117.51 (9)
H11A—C11—H11B	109.5	C4—N2—H021	122.7 (12)
C10—C11—H11C	109.5	C4—N2—H022	119.3 (11)
H11A—C11—H11C	109.5	H021—N2—H022	118.1 (16)
H11B—C11—H11C	109.5		

C6—N1—C2—N3	−1.24 (17)	N1—C6—C21—C22	−149.74 (10)
C6—N1—C2—S1	−178.13 (8)	C5—C6—C21—C22	30.48 (16)

C8—S1—C2—N3	168.96 (8)	C26—C21—C22—C23	2.90 (17)
C8—S1—C2—N1	−13.64 (10)	C6—C21—C22—C23	−176.82 (10)
N1—C2—N3—C4	2.13 (17)	C21—C22—C23—O3	179.04 (10)
S1—C2—N3—C4	179.18 (8)	C21—C22—C23—C24	−0.22 (16)
C2—N3—C4—N2	−179.21 (10)	O3—C23—C24—O4	−0.95 (14)
C2—N3—C4—C5	1.14 (15)	C22—C23—C24—O4	178.37 (10)
N2—C4—C5—C6	175.43 (11)	O3—C23—C24—C25	178.65 (10)
N3—C4—C5—C6	−4.93 (15)	C22—C23—C24—C25	−2.03 (16)
N2—C4—C5—C7	−8.73 (16)	O4—C24—C25—C26	−178.87 (10)
N3—C4—C5—C7	170.91 (10)	C23—C24—C25—C26	1.57 (17)
C2—N1—C6—C5	−2.96 (15)	C22—C21—C26—C25	−3.37 (17)
C2—N1—C6—C21	177.25 (9)	C6—C21—C26—C25	176.35 (10)
C7—C5—C6—N1	−169.69 (10)	C24—C25—C26—C21	1.15 (17)
C4—C5—C6—N1	5.90 (16)	O1—C9—O2—C10	1.39 (16)
C7—C5—C6—C21	10.08 (17)	C8—C9—O2—C10	−179.59 (9)
C4—C5—C6—C21	−174.33 (10)	C11—C10—O2—C9	−174.39 (10)
C2—S1—C8—C9	−69.51 (9)	C22—C23—O3—C27	−6.61 (16)
S1—C8—C9—O1	−36.23 (15)	C24—C23—O3—C27	172.68 (10)
S1—C8—C9—O2	144.75 (8)	C25—C24—O4—C28	10.82 (16)
N1—C6—C21—C26	30.55 (15)	C23—C24—O4—C28	−169.61 (10)
C5—C6—C21—C26	−149.23 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H021···N4^{i}	0.862 (19)	2.201 (19)	3.0368 (15)	163.4 (16)
N2—H022···O1^{ii}	0.879 (19)	2.139 (19)	2.9942 (13)	164.0 (16)
N2—H022···S1^{ii}	0.879 (19)	2.973 (17)	3.4465 (11)	115.7 (13)
C8—H8*A*···N4^{iii}	0.99	2.67	3.4693 (16)	138
C11—H11*A*···O3^{iv}	0.98	2.52	3.1459 (15)	122
C27—H27*B*···S1^{v}	0.98	2.95	3.6836 (12)	133

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