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Crystal structure and Hirshfeld surface analysis of ethyl 4-hydroxy-1-methyl-5-oxo-2-(thiophen-2-yl)-2,5-dihydro-1*H*-pyrrole-3-carboxylate

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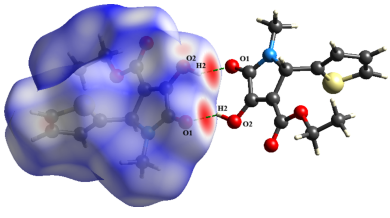
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The molecular and crystal structure of the title compound, $C_{12}H_{13}NO_4S$, has been determined *via* single-crystal X-ray diffraction. As the compound crystallizes in the centrosymmetric space group $P2_1/c$, the crystal is racemic and contains equal numbers of *R* and *S* enantiomers related by inversion symmetry. The thiophene substituent is positionally disordered over two orientations arising from rotation about the C4—C5 bond, with refined site occupancies of 0.929 (2) and 0.071 (2) for the major and minor components, respectively. The major thiophene ring is essentially planar and adopts a nearly orthogonal orientation with respect to the conjugated enaminone fragment. In the crystal packing, the title molecules are linked by intermolecular O—H···O hydrogen bonds to form one-dimensional chains, which are further supported by weak C—H···O interactions, giving rise to a three-dimensional supramolecular architecture. Hirshfeld surface analysis quantitatively revealed that the crystal packing is predominantly governed by H···H (41.5%) and H···O/O···H (31.0%) contacts, with smaller contributions from other intermolecular interactions.

1. Chemical context

Pyrrole derivatives are extensively used as building blocks in pharmaceutical design due to their versatile functionalization and ability to interact with a diverse range of biological targets, as well as their antimicrobial, anticancer, anti-inflammatory and antidiabetic activities (Amina & Redouane, 2025; Yadavalli *et al.*, 2024). The biological activities of thiophene-fused pyrroles are increased due to the presence of both heterocyclic systems (Rajender Kumar *et al.*, 2004; Prashanth *et al.*, 2025). Some derivatives are fluorescent and have been used as biomarkers for disease diagnosis (Moiseeva *et al.*, 2024; Ferreira *et al.*, 2020). Several key synthetic strategies for the synthesis of pyrroles and thiophene-fused pyrroles have been reported, including multicomponent reactions (MCR) (Inglebert *et al.*, 2013), multi-step reductive aminations (Guguloth & Gubbiyappa, 2024) and modified Clauson–Kaas pyrrole ring closures on thiophene templates (Rochais *et al.*, 2004), to advanced macrocyclic *ortho*-phenylene–pyrrole–thiophene icosamers (Matsuo *et al.*, 2025).

However, there is limited empirical structural data on thiophene-substituted pyrrole derivatives although the synthesis of pyrroles is well documented. A definitive description of the molecular geometry and the supramolecular



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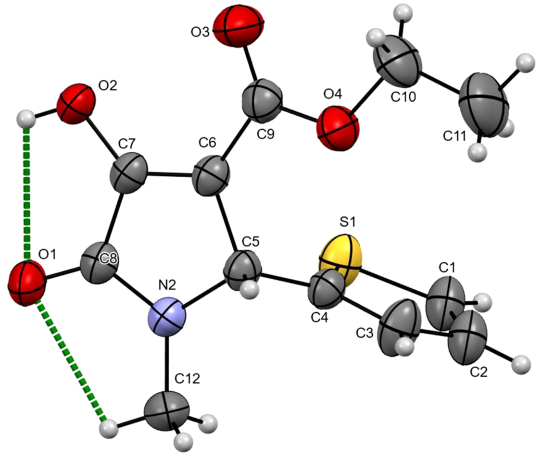


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids. The minor component of the disordered thiophene ring has been omitted for clarity. The O—H···O and C—H···O intramolecular contacts are shown as green dashed lines.

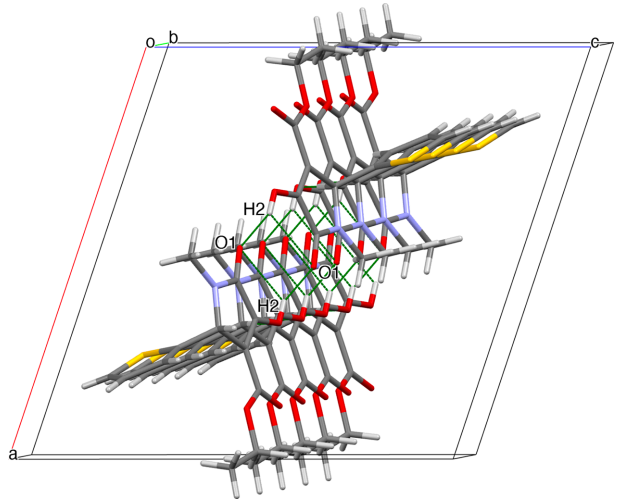
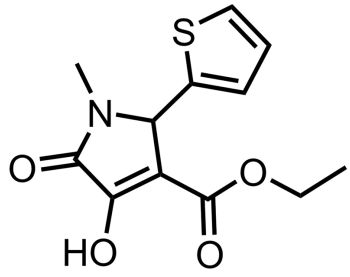


Figure 3
The crystal packing of the title compound, viewed down the *b* axis, illustrating the intermolecular O—H···O and C—H···O hydrogen-bonding interactions, shown as green lines.

architecture of ethyl 4-hydroxy-1-methyl-5-oxo-2-(thiophen-2-yl)-2,5-dihydro-1*H*-pyrrole-3-carboxylate is absent in the structural chemistry literature. Thus, the objective of this study is to determine the three-dimensional crystal structure of the title compound using single-crystal X-ray diffraction and to analyze the percentage contributions of diverse intermolecular interactions to the crystal packing using Hirshfeld surface analysis.

2. Structural commentary

The molecular structure of the title compound, showing the atom-labelling scheme, is presented in Fig. 1. The asymmetric unit comprises one crystallographically independent molecule. The molecule possesses a single stereogenic centre at atom C5. As the structure crystallizes in the centosymmetric space group $P2_1/c$, the crystal is racemic and contains equal numbers of the *R* and *S* enantiomers related by crystallographic inversion symmetry.



The thiophene substituent is positionally disordered over two orientations arising from rotation about the C4—C5 bond. The two disorder components were refined with site-occu-

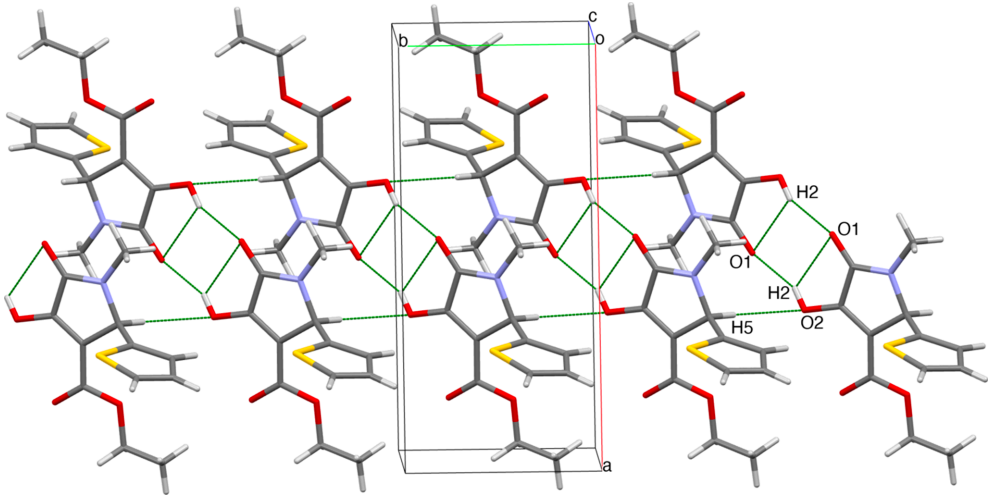


Figure 2
The crystal packing of the title compound, viewed down the *c* axis, illustrating the intermolecular O—H···O and C—H···O hydrogen-bonding interactions, shown as green lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.77 (3)	2.54 (3)	2.905 (2)	112 (3)
C12—H12A···O1	0.96	2.55	2.910 (3)	103
C12—H12A···O1^{i}	0.77 (3)	1.94 (3)	2.637 (2)	151 (3)
C5—H5···O2^{ii}	0.98	2.53	3.489 (2)	166

Symmetry codes: (i) $-x+1, y+\frac{5}{2}, -z+\frac{3}{2}$; (ii) $x, y-1, z$.

pancy factors of 0.929 (2) and 0.071 (2), respectively. For the major component, the thiophene ring (S1/C1–C4) is essentially planar, with a maximum deviation of 0.006 (1) Å for the C4 atom from the least-squares plane and it is oriented nearly perpendicular to the conjugated enaminone fragment (N2/C5–C8), with a dihedral angle of 89.94 (12)° between the planes, adopting a nearly orthogonal arrangement. The conjugated enaminone fragment is essentially planar, as indicated by the torsion angles C5—N2—C8—C7 = 1.5 (2)°, N2—C8—C7—C6 = 0.2 (2)° and C5—C6—C7—C8 = −1.7 (2)°. A weak intramolecular O2—H2···O1 contact is also present, generating an S(5) ring motif and contributing to the observed molecular conformation. In contrast, the tetrahedral stereogenic atom of C5 introduces a slight distortion into the molecular framework, as reflected by the torsion angles N2—C5—C4—S1 = 61.5 (2)° and C6—C5—C7—C8 = −55.9 (2)°. The carbonyl and ester bond lengths of C8—O1 = 1.229 (2) Å, C9—O3 = 1.201 (3) Å and C9—O4 = 1.323 (3) Å are within the expected range.

3. Supramolecular features

In the crystal packing, the molecules are linked through intermolecular O2—H2···O1 hydrogen bonds (Table 1), generating a one-dimensional hydrogen-bonded chain along the b axis. These chains are further stabilized by weak C5—H5···O2^{ii} interactions, forming the three-dimensional supramolecular architecture, as shown in Figs. 2 and 3.

4. Hirshfield surface analysis

A Hirshfeld surface analysis was performed using *CrystalExplorer21* to examine and quantify the intermolecular contacts governing the crystal packing (Spackman *et al.*, 2021).

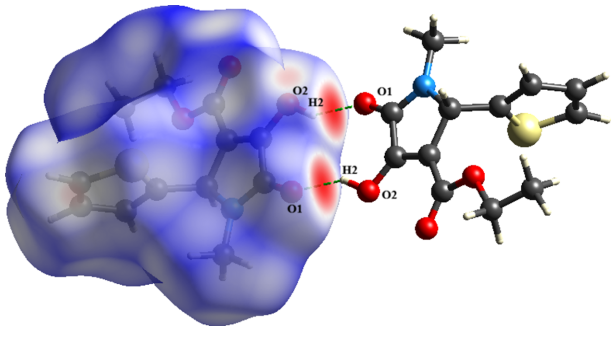


Figure 4
Hirshfeld surface of the title compound, mapped over d_{norm}.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{13}NO_4S$
M_r	267.29
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, b, c (Å)	14.3260 (4), 6.3501 (2), 14.7341 (4)
β (°)	108.740 (2)
V (Å^3)	1269.32 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.26
Crystal size (mm)	0.5 × 0.15 × 0.07
Data collection	
Diffractometer	Bruker SMART APEX CCD area detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23386, 3160, 2243
R_{int}	0.058
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.118, 1.02
No. of reflections	3160
No. of parameters	176
No. of restraints	12
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.20

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2014), *SHELXTL* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), and *OLEX2* (Dolomanov *et al.*, 2009).

Fig. 4 shows the Hirshfeld surface mapped with the normalized contact distance (d_{norm}) and reveals two intense red spots. On the d_{norm} surface, red, white and blue regions correspond to contacts shorter than, approximately equal to and longer than the sum of the van der Waals radii, respectively. Here, the two intense red spots result from the O2—H2···O1 hydrogen bonds (Table 1).

The percentage contributions of the intermolecular interactions to the total Hirshfeld surface were computed by two-dimensional fingerprint plots. As illustrated in Fig. 5, the d_i versus d_e plots show that H···H contacts make the largest contribution (41.5%). The H···O/O···H contacts contribute 31% to the total Hirshfeld surface and are characterized by a pair of prominent spikes in the two-dimensional fingerprint plot. These features are consistent with the O2—H2···O1 hydrogen bonding interaction observed in the crystal (Table 1). Other contacts contribute to a lesser extent, namely, H···C/C···H (14.5%), H···S/S···H (9.4%) and O···S/S···O (1.5%).

5. Database survey

A search of the Cambridge Structural Database (webCSD accessed August 2026; Groom *et al.*, 2016) for the title compound returned no relevant hits. However, a search with generalized pyrrole derivatives returned a number of hits, including CSD refcodes OHEJIY (Abdul Rashid *et al.*, 2024), DILYIK (Abdul Rashid *et al.*, 2023), BOQXEN (del Corte *et*

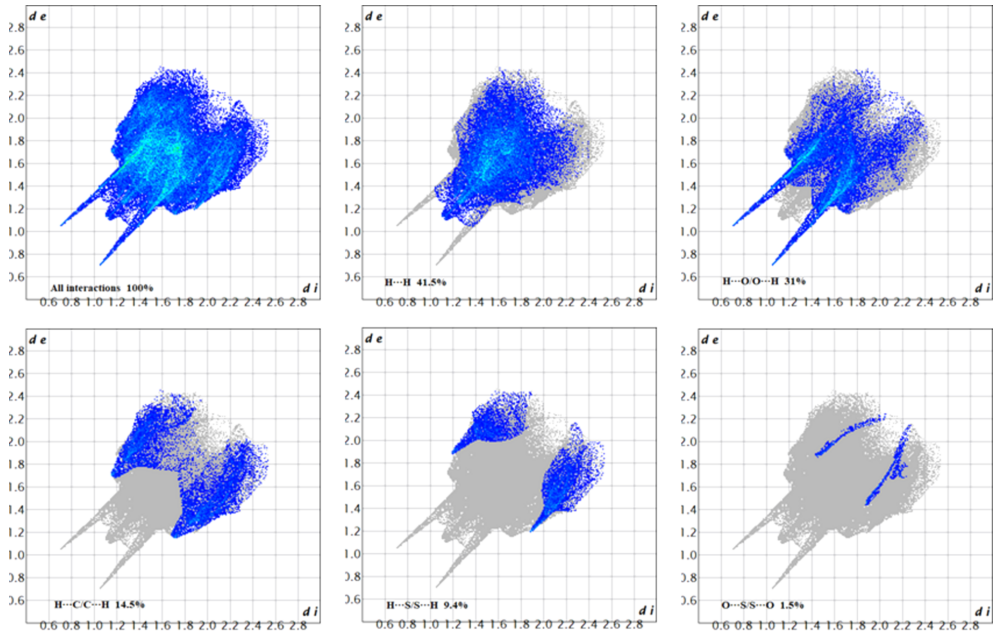


Figure 5
Comparison of the overall and prominent decomposed fingerprint plots (>1%) delineated into H···H, H···O/O···H, H···C/C···H, H···S/S···H and O···S/ S···O of the title compound.

al., 2019), EPEVED (Ahankar *et al.*, 2021), LIFBEJ (Sun *et al.*, 2011) and MEFYEF (Mal & Mukhopadhyay, 2022). The structure also is consistent with thiophene-substituted pyrrole derivatives, namely, DINBUA (Fedoseev *et al.*, 2018) and GITDEV (Saha & Das, 2017).

6. Synthesis and crystallization

The title compound was synthesized using our in-house method described by Mohammat *et al.* (2015) *via* a multiple-component reaction of methylamine, thiophene and sodium diethyl oxalacetate. A single yellow crystal of the compound, suitable for X-ray diffraction analysis, was grown by slow evaporation at room temperature from ethyl acetate/hexane (yield 0.44 g, 43%). IR (ATR): 1733 (C═O), 1663 (C═O) cm^{-1}; ^{1}H NMR (400 MHz, chloroform-*d*): δ 7.29 (*dd*, *J* = 5.0, 1.5 Hz, 1H, HC═C), 7.12–7.06 (*m*, 1H, HC═C), 6.98 (*dd*, *J* = 5.2, 3.5 Hz, 1H, HC═C), 5.33 (*s*, 1H, NCH), 4.27–4.08 (*m*, 2H, CH_2), 2.88 (*s*, 3H, NCH_3), 1.16 (*t*, *J* = 7.1 Hz, 3H, CH_3); ^{13}C NMR (101 MHz, chloroform-*d*): δ 165.19 (C═O), 163.16 (C═O), 157.99 (quat. C), 138.34 (HC═C), 127.96 (HC═C), 126.94 (HC═C), 126.34 (HC═C), 112.35 (C═C), 61.21 (CH_2), 57.91 (NCH), 27.65 (NCH_3), 14.06 (CH_3).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Carbon-bound H atoms were positioned geometrically and refined using a riding model, with C—H distances of 0.93 (aromatic), 0.97 (methylene), 0.98 (methine) and 0.96 Å (methyl). The methyl H atoms were refined as rotating groups. Isotropic displacement parameters were constrained to U_{iso}(H) = 1.2U_{eq}(C) for aromatic, methylene and methine H atoms, and to 1.5U_{eq}(C) for methyl H atoms. The hydroxyl H atom was located in a difference Fourier map and refined independently with an isotropic displacement parameter.

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supporting information

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Crystal structure and Hirshfeld surface analysis of ethyl 4-hydroxy-1-methyl-5-oxo-2-(thiophen-2-yl)-2,5-dihydro-1*H*-pyrrole-3-carboxylate

Nor Habibah Mohd Rosli, Amalina Mohd Tajuddin, Muhamad Azwan Hamali, Siti Syaida Sirat and Mohd Fazli Mohammat

Computing details

Ethyl 4-hydroxy-1-methyl-5-oxo-2-(thiophen-2-yl)-2,5-dihydro-1*H*-pyrrole-3-carboxylate

Crystal data

$C_{12}H_{13}NO_4S$
$M_r = 267.29$
Monoclinic, $P2_1/c$
$a = 14.3260$ (4) Å
$b = 6.3501$ (2) Å
$c = 14.7341$ (4) Å
$\beta = 108.740$ (2)°
$V = 1269.32$ (7) Å^3
$Z = 4$
$F(000) = 560$
$D_x = 1.399$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5165 reflections
$\theta = 2.8$–$24.0°$
$\mu = 0.26$ mm^{-1}
$T = 298$ K
Plate, colourless
0.5 × 0.15 × 0.07 mm

Data collection

Bruker SMART APEX CCD area detector diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
ω and φ scans
23386 measured reflections
3160 independent reflections
2243 reflections with $I > 2\sigma(I)$
$R_{int} = 0.058$
$\theta_{max} = 28.4°$, $\theta_{min} = 3.5°$
$h = -19 \rightarrow 19$
$k = -8 \rightarrow 8$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.118$
$S = 1.02$
3160 reflections
176 parameters
12 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.4448P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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.
The equation of the plane is of the form: P * x + Q * y + R * z - S = 0 where P, Q, R, S are constants and x, y, z are fractional coordinates. P = 10.577 (11), Q = 1.349 (6), R = 5.437 (13), S = 10.079 (3) Atom Distance x y z * S1: -0.005 (1) 0.7316 0.5380 0.2962 * C1: 0.003 (2) 0.7824 0.3487 0.2457 * C2: 0.001 (3) 0.7849 0.1612 0.2870 * C3: -0.005 (3) 0.7442 0.1626 0.3647 * C4: 0.006 (2) 0.7131 0.3639 0.3773 * P = -7.400 (12), Q = -2.756 (6), R = 12.745 (10), S = -0.384 (10) Atom Distance x y z * N2: -0.012 (2) 0.5654 0.5073 0.4069 * C5: 0.014 (2) 0.6665 0.4292 0.4508 * C6: -0.013 (2) 0.7152 0.6096 0.5160 * C7: 0.006 (2) 0.6481 0.7589 0.5107 * C8: 0.004 (2) 0.5518 0.6964 0.4411 *

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.73146 (5)	0.53827 (9)	0.29597 (5)	0.0537 (2)	0.929 (2)
O1	0.47515 (9)	0.7992 (2)	0.41956 (10)	0.0537 (4)	
O2	0.65899 (10)	0.9413 (2)	0.55704 (10)	0.0469 (3)	
O3	0.85752 (11)	0.7521 (3)	0.62993 (13)	0.0744 (5)	
O4	0.86123 (10)	0.4271 (2)	0.57403 (10)	0.0551 (4)	
N2	0.56557 (10)	0.5076 (2)	0.40703 (11)	0.0414 (4)	
C11	1.0011 (2)	0.2150 (5)	0.5940 (3)	0.0957 (9)	
H11A	0.993122	0.232038	0.527155	0.144*	
H11B	0.964010	0.094891	0.602372	0.144*	
H11C	1.069547	0.194408	0.629167	0.144*	
C10	0.96487 (16)	0.4060 (4)	0.62976 (18)	0.0692 (6)	
H10A	0.972688	0.391347	0.697333	0.083*	
H10B	1.001395	0.529001	0.621344	0.083*	
C9	0.81827 (13)	0.6095 (3)	0.57917 (13)	0.0446 (4)	
C6	0.71514 (12)	0.6098 (3)	0.51600 (12)	0.0381 (4)	
C5	0.66662 (12)	0.4295 (3)	0.45074 (12)	0.0381 (4)	
H5	0.664628	0.307015	0.490526	0.046*	
C4	0.71304 (12)	0.3640 (3)	0.37738 (12)	0.0383 (4)	
C1	0.7825 (2)	0.3461 (4)	0.24489 (18)	0.0537 (5)	0.929 (2)
H1	0.806754	0.369330	0.194303	0.064*	0.929 (2)
C2	0.78308 (18)	0.1595 (4)	0.28646 (17)	0.0537 (5)	0.929 (2)
H2A	0.806150	0.035786	0.267398	0.064*	0.929 (2)
C3	0.7444 (4)	0.1732 (5)	0.3630 (3)	0.0574 (8)	0.929 (2)
H3	0.740980	0.057679	0.400569	0.069*	0.929 (2)
C8	0.55184 (13)	0.6964 (3)	0.44110 (12)	0.0396 (4)	
C7	0.64828 (13)	0.7589 (3)	0.51072 (12)	0.0374 (4)	
C12	0.49014 (14)	0.3923 (3)	0.33459 (15)	0.0537 (5)	
H12A	0.427934	0.462546	0.322046	0.081*	
H12B	0.485397	0.252043	0.357042	0.081*	
H12C	0.507151	0.385933	0.276719	0.081*	
H2	0.606 (2)	0.996 (4)	0.5500 (17)	0.072 (8)*	
C3A	0.761 (3)	0.499 (3)	0.337 (2)	0.0537 (2)	0.071 (2)
H3A	0.777749	0.637631	0.355350	0.064*	0.071 (2)
C2A	0.782 (3)	0.393 (4)	0.260 (2)	0.0537 (5)	0.071 (2)

H2AA	0.775026	0.442555	0.199384	0.064*	0.071 (2)
C1A	0.814 (2)	0.195 (4)	0.299 (2)	0.0537 (5)	0.071 (2)
H1A	0.864381	0.118193	0.288507	0.064*	0.071 (2)
S1A	0.7427 (17)	0.1129 (18)	0.3721 (15)	0.0574 (8)	0.071 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0706 (4)	0.0410 (3)	0.0575 (4)	0.0124 (2)	0.0316 (3)	0.0121 (2)
O1	0.0443 (7)	0.0526 (8)	0.0589 (8)	0.0142 (6)	0.0091 (6)	−0.0119 (6)
O2	0.0451 (7)	0.0371 (7)	0.0558 (8)	0.0030 (6)	0.0125 (6)	−0.0123 (6)
O3	0.0545 (9)	0.0623 (10)	0.0891 (12)	0.0031 (7)	−0.0009 (8)	−0.0281 (9)
O4	0.0428 (7)	0.0519 (8)	0.0609 (8)	0.0122 (6)	0.0030 (6)	−0.0044 (6)
N2	0.0385 (8)	0.0362 (8)	0.0487 (8)	0.0009 (6)	0.0127 (6)	−0.0072 (6)
C11	0.0624 (15)	0.0839 (19)	0.133 (3)	0.0273 (14)	0.0205 (16)	0.0003 (18)
C10	0.0446 (11)	0.0753 (16)	0.0756 (15)	0.0139 (11)	0.0025 (10)	0.0026 (12)
C9	0.0442 (10)	0.0444 (10)	0.0446 (10)	0.0044 (8)	0.0133 (8)	−0.0001 (8)
C6	0.0432 (9)	0.0339 (8)	0.0379 (8)	0.0038 (7)	0.0139 (7)	0.0012 (7)
C5	0.0412 (9)	0.0307 (8)	0.0435 (9)	0.0040 (7)	0.0151 (7)	0.0018 (7)
C4	0.0409 (9)	0.0331 (9)	0.0408 (9)	0.0042 (7)	0.0129 (7)	0.0007 (7)
C1	0.0596 (9)	0.0557 (11)	0.0507 (10)	0.0180 (9)	0.0245 (8)	0.0016 (8)
C2	0.0596 (9)	0.0557 (11)	0.0507 (10)	0.0180 (9)	0.0245 (8)	0.0016 (8)
C3	0.0816 (14)	0.0372 (19)	0.0626 (16)	0.014 (2)	0.0359 (11)	0.0087 (18)
C8	0.0423 (9)	0.0367 (9)	0.0406 (9)	0.0039 (7)	0.0147 (7)	−0.0006 (7)
C7	0.0447 (9)	0.0320 (8)	0.0375 (8)	0.0015 (7)	0.0161 (7)	−0.0005 (7)
C12	0.0459 (10)	0.0533 (12)	0.0592 (12)	−0.0058 (9)	0.0133 (9)	−0.0175 (9)
C3A	0.0706 (4)	0.0410 (3)	0.0575 (4)	0.0124 (2)	0.0316 (3)	0.0121 (2)
C2A	0.0596 (9)	0.0557 (11)	0.0507 (10)	0.0180 (9)	0.0245 (8)	0.0016 (8)
C1A	0.0596 (9)	0.0557 (11)	0.0507 (10)	0.0180 (9)	0.0245 (8)	0.0016 (8)
S1A	0.0816 (14)	0.0372 (19)	0.0626 (16)	0.014 (2)	0.0359 (11)	0.0087 (18)

Geometric parameters (Å, º)

S1—C4	1.7137 (17)	C5—H5	0.9800
S1—C1	1.716 (2)	C5—C4	1.498 (2)
O1—C8	1.229 (2)	C4—C3	1.333 (4)
O2—C7	1.328 (2)	C4—C3A	1.355 (16)
O2—H2	0.81 (3)	C4—S1A	1.658 (12)
O3—C9	1.194 (2)	C1—H1	0.9300
O4—C10	1.454 (2)	C1—C2	1.333 (3)
O4—C9	1.325 (2)	C2—H2A	0.9300
N2—C5	1.469 (2)	C2—C3	1.410 (4)
N2—C8	1.338 (2)	C3—H3	0.9300
N2—C12	1.450 (2)	C8—C7	1.486 (2)
C11—H11A	0.9600	C12—H12A	0.9600
C11—H11B	0.9600	C12—H12B	0.9600
C11—H11C	0.9600	C12—H12C	0.9600
C11—C10	1.481 (4)	C3A—H3A	0.9300

C10—H10A	0.9700	C3A—C2A	1.420 (18)
C10—H10B	0.9700	C2A—H2AA	0.9300
C9—C6	1.472 (2)	C2A—C1A	1.393 (18)
C6—C5	1.513 (2)	C1A—H1A	0.9300
C6—C7	1.331 (2)	C1A—S1A	1.778 (18)

C4—S1—C1	91.76 (11)	C3A—C4—C5	123.4 (10)
C7—O2—H2	110.9 (18)	C3A—C4—S1A	114.4 (11)
C9—O4—C10	117.19 (16)	S1—C1—H1	124.1
C8—N2—C5	112.38 (14)	C2—C1—S1	111.82 (19)
C8—N2—C12	124.32 (15)	C2—C1—H1	124.1
C12—N2—C5	123.29 (14)	C1—C2—H2A	124.3
H11A—C11—H11B	109.5	C1—C2—C3	111.5 (2)
H11A—C11—H11C	109.5	C3—C2—H2A	124.3
H11B—C11—H11C	109.5	C4—C3—C2	115.0 (3)
C10—C11—H11A	109.5	C4—C3—H3	122.5
C10—C11—H11B	109.5	C2—C3—H3	122.5
C10—C11—H11C	109.5	O1—C8—N2	127.31 (17)
O4—C10—C11	106.6 (2)	O1—C8—C7	126.29 (16)
O4—C10—H10A	110.4	N2—C8—C7	106.40 (14)
O4—C10—H10B	110.4	O2—C7—C6	128.92 (17)
C11—C10—H10A	110.4	O2—C7—C8	121.08 (15)
C11—C10—H10B	110.4	C6—C7—C8	110.00 (15)
H10A—C10—H10B	108.6	N2—C12—H12A	109.5
O3—C9—O4	124.40 (17)	N2—C12—H12B	109.5
O3—C9—C6	124.76 (17)	N2—C12—H12C	109.5
O4—C9—C6	110.82 (15)	H12A—C12—H12B	109.5
C9—C6—C5	124.33 (15)	H12A—C12—H12C	109.5
C7—C6—C9	126.52 (16)	H12B—C12—H12C	109.5
C7—C6—C5	109.03 (15)	C4—C3A—H3A	125.9
N2—C5—C6	102.13 (13)	C4—C3A—C2A	108.2 (18)
N2—C5—H5	108.4	C2A—C3A—H3A	125.9
N2—C5—C4	112.38 (14)	C3A—C2A—H2AA	128.4
C6—C5—H5	108.4	C1A—C2A—C3A	103.3 (19)
C4—C5—C6	116.67 (14)	C1A—C2A—H2AA	128.4
C4—C5—H5	108.4	C2A—C1A—H1A	125.2
C5—C4—S1	121.96 (12)	C2A—C1A—S1A	109.5 (18)
C5—C4—S1A	118.7 (6)	S1A—C1A—H1A	125.2
C3—C4—S1	109.9 (2)	C4—S1A—C1A	87.2 (9)
C3—C4—C5	128.2 (2)		

S1—C4—C3—C2	−0.5 (5)	C5—N2—C8—O1	−178.65 (17)
S1—C1—C2—C3	−1.8 (4)	C5—N2—C8—C7	1.45 (19)
O1—C8—C7—O2	−0.2 (3)	C5—C6—C7—O2	178.89 (16)
O1—C8—C7—C6	−179.82 (17)	C5—C6—C7—C8	−1.51 (19)
O3—C9—C6—C5	178.93 (19)	C5—C4—C3—C2	178.6 (3)
O3—C9—C6—C7	−5.4 (3)	C5—C4—C3A—C2A	−171 (2)
O4—C9—C6—C5	−2.6 (2)	C5—C4—S1A—C1A	−166.1 (12)

O4—C9—C6—C7	173.00 (16)	C4—S1—C1—C2	1.4 (2)
N2—C5—C4—S1	61.47 (18)	C4—C3A—C2A—C1A	−43 (4)
N2—C5—C4—C3	−117.6 (4)	C1—S1—C4—C5	−179.67 (17)
N2—C5—C4—C3A	86 (2)	C1—S1—C4—C3	−0.4 (3)
N2—C5—C4—S1A	−115.8 (10)	C1—C2—C3—C4	1.6 (5)
N2—C8—C7—O2	179.72 (15)	C8—N2—C5—C6	−2.25 (18)
N2—C8—C7—C6	0.08 (19)	C8—N2—C5—C4	−128.06 (15)
C10—O4—C9—O3	−4.0 (3)	C7—C6—C5—N2	2.22 (18)
C10—O4—C9—C6	177.58 (17)	C7—C6—C5—C4	125.17 (16)
C9—O4—C10—C11	−166.2 (2)	C12—N2—C5—C6	177.25 (16)
C9—C6—C5—N2	178.53 (15)	C12—N2—C5—C4	51.4 (2)
C9—C6—C5—C4	−58.5 (2)	C12—N2—C8—O1	1.9 (3)
C9—C6—C7—O2	2.7 (3)	C12—N2—C8—C7	−178.04 (16)
C9—C6—C7—C8	−177.71 (16)	C3A—C4—S1A—C1A	−6 (2)
C6—C5—C4—S1	−56.0 (2)	C3A—C2A—C1A—S1A	38 (3)
C6—C5—C4—C3	124.9 (4)	C2A—C1A—S1A—C4	−20 (2)
C6—C5—C4—C3A	−31 (2)	S1A—C4—C3A—C2A	30 (3)
C6—C5—C4—S1A	126.8 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.77 (3)	2.54 (3)	2.905 (2)	112 (3)
C12—H12*A*···O1	0.96	2.55	2.910 (3)	103
C12—H12*A*···O1^{i}	0.77 (3)	1.94 (3)	2.637 (2)	151 (3)
C5—H5···O2^{ii}	0.98	2.53	3.489 (2)	166

Symmetry codes: (i) −*x*+1, *y*+5/2, −*z*+3/2; (ii) *x*, *y*−1, *z*.