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Crystal structure and Hirshfeld surface analysis of *N*-{[5-(4-methylphenyl)-1,2-oxazol-3-yl]methyl}-1-phenyl-*N*-(prop-2-en-1-yl)methanesulfonamide

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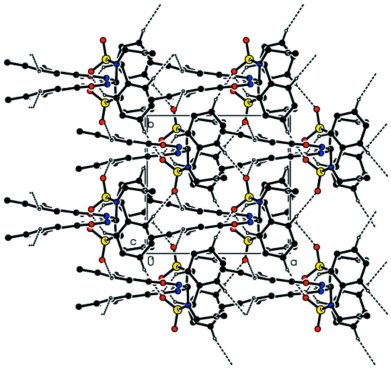
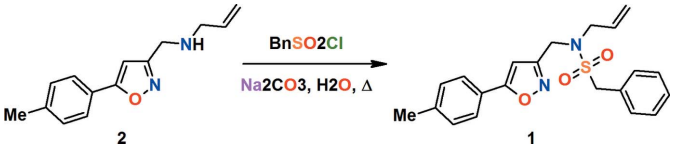
In the title compound, $C_{21}H_{22}N_2O_3S$, the 1,2-oxazole ring makes the dihedral angles of 9.16 (16) and 87.91 (17)°, respectively, with the toluene and phenyl rings, while they form a dihedral angle of 84.42 (15)° with each other. The C—S—N—C_{pr} and C—S—N—C_{me} (pr = propene, me = 3-methyl-1,2-oxazole) torsion angles are 86.8 (2) and −100.6 (3) °, respectively. In the crystal, molecules are linked by C—H···O hydrogen bonds, generating a three-dimensional network. A Hirshfeld surface analysis was performed to investigate the contributions of the different intermolecular contacts within the supramolecular structure. The major interactions are H···H (53.6%), C···H/H···C (20.8%) and O···H/H···O (17.7%).

1. Chemical context

Sulfonamide antibiotics are readily available drugs that are gradually losing their importance due to the development of bacterial resistance (Sköld, 2000). Along with the use of much less accessible antibiotics of other classes, the design of new sulfonamides to overcome this problem seems to be reasonable (Nadirova *et al.*, 2021; Naghiyev *et al.*, 2020). One of the possible methods for structural modification is the synthesis of drug analogues containing heterocycles. From this point of view, isothiazole (Kletskov *et al.*, 2020; Khalilov *et al.*, 2021) and isoxazole (Zhu *et al.*, 2018; Abdelhamid *et al.*, 2011) rings are of great interest. In particular, isoxazole derivatives possess a wide range of biological activity, so this heterocycle is considered to be one of the most privileged scaffolds in pharmaceutical chemistry (Altug *et al.*, 2017; Safavora *et al.*, 2019). Moreover, a lot of isoxazoles exhibit antibacterial properties on their own (Agrawal & Mishra, 2018; Yadigarov *et al.*, 2009), and the widely used sulfonamide antibiotic sulfamethoxazole contains an isoxazole ring. A preliminary assessment of the biological activity of newly designed isoxazole-containing structures can be carried out *in silico* using molecular docking. Data on the structural parameters of promising molecules is therefore required (Gurbanov *et al.*, 2020*a*,*b*; Ma *et al.*, 2020,2021). All this was our motive for the synthesis and accurate structure establishment of *N*-allyl-*N*-[(5-tolylisoxazol-3-yl)methyl]benzylsulfonamide (**1**), which



has not previously been characterized. It was obtained from isoxazolylallylamine (**2**) and benzyl sulfonyl chloride using the 'green chemistry' procedure developed earlier by one of us (Kolesnik *et al.*, 2022).



Allyl derivatives structurally similar to sulfonamide **1** are widely used as starting materials in organic synthesis for the construction of polyheterocyclic systems through intramolecular [4 + 2] cycloaddition reactions (Zubkov *et al.*, 2014; Krishna *et al.*, 2022).

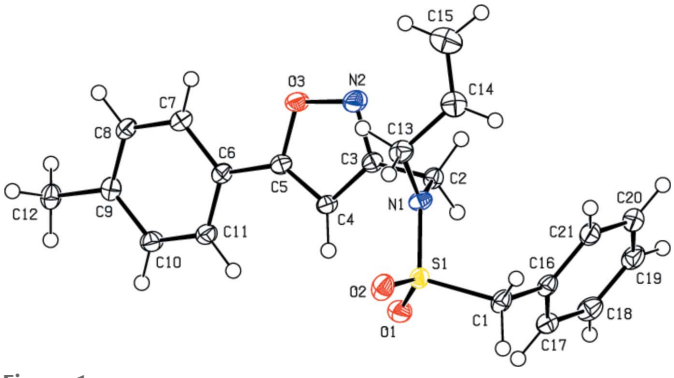


Figure 1
The title molecule with the labelling scheme and 50% probability ellipsoids.

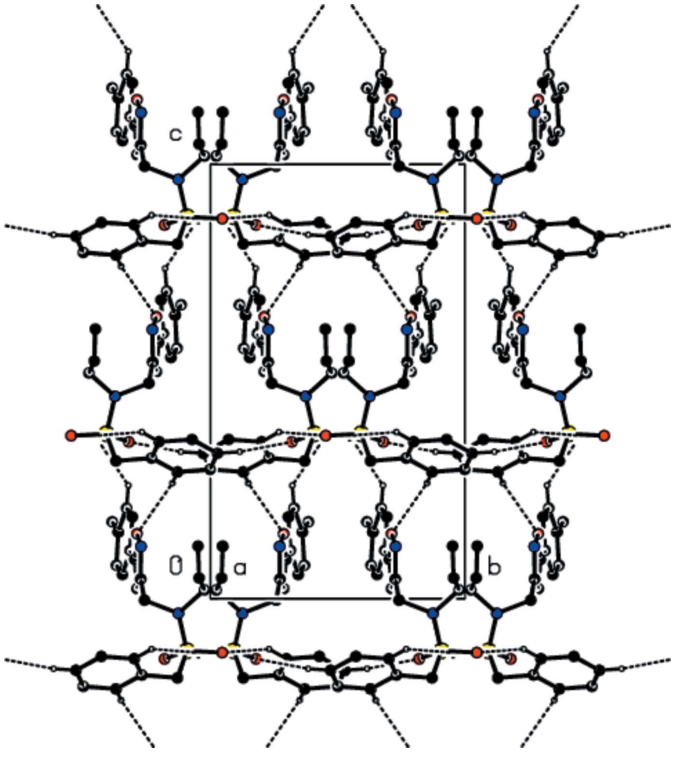


Figure 2
A view along the *a* axis of the C—H···O interactions in the title compound.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O2^{i}	0.95	2.59	3.404 (4)	143
C17—H17···O3^{ii}	0.95	2.57	3.314 (4)	135
C19—H19···O1^{iii}	0.95	2.51	3.434 (4)	165
C21—H21···O2^{iv}	0.95	2.50	3.369 (4)	152

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

2. Structural commentary

In the title compound (Fig. 1), the 1,2-oxazole ring (O3/N2/C3–C5) forms dihedral angles of 9.16 (16) and 87.91 (17) °, respectively, with the toluene and phenyl rings (C6–C11 and C16–C21) which subtend a dihedral angle of 84.42 (15)° with each other. The torsion angles C1—S1—N1—C2 and C1—S1—N1—C13 are 86.8 (2) and −100.6 (3) °, respectively.

3. Supramolecular features and Hirshfeld surface analysis

Molecules in the crystal are joined together by C—H···O hydrogen bonds, forming a three-dimensional network (Table 1; Figs. 2, 3 and 4).

The Hirshfeld surfaces were calculated and two-dimensional fingerprint plots generated using *Crystal Explorer 17.5* (Spackman *et al.*, 2021). Fig. 5 depicts the three-dimensional Hirshfeld surface projected over d_{norm} in the range −0.1677 to 1.4857 a.u. The bright-red patches surrounding O1, O2, and O3 and hydrogen atoms H8, H17, H19, and H21, which highlight their activities as donors and/or acceptors, can be connected with O1, O2, and O3 interactions, which play a significant role in the molecular packing (Tables 1 and 2).

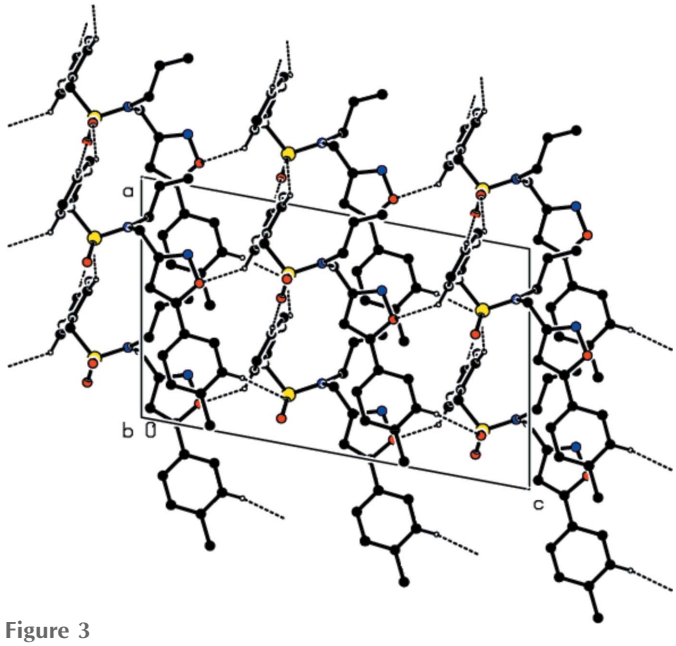


Figure 3
A view along the *b* axis of the C—H···O interactions in the title compound.

Table 2
Summary of short interatomic contacts (Å) in the title compound.

Contact	Distance	Symmetry operation
O1···H19	2.51	$-\frac{1}{2}+x, 2-y, z$
H17···O3	2.57	$x, \frac{3}{2}-y, -\frac{1}{2}+z$
O2···H21	2.50	$-\frac{1}{2}+x, 1-y, z$
O2···H8	2.59	$\frac{1}{2}+x, -\frac{1}{2}+y, -\frac{1}{2}+z$
C8···H18	2.92	$-\frac{1}{2}+x, -\frac{1}{2}+y, \frac{1}{2}+z$
H12*C*···H2*B*	2.43	$-1+x, y, z$
C16···H12*B*	2.96	$1+x, \frac{3}{2}-y, -\frac{1}{2}+z$

Fig. 6*a* depicts the overall two-dimensional fingerprint plot for the title compound. The percentage contributions to the Hirshfeld surfaces from various interatomic interactions (Table 2) include H···H (53.6%; Fig. 6*b*), C···H/H···C (20.8%; Fig. 6*c*) and O···H/H···C (17.7%; Fig. 6*d*). Other contact types, such as N···H/H···N (4.5%), C···C (1.7%), N···C/C···N (0.9%), and O···C/C···O (0.8%), account for less than 4.5% of the Hirshfeld surface and are likely to have little directional impact on the packing.

4. Database survey

Four related compounds with a methanesulfonamide unit have been reported, *viz.* *N*-(4-chlorophenyl)-1-(5-{[(2-phenylvinyl)sulfonyl]methyl}-1,3,4-oxadiazol-2-yl)methanesulfonamide (CEGKAC: Muralikrishna *et al.*, 2012), *N*-(4-fluorophenyl)methanesulfonamide (CICPIO: Gowda *et al.*, 2007*a*), *N*-(2,5-dichlorophenyl)methanesulfonamide (WIHGUQ: Gowda *et al.*, 2007*b*) and *N*-(3-methylphenyl)methanesulfonamide (VIDKOJ: Gowda *et al.*, 2007*c*).

In the crystal of CEGKAC, molecules are linked by N—H···O hydrogen bonds, generating *C*(10) chains propagating in [001]. The packing is consolidated by C—H···O, C—H···π and very weak aromatic π–π stacking interactions [centroid–centroid separation = 4.085 (2) Å]. In the crystal of CICPIO, the molecules are packed into a layer structure along the *a*-axis direction *via* N—H···O hydrogen bonds [H···O = 2.08 (2), N···O = 2.911 (6) Å and N—H···O = 164 (6)°]. In the crystal of WIHGUQ, the amide H atom is available to a receptor molecule as it lies on one side of the plane of the benzene ring, while the methanesulfonyl group is on the opposite side of the plane, similar to the arrangement in other methanesulfonanilides. The molecules are packed into chains through N—H···O and N—H···Cl hydrogen bonding. In the crystal of VIDKOJ, the molecules are linked into chains along the *c*-axis direction through N—H···O hydrogen bonds.

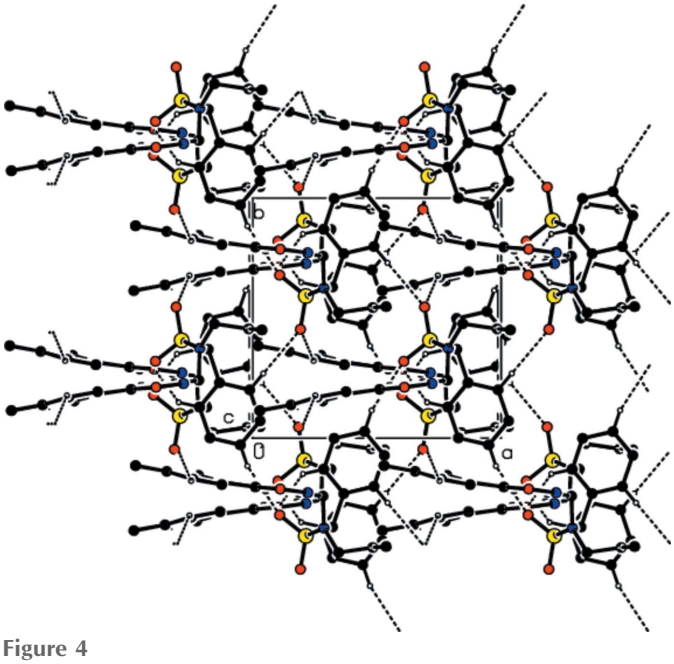


Figure 4
A view along the *c* axis of the C—H···O interactions in the title compound.

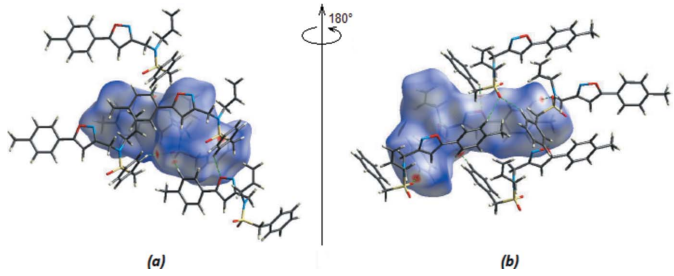


Figure 5
View of the three-dimensional Hirshfeld surface of the title compound plotted over d_{norm} in the range −0.1677 to +1.4857 a.u.

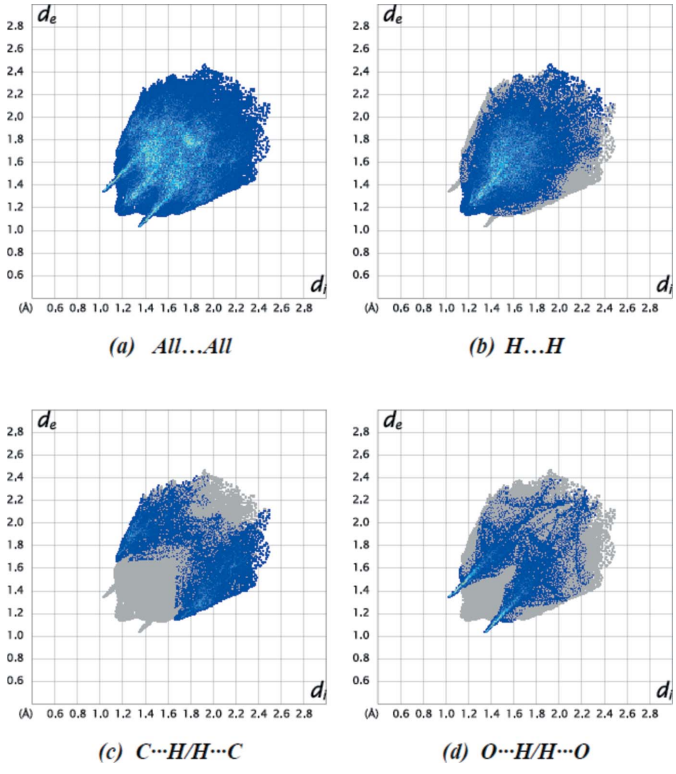


Figure 6
Two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H/H···C and (*d*) O···H/H···O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

5. Synthesis and crystallization

A mixture of 1,2-oxazolylallylamine **2** (1 mmol), benzyl sulfonyl chloride (1.2 mmol) and Na_2CO_3 (1.2 mmol) in water (15 mL) was refluxed for 4 h. After cooling, the reaction mixture was extracted with CH_2Cl_2 (3 × 10 mL). The combined organic fractions were washed with water (2 × 10 mL) and dried over Na_2SO_4. The solvent was evaporated under reduced pressure. The resulting oil was purified by flash chromatography (eluent CH_2Cl_2) and crystallized from MeOH as colourless crystals, yield 0.16 g (41%), m.p. 371–373 K. IR (KBr), ν (cm^{-1}): 1642, 1618, 1599, 1568 (1,2-oxazole), 1343 (S═O), 1151, 1128 (SO_2), 698 (N—SO_2), 541 (Aryl). ^{1}H NMR (500 MHz, $CDCl_3$, 293 K): δ = 2.40 (*s*, 3H, H12*A*, H12*B*, H12*C*), 3.71–3.73 (*d*, 2H, H13*A*, H13*B*, *J* = 6.7), 4.21 (*s*, 2H, H2*A*, H2*B*), 4.33 (*s*, 2H, H1*A*, H1*B*), 5.22–5.29 (*m*, 2H, H15*A*, H15*B*), 5.63–5.71 (*m*, 1H, H14), 6.47 (*s*, 1H, H4), 7.25–7.27 (*m*, 2H, H8, H10), 7.36–7.41 (*m*, 5H, H17, H18, H19, H20, H21), 7.64–7.65 (*d*, 2H, H7, H11, *J* = 8.2). ^{13}C NMR (126 MHz, $CDCl_3$, 293 K): δ = 21.66, 42.55, 50.58, 59.53, 98.99, 120.50, 124.64, 125.95 (2C), 129.01 (2C), 129.06, 129.85 (2C), 130.94 (2C), 132.24, 140.86, 160.95, 170.91. MS (APCI): *m*/*z* = 383 $[M + H]^+$.

6. Refinement details

Crystal data, data collection and structure refinement details are summarized in Table 3. The C-bound H atoms were positioned with idealized geometry and refined using a riding model with C—H = 0.95 Å (CH aromatic), 0.99 Å (CH_2) and 0.98 Å (CH_3). Isotropic displacement parameters for all H atoms were set equal to 1.2 or 1.5U_{eq} (parent atom). The crystal studied was refined as an inversion twin.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{22}N_2O_3S$
M_r	382.46
Crystal system, space group	Monoclinic, *Ia*
Temperature (K)	100
a, *b*, *c* (Å)	10.7979 (1), 10.2238 (10), 17.7316 (2)
β (°)	100.526 (1)
V (Å^3)	1924.55 (19)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	1.69
Crystal size (mm)	0.24 × 0.22 × 0.14
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.668, 0.779
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21251, 3572, 3542
R_{int}	0.051
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.638
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.045, 0.125, 1.09
No. of reflections	3572
No. of parameters	247
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.47, −0.58
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.00 (2)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

Acknowledgements

The authors' contributions are as follows. Conceptualization, MA and SM; synthesis, IAK, and VIP; X-ray analysis, STÇ, VNK and MA; writing (review and editing of the manuscript) STÇ, MA, IAK and SM; funding acquisition, SM; supervision, MA, VIP and SM.

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supporting information

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Crystal structure and Hirshfeld surface analysis of *N*-{[5-(4-methylphenyl)-1,2-oxazol-3-yl]methyl}-1-phenyl-*N*-(prop-2-en-1-yl)methanesulfonamide

Victor N. Khrustalev, Sevim Türktekin Çelikesir, Mehmet Akkurt, Irina A. Kolesnik, Vladimir I. Potkin and Sixberth Mlowe

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

N-{[5-(4-Methylphenyl)-1,2-oxazol-3-yl]methyl}-1-phenyl-N-(prop-2-en-1-yl)methanesulfonamide

Crystal data

$C_{21}H_{22}N_2O_3S$
$M_r = 382.46$
Monoclinic, *Ia*
$a = 10.7979$ (1) Å
$b = 10.2238$ (10) Å
$c = 17.7316$ (2) Å
$\beta = 100.526$ (1)°
$V = 1924.55$ (19) Å^3
$Z = 4$
$F(000) = 808$
$D_x = 1.320$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 18074 reflections
$\theta = 5.0$–$79.2°$
$\mu = 1.69$ mm^{-1}
$T = 100$ K
Prism, colourless
0.24 × 0.22 × 0.14 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
φ and ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
$T_{min} = 0.668$, $T_{max} = 0.779$
21251 measured reflections
3572 independent reflections
3542 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 79.6°$, $\theta_{min} = 5.0°$
$h = -13\rightarrow13$
$k = -12\rightarrow13$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.125$
$S = 1.09$
3572 reflections
247 parameters
2 restraints
Primary atom site location: SHELXT
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1004P)^2 + 0.3109P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.58$ e Å^{-3}

Extinction correction: SHELXL-2018/3 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0023 (4)
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.00 (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.

Refinement. Refined as a two-component inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.20850 (6)	0.59215 (6)	0.37939 (4)	0.0181 (2)
O1	0.1034 (2)	0.6795 (2)	0.36066 (12)	0.0253 (5)
O2	0.1867 (2)	0.4534 (2)	0.37509 (14)	0.0271 (5)
O3	0.1016 (2)	0.7878 (2)	0.64904 (11)	0.0248 (5)
N1	0.2802 (2)	0.6254 (2)	0.46571 (13)	0.0183 (5)
N2	0.2125 (3)	0.7725 (3)	0.61968 (15)	0.0259 (6)
C1	0.3167 (3)	0.6294 (3)	0.31677 (16)	0.0206 (6)
H1A	0.390384	0.570343	0.328837	0.025*
H1B	0.275212	0.612336	0.263131	0.025*
C2	0.2760 (3)	0.7586 (3)	0.49593 (15)	0.0180 (5)
H2A	0.258277	0.820906	0.452560	0.022*
H2B	0.359354	0.780818	0.526667	0.022*
C3	0.1778 (3)	0.7734 (3)	0.54474 (16)	0.0178 (5)
C4	0.0450 (3)	0.7881 (3)	0.52263 (15)	0.0179 (5)
H4	−0.003053	0.791270	0.472112	0.022*
C5	0.0023 (3)	0.7966 (3)	0.58978 (15)	0.0180 (5)
C6	−0.1207 (3)	0.8145 (3)	0.61079 (15)	0.0173 (5)
C7	−0.1342 (3)	0.8064 (3)	0.68787 (15)	0.0199 (6)
H7	−0.063522	0.785401	0.726289	0.024*
C8	−0.2503 (3)	0.8290 (3)	0.70805 (15)	0.0193 (5)
H8	−0.258482	0.822084	0.760347	0.023*
C9	−0.3554 (3)	0.8615 (3)	0.65319 (16)	0.0189 (6)
C10	−0.3414 (3)	0.8690 (3)	0.57646 (16)	0.0214 (6)
H10	−0.412186	0.890631	0.538263	0.026*
C11	−0.2261 (3)	0.8453 (3)	0.55508 (16)	0.0209 (6)
H11	−0.218664	0.850017	0.502582	0.025*
C12	−0.4808 (3)	0.8853 (3)	0.67664 (17)	0.0235 (6)
H12A	−0.470660	0.949937	0.718118	0.035*
H12B	−0.512271	0.803142	0.694488	0.035*
H12C	−0.540911	0.918217	0.632572	0.035*
C13	0.3384 (3)	0.5231 (3)	0.51956 (18)	0.0233 (6)
H13A	0.325804	0.436904	0.493807	0.028*
H13B	0.295250	0.521026	0.564246	0.028*
C14	0.4759 (3)	0.5443 (3)	0.5472 (2)	0.0264 (6)
H14	0.528386	0.555444	0.510125	0.032*

C15	0.5284 (4)	0.5485 (3)	0.6206 (2)	0.0334 (8)
H15A	0.477943	0.537711	0.658813	0.040*
H15B	0.616492	0.562376	0.635134	0.040*
C16	0.3618 (3)	0.7690 (3)	0.32347 (15)	0.0189 (6)
C17	0.2818 (3)	0.8703 (3)	0.29145 (17)	0.0221 (6)
H17	0.198709	0.850949	0.265671	0.026*
C18	0.3237 (3)	0.9990 (3)	0.29736 (18)	0.0260 (6)
H18	0.269020	1.067490	0.275926	0.031*
C19	0.4454 (4)	1.0278 (3)	0.33448 (18)	0.0265 (7)
H19	0.474088	1.115850	0.338020	0.032*
C20	0.5246 (3)	0.9281 (3)	0.36625 (19)	0.0271 (6)
H20	0.607762	0.947754	0.391695	0.033*
C21	0.4827 (3)	0.7986 (3)	0.36106 (17)	0.0223 (6)
H21	0.537283	0.730553	0.383366	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0203 (3)	0.0186 (3)	0.0162 (3)	−0.0028 (2)	0.0055 (2)	−0.0023 (2)
O1	0.0217 (11)	0.0310 (11)	0.0225 (10)	0.0011 (8)	0.0021 (8)	0.0003 (8)
O2	0.0370 (14)	0.0212 (10)	0.0251 (10)	−0.0095 (9)	0.0107 (10)	−0.0038 (9)
O3	0.0178 (10)	0.0414 (12)	0.0150 (10)	0.0038 (8)	0.0028 (8)	−0.0014 (8)
N1	0.0245 (12)	0.0164 (10)	0.0141 (10)	0.0019 (9)	0.0032 (9)	−0.0022 (9)
N2	0.0209 (12)	0.0395 (15)	0.0182 (12)	0.0047 (11)	0.0061 (10)	−0.0024 (10)
C1	0.0271 (15)	0.0194 (12)	0.0176 (11)	−0.0009 (11)	0.0099 (11)	−0.0021 (10)
C2	0.0204 (13)	0.0169 (11)	0.0175 (12)	−0.0005 (10)	0.0055 (10)	−0.0014 (9)
C3	0.0192 (13)	0.0180 (12)	0.0165 (12)	0.0013 (9)	0.0042 (10)	−0.0010 (9)
C4	0.0193 (13)	0.0199 (11)	0.0143 (11)	0.0007 (9)	0.0022 (10)	0.0008 (9)
C5	0.0201 (14)	0.0178 (11)	0.0160 (12)	0.0011 (10)	0.0031 (10)	−0.0007 (10)
C6	0.0216 (14)	0.0150 (11)	0.0160 (12)	0.0004 (9)	0.0049 (10)	−0.0005 (9)
C7	0.0241 (14)	0.0197 (13)	0.0162 (12)	0.0014 (10)	0.0044 (10)	0.0012 (10)
C8	0.0245 (14)	0.0188 (11)	0.0158 (12)	−0.0011 (10)	0.0065 (10)	0.0002 (10)
C9	0.0213 (13)	0.0146 (12)	0.0220 (13)	0.0002 (9)	0.0073 (11)	−0.0013 (9)
C10	0.0222 (14)	0.0235 (14)	0.0181 (13)	0.0012 (11)	0.0022 (10)	0.0015 (10)
C11	0.0206 (14)	0.0259 (13)	0.0164 (12)	0.0007 (10)	0.0042 (10)	0.0000 (11)
C12	0.0223 (15)	0.0256 (13)	0.0247 (14)	0.0003 (11)	0.0105 (12)	−0.0012 (12)
C13	0.0274 (15)	0.0190 (13)	0.0229 (14)	0.0014 (10)	0.0030 (11)	0.0044 (10)
C14	0.0257 (16)	0.0237 (14)	0.0297 (15)	0.0047 (11)	0.0046 (13)	0.0013 (12)
C15	0.0347 (18)	0.0248 (15)	0.0369 (18)	0.0049 (13)	−0.0035 (14)	−0.0022 (13)
C16	0.0235 (14)	0.0192 (13)	0.0156 (12)	0.0001 (10)	0.0079 (10)	−0.0015 (9)
C17	0.0242 (14)	0.0244 (14)	0.0175 (11)	−0.0017 (12)	0.0036 (11)	0.0006 (11)
C18	0.0360 (18)	0.0213 (13)	0.0212 (14)	0.0011 (12)	0.0061 (12)	0.0029 (11)
C19	0.0388 (19)	0.0216 (13)	0.0199 (13)	−0.0089 (12)	0.0076 (13)	0.0001 (10)
C20	0.0276 (16)	0.0323 (16)	0.0218 (14)	−0.0082 (13)	0.0055 (12)	0.0018 (12)
C21	0.0220 (14)	0.0255 (13)	0.0204 (13)	0.0013 (11)	0.0068 (11)	0.0033 (11)

Geometric parameters (Å, º)

S1—O1	1.434 (2)	C9—C12	1.507 (4)
S1—O2	1.438 (2)	C10—C11	1.388 (4)
S1—N1	1.620 (2)	C10—H10	0.9500
S1—C1	1.794 (3)	C11—H11	0.9500
O3—C5	1.360 (3)	C12—H12A	0.9800
O3—N2	1.399 (3)	C12—H12B	0.9800
N1—C2	1.468 (3)	C12—H12C	0.9800
N1—C13	1.477 (4)	C13—C14	1.492 (5)
N2—C3	1.313 (4)	C13—H13A	0.9900
C1—C16	1.506 (4)	C13—H13B	0.9900
C1—H1A	0.9900	C14—C15	1.322 (5)
C1—H1B	0.9900	C14—H14	0.9500
C2—C3	1.494 (4)	C15—H15A	0.9500
C2—H2A	0.9900	C15—H15B	0.9500
C2—H2B	0.9900	C16—C21	1.387 (4)
C3—C4	1.424 (4)	C16—C17	1.401 (4)
C4—C5	1.355 (4)	C17—C18	1.389 (4)
C4—H4	0.9500	C17—H17	0.9500
C5—C6	1.455 (4)	C18—C19	1.389 (5)
C6—C11	1.400 (4)	C18—H18	0.9500
C6—C7	1.403 (3)	C19—C20	1.383 (5)
C7—C8	1.385 (4)	C19—H19	0.9500
C7—H7	0.9500	C20—C21	1.397 (4)
C8—C9	1.393 (4)	C20—H20	0.9500
C8—H8	0.9500	C21—H21	0.9500
C9—C10	1.398 (4)		

O1—S1—O2	119.14 (15)	C10—C9—C12	121.4 (3)
O1—S1—N1	108.03 (13)	C11—C10—C9	121.2 (3)
O2—S1—N1	107.60 (13)	C11—C10—H10	119.4
O1—S1—C1	107.57 (14)	C9—C10—H10	119.4
O2—S1—C1	107.18 (14)	C10—C11—C6	120.1 (3)
N1—S1—C1	106.70 (14)	C10—C11—H11	120.0
C5—O3—N2	109.1 (2)	C6—C11—H11	120.0
C2—N1—C13	117.3 (2)	C9—C12—H12A	109.5
C2—N1—S1	119.87 (19)	C9—C12—H12B	109.5
C13—N1—S1	122.40 (19)	H12A—C12—H12B	109.5
C3—N2—O3	105.7 (2)	C9—C12—H12C	109.5
C16—C1—S1	112.94 (19)	H12A—C12—H12C	109.5
C16—C1—H1A	109.0	H12B—C12—H12C	109.5
S1—C1—H1A	109.0	N1—C13—C14	112.9 (3)
C16—C1—H1B	109.0	N1—C13—H13A	109.0
S1—C1—H1B	109.0	C14—C13—H13A	109.0
H1A—C1—H1B	107.8	N1—C13—H13B	109.0
N1—C2—C3	112.2 (2)	C14—C13—H13B	109.0
N1—C2—H2A	109.2	H13A—C13—H13B	107.8

C3—C2—H2A	109.2	C15—C14—C13	123.4 (3)
N1—C2—H2B	109.2	C15—C14—H14	118.3
C3—C2—H2B	109.2	C13—C14—H14	118.3
H2A—C2—H2B	107.9	C14—C15—H15A	120.0
N2—C3—C4	111.5 (3)	C14—C15—H15B	120.0
N2—C3—C2	118.9 (3)	H15A—C15—H15B	120.0
C4—C3—C2	129.6 (3)	C21—C16—C17	119.3 (3)
C5—C4—C3	104.6 (2)	C21—C16—C1	120.5 (3)
C5—C4—H4	127.7	C17—C16—C1	120.2 (3)
C3—C4—H4	127.7	C18—C17—C16	120.1 (3)
C4—C5—O3	109.2 (3)	C18—C17—H17	120.0
C4—C5—C6	134.8 (3)	C16—C17—H17	120.0
O3—C5—C6	116.0 (2)	C19—C18—C17	120.3 (3)
C11—C6—C7	119.0 (3)	C19—C18—H18	119.9
C11—C6—C5	120.7 (2)	C17—C18—H18	119.9
C7—C6—C5	120.3 (3)	C20—C19—C18	119.8 (3)
C8—C7—C6	120.1 (3)	C20—C19—H19	120.1
C8—C7—H7	119.9	C18—C19—H19	120.1
C6—C7—H7	119.9	C19—C20—C21	120.2 (3)
C7—C8—C9	121.3 (2)	C19—C20—H20	119.9
C7—C8—H8	119.3	C21—C20—H20	119.9
C9—C8—H8	119.3	C16—C21—C20	120.3 (3)
C8—C9—C10	118.3 (3)	C16—C21—H21	119.9
C8—C9—C12	120.3 (3)	C20—C21—H21	119.9

O1—S1—N1—C2	−28.6 (3)	O3—C5—C6—C7	−7.5 (4)
O2—S1—N1—C2	−158.5 (2)	C11—C6—C7—C8	−0.2 (4)
C1—S1—N1—C2	86.8 (2)	C5—C6—C7—C8	177.3 (3)
O1—S1—N1—C13	144.0 (2)	C6—C7—C8—C9	−0.8 (4)
O2—S1—N1—C13	14.2 (3)	C7—C8—C9—C10	1.0 (4)
C1—S1—N1—C13	−100.6 (3)	C7—C8—C9—C12	179.9 (3)
C5—O3—N2—C3	0.4 (3)	C8—C9—C10—C11	−0.3 (4)
O1—S1—C1—C16	58.5 (2)	C12—C9—C10—C11	−179.1 (3)
O2—S1—C1—C16	−172.3 (2)	C9—C10—C11—C6	−0.6 (4)
N1—S1—C1—C16	−57.3 (2)	C7—C6—C11—C10	0.8 (4)
C13—N1—C2—C3	−75.0 (3)	C5—C6—C11—C10	−176.6 (3)
S1—N1—C2—C3	98.1 (3)	C2—N1—C13—C14	−65.6 (3)
O3—N2—C3—C4	−0.4 (3)	S1—N1—C13—C14	121.6 (3)
O3—N2—C3—C2	−179.9 (2)	N1—C13—C14—C15	126.2 (3)
N1—C2—C3—N2	101.3 (3)	S1—C1—C16—C21	105.6 (3)
N1—C2—C3—C4	−78.2 (4)	S1—C1—C16—C17	−74.6 (3)
N2—C3—C4—C5	0.2 (3)	C21—C16—C17—C18	0.1 (4)
C2—C3—C4—C5	179.7 (3)	C1—C16—C17—C18	−179.7 (3)
C3—C4—C5—O3	0.0 (3)	C16—C17—C18—C19	0.5 (5)
C3—C4—C5—C6	178.8 (3)	C17—C18—C19—C20	−0.6 (5)
N2—O3—C5—C4	−0.2 (3)	C18—C19—C20—C21	0.1 (5)
N2—O3—C5—C6	−179.3 (2)	C17—C16—C21—C20	−0.6 (4)
C4—C5—C6—C11	−8.8 (5)	C1—C16—C21—C20	179.2 (3)

O3—C5—C6—C11	169.9 (2)	C19—C20—C21—C16	0.5 (5)
C4—C5—C6—C7	173.8 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O3	0.95	2.44	2.763 (4)	100
C8—H8···O2^{i}	0.95	2.59	3.404 (4)	143
C13—H13*A*···O2	0.99	2.36	2.867 (4)	111
C17—H17···O3^{ii}	0.95	2.57	3.314 (4)	135
C19—H19···O1^{iii}	0.95	2.51	3.434 (4)	165
C21—H21···O2^{iv}	0.95	2.50	3.369 (4)	152

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