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Crystal structure and Hirshfeld surface analysis of 4-cyano-*N*-[(4-cyanophenyl)sulfonyl]-*N*-[2-(5-methylfuran-2-yl)phenyl]benzenesulfonamide

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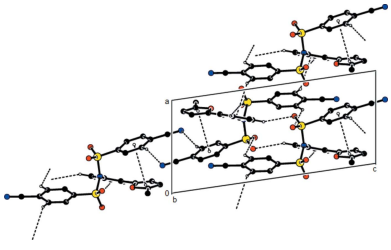
In the title compound, $C_{25}H_{17}N_3O_5S_2$, intramolecular π–π interactions [centroid-to-centroid distance = 3.5640 (9) Å] are observed between the furan and benzene rings of the 4-cyanophenyl group. In the crystal, molecules are connected *via* C—H···O and C—H···N hydrogen bonds, forming layers parallel to the (100) plane. These layers are interconnected by C—H···π interactions and weak van der Waals interactions. Hirshfeld surface analysis indicates that H···H (30.2%), N···H/H···N (22.3%), C···H/H···C (17.9%) and O···H/H···O (15.4%) interactions make the most significant contributions to the crystal packing.

1. Chemical context

The famous Hinsberg reaction, first described by Oscar Hinsberg in 1890 (Hinsberg, 1890; Hinsberg & Kessler, 1905), is a laboratory test used for the detection of primary, secondary and tertiary amines. In this reaction, the corresponding amine is shaken with benzyl or *p*-tolylsulfonyl chloride in the presence of an aqueous base. Reactions with ammonia, and primary and secondary amines are the most widespread. A primary amine will form a soluble sulfonamide salt in the presence of aqueous alkali (either KOH or NaOH). A secondary amine in the same reaction forms an insoluble sulfonamide. The most widely used sulfonylamide is sulfanilamide, an antibacterial drug that was first obtained in 1908 by the Austrian chemist Paul Josef Jakob Gelmo while he was trying to synthesize a dye for textile materials (Gelmo, 1908). Moreover, sulfonylamides are active against seizures (Thiry *et al.*, 2008), and inhibit various enzymes such as human leukocyte elastase, cathespin G and HIV-1 protease (Supuran *et al.*, 2003). Sulfonamides are also used in fungicidal (Chohan *et al.*, 2006, 2010) and insecticidal mixtures (Beesley & Peters, 1971). The number of donor and acceptor groups is a fundamental molecular descriptor to predict the oral bioavailability as well as biocatalytic activity of small drug candidates (Gurbanov *et al.*, 2020*a*,*b*, 2022; Mahmoudi *et al.*, 2017*a*,*b*). Continuing our research in the improved multiple displacement amplification (IMDA) reaction field (Mammadova *et al.*, 2023; Krishna *et al.*, 2022; Yarovaya *et al.*, 2021), in this work we have studied the interaction of 2-(α-furyl)aniline with sulfochloride containing



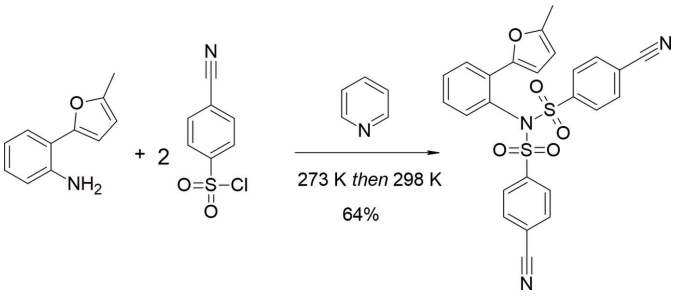
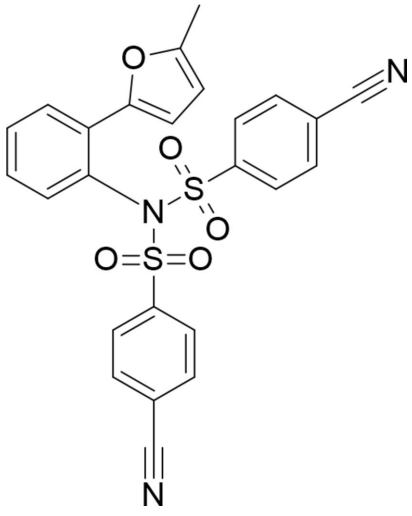


Figure 1
Reaction scheme showing the one-pot synthesis of the title compound.

an electron-withdrawing 4-cyanophenyl group. Unexpectedly, under mild reaction conditions, the product of a double sulfarylation was isolated in good yield from the reaction mixture (Fig. 1). The formation of such double sulfonamide was previously observed in the presence of strong bases (Bartsch *et al.*, 1977; Li *et al.*, 2022).



2. Structural commentary

In the title compound (Fig. 2), the angle between the planes of the phenyl rings (C12–C17 and C19–C24) of the (4-cyanophenyl)sulfonyl groups is 47.90 (7)°. The furan ring (O1/C7–C10) is inclined at angles of 39.05 (8) and 17.38 (8)° with respect to the C12–C17 and C19–C24 phenyl rings of the (4-cyanophenyl)sulfonyl groups, while it makes a dihedral angle of 20.21 (8)° with the plane of the phenyl ring (C1–C6) attached to the furan ring. The latter phenyl ring makes dihedral angles of 26.28 (7) and 36.40 (7)°, respectively, with the phenyl rings of the (4-cyanophenyl)sulfonyl groups. All geometric parameters are normal and consistent with those of related compounds listed in the *Database survey* (Section 4).

Intramolecular π–π stacking interactions [$Cg1\cdots Cg4$ = 3.5640 (9) Å; $Cg1$ and $Cg4$ are the centroids of the furan (O1/C7–C10) and benzene rings (C19–C24), respectively, of one of the two 4-cyanophenyl)sulfonyl groups, respectively; slippage = 0.793 Å], ensures the stability of the molecular configuration.

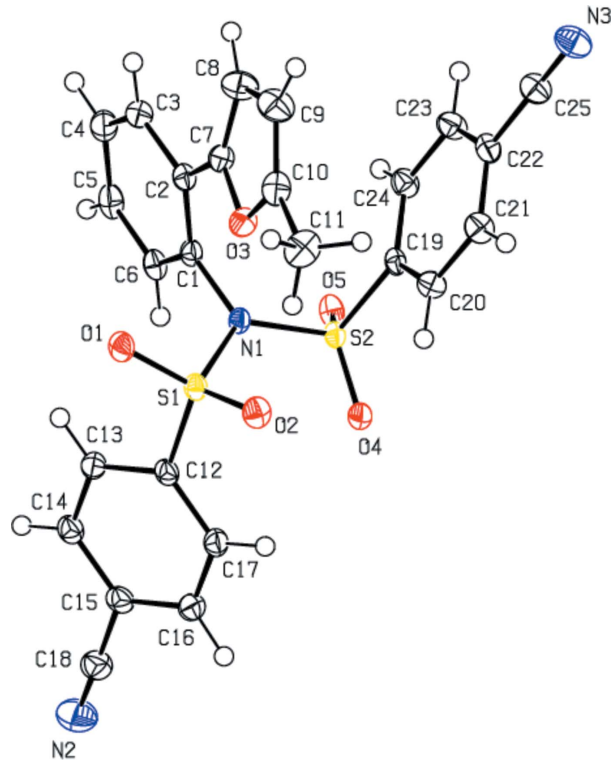


Figure 2
Molecular structure of the title compound showing the atomic labelling. Displacement ellipsoids are drawn at the 50% probability level.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked *via* C—H···O and C—H···N hydrogen bonds, forming layers parallel to the (100) plane (Table 1; Fig. 3). These layers are interconnected by C—H···π interactions and weak van der Waals interactions, thus ensuring crystal cohesion.

Hirshfeld surfaces were generated for the molecule of the title compound using *Crystal Explorer 17.5* (Spackman *et al.*,

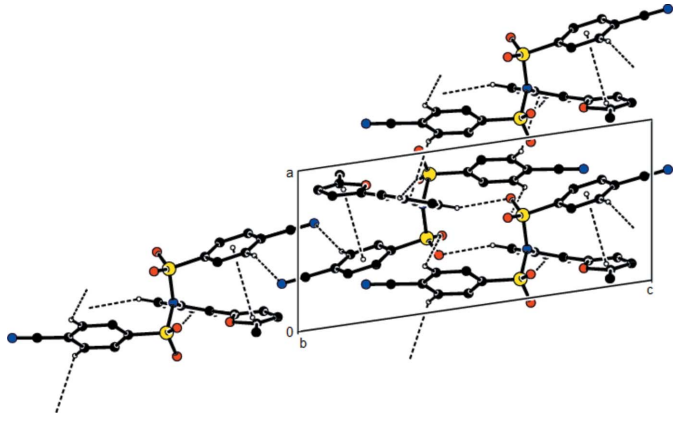


Figure 3
Crystal packing of the title compound along the *b* axis showing the C—H···O and C—H···N hydrogen bonds and C—H···π and π–π interactions.

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

*Cg*2 is the centroid of the ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{i}	0.95	2.56	3.3639 (17)	142
C6—H6···O5^{ii}	0.95	2.56	3.3744 (17)	143
C11—H11*B*···N3^{iii}	0.98	2.67	3.616 (2)	163
C16—H16···O4^{iv}	0.95	2.55	3.2115 (18)	127
C21—H21···N3^{iii}	0.95	2.54	3.433 (2)	156
C14—H14···*Cg*2^{v}	0.95	2.85	3.4945 (16)	126

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

2021). The d_{norm} mappings was performed in the range −0.3260 to +1.4294 a.u. The C—H···O and C—H···N interactions are indicated by red areas on the Hirshfeld surfaces (Fig. 4). Fingerprint plots (Fig. 5) reveal that while H···H interactions (30.2%) make the largest contributions to surface contacts (Tables 1 and 2), N···H/H···N (22.3%), C···H/H···C (17.9%) and O···H/H···O (15.4%) contacts are also important. Other, less notable interactions are O···C/C···O (6.0%), C···C (5.0%), N···N (1.2%), O···O (1.1%), N···C/C···N (0.5%), S···H/H···S (0.1%) and S···O/O···S (0.1%).

4. Database survey

Ten related compounds were found as a result of the search for '*N-(methanesulfonyl)-N-methylmethanesulfonamide*' in the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom *et al.*, 2016), *viz.* PIMGUR (Mammadova *et al.*, 2023), JOBTIF (Kim, 2014), CEGMIM (Mughal *et al.*, 2012*a*), CEGSUE (Mughal *et al.*, 2012*b*), YAXKAL (Taher & Smith, 2012*a*), EFASUB (Taher & Smith, 2012*b*), OCABUR (Abbassi *et al.*, 2011), AYUPUG (Arshad *et al.*, 2011), PONZIC (Rizzoli *et al.*, 2009) and ROGJON (Li & Song, 2008).

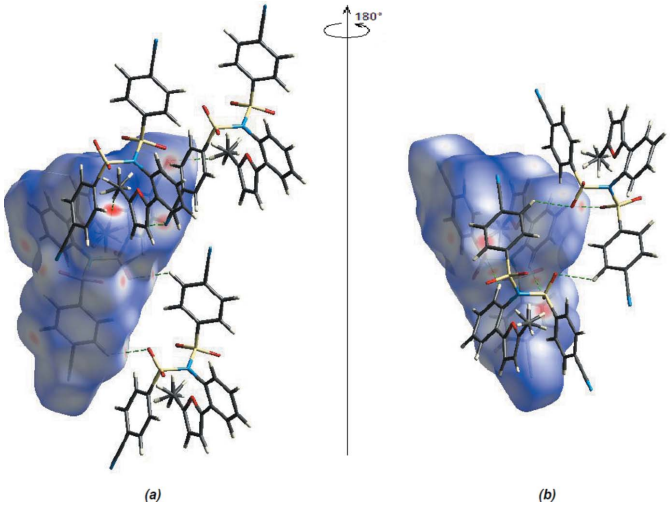


Figure 4
Front (*a*) and back (*b*) views of the three-dimensional Hirshfeld surface for the title compound. Some intermolecular C—H···O and C—H···N interactions are shown.

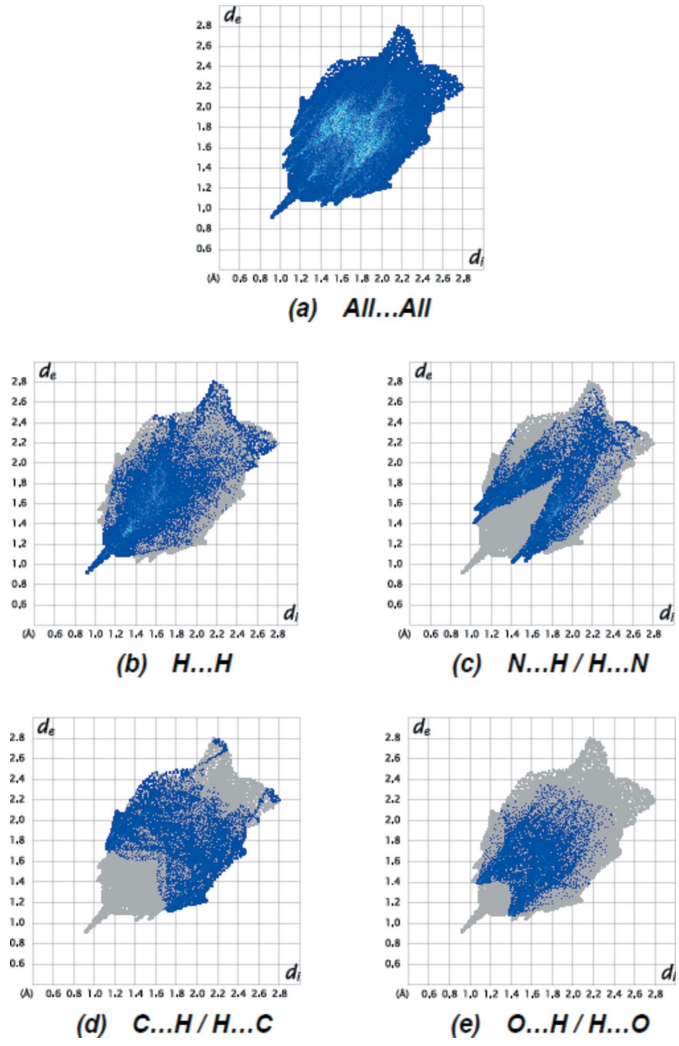


Figure 5
The two-dimensional fingerprint plots for the title compound showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) N···H/H···N, (*d*) C···H/H···C and (*e*) O···H/H···O interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

In PIMGUR (space group $P2_1/n$), C—H···O hydrogen bonds link adjacent molecules in a three-dimensional network, while π–π stacking interactions [centroid–centroid distance = 3.8745 (9) Å] between the furan and a phenyl ring of one of the two (3-nitrophenyl)sulfonyl groups result in chains parallel to the *a* axis. In JOBTIF (space group $P2_1/n$), molecules are linked by pairs of C—H···O hydrogen bonds, forming inversion dimers. In CEGMIM (space group *Pbca*), molecules are connected by C—H···O interactions into sheets in the *ab* plane. In the crystal of CEGSUE (space group $P\overline{1}$), the only directional interactions are very weak C—H···π interactions and very weak π–π stacking between parallel methylphenyl rings. In YAXKAL (space group $P\overline{1}$), molecules associate *via* pairs of N—H···N hydrogen bonds, forming a centrosymmetric eight-membered {···HNCN}$_2$ synthon. In EFASUB (space group *C*2/*c*), molecules associate *via* N—H···N and N—H···O hydrogen bonds, forming extended hydrogen-

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

Contact	Distance	Symmetry operation
C25···H11*C*	2.91	$-1+x, y, z$
H20···H4	2.37	$x, -1+y, z$
H11*E*···N2	2.76	$2-x, -y, 1-z$
H20···H16	2.44	$1-x, -y, 1-z$
H6···O5	2.56	$1-x, 1-y, 1-z$
H21···N3	2.54	$1-x, -y, -z$
H8···N3	2.73	$1-x, 1-y, -z$
H13···H13	2.40	$2-x, 1-y, 1-z$
H11*D*···H11*D*	2.02	$2-x, -y, -z$

bonded sheets that lie parallel to the *bc* plane. The N—H···N hydrogen bonds propagate along the *b*-axis direction, while the N—H···O hydrogen bonds propagate along the *c*-axis direction. The crystal structure of OCABUR (space group $P2_1/c$) features C—H···O hydrogen bonds. In the crystal structure of AYUPUG (space group $P2_1/c$), weak C—H···O interactions connect the molecules in a zigzag manner along the *a*-axis direction. In the crystal of PONZIC (space group $P\overline{1}$), molecules are linked into chains parallel to the *a* axis by intermolecular C—H···O hydrogen bonds and π–π stacking interactions. In ROGJON (space group *Pbca*), the crystal structure features weak intermolecular N—H···O, C—H···O and C—H···N hydrogen bonds and π–π interactions.

5. Synthesis and crystallization

p-Cyanobenzenesulphonyl chloride (2.33 g, 0.0115 mol) was added gradually to a solution of 2-(5-methyl-2-furyl)aniline (1.00 g, 0.00577 mol) in pyridine (7 mL) under stirring and cooling in an ice–water bath. The mixture was stirred for 7 h at r.t. and after completion of the reaction [thin-layer chromatography (TLC) monitoring; sorbfil, hexane/ethyl acetate 4:1], the mixture was poured into hydrochloric acid (6 *M*, 90 mL). The separated oil was washed with water until its crystallization. The obtained crystals were filtered off, dried, and recrystallized from an ethanol/dimethylformamide (DMF) mixture to give the target disulfonamide as a colourless solid. Single crystals were obtained by slow crystallization from an EtOH/DMF mixture (yield 64%, 1.86 g; m.p. 507–508 K). IR (KBr), ν (cm^{-1}): 1156 (ν_s SO$_2$), 1329 (ν_{as} SO$_2$), 2237 (CN). ^{1}H NMR (600.2 MHz, DMSO-d_6) (*J*, Hz): δ 8.08 (*d*, *J* = 8.6 Hz, 4H), 7.90 (*d*, *J* = 8.6 Hz, 4H), 7.72 (*dd*, *J* = 8.1, 1.5 Hz, 1H), 7.56 (*dt*, *J* = 8.6, 1.5 Hz, 1H), 7.36 (*dt*, *J* = 8.1, 1.5 Hz, 1H), 7.04 (*dd*, *J* = 8.1, 1.5 Hz, 1H), 6.61 (*d*, *J* = 3.5 Hz, 1H), 5.93 (*br.d*, *J* = 3.5 Hz, 1H), 1.96 (*s*, 3H); ^{13}C{^{1}H} NMR (150.9 MHz, DMSO-d_6): δ 153.2, 147.9 (2C), 142.9, 134.0 (4C), 133.7, 132.2, 132.0, 129.6 (4C), 128.8, 128.7, 128.6, 117.9 (2C), 117.4 (2C), 112.0, 108.6, 13.4; MS (ESI) *m*/*z*: [*M* + H]$^+$ 504. Elemental analysis calculated (%) for $C_{25}H_{17}N_3O_5S_2$ %: C 59.63, H 3.40, N 8.34, S 12.74; found: C 60.00, H 3.27, N 8.56, S 13.03.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All C-bound H atoms were positioned geometrically (C—H = 0.95 and 0.98 Å) and included as riding contributions with isotropic displacement parameters fixed at $1.2U_{eq}$(C) (1.5 for methyl groups). The hydrogen atoms of the methyl group containing the C11 atom were disordered over two positions with equal occupancies.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{17}N_3O_5S_2$
M_r	503.53
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	7.4542 (1), 9.5111 (2), 16.4378 (3)
α, β, γ (°)	88.838 (4), 81.644 (1), 81.414 (1)
V (Å^3)	1140.11 (4)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.50
Crystal size (mm)	0.29 × 0.22 × 0.15
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.481, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	29936, 4841, 4675
R_{int}	0.051
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.036, 0.095, 1.08
No. of reflections	4841
No. of parameters	316
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, −0.60

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT2016/6* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

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

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supporting information

Acta Cryst. (2023). E**79**, 747-751 [https://doi.org/10.1107/S2056989023006254]

Crystal structure and Hirshfeld surface analysis of 4-cyano-*N*-[(4-cyanophenyl)-sulfonyl]-*N*-[2-(5-methylfuran-2-yl)phenyl]benzenesulfonamide

Gunay Z. Mammadova, Elizaveta D. Yakovleva, Gleb M. Burkin, Victor N. Khrustalev, Mehmet Akkurt, Sevim Türktekin Çelikesir and Ajaya Bhattarai

Computing details

Data collection: *CrysAlis PRO* 1.171.41.117a (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* 1.171.41.117a (Rigaku OD, 2021); data reduction: *CrysAlis PRO* 1.171.41.117a (Rigaku OD, 2021); program(s) used to solve structure: *SHELXL2016/6* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016/6* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

4-Cyano-*N*-[(4-cyanophenyl)sulfonyl]-*N*-[2-(5-methylfuran-2-yl)phenyl]benzenesulfonamide

Crystal data

$C_{25}H_{17}N_3O_5S_2$
M_r = 503.53
Triclinic, $P\overline{1}$
a = 7.4542 (1) Å
b = 9.5111 (2) Å
c = 16.4378 (3) Å
α = 88.838 (4)°
β = 81.644 (1)°
γ = 81.414 (1)°
V = 1140.11 (4) Å^3
Z = 2
$F(000)$ = 520
D_x = 1.467 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 21520 reflections
θ = 2.7–77.6°
μ = 2.50 mm^{-1}
T = 100 K
Prism, colourless
0.29 × 0.22 × 0.15 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube
Detector resolution: 0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.481, T_{max} = 1.000
29936 measured reflections
4841 independent reflections
4675 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 77.9°, θ_{min} = 2.7°
h = −8→9
k = −12→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.095
S = 1.08
4841 reflections
316 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.4479P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}

Special details

Experimental. CrysAlisPro 1.171.41.117a (Rigaku OD, 2021) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.87131 (4)	0.20718 (3)	0.37143 (2)	0.01631 (10)	
S2	0.47488 (4)	0.28580 (3)	0.36436 (2)	0.01531 (10)	
O1	0.86050 (14)	0.27336 (10)	0.19206 (6)	0.0209 (2)	
O2	0.85236 (14)	0.07100 (10)	0.34200 (6)	0.0224 (2)	
O3	1.02688 (13)	0.27486 (11)	0.34195 (6)	0.0214 (2)	
O4	0.47897 (13)	0.15314 (11)	0.40679 (6)	0.0207 (2)	
O5	0.35697 (13)	0.40880 (11)	0.39862 (6)	0.0208 (2)	
N1	0.68945 (15)	0.32549 (12)	0.35205 (7)	0.0154 (2)	
N2	0.7640 (2)	0.22944 (17)	0.80753 (9)	0.0376 (3)	
N3	0.3238 (2)	0.18901 (15)	−0.04558 (8)	0.0301 (3)	
C1	0.71285 (17)	0.47104 (14)	0.33138 (8)	0.0166 (3)	
C2	0.76977 (18)	0.51151 (15)	0.25007 (9)	0.0190 (3)	
C3	0.7802 (2)	0.65682 (16)	0.23618 (10)	0.0244 (3)	
H3	0.819030	0.687961	0.182071	0.029*	
C4	0.7355 (2)	0.75524 (15)	0.29928 (10)	0.0261 (3)	
H4	0.742788	0.852707	0.287872	0.031*	
C5	0.67996 (19)	0.71301 (16)	0.37940 (10)	0.0238 (3)	
H5	0.649904	0.780898	0.422687	0.029*	
C6	0.66904 (18)	0.57071 (15)	0.39520 (9)	0.0196 (3)	
H6	0.631585	0.540682	0.449686	0.024*	
C7	0.81504 (19)	0.41619 (15)	0.17921 (9)	0.0201 (3)	
C8	0.8215 (2)	0.44092 (18)	0.09722 (10)	0.0294 (3)	
H8	0.796625	0.530602	0.071431	0.035*	
C9	0.8728 (2)	0.30600 (19)	0.05734 (9)	0.0308 (3)	
H9	0.888002	0.288669	−0.000144	0.037*	
C10	0.8957 (2)	0.20782 (17)	0.11670 (9)	0.0242 (3)	
C11	0.9513 (2)	0.05141 (18)	0.11806 (10)	0.0320 (4)	
H11A	0.951112	0.019245	0.175088	0.048*	0.5
H11B	0.864718	0.004742	0.092582	0.048*	0.5
H11C	1.074697	0.026944	0.087412	0.048*	0.5
H11D	0.975906	0.014709	0.061633	0.048*	0.5
H11E	1.062300	0.029212	0.144140	0.048*	0.5
H11F	0.852321	0.007010	0.149309	0.048*	0.5
C12	0.85015 (18)	0.20354 (14)	0.47982 (8)	0.0176 (3)	

C13	0.91148 (19)	0.31300 (14)	0.51825 (9)	0.0197 (3)
H13	0.967389	0.383552	0.486494	0.024*
C14	0.88981 (19)	0.31752 (15)	0.60333 (9)	0.0208 (3)
H14	0.928202	0.392513	0.630580	0.025*
C15	0.81124 (19)	0.21113 (15)	0.64858 (9)	0.0206 (3)
C16	0.75614 (19)	0.09909 (15)	0.60938 (9)	0.0225 (3)
H16	0.706667	0.025466	0.640954	0.027*
C17	0.77392 (19)	0.09578 (15)	0.52430 (9)	0.0204 (3)
H17	0.734758	0.021287	0.496928	0.025*
C18	0.7855 (2)	0.21874 (17)	0.73718 (10)	0.0265 (3)
C19	0.43219 (17)	0.26331 (14)	0.26310 (8)	0.0161 (3)
C20	0.47823 (19)	0.12911 (15)	0.22776 (9)	0.0201 (3)
H20	0.531585	0.051367	0.257755	0.024*
C21	0.4455 (2)	0.10992 (15)	0.14829 (9)	0.0223 (3)
H21	0.473180	0.018398	0.123514	0.027*
C22	0.37117 (19)	0.22685 (16)	0.10504 (8)	0.0203 (3)
C23	0.3246 (2)	0.36132 (16)	0.14114 (9)	0.0234 (3)
H23	0.272363	0.439559	0.111171	0.028*
C24	0.3553 (2)	0.37968 (15)	0.22120 (9)	0.0212 (3)
H24	0.324252	0.470377	0.246872	0.025*
C25	0.3437 (2)	0.20666 (16)	0.02113 (9)	0.0242 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01287 (16)	0.01633 (16)	0.01966 (17)	−0.00131 (11)	−0.00276 (12)	−0.00148 (12)
S2	0.01201 (16)	0.01925 (17)	0.01516 (16)	−0.00367 (11)	−0.00191 (11)	−0.00204 (12)
O1	0.0234 (5)	0.0214 (5)	0.0178 (5)	−0.0057 (4)	0.0000 (4)	−0.0028 (4)
O2	0.0235 (5)	0.0175 (5)	0.0260 (5)	−0.0012 (4)	−0.0044 (4)	−0.0049 (4)
O3	0.0134 (5)	0.0265 (5)	0.0241 (5)	−0.0030 (4)	−0.0020 (4)	0.0003 (4)
O4	0.0192 (5)	0.0256 (5)	0.0193 (5)	−0.0086 (4)	−0.0045 (4)	0.0028 (4)
O5	0.0143 (4)	0.0260 (5)	0.0215 (5)	−0.0012 (4)	−0.0015 (4)	−0.0081 (4)
N1	0.0119 (5)	0.0163 (5)	0.0184 (5)	−0.0034 (4)	−0.0024 (4)	−0.0002 (4)
N2	0.0433 (9)	0.0437 (8)	0.0247 (7)	−0.0043 (7)	−0.0037 (6)	0.0032 (6)
N3	0.0361 (7)	0.0327 (7)	0.0207 (6)	0.0003 (6)	−0.0065 (5)	−0.0033 (5)
C1	0.0133 (6)	0.0157 (6)	0.0214 (6)	−0.0023 (4)	−0.0044 (5)	−0.0007 (5)
C2	0.0155 (6)	0.0206 (6)	0.0220 (7)	−0.0040 (5)	−0.0055 (5)	0.0013 (5)
C3	0.0247 (7)	0.0229 (7)	0.0279 (7)	−0.0066 (5)	−0.0095 (6)	0.0056 (6)
C4	0.0239 (7)	0.0174 (6)	0.0393 (9)	−0.0028 (5)	−0.0129 (6)	0.0026 (6)
C5	0.0187 (7)	0.0204 (7)	0.0333 (8)	−0.0010 (5)	−0.0080 (6)	−0.0072 (6)
C6	0.0148 (6)	0.0214 (7)	0.0231 (7)	−0.0017 (5)	−0.0049 (5)	−0.0037 (5)
C7	0.0170 (6)	0.0225 (7)	0.0211 (7)	−0.0046 (5)	−0.0021 (5)	0.0018 (5)
C8	0.0334 (8)	0.0322 (8)	0.0208 (7)	−0.0011 (6)	−0.0024 (6)	0.0030 (6)
C9	0.0332 (8)	0.0394 (9)	0.0178 (7)	−0.0019 (7)	−0.0002 (6)	−0.0035 (6)
C10	0.0222 (7)	0.0302 (8)	0.0195 (7)	−0.0065 (6)	0.0029 (5)	−0.0076 (6)
C11	0.0368 (9)	0.0291 (8)	0.0276 (8)	−0.0056 (6)	0.0054 (7)	−0.0087 (6)
C12	0.0139 (6)	0.0173 (6)	0.0218 (6)	−0.0001 (5)	−0.0056 (5)	0.0002 (5)
C13	0.0186 (6)	0.0180 (6)	0.0236 (7)	−0.0041 (5)	−0.0055 (5)	0.0016 (5)

C14	0.0190 (7)	0.0196 (6)	0.0244 (7)	−0.0010 (5)	−0.0071 (5)	−0.0005 (5)
C15	0.0159 (6)	0.0225 (7)	0.0227 (7)	0.0009 (5)	−0.0047 (5)	0.0025 (5)
C16	0.0184 (7)	0.0223 (7)	0.0276 (7)	−0.0042 (5)	−0.0055 (5)	0.0056 (5)
C17	0.0177 (6)	0.0180 (6)	0.0269 (7)	−0.0034 (5)	−0.0072 (5)	0.0012 (5)
C18	0.0242 (7)	0.0271 (7)	0.0279 (8)	−0.0023 (6)	−0.0050 (6)	0.0039 (6)
C19	0.0116 (6)	0.0210 (6)	0.0164 (6)	−0.0038 (5)	−0.0022 (5)	−0.0020 (5)
C20	0.0202 (7)	0.0196 (6)	0.0195 (6)	0.0001 (5)	−0.0027 (5)	−0.0007 (5)
C21	0.0243 (7)	0.0214 (7)	0.0205 (7)	−0.0006 (5)	−0.0028 (5)	−0.0055 (5)
C22	0.0167 (6)	0.0277 (7)	0.0169 (6)	−0.0042 (5)	−0.0026 (5)	−0.0022 (5)
C23	0.0257 (7)	0.0223 (7)	0.0224 (7)	−0.0004 (5)	−0.0078 (5)	0.0012 (5)
C24	0.0224 (7)	0.0197 (6)	0.0217 (7)	−0.0014 (5)	−0.0058 (5)	−0.0029 (5)
C25	0.0239 (7)	0.0272 (7)	0.0206 (7)	−0.0008 (6)	−0.0027 (5)	−0.0022 (6)

Geometric parameters (Å, º)

S1—O2	1.4253 (10)	C10—C11	1.484 (2)
S1—O3	1.4287 (10)	C11—H11A	0.9800
S1—N1	1.6914 (11)	C11—H11B	0.9800
S1—C12	1.7657 (14)	C11—H11C	0.9800
S2—O5	1.4262 (10)	C11—H11D	0.9800
S2—O4	1.4277 (10)	C11—H11E	0.9800
S2—N1	1.6807 (11)	C11—H11F	0.9800
S2—C19	1.7625 (13)	C12—C17	1.3895 (19)
O1—C7	1.3699 (17)	C12—C13	1.3946 (19)
O1—C10	1.3711 (17)	C13—C14	1.385 (2)
N1—C1	1.4484 (16)	C13—H13	0.9500
N2—C18	1.148 (2)	C14—C15	1.393 (2)
N3—C25	1.147 (2)	C14—H14	0.9500
C1—C6	1.3979 (19)	C15—C16	1.398 (2)
C1—C2	1.4062 (19)	C15—C18	1.443 (2)
C2—C3	1.408 (2)	C16—C17	1.386 (2)
C2—C7	1.459 (2)	C16—H16	0.9500
C3—C4	1.382 (2)	C17—H17	0.9500
C3—H3	0.9500	C19—C24	1.3863 (19)
C4—C5	1.392 (2)	C19—C20	1.3877 (19)
C4—H4	0.9500	C20—C21	1.384 (2)
C5—C6	1.385 (2)	C20—H20	0.9500
C5—H5	0.9500	C21—C22	1.396 (2)
C6—H6	0.9500	C21—H21	0.9500
C7—C8	1.359 (2)	C22—C23	1.395 (2)
C8—C9	1.427 (2)	C22—C25	1.4442 (19)
C8—H8	0.9500	C23—C24	1.387 (2)
C9—C10	1.348 (2)	C23—H23	0.9500
C9—H9	0.9500	C24—H24	0.9500
O2—S1—O3	121.57 (6)	C10—C11—H11B	109.5
O2—S1—N1	108.74 (6)	H11A—C11—H11B	109.5
O3—S1—N1	104.43 (6)	C10—C11—H11C	109.5

O2—S1—C12	109.39 (6)	H11A—C11—H11C	109.5
O3—S1—C12	107.41 (6)	H11B—C11—H11C	109.5
N1—S1—C12	103.85 (6)	H11D—C11—H11E	109.5
O5—S2—O4	120.18 (6)	H11D—C11—H11F	109.5
O5—S2—N1	106.78 (6)	H11E—C11—H11F	109.5
O4—S2—N1	106.87 (6)	C17—C12—C13	121.92 (13)
O5—S2—C19	108.34 (6)	C17—C12—S1	120.72 (11)
O4—S2—C19	109.55 (6)	C13—C12—S1	117.36 (11)
N1—S2—C19	103.90 (6)	C14—C13—C12	119.13 (13)
C7—O1—C10	107.60 (11)	C14—C13—H13	120.4
C1—N1—S2	117.35 (9)	C12—C13—H13	120.4
C1—N1—S1	119.89 (9)	C13—C14—C15	119.42 (13)
S2—N1—S1	122.51 (7)	C13—C14—H14	120.3
C6—C1—C2	121.38 (13)	C15—C14—H14	120.3
C6—C1—N1	117.08 (12)	C14—C15—C16	120.97 (14)
C2—C1—N1	121.49 (12)	C14—C15—C18	118.91 (14)
C1—C2—C3	116.84 (13)	C16—C15—C18	120.11 (13)
C1—C2—C7	125.48 (12)	C17—C16—C15	119.79 (13)
C3—C2—C7	117.67 (13)	C17—C16—H16	120.1
C4—C3—C2	121.64 (14)	C15—C16—H16	120.1
C4—C3—H3	119.2	C16—C17—C12	118.71 (13)
C2—C3—H3	119.2	C16—C17—H17	120.6
C3—C4—C5	120.66 (14)	C12—C17—H17	120.6
C3—C4—H4	119.7	N2—C18—C15	177.81 (17)
C5—C4—H4	119.7	C24—C19—C20	122.18 (13)
C6—C5—C4	119.13 (14)	C24—C19—S2	119.24 (10)
C6—C5—H5	120.4	C20—C19—S2	118.57 (10)
C4—C5—H5	120.4	C21—C20—C19	119.19 (13)
C5—C6—C1	120.35 (14)	C21—C20—H20	120.4
C5—C6—H6	119.8	C19—C20—H20	120.4
C1—C6—H6	119.8	C20—C21—C22	119.10 (13)
C8—C7—O1	109.22 (13)	C20—C21—H21	120.5
C8—C7—C2	131.86 (14)	C22—C21—H21	120.5
O1—C7—C2	118.92 (12)	C23—C22—C21	121.32 (13)
C7—C8—C9	106.68 (14)	C23—C22—C25	120.03 (13)
C7—C8—H8	126.7	C21—C22—C25	118.65 (13)
C9—C8—H8	126.7	C24—C23—C22	119.37 (13)
C10—C9—C8	107.01 (13)	C24—C23—H23	120.3
C10—C9—H9	126.5	C22—C23—H23	120.3
C8—C9—H9	126.5	C19—C24—C23	118.81 (13)
C9—C10—O1	109.49 (13)	C19—C24—H24	120.6
C9—C10—C11	135.03 (14)	C23—C24—H24	120.6
O1—C10—C11	115.47 (13)	N3—C25—C22	179.03 (16)
C10—C11—H11A	109.5		

O5—S2—N1—C1	−33.62 (11)	C8—C9—C10—O1	0.37 (18)
O4—S2—N1—C1	−163.42 (10)	C8—C9—C10—C11	−178.47 (17)
C19—S2—N1—C1	80.78 (11)	C7—O1—C10—C9	−0.20 (16)

O5—S2—N1—S1	140.59 (8)	C7—O1—C10—C11	178.89 (13)
O4—S2—N1—S1	10.79 (9)	O2—S1—C12—C17	−16.82 (13)
C19—S2—N1—S1	−105.01 (8)	O3—S1—C12—C17	−150.62 (11)
O2—S1—N1—C1	−145.42 (10)	N1—S1—C12—C17	99.12 (12)
O3—S1—N1—C1	−14.26 (11)	O2—S1—C12—C13	163.63 (10)
C12—S1—N1—C1	98.17 (11)	O3—S1—C12—C13	29.83 (12)
O2—S1—N1—S2	40.51 (9)	N1—S1—C12—C13	−80.43 (11)
O3—S1—N1—S2	171.67 (7)	C17—C12—C13—C14	−2.4 (2)
C12—S1—N1—S2	−75.89 (9)	S1—C12—C13—C14	177.14 (10)
S2—N1—C1—C6	77.49 (14)	C12—C13—C14—C15	1.5 (2)
S1—N1—C1—C6	−96.87 (13)	C13—C14—C15—C16	0.8 (2)
S2—N1—C1—C2	−99.91 (13)	C13—C14—C15—C18	−178.59 (13)
S1—N1—C1—C2	85.72 (14)	C14—C15—C16—C17	−2.2 (2)
C6—C1—C2—C3	−0.1 (2)	C18—C15—C16—C17	177.20 (13)
N1—C1—C2—C3	177.24 (12)	C15—C16—C17—C12	1.3 (2)
C6—C1—C2—C7	−178.78 (13)	C13—C12—C17—C16	1.0 (2)
N1—C1—C2—C7	−1.5 (2)	S1—C12—C17—C16	−178.51 (10)
C1—C2—C3—C4	−0.4 (2)	O5—S2—C19—C24	23.09 (13)
C7—C2—C3—C4	178.39 (13)	O4—S2—C19—C24	155.90 (11)
C2—C3—C4—C5	0.6 (2)	N1—S2—C19—C24	−90.20 (12)
C3—C4—C5—C6	−0.3 (2)	O5—S2—C19—C20	−157.37 (11)
C4—C5—C6—C1	−0.2 (2)	O4—S2—C19—C20	−24.55 (13)
C2—C1—C6—C5	0.4 (2)	N1—S2—C19—C20	89.35 (11)
N1—C1—C6—C5	−177.05 (12)	C24—C19—C20—C21	−0.5 (2)
C10—O1—C7—C8	−0.07 (16)	S2—C19—C20—C21	180.00 (11)
C10—O1—C7—C2	179.71 (12)	C19—C20—C21—C22	1.6 (2)
C1—C2—C7—C8	158.84 (16)	C20—C21—C22—C23	−1.9 (2)
C3—C2—C7—C8	−19.9 (2)	C20—C21—C22—C25	177.80 (13)
C1—C2—C7—O1	−20.9 (2)	C21—C22—C23—C24	1.0 (2)
C3—C2—C7—O1	160.40 (12)	C25—C22—C23—C24	−178.67 (13)
O1—C7—C8—C9	0.29 (17)	C20—C19—C24—C23	−0.4 (2)
C2—C7—C8—C9	−179.45 (15)	S2—C19—C24—C23	179.11 (11)
C7—C8—C9—C10	−0.40 (19)	C22—C23—C24—C19	0.2 (2)

Hydrogen-bond geometry (Å, º)

*Cg*2 is the centroid of the ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{i}	0.95	2.56	3.3639 (17)	142
C6—H6···O5^{ii}	0.95	2.56	3.3744 (17)	143
C11—H11*B*···N3^{iii}	0.98	2.67	3.616 (2)	163
C13—H13···O3	0.95	2.56	2.9146 (18)	102
C16—H16···O4^{iv}	0.95	2.55	3.2115 (18)	127
C21—H21···N3^{iii}	0.95	2.54	3.433 (2)	156
C24—H24···O5	0.95	2.59	2.9371 (18)	102
C14—H14···*Cg*2^{v}	0.95	2.85	3.4945 (16)	126

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