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Crystal structure and Hirshfeld surface analysis of (*E*)-*N*-(2-styrylphenyl)benzenesulfonamide

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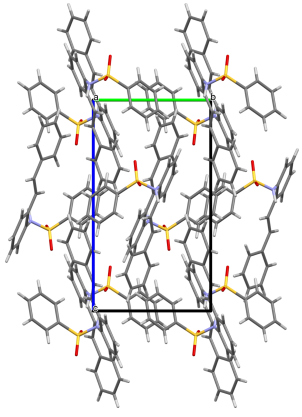
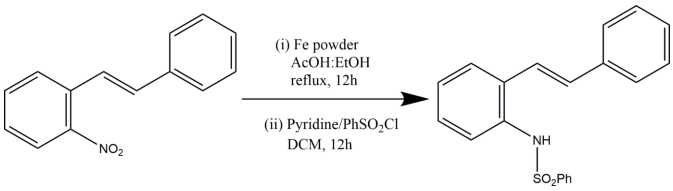
The crystal structure of the title compound $C_{20}H_{17}NO_2S$ features hydrogen-bonding and C—H$\cdots\pi$ interactions. Hirshfeld surface analysis revealed that H$\cdots$H, C$\cdots$H/H$\cdots$C and O$\cdots$H/H$\cdots$O interactions make a major contribution to the crystal packing. Docking studies were carried out to determine the binding affinity and interaction profile of the title compound with EGFR kinase, a member of the ErbB family of receptor tyrosine kinases, which is crucial for processes such as cell proliferation and differentiation. The title compound shows a strong binding affinity with EGFR kinase, with the most favourable conformation having a binding energy of −8.27 kcal mol^{-1} and a predicted IC50 of 870.34 n*M*, indicating its potential as a promising candidate for targeted lung cancer therapy.

1. Chemical context

The indole structure is widely regarded as a privileged scaffold, capable of serving as a ligand for various biological targets (Kaushik *et al.*, 2013). Indoles are prevalent across a broad spectrum of natural sources, including plants, animals and microorganisms. Numerous indole-containing compounds exhibit notable biological activities; for instance, indole-based alkaloids such as serotonin, tryptamine, and ergotamine are crucial in regulating physiological processes and significantly impact human health and behaviour. Indoles are also present in a variety of pharmaceuticals, such as antipsychotic, antidepressant and antimicrobial drugs. Beyond their biological significance, indoles are valuable as they are versatile building blocks in organic synthesis, with the indole ring being functionalized and modified to produce a diverse array of chemical compounds. Although many methods for synthesizing indole derivatives exist, there remains a strong interest in developing new and more efficient synthesis techniques. The transformation of 2-alkenylanilines into indoles has gained popularity as a straightforward approach due to the widespread availability of both anilines and alkenes (or styrenes). One such method involves C—H amination *via* transition-metal catalysts. Recently, methods that avoid the use of metals in cyclization have garnered considerable attention (Hegedus *et al.*, 1978; Larock *et al.*, 1996; Maity *et al.*, 2012; Youn *et al.*, 2015, 2016). A reaction was carried out with the aim of synthesizing 2-phenylindole from (*E*)-*N*-(2-styrylphenyl)benzenesulfonamide through PIDA/BF_3·OEt_2-mediated intramolecular cyclization and the structure of the (*E*)-*N*-(2-styrylphenyl)-benzenesulfonamide intermediate of 2-phenylindole was confirmed through X-ray diffraction analysis.





2. Structural commentary

In the title compound, the sulfur atom is bound to two oxygens, a nitrogen (which is connected to another aromatic ring) and a carbon atom, forming a tetrahedral structure between the two aromatic moieties with sulfur at the centre. Relevant bond lengths and angles are given in Table 1. For the C1–C6 ring, the weighted average bond distance is 1.3959 Å, the weighted average absolute torsion angle is 0.34° and the pseudo-rotation parameter (τ) is 0.3°. The C7–C12 ring has a weighted average bond distance of 1.3899 Å, a weighted average absolute torsion angle of 0.83° and a τ value of 0.8. Similarly, the C15–C20 ring exhibits a weighted average bond distance of 1.3925 Å, a weighted average absolute torsion angle of 1.76° and τ value of 1.8°. An intramolecular C7—H7···O2 hydrogen bond (Fig. 1, Table 2) directs the relative orientation of the C7–C12 ring in the molecular structure.

3. Supramolecular features

In the crystal, N1—H1···O1 and C6—H6···O2 hydrogen bonds and C—H···π interactions (Table 1) are observed. The packing is shown in Fig. 2.

4. Database survey

A search in the Cambridge Structural Database (CSD, Version 5.45; Groom *et al.*, 2016) for the term '(styrylphenyl)-benzenesulfonamide' gave one hit, (*Z*)-*N*-(difluoromethyl)-4-methyl-*N*-(2-styrylphenyl)benzenesulfonamide (CSD refcode HINBEO; Polley *et al.*, 2018). In this structure there is a difluromethyl group attached to the nitrogen in addition to a

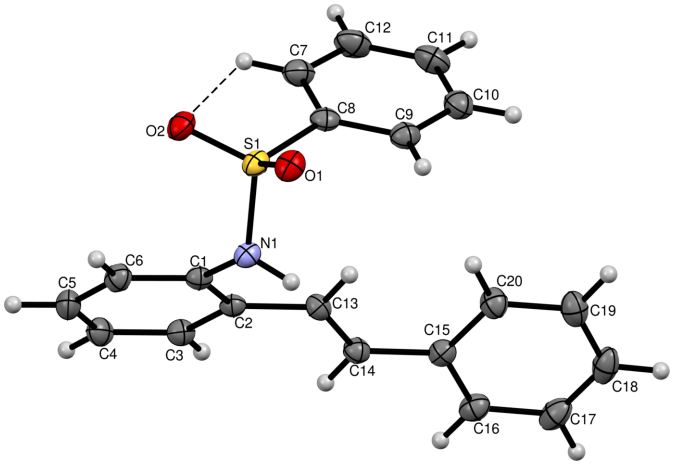


Figure 1
View of title compound showing the atom-numbering scheme with displacement ellipsoids drawn at the 50% probability level. The intramolecular C7—H7···O2 hydrogen bond is shown as a dashed line.

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.4422 (9)	S1—C8	1.7653 (12)
S1—O2	1.4300 (9)	N1—C1	1.4343 (14)
S1—N1	1.6342 (10)		
O1—S1—N1	105.29 (5)	O2—S1—C8	108.68 (6)
O1—S1—C8	107.63 (6)	N1—S1—C8	106.87 (5)
O2—S1—O1	119.83 (5)	C1—N1—S1	121.88 (8)
O2—S1—N1	107.85 (5)		

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.888 (18)	2.010 (18)	2.8907 (14)	170.8 (17)
C6—H6···O2^{ii}	0.95	2.53	3.3332 (16)	143
C7—H7···O2	0.95	2.54	2.9208 (16)	104
C12—H12···*Cg*1^{iii}	0.95	2.59	3.4333 (15)	148
C19—H19···*Cg*1^{iv}	0.95	2.81	3.5747 (15)	141

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

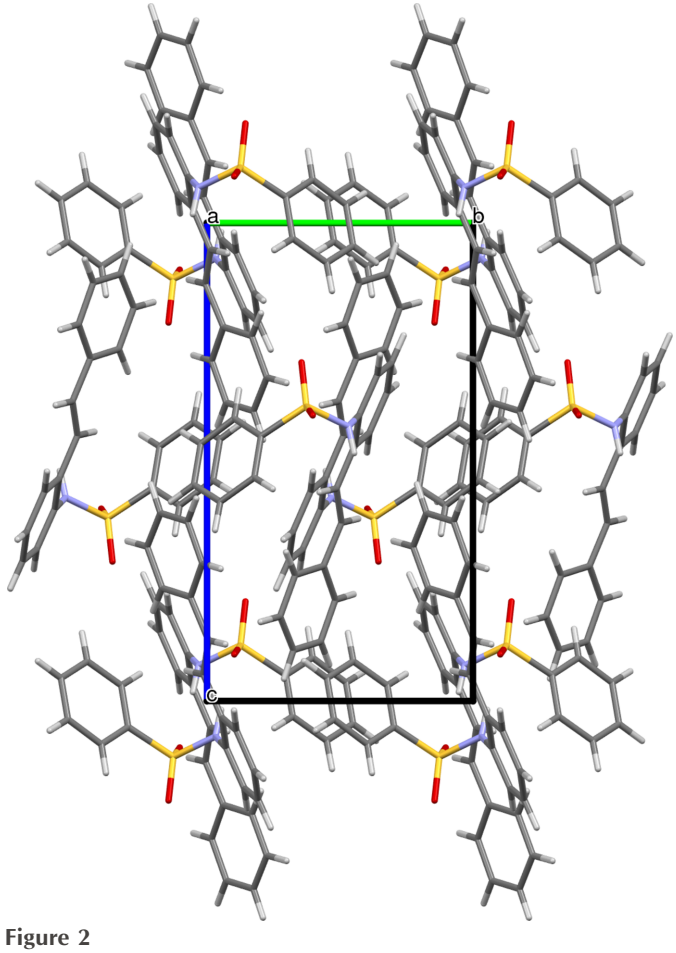


Figure 2
The crystal packing of the title compound viewed along the *a* axis.

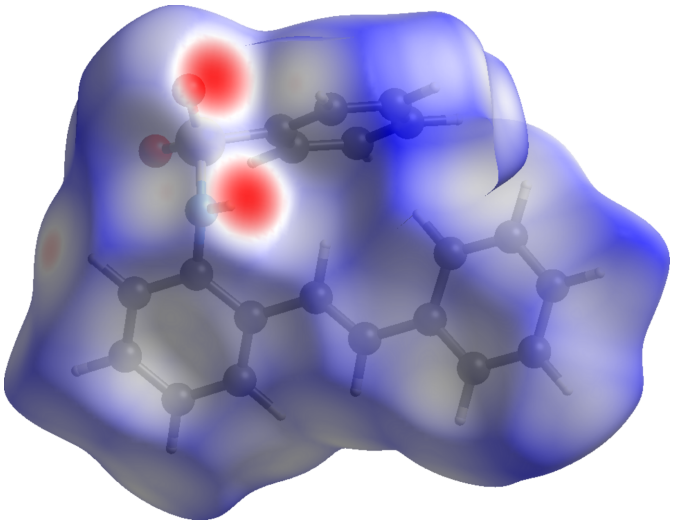


Figure 3
The Hirshfeld surface of the title compound mapped over d_{norm}.

methyl group at the *para* position of the benzene ring of benzenesulfonamide.

5. Hirshfeld surface analysis

The Hirshfeld surface analysis was carried out using *Crystal Explorer 21* (Spackman *et al.*, 2021) to study the non-covalent interactions and the interatomic contacts. The Hirshfeld surface mapped over d_{norm} with shorter contacts in red, contacts around the van der Waals separation in white and longer contacts in blue is shown in Fig. 3.

The two-dimensional fingerprint plots for significant contacts are given in Fig. 4. The contacts making the largest contributions are H···H (40.1%) due to the large number of hydrogen atoms in the molecule, C···H/H···C (37.1%) and O···H/H···O (19.7%). Contacts making minor contributions include C···C (1.4%), N···H/H···N (1.3%) and O···C/C···O (0.4%).

6. *In silico* analysis

Molecular docking studies were carried out to assess the potential of the title compound as a therapeutic agent by targeting EGFR kinase, a key protein involved in lung cancer development (Kavarthapu *et al.*, 2021). Dysregulation of EGFR, often through mutations or overexpression, is a major driver of non-small cell lung cancer (NSCLC), making it a key therapeutic target.

Docking was carried out using *AutoDock 4.2* (Morris *et al.*, 2009) software, with the EGFR kinase's high-resolution 3D crystal structure (PDB ID: 2ITY; Yun *et al.*, 2007) obtained from the Protein Data Bank (Berman *et al.*, 2000). Prior to docking, co-crystallized ligands and solvent molecules were removed using *PyMOL* (DeLano, 2002), the polar hydrogen atoms were added and the Kollman and Gasteiger charges were assigned to the protein. *AutoGrid* was used to calculate grid parameters, with a 40 × 40 × 40 point grid box and a spacing of 0.375 Å, centered on the binding site determined by the ligand-bound EGFR kinase (2ITY). Docking was conducted with the Lamarckian Genetic Algorithm (LGA) for 100 independent runs, keeping all other parameters at default. The protein was treated as rigid, while the ligand was allowed full flexibility. Docking results were evaluated based on binding interactions, binding energy (kcal mol^{-1}), and predicted inhibitory concentration (IC50). The docking results showed that (*E*)-*N*-(2-styrylphenyl)benzenesulfonamide has a strong binding affinity for EGFR kinase, with the most favourable conformation having a binding energy of −8.27 kcal mol^{-1} and a predicted IC50 of 870.34 n*M*.

Further interaction analysis shows that the ligand forms a hydrogen bond with the MET-793 residue at 3.0 Å, a crucial interaction for the stability of the ligand–protein complex (Fig. 5). Additionally, the compound engages in various non-covalent interactions, including π–alkyl with VAL-726, ALA-743, LYS-745, LEU-788, and LEU-792; π–sigma with LEU-718, THR-790, and LEU-844; pi-sulfur with CYS-797; and van der Waals with ILE-744, MET-766, PRO-794, GLY-796, and

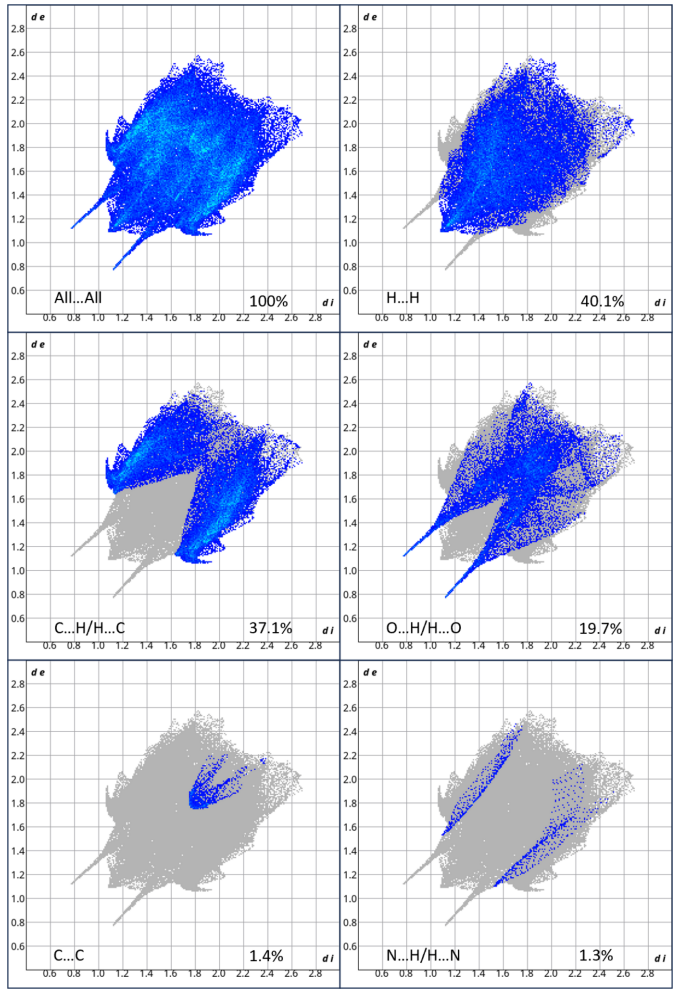


Figure 4
The various two dimensional fingerprint plots with the significant contacts labelled.

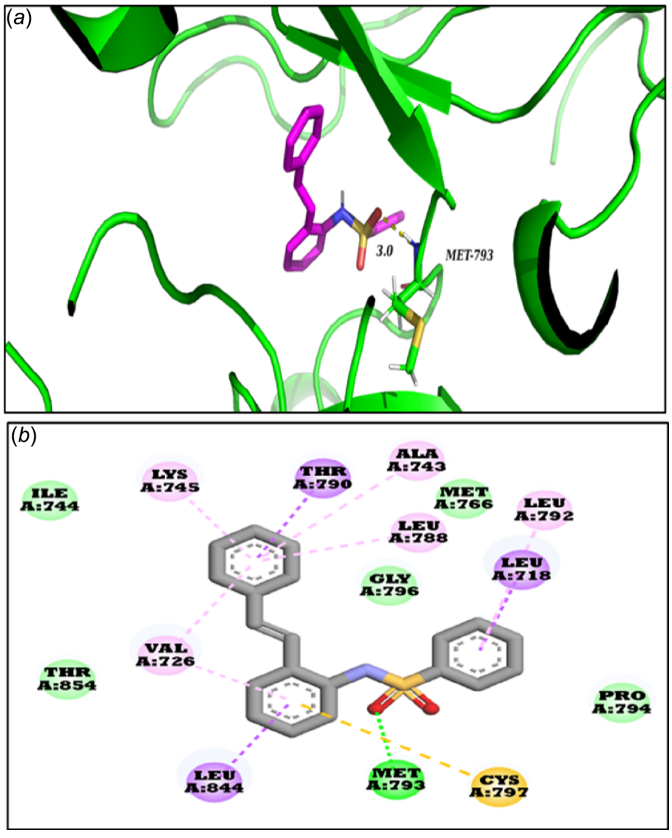


Figure 5
Molecular docking results illustrating the interaction of the title compound with EGFR kinase. (*a*) Hydrogen-bond interaction and (*b*) overall interactions (the vdW, π–alkyl, π–sigma, and π–sulfur interactions are indicated in green, pink, purple, and yellow, respectively)

THR-854. These interactions collectively enhance the ligand's stability and affinity for EGFR kinase.

Considering EGFR's critical role in NSCLC, the interaction profile suggests the potential of the title compound as a therapeutic agent. Its strong binding affinity and specific interactions with EGFR kinase highlight its promise for further development in targeted lung cancer treatment, particularly for patients with EGFR mutations.

7. Synthesis and crystallization

To a hot solution of (*E*)-1-nitro-2-styrylbenzene (2.9 g, 12.88 mmol) in 50 mL of an EtOH–AcOH mixture (4:1 ratio), Fe powder (3.5 g, 64.40 mmol) was added, and the reaction mixture was refluxed for 6 h. Once the reaction was complete, as monitored by TLC, the solution was carefully decanted to remove the iron residue and then poured over crushed ice (100 g) containing 5 mL of concentrated HCl. The resulting solid was filtered and dried over $CaCl_2$. The crude product was used directly in the next step without further purification. Subsequently, a solution of the resulting amine salts (2.2 g, 9.52 mmol) in dry DCM (20 mL) was prepared, to which benzenesulfonyl chloride (1.3 mL, 10.47 mmol) and pyridine (0.92 mL, 11.42 mmol) were slowly added. The mixture was stirred at room temperature for 8 h under a nitrogen atmosphere. After the reaction was complete, as monitored by TLC, the mixture was poured into ice–water (50 mL) containing 1 mL of concentrated HCl, extracted with DCM (2 × 20 mL), and then washed with water (2 × 20 mL) and dried over Na_2SO_4. The solvent was removed under reduced pressure, and the crude product was triturated with diethyl ether (10 mL), yielding (*E*)-*N*-(2-styrylphenyl)benzenesulfonamide (2.3 g, 61% yield over two steps) as a white solid, m.p. 399–401 K.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{17}NO_2S$
M_r	335.40
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.7320 (1), 8.2475 (1), 15.5387 (2)
β (°)	107.505 (1)
V (Å^3)	1678.33 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.80
Crystal size (mm)	0.21 × 0.14 × 0.1
Data collection	
Diffractometer	SuperNova, Dual, Cu at home/near, HyPix
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.560, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37664, 3562, 3380
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.084, 1.07
No. of reflections	3562
No. of parameters	221
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.46

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The N-bound H atom was fully refined. C-bound H atoms were positioned geometrically (C—H = 0.95 Å) with U_{iso}(H) = 1.2U_{eq}(C).

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supporting information

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Crystal structure and Hirshfeld surface analysis of (*E*)-*N*-(2-styrylphenyl)-benzenesulfonamide

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Computing details

N-{2-[(E)-2-Phenylethenyl]phenyl}benzenesulfonamide

Crystal data

$C_{20}H_{17}NO_2S$
$M_r = 335.40$
Monoclinic, $P2_1/c$
$a = 13.7320$ (1) Å
$b = 8.2475$ (1) Å
$c = 15.5387$ (2) Å
$\beta = 107.505$ (1)°
$V = 1678.33$ (3) Å^3
$Z = 4$
$F(000) = 704$
$D_x = 1.327$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 18551 reflections
$\theta = 5.1$–$77.6°$
$\mu = 1.80$ mm^{-1}
$T = 100$ K
Block, clear intense colourless
0.21 × 0.14 × 0.1 mm

Data collection

SuperNova, Dual, Cu at home/near, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2022)
$T_{min} = 0.560$, $T_{max} = 1.000$
37664 measured reflections
3562 independent reflections
3380 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 77.7°$, $\theta_{min} = 3.4°$
$h = -17\rightarrow17$
$k = -10\rightarrow10$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.084$
$S = 1.07$
3562 reflections
221 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.655P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.47127 (2)	0.62654 (3)	0.61679 (2)	0.02047 (10)
O1	0.56671 (6)	0.60255 (11)	0.59762 (6)	0.0253 (2)
O2	0.47052 (7)	0.64449 (11)	0.70812 (6)	0.0267 (2)
N1	0.40171 (7)	0.46841 (12)	0.57421 (7)	0.0195 (2)
C1	0.31138 (8)	0.42782 (14)	0.59774 (8)	0.0187 (2)
C2	0.21387 (8)	0.44410 (13)	0.53465 (8)	0.0183 (2)
C6	0.32417 (10)	0.35980 (15)	0.68241 (8)	0.0235 (3)
H6	0.390750	0.349266	0.723729	0.028*
C3	0.13033 (9)	0.38948 (14)	0.56134 (8)	0.0212 (2)
H3	0.063492	0.398483	0.520299	0.025*
C15	0.10379 (9)	0.56186 (14)	0.28252 (8)	0.0211 (2)
C13	0.20040 (8)	0.51323 (14)	0.44460 (8)	0.0197 (2)
H13	0.254825	0.576531	0.436591	0.024*
C14	0.11773 (9)	0.49428 (14)	0.37298 (8)	0.0214 (2)
H14	0.063239	0.431619	0.381352	0.026*
C8	0.41068 (9)	0.79664 (14)	0.55434 (8)	0.0217 (2)
C9	0.41757 (9)	0.82218 (15)	0.46753 (9)	0.0243 (2)
H9	0.458356	0.753136	0.443539	0.029*
C20	0.17418 (10)	0.66848 (16)	0.26366 (9)	0.0260 (3)
H20	0.232179	0.702399	0.311078	0.031*
C16	0.01775 (9)	0.51760 (15)	0.21170 (8)	0.0252 (3)
H16	−0.032413	0.449058	0.223398	0.030*
C7	0.35190 (10)	0.89704 (16)	0.59075 (9)	0.0276 (3)
H7	0.349045	0.879951	0.650404	0.033*
C4	0.14281 (10)	0.32289 (15)	0.64586 (9)	0.0247 (3)
H4	0.084878	0.287896	0.662230	0.030*
C5	0.23998 (10)	0.30723 (16)	0.70673 (8)	0.0260 (3)
H5	0.248753	0.260922	0.764550	0.031*
C18	0.07681 (11)	0.67486 (17)	0.10673 (9)	0.0306 (3)
H18	0.068938	0.710281	0.046843	0.037*
C19	0.16044 (10)	0.72510 (17)	0.17695 (9)	0.0292 (3)
H19	0.208369	0.798530	0.165462	0.035*
C10	0.36395 (10)	0.94990 (16)	0.41689 (9)	0.0280 (3)
H10	0.368583	0.969798	0.358024	0.034*
C17	0.00479 (10)	0.57280 (17)	0.12428 (9)	0.0307 (3)
H17	−0.053439	0.540529	0.076612	0.037*
C11	0.30336 (11)	1.04897 (16)	0.45224 (10)	0.0322 (3)
H11	0.265829	1.135175	0.416894	0.039*
C12	0.29735 (11)	1.02292 (16)	0.53841 (10)	0.0334 (3)

H12	0.255793	1.091263	0.561936	0.040*
H1	0.4039 (13)	0.447 (2)	0.5188 (12)	0.036 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01609 (15)	0.02539 (16)	0.01903 (16)	−0.00204 (10)	0.00389 (11)	−0.00271 (10)
O1	0.0159 (4)	0.0348 (5)	0.0244 (4)	−0.0009 (3)	0.0046 (3)	−0.0016 (4)
O2	0.0253 (4)	0.0339 (5)	0.0197 (4)	−0.0052 (4)	0.0052 (3)	−0.0049 (3)
N1	0.0165 (4)	0.0227 (5)	0.0189 (5)	0.0000 (4)	0.0046 (4)	−0.0018 (4)
C1	0.0176 (5)	0.0178 (5)	0.0212 (5)	0.0009 (4)	0.0064 (4)	−0.0017 (4)
C2	0.0184 (5)	0.0164 (5)	0.0198 (5)	0.0008 (4)	0.0056 (4)	−0.0016 (4)
C6	0.0235 (6)	0.0246 (6)	0.0210 (6)	0.0016 (4)	0.0044 (5)	0.0005 (4)
C3	0.0188 (5)	0.0216 (5)	0.0234 (6)	−0.0002 (4)	0.0069 (4)	−0.0017 (4)
C15	0.0196 (5)	0.0220 (6)	0.0211 (5)	0.0029 (4)	0.0051 (4)	−0.0006 (4)
C13	0.0177 (5)	0.0196 (5)	0.0223 (6)	0.0002 (4)	0.0067 (4)	0.0014 (4)
C14	0.0199 (5)	0.0217 (5)	0.0226 (6)	−0.0019 (4)	0.0066 (4)	0.0001 (4)
C8	0.0180 (5)	0.0203 (5)	0.0261 (6)	−0.0044 (4)	0.0054 (4)	−0.0032 (4)
C9	0.0218 (6)	0.0247 (6)	0.0268 (6)	−0.0023 (5)	0.0077 (5)	−0.0031 (5)
C20	0.0229 (6)	0.0285 (6)	0.0249 (6)	0.0001 (5)	0.0048 (5)	0.0036 (5)
C16	0.0223 (6)	0.0266 (6)	0.0248 (6)	0.0016 (5)	0.0039 (5)	−0.0026 (5)
C7	0.0293 (6)	0.0239 (6)	0.0326 (7)	−0.0036 (5)	0.0139 (5)	−0.0055 (5)
C4	0.0261 (6)	0.0247 (6)	0.0273 (6)	−0.0028 (5)	0.0142 (5)	−0.0015 (5)
C5	0.0322 (6)	0.0267 (6)	0.0203 (6)	−0.0001 (5)	0.0096 (5)	0.0028 (5)
C18	0.0362 (7)	0.0348 (7)	0.0214 (6)	0.0149 (6)	0.0093 (5)	0.0055 (5)
C19	0.0299 (6)	0.0305 (7)	0.0298 (7)	0.0063 (5)	0.0125 (5)	0.0080 (5)
C10	0.0286 (6)	0.0256 (6)	0.0291 (6)	−0.0039 (5)	0.0075 (5)	0.0013 (5)
C17	0.0303 (7)	0.0348 (7)	0.0223 (6)	0.0084 (5)	0.0009 (5)	−0.0032 (5)
C11	0.0329 (7)	0.0210 (6)	0.0422 (8)	0.0004 (5)	0.0106 (6)	0.0022 (5)
C12	0.0367 (7)	0.0221 (6)	0.0456 (8)	0.0022 (5)	0.0189 (6)	−0.0043 (6)

Geometric parameters (Å, º)

S1—O1	1.4422 (9)	C9—H9	0.9500
S1—O2	1.4300 (9)	C9—C10	1.3865 (18)
S1—N1	1.6342 (10)	C20—H20	0.9500
S1—C8	1.7653 (12)	C20—C19	1.3842 (18)
N1—C1	1.4343 (14)	C16—H16	0.9500
N1—H1	0.888 (18)	C16—C17	1.3924 (18)
C1—C2	1.4080 (15)	C7—H7	0.9500
C1—C6	1.3918 (16)	C7—C12	1.391 (2)
C2—C3	1.4061 (16)	C4—H4	0.9500
C2—C13	1.4701 (15)	C4—C5	1.3901 (18)
C6—H6	0.9500	C5—H5	0.9500
C6—C5	1.3894 (17)	C18—H18	0.9500
C3—H3	0.9500	C18—C19	1.388 (2)
C3—C4	1.3859 (17)	C18—C17	1.387 (2)
C15—C14	1.4702 (16)	C19—H19	0.9500

C15—C20	1.4013 (17)	C10—H10	0.9500
C15—C16	1.3993 (16)	C10—C11	1.3916 (19)
C13—H13	0.9500	C17—H17	0.9500
C13—C14	1.3385 (17)	C11—H11	0.9500
C14—H14	0.9500	C11—C12	1.383 (2)
C8—C9	1.3963 (17)	C12—H12	0.9500
C8—C7	1.3900 (17)		

O1—S1—N1	105.29 (5)	C10—C9—H9	120.5
O1—S1—C8	107.63 (6)	C15—C20—H20	119.5
O2—S1—O1	119.83 (5)	C19—C20—C15	120.97 (12)
O2—S1—N1	107.85 (5)	C19—C20—H20	119.5
O2—S1—C8	108.68 (6)	C15—C16—H16	119.6
N1—S1—C8	106.87 (5)	C17—C16—C15	120.79 (12)
S1—N1—H1	111.2 (11)	C17—C16—H16	119.6
C1—N1—S1	121.88 (8)	C8—C7—H7	120.6
C1—N1—H1	119.1 (11)	C8—C7—C12	118.90 (13)
C2—C1—N1	120.96 (10)	C12—C7—H7	120.6
C6—C1—N1	117.52 (10)	C3—C4—H4	120.0
C6—C1—C2	121.33 (11)	C3—C4—C5	120.09 (11)
C1—C2—C13	121.39 (10)	C5—C4—H4	120.0
C3—C2—C1	116.96 (10)	C6—C5—C4	119.53 (11)
C3—C2—C13	121.65 (10)	C6—C5—H5	120.2
C1—C6—H6	119.9	C4—C5—H5	120.2
C5—C6—C1	120.27 (11)	C19—C18—H18	120.1
C5—C6—H6	119.9	C17—C18—H18	120.1
C2—C3—H3	119.1	C17—C18—C19	119.80 (12)
C4—C3—C2	121.82 (11)	C20—C19—C18	120.18 (13)
C4—C3—H3	119.1	C20—C19—H19	119.9
C20—C15—C14	122.56 (11)	C18—C19—H19	119.9
C16—C15—C14	119.30 (11)	C9—C10—H10	120.0
C16—C15—C20	118.14 (11)	C9—C10—C11	120.03 (12)
C2—C13—H13	117.3	C11—C10—H10	120.0
C14—C13—C2	125.34 (11)	C16—C17—H17	120.0
C14—C13—H13	117.3	C18—C17—C16	120.06 (12)
C15—C14—H14	117.1	C18—C17—H17	120.0
C13—C14—C15	125.78 (11)	C10—C11—H11	119.7
C13—C14—H14	117.1	C12—C11—C10	120.53 (13)
C9—C8—S1	119.56 (9)	C12—C11—H11	119.7
C7—C8—S1	119.01 (10)	C7—C12—H12	119.9
C7—C8—C9	121.31 (12)	C11—C12—C7	120.25 (13)
C8—C9—H9	120.5	C11—C12—H12	119.9
C10—C9—C8	118.96 (12)		

S1—N1—C1—C2	110.23 (11)	C6—C1—C2—C13	−178.89 (11)
S1—N1—C1—C6	−74.82 (13)	C3—C2—C13—C14	−18.42 (18)
S1—C8—C9—C10	175.66 (9)	C3—C4—C5—C6	0.44 (19)
S1—C8—C7—C12	−174.65 (10)	C15—C20—C19—C18	−0.9 (2)

O1—S1—N1—C1	164.82 (9)	C15—C16—C17—C18	−0.97 (19)
O1—S1—C8—C9	37.47 (11)	C13—C2—C3—C4	179.40 (11)
O1—S1—C8—C7	−146.36 (10)	C14—C15—C20—C19	177.62 (12)
O2—S1—N1—C1	35.79 (10)	C14—C15—C16—C17	−176.72 (11)
O2—S1—C8—C9	168.65 (9)	C8—S1—N1—C1	−80.91 (10)
O2—S1—C8—C7	−15.19 (11)	C8—C9—C10—C11	−0.86 (18)
N1—S1—C8—C9	−75.20 (10)	C8—C7—C12—C11	−1.2 (2)
N1—S1—C8—C7	100.96 (10)	C9—C8—C7—C12	1.44 (18)
N1—C1—C2—C3	175.13 (10)	C9—C10—C11—C12	1.1 (2)
N1—C1—C2—C13	−4.13 (16)	C20—C15—C14—C13	−6.09 (19)
N1—C1—C6—C5	−175.42 (11)	C20—C15—C16—C17	2.61 (18)
C1—C2—C3—C4	0.15 (17)	C16—C15—C14—C13	173.20 (12)
C1—C2—C13—C14	160.81 (12)	C16—C15—C20—C19	−1.68 (19)
C1—C6—C5—C4	0.07 (19)	C7—C8—C9—C10	−0.41 (18)
C2—C1—C6—C5	−0.48 (18)	C19—C18—C17—C16	−1.7 (2)
C2—C3—C4—C5	−0.56 (18)	C10—C11—C12—C7	0.0 (2)
C2—C13—C14—C15	−179.52 (11)	C17—C18—C19—C20	2.6 (2)
C6—C1—C2—C3	0.37 (16)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.888 (18)	2.010 (18)	2.8907 (14)	170.8 (17)
C6—H6···O2^{ii}	0.95	2.53	3.3332 (16)	143
C7—H7···O2	0.95	2.54	2.9208 (16)	104
C12—H12···*Cg*1^{iii}	0.95	2.59	3.4333 (15)	148
C19—H19···*Cg*1^{iv}	0.95	2.81	3.5747 (15)	141

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