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Morpholin-4-ium [5-cyano-6-(4-methylphenyl)-4-(morpholin-4-yl)pyrimidin-2-yl](phenylsulfonyl)-amide

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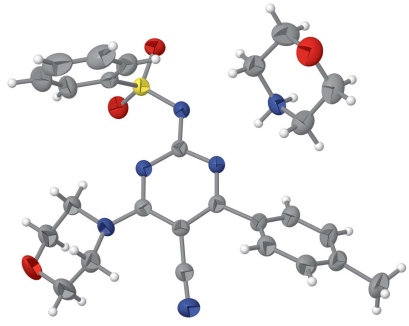
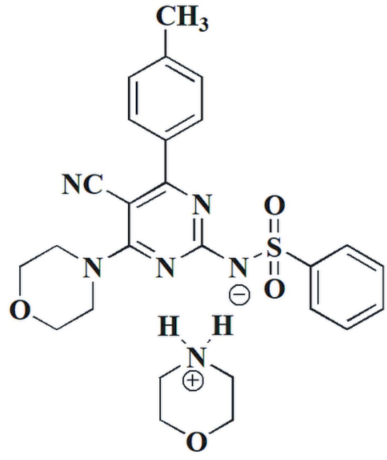
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecular salt, $C_4H_{10}NO^+\cdot C_{22}H_{20}N_5O_2S^-$, pairs of anions are linked by pairs of morpholinium cations through N—H···N and bifurcated N—H···(O,N) hydrogen bonds. Every cation donates two such bonds, one to each of the neighbouring pair of cations, generating centrosymmetric tetramers.

3D view



Chemical scheme



Structure description

Sulfonamides were pioneering medications for the treatment of bacterial infections and, despite the subsequent introduction of penicillin, they are still used as antibiotics (Gulçin & Taslimi, 2018). As part of our ongoing studies in this area (Elgemeie *et al.*, 2015*a*,*b*, 2019; Azzam *et al.*, 2019, 2017; Mohamed-Ezzat *et al.*, 2021), the structure of the title compound is now described: it crystallizes as a molecular salt comprising morpholin-4-ium ($C_4H_{10}NO^+$) cations and (benzenesulfonyl)[5-cyano-4-(morpholin-4-yl)-6-phenylpyrimidin-2-yl]azanide **5**(–H) ($C_{22}H_{20}N_5O_2S^-$) anions (Fig. 1). The sulfonamide group is deprotonated in contrast to other crystal structures containing the *N*-(pyrimidin-2-yl)benzenesulfonamide moiety, which are protonated (Singh & Baruah, 2019; Basak *et al.*, 1983): the morpholine reagent used in the last step of the synthesis accepts a proton to form the counter-ion.

In the pyrimidine ring of the anion, the longest C—N bond is C7—N2 [1.370 (2) Å], which is located opposite the longest C—C bond [C8—C9 = 1.431 (2) Å]. The other N—C bonds lie in the range 1.330 (2)–1.339 (2) Å. One phenyl ring (C1–C6) is almost perpendicular to the plane of the pyrimidine ring (N2/N3/C7–C10): the dihedral angle of 84.84 (6)° is enabled by a twist in the sulfonamide group as illustrated by the C7—N1—S1—C1 torsion angle of 63.74 (15)°. The angle between the second phenyl group (C16–

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

D—H···A	D—H	H···A	D···A	D—H···A
N6—H6A···O1^{i}	0.89	2.45	3.113 (2)	131
N6—H6A···N1^{i}	0.89	2.19	3.059 (2)	165
N6—H6B···N2	0.89	1.95	2.831 (2)	171

Symmetry code: (i) $-x+1, -y+1, -z+1$.

C21) and the pyrimidine ring is 48.19 (7)°. The two H atoms attached to the nitrogen atom of the morpholin-4-ium ion are involved in intermolecular N—H···N and N—H···(O,N) hydrogen bonds (Table 1) to the anion (Fig. 2). N2 is an acceptor of one contact whereas the other contact is bifurcated to O1 and N1. Thus, two anions adjacent to the cation are bridged through hydrogen bonding to generate centrosymmetric tetramers.

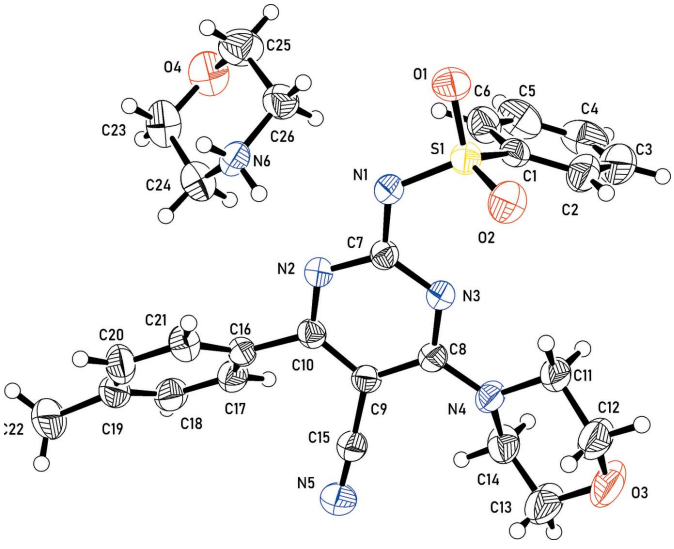


Figure 1
The asymmetric unit of **5** showing 50% probability displacement ellipsoids.

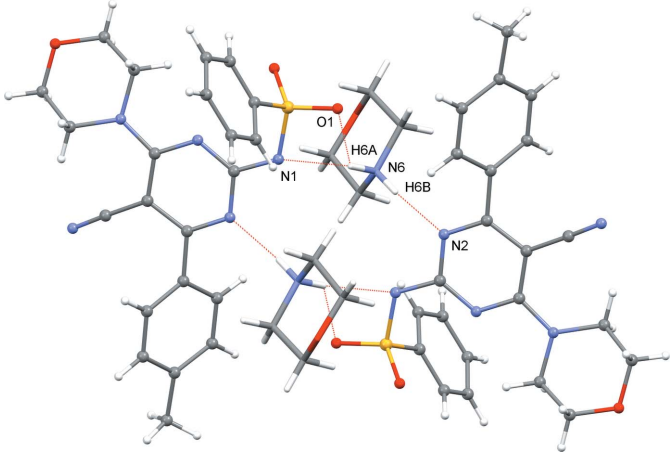


Figure 2
A segment of the crystal structure showing a tetramer of two anions and two cations with hydrogen bonds shown as red dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_{10}NO^+·C_{22}H_{20}N_5O_3S^-$
M_r	522.62
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	10.4177 (4), 11.7104 (3), 21.5388 (7)
β (°)	99.964 (3)
V (Å^3)	2588.00 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.17
Crystal size (mm)	0.59 × 0.39 × 0.22
Data collection	
Diffractometer	SuperNova, Dual, Cu at home/near, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2021)
T_{min}, T_{max}	0.468, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24156, 6299, 4792
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.695
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.130, 1.07
No. of reflections	6299
No. of parameters	335
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.42

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015) and *ORTEP-3 for Windows* (Farrugia, 2012).

Synthesis and crystallization

N-[5-Cyano-4-(4-methylphenyl)-6-oxo-1,6-dihydropyrimidin-2-yl]benzenesulfonamide, **3**, was prepared *via* a Michael addition by the reaction of *N*-(diaminomethylidene)benz-

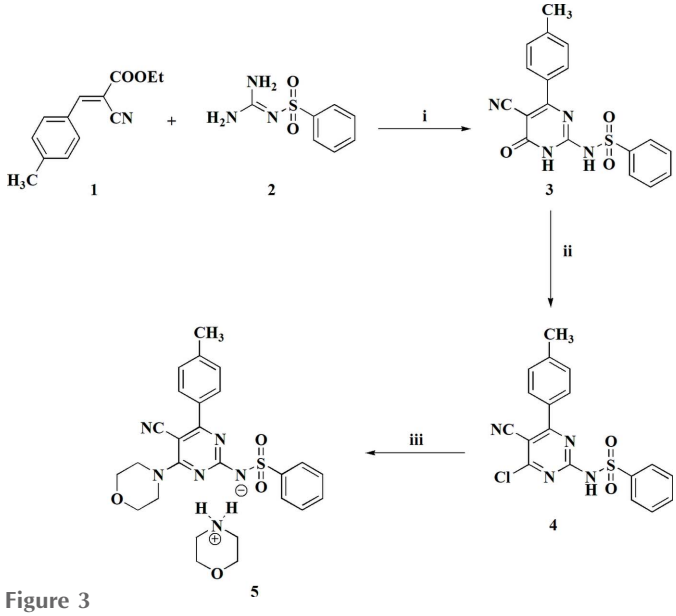


Figure 3
Reaction scheme. Reagents and conditions: (i) potassium hydroxide; dioxane; reflux; 2 h, (ii) phosphorus oxychloride; reflux; 1 h, and (iii) morpholine; potassium carbonate; dioxane; reflux; 2 h.

enesulfonamide, **2**, with ethyl (2*E*)-2-cyano-3-(4-methylphenyl)prop-2-enoate, **1**, in the presence of potassium hydroxide, with dioxane as a solvent (Azzam, 2019). *N*-[4-Chloro-5-cyano-6-(4-methylphenyl)pyrimidin-2-yl]benzenesulfonamide, **4**, was formed by treating compound **3** with phosphorous oxychloride. Finally, a solution of **4** (0.01 mol) and morpholine (0.03 mmol) in dry dioxane (20 ml) containing potassium hydroxide (0.015 mol) was refluxed for 2 h (Fig. 3). The reaction mixture was cooled and poured onto ice. After 48 hours, the solid product formed was filtered off. Recrystallization from aqueous solution produced the title salt, **5**.

Off-white crystals; yield 69%; m.p. 244–246°C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 2.35 (*s*, 3H, CH_3), 3.15–3.18 (*m*, 4H, $2CH_2$), 3.49–3.51 (*m*, 4H, $2CH_2$), 3.56–3.58 (*m*, 4H, $2CH_2$), 3.80–3.83 (*m*, 4H, $2CH_2$), 7.25 (*d*, *J* = 8.8 Hz, 2H, Ar—H), 7.41–7.48 (*m*, 3H, Ar—H), 7.54 (*d*, *J* = 8.8 Hz, 2H, Ar—H), 7.78–7.79 (*m*, 2H, Ar—H), 7.80 (*s*, 2H, NH_2). Analysis calculated for $C_{26}H_{30}N_6O_4S$: C 59.75; H 5.79; N 16.08; S 6.14. Found: C 59.69; H 5.75; N 16.20; S 6.19%.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

References

Azzam, R. A. (2019). *J. Heterocycl. Chem.* **56**, 619–627.

Azzam, R. A., Elgemeie, G. H., Elsayed, R. E. & Jones, P. G. (2017). *Acta Cryst.* E**73**, 1041–1043.

Azzam, R. A., Elgemeie, G. H., Osman, R. R. & Jones, P. G. (2019). *Acta Cryst.* E**75**, 367–371.

Basak, A. K., Mazumdar, S. K. & Chaudhuri, S. (1983). *Acta Cryst.* C**39**, 492–494.

Elgemeie, G. H., Azzam, R. A. & Elsayed, R. E. (2019). *Med. Chem. Res.* **28**, 1099–1131.

Elgemeie, G. H., Mohamed, R. A., Hussein, H. A. & Jones, P. G. (2015*a*). *Acta Cryst.* E**71**, 1322–1324.

Elgemeie, G. H., Salah, A. M., Mohamed, R. A. & Jones, P. G. (2015*b*). *Acta Cryst.* E**71**, 1319–1321.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Gulçin, I. & Taslimi, P. (2018). *Expert Opin. Ther. Pat.* **28**, 541–549.

Mohamed-Ezzat, R. A., Elgemeie, G. H. & Jones, P. G. (2021). *Acta Cryst.* E**77**, 547–550.

Rigaku OD (2021). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.

Singh, M. P. & Baruah, J. B. (2019). *ACS Omega*, **4**, 11609–11620.

full crystallographic data

IUCrData (2022). **7**, x221033 [https://doi.org/10.1107/S2414314622010331]

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Morpholin-4-ium [5-cyano-6-(4-methylphenyl)-4-(morpholin-4-yl)pyrimidin-2-yl](phenylsulfonyl)amide

Crystal data

$C_4H_{10}NO^+\cdot C_{22}H_{20}N_5O_3S^-$
M_r = 522.62
Monoclinic, $P2_1/n$
a = 10.4177 (4) Å
b = 11.7104 (3) Å
c = 21.5388 (7) Å
β = 99.964 (3)°
V = 2588.00 (15) Å^3
Z = 4
$F(000)$ = 1104
D_x = 1.341 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9606 reflections
θ = 3.8–28.7°
μ = 0.17 mm^{-1}
T = 296 K
Block, colourless
0.59 × 0.39 × 0.22 mm

Data collection

SuperNova, Dual, Cu at home/near, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2021)
T_{min} = 0.468, T_{max} = 1.000
24156 measured reflections
6299 independent reflections
4792 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 29.6°, θ_{min} = 3.4°
h = −14→13
k = −15→16
l = −29→28

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.130
S = 1.07
6299 reflections
335 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 1.057P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 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.

Refinement. Hydrogen atoms were inserted in idealized positions and a riding model was used with U_{iso}(H) set at 1.2 the values for the C or N to which they are bonded.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.39746 (16)	0.55594 (15)	0.26967 (8)	0.0364 (4)
C2	0.4004 (2)	0.6037 (2)	0.21176 (9)	0.0554 (5)
H2	0.431138	0.677645	0.208445	0.066*
C3	0.3566 (3)	0.5391 (3)	0.15822 (11)	0.0751 (8)
H3	0.355923	0.570912	0.118600	0.090*
C4	0.3144 (2)	0.4296 (3)	0.16295 (12)	0.0723 (8)
H4	0.287794	0.386557	0.126719	0.087*
C5	0.3111 (2)	0.3831 (2)	0.22091 (13)	0.0661 (7)
H5	0.281315	0.308830	0.224035	0.079*
C6	0.3517 (2)	0.44611 (17)	0.27452 (10)	0.0512 (5)
H6	0.348518	0.414928	0.313928	0.061*
C7	0.64862 (16)	0.52093 (14)	0.37849 (7)	0.0329 (4)
C8	0.80885 (17)	0.51091 (14)	0.31695 (8)	0.0338 (4)
C9	0.88299 (16)	0.43727 (14)	0.36271 (8)	0.0339 (4)
C10	0.82690 (16)	0.40889 (14)	0.41528 (8)	0.0338 (4)
C11	0.7780 (2)	0.64082 (18)	0.22731 (10)	0.0513 (5)
H11A	0.728043	0.684328	0.253162	0.062*
H11B	0.717953	0.607433	0.192622	0.062*
C12	0.8723 (3)	0.7172 (2)	0.20250 (13)	0.0690 (7)
H12A	0.824400	0.776570	0.176883	0.083*
H12B	0.928029	0.753801	0.237609	0.083*
C13	1.0217 (3)	0.5704 (3)	0.20295 (15)	0.0853 (9)
H13A	1.080848	0.605144	0.237535	0.102*
H13B	1.073593	0.529160	0.177068	0.102*
C14	0.9353 (2)	0.48884 (19)	0.22871 (10)	0.0526 (5)
H14A	0.882101	0.447882	0.194430	0.063*
H14B	0.987657	0.433602	0.255552	0.063*
C15	1.01574 (18)	0.40786 (16)	0.36277 (9)	0.0408 (4)
C16	0.89636 (17)	0.33313 (15)	0.46580 (8)	0.0365 (4)
C17	0.95107 (19)	0.23040 (16)	0.45184 (9)	0.0443 (4)
H17	0.940804	0.205576	0.410260	0.053*
C18	1.0208 (2)	0.16462 (18)	0.49937 (10)	0.0509 (5)
H18	1.055758	0.095288	0.489394	0.061*
C19	1.0396 (2)	0.20040 (19)	0.56175 (10)	0.0516 (5)
C20	0.9792 (2)	0.29990 (19)	0.57567 (9)	0.0538 (5)
H20	0.986764	0.322991	0.617454	0.065*
C21	0.9077 (2)	0.36606 (17)	0.52859 (9)	0.0455 (4)
H21	0.867217	0.432463	0.538977	0.055*
C22	1.1275 (3)	0.1340 (3)	0.61238 (13)	0.0786 (8)
H22A	1.212050	0.169081	0.620502	0.118*
H22B	1.135534	0.056836	0.598458	0.118*
H22C	1.090822	0.133863	0.650304	0.118*
C23	0.5070 (3)	0.14024 (18)	0.53116 (11)	0.0636 (6)
H23A	0.543086	0.063991	0.537983	0.076*
H23B	0.494986	0.170698	0.571640	0.076*

C24	0.6004 (2)	0.21430 (19)	0.50402 (11)	0.0567 (5)
H24A	0.682757	0.217948	0.532919	0.068*
H24B	0.616321	0.182007	0.464587	0.068*
C25	0.3288 (2)	0.2453 (2)	0.48171 (14)	0.0689 (7)
H25A	0.316172	0.275345	0.522183	0.083*
H25B	0.244099	0.240285	0.454790	0.083*
C26	0.4142 (2)	0.32545 (19)	0.45255 (11)	0.0546 (5)
H26A	0.422374	0.298634	0.410798	0.066*
H26B	0.375257	0.400904	0.448447	0.066*
O1	0.32666 (13)	0.65594 (12)	0.36557 (6)	0.0501 (3)
O2	0.50656 (15)	0.73961 (11)	0.32196 (7)	0.0514 (4)
O3	0.9501 (2)	0.65779 (19)	0.16615 (10)	0.0938 (7)
O4	0.38439 (18)	0.13440 (13)	0.49027 (8)	0.0684 (5)
S1	0.44351 (4)	0.63797 (4)	0.33901 (2)	0.03651 (13)
N1	0.53251 (14)	0.55919 (12)	0.39007 (6)	0.0361 (3)
N2	0.71172 (14)	0.44877 (12)	0.42381 (6)	0.0356 (3)
N3	0.69318 (14)	0.54979 (12)	0.32594 (6)	0.0358 (3)
N4	0.85165 (15)	0.55056 (13)	0.26502 (7)	0.0420 (4)
N5	1.12314 (18)	0.38456 (18)	0.36510 (9)	0.0609 (5)
N6	0.54503 (16)	0.33128 (13)	0.49288 (7)	0.0438 (4)
H6A	0.538585	0.363750	0.529578	0.053*
H6B	0.597821	0.373892	0.474098	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0308 (9)	0.0433 (9)	0.0350 (8)	0.0055 (7)	0.0054 (7)	−0.0001 (7)
C2	0.0581 (13)	0.0678 (13)	0.0411 (10)	−0.0057 (11)	0.0112 (9)	0.0056 (10)
C3	0.0694 (16)	0.122 (2)	0.0347 (11)	−0.0027 (16)	0.0102 (11)	−0.0037 (13)
C4	0.0519 (14)	0.100 (2)	0.0617 (15)	0.0027 (13)	−0.0006 (11)	−0.0382 (15)
C5	0.0566 (14)	0.0577 (13)	0.0773 (17)	−0.0040 (11)	−0.0074 (12)	−0.0182 (12)
C6	0.0500 (12)	0.0493 (11)	0.0509 (11)	−0.0036 (9)	−0.0009 (9)	0.0020 (9)
C7	0.0333 (9)	0.0354 (8)	0.0294 (8)	−0.0023 (7)	0.0041 (6)	−0.0007 (6)
C8	0.0346 (9)	0.0334 (8)	0.0339 (8)	−0.0013 (7)	0.0069 (7)	0.0005 (7)
C9	0.0305 (8)	0.0341 (8)	0.0369 (8)	−0.0008 (7)	0.0053 (7)	0.0010 (7)
C10	0.0336 (9)	0.0328 (8)	0.0334 (8)	−0.0042 (7)	0.0011 (7)	−0.0001 (7)
C11	0.0461 (11)	0.0605 (12)	0.0497 (11)	0.0153 (9)	0.0151 (9)	0.0198 (10)
C12	0.0693 (15)	0.0678 (15)	0.0767 (16)	0.0169 (12)	0.0319 (13)	0.0358 (13)
C13	0.0701 (17)	0.106 (2)	0.0923 (19)	0.0398 (16)	0.0503 (15)	0.0471 (17)
C14	0.0600 (13)	0.0591 (12)	0.0410 (10)	0.0185 (10)	0.0153 (9)	0.0032 (9)
C15	0.0388 (10)	0.0422 (9)	0.0420 (10)	0.0012 (8)	0.0082 (8)	0.0065 (8)
C16	0.0333 (9)	0.0389 (9)	0.0357 (9)	−0.0031 (7)	0.0017 (7)	0.0057 (7)
C17	0.0464 (11)	0.0440 (10)	0.0432 (10)	0.0017 (8)	0.0097 (8)	0.0054 (8)
C18	0.0478 (11)	0.0475 (11)	0.0592 (12)	0.0074 (9)	0.0144 (9)	0.0167 (9)
C19	0.0419 (11)	0.0552 (12)	0.0552 (12)	−0.0031 (9)	0.0013 (9)	0.0230 (10)
C20	0.0596 (13)	0.0596 (13)	0.0378 (10)	−0.0091 (10)	−0.0043 (9)	0.0067 (9)
C21	0.0495 (11)	0.0442 (10)	0.0400 (10)	−0.0004 (8)	0.0004 (8)	0.0007 (8)
C22	0.0641 (16)	0.0932 (19)	0.0734 (17)	0.0086 (14)	−0.0025 (13)	0.0425 (15)

C23	0.0891 (18)	0.0418 (11)	0.0547 (13)	−0.0095 (11)	−0.0024 (12)	−0.0006 (10)
C24	0.0597 (13)	0.0531 (12)	0.0534 (12)	0.0034 (10)	−0.0011 (10)	−0.0020 (10)
C25	0.0554 (14)	0.0606 (14)	0.0907 (18)	−0.0143 (11)	0.0129 (13)	0.0042 (13)
C26	0.0467 (12)	0.0561 (12)	0.0596 (13)	−0.0036 (9)	0.0053 (10)	0.0086 (10)
O1	0.0445 (8)	0.0598 (8)	0.0491 (8)	0.0160 (6)	0.0165 (6)	−0.0027 (6)
O2	0.0632 (9)	0.0348 (7)	0.0568 (8)	−0.0026 (6)	0.0120 (7)	0.0027 (6)
O3	0.0915 (14)	0.1168 (16)	0.0896 (13)	0.0481 (12)	0.0616 (11)	0.0614 (12)
O4	0.0789 (12)	0.0474 (8)	0.0741 (11)	−0.0195 (8)	0.0002 (9)	−0.0010 (8)
S1	0.0395 (2)	0.0355 (2)	0.0353 (2)	0.00451 (17)	0.00866 (17)	−0.00001 (17)
N1	0.0350 (8)	0.0425 (8)	0.0317 (7)	0.0021 (6)	0.0082 (6)	0.0022 (6)
N2	0.0342 (8)	0.0398 (8)	0.0328 (7)	−0.0002 (6)	0.0055 (6)	0.0040 (6)
N3	0.0339 (8)	0.0409 (8)	0.0331 (7)	0.0016 (6)	0.0074 (6)	0.0050 (6)
N4	0.0426 (9)	0.0447 (8)	0.0425 (8)	0.0106 (7)	0.0180 (7)	0.0120 (7)
N5	0.0420 (10)	0.0787 (13)	0.0635 (12)	0.0099 (9)	0.0131 (8)	0.0145 (10)
N6	0.0511 (9)	0.0461 (9)	0.0358 (8)	−0.0075 (7)	0.0116 (7)	0.0019 (7)

Geometric parameters (Å, º)

C1—C2	1.372 (3)	C14—H14B	0.9700
C1—C6	1.382 (3)	C15—N5	1.144 (2)
C1—S1	1.7708 (17)	C16—C17	1.386 (3)
C2—C3	1.389 (3)	C16—C21	1.392 (3)
C2—H2	0.9300	C17—C18	1.383 (3)
C3—C4	1.365 (4)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.389 (3)
C4—C5	1.368 (4)	C18—H18	0.9300
C4—H4	0.9300	C19—C20	1.381 (3)
C5—C6	1.374 (3)	C19—C22	1.513 (3)
C5—H5	0.9300	C20—C21	1.387 (3)
C6—H6	0.9300	C20—H20	0.9300
C7—N3	1.339 (2)	C21—H21	0.9300
C7—N1	1.353 (2)	C22—H22A	0.9600
C7—N2	1.370 (2)	C22—H22B	0.9600
C8—N3	1.333 (2)	C22—H22C	0.9600
C8—N4	1.356 (2)	C23—O4	1.423 (3)
C8—C9	1.431 (2)	C23—C24	1.495 (3)
C9—C10	1.401 (2)	C23—H23A	0.9700
C9—C15	1.425 (3)	C23—H23B	0.9700
C10—N2	1.330 (2)	C24—N6	1.490 (3)
C10—C16	1.491 (2)	C24—H24A	0.9700
C11—N4	1.466 (2)	C24—H24B	0.9700
C11—C12	1.494 (3)	C25—O4	1.421 (3)
C11—H11A	0.9700	C25—C26	1.504 (3)
C11—H11B	0.9700	C25—H25A	0.9700
C12—O3	1.405 (3)	C25—H25B	0.9700
C12—H12A	0.9700	C26—N6	1.486 (3)
C12—H12B	0.9700	C26—H26A	0.9700
C13—O3	1.423 (3)	C26—H26B	0.9700

C13—C14	1.484 (4)	O1—S1	1.4472 (14)
C13—H13A	0.9700	O2—S1	1.4375 (14)
C13—H13B	0.9700	S1—N1	1.6023 (14)
C14—N4	1.459 (2)	N6—H6A	0.8900
C14—H14A	0.9700	N6—H6B	0.8900

C2—C1—C6	120.69 (18)	C17—C18—H18	119.5
C2—C1—S1	120.00 (15)	C19—C18—H18	119.5
C6—C1—S1	119.20 (14)	C20—C19—C18	118.13 (18)
C1—C2—C3	118.5 (2)	C20—C19—C22	121.3 (2)
C1—C2—H2	120.8	C18—C19—C22	120.6 (2)
C3—C2—H2	120.8	C19—C20—C21	121.3 (2)
C4—C3—C2	120.9 (2)	C19—C20—H20	119.3
C4—C3—H3	119.5	C21—C20—H20	119.3
C2—C3—H3	119.5	C20—C21—C16	120.01 (19)
C3—C4—C5	120.1 (2)	C20—C21—H21	120.0
C3—C4—H4	120.0	C16—C21—H21	120.0
C5—C4—H4	120.0	C19—C22—H22A	109.5
C4—C5—C6	120.1 (2)	C19—C22—H22B	109.5
C4—C5—H5	120.0	H22A—C22—H22B	109.5
C6—C5—H5	120.0	C19—C22—H22C	109.5
C5—C6—C1	119.8 (2)	H22A—C22—H22C	109.5
C5—C6—H6	120.1	H22B—C22—H22C	109.5
C1—C6—H6	120.1	O4—C23—C24	111.16 (18)
N3—C7—N1	121.60 (15)	O4—C23—H23A	109.4
N3—C7—N2	124.35 (16)	C24—C23—H23A	109.4
N1—C7—N2	114.01 (15)	O4—C23—H23B	109.4
N3—C8—N4	115.94 (15)	C24—C23—H23B	109.4
N3—C8—C9	119.96 (15)	H23A—C23—H23B	108.0
N4—C8—C9	124.00 (16)	N6—C24—C23	109.7 (2)
C10—C9—C15	118.84 (15)	N6—C24—H24A	109.7
C10—C9—C8	116.65 (15)	C23—C24—H24A	109.7
C15—C9—C8	123.66 (16)	N6—C24—H24B	109.7
N2—C10—C9	122.75 (15)	C23—C24—H24B	109.7
N2—C10—C16	116.35 (16)	H24A—C24—H24B	108.2
C9—C10—C16	120.89 (16)	O4—C25—C26	111.5 (2)
N4—C11—C12	108.46 (17)	O4—C25—H25A	109.3
N4—C11—H11A	110.0	C26—C25—H25A	109.3
C12—C11—H11A	110.0	O4—C25—H25B	109.3
N4—C11—H11B	110.0	C26—C25—H25B	109.3
C12—C11—H11B	110.0	H25A—C25—H25B	108.0
H11A—C11—H11B	108.4	N6—C26—C25	109.50 (18)
O3—C12—C11	112.4 (2)	N6—C26—H26A	109.8
O3—C12—H12A	109.1	C25—C26—H26A	109.8
C11—C12—H12A	109.1	N6—C26—H26B	109.8
O3—C12—H12B	109.1	C25—C26—H26B	109.8
C11—C12—H12B	109.1	H26A—C26—H26B	108.2
H12A—C12—H12B	107.9	C12—O3—C13	110.05 (19)

O3—C13—C14	112.2 (2)	C25—O4—C23	109.80 (17)
O3—C13—H13A	109.2	O2—S1—O1	115.69 (9)
C14—C13—H13A	109.2	O2—S1—N1	114.60 (8)
O3—C13—H13B	109.2	O1—S1—N1	103.82 (8)
C14—C13—H13B	109.2	O2—S1—C1	107.62 (9)
H13A—C13—H13B	107.9	O1—S1—C1	106.78 (8)
N4—C14—C13	109.8 (2)	N1—S1—C1	107.86 (8)
N4—C14—H14A	109.7	C7—N1—S1	119.59 (12)
C13—C14—H14A	109.7	C10—N2—C7	116.83 (15)
N4—C14—H14B	109.7	C8—N3—C7	119.39 (15)
C13—C14—H14B	109.7	C8—N4—C14	125.78 (15)
H14A—C14—H14B	108.2	C8—N4—C11	119.25 (15)
N5—C15—C9	177.6 (2)	C14—N4—C11	111.35 (15)
C17—C16—C21	118.84 (16)	C26—N6—C24	110.01 (16)
C17—C16—C10	121.61 (16)	C26—N6—H6A	109.7
C21—C16—C10	119.55 (16)	C24—N6—H6A	109.7
C18—C17—C16	120.40 (19)	C26—N6—H6B	109.7
C18—C17—H17	119.8	C24—N6—H6B	109.7
C16—C17—H17	119.8	H6A—N6—H6B	108.2
C17—C18—C19	121.1 (2)		
C7—N1—S1—C1	63.74 (15)	N3—C7—N1—S1	1.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H6*A*···O1^{i}	0.89	2.45	3.113 (2)	131
N6—H6*A*···N1^{i}	0.89	2.19	3.059 (2)	165
N6—H6*B*···N2	0.89	1.95	2.831 (2)	171

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.