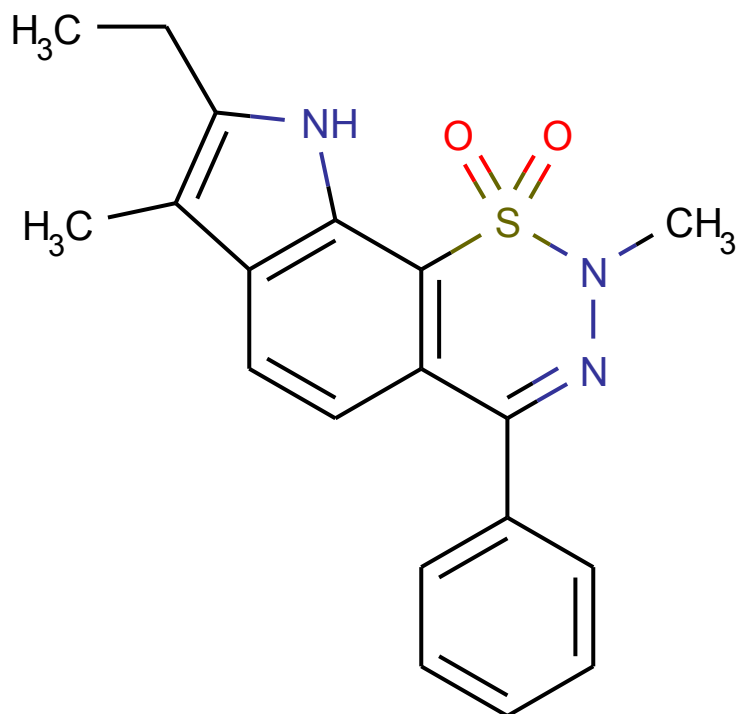


**143497**

**PGY0767\_1A**

Submitted by: Pusztai Gyongyver  
Operator: Dancso Andras

X-ray Structure Report



November 12, 2024

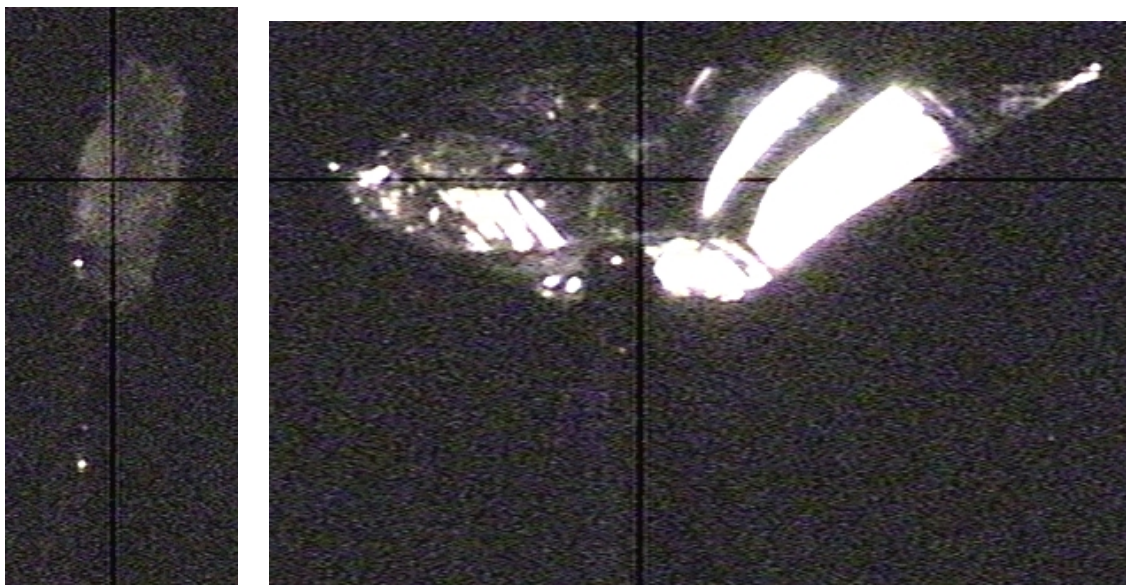


Fig. 1. The crystal

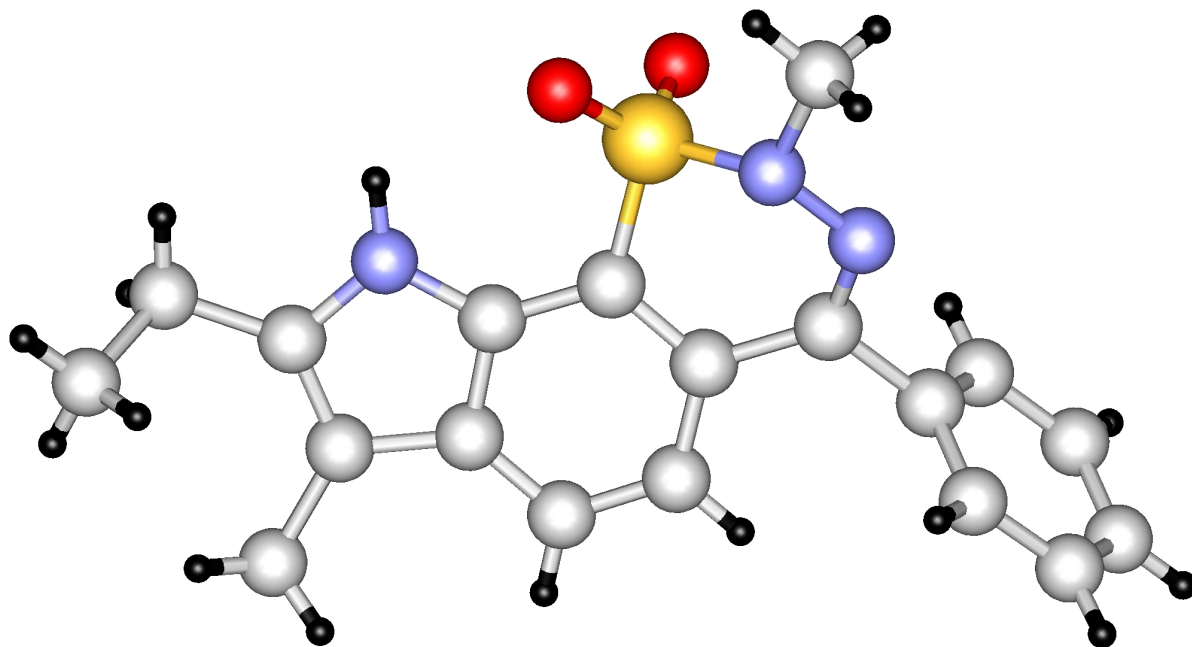


Fig. 2. The molecule (hydrogens were generated by the software)

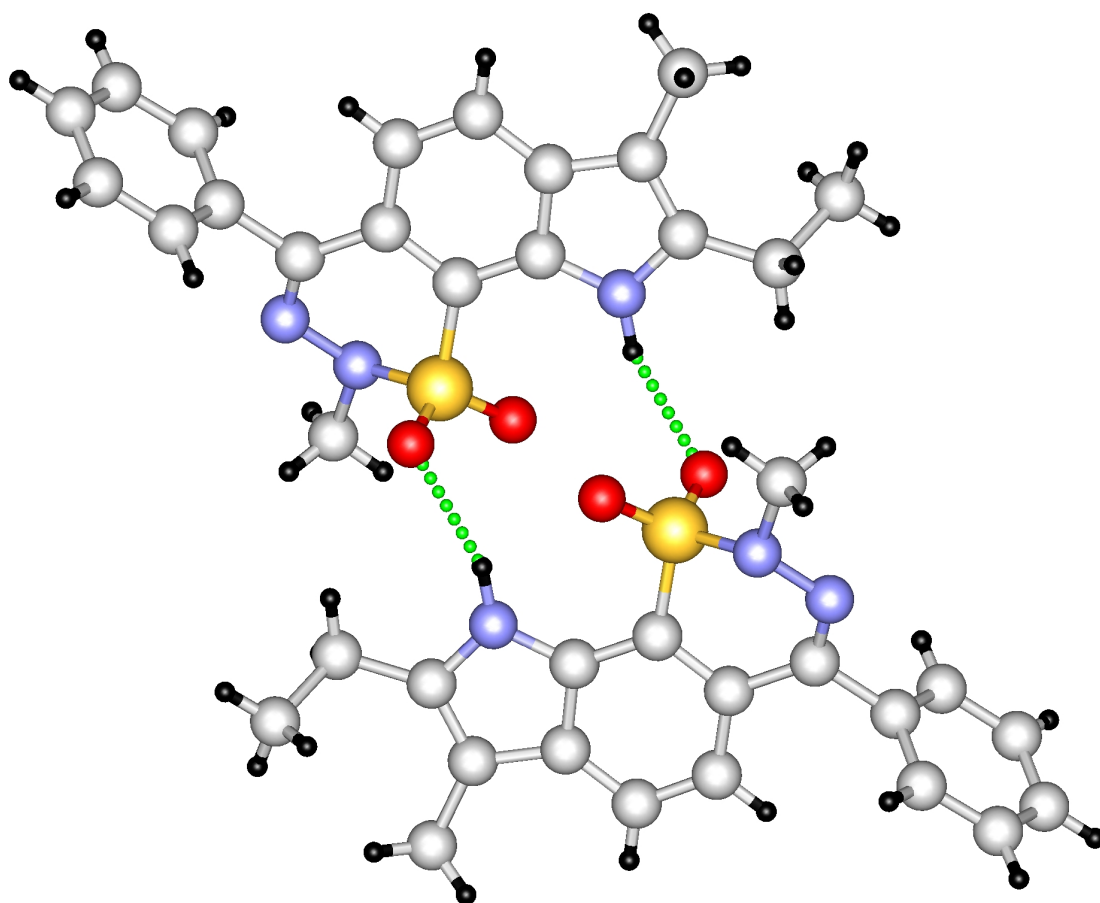


Fig. 3. Hydrogen bonds

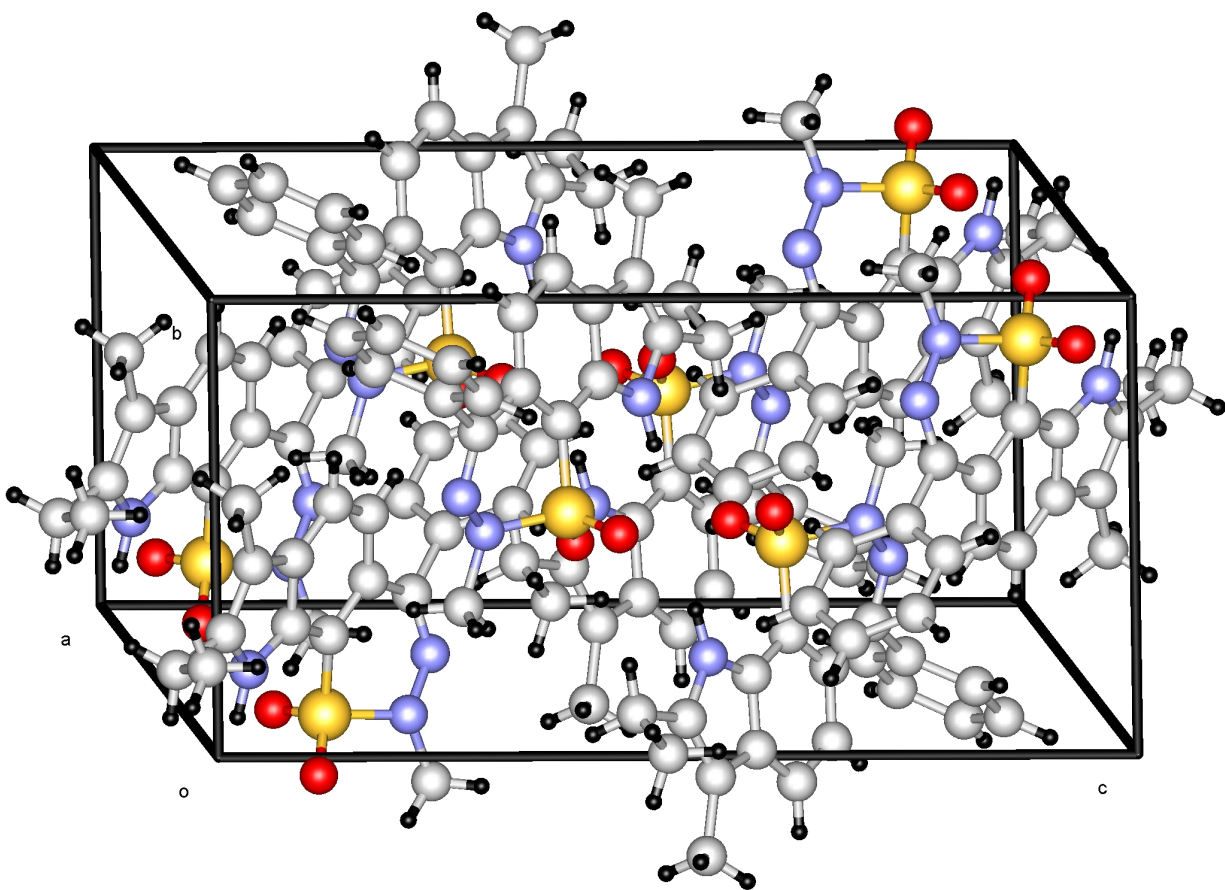


Fig. 4. Packing

## *Experimental*

### Data Collection

A colorless chunk crystal of  $C_{19}H_{19}N_3O_2S$  having approximate dimensions of 0.92 x 0.34 x 0.16 mm was mounted on a cactus needle. All measurements were made on a Rigaku RAXIS RAPID imaging plate area detector with graphite monochromated Cu-K $\alpha$  radiation.

Indexing was performed from 4 oscillations that were exposed for 60 seconds. The crystal-to-detector distance was 127.40 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

$$\begin{aligned}a &= 11.4934(5) \text{ \AA} \\b &= 8.9477(4) \text{ \AA} \quad \beta = 103.493(3)^\circ \\c &= 17.3845(8) \text{ \AA} \\V &= 1738.47(13) \text{ \AA}^3\end{aligned}$$

For  $Z = 4$  and F.W. = 353.44, the calculated density is 1.350 g/cm<sup>3</sup>. The systematic absences of:

$$\begin{aligned}h0l: l \pm 2n \\0k0: k \pm 2n\end{aligned}$$

uniquely determine the space group to be:

$$P2_1/c \text{ (\#14)}$$

The data were collected at a temperature of  $20 \pm 1^\circ\text{C}$  to a maximum  $2\theta$  value of  $143.1^\circ$ . A total of 180 oscillation images were collected. A sweep of data was done using  $\omega$  scans from  $20.0$  to  $200.0^\circ$  in  $5.0^\circ$  step, at  $\chi=0.0^\circ$  and  $\phi = 0.0^\circ$ . The exposure rate was 12.0 [sec./ $^\circ$ ]. A second sweep was performed using  $\omega$  scans from  $20.0$  to  $200.0^\circ$  in  $5.0^\circ$  step, at  $\chi=54.0^\circ$  and  $\phi = 0.0^\circ$ . The exposure rate was 12.0 [sec./ $^\circ$ ]. Another sweep was performed using  $\omega$  scans from  $20.0$  to  $200.0^\circ$  in  $5.0^\circ$  step, at  $\chi=54.0^\circ$  and  $\phi = 90.0^\circ$ . The exposure rate was 12.0 [sec./ $^\circ$ ]. Another sweep was performed using  $\omega$  scans from  $20.0$  to  $200.0^\circ$  in  $5.0^\circ$  step, at  $\chi=54.0^\circ$  and  $\phi = 180.0^\circ$ . The exposure rate was 12.0 [sec./ $^\circ$ ]. Another sweep was performed using  $\omega$  scans from  $20.0$  to  $200.0^\circ$  in  $5.0^\circ$  step, at  $\chi=54.0^\circ$  and  $\phi = 270.0^\circ$ . The exposure rate was 12.0 [sec./ $^\circ$ ]. The crystal-to-detector distance was 127.40 mm. Readout was performed in the 0.100 mm pixel mode.

## Data Reduction

Of the 19734 reflections that were collected, 3328 were unique ( $R_{\text{int}} = 0.106$ ).

The linear absorption coefficient,  $\mu$ , for Cu-K $\alpha$  radiation is 17.988 cm<sup>-1</sup>. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.358 to 0.746. The data were corrected for Lorentz and polarization effects.

## Structure Solution and Refinement

The structure was solved by direct methods<sup>1</sup> and expanded using Fourier techniques<sup>2</sup>. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement<sup>3</sup> on F was based on 10568 observed reflections ( $I > 2.00\sigma(I)$ ) and 245 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o| = 0.1199$$

$$R_w = [ \Sigma w (|F_o| - |F_c|)^2 / \Sigma w F_o^2 ]^{1/2} = 0.1559$$

The standard deviation of an observation of unit weight<sup>4</sup> was 8.84. Unit weights were used. Plots of  $\Sigma w (|F_o| - |F_c|)^2$  versus  $|F_o|$ , reflection order in data collection,  $\sin \theta/\lambda$  and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 7.91 and -9.74 e<sup>-</sup>/Å<sup>3</sup>, respectively.

Neutral atom scattering factors were taken from Cromer and Waber<sup>5</sup>. Anomalous dispersion effects were included in Fcalc<sup>6</sup>; the values for  $\Delta f'$  and  $\Delta f''$  were those of Creagh and McAuley<sup>7</sup>. The values for the mass attenuation coefficients are those of Creagh and Hubbell<sup>8</sup>. All calculations were performed using the CrystalStructure<sup>9,10</sup> crystallographic software package.

## *References*

- (1) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.
- (2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized:

$$\sum w(|F_o| - |F_c|)^2 \quad \text{where } w = \text{Least Squares weights.}$$

(4) Standard deviation of an observation of unit weight:

$$[\sum w(|F_o| - |F_c|)^2 / (N_o - N_v)]^{1/2}$$

where:  $N_o$  = number of observations

$N_v$  = number of variables

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(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

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(8) Creagh, D. C. & Hubbell, J.H.; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 3.7.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSK (2000-2005). 9009 New Trails Dr. The Woodlands TX 77381 USA.

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## EXPERIMENTAL DETAILS

### A. Crystal Data

Empirical Formula	$\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_2\text{S}$
Formula Weight	353.44
Crystal Color, Habit	colorless, chunk
Crystal Dimensions	0.92 X 0.34 X 0.16 mm
Crystal System	monoclinic
Lattice Type	Primitive
Indexing Images	4 oscillations @ 60.0 seconds
Detector Position	127.40 mm
Pixel Size	0.100 mm
Lattice Parameters	$a = 11.4934(5) \text{ \AA}$ $b = 8.9477(4) \text{ \AA}$ $c = 17.3845(8) \text{ \AA}$ $\beta = 103.493(3)^\circ$ $V = 1738.47(13) \text{ \AA}^3$
Space Group	$P2_1/c$ (#14)
Z value	4
D <sub>calc</sub>	1.350 g/cm <sup>3</sup>
F <sub>000</sub>	744.00
$\mu(\text{CuK}\alpha)$	17.988 cm <sup>-1</sup>

## B. Intensity Measurements

Diffractometer	Rigaku RAXIS-RAPID
Radiation	CuK $\alpha$ ( $\lambda$ = 1.54187 Å) graphite monochromated
Detector Aperture	280 mm x 256 mm
Data Images	180 exposures
$\omega$ oscillation Range ( $\chi$ =0.0, $\phi$ =0.0)	20.0 - 200.0°
Exposure Rate	12.0 sec./°
$\omega$ oscillation Range ( $\chi$ =54.0, $\phi$ =0.0)	20.0 - 200.0°
Exposure Rate	12.0 sec./°
$\omega$ oscillation Range ( $\chi$ =54.0, $\phi$ =90.0)	20.0 - 200.0°
Exposure Rate	12.0 sec./°
$\omega$ oscillation Range ( $\chi$ =54.0, $\phi$ =180.0)	20.0 - 200.0°
Exposure Rate	12.0 sec./°
$\omega$ oscillation Range ( $\chi$ =54.0, $\phi$ =270.0)	20.0 - 200.0°
Exposure Rate	12.0 sec./°
Detector Position	127.40 mm
Pixel Size	0.100 mm
$2\theta_{\text{max}}$	143.1°
No. of Reflections Measured	Total: 19734 Unique: 3328 ( $R_{\text{int}}$ = 0.106)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.358 - 0.746)

### C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F
Function Minimized	$\Sigma w ( Fo  -  Fc )^2$
Least Squares Weights	1
$2\theta_{\text{max}}$ cutoff	143.1 $^{\circ}$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ( $I > 2.00\sigma(I)$ )	10568
No. Variables	245
Reflection/Parameter Ratio	43.13
Residuals: R ( $I > 2.00\sigma(I)$ )	0.1199
Residuals: Rw ( $I > 2.00\sigma(I)$ )	0.1559
Goodness of Fit Indicator	8.838
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	7.91 e $^{-}/\text{\AA}^3$
Minimum peak in Final Diff. Map	-9.74 e $^{-}/\text{\AA}^3$

Table 1. Atomic coordinates and B<sub>iso</sub>/B<sub>eq</sub>

atom	x	y	z	B <sub>eq</sub>
S(1)	0.09099(16)	0.43704(19)	0.62743(11)	1.75(3)
O(2)	-0.0112(3)	0.5361(4)	0.6073(2)	2.86(12)
O(3)	0.1790(3)	0.4553(4)	0.5827(2)	1.95(11)
N(1)	0.1510(4)	0.4579(5)	0.7258(3)	2.11(14)
N(4)	-0.1381(4)	0.2622(5)	0.5169(2)	1.74(13)
N(5)	0.2384(4)	0.3539(5)	0.7616(2)	1.79(13)
C(1)	-0.0771(5)	0.0392(6)	0.5757(3)	1.69(16)
C(8)	-0.0047(5)	-0.0559(7)	0.6280(3)	2.34(17)
C(9)	0.0929(5)	-0.0000(7)	0.6791(4)	2.16(17)
C(10)	0.0489(5)	0.2497(6)	0.6281(3)	1.54(15)
C(11)	0.1217(5)	0.1534(7)	0.6809(3)	1.46(15)
C(12)	0.2223(5)	0.2173(7)	0.7407(3)	1.58(16)
C(13)	-0.1877(5)	0.0172(7)	0.5168(3)	1.92(17)
C(14)	-0.2210(5)	0.1548(7)	0.4819(3)	1.79(17)
C(15)	0.3140(5)	0.1107(6)	0.7882(4)	2.09(17)
C(16)	-0.2512(5)	-0.1357(6)	0.4977(4)	3.4(2)
C(17)	-0.0516(5)	0.1948(6)	0.5744(3)	1.52(16)
C(18)	-0.3241(5)	0.2007(7)	0.4150(3)	2.65(18)
C(19)	0.4158(6)	0.0749(7)	0.7584(4)	2.81(19)
C(20)	0.5021(6)	-0.0227(8)	0.8021(5)	3.3(2)
C(21)	0.1787(6)	0.6130(6)	0.7536(4)	3.6(2)
C(22)	-0.4476(5)	0.1539(7)	0.4330(3)	3.33(19)
C(23)	0.2946(6)	0.0515(8)	0.8610(4)	3.6(2)
C(24)	0.4865(7)	-0.0844(9)	0.8723(5)	4.8(2)
C(25)	0.3843(7)	-0.0457(9)	0.9031(4)	4.9(2)
H(1)	-0.1402	0.3654	0.5037	1.93
H(2)	-0.0233	-0.1594	0.6274	2.69
H(3)	0.1439	-0.0655	0.7148	2.44
H(4)	0.4243	0.1175	0.7100	3.41
H(5)	0.5709	-0.0474	0.7833	4.04
H(6)	0.2251	0.0762	0.8791	4.35
H(7)	0.5455	-0.1504	0.9013	5.38
H(8)	0.3767	-0.0880	0.9518	5.70
H(9)	-0.3233	0.3059	0.4078	2.85
H(10)	-0.3161	0.1523	0.3679	2.85
H(11)	-0.2224	-0.1831	0.4569	3.70
H(12)	-0.3351	-0.1208	0.4806	3.71

Table 1. Atomic coordinates and  $B_{\text{iso}}/B_{\text{eq}}$  (continued)

atom	x	y	z	$B_{\text{eq}}$
H(13)	-0.2346	-0.1969	0.5436	3.71
H(14)	0.2582	0.6370	0.7508	3.98
H(15)	0.1714	0.6218	0.8067	3.97
H(16)	0.1245	0.6799	0.7210	3.98
H(17)	-0.4680	0.0556	0.4138	3.69
H(18)	-0.5088	0.2214	0.4083	3.69
H(19)	-0.4397	0.1560	0.4886	3.70

$$B_{\text{eq}} = 8/3 \pi^2 (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$

Table 2. Anisotropic displacement parameters

atom	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
S(1)	0.0229(9)	0.0124(9)	0.0296(11)	-0.0022(9)	0.0025(8)	0.0039(9)
O(2)	0.033(2)	0.004(2)	0.061(3)	-0.002(2)	-0.009(2)	0.011(2)
O(3)	0.032(2)	0.027(2)	0.023(2)	-0.006(2)	0.021(2)	0.006(2)
N(1)	0.026(3)	0.009(3)	0.044(4)	-0.002(2)	0.005(2)	-0.002(3)
N(4)	0.023(3)	-0.002(2)	0.040(4)	-0.009(2)	-0.003(2)	0.005(2)
N(5)	0.017(3)	0.014(3)	0.032(3)	0.004(2)	-0.005(2)	0.004(2)
C(1)	0.021(3)	0.008(3)	0.031(4)	-0.006(3)	-0.003(3)	0.000(3)
C(8)	0.031(4)	0.007(3)	0.047(5)	-0.002(3)	0.001(3)	0.001(3)
C(9)	0.022(4)	0.008(3)	0.048(5)	0.006(3)	-0.001(3)	0.008(3)
C(10)	0.021(3)	-0.004(3)	0.040(4)	-0.006(2)	0.004(3)	0.001(3)
C(11)	0.013(3)	0.015(4)	0.026(4)	0.005(3)	0.001(3)	0.006(3)
C(12)	0.013(3)	0.014(4)	0.032(4)	0.008(3)	0.004(3)	0.012(3)
C(13)	0.023(4)	0.020(4)	0.029(4)	-0.001(3)	0.004(3)	-0.001(3)
C(14)	0.021(4)	0.023(4)	0.027(4)	-0.002(3)	0.011(3)	0.005(3)
C(15)	0.018(4)	0.005(3)	0.047(5)	0.001(3)	-0.012(3)	-0.009(3)
C(16)	0.030(4)	0.023(4)	0.064(6)	0.004(3)	-0.011(4)	-0.011(4)
C(17)	0.027(4)	0.004(3)	0.030(4)	-0.006(3)	0.012(3)	0.005(3)
C(18)	0.035(4)	0.028(4)	0.027(4)	-0.007(3)	-0.014(3)	0.004(3)
C(19)	0.037(4)	0.034(5)	0.037(5)	0.009(4)	0.011(4)	-0.003(4)
C(20)	0.033(5)	0.037(5)	0.057(6)	0.014(4)	0.017(4)	-0.008(4)
C(21)	0.057(5)	0.004(4)	0.064(6)	-0.001(3)	-0.006(4)	-0.008(3)
C(22)	0.014(4)	0.053(5)	0.050(5)	0.003(3)	-0.013(3)	0.002(4)
C(23)	0.036(5)	0.069(6)	0.033(5)	0.010(4)	0.008(4)	0.028(4)
C(24)	0.028(5)	0.051(6)	0.092(8)	0.021(4)	-0.011(5)	0.017(5)
C(25)	0.070(6)	0.063(6)	0.048(6)	-0.001(5)	-0.000(5)	0.043(5)

The general temperature factor expression:  $\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$

Table 3. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
S(1)	O(2)	1.448(4)	S(1)	O(3)	1.422(4)
S(1)	N(1)	1.698(5)	S(1)	C(10)	1.745(5)
N(1)	N(5)	1.404(6)	N(1)	C(21)	1.480(7)
N(4)	C(14)	1.389(7)	N(4)	C(17)	1.374(7)
N(4)	H(1)	0.950	N(5)	C(12)	1.277(8)
C(1)	C(8)	1.374(8)	C(1)	C(13)	1.448(8)
C(1)	C(17)	1.425(8)	C(8)	C(9)	1.354(8)
C(8)	H(2)	0.950	C(9)	C(11)	1.411(8)
C(9)	H(3)	0.950	C(10)	C(11)	1.388(8)
C(10)	C(17)	1.394(8)	C(11)	C(12)	1.477(8)
C(12)	C(15)	1.516(8)	C(13)	C(14)	1.386(9)
C(13)	C(16)	1.549(8)	C(14)	C(18)	1.511(8)
C(15)	C(19)	1.421(10)	C(15)	C(23)	1.436(11)
C(16)	H(11)	0.950	C(16)	H(12)	0.950
C(16)	H(13)	0.950	C(18)	C(22)	1.581(9)
C(18)	H(9)	0.950	C(18)	H(10)	0.950
C(19)	C(20)	1.404(9)	C(19)	H(4)	0.950
C(20)	C(24)	1.388(13)	C(20)	H(5)	0.950
C(21)	H(14)	0.950	C(21)	H(15)	0.950
C(21)	H(16)	0.950	C(22)	H(17)	0.950
C(22)	H(18)	0.950	C(22)	H(19)	0.950
C(23)	C(25)	1.415(10)	C(23)	H(6)	0.950
C(24)	C(25)	1.442(13)	C(24)	H(7)	0.950
C(25)	H(8)	0.950			

Table 4. Bond angles ( $^{\circ}$ )

atom	atom	atom	angle	atom	atom	atom	angle
O(2)	S(1)	O(3)	116.0(2)	O(2)	S(1)	N(1)	107.0(2)
O(2)	S(1)	C(10)	112.3(2)	O(3)	S(1)	N(1)	111.4(2)
O(3)	S(1)	C(10)	110.4(3)	N(1)	S(1)	C(10)	98.4(2)
S(1)	N(1)	N(5)	117.0(4)	S(1)	N(1)	C(21)	115.9(4)
N(5)	N(1)	C(21)	113.6(4)	C(14)	N(4)	C(17)	108.7(4)
C(14)	N(4)	H(1)	126.2	C(17)	N(4)	H(1)	125.1
N(1)	N(5)	C(12)	117.9(4)	C(8)	C(1)	C(13)	132.8(5)
C(8)	C(1)	C(17)	121.4(5)	C(13)	C(1)	C(17)	105.8(5)
C(1)	C(8)	C(9)	119.1(5)	C(1)	C(8)	H(2)	119.8
C(9)	C(8)	H(2)	121.1	C(8)	C(9)	C(11)	121.9(5)
C(8)	C(9)	H(3)	119.5	C(11)	C(9)	H(3)	118.7
S(1)	C(10)	C(11)	118.4(4)	S(1)	C(10)	C(17)	121.4(4)
C(11)	C(10)	C(17)	120.1(5)	C(9)	C(11)	C(10)	119.2(5)
C(9)	C(11)	C(12)	122.2(5)	C(10)	C(11)	C(12)	118.5(5)
N(5)	C(12)	C(11)	127.5(5)	N(5)	C(12)	C(15)	114.3(5)
C(11)	C(12)	C(15)	118.1(5)	C(1)	C(13)	C(14)	107.2(5)
C(1)	C(13)	C(16)	124.3(5)	C(14)	C(13)	C(16)	128.5(5)
N(4)	C(14)	C(13)	109.4(4)	N(4)	C(14)	C(18)	118.9(5)
C(13)	C(14)	C(18)	131.7(5)	C(12)	C(15)	C(19)	118.0(6)
C(12)	C(15)	C(23)	118.7(6)	C(19)	C(15)	C(23)	123.2(5)
C(13)	C(16)	H(11)	109.0	C(13)	C(16)	H(12)	109.6
C(13)	C(16)	H(13)	109.7	H(11)	C(16)	H(12)	109.5
H(11)	C(16)	H(13)	109.5	H(12)	C(16)	H(13)	109.5
N(4)	C(17)	C(1)	108.9(4)	N(4)	C(17)	C(10)	132.8(5)
C(1)	C(17)	C(10)	118.4(5)	C(14)	C(18)	C(22)	110.8(5)
C(14)	C(18)	H(9)	109.9	C(14)	C(18)	H(10)	108.9
C(22)	C(18)	H(9)	109.0	C(22)	C(18)	H(10)	108.8
H(9)	C(18)	H(10)	109.5	C(15)	C(19)	C(20)	118.7(6)
C(15)	C(19)	H(4)	119.8	C(20)	C(19)	H(4)	121.5
C(19)	C(20)	C(24)	120.2(7)	C(19)	C(20)	H(5)	119.9
C(24)	C(20)	H(5)	119.9	N(1)	C(21)	H(14)	109.4
N(1)	C(21)	H(15)	109.5	N(1)	C(21)	H(16)	109.6
H(14)	C(21)	H(15)	109.5	H(14)	C(21)	H(16)	109.5
H(15)	C(21)	H(16)	109.5	C(18)	C(22)	H(17)	109.6
C(18)	C(22)	H(18)	110.2	C(18)	C(22)	H(19)	108.6
H(17)	C(22)	H(18)	109.5	H(17)	C(22)	H(19)	109.5
H(18)	C(22)	H(19)	109.5	C(15)	C(23)	C(25)	115.9(7)



Table 4. Bond angles ( $^{\circ}$ ) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(15)	C(23)	H(6)	121.4	C(25)	C(23)	H(6)	122.7
C(20)	C(24)	C(25)	120.9(7)	C(20)	C(24)	H(7)	119.4
C(25)	C(24)	H(7)	119.7	C(23)	C(25)	C(24)	121.0(7)
C(23)	C(25)	H(8)	119.9	C(24)	C(25)	H(8)	119.1

Table 5. Torsion Angles( $^{\circ}$ )

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
O(2)	S(1)	N(1)	N(5)	169.1(4)	O(2)	S(1)	N(1)	C(21)	-52.6(5)
O(2)	S(1)	C(10)	C(11)	-148.0(5)	O(2)	S(1)	C(10)	C(17)	35.5(7)
O(3)	S(1)	N(1)	N(5)	-63.3(4)	O(3)	S(1)	N(1)	C(21)	75.1(5)
O(3)	S(1)	C(10)	C(11)	81.0(6)	O(3)	S(1)	C(10)	C(17)	-95.5(6)
N(1)	S(1)	C(10)	C(11)	-35.6(6)	N(1)	S(1)	C(10)	C(17)	147.9(6)
C(10)	S(1)	N(1)	N(5)	52.6(4)	C(10)	S(1)	N(1)	C(21)	-169.1(4)
S(1)	N(1)	N(5)	C(12)	-40.1(7)	C(21)	N(1)	N(5)	C(12)	-179.4(6)
C(14)	N(4)	C(17)	C(1)	1.5(7)	C(14)	N(4)	C(17)	C(10)	-178.0(7)
C(17)	N(4)	C(14)	C(13)	-0.2(6)	C(17)	N(4)	C(14)	C(18)	-178.6(6)
N(1)	N(5)	C(12)	C(11)	1.3(10)	N(1)	N(5)	C(12)	C(15)	-174.0(5)
C(8)	C(1)	C(13)	C(14)	179.4(7)	C(8)	C(1)	C(13)	C(16)	-1.9(12)
C(13)	C(1)	C(8)	C(9)	-177.3(7)	C(8)	C(1)	C(17)	N(4)	-180(179)
C(8)	C(1)	C(17)	C(10)	-0.4(9)	C(17)	C(1)	C(8)	C(9)	-0.2(8)
C(13)	C(1)	C(17)	N(4)	-2.1(7)	C(13)	C(1)	C(17)	C(10)	177.5(6)
C(17)	C(1)	C(13)	C(14)	1.9(8)	C(17)	C(1)	C(13)	C(16)	-179.4(6)
C(1)	C(8)	C(9)	C(11)	0.8(11)	C(8)	C(9)	C(11)	C(10)	-0.8(10)
C(8)	C(9)	C(11)	C(12)	174.9(6)	S(1)	C(10)	C(11)	C(9)	-176.3(5)
S(1)	C(10)	C(11)	C(12)	7.9(9)	S(1)	C(10)	C(17)	N(4)	-3.8(11)
S(1)	C(10)	C(17)	C(1)	176.7(5)	C(11)	C(10)	C(17)	N(4)	179.8(6)
C(11)	C(10)	C(17)	C(1)	0.3(8)	C(17)	C(10)	C(11)	C(9)	0.2(8)
C(17)	C(10)	C(11)	C(12)	-175.6(6)	C(9)	C(11)	C(12)	N(5)	-160.1(7)
C(9)	C(11)	C(12)	C(15)	15.0(10)	C(10)	C(11)	C(12)	N(5)	15.6(11)
C(10)	C(11)	C(12)	C(15)	-169.3(6)	N(5)	C(12)	C(15)	C(19)	-93.5(7)
N(5)	C(12)	C(15)	C(23)	86.1(7)	C(11)	C(12)	C(15)	C(19)	90.7(7)
C(11)	C(12)	C(15)	C(23)	-89.6(8)	C(1)	C(13)	C(14)	N(4)	-1.1(8)
C(1)	C(13)	C(14)	C(18)	176.9(7)	C(16)	C(13)	C(14)	N(4)	-179.7(6)
C(16)	C(13)	C(14)	C(18)	-1.6(13)	N(4)	C(14)	C(18)	C(22)	-126.0(6)
C(13)	C(14)	C(18)	C(22)	56.1(10)	C(12)	C(15)	C(19)	C(20)	179.5(5)
C(12)	C(15)	C(23)	C(25)	-179.2(6)	C(19)	C(15)	C(23)	C(25)	0.5(9)
C(23)	C(15)	C(19)	C(20)	-0.2(7)	C(15)	C(19)	C(20)	C(24)	1.0(10)
C(19)	C(20)	C(24)	C(25)	-2.2(11)	C(15)	C(23)	C(25)	C(24)	-1.6(10)
C(20)	C(24)	C(25)	C(23)	2.5(11)					

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table 6. Distances beyond the asymmetric unit out to 3.60 Å

atom	atom	distance	atom	atom	distance
S(1)	N(4)	3.273(4)	S(1)	N(5)	2.650(4)
S(1)	C(11)	2.697(6)	S(1)	C(12)	2.939(6)
S(1)	C(17)	2.743(6)	S(1)	C(21)	2.697(6)
S(1)	H(1)	3.071	S(1)	H(1) <sup>1)</sup>	3.040
S(1)	H(11) <sup>2)</sup>	3.260	S(1)	H(14)	3.094
S(1)	H(15)	3.457	S(1)	H(16)	2.688
O(2)	O(3)	2.433(6)	O(2)	O(3) <sup>1)</sup>	3.415(5)
O(2)	N(1)	2.534(6)	O(2)	N(4)	3.088(5)
O(2)	N(4) <sup>1)</sup>	3.548(7)	O(2)	C(10)	2.657(6)
O(2)	C(17)	3.121(6)	O(2)	C(21)	3.019(7)
O(2)	C(23) <sup>3)</sup>	3.430(8)	O(2)	H(1)	2.555
O(2)	H(1) <sup>1)</sup>	3.016	O(2)	H(2) <sup>4)</sup>	2.755
O(2)	H(6) <sup>3)</sup>	2.549	O(2)	H(13) <sup>4)</sup>	3.493
O(2)	H(16)	2.561	O(3)	O(2)	2.433(6)
O(3)	O(2) <sup>1)</sup>	3.415(5)	O(3)	N(1)	2.582(7)
O(3)	N(4) <sup>1)</sup>	3.038(6)	O(3)	N(5)	3.158(6)
O(3)	C(10)	2.607(7)	O(3)	C(11)	3.342(7)
O(3)	C(12)	3.419(7)	O(3)	C(16) <sup>2)</sup>	3.371(7)
O(3)	C(17)	3.507(7)	O(3)	C(18) <sup>1)</sup>	3.496(7)
O(3)	C(21)	3.289(8)	O(3)	H(1) <sup>1)</sup>	2.172
O(3)	H(5) <sup>5)</sup>	3.251	O(3)	H(7) <sup>5)</sup>	3.254
O(3)	H(9) <sup>1)</sup>	2.686	O(3)	H(11) <sup>2)</sup>	2.611
O(3)	H(13) <sup>2)</sup>	3.352	O(3)	H(14)	3.282
O(3)	H(16)	3.303	N(1)	O(2)	2.534(6)
N(1)	O(3)	2.582(7)	N(1)	C(8) <sup>3)</sup>	3.362(9)
N(1)	C(9) <sup>3)</sup>	3.591(9)	N(1)	C(10)	2.608(7)
N(1)	C(11)	2.833(8)	N(1)	C(12)	2.297(8)
N(1)	H(2) <sup>3)</sup>	3.393	N(1)	H(5) <sup>5)</sup>	3.237
N(1)	H(14)	2.006	N(1)	H(15)	2.007
N(1)	H(16)	2.009	N(4)	S(1)	3.273(4)
N(4)	O(2)	3.088(5)	N(4)	O(2) <sup>1)</sup>	3.548(7)
N(4)	O(3) <sup>1)</sup>	3.038(6)	N(4)	C(1)	2.277(7)
N(4)	C(8)	3.577(7)	N(4)	C(10)	2.537(7)
N(4)	C(13)	2.265(8)	N(4)	C(18)	2.498(7)
N(4)	H(2) <sup>2)</sup>	3.571	N(4)	H(8) <sup>3)</sup>	3.212
N(4)	H(9)	2.528	N(4)	H(10)	3.064
N(4)	H(15) <sup>6)</sup>	3.418	N(4)	H(19)	3.517

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
N(5)	S(1)	2.650(4)	N(5)	O(3)	3.158(6)
N(5)	C(10)	2.939(7)	N(5)	C(11)	2.472(7)
N(5)	C(15)	2.350(8)	N(5)	C(19)	3.232(8)
N(5)	C(20) <sup>5j</sup>	3.590(9)	N(5)	C(21)	2.412(7)
N(5)	C(23)	3.194(9)	N(5)	H(2) <sup>3j</sup>	3.473
N(5)	H(4)	3.278	N(5)	H(5) <sup>5j</sup>	2.645
N(5)	H(6)	3.242	N(5)	H(13) <sup>3j</sup>	3.426
N(5)	H(14)	2.553	N(5)	H(15)	2.689
N(5)	H(16)	3.208	N(5)	H(18) <sup>7j</sup>	3.456
C(1)	N(4)	2.277(7)	C(1)	C(1) <sup>2j</sup>	3.568(10)
C(1)	C(9)	2.352(8)	C(1)	C(10)	2.421(8)
C(1)	C(11)	2.768(8)	C(1)	C(14)	2.281(8)
C(1)	C(16)	2.650(8)	C(1)	C(21) <sup>6j</sup>	3.498(10)
C(1)	H(1)	3.192	C(1)	H(2)	2.022
C(1)	H(3)	3.211	C(1)	H(11)	3.066
C(1)	H(12)	3.360	C(1)	H(13)	2.753
C(1)	H(15) <sup>6j</sup>	2.634	C(8)	N(1) <sup>6j</sup>	3.362(9)
C(8)	N(4)	3.577(7)	C(8)	C(10)	2.803(8)
C(8)	C(11)	2.417(8)	C(8)	C(13)	2.586(8)
C(8)	C(16)	3.266(8)	C(8)	C(17)	2.440(8)
C(8)	C(21) <sup>6j</sup>	3.528(10)	C(8)	H(3)	2.000
C(8)	H(11)	3.595	C(8)	H(13)	2.986
C(8)	H(15) <sup>6j</sup>	2.916	C(8)	H(16) <sup>8j</sup>	3.048
C(9)	N(1) <sup>6j</sup>	3.591(9)	C(9)	C(1)	2.352(8)
C(9)	C(10)	2.413(8)	C(9)	C(12)	2.529(8)
C(9)	C(15)	2.965(8)	C(9)	C(17)	2.775(8)
C(9)	C(23)	3.488(8)	C(9)	H(2)	2.016
C(9)	H(6)	3.521	C(9)	H(10) <sup>2j</sup>	3.175
C(9)	H(11) <sup>2j</sup>	3.483	C(9)	H(15) <sup>6j</sup>	3.291
C(9)	H(16) <sup>8j</sup>	2.956	C(10)	O(2)	2.657(6)
C(10)	O(3)	2.607(7)	C(10)	N(1)	2.608(7)
C(10)	N(4)	2.537(7)	C(10)	N(5)	2.939(7)
C(10)	C(1)	2.421(8)	C(10)	C(8)	2.803(8)
C(10)	C(9)	2.413(8)	C(10)	C(12)	2.463(7)
C(10)	H(1)	2.878	C(10)	H(3)	3.263
C(10)	H(11) <sup>2j</sup>	2.810	C(10)	H(15) <sup>6j</sup>	3.217
C(11)	S(1)	2.697(6)	C(11)	O(3)	3.342(7)

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C(11)	N(1)	2.833(8)	C(11)	N(5)	2.472(7)
C(11)	C(1)	2.768(8)	C(11)	C(8)	2.417(8)
C(11)	C(15)	2.567(8)	C(11)	C(17)	2.411(8)
C(11)	C(19)	3.407(8)	C(11)	C(23)	3.418(8)
C(11)	H(2)	3.279	C(11)	H(3)	2.044
C(11)	H(4)	3.410	C(11)	H(6)	3.442
C(11)	H(11) <sup>2j</sup>	2.906	C(11)	H(15) <sup>6j</sup>	3.438
C(12)	S(1)	2.939(6)	C(12)	O(3)	3.419(7)
C(12)	N(1)	2.297(8)	C(12)	C(9)	2.529(8)
C(12)	C(10)	2.463(7)	C(12)	C(19)	2.519(9)
C(12)	C(21)	3.591(8)	C(12)	C(23)	2.540(9)
C(12)	H(3)	2.688	C(12)	H(4)	2.656
C(12)	H(5) <sup>5j</sup>	3.274	C(12)	H(6)	2.710
C(12)	H(11) <sup>2j</sup>	3.450	C(13)	N(4)	2.265(8)
C(13)	C(8)	2.586(8)	C(13)	C(17)	2.291(8)
C(13)	C(18)	2.644(8)	C(13)	C(22)	3.242(8)
C(13)	H(1)	3.180	C(13)	H(2)	2.841
C(13)	H(9)	3.364	C(13)	H(10)	2.926
C(13)	H(11)	2.064	C(13)	H(12)	2.072
C(13)	H(13)	2.072	C(13)	H(15) <sup>6j</sup>	3.171
C(13)	H(17)	3.318	C(13)	H(19)	3.084
C(14)	C(1)	2.281(8)	C(14)	C(16)	2.645(9)
C(14)	C(17)	2.246(8)	C(14)	C(22)	2.545(8)
C(14)	H(1)	2.096	C(14)	H(8) <sup>3j</sup>	3.285
C(14)	H(9)	2.040	C(14)	H(10)	2.029
C(14)	H(11)	3.054	C(14)	H(12)	2.791
C(14)	H(13)	3.340	C(14)	H(15) <sup>6j</sup>	3.597
C(14)	H(17)	2.946	C(14)	H(18)	3.310
C(14)	H(19)	2.544	C(15)	N(5)	2.350(8)
C(15)	C(9)	2.965(8)	C(15)	C(11)	2.567(8)
C(15)	C(20)	2.431(9)	C(15)	C(24)	2.786(9)
C(15)	C(25)	2.417(10)	C(15)	H(3)	2.602
C(15)	H(4)	2.065	C(15)	H(5)	3.293
C(15)	H(6)	2.095	C(15)	H(8)	3.287
C(15)	H(10) <sup>2j</sup>	3.596	C(15)	H(18) <sup>7j</sup>	2.963
C(16)	O(3) <sup>2j</sup>	3.371(7)	C(16)	C(1)	2.650(8)
C(16)	C(8)	3.266(8)	C(16)	C(14)	2.645(9)

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C(16)	C(18)	3.357(8)	C(16)	C(22)	3.448(8)
C(16)	H(2)	3.038	C(16)	H(6) <sup>6j</sup>	3.320
C(16)	H(7) <sup>9j</sup>	3.179	C(16)	H(10)	3.392
C(16)	H(17)	3.094	C(16)	H(19)	3.372
C(17)	S(1)	2.743(6)	C(17)	O(2)	3.121(6)
C(17)	O(3)	3.507(7)	C(17)	C(8)	2.440(8)
C(17)	C(9)	2.775(8)	C(17)	C(11)	2.411(8)
C(17)	C(13)	2.291(8)	C(17)	C(14)	2.246(8)
C(17)	H(1)	2.072	C(17)	H(2)	3.295
C(17)	H(11) <sup>2j</sup>	3.321	C(17)	H(15) <sup>6j</sup>	2.815
C(18)	O(3) <sup>1j</sup>	3.496(7)	C(18)	N(4)	2.498(7)
C(18)	C(13)	2.644(8)	C(18)	C(16)	3.357(8)
C(18)	H(1)	2.738	C(18)	H(8) <sup>3j</sup>	3.156
C(18)	H(12)	3.108	C(18)	H(14) <sup>1j</sup>	3.466
C(18)	H(17)	2.099	C(18)	H(18)	2.107
C(18)	H(19)	2.088	C(19)	N(5)	3.232(8)
C(19)	C(11)	3.407(8)	C(19)	C(12)	2.519(9)
C(19)	C(23)	2.514(11)	C(19)	C(24)	2.420(11)
C(19)	C(25)	2.835(11)	C(19)	H(3)	3.288
C(19)	H(5)	2.050	C(19)	H(5) <sup>5j</sup>	3.468
C(19)	H(6)	3.368	C(19)	H(7)	3.275
C(19)	H(10) <sup>2j</sup>	3.015	C(19)	H(17) <sup>2j</sup>	3.396
C(19)	H(18) <sup>7j</sup>	3.131	C(20)	N(5) <sup>10j</sup>	3.590(9)
C(20)	C(15)	2.431(9)	C(20)	C(23)	2.884(11)
C(20)	C(25)	2.463(13)	C(20)	H(4)	2.066
C(20)	H(4) <sup>10j</sup>	3.348	C(20)	H(7)	2.031
C(20)	H(8)	3.307	C(20)	H(9) <sup>7j</sup>	3.074
C(20)	H(10) <sup>2j</sup>	3.420	C(20)	H(14) <sup>10j</sup>	3.415
C(20)	H(18) <sup>7j</sup>	3.286	C(21)	S(1)	2.697(6)
C(21)	O(2)	3.019(7)	C(21)	O(3)	3.289(8)
C(21)	N(5)	2.412(7)	C(21)	C(1) <sup>3j</sup>	3.498(10)
C(21)	C(8) <sup>3j</sup>	3.528(10)	C(21)	C(12)	3.591(8)
C(21)	H(2) <sup>4j</sup>	3.460	C(21)	H(3) <sup>4j</sup>	2.960
C(21)	H(5) <sup>5j</sup>	3.408	C(21)	H(10) <sup>1j</sup>	3.593
C(22)	C(13)	3.242(8)	C(22)	C(14)	2.545(8)
C(22)	C(16)	3.448(8)	C(22)	H(4) <sup>2j</sup>	3.530
C(22)	H(8) <sup>3j</sup>	3.041	C(22)	H(9)	2.092

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C(22)	H(10)	2.090	C(22)	H(12)	2.811
C(22)	H(12) <sup>11)</sup>	3.214	C(22)	H(17) <sup>11)</sup>	3.571
C(22)	H(19) <sup>11)</sup>	3.470	C(23)	O(2) <sup>6)</sup>	3.430(8)
C(23)	N(5)	3.194(9)	C(23)	C(9)	3.488(8)
C(23)	C(11)	3.418(8)	C(23)	C(12)	2.540(9)
C(23)	C(19)	2.514(11)	C(23)	C(20)	2.884(11)
C(23)	C(24)	2.487(11)	C(23)	H(3)	2.916
C(23)	H(4)	3.360	C(23)	H(7)	3.336
C(23)	H(8)	2.060	C(23)	H(13) <sup>3)</sup>	2.970
C(23)	H(18) <sup>7)</sup>	3.008	C(24)	C(15)	2.786(9)
C(24)	C(19)	2.420(11)	C(24)	C(23)	2.487(11)
C(24)	H(4)	3.285	C(24)	H(4) <sup>10)</sup>	3.301
C(24)	H(5)	2.036	C(24)	H(6)	3.358
C(24)	H(8)	2.078	C(24)	H(8) <sup>12)</sup>	3.458
C(24)	H(9) <sup>7)</sup>	3.277	C(24)	H(12) <sup>13)</sup>	3.592
C(24)	H(18) <sup>7)</sup>	3.306	C(24)	H(19) <sup>6)</sup>	3.484
C(25)	C(15)	2.417(10)	C(25)	C(19)	2.835(11)
C(25)	C(20)	2.463(13)	C(25)	H(5)	3.320
C(25)	H(6)	2.087	C(25)	H(7)	2.083
C(25)	H(8) <sup>12)</sup>	3.480	C(25)	H(18) <sup>7)</sup>	3.144
C(25)	H(19) <sup>6)</sup>	3.243	H(1)	S(1)	3.071
H(1)	S(1) <sup>1)</sup>	3.040	H(1)	O(2)	2.555
H(1)	O(2) <sup>1)</sup>	3.016	H(1)	O(3) <sup>1)</sup>	2.172
H(1)	C(1)	3.192	H(1)	C(10)	2.878
H(1)	C(13)	3.180	H(1)	C(14)	2.096
H(1)	C(17)	2.072	H(1)	C(18)	2.738
H(1)	H(6) <sup>3)</sup>	3.097	H(1)	H(8) <sup>3)</sup>	3.024
H(1)	H(9)	2.419	H(1)	H(10)	3.327
H(2)	O(2) <sup>8)</sup>	2.755	H(2)	N(1) <sup>6)</sup>	3.393
H(2)	N(4) <sup>2)</sup>	3.571	H(2)	N(5) <sup>6)</sup>	3.473
H(2)	C(1)	2.022	H(2)	C(9)	2.016
H(2)	C(11)	3.279	H(2)	C(13)	2.841
H(2)	C(16)	3.038	H(2)	C(17)	3.295
H(2)	C(21) <sup>8)</sup>	3.460	H(2)	H(3)	2.312
H(2)	H(6) <sup>6)</sup>	3.296	H(2)	H(11)	3.302
H(2)	H(13)	2.546	H(2)	H(15) <sup>6)</sup>	3.383
H(2)	H(16) <sup>8)</sup>	2.512	H(3)	C(1)	3.211

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
H(3)	C(8)	2.000	H(3)	C(10)	3.263
H(3)	C(11)	2.044	H(3)	C(12)	2.688
H(3)	C(15)	2.602	H(3)	C(19)	3.288
H(3)	C(21) <sup>8)</sup>	2.960	H(3)	C(23)	2.916
H(3)	H(2)	2.312	H(3)	H(6)	3.064
H(3)	H(10) <sup>2)</sup>	2.814	H(3)	H(14) <sup>8)</sup>	2.970
H(3)	H(15) <sup>8)</sup>	3.201	H(3)	H(16) <sup>8)</sup>	2.294
H(4)	N(5)	3.278	H(4)	C(11)	3.410
H(4)	C(12)	2.656	H(4)	C(15)	2.065
H(4)	C(20)	2.066	H(4)	C(20) <sup>5)</sup>	3.348
H(4)	C(22) <sup>2)</sup>	3.530	H(4)	C(23)	3.360
H(4)	C(24)	3.285	H(4)	C(24) <sup>5)</sup>	3.301
H(4)	H(5)	2.374	H(4)	H(5) <sup>5)</sup>	3.001
H(4)	H(7) <sup>5)</sup>	2.914	H(4)	H(10) <sup>2)</sup>	2.902
H(4)	H(11) <sup>2)</sup>	3.318	H(4)	H(12) <sup>2)</sup>	3.233
H(4)	H(14) <sup>10)</sup>	3.557	H(4)	H(17) <sup>2)</sup>	2.791
H(5)	O(3) <sup>10)</sup>	3.251	H(5)	N(1) <sup>10)</sup>	3.237
H(5)	N(5) <sup>10)</sup>	2.645	H(5)	C(12) <sup>10)</sup>	3.274
H(5)	C(15)	3.293	H(5)	C(19)	2.050
H(5)	C(19) <sup>10)</sup>	3.468	H(5)	C(21) <sup>10)</sup>	3.408
H(5)	C(24)	2.036	H(5)	C(25)	3.320
H(5)	H(4)	2.374	H(5)	H(4) <sup>10)</sup>	3.001
H(5)	H(7)	2.329	H(5)	H(9) <sup>7)</sup>	3.100
H(5)	H(10) <sup>2)</sup>	3.573	H(5)	H(14) <sup>10)</sup>	2.734
H(5)	H(17) <sup>2)</sup>	3.354	H(5)	H(18) <sup>2)</sup>	3.593
H(6)	O(2) <sup>6)</sup>	2.549	H(6)	N(5)	3.242
H(6)	C(9)	3.521	H(6)	C(11)	3.442
H(6)	C(12)	2.710	H(6)	C(15)	2.095
H(6)	C(16) <sup>3)</sup>	3.320	H(6)	C(19)	3.368
H(6)	C(24)	3.358	H(6)	C(25)	2.087
H(6)	H(1) <sup>6)</sup>	3.097	H(6)	H(2) <sup>3)</sup>	3.296
H(6)	H(3)	3.064	H(6)	H(8)	2.401
H(6)	H(11) <sup>3)</sup>	3.579	H(6)	H(13) <sup>3)</sup>	2.423
H(6)	H(18) <sup>7)</sup>	3.489	H(7)	O(3) <sup>10)</sup>	3.254
H(7)	C(16) <sup>13)</sup>	3.179	H(7)	C(19)	3.275
H(7)	C(20)	2.031	H(7)	C(23)	3.336
H(7)	C(25)	2.083	H(7)	H(4) <sup>10)</sup>	2.914



Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
H(7)	H(5)	2.329	H(7)	H(8)	2.375
H(7)	H(8) <sup>12)</sup>	3.287	H(7)	H(9) <sup>7)</sup>	3.421
H(7)	H(11) <sup>13)</sup>	3.011	H(7)	H(12) <sup>13)</sup>	2.663
H(7)	H(13) <sup>13)</sup>	3.385	H(7)	H(19) <sup>6)</sup>	3.038
H(8)	N(4) <sup>6)</sup>	3.212	H(8)	C(14) <sup>6)</sup>	3.285
H(8)	C(15)	3.287	H(8)	C(18) <sup>6)</sup>	3.156
H(8)	C(20)	3.307	H(8)	C(22) <sup>6)</sup>	3.041
H(8)	C(23)	2.060	H(8)	C(24)	2.078
H(8)	C(24) <sup>12)</sup>	3.458	H(8)	C(25) <sup>12)</sup>	3.480
H(8)	H(1) <sup>6)</sup>	3.024	H(8)	H(6)	2.401
H(8)	H(7)	2.375	H(8)	H(7) <sup>12)</sup>	3.287
H(8)	H(8) <sup>12)</sup>	3.332	H(8)	H(9) <sup>6)</sup>	2.817
H(8)	H(18) <sup>6)</sup>	3.067	H(8)	H(19) <sup>6)</sup>	2.549
H(9)	O(3) <sup>1)</sup>	2.686	H(9)	N(4)	2.528
H(9)	C(13)	3.364	H(9)	C(14)	2.040
H(9)	C(20) <sup>14)</sup>	3.074	H(9)	C(22)	2.092
H(9)	C(24) <sup>14)</sup>	3.277	H(9)	H(1)	2.419
H(9)	H(5) <sup>14)</sup>	3.100	H(9)	H(7) <sup>14)</sup>	3.421
H(9)	H(8) <sup>3)</sup>	2.817	H(9)	H(10)	1.551
H(9)	H(14) <sup>1)</sup>	3.065	H(9)	H(16) <sup>1)</sup>	3.555
H(9)	H(17)	2.806	H(9)	H(18)	2.264
H(9)	H(19)	2.538	H(10)	N(4)	3.064
H(10)	C(9) <sup>2)</sup>	3.175	H(10)	C(13)	2.926
H(10)	C(14)	2.029	H(10)	C(15) <sup>2)</sup>	3.596
H(10)	C(16)	3.392	H(10)	C(19) <sup>2)</sup>	3.015
H(10)	C(20) <sup>2)</sup>	3.420	H(10)	C(21) <sup>1)</sup>	3.593
H(10)	C(22)	2.090	H(10)	H(1)	3.327
H(10)	H(3) <sup>2)</sup>	2.814	H(10)	H(4) <sup>2)</sup>	2.902
H(10)	H(5) <sup>2)</sup>	3.573	H(10)	H(9)	1.551
H(10)	H(11)	3.433	H(10)	H(12)	3.172
H(10)	H(14) <sup>1)</sup>	2.983	H(10)	H(16) <sup>1)</sup>	3.328
H(10)	H(17)	2.255	H(10)	H(18)	2.550
H(10)	H(19)	2.797	H(11)	S(1) <sup>2)</sup>	3.260
H(11)	O(3) <sup>2)</sup>	2.611	H(11)	C(1)	3.066
H(11)	C(8)	3.595	H(11)	C(9) <sup>2)</sup>	3.483
H(11)	C(10) <sup>2)</sup>	2.810	H(11)	C(11) <sup>2)</sup>	2.906
H(11)	C(12) <sup>2)</sup>	3.450	H(11)	C(13)	2.064

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
H(11)	C(14)	3.054	H(11)	C(17) <sup>2j</sup>	3.321
H(11)	H(2)	3.302	H(11)	H(4) <sup>2j</sup>	3.318
H(11)	H(6) <sup>6j</sup>	3.579	H(11)	H(7) <sup>9j</sup>	3.011
H(11)	H(10)	3.433	H(11)	H(12)	1.551
H(11)	H(13)	1.551	H(11)	H(17)	3.479
H(12)	C(1)	3.360	H(12)	C(13)	2.072
H(12)	C(14)	2.791	H(12)	C(18)	3.108
H(12)	C(22)	2.811	H(12)	C(22) <sup>11j</sup>	3.214
H(12)	C(24) <sup>9j</sup>	3.592	H(12)	H(4) <sup>2j</sup>	3.233
H(12)	H(7) <sup>9j</sup>	2.663	H(12)	H(10)	3.172
H(12)	H(11)	1.551	H(12)	H(13)	1.551
H(12)	H(17)	2.313	H(12)	H(17) <sup>11j</sup>	3.281
H(12)	H(18) <sup>11j</sup>	3.063	H(12)	H(19)	2.771
H(12)	H(19) <sup>11j</sup>	2.780	H(13)	O(2) <sup>8j</sup>	3.493
H(13)	O(3) <sup>2j</sup>	3.352	H(13)	N(5) <sup>6j</sup>	3.426
H(13)	C(1)	2.753	H(13)	C(8)	2.986
H(13)	C(13)	2.072	H(13)	C(14)	3.340
H(13)	C(23) <sup>6j</sup>	2.970	H(13)	H(2)	2.546
H(13)	H(6) <sup>6j</sup>	2.423	H(13)	H(7) <sup>9j</sup>	3.385
H(13)	H(11)	1.551	H(13)	H(12)	1.551
H(13)	H(18) <sup>11j</sup>	3.255	H(14)	S(1)	3.094
H(14)	O(3)	3.282	H(14)	N(1)	2.006
H(14)	N(5)	2.553	H(14)	C(18) <sup>1j</sup>	3.466
H(14)	C(20) <sup>5j</sup>	3.415	H(14)	H(3) <sup>4j</sup>	2.970
H(14)	H(4) <sup>5j</sup>	3.557	H(14)	H(5) <sup>5j</sup>	2.734
H(14)	H(9) <sup>1j</sup>	3.065	H(14)	H(10) <sup>1j</sup>	2.983
H(14)	H(15)	1.551	H(14)	H(16)	1.551
H(15)	S(1)	3.457	H(15)	N(1)	2.007
H(15)	N(4) <sup>3j</sup>	3.418	H(15)	N(5)	2.689
H(15)	C(1) <sup>3j</sup>	2.634	H(15)	C(8) <sup>3j</sup>	2.916
H(15)	C(9) <sup>3j</sup>	3.291	H(15)	C(10) <sup>3j</sup>	3.217
H(15)	C(11) <sup>3j</sup>	3.438	H(15)	C(13) <sup>3j</sup>	3.171
H(15)	C(14) <sup>3j</sup>	3.597	H(15)	C(17) <sup>3j</sup>	2.815
H(15)	H(2) <sup>3j</sup>	3.383	H(15)	H(3) <sup>4j</sup>	3.201
H(15)	H(14)	1.551	H(15)	H(16)	1.551
H(16)	S(1)	2.688	H(16)	O(2)	2.561
H(16)	O(3)	3.303	H(16)	N(1)	2.009

Table 6. Distances beyond the asymmetric unit out to 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
H(16)	N(5)	3.208	H(16)	C(8) <sup>4j</sup>	3.048
H(16)	C(9) <sup>4j</sup>	2.956	H(16)	H(2) <sup>4j</sup>	2.512
H(16)	H(3) <sup>4j</sup>	2.294	H(16)	H(9) <sup>1j</sup>	3.555
H(16)	H(10) <sup>1j</sup>	3.328	H(16)	H(14)	1.551
H(16)	H(15)	1.551	H(17)	C(13)	3.318
H(17)	C(14)	2.946	H(17)	C(16)	3.094
H(17)	C(18)	2.099	H(17)	C(19) <sup>2j</sup>	3.396
H(17)	C(22) <sup>11j</sup>	3.571	H(17)	H(4) <sup>2j</sup>	2.791
H(17)	H(5) <sup>2j</sup>	3.354	H(17)	H(9)	2.806
H(17)	H(10)	2.255	H(17)	H(11)	3.479
H(17)	H(12)	2.313	H(17)	H(12) <sup>11j</sup>	3.281
H(17)	H(17) <sup>11j</sup>	3.397	H(17)	H(18)	1.551
H(17)	H(19)	1.551	H(17)	H(19) <sup>11j</sup>	2.903
H(18)	N(5) <sup>14j</sup>	3.456	H(18)	C(14)	3.310
H(18)	C(15) <sup>14j</sup>	2.963	H(18)	C(18)	2.107
H(18)	C(19) <sup>14j</sup>	3.131	H(18)	C(20) <sup>14j</sup>	3.286
H(18)	C(23) <sup>14j</sup>	3.008	H(18)	C(24) <sup>14j</sup>	3.306
H(18)	C(25) <sup>14j</sup>	3.144	H(18)	H(5) <sup>2j</sup>	3.593
H(18)	H(6) <sup>14j</sup>	3.489	H(18)	H(8) <sup>3j</sup>	3.067
H(18)	H(9)	2.264	H(18)	H(10)	2.550
H(18)	H(12) <sup>11j</sup>	3.063	H(18)	H(13) <sup>11j</sup>	3.255
H(18)	H(17)	1.551	H(18)	H(19)	1.551
H(19)	N(4)	3.517	H(19)	C(13)	3.084
H(19)	C(14)	2.544	H(19)	C(16)	3.372
H(19)	C(18)	2.088	H(19)	C(22) <sup>11j</sup>	3.470
H(19)	C(24) <sup>3j</sup>	3.484	H(19)	C(25) <sup>3j</sup>	3.243
H(19)	H(7) <sup>3j</sup>	3.038	H(19)	H(8) <sup>3j</sup>	2.549
H(19)	H(9)	2.538	H(19)	H(10)	2.797
H(19)	H(12)	2.771	H(19)	H(12) <sup>11j</sup>	2.780
H(19)	H(17)	1.551	H(19)	H(17) <sup>11j</sup>	2.903
H(19)	H(18)	1.551	H(19)	H(19) <sup>11j</sup>	3.182

Symmetry Operators:

- |                          |                            |
|--------------------------|----------------------------|
| (1) -X,-Y+1,-Z+1         | (2) -X,-Y,-Z+1             |
| (3) -X,Y+1/2,-Z+1/2+1    | (4) X,Y+1,Z                |
| (5) -X+1,Y+1/2,-Z+1/2+1  | (6) -X,Y+1/2-1,-Z+1/2+1    |
| (7) X+1,-Y+1/2,Z+1/2     | (8) X,Y-1,Z                |
| (9) X-1,-Y+1/2-1,Z+1/2-1 | (10) -X+1,Y+1/2-1,-Z+1/2+1 |
| (11) -X-1,-Y,-Z+1        | (12) -X+1,-Y,-Z+2          |
| (13) X+1,-Y+1/2-1,Z+1/2  | (14) X-1,-Y+1/2,Z+1/2-1    |

Table 7. Intramolecular and Intermolecular Hydrogen bonds

D	H	A	D...A	D-H	H...A	D-H...A
N(4)	H(1)	O(2)	3.088(5)	0.950	2.555	115.7
N(4)	H(1)	O(3)[3:0:1:1]	3.038(6)	0.950	2.172	150.9

Note) 1. The symmetry operations are applied to the acceptors.  
2. Estimated standard deviations (esd's) are shown in the parentheses.  
They are not calculated when all atoms have an esd=0.0.