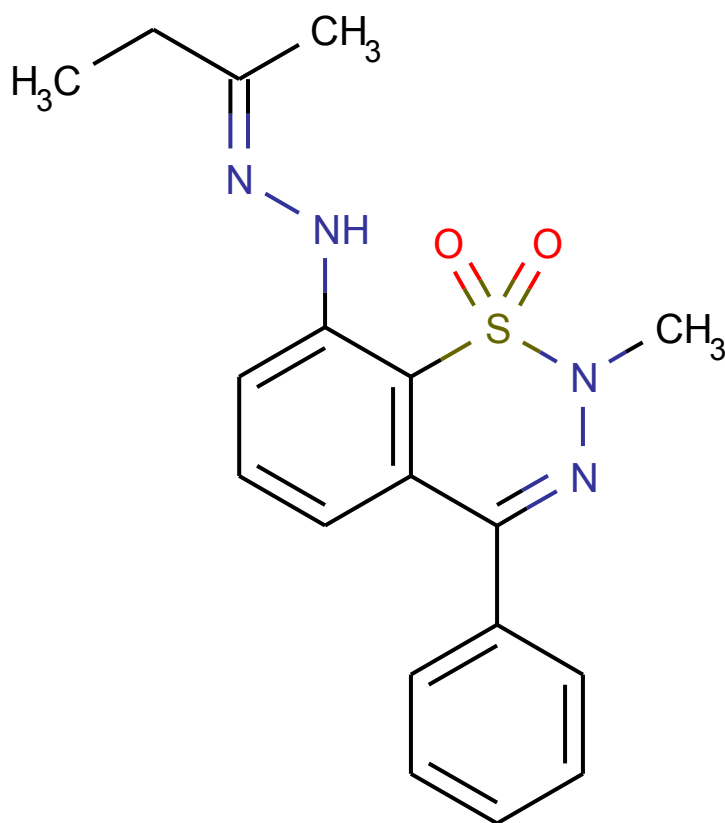


**144149**

**PGY0791\_1A**

Submitted by: Pusztai Gyongyver  
Operator: Dancso Andras

X-ray Structure Report



February 3, 2025

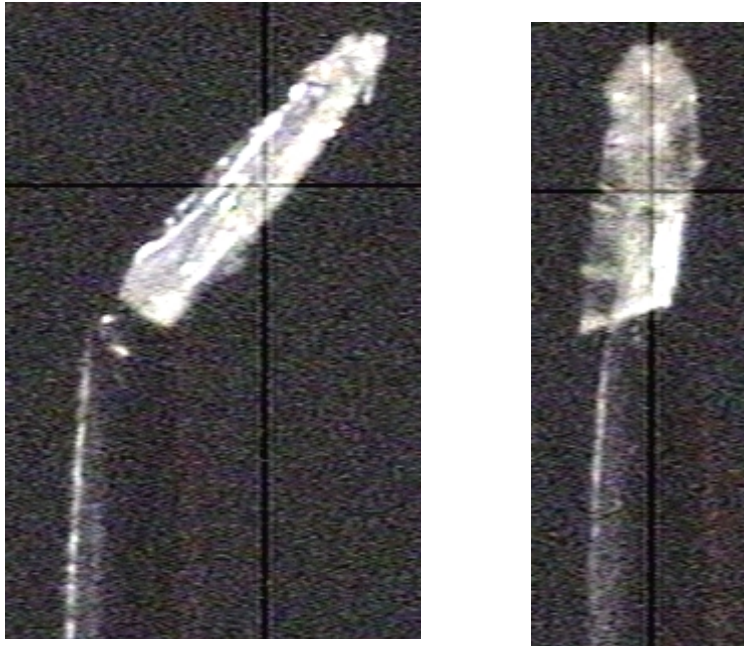


Fig. 1. The crystal

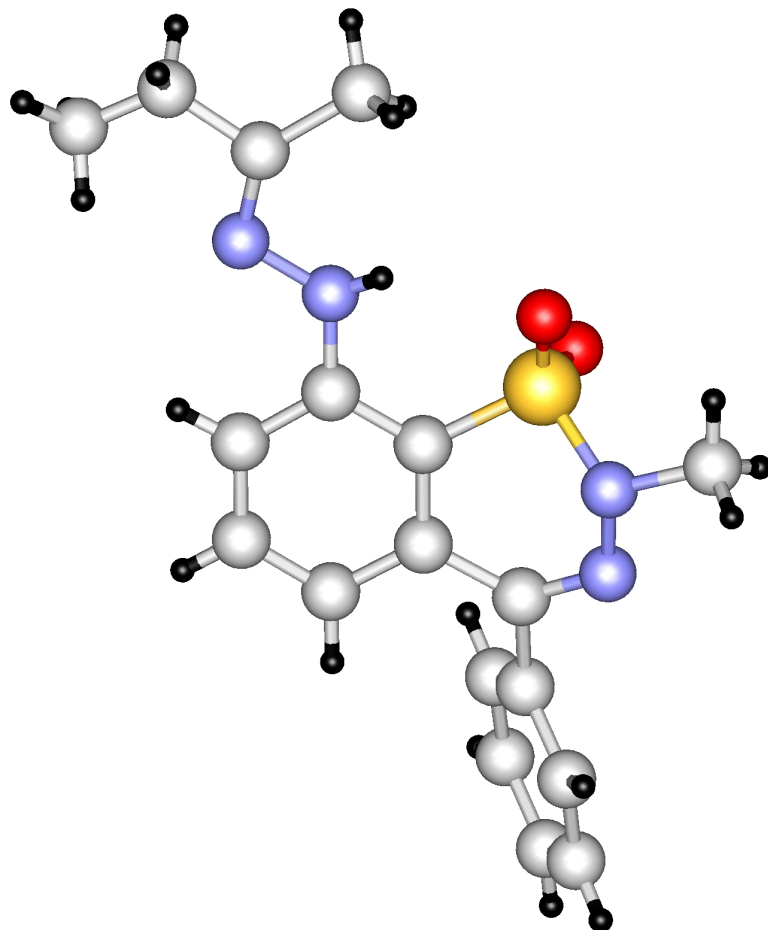


Fig. 2. The molecule (some hydrogens were generated by the software)

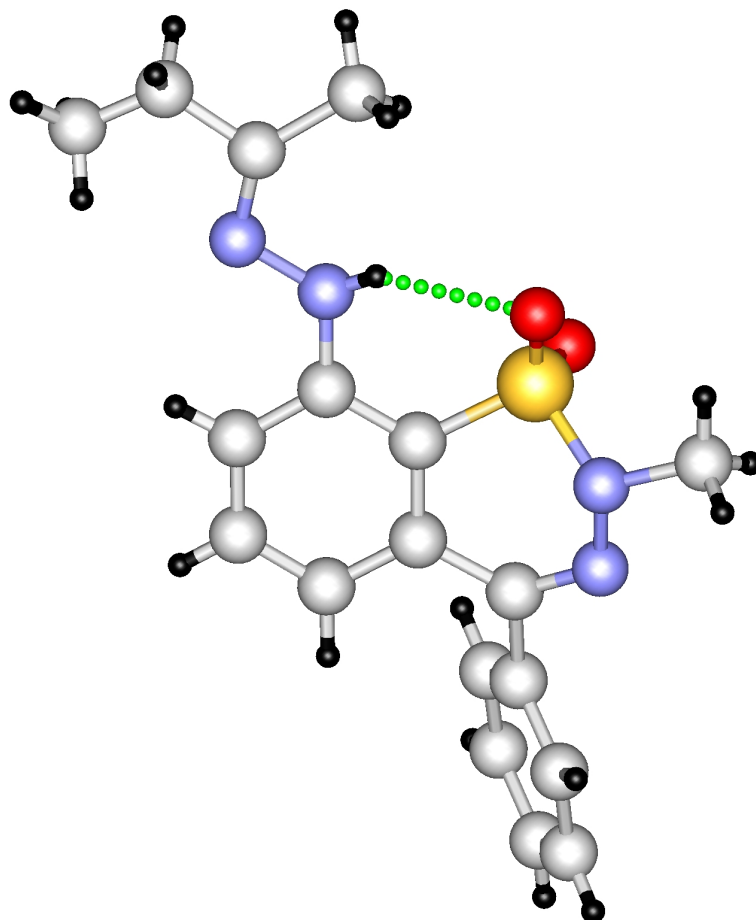


Fig. 3. Hydrogen bond

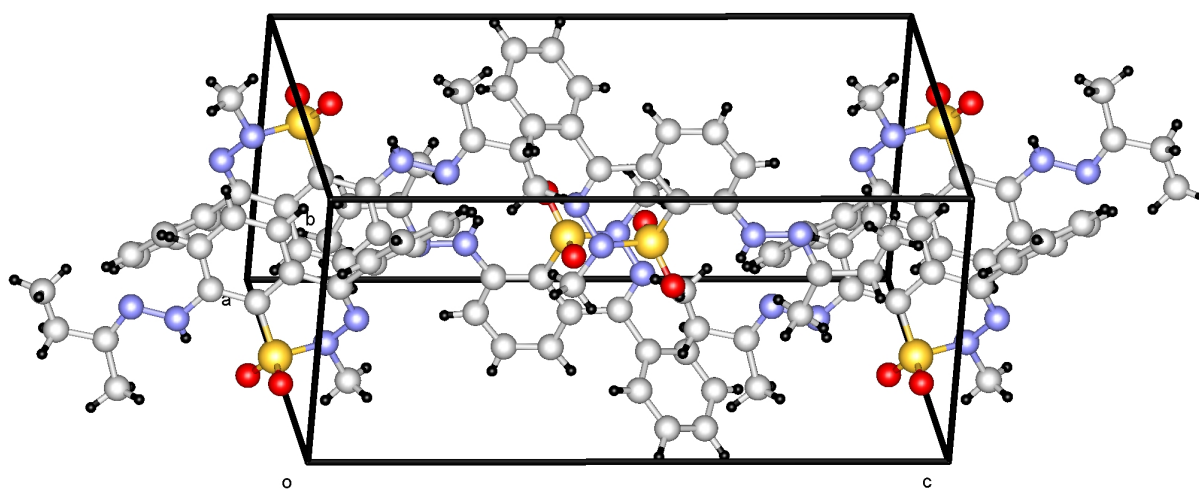


Fig. 4. Packing

## *Experimental*

### Data Collection

A colorless chunk crystal of  $C_{18}H_{20}N_4O_2S$  having approximate dimensions of 0.44 x 0.14 x 0.12 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 180 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:

$$\begin{aligned}a &= 11.2127(6) \text{ \AA} \\b &= 8.6727(4) \text{ \AA} \quad \beta = 90.6559(19)^\circ \\c &= 18.8928(9) \text{ \AA} \\V &= 1837.10(16) \text{ \AA}^3\end{aligned}$$

For  $Z = 4$  and F.W. = 356.44, the calculated density is 1.289 g/cm<sup>3</sup>. The systematic absences of:

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

uniquely determine the space group to be:

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

The data were collected at a temperature of  $20 \pm 1^\circ\text{C}$  to a maximum  $2\theta$  value of  $143.3^\circ$ . 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 60.0 [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 60.0 [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 60.0 [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 60.0 [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 60.0 [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 20280 reflections that were collected, 3536 were unique ( $R_{\text{int}} = 0.050$ ).

The linear absorption coefficient,  $\mu$ , for Cu-K $\alpha$  radiation is 17.205 cm<sup>-1</sup>. An empirical absorption correction was applied which resulted in transmission factors ranging from 0.625 to 0.818. 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. Some hydrogen atoms were refined isotropically and the rest were refined using the riding model. The final cycle of full-matrix least-squares refinement<sup>3</sup> on F was based on 11101 observed reflections ( $I > 2.00\sigma(I)$ ) and 273 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o| = 0.0623$$

$$R_w = [ \Sigma w (|F_o| - |F_c|)^2 / \Sigma w F_o^2 ]^{1/2} = 0.0585$$

The standard deviation of an observation of unit weight<sup>4</sup> was 3.08. 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 4.20 and -2.55 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  $F_{\text{calc}}$ <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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(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       | $\text{C}_{18}\text{H}_{20}\text{N}_4\text{O}_2\text{S}$  |
| Formula Weight          | 356.44  |
| Crystal Color, Habit    | colorless, chunk  |
| Crystal Dimensions      | 0.44 X 0.14 X 0.12 mm   |
| Crystal System          | monoclinic  |
| Lattice Type            | Primitive   |
| Indexing Images         | 4 oscillations @ 180.0 seconds  |
| Detector Position       | 127.40 mm   |
| Pixel Size              | 0.100 mm  |
| Lattice Parameters      | $a = 11.2127(6) \text{ \AA}$<br>$b = 8.6727(4) \text{ \AA}$<br>$c = 18.8928(9) \text{ \AA}$<br>$\beta = 90.6559(19)^\circ$<br>$V = 1837.10(16) \text{ \AA}^3$ |
| Space Group             | $P2_1/n$ (#14)  |
| Z value                 | 4   |
| D <sub>calc</sub>       | 1.289 g/cm <sup>3</sup>   |
| F <sub>000</sub>        | 752.00  |
| $\mu(\text{CuK}\alpha)$ | 17.205 cm <sup>-1</sup>   |

## B. Intensity Measurements

|   |   |
|---|---|
| Diffractometer  | Rigaku RAXIS-RAPID  |
| Radiation   | CuK $\alpha$ ( $\lambda$ = 1.54187 Å)<br>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 $^{\circ}$   |
| Exposure Rate   | 60.0 sec./ $^{\circ}$   |
| $\omega$ oscillation Range ( $\chi$ =54.0, $\phi$ =0.0)   | 20.0 - 200.0 $^{\circ}$   |
| Exposure Rate   | 60.0 sec./ $^{\circ}$   |
| $\omega$ oscillation Range ( $\chi$ =54.0, $\phi$ =90.0)  | 20.0 - 200.0 $^{\circ}$   |
| Exposure Rate   | 60.0 sec./ $^{\circ}$   |
| $\omega$ oscillation Range ( $\chi$ =54.0, $\phi$ =180.0) | 20.0 - 200.0 $^{\circ}$   |
| Exposure Rate   | 60.0 sec./ $^{\circ}$   |
| $\omega$ oscillation Range ( $\chi$ =54.0, $\phi$ =270.0) | 20.0 - 200.0 $^{\circ}$   |
| Exposure Rate   | 60.0 sec./ $^{\circ}$   |
| Detector Position   | 127.40 mm   |
| Pixel Size  | 0.100 mm  |
| $2\theta_{\text{max}}$                                    | 143.3 $^{\circ}$  |
| No. of Reflections Measured                               | Total: 20280<br>Unique: 3536 ( $R_{\text{int}}$ = 0.050)              |
| Corrections   | Lorentz-polarization<br>Absorption<br>(trans. factors: 0.625 - 0.818) |

### 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            | 143.3 $^{\circ}$               |
| Anomalous Dispersion                     | All non-hydrogen atoms         |
| No. Observations ( $I > 2.00\sigma(I)$ ) | 11101                          |
| No. Variables                            | 273                            |
| Reflection/Parameter Ratio               | 40.66                          |
| Residuals: R ( $I > 2.00\sigma(I)$ )     | 0.0623                         |
| Residuals: Rw ( $I > 2.00\sigma(I)$ )    | 0.0585                         |
| Goodness of Fit Indicator                | 3.079                          |
| Max Shift/Error in Final Cycle           | 0.000                          |
| Maximum peak in Final Diff. Map          | 4.20 e $^{-}/\text{\AA}^3$     |
| Minimum peak in Final Diff. Map          | -2.55 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)  | 0.29553(9)  | 0.19649(11) | 0.96997(4)  | 6.21(2)         |
| O(2)  | 0.16839(18) | 0.1817(2)   | 0.96694(10) | 7.92(6)         |
| O(3)  | 0.36482(19) | 0.0766(2)   | 0.93825(10) | 8.09(6)         |
| N(1)  | 0.3820(2)   | 0.2817(4)   | 0.82149(19) | 8.77(11)        |
| N(2)  | 0.4122(2)   | 0.3053(4)   | 0.75221(14) | 8.84(10)        |
| N(4)  | 0.34403(19) | 0.2149(3)   | 1.05291(12) | 5.75(7)         |
| N(5)  | 0.2982(2)   | 0.3378(3)   | 1.09190(11) | 5.51(7)         |
| C(1)  | 0.3207(2)   | 0.5000(3)   | 0.98683(16) | 4.77(8)         |
| C(2)  | 0.2387(2)   | 0.5935(3)   | 1.10455(16) | 4.77(9)         |
| C(8)  | 0.3358(2)   | 0.3767(3)   | 0.93909(17) | 5.05(8)         |
| C(10) | 0.2875(2)   | 0.4678(3)   | 1.06008(16) | 4.83(8)         |
| C(11) | 0.1365(3)   | 0.6706(4)   | 1.0837(2)   | 6.08(11)        |
| C(12) | 0.2873(3)   | 0.6288(4)   | 1.16982(19) | 6.25(11)        |
| C(14) | 0.0841(3)   | 0.7792(4)   | 1.1267(2)   | 6.95(12)        |
| C(15) | 0.3420(2)   | 0.6482(4)   | 0.96394(18) | 5.97(10)        |
| C(16) | 0.1345(4)   | 0.8136(4)   | 1.1910(2)   | 7.16(12)        |
| C(17) | 0.3771(3)   | 0.6698(4)   | 0.8951(2)   | 7.15(12)        |
| C(18) | 0.3705(2)   | 0.4015(4)   | 0.8686(2)   | 6.28(11)        |
| C(19) | 0.4555(4)   | 0.1896(6)   | 0.6433(3)   | 15.0(2)         |
| C(20) | 0.3905(3)   | 0.5510(5)   | 0.8480(2)   | 7.16(12)        |
| C(21) | 0.2358(4)   | 0.7398(4)   | 1.2129(2)   | 7.45(13)        |
| C(22) | 0.3472(2)   | 0.0696(3)   | 1.09288(14) | 7.92(10)        |
| C(23) | 0.4311(3)   | 0.1689(7)   | 0.71890(19) | 12.20(18)       |
| C(24) | 0.4077(3)   | -0.0002(4)  | 0.74086(18) | 12.72(15)       |
| C(25) | 0.4658(4)   | 0.3279(5)   | 0.6181(2)   | 15.7(2)         |
| H(1)  | 0.3342(18)  | 0.732(2)    | 0.9983(10)  | 4.8(6)          |
| H(2)  | 0.3836(16)  | 0.769(2)    | 0.8808(9)   | 2.7(5)          |
| H(3)  | 0.409(2)    | 0.574(3)    | 0.8021(13)  | 7.4(9)          |
| H(4)  | 0.392(2)    | 0.201(2)    | 0.8393(11)  | 2.4(6)          |
| H(5)  | 0.273(2)    | 0.762(2)    | 1.2540(12)  | 6.4(8)          |
| H(6)  | 0.098(2)    | 0.892(2)    | 1.2209(13)  | 7.9(9)          |
| H(7)  | 0.011(2)    | 0.836(3)    | 1.1084(13)  | 8.3(9)          |
| H(8)  | 0.1004(19)  | 0.646(2)    | 1.0402(11)  | 5.5(7)          |
| H(9)  | 0.3585(18)  | 0.581(2)    | 1.1822(10)  | 4.0(7)          |
| H(10) | 0.5301      | 0.1436      | 0.6326      | 17.99           |
| H(11) | 0.3939      | 0.1389      | 0.6174      | 17.99           |
| H(12) | 0.2731      | 0.0562      | 1.1160      | 9.56            |

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

| atom  | x      | y       | z      | $B_{\text{eq}}$ |
|-------|--------|---------|--------|-----------------|
| H(13) | 0.4096 | 0.0743  | 1.1272 | 9.55            |
| H(14) | 0.3605 | -0.0148 | 1.0619 | 9.54            |
| H(15) | 0.4715 | -0.0407 | 0.7687 | 15.30           |
| H(16) | 0.3940 | -0.0650 | 0.7010 | 15.23           |
| H(17) | 0.3377 | 0.0045  | 0.7686 | 15.24           |
| H(18) | 0.3881 | 0.3597  | 0.6040 | 18.89           |
| H(19) | 0.5180 | 0.3351  | 0.5790 | 18.88           |
| H(20) | 0.4941 | 0.3925  | 0.6553 | 18.89           |

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

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)  | 0.0914(7)       | 0.0714(6)       | 0.0729(5)       | 0.0010(6)       | -0.0015(4)      | -0.0082(5)      |
| O(2)  | 0.0787(15)      | 0.1065(17)      | 0.1153(17)      | -0.0202(14)     | -0.0143(12)     | -0.0079(13)     |
| O(3)  | 0.144(2)        | 0.0783(15)      | 0.0854(15)      | 0.0223(14)      | 0.0077(13)      | -0.0176(12)     |
| N(1)  | 0.154(2)        | 0.101(3)        | 0.079(2)        | 0.049(2)        | 0.006(2)        | -0.004(2)       |
| N(2)  | 0.103(2)        | 0.188(3)        | 0.0453(18)      | 0.014(2)        | 0.0116(16)      | -0.003(2)       |
| N(4)  | 0.0869(18)      | 0.0604(18)      | 0.0712(17)      | 0.0008(16)      | -0.0021(14)     | 0.0031(16)      |
| N(5)  | 0.0866(18)      | 0.0598(19)      | 0.0630(16)      | 0.0039(16)      | -0.0003(14)     | -0.0022(15)     |
| C(1)  | 0.059(2)        | 0.059(2)        | 0.063(2)        | -0.0070(18)     | 0.0051(17)      | 0.0085(19)      |
| C(2)  | 0.069(2)        | 0.060(2)        | 0.053(2)        | -0.0115(19)     | 0.0030(18)      | 0.0039(17)      |
| C(8)  | 0.063(2)        | 0.069(2)        | 0.060(2)        | 0.0022(17)      | 0.0048(16)      | -0.0004(18)     |
| C(10) | 0.067(2)        | 0.053(2)        | 0.063(2)        | -0.0045(18)     | -0.0036(17)     | 0.0001(18)      |
| C(11) | 0.079(2)        | 0.085(3)        | 0.067(2)        | 0.000(2)        | -0.006(2)       | -0.012(2)       |
| C(12) | 0.090(3)        | 0.086(3)        | 0.061(2)        | 0.007(2)        | -0.006(2)       | 0.001(2)        |
| C(14) | 0.087(3)        | 0.086(3)        | 0.091(2)        | 0.008(2)        | -0.002(2)       | -0.009(2)       |
| C(15) | 0.089(2)        | 0.077(3)        | 0.061(2)        | -0.016(2)       | 0.0173(19)      | -0.007(2)       |
| C(16) | 0.101(3)        | 0.081(3)        | 0.091(3)        | -0.005(2)       | 0.027(2)        | -0.021(2)       |
| C(17) | 0.105(2)        | 0.066(3)        | 0.101(3)        | -0.010(2)       | 0.025(2)        | 0.022(2)        |
| C(18) | 0.077(2)        | 0.083(3)        | 0.078(2)        | 0.009(2)        | 0.014(2)        | 0.008(2)        |
| C(19) | 0.119(3)        | 0.200(6)        | 0.251(7)        | 0.005(4)        | 0.026(4)        | -0.037(5)       |
| C(20) | 0.097(2)        | 0.106(3)        | 0.069(2)        | 0.003(2)        | 0.027(2)        | 0.003(3)        |
| C(21) | 0.125(3)        | 0.101(3)        | 0.057(2)        | -0.015(2)       | 0.002(2)        | -0.012(2)       |
| C(22) | 0.129(3)        | 0.071(2)        | 0.101(2)        | 0.013(2)        | 0.001(2)        | 0.010(2)        |
| C(23) | 0.157(3)        | 0.280(7)        | 0.028(2)        | 0.030(4)        | 0.024(2)        | -0.054(3)       |
| C(24) | 0.278(5)        | 0.114(3)        | 0.092(3)        | 0.101(3)        | 0.012(3)        | 0.019(2)        |
| C(25) | 0.284(6)        | 0.185(5)        | 0.128(4)        | -0.093(5)       | 0.075(3)        | -0.044(4)       |

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)  | 1.432(2) | S(1)  | O(3)  | 1.433(2) |
| S(1)  | N(4)  | 1.660(2) | S(1)  | C(8)  | 1.730(3) |
| N(1)  | N(2)  | 1.371(4) | N(1)  | C(18) | 1.375(5) |
| N(1)  | H(4)  | 0.78(2)  | N(2)  | C(23) | 1.358(7) |
| N(4)  | N(5)  | 1.397(3) | N(4)  | C(22) | 1.470(3) |
| N(5)  | C(10) | 1.282(4) | C(1)  | C(8)  | 1.410(4) |
| C(1)  | C(10) | 1.464(4) | C(1)  | C(15) | 1.378(5) |
| C(2)  | C(10) | 1.485(4) | C(2)  | C(11) | 1.381(4) |
| C(2)  | C(12) | 1.377(4) | C(8)  | C(18) | 1.408(4) |
| C(11) | C(14) | 1.378(5) | C(11) | H(8)  | 0.94(2)  |
| C(12) | C(21) | 1.390(5) | C(12) | H(9)  | 0.93(2)  |
| C(14) | C(16) | 1.368(5) | C(14) | H(7)  | 1.01(2)  |
| C(15) | C(17) | 1.376(5) | C(15) | H(1)  | 0.98(2)  |
| C(16) | C(21) | 1.364(6) | C(16) | H(6)  | 0.98(2)  |
| C(17) | C(20) | 1.370(6) | C(17) | H(2)  | 0.90(2)  |
| C(18) | C(20) | 1.373(6) | C(19) | C(23) | 1.469(7) |
| C(19) | C(25) | 1.296(7) | C(19) | H(10) | 0.950    |
| C(19) | H(11) | 0.950    | C(20) | H(3)  | 0.92(2)  |
| C(21) | H(5)  | 0.90(2)  | C(22) | H(12) | 0.950    |
| C(22) | H(13) | 0.950    | C(22) | H(14) | 0.950    |
| C(23) | C(24) | 1.547(7) | C(24) | H(15) | 0.950    |
| C(24) | H(16) | 0.950    | C(24) | H(17) | 0.950    |
| C(25) | H(18) | 0.950    | C(25) | H(19) | 0.950    |
| C(25) | H(20) | 0.950    |       |       |          |

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

| atom  | atom  | atom  | angle      | atom  | atom  | atom  | angle      |
|-------|-------|-------|------------|-------|-------|-------|------------|
| O(2)  | S(1)  | O(3)  | 117.56(13) | O(2)  | S(1)  | N(4)  | 111.19(11) |
| O(2)  | S(1)  | C(8)  | 109.30(13) | O(3)  | S(1)  | N(4)  | 106.93(12) |
| O(3)  | S(1)  | C(8)  | 111.70(13) | N(4)  | S(1)  | C(8)  | 98.48(14)  |
| N(2)  | N(1)  | C(18) | 122.1(3)   | N(2)  | N(1)  | H(4)  | 120.7(16)  |
| C(18) | N(1)  | H(4)  | 114.1(16)  | N(1)  | N(2)  | C(23) | 110.7(3)   |
| S(1)  | N(4)  | N(5)  | 116.90(18) | S(1)  | N(4)  | C(22) | 114.08(19) |
| N(5)  | N(4)  | C(22) | 113.0(2)   | N(4)  | N(5)  | C(10) | 117.1(2)   |
| C(8)  | C(1)  | C(10) | 119.6(2)   | C(8)  | C(1)  | C(15) | 118.9(2)   |
| C(10) | C(1)  | C(15) | 121.4(2)   | C(10) | C(2)  | C(11) | 120.3(2)   |
| C(10) | C(2)  | C(12) | 121.7(2)   | C(11) | C(2)  | C(12) | 117.8(3)   |
| S(1)  | C(8)  | C(1)  | 115.8(2)   | S(1)  | C(8)  | C(18) | 122.2(2)   |
| C(1)  | C(8)  | C(18) | 121.7(3)   | N(5)  | C(10) | C(1)  | 126.0(2)   |
| N(5)  | C(10) | C(2)  | 114.4(2)   | C(1)  | C(10) | C(2)  | 119.6(2)   |
| C(2)  | C(11) | C(14) | 121.4(3)   | C(2)  | C(11) | H(8)  | 119.4(14)  |
| C(14) | C(11) | H(8)  | 119.2(14)  | C(2)  | C(12) | C(21) | 121.0(3)   |
| C(2)  | C(12) | H(9)  | 117.3(13)  | C(21) | C(12) | H(9)  | 121.5(13)  |
| C(11) | C(14) | C(16) | 119.9(3)   | C(11) | C(14) | H(7)  | 118.7(14)  |
| C(16) | C(14) | H(7)  | 121.4(14)  | C(1)  | C(15) | C(17) | 118.4(3)   |
| C(1)  | C(15) | H(1)  | 117.9(12)  | C(17) | C(15) | H(1)  | 123.6(12)  |
| C(14) | C(16) | C(21) | 120.1(3)   | C(14) | C(16) | H(6)  | 119.7(15)  |
| C(21) | C(16) | H(6)  | 120.3(15)  | C(15) | C(17) | C(20) | 123.1(3)   |
| C(15) | C(17) | H(2)  | 116.0(12)  | C(20) | C(17) | H(2)  | 120.7(12)  |
| N(1)  | C(18) | C(8)  | 121.7(3)   | N(1)  | C(18) | C(20) | 120.9(3)   |
| C(8)  | C(18) | C(20) | 117.4(3)   | C(23) | C(19) | C(25) | 119.3(5)   |
| C(23) | C(19) | H(10) | 109.3      | C(23) | C(19) | H(11) | 107.6      |
| C(25) | C(19) | H(10) | 103.2      | C(25) | C(19) | H(11) | 107.9      |
| H(10) | C(19) | H(11) | 109.5      | C(17) | C(20) | C(18) | 120.5(3)   |
| C(17) | C(20) | H(3)  | 118.5(16)  | C(18) | C(20) | H(3)  | 120.9(16)  |
| C(12) | C(21) | C(16) | 119.8(3)   | C(12) | C(21) | H(5)  | 117.3(15)  |
| C(16) | C(21) | H(5)  | 122.8(15)  | N(4)  | C(22) | H(12) | 109.0      |
| N(4)  | C(22) | H(13) | 109.1      | N(4)  | C(22) | H(14) | 110.3      |
| H(12) | C(22) | H(13) | 109.5      | H(12) | C(22) | H(14) | 109.5      |
| H(13) | C(22) | H(14) | 109.5      | N(2)  | C(23) | C(19) | 112.1(4)   |
| N(2)  | C(23) | C(24) | 132.4(3)   | C(19) | C(23) | C(24) | 114.3(4)   |
| C(23) | C(24) | H(15) | 111.7      | C(23) | C(24) | H(16) | 112.0      |
| C(23) | C(24) | H(17) | 104.6      | H(15) | C(24) | H(16) | 109.5      |
| H(15) | C(24) | H(17) | 109.5      | H(16) | C(24) | H(17) | 109.5      |

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

| atom  | atom  | atom  | angle | atom  | atom  | atom  | angle |
|-------|-------|-------|-------|-------|-------|-------|-------|
| C(19) | C(25) | H(18) | 106.7 | C(19) | C(25) | H(19) | 113.9 |
| C(19) | C(25) | H(20) | 107.8 | H(18) | C(25) | H(19) | 109.5 |
| H(18) | C(25) | H(20) | 109.5 | H(19) | C(25) | H(20) | 109.5 |



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

| atom1 | atom2 | atom3 | atom4 | angle      | atom1 | atom2 | atom3 | atom4 | angle       |
|-------|-------|-------|-------|------------|-------|-------|-------|-------|-------------|
| O(2)  | S(1)  | N(4)  | N(5)  | -57.5(2)   | O(2)  | S(1)  | N(4)  | C(22) | 77.4(2)     |
| O(2)  | S(1)  | C(8)  | C(1)  | 77.9(2)    | O(2)  | S(1)  | C(8)  | C(18) | -96.1(2)    |
| O(3)  | S(1)  | N(4)  | N(5)  | 172.95(19) | O(3)  | S(1)  | N(4)  | C(22) | -52.1(2)    |
| O(3)  | S(1)  | C(8)  | C(1)  | -150.2(2)  | O(3)  | S(1)  | C(8)  | C(18) | 35.7(2)     |
| N(4)  | S(1)  | C(8)  | C(1)  | -38.1(2)   | N(4)  | S(1)  | C(8)  | C(18) | 147.8(2)    |
| C(8)  | S(1)  | N(4)  | N(5)  | 57.1(2)    | C(8)  | S(1)  | N(4)  | C(22) | -168.00(19) |
| N(2)  | N(1)  | C(18) | C(8)  | 178.0(2)   | N(2)  | N(1)  | C(18) | C(20) | -0.8(5)     |
| C(18) | N(1)  | N(2)  | C(23) | 173.0(3)   | N(1)  | N(2)  | C(23) | C(19) | 176.0(3)    |
| N(1)  | N(2)  | C(23) | C(24) | 10.1(5)    | S(1)  | N(4)  | N(5)  | C(10) | -41.8(3)    |
| C(22) | N(4)  | N(5)  | C(10) | -177.2(2)  | N(4)  | N(5)  | C(10) | C(1)  | -0.9(4)     |
| N(4)  | N(5)  | C(10) | C(2)  | -179.8(2)  | C(8)  | C(1)  | C(10) | N(5)  | 18.4(4)     |
| C(8)  | C(1)  | C(10) | C(2)  | -162.8(2)  | C(10) | C(1)  | C(8)  | S(1)  | 7.5(3)      |
| C(10) | C(1)  | C(8)  | C(18) | -178.4(2)  | C(8)  | C(1)  | C(15) | C(17) | 0.1(3)      |
| C(15) | C(1)  | C(8)  | S(1)  | -175.0(2)  | C(15) | C(1)  | C(8)  | C(18) | -0.9(4)     |
| C(10) | C(1)  | C(15) | C(17) | 177.6(2)   | C(15) | C(1)  | C(10) | N(5)  | -159.1(2)   |
| C(15) | C(1)  | C(10) | C(2)  | 19.7(4)    | C(10) | C(2)  | C(11) | C(14) | 174.8(3)    |
| C(11) | C(2)  | C(10) | N(5)  | -122.6(3)  | C(11) | C(2)  | C(10) | C(1)  | 58.5(4)     |
| C(10) | C(2)  | C(12) | C(21) | -175.6(3)  | C(12) | C(2)  | C(10) | N(5)  | 52.2(4)     |
| C(12) | C(2)  | C(10) | C(1)  | -126.8(3)  | C(11) | C(2)  | C(12) | C(21) | -0.8(5)     |
| C(12) | C(2)  | C(11) | C(14) | -0.1(4)    | S(1)  | C(8)  | C(18) | N(1)  | -4.4(4)     |
| S(1)  | C(8)  | C(18) | C(20) | 174.4(2)   | C(1)  | C(8)  | C(18) | N(1)  | -178.1(2)   |
| C(1)  | C(8)  | C(18) | C(20) | 0.7(4)     | C(2)  | C(11) | C(14) | C(16) | 0.8(5)      |
| C(2)  | C(12) | C(21) | C(16) | 1.1(6)     | C(11) | C(14) | C(16) | C(21) | -0.5(6)     |
| C(1)  | C(15) | C(17) | C(20) | 0.8(5)     | C(14) | C(16) | C(21) | C(12) | -0.4(6)     |
| C(15) | C(17) | C(20) | C(18) | -1.0(5)    | N(1)  | C(18) | C(20) | C(17) | 179.1(3)    |
| C(8)  | C(18) | C(20) | C(17) | 0.2(4)     | C(25) | C(19) | C(23) | N(2)  | 5.3(6)      |
| C(25) | C(19) | C(23) | C(24) | 173.9(4)   |       |       |       |       |             |

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  |
|-------|----------------------|-----------|-------|----------------------|-----------|
| O(2)  | C(14) <sup>11</sup>  | 3.338(4)  | O(2)  | H(7) <sup>11</sup>   | 2.45(2)   |
| O(2)  | H(8) <sup>11</sup>   | 3.36(2)   | O(2)  | H(18) <sup>21</sup>  | 3.159     |
| O(2)  | H(19) <sup>31</sup>  | 2.725     | O(3)  | C(22) <sup>41</sup>  | 3.525(3)  |
| O(3)  | H(1) <sup>51</sup>   | 3.21(2)   | O(3)  | H(2) <sup>51</sup>   | 2.89(2)   |
| O(3)  | H(13) <sup>41</sup>  | 3.116     | O(3)  | H(14) <sup>41</sup>  | 3.126     |
| O(3)  | H(18) <sup>21</sup>  | 3.487     | N(1)  | H(9) <sup>61</sup>   | 3.14(2)   |
| N(1)  | H(16) <sup>71</sup>  | 3.390     | N(1)  | H(17) <sup>71</sup>  | 3.549     |
| N(2)  | H(5) <sup>61</sup>   | 3.58(2)   | N(2)  | H(6) <sup>81</sup>   | 3.41(2)   |
| N(2)  | H(9) <sup>61</sup>   | 3.01(2)   | N(2)  | H(17) <sup>71</sup>  | 3.311     |
| N(4)  | C(17) <sup>61</sup>  | 3.416(4)  | N(4)  | H(2) <sup>61</sup>   | 3.290(18) |
| N(5)  | H(5) <sup>91</sup>   | 3.10(2)   | N(5)  | H(10) <sup>31</sup>  | 3.115     |
| N(5)  | H(19) <sup>31</sup>  | 3.487     | C(1)  | H(11) <sup>71</sup>  | 3.318     |
| C(2)  | H(10) <sup>31</sup>  | 3.164     | C(8)  | H(11) <sup>71</sup>  | 3.588     |
| C(10) | H(10) <sup>31</sup>  | 3.352     | C(11) | H(10) <sup>31</sup>  | 3.119     |
| C(12) | H(5) <sup>91</sup>   | 3.56(2)   | C(12) | H(6) <sup>91</sup>   | 3.17(2)   |
| C(14) | O(2) <sup>11</sup>   | 3.338(4)  | C(14) | H(12) <sup>101</sup> | 3.211     |
| C(14) | H(16) <sup>31</sup>  | 3.169     | C(14) | H(19) <sup>111</sup> | 3.541     |
| C(14) | H(20) <sup>111</sup> | 3.071     | C(15) | H(11) <sup>71</sup>  | 3.045     |
| C(15) | H(14) <sup>101</sup> | 3.464     | C(15) | H(18) <sup>71</sup>  | 3.405     |
| C(16) | H(3) <sup>111</sup>  | 3.45(2)   | C(16) | H(9) <sup>121</sup>  | 3.34(2)   |
| C(16) | H(12) <sup>101</sup> | 2.983     | C(16) | H(15) <sup>31</sup>  | 3.340     |
| C(16) | H(16) <sup>31</sup>  | 3.460     | C(16) | H(20) <sup>111</sup> | 3.067     |
| C(17) | N(4) <sup>61</sup>   | 3.416(4)  | C(17) | H(11) <sup>71</sup>  | 3.057     |
| C(17) | H(13) <sup>61</sup>  | 3.292     | C(17) | H(18) <sup>71</sup>  | 3.399     |
| C(18) | H(9) <sup>61</sup>   | 3.20(2)   | C(18) | H(16) <sup>71</sup>  | 3.243     |
| C(18) | H(17) <sup>71</sup>  | 3.581     | C(19) | H(8) <sup>21</sup>   | 3.53(2)   |
| C(20) | H(6) <sup>81</sup>   | 3.40(2)   | C(20) | H(9) <sup>61</sup>   | 3.10(2)   |
| C(20) | H(11) <sup>71</sup>  | 3.349     | C(20) | H(16) <sup>71</sup>  | 3.460     |
| C(20) | H(17) <sup>71</sup>  | 3.381     | C(21) | H(12) <sup>101</sup> | 3.328     |
| C(21) | H(15) <sup>31</sup>  | 3.598     | C(22) | O(3) <sup>41</sup>   | 3.525(3)  |
| C(22) | H(1) <sup>51</sup>   | 3.43(2)   | C(22) | H(2) <sup>61</sup>   | 3.361(19) |
| C(22) | H(15) <sup>41</sup>  | 3.304     | C(23) | H(5) <sup>61</sup>   | 3.40(2)   |
| C(24) | H(2) <sup>51</sup>   | 3.332(19) | C(24) | H(13) <sup>41</sup>  | 3.272     |
| C(25) | H(6) <sup>81</sup>   | 3.43(2)   | C(25) | H(7) <sup>81</sup>   | 2.96(2)   |
| C(25) | H(8) <sup>21</sup>   | 3.45(2)   | C(25) | H(12) <sup>131</sup> | 3.590     |
| H(1)  | O(3) <sup>101</sup>  | 3.21(2)   | H(1)  | C(22) <sup>101</sup> | 3.43(2)   |
| H(1)  | H(11) <sup>71</sup>  | 3.441     | H(1)  | H(14) <sup>101</sup> | 2.517     |

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

| atom  | atom                 | distance  | atom  | atom                 | distance  |
|-------|----------------------|-----------|-------|----------------------|-----------|
| H(1)  | H(18) <sup>7j</sup>  | 3.325     | H(2)  | O(3) <sup>10j</sup>  | 2.89(2)   |
| H(2)  | N(4) <sup>6j</sup>   | 3.290(18) | H(2)  | C(22) <sup>6j</sup>  | 3.361(19) |
| H(2)  | C(24) <sup>10j</sup> | 3.332(19) | H(2)  | H(11) <sup>7j</sup>  | 3.309     |
| H(2)  | H(13) <sup>6j</sup>  | 2.695     | H(2)  | H(15) <sup>10j</sup> | 2.871     |
| H(2)  | H(17) <sup>10j</sup> | 2.987     | H(2)  | H(18) <sup>7j</sup>  | 3.164     |
| H(3)  | C(16) <sup>8j</sup>  | 3.45(2)   | H(3)  | H(6) <sup>8j</sup>   | 2.65(3)   |
| H(3)  | H(9) <sup>6j</sup>   | 2.95(3)   | H(3)  | H(15) <sup>10j</sup> | 3.473     |
| H(3)  | H(17) <sup>7j</sup>  | 3.115     | H(4)  | H(9) <sup>6j</sup>   | 3.41(3)   |
| H(4)  | H(13) <sup>4j</sup>  | 3.323     | H(5)  | N(2) <sup>6j</sup>   | 3.58(2)   |
| H(5)  | N(5) <sup>12j</sup>  | 3.10(2)   | H(5)  | C(12) <sup>12j</sup> | 3.56(2)   |
| H(5)  | C(23) <sup>6j</sup>  | 3.40(2)   | H(5)  | H(6) <sup>9j</sup>   | 3.54(3)   |
| H(5)  | H(9) <sup>12j</sup>  | 3.37(3)   | H(5)  | H(10) <sup>6j</sup>  | 3.166     |
| H(5)  | H(12) <sup>12j</sup> | 3.083     | H(5)  | H(13) <sup>12j</sup> | 3.461     |
| H(5)  | H(20) <sup>6j</sup>  | 3.381     | H(6)  | N(2) <sup>11j</sup>  | 3.41(2)   |
| H(6)  | C(12) <sup>12j</sup> | 3.17(2)   | H(6)  | C(20) <sup>11j</sup> | 3.40(2)   |
| H(6)  | C(25) <sup>11j</sup> | 3.43(2)   | H(6)  | H(3) <sup>11j</sup>  | 2.65(3)   |
| H(6)  | H(5) <sup>12j</sup>  | 3.54(3)   | H(6)  | H(9) <sup>12j</sup>  | 2.50(3)   |
| H(6)  | H(12) <sup>10j</sup> | 3.143     | H(6)  | H(15) <sup>3j</sup>  | 3.488     |
| H(6)  | H(20) <sup>11j</sup> | 2.519     | H(7)  | O(2) <sup>1j</sup>   | 2.45(2)   |
| H(7)  | C(25) <sup>11j</sup> | 2.96(2)   | H(7)  | H(12) <sup>10j</sup> | 3.507     |
| H(7)  | H(16) <sup>3j</sup>  | 3.219     | H(7)  | H(18) <sup>11j</sup> | 2.977     |
| H(7)  | H(19) <sup>7j</sup>  | 3.551     | H(7)  | H(19) <sup>11j</sup> | 2.907     |
| H(7)  | H(20) <sup>11j</sup> | 2.523     | H(8)  | O(2) <sup>1j</sup>   | 3.36(2)   |
| H(8)  | C(19) <sup>7j</sup>  | 3.53(2)   | H(8)  | C(25) <sup>7j</sup>  | 3.45(2)   |
| H(8)  | H(10) <sup>7j</sup>  | 3.561     | H(8)  | H(10) <sup>3j</sup>  | 3.167     |
| H(8)  | H(11) <sup>7j</sup>  | 2.979     | H(8)  | H(18) <sup>7j</sup>  | 3.296     |
| H(8)  | H(19) <sup>7j</sup>  | 3.072     | H(9)  | N(1) <sup>6j</sup>   | 3.14(2)   |
| H(9)  | N(2) <sup>6j</sup>   | 3.01(2)   | H(9)  | C(16) <sup>9j</sup>  | 3.34(2)   |
| H(9)  | C(18) <sup>6j</sup>  | 3.20(2)   | H(9)  | C(20) <sup>6j</sup>  | 3.10(2)   |
| H(9)  | H(3) <sup>6j</sup>   | 2.95(3)   | H(9)  | H(4) <sup>6j</sup>   | 3.41(3)   |
| H(9)  | H(5) <sup>9j</sup>   | 3.37(3)   | H(9)  | H(6) <sup>9j</sup>   | 2.50(3)   |
| H(9)  | H(20) <sup>6j</sup>  | 3.477     | H(10) | N(5) <sup>13j</sup>  | 3.115     |
| H(10) | C(2) <sup>13j</sup>  | 3.164     | H(10) | C(10) <sup>13j</sup> | 3.352     |
| H(10) | C(11) <sup>13j</sup> | 3.119     | H(10) | H(5) <sup>6j</sup>   | 3.166     |
| H(10) | H(8) <sup>2j</sup>   | 3.561     | H(10) | H(8) <sup>13j</sup>  | 3.167     |
| H(11) | C(1) <sup>2j</sup>   | 3.318     | H(11) | C(8) <sup>2j</sup>   | 3.588     |
| H(11) | C(15) <sup>2j</sup>  | 3.045     | H(11) | C(17) <sup>2j</sup>  | 3.057     |

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

| atom  | atom                 | distance | atom  | atom                 | distance |
|-------|----------------------|----------|-------|----------------------|----------|
| H(11) | C(20) <sup>2)</sup>  | 3.349    | H(11) | H(1) <sup>2)</sup>   | 3.441    |
| H(11) | H(2) <sup>2)</sup>   | 3.309    | H(11) | H(8) <sup>2)</sup>   | 2.979    |
| H(12) | C(14) <sup>5)</sup>  | 3.211    | H(12) | C(16) <sup>5)</sup>  | 2.983    |
| H(12) | C(21) <sup>5)</sup>  | 3.328    | H(12) | C(25) <sup>3)</sup>  | 3.590    |
| H(12) | H(5) <sup>9)</sup>   | 3.083    | H(12) | H(6) <sup>5)</sup>   | 3.143    |
| H(12) | H(7) <sup>5)</sup>   | 3.507    | H(12) | H(15) <sup>4)</sup>  | 3.581    |
| H(12) | H(19) <sup>3)</sup>  | 3.085    | H(12) | H(20) <sup>3)</sup>  | 3.254    |
| H(13) | O(3) <sup>4)</sup>   | 3.116    | H(13) | C(17) <sup>6)</sup>  | 3.292    |
| H(13) | C(24) <sup>4)</sup>  | 3.272    | H(13) | H(2) <sup>6)</sup>   | 2.695    |
| H(13) | H(4) <sup>4)</sup>   | 3.323    | H(13) | H(5) <sup>9)</sup>   | 3.461    |
| H(13) | H(15) <sup>4)</sup>  | 2.381    | H(13) | H(17) <sup>4)</sup>  | 3.499    |
| H(14) | O(3) <sup>4)</sup>   | 3.126    | H(14) | C(15) <sup>5)</sup>  | 3.464    |
| H(14) | H(1) <sup>5)</sup>   | 2.517    | H(15) | C(16) <sup>13)</sup> | 3.340    |
| H(15) | C(21) <sup>13)</sup> | 3.598    | H(15) | C(22) <sup>4)</sup>  | 3.304    |
| H(15) | H(2) <sup>5)</sup>   | 2.871    | H(15) | H(3) <sup>5)</sup>   | 3.473    |
| H(15) | H(6) <sup>13)</sup>  | 3.488    | H(15) | H(12) <sup>4)</sup>  | 3.581    |
| H(15) | H(13) <sup>4)</sup>  | 2.381    | H(16) | N(1) <sup>2)</sup>   | 3.390    |
| H(16) | C(14) <sup>13)</sup> | 3.169    | H(16) | C(16) <sup>13)</sup> | 3.460    |
| H(16) | C(18) <sup>2)</sup>  | 3.243    | H(16) | C(20) <sup>2)</sup>  | 3.460    |
| H(16) | H(7) <sup>13)</sup>  | 3.219    | H(17) | N(1) <sup>2)</sup>   | 3.549    |
| H(17) | N(2) <sup>2)</sup>   | 3.311    | H(17) | C(18) <sup>2)</sup>  | 3.581    |
| H(17) | C(20) <sup>2)</sup>  | 3.381    | H(17) | H(2) <sup>5)</sup>   | 2.987    |
| H(17) | H(3) <sup>2)</sup>   | 3.115    | H(17) | H(13) <sup>4)</sup>  | 3.499    |
| H(18) | O(2) <sup>7)</sup>   | 3.159    | H(18) | O(3) <sup>7)</sup>   | 3.487    |
| H(18) | C(15) <sup>2)</sup>  | 3.405    | H(18) | C(17) <sup>2)</sup>  | 3.399    |
| H(18) | H(1) <sup>2)</sup>   | 3.325    | H(18) | H(2) <sup>2)</sup>   | 3.164    |
| H(18) | H(7) <sup>8)</sup>   | 2.977    | H(18) | H(8) <sup>2)</sup>   | 3.296    |
| H(19) | O(2) <sup>13)</sup>  | 2.725    | H(19) | N(5) <sup>13)</sup>  | 3.487    |
| H(19) | C(14) <sup>8)</sup>  | 3.541    | H(19) | H(7) <sup>2)</sup>   | 3.551    |
| H(19) | H(7) <sup>8)</sup>   | 2.907    | H(19) | H(8) <sup>2)</sup>   | 3.072    |
| H(19) | H(12) <sup>13)</sup> | 3.085    | H(20) | C(14) <sup>8)</sup>  | 3.071    |
| H(20) | C(16) <sup>8)</sup>  | 3.067    | H(20) | H(5) <sup>6)</sup>   | 3.381    |
| H(20) | H(6) <sup>8)</sup>   | 2.519    | H(20) | H(7) <sup>8)</sup>   | 2.523    |
| H(20) | H(9) <sup>6)</sup>   | 3.477    | H(20) | H(12) <sup>13)</sup> | 3.254    |

Symmetry Operators:

- |                             |                             |
|-----------------------------|-----------------------------|
| (1) -X,-Y+1,-Z+2            | (2) -X+1/2,Y+1/2-1,-Z+1/2+1 |
| (3) X+1/2-1,-Y+1/2,Z+1/2    | (4) -X+1,-Y,-Z+2            |
| (5) X,Y-1,Z                 | (6) -X+1,-Y+1,-Z+2          |
| (7) -X+1/2,Y+1/2,-Z+1/2+1   | (8) X+1/2,-Y+1/2+1,Z+1/2-1  |
| (9) -X+1/2,Y+1/2-1,-Z+1/2+2 | (10) X,Y+1,Z                |
| (11) X+1/2-1,-Y+1/2+1,Z+1/2 | (12) -X+1/2,Y+1/2,-Z+1/2+2  |
| (13) X+1/2,-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(1) | H(4) | O(3) | 2.842(4) | 0.78(2) | 2.18(2) | 142(2)  |

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.