# organic compounds

# Methyl 5-[*N*,*N*-bis(methoxycarbonyl-methyl)amino]-4-cyano-2-methoxy-carbonyl-3-thiopheneethanoate

## Qiang Wang, Zhong-Shu Li and Bai-Wang Sun*

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In the title compound, $C_{16}H_{18}N_2O_8S$, derived from ranelic acid, there is a highly substituted thiophene ring. The crystal structure involves intermolecular C—H⋯O and C—H⋯S hydrogen bonds.

## Related literature

For related literature, see: Bonnelye *et al.* (2008); Fonseca (2008).
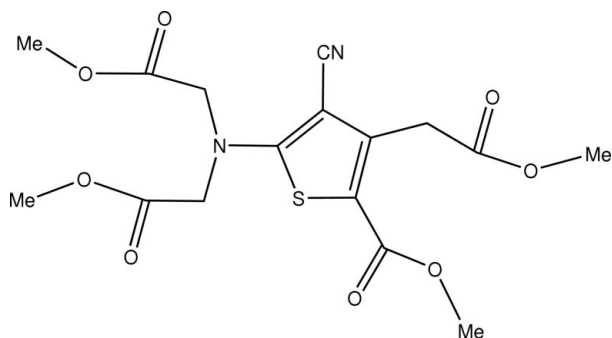


## Experimental

### Crystal data

| | |
|---|---|
| $C_{16}H_{18}N_2O_8S$ | $\gamma = 95.81\ (3)°$ |
| $M_r = 398.38$ | $V = 944.5\ (3)$ Å$^3$ |
| Triclinic, $P\bar{1}$ | $Z = 2$ |
| $a = 9.7164\ (19)$ Å | Mo $K\alpha$ radiation |
| $b = 9.790\ (2)$ Å | $\mu = 0.22$ mm$^{-1}$ |
| $c = 10.170\ (2)$ Å | $T = 293\ (2)$ K |
| $\alpha = 98.05\ (3)°$ | $0.25 \times 0.20 \times 0.18$ mm |
| $\beta = 96.71\ (3)°$ | |

### Data collection

| | |
|---|---|
| Rigaku SCXmini diffractometer | 9976 measured reflections |
| Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005) | 4313 independent reflections |
| $T_{min} = 0.942$, $T_{max} = 0.988$ | 3561 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.027$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.130$ | |
| $S = 1.03$ | |
| 4313 reflections | $\Delta\rho_{max} = 0.33$ e Å$^{-3}$ |
| 246 parameters | $\Delta\rho_{min} = -0.38$ e Å$^{-3}$ |

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C3—H3$A$⋯O3$^i$ | 0.97 | 2.51 | 3.355 (3) | 146 |
| C16—H16$A$⋯O5$^{ii}$ | 0.96 | 2.57 | 3.421 (3) | 148 |
| C16—H16$C$⋯S$^{ii}$ | 0.96 | 2.87 | 3.727 (3) | 149 |

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2258).

## References

Bonnelye, E., Chabadel, A., Saltel, F. & Jurdic, P. (2008). *Bone*, **42**, 129–138.
Fonseca, J. E. (2008). *Rheumatology*, **47**, iv17–iv19.
Rigaku. (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# Methyl 5-[*N*,*N*-bis(methoxycarbonylmethyl)amino]-4-cyano-2-methoxy-carbonyl-3-thiopheneethanoate

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### S1. Comment

The title compound, (I), $C_{16}H_{18}O_8N_2S$, is an important intermediate in the synthesis of strontium ranelate, a medicine for the treatment of osteoporosis (Bonnelye *et al.*, 2008; Fonseca, 2008). Strontium ranelate is composed of two stable strontium ions combined with the anion of organic ranelic acid. The ranelic acid is a carrier that makes the treatment palatable, and the strontium is the active component with regard to the bone. We report here the crystal structure of the title compound. The molecular structure of (I) is shown in Fig. 1 and geometric parameters are given in Table 1. In the crystal (Fig. 2 and Table 2), there are intermolecular C—H···O and C—H···S hydrogen bonds leading to a one-dimensional structure.

### S2. Experimental

All chemicals used (reagent grade) were commercially available. Methyl 5-[bis(methoxycarbonylmethyl)amino]-4-cyano-3-(methoxycarbonyl)-2-thiophene- carboxylate (0.426 g, 0.1 mmol) was added to a solution containing ethanol (8 ml) and acetone (4 ml). The mixture was stirred at room temperature for 10 min and then filtered off. Colorless crystals suitable for X-ray analysis were obtained by slow evaporation at room temperature over several days.

### S3. Refinement

All H atoms attached to C and N atom were fixed geometrically and treated as riding with C—H = 0.97 Å with $U_{iso}(H)$ =1.2$U_{eq}(C)$.
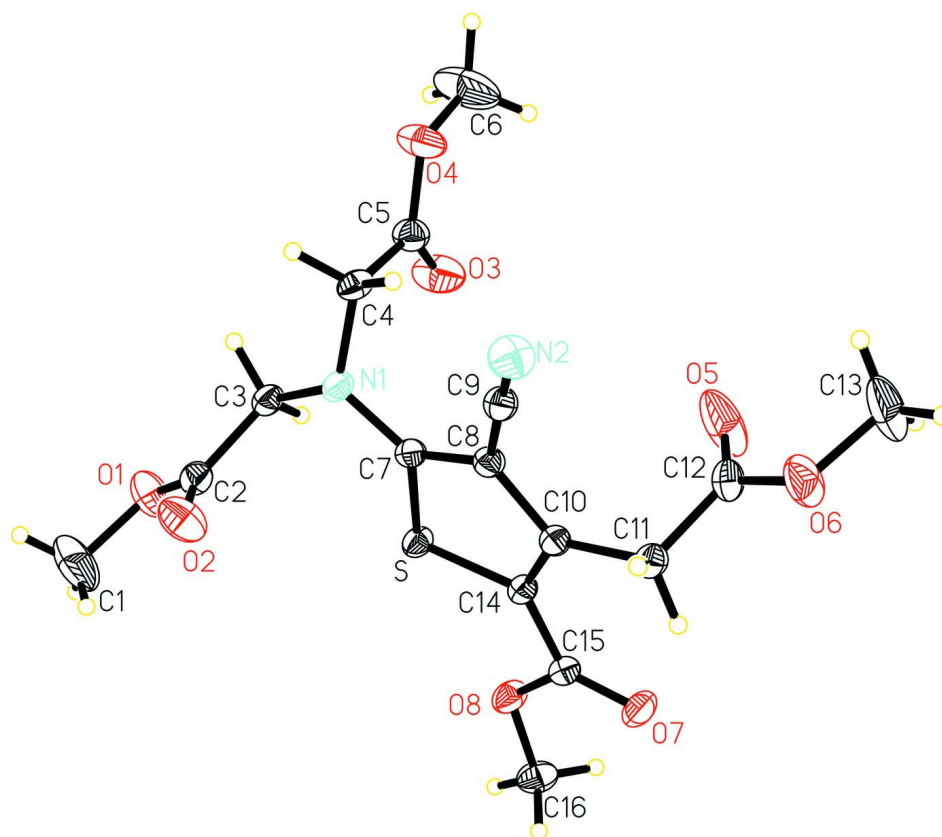
**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.
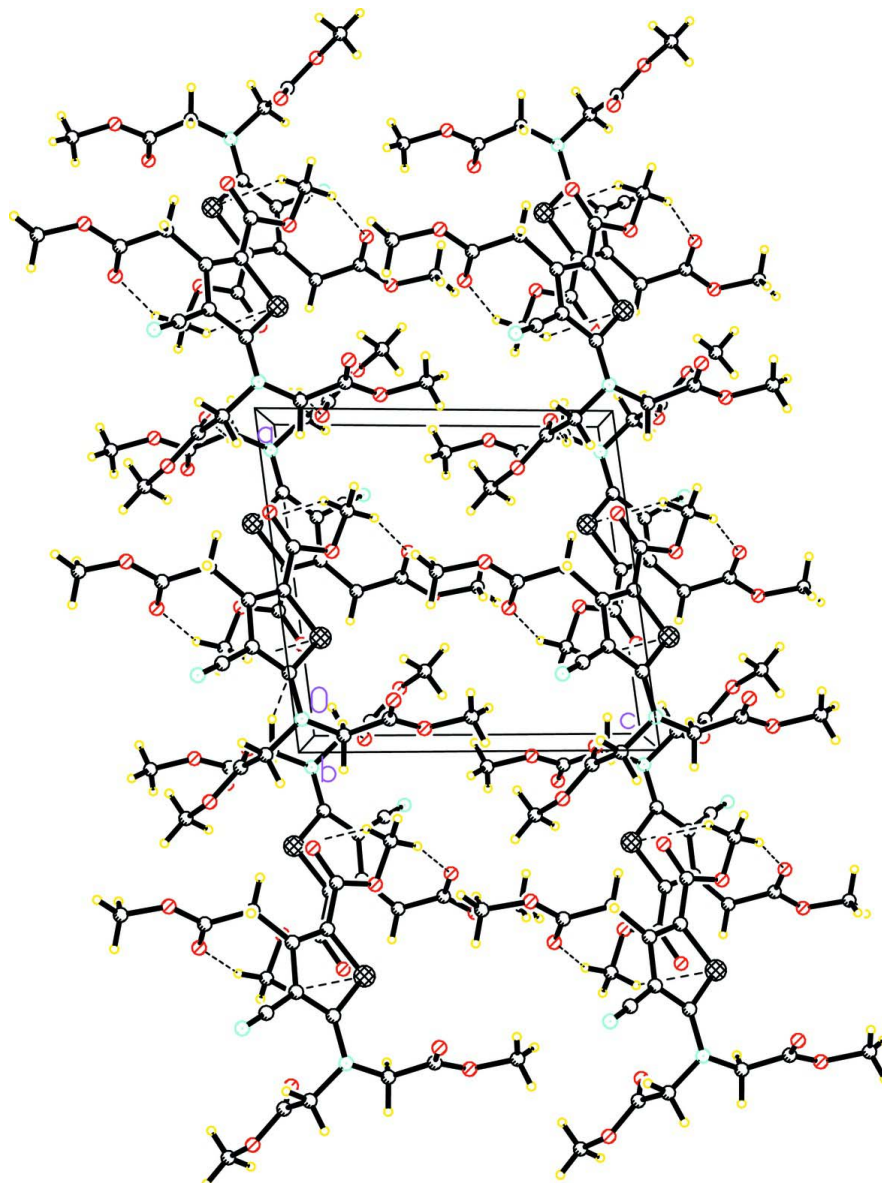
**Figure 2**

Crystal packing of the compound (I) viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

**methyl 5-[*N,N*-bis(methoxycarbonylmethyl)amino]-4-cyano-2- methoxycarbonyl-3-thiophene-ethanoate**

*Crystal data*

| | |
|---|---|
| $C_{16}H_{18}N_2O_8S$ | $\gamma = 95.81\ (3)°$ |
| $M_r = 398.38$ | $V = 944.5\ (3)\ Å^3$ |
| Triclinic, $P\bar{1}$ | $Z = 2$ |
| Hall symbol: -P 1 | $F(000) = 416$ |
| $a = 9.7164\ (19)$ Å | $D_x = 1.401$ Mg m$^{-3}$ |
| $b = 9.790\ (2)$ Å | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $c = 10.170\ (2)$ Å | Cell parameters from 6733 reflections |
| $\alpha = 98.05\ (3)°$ | $\theta = 3.3–27.3°$ |
| $\beta = 96.71\ (3)°$ | $\mu = 0.22$ mm$^{-1}$ |

$T = 293$ K

Prism, colorless

$0.25 \times 0.20 \times 0.18$ mm

*Data collection*

| | |
|---|---|
| Rigaku SCXmini diffractometer | 9976 measured reflections |
| Radiation source: fine-focus sealed tube | 4313 independent reflections |
| Graphite monochromator | 3561 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 8.192 pixels mm$^{-1}$ | $R_{int} = 0.027$ |
| $\omega$ scans | $\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$ |
| Absorption correction: multi-scan | $h = -12 \rightarrow 12$ |
| (*CrystalClear*; Rigaku, 2005) | $k = -12 \rightarrow 12$ |
| $T_{min} = 0.942$, $T_{max} = 0.988$ | $l = -13 \rightarrow 13$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | |
| $wR(F^2) = 0.130$ | |
| $S = 1.03$ | H atoms treated by a mixture of independent and constrained refinement |
| 4313 reflections | |
| 246 parameters | $w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.411P]$ |
| 0 restraints | where $P = (F_o^2 + 2F_c^2)/3$ |
| Primary atom site location: structure-invariant direct methods | $(\Delta/\sigma)_{max} < 0.001$ |
| | $\Delta\rho_{max} = 0.33$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -0.38$ e Å$^{-3}$ |

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness of fit $S$ are based on $F^2$, conventional $R$-factors $R$ are based on $F$, with $F$ set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. $R$-factors based on $F^2$ are statistically about twice as large as those based on $F$, and $R$- factors based on ALL data will be even larger.

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

| | $x$ | $y$ | $z$ | $U_{iso}*/U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.0925 (5) | 0.8277 (4) | 0.4871 (3) | 0.0967 (13) |
| H1A | 0.165 (3) | 0.894 (3) | 0.4933 (6) | 0.145* |
| H1B | 0.116 (3) | 0.7635 (17) | 0.5387 (14) | 0.145* |
| H1C | 0.018 (2) | 0.866 (3) | 0.5154 (12) | 0.145* |
| C2 | 0.0887 (2) | 0.8372 (2) | 0.2560 (2) | 0.0414 (5) |
| C3 | 0.03705 (19) | 0.7542 (2) | 0.11943 (19) | 0.0374 (4) |
| H3A | 0.0661 | 0.6620 | 0.1164 | 0.045* |
| H3B | −0.0642 | 0.7441 | 0.1059 | 0.045* |
| C4 | −0.01502 (19) | 0.8243 (2) | −0.1025 (2) | 0.0366 (4) |
| H4A | 0.0231 | 0.8874 | −0.1582 | 0.044* |
| H4B | −0.0962 | 0.8606 | −0.0702 | 0.044* |
| C5 | −0.0589 (2) | 0.6829 (2) | −0.1857 (2) | 0.0427 (5) |
| C6 | −0.2176 (5) | 0.5578 (4) | −0.3673 (4) | 0.1086 (14) |

| | | | |
|---|---|---|---|
| H6A | −0.2891 | 0.5740 | −0.4348 | 0.163* |
| H6B | −0.2567 | 0.4957 | −0.3126 | 0.163* |
| H6C | −0.1448 | 0.5171 | −0.4094 | 0.163* |
| C7 | 0.22416 (18) | 0.80692 (18) | −0.00849 (18) | 0.0312 (4) |
| C8 | 0.30195 (18) | 0.86329 (19) | −0.09923 (18) | 0.0321 (4) |
| C9 | 0.2567 (2) | 0.9617 (2) | −0.18082 (19) | 0.0369 (4) |
| C10 | 0.43987 (18) | 0.82416 (19) | −0.09451 (18) | 0.0335 (4) |
| C11 | 0.5374 (2) | 0.8694 (2) | −0.18941 (19) | 0.0404 (4) |
| H11A | 0.5404 | 0.9690 | −0.1876 | 0.048* |
| H11B | 0.6307 | 0.8498 | −0.1592 | 0.048* |
| C12 | 0.4935 (2) | 0.7974 (2) | −0.3310 (2) | 0.0446 (5) |
| C13 | 0.5241 (4) | 0.8027 (4) | −0.5571 (3) | 0.0940 (11) |
| H13A | 0.5736 | 0.8606 | −0.6092 | 0.141* |
| H13B | 0.4257 | 0.7956 | −0.5864 | 0.141* |
| H13C | 0.5541 | 0.7119 | −0.5686 | 0.141* |
| C14 | 0.46807 (18) | 0.7442 (2) | 0.00257 (18) | 0.0335 (4) |
| C15 | 0.59750 (19) | 0.6869 (2) | 0.04245 (19) | 0.0360 (4) |
| C16 | 0.7100 (2) | 0.5700 (2) | 0.2060 (2) | 0.0501 (5) |
| H16A | 0.6891 | 0.5245 | 0.2802 | 0.075* |
| H16B | 0.7815 | 0.6466 | 0.2366 | 0.075* |
| H16C | 0.7418 | 0.5053 | 0.1396 | 0.075* |
| O1 | 0.0564 (2) | 0.76176 (18) | 0.34904 (16) | 0.0637 (5) |
| O2 | 0.1471 (2) | 0.95261 (18) | 0.27677 (18) | 0.0673 (5) |
| O3 | −0.0096 (2) | 0.57999 (18) | −0.1647 (2) | 0.0719 (6) |
| O4 | −0.15997 (19) | 0.68911 (18) | −0.28405 (17) | 0.0626 (5) |
| O5 | 0.4141 (3) | 0.6943 (2) | −0.3638 (2) | 0.1020 (9) |
| O6 | 0.5525 (2) | 0.8633 (2) | −0.41698 (17) | 0.0695 (5) |
| O7 | 0.70142 (14) | 0.69773 (18) | −0.01103 (16) | 0.0520 (4) |
| O8 | 0.58547 (14) | 0.62078 (16) | 0.14789 (15) | 0.0438 (3) |
| N1 | 0.08891 (15) | 0.81812 (17) | 0.01103 (16) | 0.0346 (3) |
| N2 | 0.2253 (2) | 1.0438 (2) | −0.2444 (2) | 0.0535 (5) |
| S | 0.32536 (5) | 0.71175 (5) | 0.08736 (5) | 0.03457 (14) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.151 (4) | 0.103 (3) | 0.0364 (14) | 0.029 (2) | 0.0078 (17) | 0.0058 (15) |
| C2 | 0.0371 (10) | 0.0491 (12) | 0.0399 (11) | 0.0130 (9) | 0.0055 (8) | 0.0071 (9) |
| C3 | 0.0266 (9) | 0.0471 (11) | 0.0394 (10) | 0.0020 (7) | 0.0078 (7) | 0.0087 (8) |
| C4 | 0.0280 (9) | 0.0392 (10) | 0.0447 (11) | 0.0078 (7) | 0.0016 (8) | 0.0136 (8) |
| C5 | 0.0412 (11) | 0.0444 (11) | 0.0418 (11) | 0.0083 (9) | −0.0004 (8) | 0.0071 (9) |
| C6 | 0.132 (3) | 0.080 (2) | 0.088 (2) | 0.010 (2) | −0.054 (2) | −0.0192 (19) |
| C7 | 0.0275 (8) | 0.0346 (9) | 0.0308 (9) | 0.0026 (7) | 0.0019 (7) | 0.0052 (7) |
| C8 | 0.0301 (9) | 0.0364 (9) | 0.0297 (9) | 0.0015 (7) | 0.0031 (7) | 0.0069 (7) |
| C9 | 0.0335 (9) | 0.0429 (10) | 0.0348 (10) | 0.0016 (8) | 0.0064 (7) | 0.0084 (8) |
| C10 | 0.0292 (9) | 0.0388 (10) | 0.0312 (9) | −0.0010 (7) | 0.0047 (7) | 0.0039 (8) |
| C11 | 0.0329 (10) | 0.0530 (12) | 0.0366 (10) | −0.0014 (8) | 0.0081 (8) | 0.0128 (9) |
| C12 | 0.0494 (12) | 0.0491 (12) | 0.0391 (11) | 0.0046 (10) | 0.0171 (9) | 0.0112 (9) |

| | | | | | |
|---|---|---|---|---|---|
| C13 | 0.137 (3) | 0.106 (3) | 0.0417 (15) | −0.002 (2) | 0.0369 (17) | 0.0125 (16) |
| C14 | 0.0259 (8) | 0.0432 (10) | 0.0318 (9) | 0.0027 (7) | 0.0055 (7) | 0.0068 (8) |
| C15 | 0.0280 (9) | 0.0429 (10) | 0.0358 (10) | 0.0015 (7) | 0.0030 (7) | 0.0045 (8) |
| C16 | 0.0396 (11) | 0.0547 (13) | 0.0573 (13) | 0.0102 (9) | −0.0046 (10) | 0.0188 (11) |
| O1 | 0.0920 (13) | 0.0632 (11) | 0.0376 (8) | 0.0077 (9) | 0.0124 (8) | 0.0119 (8) |
| O2 | 0.0858 (13) | 0.0538 (10) | 0.0547 (10) | −0.0060 (9) | −0.0015 (9) | 0.0011 (8) |
| O3 | 0.0808 (13) | 0.0454 (9) | 0.0806 (13) | 0.0218 (9) | −0.0235 (10) | −0.0024 (9) |
| O4 | 0.0680 (11) | 0.0608 (10) | 0.0513 (10) | 0.0112 (8) | −0.0206 (8) | 0.0029 (8) |
| O5 | 0.161 (2) | 0.0805 (14) | 0.0505 (11) | −0.0555 (15) | 0.0369 (13) | −0.0065 (10) |
| O6 | 0.0858 (13) | 0.0810 (12) | 0.0413 (9) | −0.0148 (10) | 0.0204 (9) | 0.0163 (9) |
| O7 | 0.0305 (7) | 0.0792 (11) | 0.0519 (9) | 0.0127 (7) | 0.0118 (6) | 0.0202 (8) |
| O8 | 0.0322 (7) | 0.0563 (9) | 0.0478 (8) | 0.0104 (6) | 0.0060 (6) | 0.0207 (7) |
| N1 | 0.0255 (7) | 0.0430 (9) | 0.0366 (8) | 0.0047 (6) | 0.0049 (6) | 0.0094 (7) |
| N2 | 0.0579 (12) | 0.0532 (11) | 0.0536 (11) | 0.0069 (9) | 0.0061 (9) | 0.0237 (9) |
| S | 0.0279 (2) | 0.0437 (3) | 0.0358 (3) | 0.00654 (18) | 0.00741 (17) | 0.0147 (2) |

## Geometric parameters (Å, º)

| | | | |
|---|---|---|---|
| C1—O1 | 1.448 (3) | C8—C9 | 1.427 (3) |
| C1—H1A | 0.9033 | C8—C10 | 1.428 (3) |
| C1—H1B | 0.9033 | C9—N2 | 1.143 (3) |
| C1—H1C | 0.9033 | C10—C14 | 1.363 (3) |
| C2—O2 | 1.191 (3) | C10—C11 | 1.508 (3) |
| C2—O1 | 1.325 (3) | C11—C12 | 1.504 (3) |
| C2—C3 | 1.510 (3) | C11—H11A | 0.9700 |
| C3—N1 | 1.456 (2) | C11—H11B | 0.9700 |
| C3—H3A | 0.9700 | C12—O5 | 1.189 (3) |
| C3—H3B | 0.9700 | C12—O6 | 1.308 (3) |
| C4—N1 | 1.455 (2) | C13—O6 | 1.448 (3) |
| C4—C5 | 1.511 (3) | C13—H13A | 0.9600 |
| C4—H4A | 0.9700 | C13—H13B | 0.9600 |
| C4—H4B | 0.9700 | C13—H13C | 0.9600 |
| C5—O3 | 1.193 (3) | C14—C15 | 1.466 (3) |
| C5—O4 | 1.330 (2) | C14—S | 1.7420 (18) |
| C6—O4 | 1.457 (3) | C15—O7 | 1.204 (2) |
| C6—H6A | 0.9600 | C15—O8 | 1.338 (2) |
| C6—H6B | 0.9600 | C16—O8 | 1.448 (2) |
| C6—H6C | 0.9600 | C16—H16A | 0.9600 |
| C7—N1 | 1.365 (2) | C16—H16B | 0.9600 |
| C7—C8 | 1.396 (2) | C16—H16C | 0.9600 |
| C7—S | 1.7323 (19) | | |
| | | | |
| O1—C1—H1A | 109.5 | C14—C10—C11 | 126.48 (17) |
| O1—C1—H1B | 109.5 | C8—C10—C11 | 121.39 (17) |
| H1A—C1—H1B | 109.5 | C12—C11—C10 | 112.45 (16) |
| O1—C1—H1C | 109.5 | C12—C11—H11A | 109.1 |
| H1A—C1—H1C | 109.5 | C10—C11—H11A | 109.1 |
| H1B—C1—H1C | 109.5 | C12—C11—H11B | 109.1 |

| | | | |
|---|---|---|---|
| O2—C2—O1 | 125.5 (2) | C10—C11—H11B | 109.1 |
| O2—C2—C3 | 125.5 (2) | H11A—C11—H11B | 107.8 |
| O1—C2—C3 | 108.99 (18) | O5—C12—O6 | 122.9 (2) |
| N1—C3—C2 | 112.93 (16) | O5—C12—C11 | 125.5 (2) |
| N1—C3—H3A | 109.0 | O6—C12—C11 | 111.64 (19) |
| C2—C3—H3A | 109.0 | O6—C13—H13A | 109.5 |
| N1—C3—H3B | 109.0 | O6—C13—H13B | 109.5 |
| C2—C3—H3B | 109.0 | H13A—C13—H13B | 109.5 |
| H3A—C3—H3B | 107.8 | O6—C13—H13C | 109.5 |
| N1—C4—C5 | 111.64 (16) | H13A—C13—H13C | 109.5 |
| N1—C4—H4A | 109.3 | H13B—C13—H13C | 109.5 |
| C5—C4—H4A | 109.3 | C10—C14—C15 | 129.21 (17) |
| N1—C4—H4B | 109.3 | C10—C14—S | 112.01 (14) |
| C5—C4—H4B | 109.3 | C15—C14—S | 118.78 (14) |
| H4A—C4—H4B | 108.0 | O7—C15—O8 | 124.03 (18) |
| O3—C5—O4 | 125.0 (2) | O7—C15—C14 | 125.19 (18) |
| O3—C5—C4 | 124.21 (19) | O8—C15—C14 | 110.78 (16) |
| O4—C5—C4 | 110.76 (17) | O8—C16—H16A | 109.5 |
| O4—C6—H6A | 109.5 | O8—C16—H16B | 109.5 |
| O4—C6—H6B | 109.5 | H16A—C16—H16B | 109.5 |
| H6A—C6—H6B | 109.5 | O8—C16—H16C | 109.5 |
| O4—C6—H6C | 109.5 | H16A—C16—H16C | 109.5 |
| H6A—C6—H6C | 109.5 | H16B—C16—H16C | 109.5 |
| H6B—C6—H6C | 109.5 | C2—O1—C1 | 116.7 (2) |
| N1—C7—C8 | 129.48 (17) | C5—O4—C6 | 116.3 (2) |
| N1—C7—S | 120.44 (14) | C12—O6—C13 | 117.7 (2) |
| C8—C7—S | 110.07 (13) | C15—O8—C16 | 116.74 (16) |
| C7—C8—C9 | 124.59 (17) | C7—N1—C4 | 119.77 (16) |
| C7—C8—C10 | 113.62 (16) | C7—N1—C3 | 117.45 (15) |
| C9—C8—C10 | 121.51 (16) | C4—N1—C3 | 115.49 (15) |
| N2—C9—C8 | 177.3 (2) | C7—S—C14 | 92.11 (9) |
| C14—C10—C8 | 112.12 (16) | | |
| | | | |
| O2—C2—C3—N1 | 11.3 (3) | S—C14—C15—O7 | 177.27 (17) |
| O1—C2—C3—N1 | −169.76 (17) | C10—C14—C15—O8 | 176.21 (19) |
| N1—C4—C5—O3 | −3.4 (3) | S—C14—C15—O8 | −3.1 (2) |
| N1—C4—C5—O4 | 176.17 (17) | O2—C2—O1—C1 | 1.7 (4) |
| N1—C7—C8—C9 | 8.5 (3) | C3—C2—O1—C1 | −177.2 (2) |
| S—C7—C8—C9 | −171.41 (15) | O3—C5—O4—C6 | 3.0 (4) |
| N1—C7—C8—C10 | −177.50 (17) | C4—C5—O4—C6 | −176.6 (3) |
| S—C7—C8—C10 | 2.6 (2) | O5—C12—O6—C13 | −3.2 (4) |
| C7—C8—C9—N2 | 129 (5) | C11—C12—O6—C13 | 177.7 (2) |
| C10—C8—C9—N2 | −45 (5) | O7—C15—O8—C16 | 5.2 (3) |
| C7—C8—C10—C14 | −2.7 (2) | C14—C15—O8—C16 | −174.41 (17) |
| C9—C8—C10—C14 | 171.57 (17) | C8—C7—N1—C4 | 34.7 (3) |
| C7—C8—C10—C11 | 177.14 (16) | S—C7—N1—C4 | −145.47 (15) |
| C9—C8—C10—C11 | −8.6 (3) | C8—C7—N1—C3 | −176.48 (18) |
| C14—C10—C11—C12 | 109.2 (2) | S—C7—N1—C3 | 3.4 (2) |

| | | | |
|---|---|---|---|
| C8—C10—C11—C12 | −70.6 (2) | C5—C4—N1—C7 | 76.6 (2) |
| C10—C11—C12—O5 | −17.2 (4) | C5—C4—N1—C3 | −72.8 (2) |
| C10—C11—C12—O6 | 161.94 (19) | C2—C3—N1—C7 | 76.1 (2) |
| C8—C10—C14—C15 | −177.92 (18) | C2—C3—N1—C4 | −133.71 (17) |
| C11—C10—C14—C15 | 2.3 (3) | N1—C7—S—C14 | 178.60 (15) |
| C8—C10—C14—S | 1.4 (2) | C8—C7—S—C14 | −1.50 (14) |
| C11—C10—C14—S | −178.35 (15) | C10—C14—S—C7 | 0.03 (15) |
| C10—C14—C15—O7 | −3.4 (3) | C15—C14—S—C7 | 179.46 (15) |

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| C3—H3A···O3[i] | 0.97 | 2.51 | 3.355 (3) | 146 |
| C16—H16A···O5[ii] | 0.96 | 2.57 | 3.421 (3) | 148 |
| C16—H16C···S[ii] | 0.96 | 2.87 | 3.727 (3) | 149 |

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