



# Crystal structure of *N*-[2-(cyclohexylsulfanyl)ethyl]quinolinic acid imide

Hyunjin Park, Myong Yong Choi,\* Cheol Joo Moon and Tae Ho Kim\*

Department of Chemistry (BK21 plus) and Research Institute of Natural Sciences, Gyeongsang National University, Jinju 52828, Republic of Korea. \*Correspondence e-mail: mychoi@gnu.ac.kr, thkim@gnu.ac.kr

Received 13 June 2017

Accepted 22 August 2017

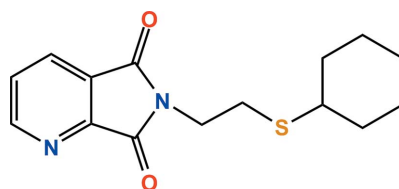
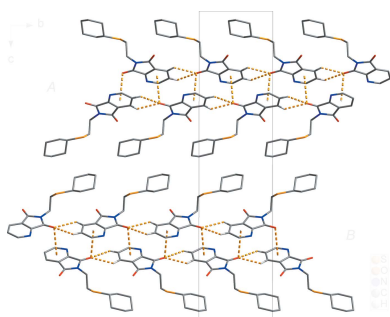
Edited by W. T. A. Harrison, University of Aberdeen, Scotland

**Keywords:** crystal structure; theoretical calculations; quinolinic acid imide; hydrogen bonding.**CCDC reference:** 1570205**Supporting information:** this article has supporting information at journals.iucr.org/e

The title compound, C<sub>15</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>S {systematic name: 6-[2-(cyclohexylsulfanyl)ethyl]-5*H*-pyrrolo[3,4-*b*]pyridine-5,7(6*H*)-dione}, was obtained from the reaction of pyridine-2,3-dicarboxylic anhydride (synonym: quinolinic anhydride) with 2-(cyclohexylsulfanyl)ethylamine. The dihedral angle between the mean plane of the cyclohexyl ring and the quinolinic acid imide ring is 25.43 (11)°. In the crystal, each molecule forms two C—H···O hydrogen bonds and one weak C—O···π [O···ring centroid = 3.255 (2) Å] interaction with neighbouring molecules to generate a ladder structure along the *b*-axis direction. The ladders are linked by weak C—O···π [O···ring centroid = 3.330 (2) Å] interactions, resulting in sheets extending parallel to the *ab* plane. The molecular structure is broadly consistent with theoretical calculations performed by density functional theory (DFT).

## 1. Chemical context

Quinolinic anhydrides have been used extensively as versatile intermediates in the synthesis of various heterocyclic systems, such as aphthiridines, nicotinamides and isotonic derivatives. Recently, they have been exploited in antiviral, dementia, anti-allergy and antitumor targets (Metobo *et al.*, 2013). In addition, it is expected that various metal complexes may be formed because they are composed of N/S-donor atoms. In particular, our group reported copper(I) coordination polymers with N/S-donor-atom ligands, which showed their various luminescence and reversible/irreversible structural transformations (Jeon *et al.*, 2014; Cho *et al.*, 2015). As part of our ongoing studies in this area, we designed and synthesized a new N/S-donor ligand, namely *N*-[2-(cyclohexylsulfanyl)ethyl]quinolinic acid imide, which was prepared from the reaction of quinolinic anhydride with 2-(cyclohexylsulfanyl)ethylamine. Herein, we report its crystal structure.



## 2. Structural commentary

The crystal structure of the title compound is shown in Fig. 1. The cyclohexyl ring adopts a chair conformation, with the exocyclic C—S bond in an equatorial orientation; the dihedral angle between the mean plane (r.m.s. deviation = 0.2317 Å) of

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2\cdots O1^i$	0.95	2.50	3.119 (3)	123
$C3-H3\cdots O1^i$	0.95	2.55	3.129 (3)	119

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

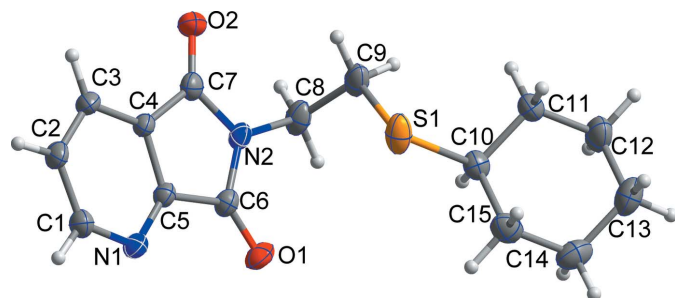
the cyclohexyl ring and the quinolinic acid imide ring is  $25.43(11)^\circ$ . All bond lengths and angles are normal and comparable to those observed in similar crystal structures (Garduño-Beltrán *et al.*, 2009; Inoue *et al.*, 2009).

### 3. Supramolecular features

In the crystal, molecules are linked by  $C2-H2\cdots O1^i$  and  $C3-H3\cdots O1^i$  hydrogen bonds [ $H\cdots O = 2.50$  and  $2.55$  Å, respectively; symmetry code: (i)  $x, y + 1, z$ ; Table 1], and weak  $C6-O1\cdots Cg1^{ii}$  ( $Cg1$  is the centroid of the  $N1/C1-C5$  ring) interactions [ $O\cdots\pi = 3.255(2)$  Å; symmetry code: (ii)  $1 - x, -\frac{1}{2} + y, \frac{1}{2} - z$ ], forming a one-dimensional ladder structure along the  $b$  axis. The ladders are packed in an  $ABAB$  pattern along the  $c$  axis (yellow dashed lines in Fig. 2). In addition, the ladders are linked by  $C7-O2\cdots Cg1^{iii}$  interactions [ $O\cdots\pi = 3.330(2)$  Å; symmetry code: (iii)  $-1 + x, y, z$ ], resulting in the formation of a two-dimensional network structure lying parallel to the  $ab$  plane (red dashed lines in Fig. 3).

### 4. Theoretical calculations

To support the experimental data based on the diffraction study, computational calculations on the  $N$ -[2-(cyclohexylsulfanyl)ethyl]quinolinic acid imide molecule were performed using the *GAUSSIAN09* software package (Frisch *et al.*, 2009). Full geometry optimizations were calculated at the DFT level of theory using a basis set of 6-311++G(d,p). The optimized parameters, such as bond lengths and angles, are in generally good agreement (the largest bond-length deviation is less than 0.03 Å) with the experimental crystallographic data (Table 2). The calculated and experimental torsion angles for  $N2-C8-C9-S1$  ( $C8-C9-S1-C10$ ) are  $53.64(65.80)$  and  $64.2(3)^\circ$  [ $97.4(2)^\circ$ ], respectively. The calculated and experimental dihedral angle between the ring systems were  $25.34$  and



**Figure 1**  
 The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

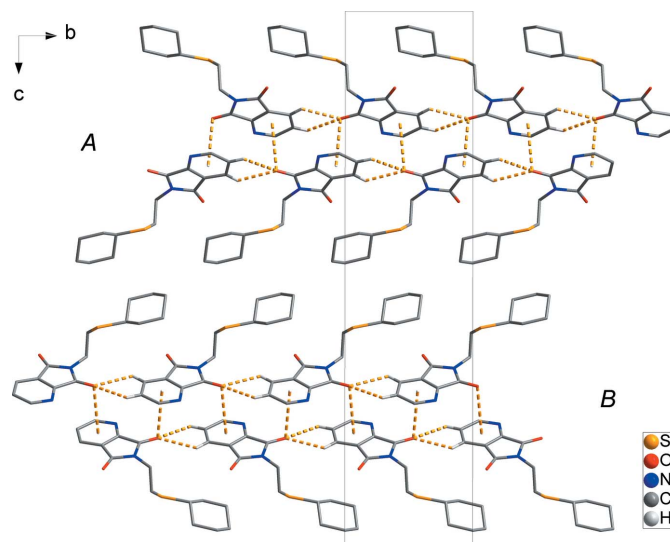
**Table 2**  
 Experimental and calculated bond lengths (Å).

Bond	X-ray	B3LYP (6-311++G(d,p))	Difference
S1-C9	1.813 (3)	1.830	-0.017
S1-C10	1.827 (3)	1.853	-0.026
O1-C6	1.212 (3)	1.205	0.007
O2-C7	1.209 (3)	1.210	0.001
N1-C5	1.325 (3)	1.324	0.001
N1-C1	1.342 (4)	1.342	0.000
N2-C6	1.394 (3)	1.407	-0.013
N2-C7	1.395 (4)	1.399	-0.004
N2-C8	1.460 (3)	1.456	0.004
C1-C2	1.382 (4)	1.400	-0.018
C2-C3	1.381 (4)	1.396	-0.015
C3-C4	1.380 (4)	1.385	-0.005
C4-C5	1.376 (4)	1.392	-0.016
C4-C7	1.490 (4)	1.492	-0.002
C5-C6	1.497 (4)	1.508	-0.011
C8-C9	1.522 (4)	1.536	-0.014
C10-C11	1.516 (4)	1.534	-0.018
C10-C15	1.530 (4)	1.536	-0.006
C11-C12	1.523 (4)	1.539	-0.016
C12-C13	1.523 (4)	1.534	-0.011
C13-C14	1.514 (4)	1.535	-0.021
C14-C15	1.524 (5)	1.537	-0.013

$25.43(11)^\circ$ , respectively. However, several relatively large differences between the experimental and theoretical data (see Table 2) may be due to the packing effects induced by the intermolecular interactions in the crystal.

### 5. Synthesis and crystallization

A mixture of quinolinic anhydride (0.67 g, 5.0 mmol) and 2-(cyclohexylsulfanyl)ethylamine (0.83 g, 5.3 mmol) in toluene (15 ml) was heated at 433 K with stirring for 8 h. The crude product was extracted with dichloromethane. The dichloromethane layer was dried with anhydrous  $Na_2SO_4$  and



**Figure 2**  
 The crystal packing of the title compound, indicating the  $C-H\cdots O$  hydrogen bonds and  $C-O\cdots\pi$  interactions (yellow dashed lines) [symmetry codes: (i)  $x, y + 1, z$ ; (ii)  $1 - x, -\frac{1}{2} + y, \frac{1}{2} - z$ ], which results in a one-dimensional ladder structure along the  $b$  axis.

evaporated to give a crude solid. The reaction mixture was then concentrated and purified by chromatography on silica gel (MeCOOEt/*n*-C<sub>6</sub>H<sub>14</sub> = 30/70 v/v, *R<sub>F</sub>* = 0.28) (Kang *et al.*, 2015). Colourless plates were obtained by slow evaporation of a hexane solution of the title compound. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>): δ 7.40 (*dd*, H, Py), 8.02 (*t*, H, Py), 7.52 (*dd*, H, Py), 3.74 (*t*, 2H, NCH<sub>2</sub>), 2.64 (*t*, 2H, CH<sub>2</sub>S), 2.56 (*d*, H, SCH), 1.82–1.04 [*m*, 10H, (CH<sub>2</sub>)<sub>5</sub>]; <sup>13</sup>C NMR (75.4 MHz, CDCl<sub>3</sub>): δ 166.84, 166.47, 155.60, 144.65, 139.31, 125.76, 116.76, 42.95, 37.89, 33.36, 27.71, 25.91, 25.68

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and refined using a riding model, with C–H = 0.95 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for aromatic C–H groups, C–H = 0.99 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for CH<sub>2</sub> groups, and C–H = 1.00 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for *Csp*<sup>3</sup>–H groups.

## Acknowledgements

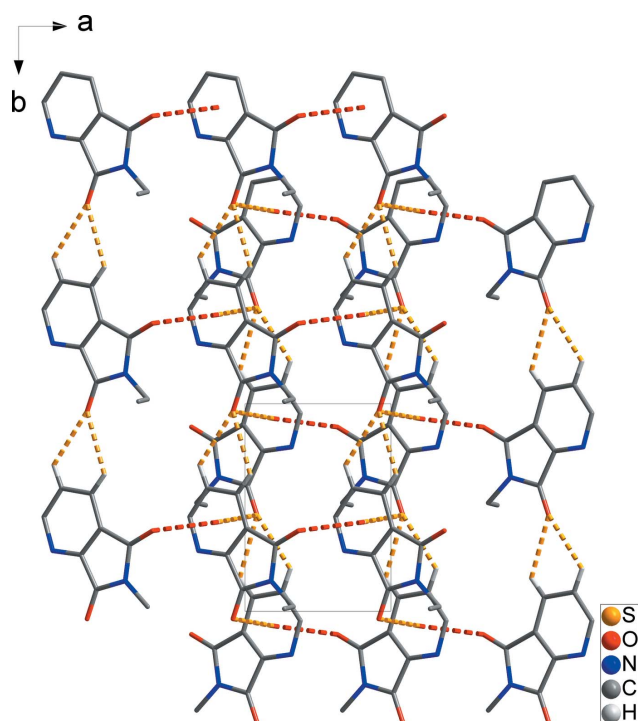
The main calculations were carried out by the Supercomputing Center/Korea Institute of Science and Technology Information (KISTI) (KSC-2017-C1-0002).

## Funding information

Funding for this research was provided by: National Research Foundation of Korea (Basic Science Research Program through the National Research Foundation of Korea (NRF); grant No. 2015R1D1A3A01020410; grant No. 2016R1D1A1B03934376) and by the Korea government (MSIP) (2017M2B2A9A02049940).

## References

- Brandenburg, K. (2010). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2014). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Cho, S., Jeon, Y., Lee, S., Kim, J. & Kim, T. H. (2015). *Chem. Eur. J.* **21**, 1439–1443.
- Frisch, M. J., *et al.* (2009). *GAUSSIAN09*. Gaussian Inc., Wallingford, CT, USA. <http://www.gaussian.com>.
- Garduño-Beltrán, O., Román-Bravo, P., Medrano, F. & Tlahuext, H. (2009). *Acta Cryst.* **E65**, o2581.
- Inoue, S., Shiota, H., Fukumoto, Y. & Chatani, N. (2009). *J. Am. Chem. Soc.* **131**, 6898–6899.
- Jeon, Y., Cheon, S., Cho, S., Lee, K. Y., Kim, T. H. & Kim, J. (2014). *Cryst. Growth Des.* **14**, 2105–2109.
- Kang, G., Jeon, Y., Lee, K. Y., Kim, J. & Kim, T. H. (2015). *Cryst. Growth Des.* **15**, 5183–5187.
- Metobo, S. E., Jabri, S. Y., Aktoudianakis, E., Evans, J., Jin, H. & Kim, C. U. (2013). *Tetrahedron Lett.* **54**, 6782–6784.
- Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* **B69**, 249–259.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.



**Figure 3**  
The packing diagram, showing the two-dimensional network structure formed by C–O···π interactions (red dashed lines) [symmetry code: (iii)  $-1 + x, y, z$ ]. H atoms and cyclohexanesulfanyl groups not involved in intermolecular interactions have been omitted for clarity.

**Table 3**  
Experimental details.

Crystal data	
Chemical formula	C <sub>15</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub> S
<i>M<sub>r</sub></i>	290.37
Crystal system, space group	Orthorhombic, <i>P</i> <sub>2</sub> 1 <sub>2</sub> 1
Temperature (K)	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.5322 (2), 7.8707 (3), 32.9092 (14)
<i>V</i> (Å <sup>3</sup> )	1432.94 (10)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.23
Crystal size (mm)	0.28 × 0.10 × 0.09
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2014)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.690, 0.746
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	11035, 2536, 2302
<i>R</i> <sub>int</sub>	0.046
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.595
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.034, 0.072, 1.04
No. of reflections	2536
No. of parameters	181
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.20, -0.19
Absolute structure	Flack <i>x</i> determined using 839 quotients [( <i>I</i> <sup>+</sup> ) - ( <i>I</i> <sup>-</sup> )] / [( <i>I</i> <sup>+</sup> ) + ( <i>I</i> <sup>-</sup> )] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.05 (5)

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010), *SHELXTL* (Sheldrick, 2008) and *PUBLICIF* (Westrip, 2010).

## supporting information

*Acta Cryst.* (2017). E73, 1372-1374 [https://doi.org/10.1107/S2056989017012142]

## Crystal structure of *N*-[2-(cyclohexylsulfanyl)ethyl]quinolinic acid imide

Hyunjin Park, Myong Yong Choi, Cheol Joo Moon and Tae Ho Kim

### Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

### 6-[2-(Cyclohexylsulfanyl)ethyl]-5*H*-pyrrolo[3,4-*b*]pyridine-5,7(6*H*)-dione

#### Crystal data

$C_{15}H_{18}N_2O_2S$

$M_r = 290.37$

Orthorhombic,  $P2_12_12_1$

$a = 5.5322$  (2) Å

$b = 7.8707$  (3) Å

$c = 32.9092$  (14) Å

$V = 1432.94$  (10) Å<sup>3</sup>

$Z = 4$

$F(000) = 616$

$D_x = 1.346$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2024 reflections

$\theta = 2.5$ – $27.2^\circ$

$\mu = 0.23$  mm<sup>-1</sup>

$T = 173$  K

Plate, colourless

$0.28 \times 0.10 \times 0.09$  mm

#### Data collection

Bruker APEXII CCD  
diffractometer

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2014)

$T_{\min} = 0.690$ ,  $T_{\max} = 0.746$

11035 measured reflections

2536 independent reflections

2302 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 1.2^\circ$

$h = -6 \rightarrow 6$

$k = -8 \rightarrow 9$

$l = -39 \rightarrow 39$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.072$

$S = 1.04$

2536 reflections

181 parameters

0 restraints

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 0.3497P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.20$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.19$  e Å<sup>-3</sup>

Absolute structure: Flack  $x$  determined using

839 quotients  $[(I^+)-(I^-)]/[(I^+)+(I^-)]$  (Parsons *et al.*, 2013)

Absolute structure parameter: 0.05 (5)

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.53243 (13)	0.93377 (11)	0.09181 (3)	0.0414 (2)
O1	0.5825 (3)	0.9636 (2)	0.20137 (6)	0.0362 (5)
O2	0.1331 (3)	1.3885 (3)	0.14389 (6)	0.0360 (5)
N1	0.8186 (4)	1.2919 (3)	0.22791 (7)	0.0292 (6)
N2	0.3211 (4)	1.1461 (3)	0.16766 (7)	0.0268 (5)
C1	0.8794 (5)	1.4552 (4)	0.23364 (8)	0.0306 (7)
H1	1.0179	1.4779	0.2498	0.037*
C2	0.7561 (5)	1.5929 (4)	0.21783 (8)	0.0320 (7)
H2	0.8111	1.7050	0.2233	0.038*
C3	0.5532 (5)	1.5678 (3)	0.19413 (8)	0.0301 (6)
H3	0.4639	1.6597	0.1829	0.036*
C4	0.4884 (5)	1.4006 (3)	0.18778 (7)	0.0235 (6)
C5	0.6241 (5)	1.2727 (3)	0.20487 (8)	0.0234 (6)
C6	0.5174 (5)	1.1058 (3)	0.19241 (8)	0.0262 (6)
C7	0.2900 (5)	1.3212 (4)	0.16376 (8)	0.0281 (7)
C8	0.1681 (5)	1.0227 (4)	0.14678 (9)	0.0335 (7)
H8A	-0.0035	1.0559	0.1499	0.040*
H8B	0.1895	0.9095	0.1594	0.040*
C9	0.2300 (5)	1.0119 (4)	0.10179 (9)	0.0369 (8)
H9A	0.2130	1.1263	0.0896	0.044*
H9B	0.1120	0.9361	0.0883	0.044*
C10	0.4745 (5)	0.7095 (3)	0.08142 (8)	0.0278 (6)
H10	0.3597	0.6645	0.1023	0.033*
C11	0.3645 (5)	0.6857 (4)	0.03962 (8)	0.0318 (7)
H11A	0.4706	0.7395	0.0191	0.038*
H11B	0.2057	0.7435	0.0387	0.038*
C12	0.3313 (6)	0.4988 (4)	0.02908 (10)	0.0448 (9)
H12A	0.2117	0.4476	0.0478	0.054*
H12B	0.2676	0.4887	0.0011	0.054*
C13	0.5693 (6)	0.4026 (4)	0.03229 (10)	0.0463 (8)
H13A	0.5408	0.2803	0.0271	0.056*
H13B	0.6831	0.4450	0.0114	0.056*
C14	0.6795 (6)	0.4253 (4)	0.07406 (10)	0.0438 (8)
H14A	0.8382	0.3672	0.0750	0.053*
H14B	0.5734	0.3716	0.0946	0.053*
C15	0.7133 (5)	0.6123 (4)	0.08458 (9)	0.0388 (8)
H15A	0.8329	0.6633	0.0658	0.047*
H15B	0.7773	0.6223	0.1126	0.047*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0268 (4)	0.0445 (5)	0.0529 (5)	-0.0066 (4)	0.0022 (3)	-0.0203 (4)
O1	0.0412 (12)	0.0199 (11)	0.0474 (12)	0.0036 (10)	-0.0046 (10)	0.0019 (10)
O2	0.0354 (11)	0.0345 (12)	0.0380 (11)	0.0093 (10)	-0.0109 (9)	-0.0026 (10)
N1	0.0318 (13)	0.0227 (14)	0.0332 (13)	0.0016 (11)	-0.0039 (11)	-0.0014 (11)
N2	0.0258 (12)	0.0212 (13)	0.0333 (13)	-0.0014 (11)	-0.0006 (11)	-0.0047 (10)
C1	0.0334 (15)	0.0274 (17)	0.0310 (16)	0.0000 (14)	-0.0036 (12)	-0.0047 (13)
C2	0.0432 (17)	0.0200 (17)	0.0329 (16)	-0.0009 (14)	-0.0028 (13)	-0.0022 (13)
C3	0.0408 (15)	0.0212 (15)	0.0282 (14)	0.0072 (14)	-0.0074 (13)	-0.0001 (12)
C4	0.0302 (14)	0.0186 (14)	0.0217 (13)	0.0009 (13)	-0.0013 (11)	-0.0016 (11)
C5	0.0263 (13)	0.0186 (15)	0.0252 (14)	0.0002 (12)	0.0010 (12)	-0.0010 (12)
C6	0.0275 (14)	0.0215 (15)	0.0297 (14)	0.0013 (13)	0.0031 (12)	-0.0012 (12)
C7	0.0304 (15)	0.0289 (17)	0.0251 (14)	0.0027 (14)	0.0033 (12)	-0.0035 (13)
C8	0.0253 (14)	0.0272 (17)	0.0478 (18)	-0.0047 (13)	0.0013 (14)	-0.0099 (14)
C9	0.0290 (14)	0.0363 (18)	0.0455 (18)	0.0024 (13)	-0.0079 (13)	-0.0159 (14)
C10	0.0245 (14)	0.0323 (16)	0.0265 (14)	-0.0028 (13)	0.0030 (12)	-0.0022 (12)
C11	0.0361 (16)	0.0329 (18)	0.0265 (15)	0.0029 (14)	-0.0032 (13)	-0.0027 (13)
C12	0.0435 (19)	0.039 (2)	0.052 (2)	0.0007 (16)	-0.0084 (16)	-0.0145 (16)
C13	0.0491 (19)	0.0342 (19)	0.056 (2)	0.0052 (17)	0.0069 (16)	-0.0118 (16)
C14	0.0379 (17)	0.042 (2)	0.051 (2)	0.0103 (18)	0.0047 (15)	0.0076 (17)
C15	0.0307 (15)	0.049 (2)	0.0372 (17)	0.0036 (15)	-0.0018 (13)	-0.0023 (16)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

S1—C9	1.813 (3)	C8—H8B	0.9900
S1—C10	1.827 (3)	C9—H9A	0.9900
O1—C6	1.212 (3)	C9—H9B	0.9900
O2—C7	1.209 (3)	C10—C11	1.516 (4)
N1—C5	1.325 (3)	C10—C15	1.530 (4)
N1—C1	1.342 (4)	C10—H10	1.0000
N2—C6	1.394 (3)	C11—C12	1.523 (4)
N2—C7	1.395 (4)	C11—H11A	0.9900
N2—C8	1.460 (3)	C11—H11B	0.9900
C1—C2	1.382 (4)	C12—C13	1.523 (4)
C1—H1	0.9500	C12—H12A	0.9900
C2—C3	1.381 (4)	C12—H12B	0.9900
C2—H2	0.9500	C13—C14	1.514 (4)
C3—C4	1.380 (4)	C13—H13A	0.9900
C3—H3	0.9500	C13—H13B	0.9900
C4—C5	1.376 (4)	C14—C15	1.524 (5)
C4—C7	1.490 (4)	C14—H14A	0.9900
C5—C6	1.497 (4)	C14—H14B	0.9900
C8—C9	1.522 (4)	C15—H15A	0.9900
C8—H8A	0.9900	C15—H15B	0.9900
C9—S1—C10	101.54 (14)	H9A—C9—H9B	107.7



C5—N1—C1	113.2 (2)	C11—C10—C15	110.3 (2)
C6—N2—C7	112.0 (2)	C11—C10—S1	111.1 (2)
C6—N2—C8	125.1 (2)	C15—C10—S1	108.6 (2)
C7—N2—C8	122.8 (2)	C11—C10—H10	109.0
N1—C1—C2	125.0 (3)	C15—C10—H10	109.0
N1—C1—H1	117.5	S1—C10—H10	109.0
C2—C1—H1	117.5	C10—C11—C12	112.0 (2)
C3—C2—C1	120.1 (3)	C10—C11—H11A	109.2
C3—C2—H2	120.0	C12—C11—H11A	109.2
C1—C2—H2	120.0	C10—C11—H11B	109.2
C4—C3—C2	115.7 (3)	C12—C11—H11B	109.2
C4—C3—H3	122.2	H11A—C11—H11B	107.9
C2—C3—H3	122.2	C13—C12—C11	111.1 (3)
C5—C4—C3	119.6 (2)	C13—C12—H12A	109.4
C5—C4—C7	108.2 (2)	C11—C12—H12A	109.4
C3—C4—C7	132.2 (2)	C13—C12—H12B	109.4
N1—C5—C4	126.4 (2)	C11—C12—H12B	109.4
N1—C5—C6	125.3 (2)	H12A—C12—H12B	108.0
C4—C5—C6	108.3 (2)	C14—C13—C12	110.6 (3)
O1—C6—N2	125.7 (2)	C14—C13—H13A	109.5
O1—C6—C5	128.7 (2)	C12—C13—H13A	109.5
N2—C6—C5	105.5 (2)	C14—C13—H13B	109.5
O2—C7—N2	124.8 (3)	C12—C13—H13B	109.5
O2—C7—C4	129.2 (3)	H13A—C13—H13B	108.1
N2—C7—C4	106.0 (2)	C13—C14—C15	111.7 (3)
N2—C8—C9	111.4 (2)	C13—C14—H14A	109.3
N2—C8—H8A	109.4	C15—C14—H14A	109.3
C9—C8—H8A	109.4	C13—C14—H14B	109.3
N2—C8—H8B	109.4	C15—C14—H14B	109.3
C9—C8—H8B	109.4	H14A—C14—H14B	107.9
H8A—C8—H8B	108.0	C14—C15—C10	111.2 (3)
C8—C9—S1	113.7 (2)	C14—C15—H15A	109.4
C8—C9—H9A	108.8	C10—C15—H15A	109.4
S1—C9—H9A	108.8	C14—C15—H15B	109.4
C8—C9—H9B	108.8	C10—C15—H15B	109.4
S1—C9—H9B	108.8	H15A—C15—H15B	108.0
C5—N1—C1—C2	0.3 (4)	C6—N2—C7—C4	1.1 (3)
N1—C1—C2—C3	0.1 (4)	C8—N2—C7—C4	-177.0 (2)
C1—C2—C3—C4	-0.3 (4)	C5—C4—C7—O2	-179.3 (3)
C2—C3—C4—C5	0.2 (4)	C3—C4—C7—O2	-0.8 (5)
C2—C3—C4—C7	-178.2 (3)	C5—C4—C7—N2	-0.6 (3)
C1—N1—C5—C4	-0.4 (4)	C3—C4—C7—N2	177.9 (3)
C1—N1—C5—C6	178.4 (3)	C6—N2—C8—C9	-103.0 (3)
C3—C4—C5—N1	0.2 (4)	C7—N2—C8—C9	74.9 (3)
C7—C4—C5—N1	179.0 (2)	N2—C8—C9—S1	64.2 (3)
C3—C4—C5—C6	-178.8 (2)	C10—S1—C9—C8	97.4 (2)
C7—C4—C5—C6	0.0 (3)	C9—S1—C10—C11	75.0 (2)

C7—N2—C6—O1	178.8 (3)	C9—S1—C10—C15	-163.5 (2)
C8—N2—C6—O1	-3.1 (4)	C15—C10—C11—C12	55.5 (3)
C7—N2—C6—C5	-1.1 (3)	S1—C10—C11—C12	175.9 (2)
C8—N2—C6—C5	176.9 (2)	C10—C11—C12—C13	-56.0 (4)
N1—C5—C6—O1	1.7 (4)	C11—C12—C13—C14	55.3 (4)
C4—C5—C6—O1	-179.3 (3)	C12—C13—C14—C15	-55.8 (4)
N1—C5—C6—N2	-178.4 (2)	C13—C14—C15—C10	56.0 (3)
C4—C5—C6—N2	0.6 (3)	C11—C10—C15—C14	-55.2 (3)
C6—N2—C7—O2	179.9 (3)	S1—C10—C15—C14	-177.1 (2)
C8—N2—C7—O2	1.8 (4)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...O1 <sup>i</sup>	0.95	2.50	3.119 (3)	123
C3—H3...O1 <sup>i</sup>	0.95	2.55	3.129 (3)	119

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