Crystal structures of two 1,3-thiazolidin-4-one derivatives featuring sulfide and sulfone functional groups

Hemant P. Yennawar,[a] Lee J. Silverberg,[b] Kevin Cannon,[c] Deepa Gandla,[d] Sandeep K. Kondaveeti,[d] Michael J. Zdilla[d] and Ahmed Nuriye[c]*

[a]Department of Biochemistry and Molecular Biology, The Pennsylvania State University, University Park, Pennsylvania, 16802, USA, [b]Department of Chemistry, The Pennsylvania State University, Schuylkill Campus, 200 University Drive, Schuylkill Haven, Pennsylvania, 17972, USA, [c]Department of Chemistry, The Pennsylvania State University, Abington College, 1600 Woodland Road, Abington, Pennsylvania, 19001, USA, and [d]Department of Chemistry, Temple University, 1901 North 13th Street, Philadelphia, Pennsylvania, 19122, USA. *Correspondence e-mail: auy3@psu.edu

The crystal structures of two closely related compounds, 1-cyclohexyl-2-(2-nitrophenyl)-1,3-thiazolidin-4-one, $C_{15}H_{18}N_2O_3S$, **(1)** and 1-cyclohexyl-2-(2-nitrophenyl)-1,3-thiazolidin-4-one 1,1-dioxide, $C_{15}H_{18}N_2O_5S$, **(2)**, are presented. These compounds are comprised of three types of rings: thiazolidinone, nitrophenyl and cyclohexyl. In both structures, the rings are close to mutually perpendicular, with interplanar dihedral angles greater than 80° in each case. The thiazolidinone rings in both structures exhibit envelope puckering with the S atom as flap and the cyclohexyl rings are in their expected chair conformations. The two structures superpose fairly well, except for the orientation of the nitro groups with respect to their host phenyl ring, with a difference of about 10° between **1** and **2**. The extended structure of **1** has two kinds of weak C—H···O interactions, giving rise to a closed ring formation involving three symmetry-related molecules. Structure **2** has four C—H···O interactions, two of which are exclusively between symmetry-related thiazolidinone dioxide moieties and have a parallel 'give-and-take-fashion' counterpart. In the other two interactions, the nitrophenyl ring and the cyclohexane ring each offer an H atom to the two O atoms on the sulfone group. Additionally, a C—H···π interaction between a C—H group of the cyclohexane ring and the nitrophenyl ring of an adjacent molecule helps to consolidate the structure.
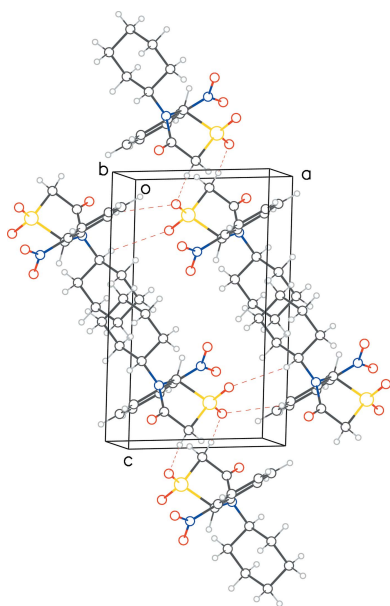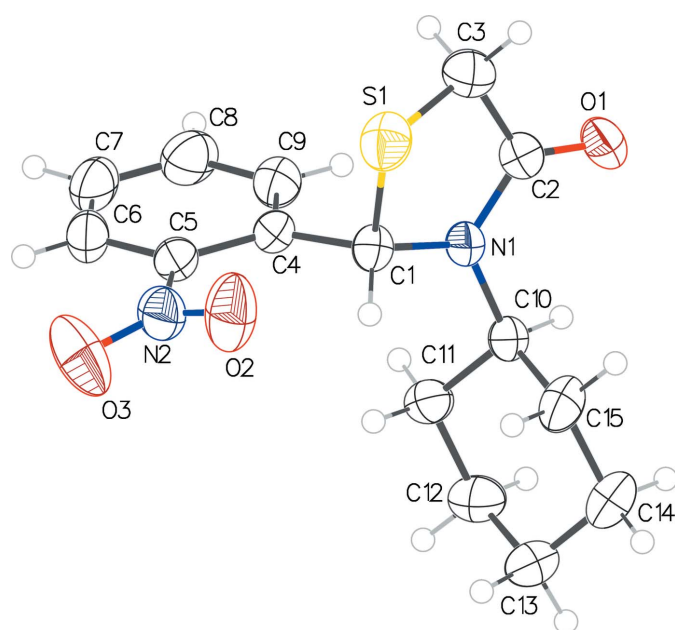
1. Chemical context

The title compounds were synthesized as a part of our ongoing work on the synthesis of new types of 2,3-disubstituted 1,3-thiazolidin-4-ones. We have reported the crystal structures of a number of these compounds before (Nuriye *et al.*, 2018; Yennawar *et al.*, 2015). These compounds are synthesized by a tandem nucleophilic addition-carbonyl condensation of thioglycolic acid with the desired *in situ*-generated imine. The variation in substitution pattern is set during the synthesis of the imine where alkyl or aryl amines are condensed with an aldehyde (Surrey, 1947; von Erlenmeyer & Oberlin, 1947). In addition, the S atom in the thiazolidinone ring can be oxidized to the sulfoxide or the sulfone to produce structures with different properties. Thiazolidinones have well documented biological activity (Thakare *et al.*, 2018; Brown, 1961; Abdel Rahman *et al.*, 1990; Joshi *et al.*, 2014; Suryawanshi *et al.*, 2017; Kaushal & Kaur, 2016; Kumar *et al.*, 2015; Tripathi *et al.*, 2014; Jain *et al.*, 2012; Abhinit *et al.* 2009; Hamama *et al.*, 2008; Singh *et al.*, 1981). The synthesis and characterization of these

compounds could be valuable in investigations for the practical applications of their activities. To the best of our knowledge, only two crystal structures of thiazolidinone sulfones have been reported in the literature (Orsini *et al.*, 1995; Glasl *et al.*, 1997). The compounds presented in this paper both feature an *ortho*-nitrophenyl ring at position 2 and a cyclohexane ring at the 3-position of the thiazolidinone ring. Compound **1** is a sulfide, while compound **2** contains a fully oxidized sulfone functional group.
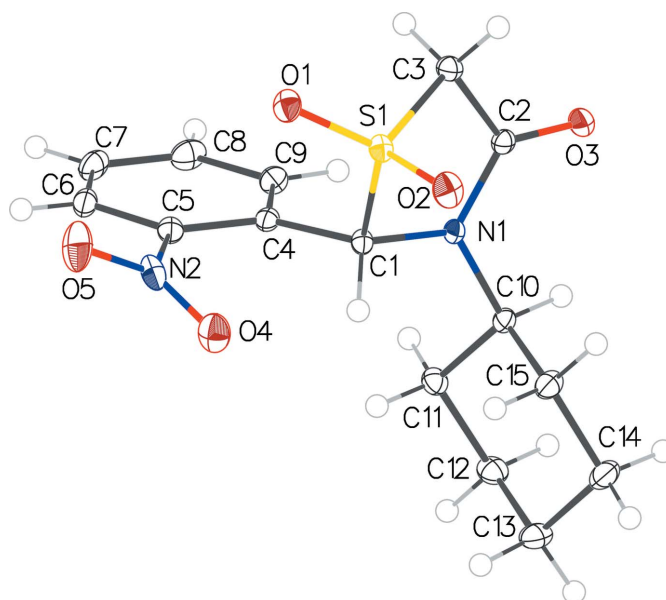
1   **2**
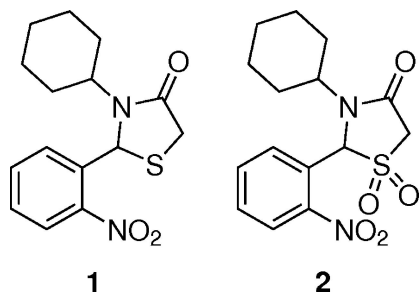
2. Structural commentary

Compound **2** is the dioxide version of **1**, both comprising of three types of rings, a thiazolidinone (*A*), a nitrophenyl (*B*) and a cyclohexyl (*C*) ring. In each structure, the interplanar dihedral angles between the three pairs of rings are close to orthogonal, with values of (in ascending order) $A/C =$ 84.04 (9), $B/C =$ 84.98 (10) and $A/B =$ 85.85 (9)°. The corresponding data for **2** span a slightly wider range: $B/C =$ 80.74 (6), $A/B =$ 83.12 (6) and $A/C =$ 87.96 (6)° (Figs. 1 and 2). In both structures, the thiazolidinone rings exhibit an envelope pucker conformation with the sulfur atom as a flap. The cyclohexyl rings are in the most stable chair conformation in both

Figure 2
The molecular structure of **2** with displacement ellipsoids drawn at the 50% probability level.

structures. An overlay of the two structures (Fig. 3) shows that they overlap well. Fig. 3 also shows that the nitro group plane in **2** is twisted further away by *ca* 10° from the nitrophenyl ring plane as compared to that in **1**; the dihedral angles between the nitro group plane and the host phenyl ring plane were found to be 18.3 (5)° in **1** and 28.3 (5)° in **2**.
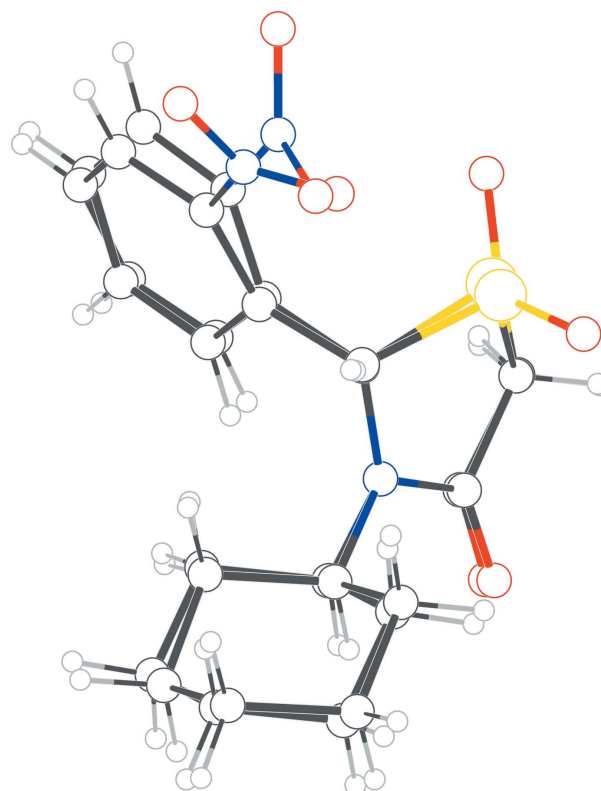

Figure 1
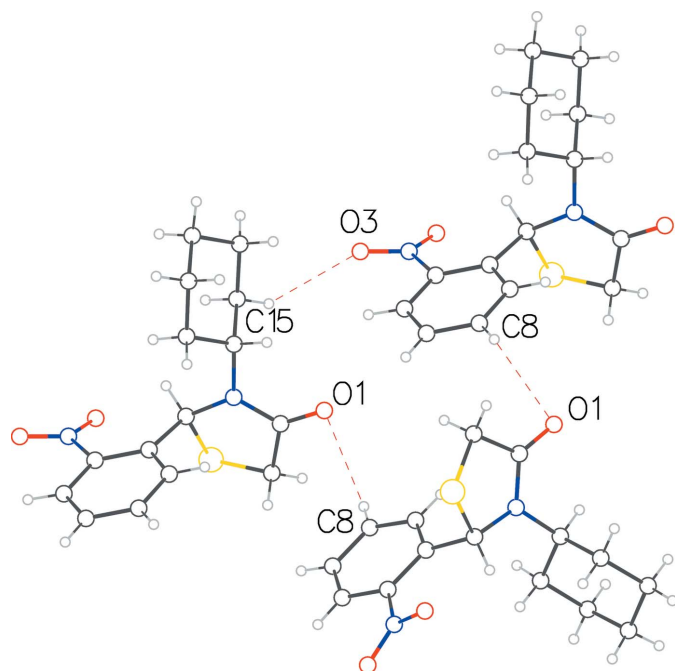The molecular structure of **1** with displacement ellipsoids drawn at the 50% probability level.

Figure 3
Overlay image of the two title molecules showing the difference in the orientation of the nitro group with respect to the nitrophenyl ring plane.

Looking at the thiazolidinone ring systems, the C1—N1 and C1—S1 bond lengths are 1.438 (3) and 1.839 (3) Å, respectively, for structure **1** and 1.4527 (13) and 1.8382 (12) Å for structure **2**. The N—C—S bond angle is found to be 105.22 (12)° in structure **1** and 101.36 (7)° in structure **2** indicating a compression of the N—C—S bond angle going from the sulfide to the sulfone. Bond length and angle values in the thiazolidinone ring of the sulfide appear to be typical and match data that we have previously reported (Nuriye *et al.*, 2018). Although structural data for the sulfone are scarce, the data reported by Orsini *et al.* (1995) matches our findings.

3. Supramolecular features

In structure **1**, two weak C—H···O type interactions (Table 1) result in a closed-ring formation of three symmetry-related molecules (Fig. 4). One of the nitrophenyl-ring carbon atoms donates its H atom to the oxygen atom on the thiazolidinone ring of a neighboring molecule [C8···O1 = 3.411 (5) Å, C—H···O = 140°], which then interacts with a third symmetry-related molecule through a *symmetry-equivalent* contact. Finally, this third molecule donates one of its cyclohexane protons to the nitrophenyl oxygen atom of the first molecule [C15···O3 = 3.437 (5) Å, 138°], thus completing the three-molecule ring arrangement. In the extended structure, the molecules arrange themselves in distinct layers in (020) planes. Perpendicular to *c*, the longest axis, there is an alternating pattern of hydrophobic and hydrophilic surfaces of the molecules, as is evident in the packing diagram (Fig. 5).

In structure **2**, we observe four C—H···O type interactions (Table 2). Two of these involve the thiazolidinone dioxide moieties exclusively and have parallel 'give-and-take' type

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1[i]	0.93	2.65	3.411 (5)	140
C15—H15B···O3[ii]	0.97	2.66	3.437 (5)	138

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (ii) $x + 1, y, z$.

counterparts [C···O = 3.4594 (16) Å, 161° and 3.3068 (16) Å, 157°], forming continuous chains propagating along the *b*-axis direction. The remaining two interactions are weaker and involve the carbon atoms of nitrophenyl rings and cyclohexane rings of one molecule offering protons to the oxygen pair of the dioxide group [C9···O1 3.5144 (16) Å, 132.6° and 3.4381 (16) Å, 129°] of a symmetry-related molecule. Similar to packing of **1**, the molecules are arranged in distinct layers but this time in ($\bar{2}$02) planes. Also seen is the alternating pattern of hydrophobic and hydrophilic surfaces perpendicular to the *c*-axis direction (Fig. 6).

Figure 5
View down the *a* axis of the packing of **1**. The layering of molecules in the (020) plane as well as the alternating pattern of hydrophobic and hydrophilic regions perpendicular to *c* axis can be seen.
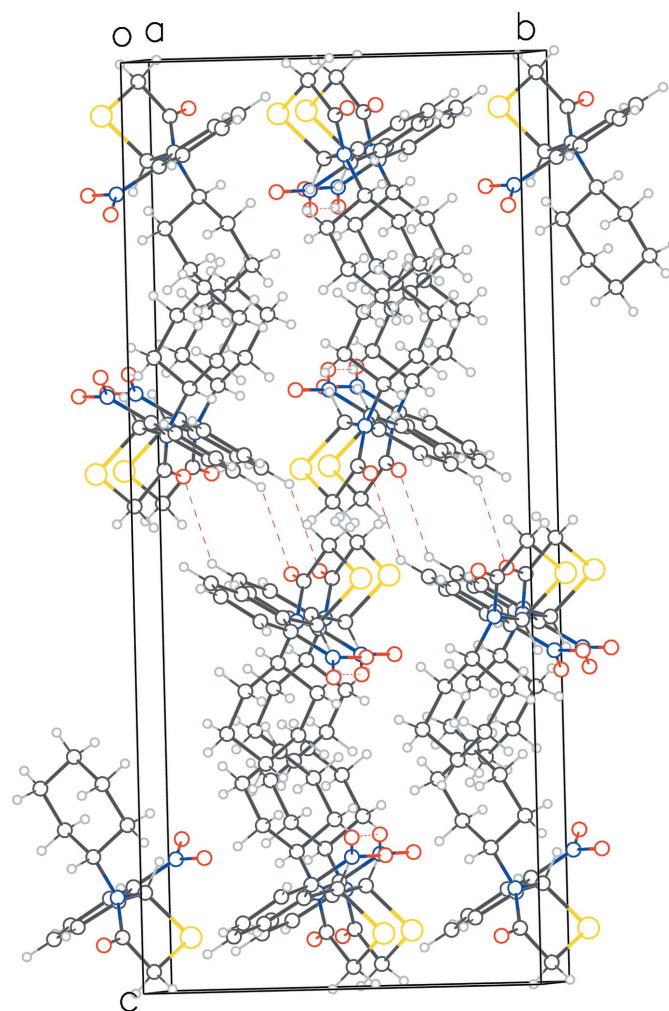

Figure 4
Hydrogen-bond interactions between three symmetry-related molecules of **1** forming a closed-ring system.
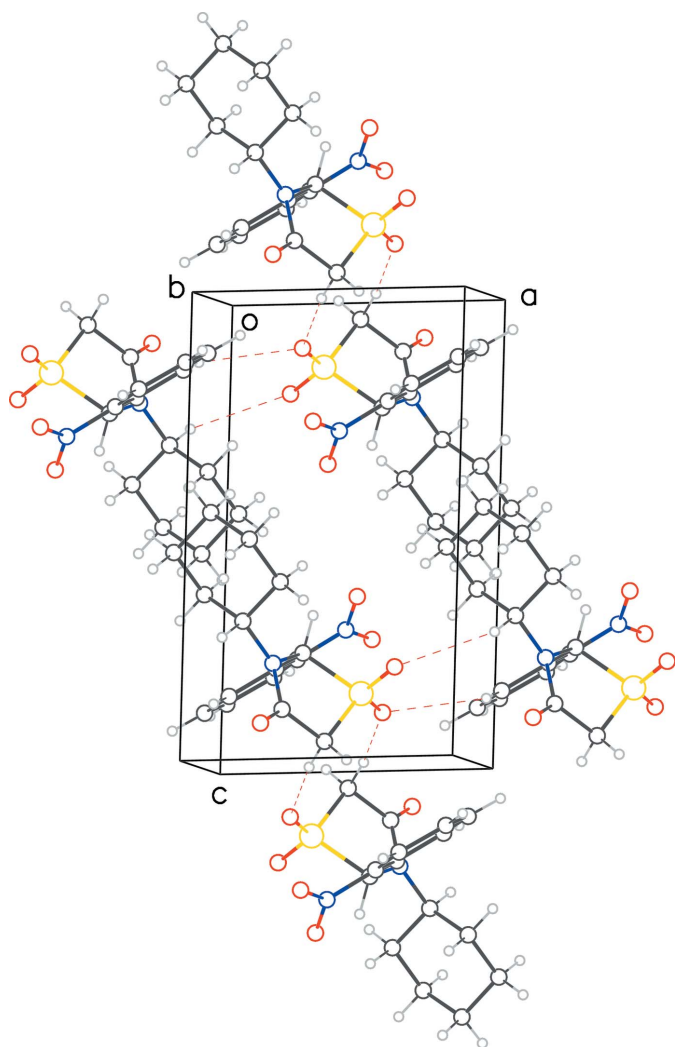
Figure 6
View down the *b* axis of the packing arrangement of **2**. The layering of molecules in the ($\bar{2}$02) plane as well as the alternating pattern of hydrophobic and hydrophilic regions perpendicular to the *c* axis can be seen.

4. Synthesis and crystallization

1-Cyclohexyl-2-(2-nitrophenyl)-1,3-thiazolidin-4-one:
Following the reported method (Cannon *et al.*, 2015), 2-nitrobenzaldehyde (0.725 g, 4.80 mmol) was dissolved in CH$_2$Cl$_2$ (20 ml) and anhydrous MgSO$_4$ (3.0 g) and cyclohexyamine (0.5 g, 5 mmol) were added sequentially and stirred for 4 h at r.t. under nitrogen. The MgSO$_4$ was filtered off and the reaction was concentrated *in vacuo* to give 0.9826 g of an orange oil, which solidified upon sitting in a freezer and remained solid upon warming up to room temperature.

The crude imine was resuspended in toluene (25 ml) and thioglycolic acid (0.55 g, 6.0 mmol) was added and the reaction was heated at reflux for 1.5 h with a Dean–Stark trap attached. The reaction was then cooled to room temperature and washed with aqueous NaHCO$_3$ (2 × 35 ml). The combined organic layers were dried over anhydrous Na$_2$SO$_4$, filtered, and concentrated under reduced pressure to give an orange oil. The crude substance was purified by flash column chro-

Table 2
Hydrogen-bond geometry (Å, °) for **2**.

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
C3—H3$A\cdots$O1^i	0.99	2.51	3.4594 (16)	161
C3—H3$B\cdots$O3^{ii}	0.99	2.37	3.3068 (16)	157
C9—H9$\cdots$O1^{iii}	0.95	2.80	3.5144 (16)	133
C10—H10$\cdots$O2^{iii}	1.00	2.72	3.4381 (16)	129

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, -y+2, -z+2$; (iii) $x-1, y, z$.

matography on silica gel (15 g) using 20–60% ethyl acetate in hexanes as the eluent to yield a yellow solid (0.720 g). The solid was recrystallized from ethanol solution to give a pale-yellow solid (0.508 g, 36.4% over two steps). mp 373–383 K; IR: cm^{-1} 1671.1 (C=O); ^{1}H NMR (CDCl$_3$): 8.08–7.46 (4H, *m*, aromatics), 6.25 (1H, C2), 3.94 (1H, *tt*, *J* = 12.2 Hz, and *J* = 3.6 Hz, NCH), 3.76 (1H, *dd*, C5, *J* = 0.7 Hz, and *J* = 15.7 Hz), 3.47 (1H, *d*, C5, *J* = 15.7 Hz), 1.96–0.86 (10H, *m*, cyclohexyls); ^{13}C NMR: 172.95 (C4), 146.05, 139.12, 134.02, 129.04, 126.72, 125.68, 58.82 (C2), 55.74, 32.20(C5), 31.25, 30.29, 25.89, 25.70, 25.19; MS: (*m/z*) 306 (*M*$^+$) C$_{15}$H$_{18}$O$_3$N$_2$S (306.10).

Crystals for X-ray data collection were grown by dissolving 0.101 g of the solid in hot ethanol and slow evaporation of the solvent.

1-Cyclohexyl-2-(2-nitrophenyl)-1,3-thiazolidin-4-one 1,1-dioxide: 1-Cyclohexyl-2-(2-nitrophenyl)-1,3-thiazolidin-4-one (0.553 mmol) was dissolved in glacial acetic acid (2.4 ml), to which an aqueous solution of KMnO$_4$ (175 mg, 1.11 mmol, in 3.0 ml water) was added dropwise at room temperature with vigorous stirring, and stirred for an additional 5 min. Solid sodium bisulfite (NaHSO$_3$/Na$_2$S$_2$O$_5$) was then added until the solution remained colorless; 3.0 ml of water was then added and the mixture was stirred for a further 10 min. The resulting solid precipitate was filtered and rinsed with water. The resulting powder was purified by recrystallization from CH$_3$OH solution. Yield (64%); m.p. 471–472 K; IR: cm^{-1} 1689.6 (C=O), 1326.9, 1308.1, 1162.7 (S=O); ^{1}H NMR (CDCl$_3$): 8.38 (1H, *dd*, *J* = 8.0, and J = 1.2 Hz, aromatic), 7.78 (1H, *dddd*, *J* = 8.0, 8.0, 1.2, 0.8 Hz, aromatic), 7.68 (1H, *ddd*, *J* = 8.0, 8.0, 1.2 Hz, aromatic), 7.54 (1H, *dd*, *J* = 7.6, 1.2 Hz, aromatic), 6.77 (1H, *s*, C2), 4.41 (1H, *tt*, *J* = 12.0, and *J* = 3.6 Hz, NCH), 3.76 (*dd*, *J* = 16.0 Hz, and *J* = 0.4 Hz, 1H), 3.69 (*d*, *J* = 16.4 Hz, 1 H), 1.96–0.82 (10 H, *m*, cyclohexyls); ^{13}C NMR: 163.41 (C4), 147.80, 134.43, 131.22, 128.82, 126.92 75.77, 54.52, 50.16, 31.39, 29.67, 25.50, 25.16, 24.84; MS: (*m/z*) 339 ([*M* + H]$^+$) C$_{15}$H$_{18}$O$_5$N$_2$S (338.09).

Crystals for X-ray data collection were grown by slow evaporation of a hot methanol solution of the compound.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms were placed geometrically and allowed to ride on their parent C atoms during refinement, with C—H distances of 0.93 Å (aromatic),

Table 3
Experimental details.

	1	2
Crystal data		
Chemical formula	$C_{15}H_{18}N_2O_3S$	$C_{15}H_{18}N_2O_5S$
M_r	306.37	338.37
Crystal system, space group	Orthorhombic, $Pbca$	Triclinic, $P\bar{1}$
Temperature (K)	298	100
a, b, c (Å)	9.582 (13), 11.444 (15), 26.69 (4)	7.114 (2), 9.401 (3), 12.038 (3)
α, β, γ (°)	90, 90, 90	94.808 (5), 92.110 (5), 107.198 (5)
V (Å^3)	2927 (7)	764.8 (4)
Z	8	2
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.23	0.24
Crystal size (mm)	$0.27 \times 0.25 \times 0.2$	$0.29 \times 0.11 \times 0.06$
Data collection		
Diffractometer	Bruker SMART CCD area detector	Bruker SMART CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2001)	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.732, 0.955	0.815, 0.989
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24930, 3685, 2924	9076, 3728, 3475
R_{int}	0.029	0.015
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.673	0.663
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.135, 1.08	0.030, 0.082, 1.05
No. of reflections	3685	3728
No. of parameters	190	208
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.35, −0.17	0.45, −0.34

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *COSMO* and *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* and *SHELXL2016* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

0.97 Å (methylene) and 0.98 Å (methyl), with $U_{iso}(H) = 1.2U_{eq}$(aromatic or methylene C) or $1.5U_{eq}$(methyl C).

References

Abdel Rahman, R. M., El Gendy, Z. & Mahmoud, M. B. (1990). *J. Indian Chem. Soc.* **67**, 61.

Abhinit, M., Ghodke, M. & Pratima, N. A. (2009). *Int. J. Pharm. Pharm. Sci.* **1**, 47–64.

Brown, F. (1961). *Chem. Rev.* **61**, 463–521.

Bruker (2001). *SMART, SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2013). *COSMO, SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Cannon, K. C., Gandla, D., Lauro, S., Silverberg, L. J., Tierney, J. & Lagalante, A. (2015). *Int. J. Chem.* **7**, 73–84.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

Erlenmeyer, H. & Oberlin, V. (1947). *Helv. Chim. Acta*, **30**, 1329–1335.

Glasl, D., Otto, H. & Rihs, G. (1997). *Helv. Chim. Acta*, **80**, 671–683.

Hamama, W. S., Ismail, M. A., Shaaban, S. & Zoorob, H. H. (2008). *J. Het. Chem.* **45**, 939–956.

Jain, A. K., Vaidya, A., Ravichandran, V., Kashaw, S. K. & Agrawal, R. A. (2012). *Bioorg. Med. Chem.* **20**, 3378–3395.

Joshi, A., Anderson, C., Binch, H., Hadida, S., Yoo, S., Bergeron, D., Decker, C., terHaar, E., Moore, J., Garcia-Guzman, M. & Termin, A. (2014). *Bioorg. Med. Chem. Lett.* **24**, 845–849.

Kaushal, M. & Kaur, A. (2016). *World J. Pharm. Res.* **5**, 1966–1977.

Kumar, D., Kumar, V., Mundlia, J., Pradhan, D. & Malik, S. (2015). *Cent. Nerv. Syst. Agent. Med. Chem.* **15**, 23–27.

Nuriye, A., Yennawar, H., Cannon, K. & Tierney, J. (2018). *Acta Cryst.* E**74**, 1509–1512.

Orsini, F., Bombieri, G., Benetollo, F., Vigorita, M. G. & Previtera, T. (1995). *J. Chem. Crystallogr.* **25**, 589–595.

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

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

Singh, S. P., Parmar, S. S., Raman, R. & Stenberg, V. I. (1981). *Chem. Rev.* **81**, 175–203.

Surrey, A. R. (1947). *J. Am. Chem. Soc.* **69**, 2911–2912.

Suryawanshi, R., Jadhav, S., Makwana, N., Desai, D., Chaturbhuj, D., Sonawani, A., Idicula-Thomas, S., Murugesan, V., Katti, S. B., Tripathy, S., Paranjape, R. & Kulkarni, S. (2017). *Bioorg. Chem.* **71**, 211–218.

Thakare, M. P., Shaikh, R. & Tayade, D. (2018). *Heterocycl. Lett.* **8**, 493–506.

Tripathi, A. C., Gupta, S. J., Fatima, G. N., Sonar, P. K., Verma, A. & Saraf, S. K. (2014). *Eur. J. Med. Chem.* **72**, 52–77.

Yennawar, H. P., Tierney, J., Hullihen, P. D. & Silverberg, L. J. (2015). *Acta Cryst.* E**71**, 264–267.

supporting information

Crystal structures of two 1,3-thiazolidin-4-one derivatives featuring sulfide and sulfone functional groups

Hemant P. Yennawar, Lee J. Silverberg, Kevin Cannon, Deepa Gandla, Sandeep K. Kondaveeti, Michael J. Zdilla and Ahmed Nuriye

Computing details

Data collection: *SMART* (Bruker, 2001) for (1); *COSMO* (Bruker, 2013) for (2). Cell refinement: *SAINT* (Bruker, 2001) for (1); *SAINT* (Bruker, 2013) for (2). Data reduction: *SAINT* (Bruker, 2001) for (1); *SAINT* (Bruker, 2013) for (2). For both structures, program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008). Program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015) for (1); *SHELXL2014* (Sheldrick, 2015) for (2). For both structures, molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

1-Cyclohexyl-2-(2-nitrophenyl)-1,3-thiazolidin-4-one (1)

Crystal data

$C_{15}H_{18}N_2O_3S$	$D_x = 1.391$ Mg m^{-3}
$M_r = 306.37$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 5287 reflections
$a = 9.582$ (13) Å	$\theta = 2.6–24.3°$
$b = 11.444$ (15) Å	$\mu = 0.23$ mm^{-1}
$c = 26.69$ (4) Å	$T = 298$ K
$V = 2927$ (7) Å^3	Plate, colorless
$Z = 8$	$0.27 \times 0.25 \times 0.2$ mm
$F(000) = 1296$	

Data collection

Bruker SMART CCD area detector diffractometer	3685 independent reflections
	2924 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.029$
phi and ω scans	$\theta_{max} = 28.6°$, $\theta_{min} = 2.6°$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -12\rightarrow12$
	$k = -13\rightarrow15$
$T_{min} = 0.732$, $T_{max} = 0.955$	$l = -34\rightarrow35$
24930 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.135$	$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2 + 0.9885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	
3685 reflections	$(\Delta/\sigma)_{max} = 0.001$
190 parameters	$\Delta\rho_{max} = 0.35$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details

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

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

	x	y	z	U_{iso}*/U_{eq}
S1	0.64305 (5)	0.59741 (4)	0.55845 (2)	0.05141 (17)
O1	0.95808 (13)	0.40036 (13)	0.55305 (5)	0.0543 (4)
O2	0.43309 (16)	0.62101 (16)	0.64290 (7)	0.0743 (5)
O3	0.23757 (18)	0.55133 (18)	0.66333 (8)	0.0905 (6)
N1	0.76951 (13)	0.42423 (13)	0.60346 (5)	0.0360 (3)
N2	0.34792 (16)	0.54315 (17)	0.64206 (6)	0.0524 (4)
C1	0.63847 (16)	0.48476 (15)	0.60757 (7)	0.0374 (4)
H1	0.631265	0.521843	0.640564	0.045*
C2	0.84294 (17)	0.43948 (18)	0.56067 (7)	0.0417 (4)
C3	0.7632 (2)	0.5110 (2)	0.52278 (7)	0.0533 (5)
H3A	0.713666	0.460539	0.499625	0.064*
H3B	0.826129	0.560651	0.503872	0.064*
C4	0.51274 (17)	0.40812 (15)	0.59855 (6)	0.0371 (4)
C5	0.37756 (17)	0.43693 (18)	0.61324 (7)	0.0418 (4)
C6	0.26504 (19)	0.3690 (2)	0.60127 (8)	0.0533 (5)
H6	0.176194	0.390377	0.611901	0.064*
C7	0.2834 (2)	0.2698 (2)	0.57371 (8)	0.0603 (6)
H7	0.206700	0.224720	0.564627	0.072*
C8	0.4151 (2)	0.2367 (2)	0.55939 (8)	0.0585 (5)
H8	0.428365	0.168290	0.541158	0.070*
C9	0.5272 (2)	0.30517 (18)	0.57219 (7)	0.0470 (4)
H9	0.616167	0.281283	0.562734	0.056*
C10	0.83474 (16)	0.37054 (16)	0.64788 (6)	0.0359 (4)
H10	0.911045	0.320833	0.635901	0.043*
C11	0.73624 (19)	0.29343 (17)	0.67713 (6)	0.0438 (4)
H11A	0.701899	0.231608	0.655539	0.053*
H11B	0.656828	0.339271	0.688165	0.053*
C12	0.8082 (2)	0.2396 (2)	0.72259 (7)	0.0544 (5)
H12A	0.740381	0.195440	0.741803	0.065*
H12B	0.879757	0.185814	0.711273	0.065*
C13	0.8736 (2)	0.3306 (2)	0.75583 (7)	0.0580 (6)
H13A	0.924527	0.292580	0.782674	0.070*
H13B	0.801130	0.378481	0.770746	0.070*
C14	0.9720 (2)	0.4073 (2)	0.72616 (8)	0.0602 (6)
H14A	1.050130	0.360810	0.714471	0.072*
H14B	1.008345	0.468373	0.747720	0.072*
C15	0.89855 (19)	0.46261 (18)	0.68135 (8)	0.0498 (5)
H15A	0.825973	0.514902	0.693159	0.060*
H15B	0.965152	0.508361	0.662267	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0457 (3)	0.0450 (3)	0.0635 (3)	0.0006 (2)	−0.0051 (2)	0.0116 (2)
O1	0.0367 (7)	0.0788 (10)	0.0473 (8)	0.0056 (6)	0.0121 (5)	0.0074 (7)
O2	0.0446 (8)	0.0696 (11)	0.1087 (14)	0.0105 (8)	−0.0022 (8)	−0.0240 (10)
O3	0.0650 (10)	0.0923 (14)	0.1142 (15)	0.0137 (10)	0.0447 (11)	−0.0008 (12)
N1	0.0265 (6)	0.0465 (8)	0.0350 (7)	0.0030 (6)	0.0009 (5)	0.0024 (6)
N2	0.0391 (8)	0.0655 (11)	0.0525 (10)	0.0153 (8)	0.0033 (7)	0.0072 (8)
C1	0.0293 (7)	0.0437 (9)	0.0392 (9)	0.0029 (7)	−0.0013 (6)	0.0000 (7)
C2	0.0358 (8)	0.0510 (10)	0.0384 (9)	−0.0043 (7)	0.0015 (7)	0.0026 (8)
C3	0.0499 (10)	0.0674 (13)	0.0427 (10)	−0.0001 (10)	0.0020 (8)	0.0133 (9)
C4	0.0297 (7)	0.0488 (10)	0.0328 (8)	0.0009 (7)	−0.0028 (6)	0.0050 (7)
C5	0.0335 (8)	0.0559 (11)	0.0361 (9)	0.0031 (7)	−0.0018 (7)	0.0113 (8)
C6	0.0319 (8)	0.0767 (15)	0.0514 (11)	−0.0066 (9)	−0.0026 (8)	0.0171 (10)
C7	0.0471 (11)	0.0782 (16)	0.0557 (12)	−0.0246 (11)	−0.0119 (9)	0.0133 (12)
C8	0.0618 (13)	0.0614 (13)	0.0522 (12)	−0.0143 (11)	−0.0078 (10)	−0.0044 (10)
C9	0.0401 (9)	0.0551 (11)	0.0458 (10)	−0.0031 (8)	−0.0012 (8)	−0.0047 (9)
C10	0.0277 (7)	0.0446 (9)	0.0354 (8)	0.0052 (6)	0.0010 (6)	0.0004 (7)
C11	0.0447 (9)	0.0524 (11)	0.0341 (9)	−0.0078 (8)	−0.0021 (7)	−0.0002 (8)
C12	0.0598 (11)	0.0640 (13)	0.0395 (10)	−0.0026 (10)	−0.0014 (9)	0.0090 (9)
C13	0.0509 (11)	0.0862 (16)	0.0368 (10)	0.0024 (11)	−0.0085 (8)	−0.0009 (10)
C14	0.0443 (10)	0.0800 (16)	0.0564 (12)	−0.0056 (10)	−0.0177 (9)	−0.0020 (11)
C15	0.0384 (9)	0.0538 (12)	0.0570 (12)	−0.0061 (8)	−0.0118 (8)	−0.0006 (9)

Geometric parameters (Å, º)

S1—C1	1.839 (3)	C8—H8	0.9300
S1—C3	1.792 (3)	C8—C9	1.373 (3)
O1—C2	1.208 (2)	C9—H9	0.9300
O2—N2	1.209 (3)	C10—H10	0.9800
O3—N2	1.204 (2)	C10—C11	1.510 (3)
N1—C1	1.438 (3)	C10—C15	1.511 (3)
N1—C2	1.353 (3)	C11—H11A	0.9700
N1—C10	1.474 (2)	C11—H11B	0.9700
N2—C5	1.466 (3)	C11—C12	1.525 (3)
C1—H1	0.9800	C12—H12A	0.9700
C1—C4	1.509 (3)	C12—H12B	0.9700
C2—C3	1.508 (3)	C12—C13	1.505 (3)
C3—H3A	0.9700	C13—H13A	0.9700
C3—H3B	0.9700	C13—H13B	0.9700
C4—C5	1.393 (3)	C13—C14	1.511 (3)
C4—C9	1.379 (3)	C14—H14A	0.9700
C5—C6	1.367 (3)	C14—H14B	0.9700
C6—H6	0.9300	C14—C15	1.525 (3)
C6—C7	1.364 (4)	C15—H15A	0.9700
C7—H7	0.9300	C15—H15B	0.9700
C7—C8	1.372 (4)		

C3—S1—C1	90.40 (12)	C8—C9—C4	122.42 (19)
C1—N1—C10	120.64 (14)	C8—C9—H9	118.8
C2—N1—C1	117.15 (15)	N1—C10—H10	107.2
C2—N1—C10	120.80 (16)	N1—C10—C11	113.22 (15)
O2—N2—C5	119.36 (17)	N1—C10—C15	110.87 (17)
O3—N2—O2	121.8 (2)	C11—C10—H10	107.2
O3—N2—C5	118.8 (2)	C11—C10—C15	110.80 (17)
S1—C1—H1	109.8	C15—C10—H10	107.2
N1—C1—S1	105.22 (12)	C10—C11—H11A	109.4
N1—C1—H1	109.8	C10—C11—H11B	109.4
N1—C1—C4	113.88 (17)	C10—C11—C12	111.39 (17)
C4—C1—S1	108.22 (12)	H11A—C11—H11B	108.0
C4—C1—H1	109.8	C12—C11—H11A	109.4
O1—C2—N1	124.72 (17)	C12—C11—H11B	109.4
O1—C2—C3	123.40 (17)	C11—C12—H12A	109.2
N1—C2—C3	111.88 (17)	C11—C12—H12B	109.2
S1—C3—H3A	110.6	H12A—C12—H12B	107.9
S1—C3—H3B	110.6	C13—C12—C11	112.2 (2)
C2—C3—S1	105.59 (16)	C13—C12—H12A	109.2
C2—C3—H3A	110.6	C13—C12—H12B	109.2
C2—C3—H3B	110.6	C12—C13—H13A	109.5
H3A—C3—H3B	108.8	C12—C13—H13B	109.5
C5—C4—C1	124.04 (18)	C12—C13—C14	110.66 (19)
C9—C4—C1	119.83 (16)	H13A—C13—H13B	108.1
C9—C4—C5	116.05 (17)	C14—C13—H13A	109.5
C4—C5—N2	121.60 (17)	C14—C13—H13B	109.5
C6—C5—N2	116.18 (18)	C13—C14—H14A	109.4
C6—C5—C4	122.2 (2)	C13—C14—H14B	109.4
C5—C6—H6	120.1	C13—C14—C15	111.34 (18)
C7—C6—C5	119.84 (19)	H14A—C14—H14B	108.0
C7—C6—H6	120.1	C15—C14—H14A	109.4
C6—C7—H7	120.0	C15—C14—H14B	109.4
C6—C7—C8	119.92 (19)	C10—C15—C14	111.15 (19)
C8—C7—H7	120.0	C10—C15—H15A	109.4
C7—C8—H8	120.3	C10—C15—H15B	109.4
C7—C8—C9	119.5 (2)	C14—C15—H15A	109.4
C9—C8—H8	120.3	C14—C15—H15B	109.4
C4—C9—H9	118.8	H15A—C15—H15B	108.0

S1—C1—C4—C5	−81.4 (2)	C2—N1—C1—C4	102.13 (19)
S1—C1—C4—C9	95.38 (19)	C2—N1—C10—C11	−143.59 (18)
O1—C2—C3—S1	−155.76 (17)	C2—N1—C10—C15	91.2 (2)
O2—N2—C5—C4	18.2 (3)	C3—S1—C1—N1	25.72 (13)
O2—N2—C5—C6	−161.08 (19)	C3—S1—C1—C4	−96.37 (16)
O3—N2—C5—C4	−163.46 (19)	C4—C5—C6—C7	−0.5 (3)
O3—N2—C5—C6	17.2 (3)	C5—C4—C9—C8	2.3 (3)
N1—C1—C4—C5	162.03 (16)	C5—C6—C7—C8	2.0 (3)

N1—C1—C4—C9	−21.2 (2)	C6—C7—C8—C9	−1.3 (3)
N1—C2—C3—S1	24.8 (2)	C7—C8—C9—C4	−1.0 (3)
N1—C10—C11—C12	179.86 (15)	C9—C4—C5—N2	179.17 (16)
N1—C10—C15—C14	−177.41 (15)	C9—C4—C5—C6	−1.6 (3)
N2—C5—C6—C7	178.77 (17)	C10—N1—C1—S1	150.33 (13)
C1—S1—C3—C2	−28.32 (15)	C10—N1—C1—C4	−91.31 (19)
C1—N1—C2—O1	175.24 (18)	C10—N1—C2—O1	8.7 (3)
C1—N1—C2—C3	−5.3 (2)	C10—N1—C2—C3	−171.82 (16)
C1—N1—C10—C11	50.3 (2)	C10—C11—C12—C13	54.7 (2)
C1—N1—C10—C15	−74.9 (2)	C11—C10—C15—C14	56.0 (2)
C1—C4—C5—N2	−4.0 (3)	C11—C12—C13—C14	−54.6 (2)
C1—C4—C5—C6	175.29 (17)	C12—C13—C14—C15	55.4 (3)
C1—C4—C9—C8	−174.68 (18)	C13—C14—C15—C10	−56.6 (2)
C2—N1—C1—S1	−16.23 (18)	C15—C10—C11—C12	−54.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^i	0.93	2.65	3.411 (5)	140
C15—H15B···O3^{ii}	0.97	2.66	3.437 (5)	138

Symmetry codes: (i) $x-1/2$, $-y+1/2$, $-z+1$; (ii) $x+1$, y, z.

1-Cyclohexyl-2-(2-nitrophenyl)-1,3-thiazolidin-4-one 1,1-dioxide (2)

Crystal data

$C_{15}H_{18}N_2O_5S$	$Z = 2$
$M_r = 338.37$	$F(000) = 356$
Triclinic, $P\overline{1}$	$D_x = 1.469$ Mg m^{-3}
$a = 7.114$ (2) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 9.401$ (3) Å	Cell parameters from 1021 reflections
$c = 12.038$ (3) Å	$\theta = 2.6$–25.0°
$\alpha = 94.808$ (5)°	$\mu = 0.24$ mm^{-1}
$\beta = 92.110$ (5)°	$T = 100$ K
$\gamma = 107.198$ (5)°	Block, colorless
$V = 764.8$ (4) Å^3	$0.29 \times 0.11 \times 0.06$ mm

Data collection

Bruker SMART CCD area detector diffractometer	9076 measured reflections
Radiation source: fine-focus sealed tube	3728 independent reflections
Graphite monochromator	3475 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{int} = 0.015$
Absorption correction: multi-scan (SADABS; Bruker, 2013)	$\theta_{max} = 28.1°$, $\theta_{min} = 1.7°$
$T_{min} = 0.815$, $T_{max} = 0.989$	$h = -9 \rightarrow 9$
	$k = -12 \rightarrow 12$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.030$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.082$	
$S = 1.05$	H-atom parameters constrained
3728 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.4077P]$ where $P = (F_o^2 + 2F_c^2)/3$
208 parameters	
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.45$ e Å^{-3}
	$\Delta\rho_{min} = -0.34$ e Å^{-3}

Special details

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

Refinement. 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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	0.60965 (4)	0.67214 (3)	0.85449 (2)	0.01180 (8)
O1	0.67190 (12)	0.55058 (9)	0.89218 (7)	0.01731 (18)
O2	0.74722 (12)	0.78778 (9)	0.80246 (8)	0.01862 (18)
O3	0.27805 (12)	0.90586 (9)	0.92007 (7)	0.01539 (17)
O4	0.54722 (14)	0.41291 (10)	0.63921 (8)	0.0228 (2)
O5	0.57817 (15)	0.22722 (11)	0.72569 (10)	0.0296 (2)
N1	0.29029 (13)	0.71982 (10)	0.78749 (8)	0.01082 (18)
N2	0.49472 (15)	0.32058 (11)	0.70700 (9)	0.0170 (2)
C1	0.38198 (15)	0.60257 (11)	0.76329 (9)	0.0105 (2)
H1	0.4147	0.5983	0.6832	0.013*
C2	0.34073 (16)	0.80345 (12)	0.88860 (9)	0.0114 (2)
C3	0.49252 (16)	0.75554 (12)	0.95740 (9)	0.0136 (2)
H3A	0.4276	0.6827	1.0094	0.016*
H3B	0.5881	0.8429	1.0007	0.016*
C4	0.26158 (16)	0.44866 (12)	0.79064 (9)	0.0112 (2)
C5	0.31876 (16)	0.31896 (12)	0.76822 (9)	0.0130 (2)
C6	0.21380 (18)	0.18142 (13)	0.80081 (10)	0.0166 (2)
H6	0.2592	0.0968	0.7858	0.020*
C7	0.04245 (19)	0.16798 (14)	0.85541 (11)	0.0198 (2)
H7	−0.0318	0.0740	0.8773	0.024*
C8	−0.01917 (18)	0.29359 (14)	0.87772 (10)	0.0193 (2)
H8	−0.1375	0.2850	0.9143	0.023*
C9	0.08976 (17)	0.43194 (13)	0.84728 (10)	0.0146 (2)
H9	0.0464	0.5169	0.8654	0.018*
C10	0.18316 (16)	0.76881 (12)	0.69763 (9)	0.0117 (2)

H10	0.1191	0.8408	0.7335	0.014*
C11	0.02037 (16)	0.63935 (12)	0.63537 (9)	0.0137 (2)
H11A	−0.0743	0.5895	0.6886	0.016*
H11B	0.0783	0.5647	0.5997	0.016*
C12	−0.08705 (17)	0.69932 (13)	0.54591 (10)	0.0167 (2)
H12A	−0.1903	0.6151	0.5043	0.020*
H12B	−0.1522	0.7688	0.5824	0.020*
C13	0.05666 (19)	0.78087 (14)	0.46475 (10)	0.0190 (2)
H13A	−0.0150	0.8207	0.4090	0.023*
H13B	0.1151	0.7098	0.4244	0.023*
C14	0.22021 (18)	0.90929 (13)	0.52708 (10)	0.0188 (2)
H14A	0.1627	0.9848	0.5618	0.023*
H14B	0.3150	0.9582	0.4735	0.023*
C15	0.32904 (17)	0.85282 (13)	0.61788 (10)	0.0156 (2)
H15A	0.3984	0.7854	0.5827	0.019*
H15B	0.4287	0.9387	0.6602	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.00952 (13)	0.01062 (13)	0.01482 (14)	0.00278 (9)	−0.00059 (9)	0.00021 (9)
O1	0.0150 (4)	0.0156 (4)	0.0222 (4)	0.0069 (3)	−0.0040 (3)	0.0006 (3)
O2	0.0134 (4)	0.0156 (4)	0.0239 (4)	−0.0002 (3)	0.0037 (3)	0.0016 (3)
O3	0.0187 (4)	0.0137 (4)	0.0148 (4)	0.0072 (3)	0.0002 (3)	−0.0008 (3)
O4	0.0229 (4)	0.0203 (4)	0.0274 (5)	0.0086 (4)	0.0096 (4)	0.0034 (4)
O5	0.0233 (5)	0.0216 (5)	0.0491 (6)	0.0149 (4)	0.0014 (4)	0.0033 (4)
N1	0.0128 (4)	0.0093 (4)	0.0114 (4)	0.0050 (3)	−0.0005 (3)	0.0008 (3)
N2	0.0142 (4)	0.0121 (4)	0.0240 (5)	0.0047 (4)	−0.0021 (4)	−0.0039 (4)
C1	0.0104 (4)	0.0090 (5)	0.0123 (5)	0.0033 (4)	0.0000 (4)	0.0008 (4)
C2	0.0116 (5)	0.0102 (5)	0.0115 (5)	0.0015 (4)	0.0010 (4)	0.0024 (4)
C3	0.0154 (5)	0.0142 (5)	0.0119 (5)	0.0062 (4)	−0.0010 (4)	−0.0001 (4)
C4	0.0109 (5)	0.0104 (5)	0.0115 (5)	0.0022 (4)	−0.0022 (4)	0.0014 (4)
C5	0.0116 (5)	0.0121 (5)	0.0144 (5)	0.0031 (4)	−0.0030 (4)	0.0003 (4)
C6	0.0201 (5)	0.0104 (5)	0.0179 (5)	0.0030 (4)	−0.0065 (4)	0.0017 (4)
C7	0.0213 (6)	0.0147 (5)	0.0190 (6)	−0.0023 (4)	−0.0036 (4)	0.0065 (4)
C8	0.0160 (5)	0.0221 (6)	0.0176 (6)	0.0010 (4)	0.0028 (4)	0.0062 (5)
C9	0.0143 (5)	0.0151 (5)	0.0147 (5)	0.0047 (4)	0.0007 (4)	0.0022 (4)
C10	0.0131 (5)	0.0104 (5)	0.0122 (5)	0.0046 (4)	−0.0015 (4)	0.0015 (4)
C11	0.0130 (5)	0.0122 (5)	0.0145 (5)	0.0025 (4)	−0.0009 (4)	−0.0002 (4)
C12	0.0153 (5)	0.0189 (5)	0.0156 (5)	0.0062 (4)	−0.0030 (4)	−0.0011 (4)
C13	0.0228 (6)	0.0224 (6)	0.0130 (5)	0.0089 (5)	−0.0028 (4)	0.0022 (4)
C14	0.0224 (6)	0.0173 (5)	0.0169 (5)	0.0052 (5)	−0.0017 (4)	0.0067 (4)
C15	0.0155 (5)	0.0147 (5)	0.0160 (5)	0.0029 (4)	−0.0007 (4)	0.0047 (4)

Geometric parameters (Å, º)

S1—O1	1.4419 (9)	C7—C8	1.3858 (18)
S1—O2	1.4360 (9)	C8—H8	0.9500

S1—C1	1.8382 (12)	C8—C9	1.3896 (16)
S1—C3	1.7729 (12)	C9—H9	0.9500
O3—C2	1.2143 (14)	C10—H10	1.0000
O4—N2	1.2281 (14)	C10—C11	1.5276 (15)
O5—N2	1.2267 (14)	C10—C15	1.5291 (16)
N1—C1	1.4527 (13)	C11—H11A	0.9900
N1—C2	1.3671 (14)	C11—H11B	0.9900
N1—C10	1.4810 (14)	C11—C12	1.5354 (16)
N2—C5	1.4726 (15)	C12—H12A	0.9900
C1—H1	1.0000	C12—H12B	0.9900
C1—C4	1.5177 (15)	C12—C13	1.5242 (17)
C2—C3	1.5294 (15)	C13—H13A	0.9900
C3—H3A	0.9900	C13—H13B	0.9900
C3—H3B	0.9900	C13—C14	1.5257 (17)
C4—C5	1.4040 (15)	C14—H14A	0.9900
C4—C9	1.3963 (16)	C14—H14B	0.9900
C5—C6	1.3853 (16)	C14—C15	1.5342 (16)
C6—H6	0.9500	C15—H15A	0.9900
C6—C7	1.3841 (18)	C15—H15B	0.9900
C7—H7	0.9500		
O1—S1—C1	111.35 (5)	C9—C8—H8	119.5
O1—S1—C3	113.14 (6)	C4—C9—H9	119.3
O2—S1—O1	119.26 (6)	C8—C9—C4	121.39 (11)
O2—S1—C1	108.34 (5)	C8—C9—H9	119.3
O2—S1—C3	109.11 (6)	N1—C10—H10	107.5
C3—S1—C1	92.26 (5)	N1—C10—C11	112.55 (9)
C1—N1—C10	120.68 (9)	N1—C10—C15	109.90 (9)
C2—N1—C1	117.45 (9)	C11—C10—H10	107.5
C2—N1—C10	120.48 (9)	C11—C10—C15	111.61 (9)
O4—N2—C5	118.45 (10)	C15—C10—H10	107.5
O5—N2—O4	123.92 (11)	C10—C11—H11A	109.8
O5—N2—C5	117.62 (11)	C10—C11—H11B	109.8
S1—C1—H1	110.0	C10—C11—C12	109.49 (9)
N1—C1—S1	101.36 (7)	H11A—C11—H11B	108.2
N1—C1—H1	110.0	C12—C11—H11A	109.8
N1—C1—C4	114.61 (9)	C12—C11—H11B	109.8
C4—C1—S1	110.64 (7)	C11—C12—H12A	109.5
C4—C1—H1	110.0	C11—C12—H12B	109.5
O3—C2—N1	124.96 (10)	H12A—C12—H12B	108.1
O3—C2—C3	123.40 (10)	C13—C12—C11	110.88 (10)
N1—C2—C3	111.61 (9)	C13—C12—H12A	109.5
S1—C3—H3A	111.1	C13—C12—H12B	109.5
S1—C3—H3B	111.1	C12—C13—H13A	109.5
C2—C3—S1	103.22 (8)	C12—C13—H13B	109.5
C2—C3—H3A	111.1	C12—C13—C14	110.58 (10)
C2—C3—H3B	111.1	H13A—C13—H13B	108.1
H3A—C3—H3B	109.1	C14—C13—H13A	109.5

C5—C4—C1	123.62 (10)	C14—C13—H13B	109.5
C9—C4—C1	120.00 (10)	C13—C14—H14A	109.4
C9—C4—C5	116.27 (10)	C13—C14—H14B	109.4
C4—C5—N2	121.73 (10)	C13—C14—C15	111.06 (10)
C6—C5—N2	115.57 (10)	H14A—C14—H14B	108.0
C6—C5—C4	122.70 (11)	C15—C14—H14A	109.4
C5—C6—H6	120.2	C15—C14—H14B	109.4
C7—C6—C5	119.66 (11)	C10—C15—C14	110.26 (10)
C7—C6—H6	120.2	C10—C15—H15A	109.6
C6—C7—H7	120.5	C10—C15—H15B	109.6
C6—C7—C8	119.05 (11)	C14—C15—H15A	109.6
C8—C7—H7	120.5	C14—C15—H15B	109.6
C7—C8—H8	119.5	H15A—C15—H15B	108.1
C7—C8—C9	120.90 (12)		
S1—C1—C4—C5	−69.60 (12)	C1—C4—C5—C6	175.39 (10)
S1—C1—C4—C9	106.31 (10)	C1—C4—C9—C8	−177.24 (10)
O1—S1—C1—N1	148.94 (7)	C2—N1—C1—S1	−24.61 (11)
O1—S1—C1—C4	26.96 (9)	C2—N1—C1—C4	94.57 (11)
O1—S1—C3—C2	−147.19 (7)	C2—N1—C10—C11	−138.49 (10)
O2—S1—C1—N1	−78.01 (8)	C2—N1—C10—C15	96.45 (12)
O2—S1—C1—C4	160.01 (7)	C3—S1—C1—N1	32.98 (7)
O2—S1—C3—C2	77.52 (8)	C3—S1—C1—C4	−88.99 (8)
O3—C2—C3—S1	−153.99 (9)	C4—C5—C6—C7	1.63 (17)
O4—N2—C5—C4	−28.26 (16)	C5—C4—C9—C8	−1.03 (16)
O4—N2—C5—C6	151.15 (11)	C5—C6—C7—C8	−0.87 (17)
O5—N2—C5—C4	152.98 (11)	C6—C7—C8—C9	−0.79 (18)
O5—N2—C5—C6	−27.60 (15)	C7—C8—C9—C4	1.78 (18)
N1—C1—C4—C5	176.56 (10)	C9—C4—C5—N2	178.71 (10)
N1—C1—C4—C9	−7.52 (14)	C9—C4—C5—C6	−0.67 (16)
N1—C2—C3—S1	24.31 (11)	C10—N1—C1—S1	141.97 (8)
N1—C10—C11—C12	178.54 (9)	C10—N1—C1—C4	−98.85 (11)
N1—C10—C15—C14	−177.81 (9)	C10—N1—C2—O3	12.62 (16)
N2—C5—C6—C7	−177.78 (10)	C10—N1—C2—C3	−165.64 (9)
C1—S1—C3—C2	−32.79 (8)	C10—C11—C12—C13	57.68 (12)
C1—N1—C2—O3	179.23 (10)	C11—C10—C15—C14	56.59 (12)
C1—N1—C2—C3	0.97 (13)	C11—C12—C13—C14	−57.84 (13)
C1—N1—C10—C11	55.34 (13)	C12—C13—C14—C15	56.73 (13)
C1—N1—C10—C15	−69.72 (12)	C13—C14—C15—C10	−55.78 (13)
C1—C4—C5—N2	−5.23 (16)	C15—C10—C11—C12	−57.33 (12)

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···O1[i]	0.99	2.51	3.4594 (16)	161
C3—H3B···O3[ii]	0.99	2.37	3.3068 (16)	157

C9—H9···O1[iii]	0.95	2.80	3.5144 (16)	133
C10—H10···O2[iii]	1.00	2.72	3.4381 (16)	129

Symmetry codes: (i) −x+1, −y+1, −z+2; (ii) −x+1, −y+2, −z+2; (iii) x−1, y, z.