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5-Propyl-6-(*p*-tolylsulfanyl)pyrimidine-2,4(1*H*,3*H*)-dione

Fatmah A. M. Al-Omary,[a] Hazem A. Ghabbour,[a] Ali A. El-Emam,[a]‡ C. S. Chidan Kumar[b]§ and Hoong-Kun Fun[a]*¶

[a]Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, PO Box 2457, Riaydh 11451, Saudi Arabia, and [b]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hfun.c@ksu.edu.sa

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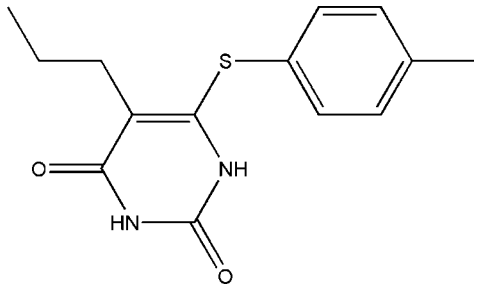
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.044; wR factor = 0.126; data-to-parameter ratio = 14.8.

In the title pymiridine-2,4-dione derivative, $C_{14}H_{16}N_2O_2S$, the dihedral angle between the six-membered rings is 66.69 (10)°. The molecule is twisted about the C_p—S (p = pyrimidine) bond, with a C—S—C—N torsion angle of −19.57 (16)°. In the crystal, adjacent molecules form inversion dimers through pairs of strong N—H···O hydrogen bonds, generating an $R_2^2(8)$ ring motif. The dimers are connected into chains extending along the *c*-axis direction through additional N—H···O hydrogen bonds.

Related literature

For the pharmacological activity of pyrimidine-2,4-dione derivatives, see: Al-Abdullah *et al.* (2011); El-Emam *et al.* (2004); Hopkins *et al.* (1996); Klein *et al.* (2001); Miyasaka *et al.* (1989); Nencka *et al.* (2006); Russ *et al.* (2003); Tanaka *et al.* (1995); For related pyrimidine-2,4-dione structures, see: El-Brollosy *et al.* (2009); Wang *et al.* (2006). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For reference bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{14}H_{16}N_2O_2S$
M_r = 276.35
Monoclinic, $P2_1/c$
a = 11.8356 (3) Å
b = 10.3040 (2) Å
c = 13.3999 (3) Å
β = 119.850 (2)°
V = 1417.37 (6) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.03 mm^{-1}
T = 293 K
0.82 × 0.71 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.287, T_{max} = 0.855
9643 measured reflections
2658 independent reflections
2450 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 1.06
2658 reflections
180 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*N*2···O1^{i}	0.84 (2)	1.98 (2)	2.815 (2)	173 (2)
N1—H1*N*1···O2^{ii}	0.79 (2)	2.17 (2)	2.8988 (18)	155 (2)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SJ5382).

References

Al-Abdullah, E. S., Al-Obaid, A. M., Al-Deeb, O. A., Habib, E. E. & El-Emam, A. A. (2011). *Eur. J. Med. Chem.* **46**, 4642–4647.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chamg, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2009). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
El-Brollosy, N. R., Al-Deeb, O. A., El-Emam, A. A., Pedersen, E. B., La Colla, P., Collu, G., Sanna, G. & Loddo, R. (2009). *Arch. Pharm.* **342**, 663–670.
El-Emam, A. A., Massoud, M. A., El-Bendary, E. R. & El-Sayed, M. A. (2004). *Bull. Korean Chem. Soc.* **25**, 991–996.

‡ Additonal correspondence author, e-mail: elemam5@hotmail.com.
§ Thomson Reuters ResearcherID: C-3194-2011.
¶ Thomson Reuters ResearcherID: A-3561-2009.

Hopkins, A. L., Ren, J., Esnouf, R. M., Willcox, B. E., Jones, E. Y., Ross, C., Miyasaka, T., Walker, R. T., Tanaka, H., Stammers, D. K. & Stuart, D. I. (1996). *J. Med. Chem.* **39**, 1589–1600.
Klein, R. S., Lenzi, M., Lim, T. H., Hotchkiss, K. A., Wilson, P. & Schwartz, E. L. (2001). *Biochem. Pharmacol.* **62**, 1257–1263.
Miyasaka, T., Tanaka, H., Baba, M., Hayakawa, H., Walker, R. T., Balzarini, J. & Clercq, E. D. (1989). *J. Med. Chem.* **32**, 2507–2509.
Nencka, R., Votruba, I., Hrebabecky, H., Tloust'ova, E., Horska, K., Masojidkova, M. & Holý, A. (2006). *Bioorg. Med. Chem. Lett.* **16**, 1335–1337.
Russ, P., Schelling, P., Scapozza, L., Folkers, G., De Clercq, E. & Marquez, V. E. (2003). *J. Med. Chem.* **46**, 5045–5054.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Tanaka, H., Takashima, H., Ubasawa, M., Sekiya, K., Inouye, N., Baba, M., Shigeta, S., Walker, R. T., Clercq, E. D. & Miyasaka, T. (1995). *J. Med. Chem.* **38**, 2860–2865.
Wang, X., Lou, Q., Guo, Y., Xu, Y., Zhang, Z. & Liu, J. (2006). *Org. Biomol. Chem.* **4**, 3252–3258.

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5-Propyl-6-(*p*-tolylsulfanyl)pyrimidine-2,4(1*H*,3*H*)-dione

Fatmah A. M. Al-Omary, Hazem A. Ghabbour, Ali A. El-Emam, C. S. Chidan Kumar and Hoong-Kun Fun

S1. Comment

Pyrimidine-2,4-diones and their related derivatives have long been known for their diverse chemotherapeutic activities including antiviral activity against the HIV (Miyasaka *et al.*, 1989; Tanaka *et al.*, 1995; Hopkins *et al.*, 1996; El-Emam *et al.*, 2004), and HSV viruses (Russ *et al.*, 2003). In addition, potent anticancer activity was observed for several pyrimidine-2,4-diones (Klein *et al.*, 2001; Nencka *et al.*, 2006). In continuation to our interest in the chemical and pharmacological properties of pyrimidine and uracil derivatives (Al-Abdullah *et al.*, 2011; El-Brollosy *et al.*, 2009), we have synthesized the title compound (I) as a potential chemotherapeutic agent.

The title compound (I) is a derivative of pymiridine-2,4-dione. The heterocycle contains the structural unit CON_2H_2CO, forming the dihedral angle of 66.69 (10)° with the adjacent benzene ring. The molecule is bent (Fig. 1) at the S atom with a C–S–C–N torsion angle of -19.57 (16)°. The bond lengths (Allen *et al.*, 1987) and angles in the title compound are within normal ranges and are comparable with those reported earlier (El-Brollosy *et al.*, 2009; Wang *et al.*, 2006). The crystal structure features for two types of intermolecular N–H···O hydrogen bonds (Table 1). Two adjacent molecules form inversion-related dimers through strong N2–H2A···O1 hydrogen bonds (symmetry code: -*x* + 1, -*y*, -*z* + 1), generating an $R_2^2(8)$ ring motif (Bernstein *et al.*, 1995) (Fig. 2). These dimers are further connected into chains extending along *c* axis through additional N1–H1N1···O2 hydrogen bonds (symmetry code: *x*, -*y* +1/2, *z* + 1/2) (Fig. 2). Crystal stability is mainly consolidated by these hydrogen bonding interactions forming two-dimensional networks parallel to the *bc* plane.

S2. Experimental

A mixture of 6-chloro-5-propyluracil (943 mg, 0.005 mol), *p*-thiocresol (621 mg, 0.005 mol) and potassium hydroxide (281 mg, 0.005 mol), in ethanol (10 ml), was heated under reflux for 3 h. The solvent was then distilled off *in vacuo* and the residue was washed with cold water, dried and crystallized from ethanol to yield 995 mg (72%) of the title compound ($C_{14}H_{16}N_2O_2S$) as colorless needle-like crystals. M·P.: 446–448 K.

^{1}H NMR (DMSO-d_6, 500.13 MHz): δ 0.84 (t, 3H, CH_2CH_3, J = 7.0 Hz), 1.38–1.40 (m, 2H, CH_2CH_3), 2.31 (s, 3H, Ar—CH_3), 2.44 (t, 2H, $CH_2CH_2CH_3$, J = 7.0 Hz), 7.22 (d, 2H, Ar—H, J = 7.0 Hz), 7.30 (d, 2H, Ar—H, J = 7.0 Hz), 10.74 (s, 1H, NH), 11.21 (s, 1H, NH). ^{13}C NMR (DMSO-d_6, 125.76 MHz): δ 13.73 (CH_2CH_3), 20.54 (CH_2CH_3), 22.05 ($CH_2CH_2CH_3$), 28.11 (Ar—CH_3), 116.60 (pyrimidine C-5), 128.10, 130.01, 130.18, 130.55 (Ar—C), 143.84 (pyrimidine C-6), 150.46 (C=O), 163.19 (C=O).

S3. Refinement

The nitrogen-bound H-atoms were located in a difference Fourier map and were refined freely. Other H atoms were positioned geometrically (C=H 0.93–0.97 Å) and refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C) for

methyl H atoms. A rotating group model was used for the methyl group.

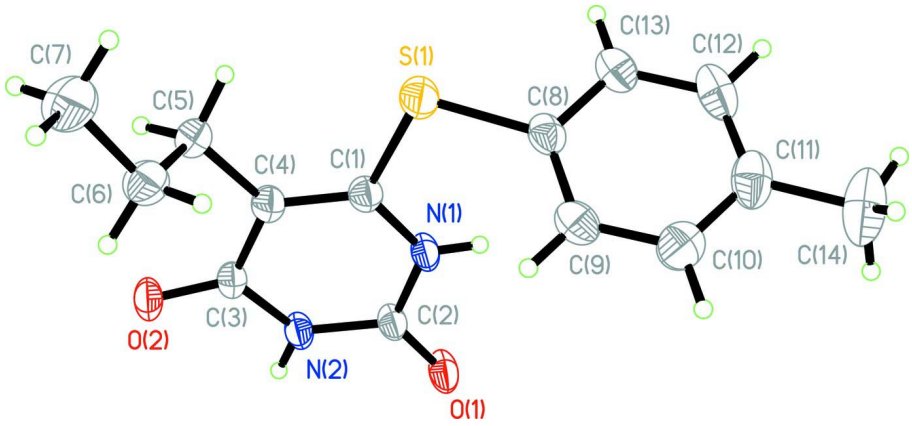

Figure 1

The molecular structure of the title compound with the atom labelling scheme and 30% probability displacement ellipsoids.

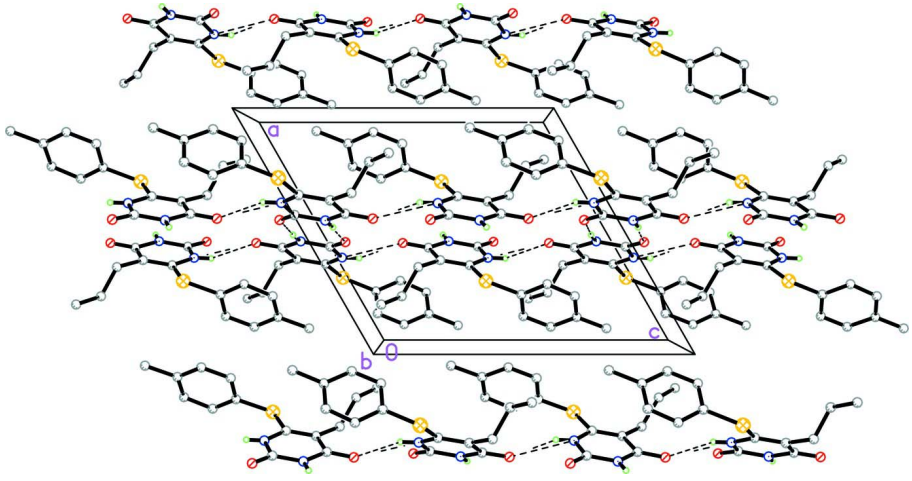

Figure 2

Crystal packing of the title compound, viewed along the *b* axis, showing the N1–H1N1···O2 and N2–H2N2···O1 intermolecular hydrogen bonds as dashed lines. H-atoms not involved in the hydrogen bonding are omited for clarity.

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Crystal data

$C_{14}H_{16}N_2O_2S$
$M_r = 276.35$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.8356$ (3) Å
$b = 10.3040$ (2) Å
$c = 13.3999$ (3) Å
$\beta = 119.850$ (2)°
$V = 1417.37$ (6) Å^3
$Z = 4$

$F(000) = 584$
$D_x = 1.295$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 5622 reflections
$\theta = 3.8$–$69.5°$
$\mu = 2.03$ mm^{-1}
$T = 293$ K
Needle, colourless
0.82 × 0.71 × 0.08 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.287, T_{max} = 0.855
9643 measured reflections
2658 independent reflections
2450 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 69.9°, θ_{min} = 4.3°
h = −14→14
k = −12→10
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 1.06
2658 reflections
180 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0707P)^2 + 0.439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.28497 (6)	0.53022 (5)	0.47950 (5)	0.0610 (2)
O1	0.45217 (15)	0.07980 (13)	0.58320 (11)	0.0594 (4)
N1	0.38171 (14)	0.28614 (14)	0.53086 (12)	0.0434 (3)
C1	0.35088 (16)	0.38803 (16)	0.45499 (14)	0.0426 (4)
O2	0.44741 (15)	0.24368 (14)	0.26889 (11)	0.0584 (4)
N2	0.45477 (15)	0.16770 (15)	0.42914 (12)	0.0441 (3)
C2	0.43133 (16)	0.17195 (16)	0.51850 (13)	0.0418 (4)
C3	0.42669 (17)	0.26374 (17)	0.34806 (14)	0.0438 (4)
C4	0.37290 (17)	0.38287 (17)	0.36542 (14)	0.0460 (4)
C5	0.3446 (2)	0.49234 (19)	0.28137 (16)	0.0529 (4)
H5A	0.4150	0.4980	0.2642	0.063*
H5B	0.3424	0.5733	0.3173	0.063*
C6	0.2176 (2)	0.4763 (2)	0.17021 (19)	0.0625 (5)
H6A	0.1478	0.4628	0.1872	0.075*
H6B	0.2225	0.4002	0.1300	0.075*

C7	0.1865 (3)	0.5949 (3)	0.0927 (2)	0.0891 (8)
H7A	0.1054	0.5816	0.0229	0.134*
H7B	0.2547	0.6076	0.0746	0.134*
H7C	0.1800	0.6702	0.1317	0.134*
C8	0.22523 (18)	0.47959 (18)	0.57142 (16)	0.0489 (4)
C9	0.1270 (2)	0.3881 (2)	0.53692 (18)	0.0586 (5)
H9A	0.0937	0.3477	0.4657	0.070*
C10	0.0791 (2)	0.3573 (2)	0.6090 (2)	0.0669 (6)
H10A	0.0149	0.2941	0.5866	0.080*
C11	0.1244 (2)	0.4185 (3)	0.7138 (2)	0.0694 (6)
C12	0.2192 (2)	0.5123 (3)	0.74454 (19)	0.0720 (6)
H12A	0.2485	0.5565	0.8136	0.086*
C13	0.2718 (2)	0.5423 (2)	0.67553 (18)	0.0587 (5)
H13A	0.3376	0.6040	0.6990	0.070*
C14	0.0734 (3)	0.3817 (4)	0.7929 (3)	0.1124 (13)
H14A	0.0086	0.3151	0.7575	0.169*
H14B	0.0353	0.4564	0.8074	0.169*
H14C	0.1438	0.3501	0.8643	0.169*
H2N2	0.483 (2)	0.096 (2)	0.4206 (19)	0.055 (6)*
H1N1	0.3791 (19)	0.291 (2)	0.5883 (19)	0.046 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0879 (4)	0.0444 (3)	0.0701 (4)	0.0183 (2)	0.0541 (3)	0.0103 (2)
O1	0.0977 (10)	0.0498 (7)	0.0494 (7)	0.0248 (7)	0.0507 (7)	0.0134 (6)
N1	0.0588 (8)	0.0447 (8)	0.0356 (7)	0.0101 (6)	0.0303 (6)	0.0027 (6)
C1	0.0483 (8)	0.0411 (9)	0.0399 (8)	0.0035 (7)	0.0231 (7)	0.0013 (7)
O2	0.0888 (9)	0.0579 (8)	0.0487 (7)	0.0058 (7)	0.0494 (7)	0.0040 (6)
N2	0.0609 (8)	0.0421 (8)	0.0392 (7)	0.0091 (6)	0.0323 (7)	0.0029 (6)
C2	0.0523 (8)	0.0434 (9)	0.0335 (7)	0.0081 (7)	0.0243 (7)	0.0018 (7)
C3	0.0545 (9)	0.0461 (9)	0.0367 (8)	−0.0002 (7)	0.0271 (7)	0.0009 (7)
C4	0.0560 (9)	0.0443 (9)	0.0414 (8)	0.0019 (7)	0.0270 (7)	0.0026 (7)
C5	0.0677 (11)	0.0465 (9)	0.0514 (10)	−0.0021 (8)	0.0348 (9)	0.0033 (8)
C6	0.0705 (12)	0.0537 (11)	0.0591 (12)	0.0046 (9)	0.0291 (10)	0.0076 (9)
C7	0.108 (2)	0.0711 (16)	0.0669 (14)	0.0175 (14)	0.0272 (14)	0.0261 (12)
C8	0.0557 (10)	0.0460 (10)	0.0498 (10)	0.0145 (7)	0.0299 (8)	0.0031 (7)
C9	0.0604 (11)	0.0551 (11)	0.0600 (11)	0.0097 (9)	0.0298 (9)	−0.0052 (9)
C10	0.0603 (11)	0.0616 (12)	0.0860 (15)	0.0110 (9)	0.0417 (11)	0.0096 (11)
C11	0.0625 (12)	0.0885 (16)	0.0680 (13)	0.0275 (12)	0.0407 (11)	0.0210 (12)
C12	0.0752 (14)	0.0937 (17)	0.0485 (11)	0.0216 (13)	0.0318 (10)	−0.0030 (11)
C13	0.0596 (11)	0.0623 (12)	0.0544 (11)	0.0090 (9)	0.0285 (9)	−0.0054 (9)
C14	0.099 (2)	0.167 (4)	0.102 (2)	0.038 (2)	0.0731 (19)	0.044 (2)

Geometric parameters (Å, º)

S1—C1	1.7658 (17)	C6—H6B	0.9700
S1—C8	1.7766 (19)	C7—H7A	0.9600

O1—C2	1.225 (2)	C7—H7B	0.9600
N1—C2	1.361 (2)	C7—H7C	0.9600
N1—C1	1.378 (2)	C8—C13	1.379 (3)
N1—H1N1	0.79 (2)	C8—C9	1.385 (3)
C1—C4	1.350 (2)	C9—C10	1.378 (3)
O2—C3	1.220 (2)	C9—H9A	0.9300
N2—C2	1.358 (2)	C10—C11	1.381 (4)
N2—C3	1.382 (2)	C10—H10A	0.9300
N2—H2N2	0.84 (3)	C11—C12	1.378 (4)
C3—C4	1.454 (2)	C11—C14	1.508 (3)
C4—C5	1.509 (2)	C12—C13	1.383 (3)
C5—C6	1.509 (3)	C12—H12A	0.9300
C5—H5A	0.9700	C13—H13A	0.9300
C5—H5B	0.9700	C14—H14A	0.9600
C6—C7	1.526 (3)	C14—H14B	0.9600
C6—H6A	0.9700	C14—H14C	0.9600

C1—S1—C8	104.50 (8)	C6—C7—H7A	109.5
C2—N1—C1	122.71 (14)	C6—C7—H7B	109.5
C2—N1—H1N1	114.1 (16)	H7A—C7—H7B	109.5
C1—N1—H1N1	122.9 (16)	C6—C7—H7C	109.5
C4—C1—N1	121.90 (15)	H7A—C7—H7C	109.5
C4—C1—S1	119.78 (13)	H7B—C7—H7C	109.5
N1—C1—S1	118.30 (12)	C13—C8—C9	120.23 (19)
C2—N2—C3	126.53 (15)	C13—C8—S1	117.82 (16)
C2—N2—H2N2	114.9 (16)	C9—C8—S1	121.72 (15)
C3—N2—H2N2	118.3 (16)	C10—C9—C8	119.5 (2)
O1—C2—N2	122.78 (15)	C10—C9—H9A	120.3
O1—C2—N1	122.06 (14)	C8—C9—H9A	120.3
N2—C2—N1	115.16 (14)	C9—C10—C11	121.3 (2)
O2—C3—N2	119.25 (16)	C9—C10—H10A	119.3
O2—C3—C4	125.16 (16)	C11—C10—H10A	119.3
N2—C3—C4	115.59 (14)	C12—C11—C10	118.1 (2)
C1—C4—C3	117.98 (15)	C12—C11—C14	121.2 (3)
C1—C4—C5	124.38 (16)	C10—C11—C14	120.8 (3)
C3—C4—C5	117.64 (15)	C11—C12—C13	121.8 (2)
C4—C5—C6	113.39 (16)	C11—C12—H12A	119.1
C4—C5—H5A	108.9	C13—C12—H12A	119.1
C6—C5—H5A	108.9	C8—C13—C12	119.0 (2)
C4—C5—H5B	108.9	C8—C13—H13A	120.5
C6—C5—H5B	108.9	C12—C13—H13A	120.5
H5A—C5—H5B	107.7	C11—C14—H14A	109.5
C5—C6—C7	111.6 (2)	C11—C14—H14B	109.5
C5—C6—H6A	109.3	H14A—C14—H14B	109.5
C7—C6—H6A	109.3	C11—C14—H14C	109.5
C5—C6—H6B	109.3	H14A—C14—H14C	109.5
C7—C6—H6B	109.3	H14B—C14—H14C	109.5
H6A—C6—H6B	108.0		

C2—N1—C1—C4	−2.7 (3)	N2—C3—C4—C5	178.08 (16)
C2—N1—C1—S1	179.11 (13)	C1—C4—C5—C6	−99.1 (2)
C8—S1—C1—C4	162.19 (15)	C3—C4—C5—C6	80.5 (2)
C8—S1—C1—N1	−19.57 (16)	C4—C5—C6—C7	174.6 (2)
C3—N2—C2—O1	175.69 (18)	C1—S1—C8—C13	123.21 (15)
C3—N2—C2—N1	−3.8 (3)	C1—S1—C8—C9	−62.23 (17)
C1—N1—C2—O1	−176.24 (17)	C13—C8—C9—C10	−2.0 (3)
C1—N1—C2—N2	3.3 (2)	S1—C8—C9—C10	−176.42 (15)
C2—N2—C3—O2	−176.34 (17)	C8—C9—C10—C11	1.8 (3)
C2—N2—C3—C4	3.4 (3)	C9—C10—C11—C12	0.3 (3)
N1—C1—C4—C3	2.1 (3)	C9—C10—C11—C14	−178.5 (2)
S1—C1—C4—C3	−179.72 (13)	C10—C11—C12—C13	−2.2 (3)
N1—C1—C4—C5	−178.32 (17)	C14—C11—C12—C13	176.6 (2)
S1—C1—C4—C5	−0.1 (2)	C9—C8—C13—C12	0.1 (3)
O2—C3—C4—C1	177.39 (17)	S1—C8—C13—C12	174.76 (16)
N2—C3—C4—C1	−2.3 (2)	C11—C12—C13—C8	2.0 (3)
O2—C3—C4—C5	−2.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*2···O1^{i}	0.84 (2)	1.98 (2)	2.815 (2)	173 (2)
N1—H1*N*1···O2^{ii}	0.79 (2)	2.17 (2)	2.8988 (18)	155 (2)

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