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4-Hydroxy-6-(4-methoxyphenyl)-4-phenyl-1,3-diazinane-2-thione

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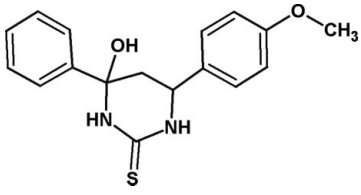
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.115; data-to-parameter ratio = 16.5.

In the title compound, $C_{17}H_{18}N_2O_2S$, the 1,3-diazinane-2-thione ring system is not coplanar with the benzene ring and methoxyphenyl ring system, the dihedral angle between the planes being 65.58 (13) and 89.18 (10)°, respectively. The crystal structure is characterized by intermolecular O—H···S, N—H···S, N—H···O and C—H···S hydrogen bonding.

Related literature

For general background to pyrimidines, see: Cheng (1969); Scott *et al.* (1959); Jonak *et al.* (1972); Falco *et al.* (1961); Ram (1990); Howells *et al.* (1981); Pershin *et al.* (1972); Matolcsy (1971); Prikazchikova *et al.* (1975). For the synthesis, see: Paghdar *et al.* (2007). For a related structure, see: Yamin *et al.* (2005).



Experimental

Crystal data

$C_{17}H_{18}N_2O_2S$
M_r = 314.39
Monoclinic, $P2_1/c$
a = 12.6016 (3) Å
b = 6.3375 (1) Å
c = 20.6637 (4) Å
β = 97.890 (2)°
V = 1634.64 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 295 K
0.18 × 0.16 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2010)
T_{min} = 0.963, T_{max} = 1.000
18135 measured reflections
3547 independent reflections
2566 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.115
S = 1.08
3547 reflections
215 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···S1^{i}	0.88 (3)	2.51 (3)	3.3688 (18)	169 (2)
C14—H14···S1^{i}	1.030 (19)	2.695 (18)	3.666 (2)	157.0 (14)
N4—H4···S1^{ii}	0.86	2.47	3.2990 (19)	163
N5—H5···O3^{iii}	0.86	2.18	3.032 (2)	169
C20—H20···S1^{iv}	0.93	2.86	3.772 (2)	166

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+2, -z+1$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank Professor T. N. Guru Row and Mr Venkatesha R. Hathwar, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, for their help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2177).

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Acta Cryst. (2011). E**67**, o815 [doi:10.1107/S1600536811008002]

4-Hydroxy-6-(4-methoxyphenyl)-4-phenyl-1,3-diazinane-2-thione

H. C. Devarajegowda, K. R. Roopashree, Irfan Ali Mohammed, Mahalakshmi and Ravish Sankolli

S1. Comment

Pyrimidines, being an integral part of DNA and RNA, exhibit diverse pharmacological properties as effective bactericide, fungicide, viricide, insecticide, and medicinal agents (Cheng, 1969; Scott *et al.*, 1959). Certain pyrimidines and annulated pyrimidine derivatives are also known to display anticancer, antimalarial, antileishmanial and antifilarial activities (Jonak *et al.*, 1972; Falco *et al.* 1961; Ram, 1990; Howells *et al.*, 1981). Pyrimidines and thio-pyrimidines play an essential role in several biological processes and have a considerable chemical and pharmacological importance. In particular, the pyrimidine nucleus can be found in a broad variety of antibacterial and antitumor agents as well as in agrochemical and veterinary products (Pershin *et al.*, 1972; Matolcsy, 1971; Prikazchikova *et al.*, 1975).

The asymmetric unit of the 4-hydroxy-6-(4-methoxyphenyl)-4-phenyl tetrahydropyrimidine-2(1*H*)-thione contains one molecule (Fig. 1). The thio-tetrahydropyrimidine ring system is not coplanar with the benzene ring and methoxyphenyl ring system; the dihedral angle between the two planes 65.58 (13)° and 89.18 (10)° respectively. The crystal structure shows intermolecular O2—H2···S1, N4—H4···S1, N5—H5···O3, C14—H14···S1 & C20—H20···S1 and C6—H6···S1 intramolecular hydrogen bonds. Bond distances and bond angles within the aromatic rings are in agreement with those observed in a related structure (Yamin *et al.*, 2005).

S2. Experimental

A general procedure for the synthesis of 4-hydroxy-6-(4-methoxyphenyl)- 4-phenyl-3,4-dihydropyrimidine-2(1*H*)-thione is given in Paghdar *et al.*, 2007. An equimolar mixture of (2E)-1,3-diphenylprop-2-en-1-one and thiourea (0.01 mol) were dissolved in minimum amount of ethanol. Potassium hydroxide solution (2.5 ml) was added slowly and the mixture stirred for 10 h until the entire mixture becomes very cloudy. Then the mixture was neutralized with 10% HCl and poured slowly into 100 ml of cold water with constant stirring. The precipitate obtained was filtered, washed and recrystallized from ethanol.

S3. Refinement

All H atoms were positioned at calculated positions with O—H = 0.88 Å, N—H = 0.86 Å, C—H = 0.93 Å for aromatic H and 0.96 Å for methyl H and refined a riding model $U_{iso}(H)$ = 1.5$U_{eq}(C)$ for methyl H and 1.2$U_{eq}(C)$ for other and also refined independently fixing C14 with C—H = 0.1.036 Å and C13 with C—H = 0.96 Å & 0.99 Å respectively.

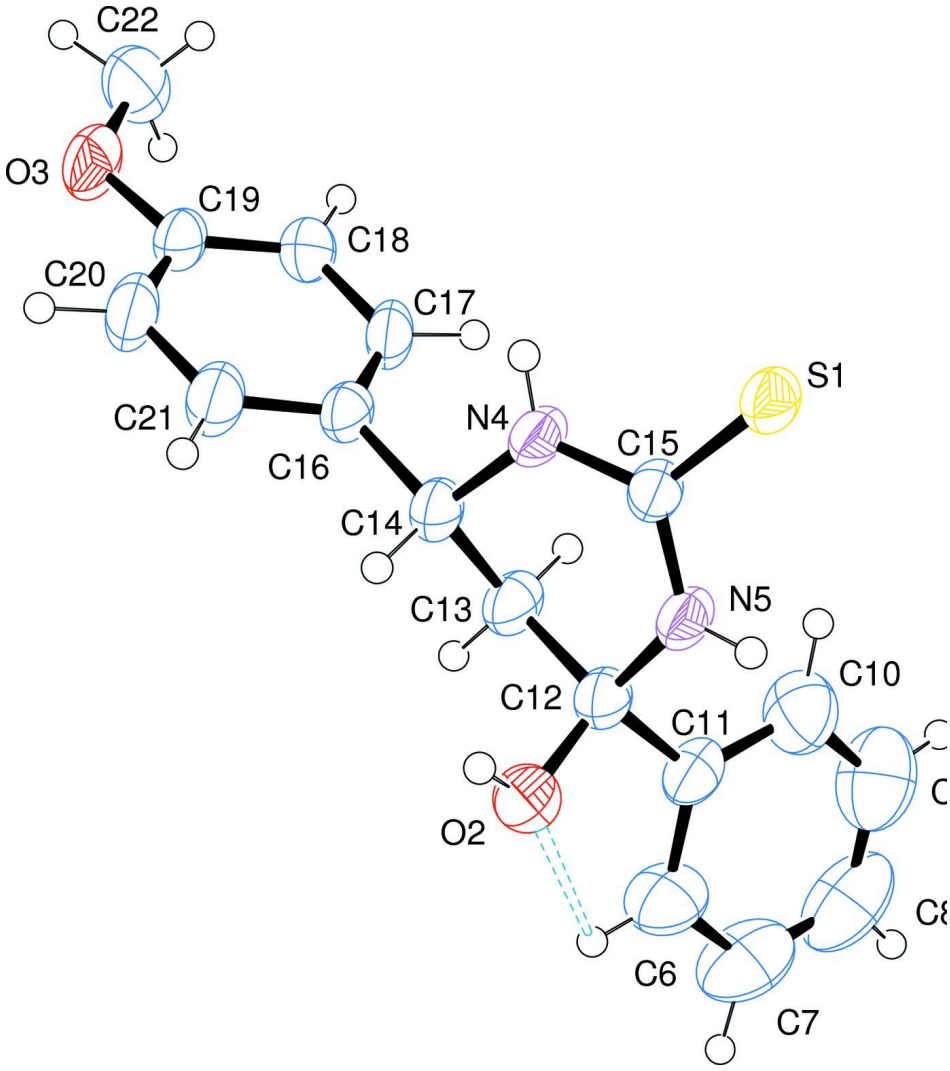

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds

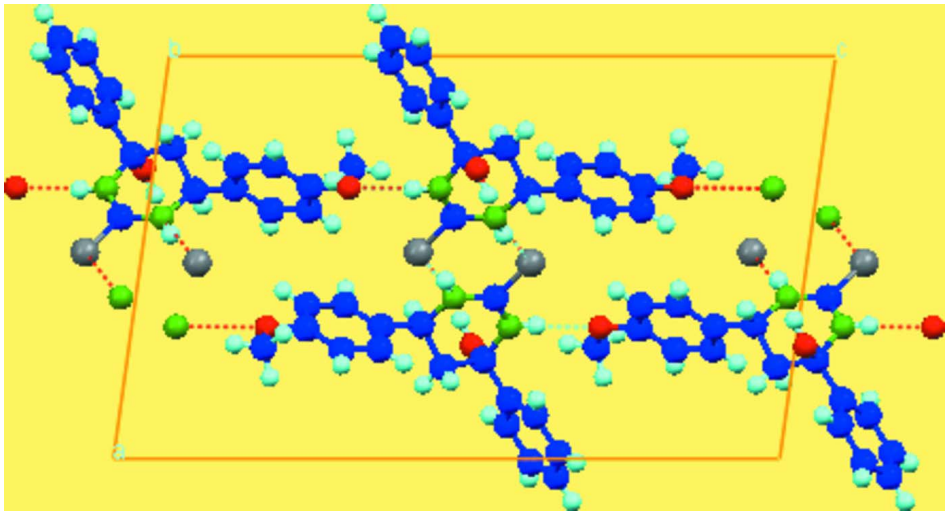

Figure 2

A packing view of the structure down the axis *b*.

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Crystal data

$C_{17}H_{18}N_2O_2S$
$M_r = 314.39$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.6016$ (3) Å
$b = 6.3375$ (1) Å
$c = 20.6637$ (4) Å
$\beta = 97.890$ (2)°
$V = 1634.64$ (6) Å^3
$Z = 4$
$F(000) = 664$
$D_x = 1.278$ Mg m^{-3}
Melting point: 392 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3547 reflections
$\theta = 2.4$–27.0°
$\mu = 0.21$ mm^{-1}
$T = 295$ K
Plate, colourless
0.18 × 0.16 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0839 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2010)
$T_{min} = 0.963$, $T_{max} = 1.000$
18135 measured reflections
3547 independent reflections
2566 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.4°$
$h = -16 \rightarrow 16$
$k = -8 \rightarrow 7$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.115$
$S = 1.08$
3547 reflections
215 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

$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 0.3347P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Special details

Experimental. *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.33.55 (release 05–01–2010 CrysAlis171. NET) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	0.48694 (4)	0.81337 (8)	0.41473 (2)	0.04465 (17)
O2	0.28051 (14)	0.2485 (2)	0.48527 (8)	0.0550 (4)
O3	0.32640 (13)	1.1217 (2)	0.79728 (7)	0.0595 (4)
N4	0.40048 (13)	0.7486 (3)	0.52278 (7)	0.0431 (4)
H4	0.4430	0.8470	0.5390	0.052*
N5	0.32830 (12)	0.5582 (2)	0.43340 (7)	0.0430 (4)
H5	0.3310	0.5243	0.3934	0.052*
C6	0.08485 (19)	0.2493 (4)	0.41656 (13)	0.0669 (7)
H6	0.1074	0.1390	0.4448	0.080*
C7	−0.0087 (2)	0.2288 (5)	0.37313 (17)	0.0873 (9)
H7	−0.0479	0.1044	0.3725	0.105*
C8	−0.0434 (2)	0.3852 (7)	0.33198 (16)	0.0943 (10)
H8	−0.1061	0.3690	0.3029	0.113*
C9	0.0139 (2)	0.5698 (6)	0.33308 (15)	0.0935 (9)
H9	−0.0101	0.6793	0.3049	0.112*
C10	0.1081 (2)	0.5928 (4)	0.37639 (13)	0.0715 (7)
H10	0.1466	0.7182	0.3770	0.086*
C11	0.14488 (16)	0.4324 (3)	0.41824 (10)	0.0464 (5)
C12	0.24682 (15)	0.4557 (3)	0.46603 (9)	0.0423 (5)
C13	0.22823 (17)	0.5908 (4)	0.52483 (10)	0.0474 (5)
C14	0.33350 (16)	0.6441 (3)	0.56604 (9)	0.0421 (5)
C15	0.39945 (14)	0.7009 (3)	0.46044 (9)	0.0369 (4)
C16	0.32722 (15)	0.7792 (3)	0.62573 (9)	0.0397 (4)
C17	0.27293 (16)	0.9682 (3)	0.62387 (9)	0.0454 (5)
H17	0.2372	1.0162	0.5842	0.055*
C18	0.27031 (16)	1.0888 (3)	0.67978 (9)	0.0456 (5)
H18	0.2329	1.2157	0.6776	0.055*
C19	0.32394 (16)	1.0182 (3)	0.73856 (9)	0.0442 (5)
C20	0.38044 (19)	0.8316 (4)	0.74086 (10)	0.0568 (6)
H20	0.4175	0.7849	0.7803	0.068*

C21	0.38211 (18)	0.7138 (3)	0.68487 (10)	0.0521 (5)
H21	0.4208	0.5885	0.6869	0.063*
C22	0.2770 (3)	1.3220 (4)	0.79812 (12)	0.0780 (8)
H22A	0.2851	1.3747	0.8421	0.117*
H22B	0.2022	1.3093	0.7818	0.117*
H22C	0.3101	1.4179	0.7710	0.117*
H2	0.345 (2)	0.244 (4)	0.5073 (14)	0.081 (9)*
H13A	0.1920 (17)	0.726 (3)	0.5100 (10)	0.054 (6)*
H13B	0.1841 (16)	0.512 (3)	0.5504 (10)	0.054 (6)*
H14	0.3700 (14)	0.504 (3)	0.5815 (9)	0.045 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0494 (3)	0.0552 (3)	0.0309 (3)	−0.0148 (2)	0.0107 (2)	−0.0048 (2)
O2	0.0585 (10)	0.0531 (9)	0.0499 (9)	−0.0108 (8)	−0.0050 (8)	0.0045 (7)
O3	0.0839 (11)	0.0644 (10)	0.0302 (7)	0.0027 (8)	0.0081 (7)	−0.0087 (7)
N4	0.0473 (9)	0.0555 (10)	0.0274 (8)	−0.0184 (8)	0.0085 (7)	−0.0080 (7)
N5	0.0476 (9)	0.0550 (10)	0.0273 (8)	−0.0169 (8)	0.0091 (7)	−0.0080 (7)
C6	0.0521 (14)	0.0733 (16)	0.0741 (17)	−0.0193 (12)	0.0038 (12)	−0.0066 (13)
C7	0.0505 (16)	0.109 (2)	0.099 (2)	−0.0249 (16)	−0.0020 (16)	−0.028 (2)
C8	0.0495 (16)	0.148 (3)	0.079 (2)	−0.002 (2)	−0.0135 (14)	−0.032 (2)
C9	0.0699 (19)	0.129 (3)	0.074 (2)	0.0122 (19)	−0.0166 (15)	0.0102 (19)
C10	0.0617 (15)	0.0838 (17)	0.0648 (17)	−0.0053 (14)	−0.0065 (13)	0.0077 (14)
C11	0.0424 (11)	0.0614 (13)	0.0356 (10)	−0.0074 (10)	0.0068 (9)	−0.0083 (9)
C12	0.0442 (11)	0.0490 (11)	0.0338 (10)	−0.0113 (9)	0.0061 (8)	−0.0011 (9)
C13	0.0492 (12)	0.0613 (14)	0.0335 (11)	−0.0173 (11)	0.0122 (9)	−0.0069 (10)
C14	0.0493 (11)	0.0496 (12)	0.0278 (10)	−0.0084 (10)	0.0072 (8)	−0.0008 (8)
C15	0.0373 (10)	0.0436 (10)	0.0293 (9)	−0.0026 (8)	0.0028 (8)	−0.0008 (8)
C16	0.0418 (10)	0.0504 (11)	0.0276 (9)	−0.0110 (9)	0.0076 (8)	−0.0007 (8)
C17	0.0509 (12)	0.0593 (13)	0.0251 (9)	−0.0048 (10)	0.0015 (8)	0.0054 (9)
C18	0.0528 (12)	0.0487 (11)	0.0362 (11)	−0.0010 (10)	0.0093 (9)	0.0011 (9)
C19	0.0541 (12)	0.0522 (12)	0.0273 (9)	−0.0091 (10)	0.0091 (9)	−0.0020 (8)
C20	0.0732 (15)	0.0646 (14)	0.0294 (11)	0.0062 (12)	−0.0038 (10)	0.0006 (10)
C21	0.0633 (14)	0.0564 (13)	0.0352 (11)	0.0064 (11)	0.0016 (10)	−0.0011 (9)
C22	0.134 (3)	0.0563 (15)	0.0468 (14)	−0.0004 (15)	0.0242 (15)	−0.0084 (11)

Geometric parameters (Å, º)

S1—C15	1.7033 (18)	C10—H10	0.9300
O2—C12	1.420 (2)	C11—C12	1.516 (3)
O2—H2	0.87 (3)	C12—C13	1.531 (3)
O3—C19	1.376 (2)	C13—C14	1.513 (3)
O3—C22	1.415 (3)	C13—H13A	1.00 (2)
N4—C15	1.321 (2)	C13—H13B	0.96 (2)
N4—C14	1.469 (2)	C14—C16	1.513 (3)
N4—H4	0.8600	C14—H14	1.029 (19)
N5—C15	1.340 (2)	C16—C17	1.377 (3)

N5—C12	1.456 (2)	C16—C21	1.382 (3)
N5—H5	0.8600	C17—C18	1.390 (3)
C6—C11	1.383 (3)	C17—H17	0.9300
C6—C7	1.386 (4)	C18—C19	1.381 (3)
C6—H6	0.9300	C18—H18	0.9300
C7—C8	1.340 (4)	C19—C20	1.378 (3)
C7—H7	0.9300	C20—C21	1.379 (3)
C8—C9	1.374 (5)	C20—H20	0.9300
C8—H8	0.9300	C21—H21	0.9300
C9—C10	1.393 (4)	C22—H22A	0.9600
C9—H9	0.9300	C22—H22B	0.9600
C10—C11	1.373 (3)	C22—H22C	0.9600

C12—O2—H2	113.2 (17)	C12—C13—H13B	108.1 (12)
C19—O3—C22	118.80 (17)	H13A—C13—H13B	109.9 (17)
C15—N4—C14	124.10 (16)	N4—C14—C16	109.86 (15)
C15—N4—H4	117.9	N4—C14—C13	106.90 (16)
C14—N4—H4	117.9	C16—C14—C13	116.45 (17)
C15—N5—C12	125.57 (15)	N4—C14—H14	107.9 (10)
C15—N5—H5	117.2	C16—C14—H14	107.9 (11)
C12—N5—H5	117.2	C13—C14—H14	107.6 (11)
C11—C6—C7	120.6 (3)	N4—C15—N5	118.50 (16)
C11—C6—H6	119.7	N4—C15—S1	121.63 (14)
C7—C6—H6	119.7	N5—C15—S1	119.87 (13)
C8—C7—C6	121.1 (3)	C17—C16—C21	118.15 (18)
C8—C7—H7	119.4	C17—C16—C14	123.44 (17)
C6—C7—H7	119.4	C21—C16—C14	118.37 (19)
C7—C8—C9	119.6 (3)	C16—C17—C18	121.58 (18)
C7—C8—H8	120.2	C16—C17—H17	119.2
C9—C8—H8	120.2	C18—C17—H17	119.2
C8—C9—C10	120.0 (3)	C19—C18—C17	119.23 (19)
C8—C9—H9	120.0	C19—C18—H18	120.4
C10—C9—H9	120.0	C17—C18—H18	120.4
C11—C10—C9	120.7 (3)	O3—C19—C20	115.45 (18)
C11—C10—H10	119.6	O3—C19—C18	124.77 (19)
C9—C10—H10	119.6	C20—C19—C18	119.79 (18)
C10—C11—C6	118.0 (2)	C19—C20—C21	120.2 (2)
C10—C11—C12	121.35 (19)	C19—C20—H20	119.9
C6—C11—C12	120.7 (2)	C21—C20—H20	119.9
O2—C12—N5	109.84 (16)	C20—C21—C16	121.1 (2)
O2—C12—C11	106.63 (16)	C20—C21—H21	119.5
N5—C12—C11	109.27 (15)	C16—C21—H21	119.5
O2—C12—C13	111.57 (17)	O3—C22—H22A	109.5
N5—C12—C13	108.21 (15)	O3—C22—H22B	109.5
C11—C12—C13	111.30 (16)	H22A—C22—H22B	109.5
C14—C13—C12	110.72 (17)	O3—C22—H22C	109.5
C14—C13—H13A	108.1 (12)	H22A—C22—H22C	109.5
C12—C13—H13A	110.4 (12)	H22B—C22—H22C	109.5

C14—C13—H13B	109.6 (12)		
C11—C6—C7—C8	−0.2 (4)	C12—C13—C14—N4	56.3 (2)
C6—C7—C8—C9	−0.5 (5)	C12—C13—C14—C16	179.46 (17)
C7—C8—C9—C10	0.5 (5)	C14—N4—C15—N5	4.5 (3)
C8—C9—C10—C11	0.1 (4)	C14—N4—C15—S1	−174.57 (15)
C9—C10—C11—C6	−0.8 (4)	C12—N5—C15—N4	3.2 (3)
C9—C10—C11—C12	−179.5 (2)	C12—N5—C15—S1	−177.72 (15)
C7—C6—C11—C10	0.9 (4)	N4—C14—C16—C17	69.8 (2)
C7—C6—C11—C12	179.6 (2)	C13—C14—C16—C17	−51.9 (3)
C15—N5—C12—O2	−101.5 (2)	N4—C14—C16—C21	−107.7 (2)
C15—N5—C12—C11	141.84 (19)	C13—C14—C16—C21	130.6 (2)
C15—N5—C12—C13	20.5 (3)	C21—C16—C17—C18	−1.7 (3)
C10—C11—C12—O2	−161.1 (2)	C14—C16—C17—C18	−179.17 (18)
C6—C11—C12—O2	20.3 (2)	C16—C17—C18—C19	0.4 (3)
C10—C11—C12—N5	−42.4 (3)	C22—O3—C19—C20	175.4 (2)
C6—C11—C12—N5	138.9 (2)	C22—O3—C19—C18	−4.4 (3)
C10—C11—C12—C13	77.0 (3)	C17—C18—C19—O3	−179.22 (18)
C6—C11—C12—C13	−101.6 (2)	C17—C18—C19—C20	1.0 (3)
O2—C12—C13—C14	70.8 (2)	O3—C19—C20—C21	179.17 (19)
N5—C12—C13—C14	−50.2 (2)	C18—C19—C20—C21	−1.0 (3)
C11—C12—C13—C14	−170.27 (18)	C19—C20—C21—C16	−0.3 (3)
C15—N4—C14—C16	−161.66 (18)	C17—C16—C21—C20	1.6 (3)
C15—N4—C14—C13	−34.5 (3)	C14—C16—C21—C20	179.26 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···S1^{i}	0.88 (3)	2.51 (3)	3.3688 (18)	169 (2)
C14—H14···S1^{i}	1.030 (19)	2.695 (18)	3.666 (2)	157.0 (14)
N4—H4···S1^{ii}	0.86	2.47	3.2990 (19)	163
N5—H5···O3^{iii}	0.86	2.18	3.032 (2)	169
C20—H20···S1^{iv}	0.93	2.86	3.772 (2)	166
C6—H6···O2	0.93	2.33	2.671 (3)	101

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) *x*, −*y*+3/2, *z*−1/2; (iv) *x*, −*y*+3/2, *z*+1/2.