Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-2-[4-*tert*-Butyl-5-(2,4,5-trimethoxybenzyl)thiazol-2-yliminomethyl]phenol

Ai-Xi Hu,[a]* Gao Cao[b] and Ying-Qi Ma[b]

[a]College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, People's Republic of China, and [b]School of Chemical and Energy Engineering, South China University of Technology, Guangzhou 510640, People's Republic of China
Correspondence e-mail: axhu0731@yahoo.com.cn

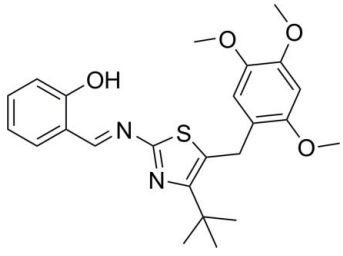
Received 22 November 2007; accepted 27 November 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.131; data-to-parameter ratio = 15.8.

In the title compound, $C_{24}H_{28}N_2O_4S$, the dihedral angle between the phenol ring and the thiazole ring system is 10.6 (1)°, and the trimethoxyphenyl group is approximately perpendicular to the thiazole ring, the dihedral angle being 84.7 (2)°. There is a strong intramolecular hydrogen-bonding interaction between the Schiff base and the hydroxy group.

Related literature

For general background, see: Modi *et al.* (1971); More *et al.* (2001).



Experimental

Crystal data

$C_{24}H_{28}N_2O_4S$
M_r = 440.54
Triclinic, $P\overline{1}$
a = 10.9137 (6) Å
b = 11.0904 (6) Å
c = 11.1260 (6) Å
α = 64.933 (1)°
β = 72.383 (1)°
γ = 83.202 (1)°
V = 1162.54 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 293 (2) K
0.48 × 0.44 × 0.42 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.922, T_{max} = 0.932
9103 measured reflections
4524 independent reflections
3450 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.131
S = 1.05
4524 reflections
287 parameters
24 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.82	1.89	2.612 (2)	147

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2213).

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More, P. G., Bhalvankar, R. B. & Pattar, S. C. (2001). *J. Indian Chem. Soc.* **78**, 474–475.
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supporting information

Acta Cryst. (2008). E**64**, o191 [https://doi.org/10.1107/S1600536807063921]

(*E*)-2-[4-*tert*-Butyl-5-(2,4,5-trimethoxybenzyl)thiazol-2-yliminomethyl]phenol

Ai-Xi Hu, Gao Cao and Ying-Qi Ma

S1. Comment

Thiazoles exhibit a wide range of biological activities and Schiff bases play an important role in many biological processes (More *et al.*, 2001). Schiff bases from benzaldehyde nitrogen mustards and *p*-aminophenylthiazole were reported to have significant anticancer activity (Modi *et al.*, 1971). As part of our research program concerning the anticancer behaviour of thiazole Schiff bases, the title compound (I) has been synthesized and characterized (Fig. 1).

Geometric parameters are in the normal ranges. The length of C=N double bond is 1.280 (3) Å. The dihedral angle between the phenol group and the thiazole ring system is 10.6 (1)°, and the 2,4,5-trimethoxybenzyl group is approximately perpendicular to the thiazole ring with a dihedral angle of 84.7 (2)°. There is a strong intramolecular hydrogen bond between the nitrogen atom of Schiff base and the hydroxy group (Table 1). Packing diagram of (I) in a unit cell is shown in Fig. 2.

S2. Experimental

A solution of thiourea (0.03 mol) and 2-bromo-4,4-dimethyl-1-(2,4,5-trimethoxyphenyl)pentan-3-one (0.03 mol) in ethanol (70 ml) was refluxed for 8 h (monitoring by TLC). Then excess of the solvent was evaporated, the residue was made alkaline by ammonia, filtered and the solid recrystallized from ethanol, dried to give 4-*tert*-butyl-5-(2,4,5-trimethoxybenzyl)thiazol-2-amine. Then a mixture of appropriate aminothiazole (10 mmol), appropriate salicylaldehyde (10 mmol) in ethanol (50 ml) and piperidine (3–4 drops) was refluxed in a water-bath at 353 K for about 6.5 h. After the reaction was over, the reaction mixture was cooled and the crystals separated were filtered and recrystallized from ethanol to give (I). Yield: 87.3%. m.p. 425–426 K.

Crystals suitable for X-ray structure determination were obtained by slow evaporation of an ethanol solution at room temperature.

S3. Refinement

The hydroxy H atom was positioned geometrically (O—H = 0.82 Å) and refined as riding [U_{iso}(H) = 1.5 U_{eq}(O)]. Methyl H atoms were positioned geometrically (C—H = 0.96 Å) and torsion angles refined to fit the electron density [U_{iso}(H) = 1.5 U_{eq}(C)]. Other H atoms were placed in calculated positions (methylene C—H = 0.97 Å, C4—H4 = 0.93 Å and aromatic C—H = 0.93 Å) and refined as riding [U_{iso}(H) = 1.2 U_{eq}(C)].

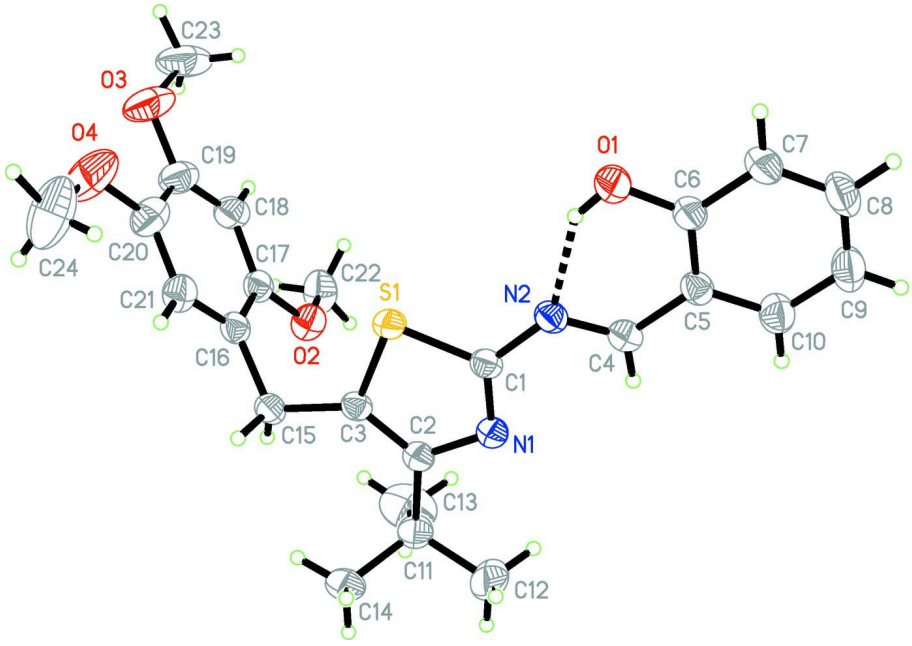

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

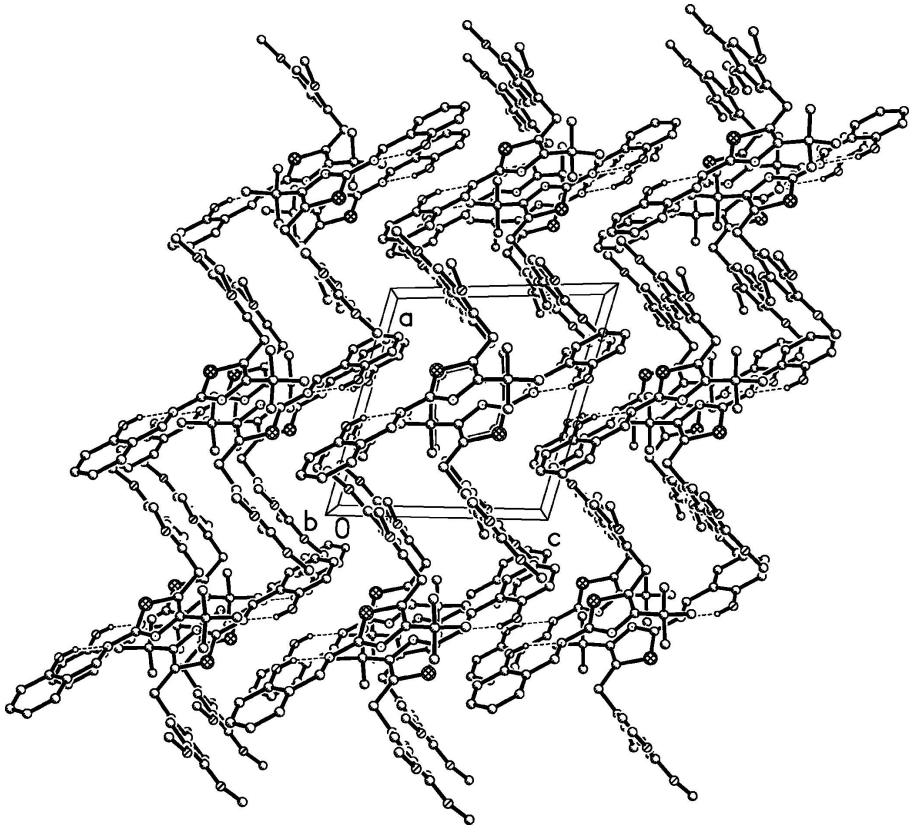

Figure 2

A packing diagram for (I). H atoms bonded to C atoms have been omitted for clarity. Dashed lines indicate hydrogen bonds.

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$F(000) = 468$
$D_x = 1.259$ Mg m^{-3}
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Cell parameters from 4266 reflections
$\theta = 2.3$–$26.9°$
$\mu = 0.17$ mm^{-1}
$T = 293$ K
Block, yellow
0.48 × 0.44 × 0.42 mm

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Bruker SMART 1K CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.922$, $T_{max} = 0.932$
9103 measured reflections
4524 independent reflections
3450 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.0°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.131$
$S = 1.05$
4524 reflections
287 parameters
24 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.4082P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Experimental. Spectroscopic analysis: ^{1}H-NMR ($CDCl_3$, 400 MHz) (p.p.m.): 1.48(s, 9H, $(CH_3)_3$), 3.80, 3.82, 3.91(3×s, 9H, 3×CH_3O), 4.19(s, 2H, CH_2), 6.55, 6.69(2×s, 2H, 2,4,5-$(OCH_3)_3C_6H_2$), 6.93(dd, J = 8.0 Hz, J= 8.0 Hz, 1H, 2-$HOC_6H_4$5-H), 6.99(d, J= 8.0 Hz, 1H, 2-$HOC_6H_4$3-H), 7.39(ddd, J = 8.0 Hz, J = 8.0 Hz, J = 1.6 Hz, 1H, 2-$HOC_6H_4$4-H), 7.42(dd, J = 8.0 Hz, J = 1.6 Hz, 1H, 2-$HOC_6H_4$6-H), 9.02(s, 1H, N=CH), 12.32(s, 1H, OH).

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	0.63017 (5)	0.60302 (5)	0.32907 (5)	0.05115 (17)
C1	0.52224 (18)	0.72677 (19)	0.33490 (19)	0.0465 (4)
C2	0.59138 (19)	0.6896 (2)	0.5140 (2)	0.0488 (5)
C3	0.66530 (17)	0.59963 (19)	0.47095 (18)	0.0445 (4)
C4	0.39884 (19)	0.8906 (2)	0.2148 (2)	0.0511 (5)
H4	0.3968	0.9315	0.2731	0.061*
C5	0.33379 (19)	0.9527 (2)	0.1080 (2)	0.0502 (5)
C6	0.3394 (2)	0.9001 (2)	0.0126 (2)	0.0556 (5)
C7	0.2783 (2)	0.9653 (3)	−0.0905 (2)	0.0715 (7)
H7	0.2832	0.9316	−0.1554	0.086*
C8	0.2110 (2)	1.0789 (3)	−0.0969 (3)	0.0781 (7)
H8	0.1704	1.1215	−0.1663	0.094*
C9	0.2023 (3)	1.1309 (3)	−0.0031 (3)	0.0786 (7)
H9	0.1552	1.2075	−0.0077	0.094*
C10	0.2638 (2)	1.0689 (2)	0.0975 (3)	0.0677 (6)
H10	0.2589	1.1050	0.1605	0.081*
C11	0.5924 (3)	0.7197 (3)	0.6354 (2)	0.0701 (6)
C12	0.4742 (4)	0.7988 (4)	0.6703 (3)	0.1338 (15)
H12A	0.4741	0.8808	0.5914	0.201*
H12B	0.4755	0.8177	0.7465	0.201*
H12C	0.3983	0.7479	0.6951	0.201*
C13	0.7146 (4)	0.7995 (4)	0.5940 (4)	0.1271 (13)
H13A	0.7884	0.7490	0.5703	0.191*
H13B	0.7181	0.8176	0.6700	0.191*
H13C	0.7140	0.8819	0.5157	0.191*
C14	0.5886 (3)	0.5915 (3)	0.7651 (2)	0.0854 (8)
H14A	0.5159	0.5380	0.7854	0.128*
H14B	0.5814	0.6133	0.8417	0.128*
H14C	0.6662	0.5427	0.7495	0.128*
C15	0.76608 (18)	0.5036 (2)	0.5243 (2)	0.0509 (5)
H15A	0.8073	0.5396	0.5681	0.061*
H15B	0.7246	0.4202	0.5939	0.061*
C16	0.86707 (18)	0.4771 (2)	0.4116 (2)	0.0496 (5)
C17	0.95846 (18)	0.5741 (2)	0.3172 (2)	0.0519 (5)
C18	1.0483 (2)	0.5553 (3)	0.2080 (2)	0.0637 (6)
H18	1.1078	0.6221	0.1439	0.076*
C19	1.0488 (2)	0.4373 (3)	0.1951 (3)	0.0732 (7)
C20	0.9608 (3)	0.3373 (3)	0.2909 (3)	0.0752 (7)
C21	0.8698 (2)	0.3587 (2)	0.3973 (2)	0.0625 (6)
H21	0.8094	0.2924	0.4603	0.075*
C22	1.0551 (2)	0.7806 (2)	0.2629 (3)	0.0811 (8)
H22A	1.1336	0.7361	0.2775	0.122*
H22B	1.0411	0.8510	0.2941	0.122*
H22C	1.0608	0.8173	0.1662	0.122*
C23	1.2105 (3)	0.5148 (4)	−0.0208 (3)	0.1211 (13)

H23A	1.1569	0.5858	−0.0623	0.182*
H23B	1.2617	0.4832	−0.0883	0.182*
H23C	1.2658	0.5469	0.0121	0.182*
C24	0.8942 (5)	0.1181 (4)	0.3630 (6)	0.1547 (19)
H24A	0.9150	0.0846	0.4494	0.232*
H24B	0.9070	0.0496	0.3294	0.232*
H24C	0.8061	0.1453	0.3764	0.232*
N1	0.51002 (16)	0.76202 (17)	0.43512 (16)	0.0512 (4)
N2	0.45913 (15)	0.78106 (17)	0.23124 (16)	0.0501 (4)
O1	0.40160 (19)	0.78624 (19)	0.01767 (18)	0.0806 (5)
H1	0.4365	0.7590	0.0800	0.121*
O2	0.95144 (14)	0.68869 (15)	0.33783 (16)	0.0659 (4)
O3	1.1324 (2)	0.4094 (3)	0.0912 (2)	0.1084 (7)
O4	0.9706 (3)	0.2228 (3)	0.2707 (3)	0.1280 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0522 (3)	0.0601 (3)	0.0439 (3)	0.0063 (2)	−0.0152 (2)	−0.0243 (2)
C1	0.0443 (10)	0.0521 (11)	0.0390 (10)	−0.0018 (8)	−0.0105 (8)	−0.0152 (8)
C2	0.0509 (11)	0.0518 (11)	0.0431 (10)	0.0017 (9)	−0.0144 (9)	−0.0184 (9)
C3	0.0404 (9)	0.0503 (10)	0.0389 (9)	−0.0028 (8)	−0.0095 (8)	−0.0150 (8)
C4	0.0526 (11)	0.0547 (12)	0.0458 (11)	−0.0039 (9)	−0.0146 (9)	−0.0187 (9)
C5	0.0462 (10)	0.0526 (11)	0.0457 (10)	−0.0030 (9)	−0.0130 (8)	−0.0135 (9)
C6	0.0506 (11)	0.0651 (13)	0.0473 (11)	0.0059 (10)	−0.0158 (9)	−0.0195 (10)
C7	0.0700 (15)	0.0908 (18)	0.0557 (13)	0.0123 (13)	−0.0288 (12)	−0.0274 (13)
C8	0.0658 (15)	0.0885 (19)	0.0678 (15)	0.0092 (14)	−0.0341 (13)	−0.0122 (14)
C9	0.0777 (17)	0.0661 (15)	0.0836 (18)	0.0169 (13)	−0.0337 (14)	−0.0194 (14)
C10	0.0745 (15)	0.0587 (13)	0.0707 (15)	0.0070 (11)	−0.0277 (12)	−0.0240 (12)
C11	0.0889 (17)	0.0793 (16)	0.0610 (14)	0.0212 (13)	−0.0340 (12)	−0.0425 (12)
C12	0.185 (3)	0.166 (3)	0.097 (2)	0.108 (3)	−0.078 (2)	−0.098 (2)
C13	0.174 (3)	0.130 (3)	0.116 (3)	−0.041 (3)	−0.054 (3)	−0.067 (2)
C14	0.100 (2)	0.112 (2)	0.0506 (13)	0.0261 (16)	−0.0310 (13)	−0.0392 (14)
C15	0.0459 (10)	0.0548 (11)	0.0438 (10)	0.0023 (9)	−0.0125 (8)	−0.0130 (9)
C16	0.0422 (10)	0.0548 (11)	0.0469 (11)	0.0054 (9)	−0.0157 (8)	−0.0153 (9)
C17	0.0420 (10)	0.0581 (12)	0.0516 (11)	0.0053 (9)	−0.0159 (9)	−0.0181 (10)
C18	0.0456 (11)	0.0832 (16)	0.0547 (13)	0.0020 (11)	−0.0095 (10)	−0.0245 (12)
C19	0.0590 (14)	0.104 (2)	0.0664 (15)	0.0146 (14)	−0.0160 (12)	−0.0484 (15)
C20	0.0733 (16)	0.0789 (17)	0.0897 (18)	0.0105 (13)	−0.0240 (14)	−0.0513 (15)
C21	0.0590 (13)	0.0573 (13)	0.0682 (14)	0.0010 (10)	−0.0163 (11)	−0.0241 (11)
C22	0.0606 (14)	0.0619 (15)	0.099 (2)	−0.0083 (12)	−0.0180 (14)	−0.0138 (14)
C23	0.084 (2)	0.209 (4)	0.074 (2)	0.005 (2)	0.0011 (17)	−0.077 (3)
C24	0.153 (4)	0.088 (3)	0.252 (6)	0.015 (3)	−0.062 (4)	−0.097 (3)
N1	0.0518 (9)	0.0570 (10)	0.0465 (9)	0.0069 (8)	−0.0162 (7)	−0.0228 (8)
N2	0.0473 (9)	0.0575 (10)	0.0437 (9)	0.0004 (8)	−0.0152 (7)	−0.0173 (8)
O1	0.0993 (13)	0.0948 (13)	0.0727 (11)	0.0399 (10)	−0.0488 (10)	−0.0505 (10)
O2	0.0539 (9)	0.0601 (9)	0.0748 (10)	−0.0058 (7)	−0.0072 (7)	−0.0250 (8)
O3	0.0873 (14)	0.157 (2)	0.0968 (15)	0.0142 (14)	−0.0022 (12)	−0.0863 (16)

O4	0.133 (2)	0.1112 (18)	0.165 (2)	0.0027 (15)	−0.0126 (17)	−0.1002 (19)

Geometric parameters (Å, º)

S1—C1	1.709 (2)	C14—H14A	0.9600
S1—C3	1.7184 (19)	C14—H14B	0.9600
C1—N1	1.297 (2)	C14—H14C	0.9600
C1—N2	1.400 (2)	C15—C16	1.507 (3)
C2—C3	1.363 (3)	C15—H15A	0.9700
C2—N1	1.382 (2)	C15—H15B	0.9700
C2—C11	1.525 (3)	C16—C21	1.384 (3)
C3—C15	1.509 (3)	C16—C17	1.385 (3)
C4—N2	1.280 (3)	C17—O2	1.373 (3)
C4—C5	1.446 (3)	C17—C18	1.388 (3)
C4—H4	0.9300	C18—C19	1.375 (3)
C5—C6	1.396 (3)	C18—H18	0.9300
C5—C10	1.397 (3)	C19—O3	1.365 (3)
C6—O1	1.349 (3)	C19—C20	1.386 (4)
C6—C7	1.389 (3)	C20—O4	1.367 (3)
C7—C8	1.367 (3)	C20—C21	1.384 (3)
C7—H7	0.9300	C21—H21	0.9300
C8—C9	1.367 (4)	C22—O2	1.413 (3)
C8—H8	0.9300	C22—H22A	0.9600
C9—C10	1.367 (3)	C22—H22B	0.9600
C9—H9	0.9300	C22—H22C	0.9600
C10—H10	0.9300	C23—O3	1.416 (4)
C11—C12	1.517 (4)	C23—H23A	0.9600
C11—C13	1.529 (4)	C23—H23B	0.9600
C11—C14	1.532 (4)	C23—H23C	0.9600
C12—H12A	0.9600	C24—O4	1.341 (5)
C12—H12B	0.9600	C24—H24A	0.9600
C12—H12C	0.9600	C24—H24B	0.9600
C13—H13A	0.9600	C24—H24C	0.9600
C13—H13B	0.9600	O1—H1	0.8200
C13—H13C	0.9600		

C1—S1—C3	89.45 (9)	C11—C14—H14C	109.5
N1—C1—N2	127.00 (18)	H14A—C14—H14C	109.5
N1—C1—S1	115.35 (14)	H14B—C14—H14C	109.5
N2—C1—S1	117.64 (14)	C16—C15—C3	112.66 (16)
C3—C2—N1	114.89 (17)	C16—C15—H15A	109.1
C3—C2—C11	127.01 (18)	C3—C15—H15A	109.1
N1—C2—C11	118.08 (18)	C16—C15—H15B	109.1
C2—C3—C15	132.31 (18)	C3—C15—H15B	109.1
C2—C3—S1	109.68 (14)	H15A—C15—H15B	107.8
C15—C3—S1	118.01 (14)	C21—C16—C17	118.45 (19)
N2—C4—C5	121.83 (19)	C21—C16—C15	121.81 (19)
N2—C4—H4	119.1	C17—C16—C15	119.72 (19)

C5—C4—H4	119.1	O2—C17—C16	115.65 (18)
C6—C5—C10	118.15 (19)	O2—C17—C18	123.3 (2)
C6—C5—C4	121.68 (19)	C16—C17—C18	121.0 (2)
C10—C5—C4	120.2 (2)	C19—C18—C17	119.6 (2)
O1—C6—C7	118.3 (2)	C19—C18—H18	120.2
O1—C6—C5	122.07 (18)	C17—C18—H18	120.2
C7—C6—C5	119.6 (2)	O3—C19—C18	124.1 (3)
C8—C7—C6	120.2 (2)	O3—C19—C20	115.6 (3)
C8—C7—H7	119.9	C18—C19—C20	120.3 (2)
C6—C7—H7	119.9	O4—C20—C21	124.6 (3)
C9—C8—C7	121.2 (2)	O4—C20—C19	115.9 (2)
C9—C8—H8	119.4	C21—C20—C19	119.4 (2)
C7—C8—H8	119.4	C20—C21—C16	121.2 (2)
C8—C9—C10	119.1 (2)	C20—C21—H21	119.4
C8—C9—H9	120.4	C16—C21—H21	119.4
C10—C9—H9	120.4	O2—C22—H22A	109.5
C9—C10—C5	121.7 (2)	O2—C22—H22B	109.5
C9—C10—H10	119.2	H22A—C22—H22B	109.5
C5—C10—H10	119.2	O2—C22—H22C	109.5
C12—C11—C2	109.8 (2)	H22A—C22—H22C	109.5
C12—C11—C13	110.4 (3)	H22B—C22—H22C	109.5
C2—C11—C13	108.1 (2)	O3—C23—H23A	109.5
C12—C11—C14	107.2 (2)	O3—C23—H23B	109.5
C2—C11—C14	111.3 (2)	H23A—C23—H23B	109.5
C13—C11—C14	110.0 (2)	O3—C23—H23C	109.5
C11—C12—H12A	109.5	H23A—C23—H23C	109.5
C11—C12—H12B	109.5	H23B—C23—H23C	109.5
H12A—C12—H12B	109.5	O4—C24—H24A	109.5
C11—C12—H12C	109.5	O4—C24—H24B	109.5
H12A—C12—H12C	109.5	H24A—C24—H24B	109.5
H12B—C12—H12C	109.5	O4—C24—H24C	109.5
C11—C13—H13A	109.5	H24A—C24—H24C	109.5
C11—C13—H13B	109.5	H24B—C24—H24C	109.5
H13A—C13—H13B	109.5	C1—N1—C2	110.61 (17)
C11—C13—H13C	109.5	C4—N2—C1	119.30 (17)
H13A—C13—H13C	109.5	C6—O1—H1	109.5
H13B—C13—H13C	109.5	C17—O2—C22	118.54 (18)
C11—C14—H14A	109.5	C19—O3—C23	117.8 (3)
C11—C14—H14B	109.5	C24—O4—C20	119.8 (3)
H14A—C14—H14B	109.5		

C3—S1—C1—N1	−1.29 (16)	C3—C15—C16—C17	73.2 (2)
C3—S1—C1—N2	177.33 (15)	C21—C16—C17—O2	−179.37 (18)
N1—C2—C3—C15	179.01 (18)	C15—C16—C17—O2	2.1 (3)
C11—C2—C3—C15	0.7 (4)	C21—C16—C17—C18	2.1 (3)
N1—C2—C3—S1	−1.1 (2)	C15—C16—C17—C18	−176.49 (18)
C11—C2—C3—S1	−179.50 (18)	O2—C17—C18—C19	179.9 (2)
C1—S1—C3—C2	1.31 (15)	C16—C17—C18—C19	−1.7 (3)

C1—S1—C3—C15	−178.82 (15)	C17—C18—C19—O3	179.6 (2)
N2—C4—C5—C6	−3.6 (3)	C17—C18—C19—C20	−0.4 (4)
N2—C4—C5—C10	176.90 (19)	O3—C19—C20—O4	1.3 (4)
C10—C5—C6—O1	−178.0 (2)	C18—C19—C20—O4	−178.8 (2)
C4—C5—C6—O1	2.4 (3)	O3—C19—C20—C21	−178.0 (2)
C10—C5—C6—C7	1.3 (3)	C18—C19—C20—C21	2.0 (4)
C4—C5—C6—C7	−178.2 (2)	O4—C20—C21—C16	179.3 (3)
O1—C6—C7—C8	178.1 (2)	C19—C20—C21—C16	−1.6 (4)
C5—C6—C7—C8	−1.3 (4)	C17—C16—C21—C20	−0.4 (3)
C6—C7—C8—C9	0.1 (4)	C15—C16—C21—C20	178.1 (2)
C7—C8—C9—C10	1.0 (4)	N2—C1—N1—C2	−177.61 (18)
C8—C9—C10—C5	−0.9 (4)	S1—C1—N1—C2	0.9 (2)
C6—C5—C10—C9	−0.2 (3)	C3—C2—N1—C1	0.2 (2)
C4—C5—C10—C9	179.3 (2)	C11—C2—N1—C1	178.72 (19)
C3—C2—C11—C12	−165.6 (3)	C5—C4—N2—C1	178.90 (17)
N1—C2—C11—C12	16.0 (3)	N1—C1—N2—C4	12.8 (3)
C3—C2—C11—C13	73.8 (3)	S1—C1—N2—C4	−165.62 (15)
N1—C2—C11—C13	−104.5 (3)	C16—C17—O2—C22	168.02 (19)
C3—C2—C11—C14	−47.1 (3)	C18—C17—O2—C22	−13.5 (3)
N1—C2—C11—C14	134.6 (2)	C18—C19—O3—C23	−9.7 (4)
C2—C3—C15—C16	−150.2 (2)	C20—C19—O3—C23	170.2 (3)
S1—C3—C15—C16	30.0 (2)	C21—C20—O4—C24	−4.7 (5)
C3—C15—C16—C21	−105.3 (2)	C19—C20—O4—C24	176.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.82	1.89	2.612 (2)	147