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5-Acetyl-2-{[(1*H*-benzimidazol-2-yl)methyl]sulfanyl}-4-(4-methoxyphenyl)-6-methylpyridine-3-carbonitrile

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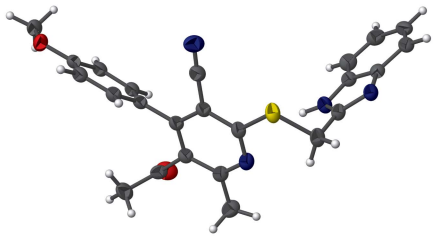
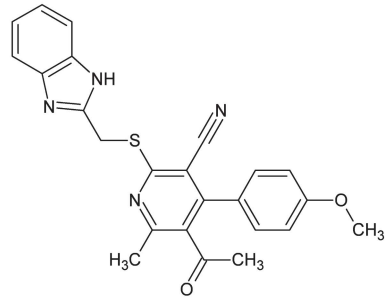
In the title compound, $C_{24}H_{20}N_4O_2S$, the benzimidiazole moiety is essentially planar within 0.020 (1) Å (r.m.s. deviation = 0.012 Å). Its mean plane makes a dihedral angle of 85.80 (3)° with the plane of the central pyridine ring while the methoxyphenyl ring makes a dihedral angle of 57.28 (4)° with this plane. In the crystal, N—H···N hydrogen bonds form sheets parallel to (010).

3D view



Chemical scheme



Structure description

The pharmacological activities exhibited by 3-cyanopyridine-2(1*H*)-thiones (Litvinov, 2003) and benzimidazoles (Ingle & Magar, 2011; Alamgir *et al.*, 2007) have been reviewed. The benzimidazole scaffold is a useful structural modification for the development of molecules of pharmaceutical or biological interest. Appropriately substituted benzimidazole derivatives have found diverse therapeutic applications such as in anti-ulcer, antihypertensive, antiviral, antifungal, anticancer and antihistaminic agents (Ingle & Magar, 2011). The optimization of benzimidazole-based structures has resulted in various drugs that are currently on the market, such as omeprazole (proton pump inhibitor), pimobendan (ionodilator), and mebendazole (anthelmintic) (Ingle & Magar, 2011). In view of the above observations, we undertook the synthesis of the title compound, which is structurally related to omeprazole, and determine its crystal structure.

In the title compound (Fig. 1), the benzimidiazolyl ring system (N3/N4/C18–C24) is essentially planar (r.m.s. deviation = 0.012 Å) and its mean plane makes a dihedral angle

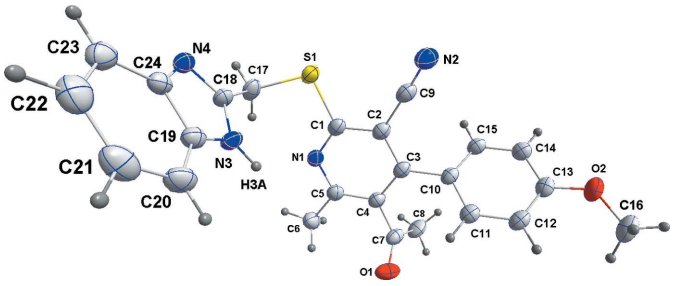


Figure 1
The title molecule with the atom-labeling scheme and 50% probability ellipsoids.

of 85.80 (3)° with that of the central pyridine ring (N1/C1–C5) while the C10—C15 ring makes a dihedral angle of 57.28 (4)° with the pyridine ring plane. The packing consists of layers parallel to (010) which are formed by N3—H3*A*···N4 hydrogen bonds (Table 1 and Fig. 2).

Synthesis and crystallization

To a suspension of 5-acetyl-3-cyano-4-(4-methoxyphenyl)-6-methylpyridine-2(1*H*)-thione (3.0 g, 10 mmol) and 2-chloromethyl-1*H*-benzimidazole (1.66 g, 10 mmol) in ethanol (30 ml), sodium acetate trihydrate (1.5 g, 11 mmol) was added. The resulting mixture was heated under reflux for 3 h and then allowed to cool. The solid that formed was collected by filtration and recrystallized from ethanol to give the title compound in the form of colourless plates. Yield: (3.6 g) 84%, m.p. 501–503 K. IR: 3200 (NH), 2200 (C≡N), 1690 (C═O) cm.$^{-1}$ ^{1}H NMR ($CDCl_3$): δ = 6.9–7.7 (*m*, 9H, Ar—H and NH), 4.8 (2H, SCH_2) 3.8 (*s*, 3H, OCH_2), 2.6 (s, 3H, CH_3 at C-6), 1.8 (*s*, 3H, $COCH_3$).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

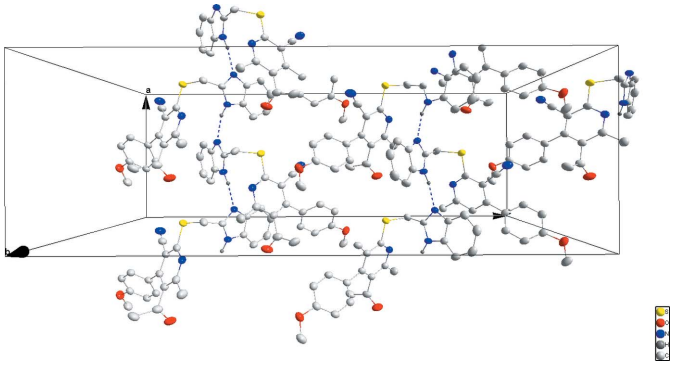


Figure 2
A portion of one layer projected onto (010), showing the N—H···N hydrogen bonds as dotted lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N4^{i}	0.92 (2)	1.98 (2)	2.8441 (16)	157.1 (17)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{20}N_4O_2S$
M_r	428.50
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	150
a, *b*, *c* (Å)	9.8513 (2), 15.0619 (2), 28.9310 (4)
V (Å^3)	4292.76 (12)
Z	8
Radiation type	Cu *Kα*
μ (mm^{-1})	1.57
Crystal size (mm)	0.24 × 0.15 × 0.06
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.79, 0.92
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31421, 4292, 3787
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.034, 0.091, 1.02
No. of reflections	4292
No. of parameters	288
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.40

Computer programs: *APEX2* and *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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full crystallographic data

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Crystal data

$C_{24}H_{20}N_4O_2S$
M_r = 428.50
Orthorhombic, *Pbca*
a = 9.8513 (2) Å
b = 15.0619 (2) Å
c = 28.9310 (4) Å
V = 4292.76 (12) Å^3
Z = 8
F(000) = 1792
D_x = 1.326 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9822 reflections
θ = 4.2–74.4°
μ = 1.57 mm^{-1}
T = 150 K
Plate, colourless
0.24 × 0.15 × 0.06 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2015)
T_{min} = 0.79, T_{max} = 0.92
31421 measured reflections
4292 independent reflections
3787 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 74.5°, θ_{min} = 3.1°
h = −11→11
k = −17→15
l = −36→36

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.02
4292 reflections
288 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 1.5046P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00051 (6)

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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. H-atoms were placed in calculated positions (C—H = 0.95 - 0.99 Å) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached carbon atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	−0.00897 (3)	0.77846 (3)	0.34587 (2)	0.03530 (11)
O1	0.66262 (11)	0.84216 (8)	0.36572 (5)	0.0513 (3)
O2	0.59674 (11)	0.57979 (7)	0.55315 (3)	0.0394 (3)
N1	0.23056 (12)	0.85965 (8)	0.33336 (4)	0.0321 (3)
N2	0.08106 (13)	0.62965 (9)	0.43416 (5)	0.0455 (3)
N3	0.12589 (12)	0.71895 (8)	0.24456 (4)	0.0309 (3)
H3A	0.208 (2)	0.7306 (12)	0.2581 (6)	0.051 (5)*
N4	−0.09632 (11)	0.71505 (8)	0.22875 (4)	0.0293 (2)
C1	0.16353 (14)	0.79895 (9)	0.35781 (4)	0.0296 (3)
C2	0.22340 (13)	0.75185 (9)	0.39439 (5)	0.0287 (3)
C3	0.35819 (13)	0.76988 (8)	0.40657 (5)	0.0283 (3)
C4	0.42723 (13)	0.83401 (9)	0.38087 (5)	0.0298 (3)
C5	0.36018 (14)	0.87725 (9)	0.34441 (5)	0.0316 (3)
C6	0.42829 (16)	0.94884 (11)	0.31656 (6)	0.0425 (4)
H6A	0.3670	0.9688	0.2920	0.064*
H6B	0.5118	0.9253	0.3028	0.064*
H6C	0.4505	0.9990	0.3368	0.064*
C7	0.57174 (14)	0.85996 (9)	0.39216 (5)	0.0355 (3)
C8	0.59363 (16)	0.91238 (11)	0.43550 (6)	0.0453 (4)
H8A	0.6909	0.9236	0.4396	0.068*
H8B	0.5591	0.8788	0.4620	0.068*
H8C	0.5452	0.9691	0.4332	0.068*
C9	0.14601 (14)	0.68374 (9)	0.41719 (5)	0.0332 (3)
C10	0.42457 (13)	0.72017 (8)	0.44466 (5)	0.0284 (3)
C11	0.54249 (14)	0.67169 (9)	0.43662 (5)	0.0300 (3)
H11	0.5826	0.6722	0.4068	0.036*
C12	0.60228 (13)	0.62245 (9)	0.47188 (5)	0.0314 (3)
H12	0.6812	0.5881	0.4659	0.038*
C13	0.54578 (14)	0.62381 (9)	0.51590 (5)	0.0308 (3)

C14	0.42925 (14)	0.67349 (9)	0.52454 (5)	0.0324 (3)
H14	0.3917	0.6752	0.5548	0.039*
C15	0.36845 (14)	0.72015 (9)	0.48920 (5)	0.0312 (3)
H15	0.2876	0.7527	0.4951	0.037*
C16	0.71090 (17)	0.52355 (10)	0.54614 (6)	0.0424 (4)
H16A	0.6868	0.4763	0.5244	0.064*
H16B	0.7382	0.4973	0.5757	0.064*
H16C	0.7863	0.5584	0.5335	0.064*
C17	−0.02451 (15)	0.82366 (10)	0.28796 (5)	0.0354 (3)
H17A	−0.1168	0.8483	0.2836	0.042*
H17B	0.0416	0.8726	0.2839	0.042*
C18	0.00095 (13)	0.75384 (9)	0.25283 (5)	0.0289 (3)
C19	0.10824 (13)	0.65117 (9)	0.21295 (5)	0.0297 (3)
C20	0.19937 (15)	0.59179 (10)	0.19302 (5)	0.0382 (3)
H20	0.2938	0.5939	0.1996	0.046*
C21	0.14543 (17)	0.52975 (10)	0.16320 (5)	0.0416 (4)
H21	0.2043	0.4879	0.1489	0.050*
C22	0.00667 (17)	0.52663 (10)	0.15334 (5)	0.0393 (3)
H22	−0.0265	0.4827	0.1327	0.047*
C23	−0.08347 (15)	0.58610 (10)	0.17298 (5)	0.0345 (3)
H23	−0.1777	0.5840	0.1661	0.041*
C24	−0.03096 (13)	0.64929 (9)	0.20332 (4)	0.0277 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02532 (18)	0.0480 (2)	0.03263 (19)	0.00303 (13)	−0.00383 (13)	−0.00463 (14)
O1	0.0310 (6)	0.0510 (7)	0.0721 (8)	−0.0016 (5)	0.0109 (5)	−0.0021 (6)
O2	0.0453 (6)	0.0365 (6)	0.0364 (5)	0.0089 (4)	−0.0109 (4)	−0.0001 (4)
N1	0.0295 (6)	0.0365 (6)	0.0303 (5)	0.0066 (5)	0.0001 (5)	−0.0021 (5)
N2	0.0356 (7)	0.0373 (7)	0.0637 (9)	−0.0027 (6)	−0.0052 (6)	0.0071 (6)
N3	0.0204 (6)	0.0363 (6)	0.0359 (6)	0.0033 (4)	−0.0025 (4)	−0.0043 (5)
N4	0.0225 (5)	0.0344 (6)	0.0310 (5)	0.0030 (4)	−0.0022 (4)	−0.0015 (5)
C1	0.0272 (7)	0.0320 (7)	0.0296 (6)	0.0052 (5)	−0.0016 (5)	−0.0067 (5)
C2	0.0271 (7)	0.0265 (6)	0.0326 (6)	0.0032 (5)	−0.0016 (5)	−0.0042 (5)
C3	0.0270 (7)	0.0255 (7)	0.0324 (6)	0.0041 (5)	−0.0021 (5)	−0.0047 (5)
C4	0.0266 (7)	0.0287 (7)	0.0341 (7)	0.0030 (5)	−0.0011 (5)	−0.0029 (5)
C5	0.0302 (7)	0.0316 (7)	0.0330 (7)	0.0052 (5)	0.0012 (5)	−0.0020 (5)
C6	0.0398 (8)	0.0447 (9)	0.0430 (8)	0.0019 (7)	0.0034 (7)	0.0088 (7)
C7	0.0279 (7)	0.0285 (7)	0.0500 (8)	0.0018 (5)	−0.0028 (6)	0.0055 (6)
C8	0.0347 (8)	0.0413 (9)	0.0600 (10)	−0.0014 (6)	−0.0149 (7)	−0.0053 (7)
C9	0.0271 (7)	0.0307 (7)	0.0419 (7)	0.0036 (5)	−0.0049 (6)	−0.0029 (6)
C10	0.0259 (7)	0.0244 (7)	0.0349 (7)	0.0001 (5)	−0.0052 (5)	−0.0030 (5)
C11	0.0283 (7)	0.0277 (7)	0.0340 (6)	0.0006 (5)	−0.0026 (5)	−0.0041 (5)
C12	0.0267 (6)	0.0277 (7)	0.0397 (7)	0.0030 (5)	−0.0063 (5)	−0.0060 (5)
C13	0.0327 (7)	0.0251 (7)	0.0345 (7)	−0.0011 (5)	−0.0086 (5)	−0.0021 (5)
C14	0.0330 (7)	0.0311 (7)	0.0332 (7)	−0.0012 (5)	−0.0019 (5)	−0.0041 (5)
C15	0.0273 (7)	0.0293 (7)	0.0369 (7)	0.0021 (5)	−0.0024 (5)	−0.0044 (5)

C16	0.0447 (9)	0.0339 (8)	0.0486 (9)	0.0090 (6)	−0.0169 (7)	−0.0021 (6)
C17	0.0309 (7)	0.0395 (8)	0.0358 (7)	0.0107 (6)	−0.0077 (6)	−0.0061 (6)
C18	0.0217 (6)	0.0348 (7)	0.0304 (6)	0.0046 (5)	−0.0026 (5)	0.0006 (5)
C19	0.0262 (6)	0.0310 (7)	0.0319 (6)	0.0021 (5)	0.0016 (5)	0.0013 (5)
C20	0.0304 (7)	0.0409 (8)	0.0433 (8)	0.0094 (6)	0.0047 (6)	−0.0003 (6)
C21	0.0503 (9)	0.0339 (8)	0.0405 (8)	0.0109 (7)	0.0088 (7)	−0.0003 (6)
C22	0.0545 (10)	0.0286 (7)	0.0346 (7)	−0.0036 (6)	0.0012 (6)	−0.0016 (6)
C23	0.0342 (7)	0.0342 (7)	0.0352 (7)	−0.0055 (6)	−0.0019 (6)	0.0020 (6)
C24	0.0255 (6)	0.0287 (7)	0.0288 (6)	0.0010 (5)	0.0020 (5)	0.0027 (5)

Geometric parameters (Å, º)

S1—C1	1.7614 (14)	C8—H8C	0.9800
S1—C17	1.8149 (15)	C10—C11	1.3917 (19)
O1—C7	1.2076 (19)	C10—C15	1.4021 (19)
O2—C13	1.3613 (16)	C11—C12	1.3920 (19)
O2—C16	1.4224 (18)	C11—H11	0.9500
N1—C1	1.3314 (18)	C12—C13	1.390 (2)
N1—C5	1.3427 (18)	C12—H12	0.9500
N2—C9	1.146 (2)	C13—C14	1.393 (2)
N3—C18	1.3596 (17)	C14—C15	1.378 (2)
N3—C19	1.3815 (18)	C14—H14	0.9500
N3—H3A	0.92 (2)	C15—H15	0.9500
N4—C18	1.3209 (18)	C16—H16A	0.9800
N4—C24	1.3917 (17)	C16—H16B	0.9800
C1—C2	1.4039 (19)	C16—H16C	0.9800
C2—C3	1.4004 (19)	C17—C18	1.4838 (19)
C2—C9	1.438 (2)	C17—H17A	0.9900
C3—C4	1.3958 (19)	C17—H17B	0.9900
C3—C10	1.4841 (18)	C19—C20	1.3922 (19)
C4—C5	1.4046 (19)	C19—C24	1.3995 (18)
C4—C7	1.5120 (19)	C20—C21	1.378 (2)
C5—C6	1.504 (2)	C20—H20	0.9500
C6—H6A	0.9800	C21—C22	1.397 (2)
C6—H6B	0.9800	C21—H21	0.9500
C6—H6C	0.9800	C22—C23	1.383 (2)
C7—C8	1.497 (2)	C22—H22	0.9500
C8—H8A	0.9800	C23—C24	1.3942 (19)
C8—H8B	0.9800	C23—H23	0.9500
C1—S1—C17	101.35 (7)	C13—C12—H12	120.2
C13—O2—C16	117.95 (12)	C11—C12—H12	120.2
C1—N1—C5	118.73 (12)	O2—C13—C12	124.79 (13)
C18—N3—C19	106.75 (11)	O2—C13—C14	115.05 (12)
C18—N3—H3A	130.7 (12)	C12—C13—C14	120.16 (12)
C19—N3—H3A	122.3 (12)	C15—C14—C13	119.94 (13)
C18—N4—C24	104.95 (11)	C15—C14—H14	120.0
N1—C1—C2	122.62 (12)	C13—C14—H14	120.0

N1—C1—S1	119.65 (10)	C14—C15—C10	120.71 (13)
C2—C1—S1	117.69 (11)	C14—C15—H15	119.6
C3—C2—C1	119.35 (13)	C10—C15—H15	119.6
C3—C2—C9	121.70 (12)	O2—C16—H16A	109.5
C1—C2—C9	118.91 (12)	O2—C16—H16B	109.5
C4—C3—C2	117.52 (12)	H16A—C16—H16B	109.5
C4—C3—C10	122.00 (12)	O2—C16—H16C	109.5
C2—C3—C10	120.46 (12)	H16A—C16—H16C	109.5
C3—C4—C5	119.45 (12)	H16B—C16—H16C	109.5
C3—C4—C7	121.51 (12)	C18—C17—S1	110.62 (10)
C5—C4—C7	119.02 (12)	C18—C17—H17A	109.5
N1—C5—C4	122.31 (13)	S1—C17—H17A	109.5
N1—C5—C6	115.99 (12)	C18—C17—H17B	109.5
C4—C5—C6	121.66 (13)	S1—C17—H17B	109.5
C5—C6—H6A	109.5	H17A—C17—H17B	108.1
C5—C6—H6B	109.5	N4—C18—N3	113.14 (12)
H6A—C6—H6B	109.5	N4—C18—C17	123.51 (12)
C5—C6—H6C	109.5	N3—C18—C17	123.20 (12)
H6A—C6—H6C	109.5	N3—C19—C20	131.89 (13)
H6B—C6—H6C	109.5	N3—C19—C24	105.67 (11)
O1—C7—C8	122.73 (14)	C20—C19—C24	122.44 (13)
O1—C7—C4	120.25 (14)	C21—C20—C19	116.50 (14)
C8—C7—C4	116.92 (13)	C21—C20—H20	121.8
C7—C8—H8A	109.5	C19—C20—H20	121.8
C7—C8—H8B	109.5	C20—C21—C22	121.85 (14)
H8A—C8—H8B	109.5	C20—C21—H21	119.1
C7—C8—H8C	109.5	C22—C21—H21	119.1
H8A—C8—H8C	109.5	C23—C22—C21	121.49 (14)
H8B—C8—H8C	109.5	C23—C22—H22	119.3
N2—C9—C2	177.63 (16)	C21—C22—H22	119.3
C11—C10—C15	118.86 (12)	C22—C23—C24	117.55 (13)
C11—C10—C3	120.55 (12)	C22—C23—H23	121.2
C15—C10—C3	120.58 (12)	C24—C23—H23	121.2
C10—C11—C12	120.68 (13)	N4—C24—C23	130.31 (12)
C10—C11—H11	119.7	N4—C24—C19	109.49 (11)
C12—C11—H11	119.7	C23—C24—C19	120.17 (13)
C13—C12—C11	119.62 (13)		

C5—N1—C1—C2	−0.72 (19)	C10—C11—C12—C13	−1.9 (2)
C5—N1—C1—S1	176.93 (10)	C16—O2—C13—C12	−4.4 (2)
C17—S1—C1—N1	19.43 (12)	C16—O2—C13—C14	176.31 (12)
C17—S1—C1—C2	−162.81 (10)	C11—C12—C13—O2	−178.69 (12)
N1—C1—C2—C3	1.2 (2)	C11—C12—C13—C14	0.6 (2)
S1—C1—C2—C3	−176.50 (10)	O2—C13—C14—C15	−179.48 (12)
N1—C1—C2—C9	−176.39 (12)	C12—C13—C14—C15	1.2 (2)
S1—C1—C2—C9	5.92 (17)	C13—C14—C15—C10	−1.7 (2)
C1—C2—C3—C4	−0.78 (18)	C11—C10—C15—C14	0.4 (2)
C9—C2—C3—C4	176.73 (12)	C3—C10—C15—C14	179.48 (12)

C1—C2—C3—C10	−179.13 (12)	C1—S1—C17—C18	91.64 (11)
C9—C2—C3—C10	−1.62 (19)	C24—N4—C18—N3	0.80 (15)
C2—C3—C4—C5	−0.01 (19)	C24—N4—C18—C17	−174.81 (13)
C10—C3—C4—C5	178.31 (12)	C19—N3—C18—N4	−0.81 (16)
C2—C3—C4—C7	178.31 (12)	C19—N3—C18—C17	174.82 (13)
C10—C3—C4—C7	−3.4 (2)	S1—C17—C18—N4	103.92 (14)
C1—N1—C5—C4	−0.13 (19)	S1—C17—C18—N3	−71.25 (16)
C1—N1—C5—C6	−177.84 (12)	C18—N3—C19—C20	−178.33 (15)
C3—C4—C5—N1	0.5 (2)	C18—N3—C19—C24	0.44 (15)
C7—C4—C5—N1	−177.87 (12)	N3—C19—C20—C21	178.13 (14)
C3—C4—C5—C6	178.07 (13)	C24—C19—C20—C21	−0.5 (2)
C7—C4—C5—C6	−0.3 (2)	C19—C20—C21—C22	0.2 (2)
C3—C4—C7—O1	112.49 (16)	C20—C21—C22—C23	0.2 (2)
C5—C4—C7—O1	−69.18 (19)	C21—C22—C23—C24	−0.3 (2)
C3—C4—C7—C8	−70.98 (18)	C18—N4—C24—C23	177.89 (14)
C5—C4—C7—C8	107.35 (16)	C18—N4—C24—C19	−0.49 (15)
C4—C3—C10—C11	−56.59 (18)	C22—C23—C24—N4	−178.18 (13)
C2—C3—C10—C11	121.69 (14)	C22—C23—C24—C19	0.0 (2)
C4—C3—C10—C15	124.37 (14)	N3—C19—C24—N4	0.02 (15)
C2—C3—C10—C15	−57.35 (17)	C20—C19—C24—N4	178.94 (12)
C15—C10—C11—C12	1.36 (19)	N3—C19—C24—C23	−178.55 (12)
C3—C10—C11—C12	−177.70 (12)	C20—C19—C24—C23	0.4 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N4^{i}	0.92 (2)	1.98 (2)	2.8441 (16)	157.1 (17)

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