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(*Z*)-*N*-[3-(2-Methoxyphenyl)-4-phenyl-2,3-dihydrothiazol-2-ylidene]-2-methylbenzamide

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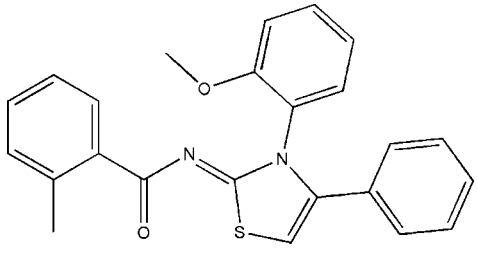
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.102; data-to-parameter ratio = 17.8.

In the title molecule, $C_{24}H_{20}N_2O_2S$, the thiazole and amide groups are essentially coplanar. The thiazole ring forms dihedral angles of 61.62 (4) and 26.75 (5)° with the benzene rings of the methoxyphenyl and methylphenyl groups, respectively, and 33.69 (6)° with the phenyl ring. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds, forming a three-dimensional network.

Related literature

For related literature, see: Arcadi *et al.* (2003); Bonde & Gaikwad (2004); Kim *et al.* (2007); Lee & Sim (2000); Saeed & Parvez (2006); Shehata *et al.* (1996); Venkatachalan *et al.* (2001).



Experimental

Crystal data

$C_{24}H_{20}N_2O_2S$
M_r = 400.48
Monoclinic, $P2_1/n$
a = 9.7826 (18) Å
b = 15.010 (3) Å
c = 13.917 (3) Å
β = 105.092 (4)°
V = 1973.1 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 153 (2) K
0.50 × 0.40 × 0.25 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.912, T_{max} = 0.955
16940 measured reflections
4697 independent reflections
4150 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.04
4697 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···N1	0.95	2.42	2.7572 (18)	101
C14—H14A···O1^{i}	0.95	2.52	3.4635 (19)	171
C22—H22A···O1^{ii}	0.95	2.48	3.4240 (18)	170

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2546).

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S1. Comment

2-Imino derivatives of 1,3-thiazolines posses a wide range of pharmacological and synthetic applications. Thus, these show potent bioactivities ranging from antitubercular (Shehata *et al.*, 1996) to anti-HIV (Venkatachalan *et al.*, 2001) activities. Iminothiazolines containing a pyrazine ring show significant antibacterial and antimicrobial activity (Bonde & Gaikwad 2004), derivatives of rhodanine show antibacterial, anti-inflammatory and antiviral activities (Lee & Sim *et al.*, 2000) and bis-thiazoline derivatives show marked anti-cancer activity against human cell lines (Arcadi *et al.*, 2003). A 2-imino-1,3-thiazoline derivative KHG22394 acts as a skin whitening agent (Kim *et al.*, 2007).

S2. Experimental

The title compound was prepared according to the method reported earlier (Saeed & Parvez 2006). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution. Full spectroscopic and physical characterization will be reported elsewhere.

S3. Refinement

Hydrogen atoms were located in difference syntheses, refined at idealized positions riding on the C (C–H = 0.95–0.98 Å) atoms with isotropic displacement parameters U_{iso}(H) = 1.2U(C_{eq}) and 1.5(methyl-C). Methyl H atoms were refined on the basis of rigid groups allowed to rotate but not tip.

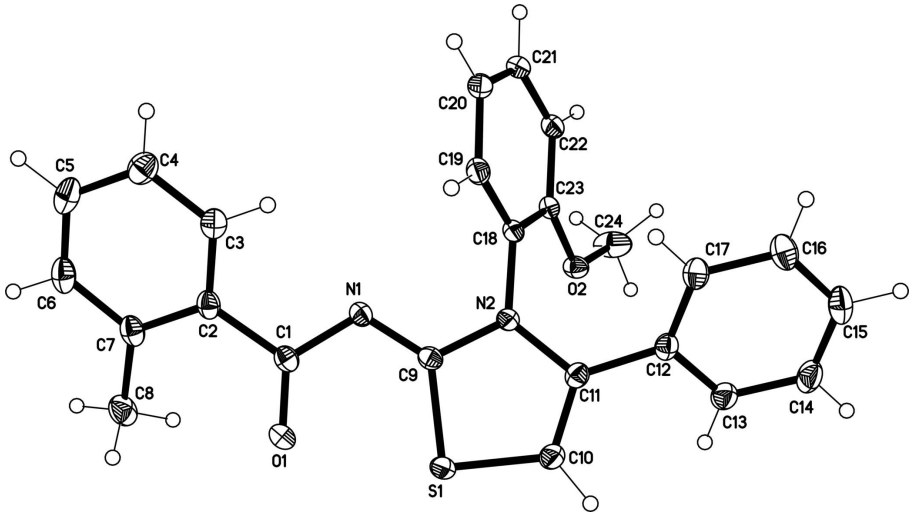

Figure 1

Molecular structure of title compound. Displacement ellipsoids are drawn at the 50% probability level.

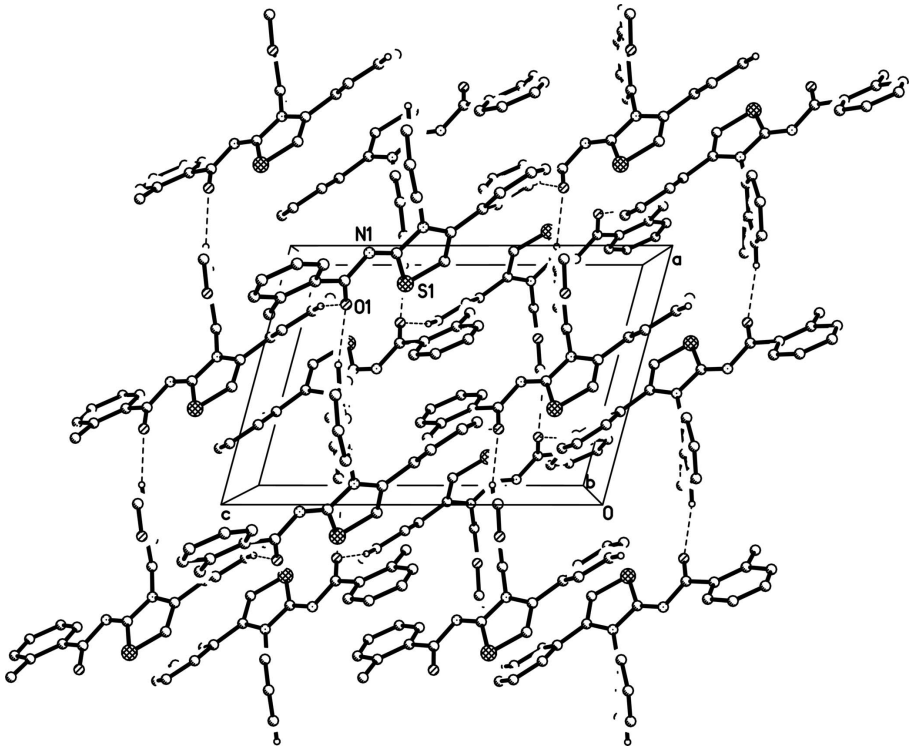

Figure 2

Crystal packing viewed along [010] with intermolecular hydrogen bonding pattern indicated as dashed lines. H-atoms not involved in hydrogen bonding are omitted.

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$c = 13.917\ (3)$ Å
$\beta = 105.092\ (4)°$
$V = 1973.1\ (6)$ Å^3
$Z = 4$
$F(000) = 840$
$D_x = 1.348$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 989 reflections
$\theta = 2.6–28.3°$
$\mu = 0.19$ mm^{-1}
$T = 153$ K
Prism, colourless
0.50 × 0.40 × 0.25 mm

Data collection

Bruker AXS SMART APEX diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.912$, $T_{max} = 0.955$
16940 measured reflections
4697 independent reflections
4150 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.0°$
$h = -11\rightarrow12$
$k = -19\rightarrow19$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.102$
$S = 1.04$
4697 reflections
264 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.8403P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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	0.63733 (3)	0.65129 (2)	0.82089 (3)	0.02247 (10)
O1	0.72271 (10)	0.57226 (7)	0.68165 (8)	0.0258 (2)
O2	0.16287 (9)	0.62604 (6)	0.76469 (7)	0.0212 (2)
N1	0.52745 (11)	0.50297 (7)	0.71108 (8)	0.0196 (2)
N2	0.42303 (11)	0.55761 (7)	0.83194 (8)	0.0177 (2)
C1	0.63503 (13)	0.51125 (9)	0.66513 (10)	0.0202 (3)
C2	0.64098 (13)	0.43708 (9)	0.59434 (10)	0.0214 (3)
C3	0.58372 (15)	0.35480 (9)	0.61069 (11)	0.0260 (3)
H3A	0.5418	0.3486	0.6647	0.031*
C4	0.58680 (16)	0.28229 (10)	0.55010 (11)	0.0301 (3)
H4A	0.5488	0.2266	0.5628	0.036*
C5	0.64615 (16)	0.29210 (10)	0.47064 (11)	0.0316 (3)
H5A	0.6477	0.2431	0.4278	0.038*
C6	0.70292 (16)	0.37264 (11)	0.45352 (11)	0.0303 (3)
H6A	0.7434	0.3779	0.3987	0.036*
C7	0.70292 (14)	0.44716 (10)	0.51435 (10)	0.0243 (3)
C8	0.76269 (16)	0.53331 (11)	0.48825 (11)	0.0313 (3)
H8A	0.8577	0.5423	0.5322	0.047*
H8B	0.7013	0.5827	0.4966	0.047*
H8C	0.7680	0.5311	0.4189	0.047*
C9	0.52416 (13)	0.56139 (8)	0.77971 (9)	0.0184 (2)
C10	0.54693 (14)	0.67709 (9)	0.90914 (10)	0.0237 (3)
H10A	0.5729	0.7248	0.9551	0.028*
C11	0.43667 (13)	0.62292 (8)	0.90605 (9)	0.0197 (2)
C12	0.34425 (13)	0.62715 (9)	0.97466 (9)	0.0206 (3)

C13	0.31678 (15)	0.71102 (10)	1.00913 (11)	0.0265 (3)
H13A	0.3513	0.7630	0.9843	0.032*
C14	0.23944 (16)	0.71898 (11)	1.07930 (11)	0.0317 (3)
H14A	0.2232	0.7761	1.1036	0.038*
C15	0.18594 (17)	0.64354 (11)	1.11381 (12)	0.0331 (3)
H15A	0.1326	0.6489	1.1616	0.040*
C16	0.21014 (16)	0.56054 (11)	1.07879 (11)	0.0306 (3)
H16A	0.1716	0.5091	1.1016	0.037*
C17	0.29047 (15)	0.55166 (9)	1.01040 (10)	0.0247 (3)
H17A	0.3087	0.4942	0.9880	0.030*
C18	0.30424 (13)	0.49851 (8)	0.79994 (9)	0.0180 (2)
C19	0.32421 (14)	0.40723 (9)	0.80007 (10)	0.0218 (3)
H19A	0.4162	0.3828	0.8251	0.026*
C20	0.20894 (16)	0.35139 (9)	0.76347 (11)	0.0252 (3)
H20A	0.2219	0.2887	0.7618	0.030*
C21	0.07491 (15)	0.38805 (9)	0.72938 (10)	0.0254 (3)
H21A	−0.0038	0.3498	0.7047	0.031*
C22	0.05328 (14)	0.47927 (9)	0.73060 (10)	0.0223 (3)
H22A	−0.0395	0.5032	0.7086	0.027*
C23	0.16958 (13)	0.53563 (8)	0.76461 (9)	0.0182 (2)
C24	0.02588 (16)	0.66550 (10)	0.73440 (16)	0.0415 (4)
H24A	−0.0176	0.6510	0.6645	0.062*
H24B	0.0344	0.7303	0.7422	0.062*
H24C	−0.0334	0.6423	0.7757	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01853 (16)	0.02102 (16)	0.02916 (18)	−0.00347 (11)	0.00855 (13)	−0.00330 (12)
O1	0.0212 (5)	0.0285 (5)	0.0302 (5)	−0.0048 (4)	0.0112 (4)	−0.0021 (4)
O2	0.0164 (4)	0.0192 (4)	0.0274 (5)	0.0005 (3)	0.0045 (4)	0.0000 (4)
N1	0.0162 (5)	0.0221 (5)	0.0212 (5)	−0.0002 (4)	0.0064 (4)	−0.0009 (4)
N2	0.0153 (5)	0.0183 (5)	0.0199 (5)	−0.0009 (4)	0.0053 (4)	−0.0015 (4)
C1	0.0174 (6)	0.0235 (6)	0.0197 (6)	0.0018 (5)	0.0049 (5)	0.0030 (5)
C2	0.0167 (6)	0.0278 (6)	0.0192 (6)	0.0047 (5)	0.0041 (5)	0.0001 (5)
C3	0.0260 (7)	0.0278 (7)	0.0252 (7)	0.0022 (5)	0.0085 (5)	−0.0014 (5)
C4	0.0310 (7)	0.0269 (7)	0.0307 (7)	0.0045 (6)	0.0051 (6)	−0.0015 (6)
C5	0.0324 (8)	0.0340 (8)	0.0263 (7)	0.0113 (6)	0.0039 (6)	−0.0068 (6)
C6	0.0277 (7)	0.0432 (8)	0.0209 (7)	0.0085 (6)	0.0081 (6)	−0.0014 (6)
C7	0.0180 (6)	0.0352 (7)	0.0191 (6)	0.0048 (5)	0.0040 (5)	0.0018 (5)
C8	0.0310 (8)	0.0423 (8)	0.0227 (7)	−0.0043 (6)	0.0108 (6)	0.0020 (6)
C9	0.0149 (5)	0.0196 (6)	0.0203 (6)	0.0003 (4)	0.0036 (5)	0.0016 (5)
C10	0.0215 (6)	0.0227 (6)	0.0273 (7)	−0.0009 (5)	0.0071 (5)	−0.0060 (5)
C11	0.0188 (6)	0.0201 (6)	0.0192 (6)	0.0023 (5)	0.0034 (5)	−0.0016 (5)
C12	0.0173 (6)	0.0261 (6)	0.0171 (6)	0.0025 (5)	0.0023 (5)	−0.0024 (5)
C13	0.0239 (7)	0.0267 (7)	0.0294 (7)	0.0000 (5)	0.0079 (6)	−0.0057 (5)
C14	0.0297 (7)	0.0349 (8)	0.0318 (8)	0.0049 (6)	0.0105 (6)	−0.0110 (6)
C15	0.0308 (8)	0.0453 (9)	0.0266 (7)	0.0087 (7)	0.0138 (6)	−0.0007 (6)

C16	0.0323 (8)	0.0359 (8)	0.0260 (7)	0.0055 (6)	0.0118 (6)	0.0072 (6)
C17	0.0261 (7)	0.0265 (7)	0.0218 (6)	0.0053 (5)	0.0067 (5)	0.0012 (5)
C18	0.0174 (6)	0.0209 (6)	0.0169 (6)	−0.0031 (5)	0.0069 (5)	−0.0012 (4)
C19	0.0234 (6)	0.0220 (6)	0.0221 (6)	0.0009 (5)	0.0101 (5)	0.0011 (5)
C20	0.0327 (7)	0.0184 (6)	0.0289 (7)	−0.0034 (5)	0.0159 (6)	−0.0015 (5)
C21	0.0259 (7)	0.0266 (7)	0.0271 (7)	−0.0098 (5)	0.0129 (6)	−0.0064 (5)
C22	0.0181 (6)	0.0267 (6)	0.0236 (6)	−0.0034 (5)	0.0080 (5)	−0.0027 (5)
C23	0.0195 (6)	0.0199 (6)	0.0169 (6)	−0.0017 (5)	0.0077 (5)	−0.0005 (4)
C24	0.0209 (7)	0.0249 (7)	0.0752 (13)	0.0040 (6)	0.0063 (8)	−0.0046 (8)

Geometric parameters (Å, º)

S1—C10	1.7337 (14)	C10—H10A	0.9500
S1—C9	1.7449 (13)	C11—C12	1.4774 (17)
O1—C1	1.2347 (16)	C12—C17	1.3943 (19)
O2—C23	1.3587 (15)	C12—C13	1.3980 (18)
O2—C24	1.4248 (17)	C13—C14	1.3875 (19)
N1—C9	1.3032 (17)	C13—H13A	0.9500
N1—C1	1.3720 (16)	C14—C15	1.385 (2)
N2—C9	1.3730 (16)	C14—H14A	0.9500
N2—C11	1.4039 (16)	C15—C16	1.381 (2)
N2—C18	1.4373 (16)	C15—H15A	0.9500
C1—C2	1.4978 (18)	C16—C17	1.3896 (19)
C2—C3	1.3991 (19)	C16—H16A	0.9500
C2—C7	1.4073 (18)	C17—H17A	0.9500
C3—C4	1.382 (2)	C18—C19	1.3840 (18)
C3—H3A	0.9500	C18—C23	1.3965 (18)
C4—C5	1.384 (2)	C19—C20	1.3909 (19)
C4—H4A	0.9500	C19—H19A	0.9500
C5—C6	1.377 (2)	C20—C21	1.387 (2)
C5—H5A	0.9500	C20—H20A	0.9500
C6—C7	1.403 (2)	C21—C22	1.386 (2)
C6—H6A	0.9500	C21—H21A	0.9500
C7—C8	1.502 (2)	C22—C23	1.3978 (18)
C8—H8A	0.9800	C22—H22A	0.9500
C8—H8B	0.9800	C24—H24A	0.9800
C8—H8C	0.9800	C24—H24B	0.9800
C10—C11	1.3425 (18)	C24—H24C	0.9800
C10—S1—C9	90.48 (6)	C17—C12—C13	119.04 (12)
C23—O2—C24	117.19 (11)	C17—C12—C11	123.15 (12)
C9—N1—C1	116.67 (11)	C13—C12—C11	117.71 (12)
C9—N2—C11	114.60 (10)	C14—C13—C12	120.51 (14)
C9—N2—C18	119.83 (10)	C14—C13—H13A	119.7
C11—N2—C18	124.97 (10)	C12—C13—H13A	119.7
O1—C1—N1	124.08 (12)	C15—C14—C13	119.89 (14)
O1—C1—C2	121.99 (11)	C15—C14—H14A	120.1
N1—C1—C2	113.90 (11)	C13—C14—H14A	120.1

C3—C2—C7	119.77 (13)	C16—C15—C14	120.03 (13)
C3—C2—C1	117.61 (12)	C16—C15—H15A	120.0
C7—C2—C1	122.61 (12)	C14—C15—H15A	120.0
C4—C3—C2	121.52 (13)	C15—C16—C17	120.52 (14)
C4—C3—H3A	119.2	C15—C16—H16A	119.7
C2—C3—H3A	119.2	C17—C16—H16A	119.7
C3—C4—C5	118.94 (14)	C16—C17—C12	119.97 (13)
C3—C4—H4A	120.5	C16—C17—H17A	120.0
C5—C4—H4A	120.5	C12—C17—H17A	120.0
C6—C5—C4	120.24 (13)	C19—C18—C23	121.02 (12)
C6—C5—H5A	119.9	C19—C18—N2	120.54 (11)
C4—C5—H5A	119.9	C23—C18—N2	118.38 (11)
C5—C6—C7	122.17 (13)	C18—C19—C20	119.70 (13)
C5—C6—H6A	118.9	C18—C19—H19A	120.2
C7—C6—H6A	118.9	C20—C19—H19A	120.2
C6—C7—C2	117.34 (13)	C21—C20—C19	119.36 (12)
C6—C7—C8	118.64 (13)	C21—C20—H20A	120.3
C2—C7—C8	123.96 (13)	C19—C20—H20A	120.3
C7—C8—H8A	109.5	C22—C21—C20	121.43 (12)
C7—C8—H8B	109.5	C22—C21—H21A	119.3
H8A—C8—H8B	109.5	C20—C21—H21A	119.3
C7—C8—H8C	109.5	C21—C22—C23	119.25 (13)
H8A—C8—H8C	109.5	C21—C22—H22A	120.4
H8B—C8—H8C	109.5	C23—C22—H22A	120.4
N1—C9—N2	121.26 (11)	O2—C23—C18	116.08 (11)
N1—C9—S1	128.79 (10)	O2—C23—C22	124.72 (12)
N2—C9—S1	109.95 (9)	C18—C23—C22	119.19 (12)
C11—C10—S1	113.32 (10)	O2—C24—H24A	109.5
C11—C10—H10A	123.3	O2—C24—H24B	109.5
S1—C10—H10A	123.3	H24A—C24—H24B	109.5
C10—C11—N2	111.61 (11)	O2—C24—H24C	109.5
C10—C11—C12	125.11 (12)	H24A—C24—H24C	109.5
N2—C11—C12	123.21 (11)	H24B—C24—H24C	109.5

C9—N1—C1—O1	−3.59 (19)	C18—N2—C11—C12	12.82 (19)
C9—N1—C1—C2	174.37 (11)	C10—C11—C12—C17	−142.16 (15)
O1—C1—C2—C3	152.58 (13)	N2—C11—C12—C17	34.49 (19)
N1—C1—C2—C3	−25.43 (17)	C10—C11—C12—C13	34.2 (2)
O1—C1—C2—C7	−26.54 (19)	N2—C11—C12—C13	−149.19 (13)
N1—C1—C2—C7	155.46 (12)	C17—C12—C13—C14	1.2 (2)
C7—C2—C3—C4	0.3 (2)	C11—C12—C13—C14	−175.25 (13)
C1—C2—C3—C4	−178.89 (13)	C12—C13—C14—C15	−1.6 (2)
C2—C3—C4—C5	−1.0 (2)	C13—C14—C15—C16	0.3 (2)
C3—C4—C5—C6	0.9 (2)	C14—C15—C16—C17	1.3 (2)
C4—C5—C6—C7	−0.2 (2)	C15—C16—C17—C12	−1.7 (2)
C5—C6—C7—C2	−0.5 (2)	C13—C12—C17—C16	0.4 (2)
C5—C6—C7—C8	−177.96 (14)	C11—C12—C17—C16	176.67 (13)
C3—C2—C7—C6	0.48 (19)	C9—N2—C18—C19	63.62 (16)

C1—C2—C7—C6	179.58 (12)	C11—N2—C18—C19	−125.79 (13)
C3—C2—C7—C8	177.79 (13)	C9—N2—C18—C23	−113.51 (13)
C1—C2—C7—C8	−3.1 (2)	C11—N2—C18—C23	57.08 (17)
C1—N1—C9—N2	−178.30 (11)	C23—C18—C19—C20	0.75 (19)
C1—N1—C9—S1	1.15 (18)	N2—C18—C19—C20	−176.30 (11)
C11—N2—C9—N1	177.57 (11)	C18—C19—C20—C21	−1.45 (19)
C18—N2—C9—N1	−10.90 (18)	C19—C20—C21—C22	0.3 (2)
C11—N2—C9—S1	−1.97 (13)	C20—C21—C22—C23	1.6 (2)
C18—N2—C9—S1	169.55 (9)	C24—O2—C23—C18	−176.49 (13)
C10—S1—C9—N1	−177.59 (13)	C24—O2—C23—C22	4.66 (19)
C10—S1—C9—N2	1.91 (10)	C19—C18—C23—O2	−177.78 (11)
C9—S1—C10—C11	−1.49 (11)	N2—C18—C23—O2	−0.66 (16)
S1—C10—C11—N2	0.64 (15)	C19—C18—C23—C22	1.13 (18)
S1—C10—C11—C12	177.62 (10)	N2—C18—C23—C22	178.25 (11)
C9—N2—C11—C10	0.89 (16)	C21—C22—C23—O2	176.52 (12)
C18—N2—C11—C10	−170.13 (12)	C21—C22—C23—C18	−2.29 (19)
C9—N2—C11—C12	−176.15 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···N1	0.95	2.42	2.7572 (18)	101
C14—H14*A*···O1^{i}	0.95	2.52	3.4635 (19)	171
C22—H22*A*···O1^{ii}	0.95	2.48	3.4240 (18)	170

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