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

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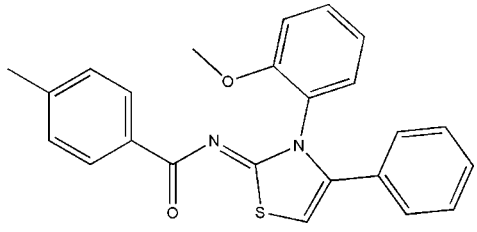
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.103; data-to-parameter ratio = 14.1.

Geometric parameters of the title compound, $C_{24}H_{20}N_2O_2S$, are in the usual ranges. The central heterocycle makes dihedral angles of 41.29 (4) and 72.94 (5)° with the phenyl ring and the methoxyphenyl ring, respectively.

Related literature

For related literature, see: Arcadi *et al.* (2003); Bae *et al.* (2005); Bonde & Gaikwad (2004); Kim *et al.* (2007); Lee & Sim (2000); Manaka *et al.* (2005); Saeed & Parvez (2006); Sanemitsu *et al.* (2006); Shehata *et al.* (1996); Shih & Ke (2004); Venkatachalan *et al.* (2001).



Experimental

Crystal data

$C_{24}H_{20}N_2O_2S$
M_r = 400.48
Monoclinic, $P2_1/c$
a = 10.1305 (10) Å
b = 20.0583 (14) Å
c = 10.0959 (10) Å
β = 102.710 (8)°
V = 2001.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 173 (2) K
0.33 × 0.23 × 0.22 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.942, T_{max} = 0.951
11964 measured reflections
3728 independent reflections
3095 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.05
3728 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2195).

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

Aamer Saeed, Sabah Zaman and Michael Bolte

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 act as a skin whitening agent (Kim *et al.*, 2007). 4-Phenyl-2-hyrazono?thiazolines exhibit potent DPPH radical scavenging activity (Shih & Ke, 2004). 3-Alkyl-3*H*-thiazoline derivative PS-028 acts as potent and selective GPllb/llla antagonist (Manaka *et al.*, 2005). 2-Acylimino-1,3-thiazolines show bleaching herbicidal activity (Sanemitsu *et al.*, 2006) and 2-phenylimino-1,3-thiazolines show significant antifungal activity against rice blast fungus Pyricularia oryzae (Bae *et al.*, 2005).

Geometric parameters of the title compound are in the usual ranges. The dihedral angles between the central heterocycle and the phenyl ring is 41.29 (4)and 72.94 (5)° for the methoxyphenyl ring.

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

All H atoms were located in a difference map. They were geometrically positioned and refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 U_{eq}(C_{methyl})] using a riding model with C—H ranging from 0.95Å to 0.98 Å.

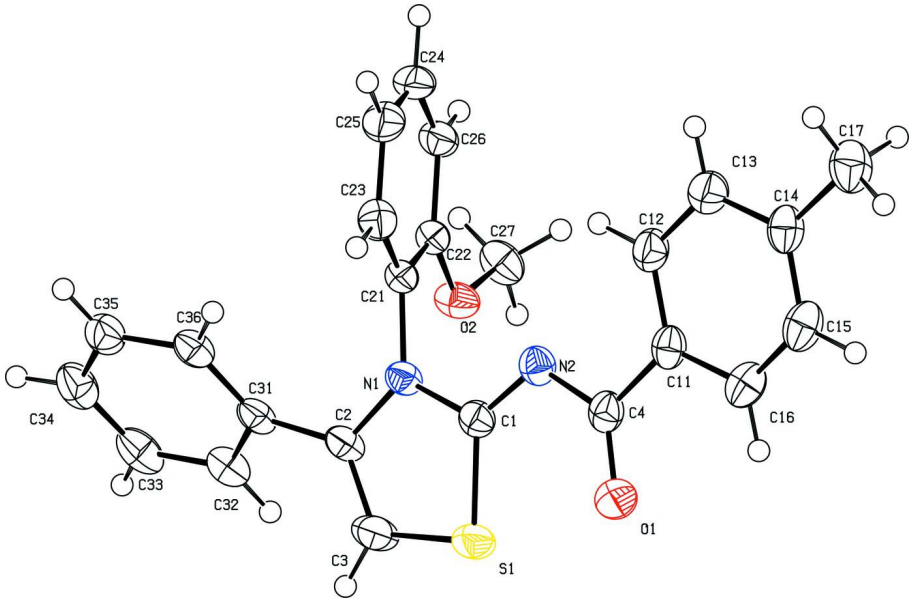

Figure 1

Molecular structure of title compound with displacement ellipsoids at the 50% probability level.

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

Crystal data

$C_{24}H_{20}N_2O_2S$
$M_r = 400.48$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
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$b = 20.0583\ (14)$ Å
$c = 10.0959\ (10)$ Å
$\beta = 102.710\ (8)°$
$V = 2001.2\ (3)$ Å^3
$Z = 4$
$F(000) = 840$
$D_x = 1.329$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10726 reflections
$\theta = 3.8–25.8°$
$\mu = 0.19$ mm^{-1}
$T = 173$ K
Block, colourless
0.33 × 0.23 × 0.22 mm

Data collection

Stoe IPDSII two-circle diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
$T_{min} = 0.942$, $T_{max} = 0.951$
11964 measured reflections
3728 independent reflections
3095 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 25.6°$, $\theta_{min} = 3.7°$
$h = -12\rightarrow11$
$k = -21\rightarrow24$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.103$
$S = 1.05$
3728 reflections
264 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2 + 0.2151P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.98050 (4)	0.70737 (2)	0.51355 (5)	0.04086 (15)
O1	1.10348 (11)	0.68440 (6)	0.31286 (12)	0.0397 (3)
O2	0.72991 (11)	0.52503 (5)	0.53280 (10)	0.0332 (3)
N1	0.75221 (12)	0.64830 (6)	0.43148 (12)	0.0265 (3)
N2	0.89232 (13)	0.63407 (6)	0.27787 (12)	0.0295 (3)
C1	0.87220 (15)	0.65906 (7)	0.39275 (15)	0.0281 (3)
C2	0.74474 (16)	0.67752 (8)	0.55719 (15)	0.0305 (3)
C3	0.86066 (19)	0.70950 (9)	0.61315 (18)	0.0434 (4)
H3	0.8755	0.7311	0.6989	0.052*
C4	1.01248 (15)	0.64968 (7)	0.24281 (15)	0.0303 (3)
C11	1.02529 (15)	0.62264 (8)	0.10802 (15)	0.0301 (3)
C12	0.91665 (16)	0.59116 (8)	0.02041 (16)	0.0347 (4)
H12	0.8335	0.5851	0.0478	0.042*
C13	0.92970 (18)	0.56869 (9)	−0.10637 (17)	0.0396 (4)
H13	0.8548	0.5478	−0.1649	0.047*
C14	1.05099 (17)	0.57628 (9)	−0.14929 (16)	0.0354 (4)
C15	1.15848 (17)	0.60780 (10)	−0.06097 (17)	0.0397 (4)
H15	1.2418	0.6135	−0.0881	0.048*
C16	1.14651 (16)	0.63095 (9)	0.06546 (17)	0.0372 (4)
H16	1.2210	0.6525	0.1232	0.045*
C17	1.0679 (2)	0.54980 (10)	−0.28494 (17)	0.0462 (4)
H17A	1.0897	0.5022	−0.2767	0.069*
H17B	1.1415	0.5738	−0.3130	0.069*
H17C	0.9836	0.5563	−0.3530	0.069*
C21	0.65588 (14)	0.60120 (7)	0.35548 (14)	0.0254 (3)
C22	0.64954 (14)	0.53698 (7)	0.40723 (14)	0.0259 (3)
C23	0.56515 (16)	0.48964 (8)	0.32885 (15)	0.0329 (4)
H23	0.5586	0.4459	0.3629	0.040*
C24	0.49103 (17)	0.50720 (9)	0.20088 (16)	0.0379 (4)
H24	0.4345	0.4749	0.1473	0.045*
C25	0.49813 (17)	0.57099 (9)	0.14992 (16)	0.0387 (4)
H25	0.4464	0.5822	0.0624	0.046*

C26	0.58140 (16)	0.61869 (8)	0.22749 (14)	0.0326 (4)
H26	0.5871	0.6625	0.1933	0.039*
C27	0.74026 (19)	0.45719 (8)	0.58037 (16)	0.0369 (4)
H27A	0.6506	0.4411	0.5872	0.055*
H27B	0.8019	0.4551	0.6699	0.055*
H27C	0.7753	0.4291	0.5164	0.055*
C31	0.62025 (16)	0.67828 (7)	0.61048 (15)	0.0297 (3)
C32	0.63140 (18)	0.67578 (8)	0.75194 (15)	0.0358 (4)
H32	0.7170	0.6677	0.8107	0.043*
C33	0.5178 (2)	0.68500 (8)	0.80611 (17)	0.0415 (4)
H33	0.5264	0.6827	0.9016	0.050*
C34	0.3918 (2)	0.69747 (9)	0.72213 (18)	0.0414 (4)
H34	0.3151	0.7050	0.7600	0.050*
C35	0.37924 (18)	0.69885 (8)	0.58204 (17)	0.0367 (4)
H35	0.2933	0.7068	0.5238	0.044*
C36	0.49179 (16)	0.68870 (7)	0.52706 (15)	0.0313 (3)
H36	0.4815	0.6888	0.4312	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0358 (2)	0.0385 (3)	0.0506 (3)	−0.01358 (18)	0.01446 (18)	−0.01702 (18)
O1	0.0342 (6)	0.0394 (7)	0.0465 (7)	−0.0054 (5)	0.0112 (5)	−0.0059 (5)
O2	0.0418 (6)	0.0246 (5)	0.0292 (5)	−0.0013 (5)	−0.0009 (5)	0.0015 (4)
N1	0.0299 (6)	0.0224 (6)	0.0278 (6)	−0.0030 (5)	0.0074 (5)	−0.0025 (5)
N2	0.0315 (7)	0.0266 (6)	0.0318 (6)	0.0011 (5)	0.0098 (5)	0.0012 (5)
C1	0.0300 (8)	0.0209 (7)	0.0335 (7)	0.0003 (6)	0.0075 (6)	0.0014 (6)
C2	0.0381 (8)	0.0246 (7)	0.0301 (7)	−0.0034 (7)	0.0102 (6)	−0.0061 (6)
C3	0.0458 (10)	0.0424 (10)	0.0444 (9)	−0.0146 (8)	0.0153 (8)	−0.0194 (8)
C4	0.0290 (8)	0.0249 (8)	0.0377 (8)	0.0040 (6)	0.0089 (6)	0.0051 (6)
C11	0.0295 (8)	0.0274 (8)	0.0347 (8)	0.0062 (6)	0.0098 (6)	0.0071 (6)
C12	0.0290 (8)	0.0376 (9)	0.0402 (9)	0.0020 (7)	0.0131 (6)	−0.0002 (7)
C13	0.0342 (9)	0.0455 (10)	0.0393 (9)	0.0014 (7)	0.0088 (7)	−0.0037 (7)
C14	0.0354 (8)	0.0383 (9)	0.0344 (8)	0.0095 (7)	0.0120 (7)	0.0077 (7)
C15	0.0326 (8)	0.0507 (11)	0.0392 (9)	0.0038 (8)	0.0155 (7)	0.0099 (7)
C16	0.0298 (8)	0.0444 (10)	0.0382 (8)	0.0011 (7)	0.0090 (7)	0.0071 (7)
C17	0.0479 (10)	0.0561 (12)	0.0390 (9)	0.0069 (9)	0.0192 (8)	0.0026 (8)
C21	0.0251 (7)	0.0268 (7)	0.0249 (7)	−0.0006 (6)	0.0065 (5)	−0.0047 (5)
C22	0.0259 (7)	0.0269 (8)	0.0252 (7)	0.0000 (6)	0.0062 (6)	−0.0033 (5)
C23	0.0337 (8)	0.0296 (8)	0.0367 (8)	−0.0051 (7)	0.0103 (7)	−0.0074 (6)
C24	0.0332 (9)	0.0449 (10)	0.0342 (8)	−0.0064 (7)	0.0049 (7)	−0.0146 (7)
C25	0.0347 (9)	0.0527 (11)	0.0261 (7)	0.0031 (8)	0.0007 (6)	−0.0055 (7)
C26	0.0350 (8)	0.0357 (9)	0.0269 (7)	0.0044 (7)	0.0065 (6)	0.0011 (6)
C27	0.0517 (10)	0.0259 (8)	0.0336 (8)	0.0036 (7)	0.0102 (7)	0.0035 (6)
C31	0.0389 (8)	0.0202 (7)	0.0319 (7)	−0.0040 (6)	0.0118 (6)	−0.0053 (6)
C32	0.0468 (10)	0.0290 (8)	0.0317 (8)	−0.0007 (7)	0.0091 (7)	−0.0047 (6)
C33	0.0645 (12)	0.0316 (9)	0.0333 (8)	−0.0023 (8)	0.0212 (8)	−0.0042 (7)
C34	0.0509 (10)	0.0318 (9)	0.0492 (10)	−0.0048 (8)	0.0277 (8)	−0.0057 (7)

C35	0.0385 (9)	0.0293 (8)	0.0443 (9)	−0.0025 (7)	0.0134 (7)	−0.0043 (7)
C36	0.0410 (9)	0.0233 (7)	0.0311 (8)	−0.0030 (7)	0.0110 (6)	−0.0025 (6)

Geometric parameters (Å, º)

S1—C3	1.7390 (19)	C17—H17B	0.9800
S1—C1	1.7439 (15)	C17—H17C	0.9800
O1—C4	1.2442 (19)	C21—C26	1.3903 (19)
O2—C22	1.3687 (17)	C21—C22	1.397 (2)
O2—C27	1.4392 (18)	C22—C23	1.400 (2)
N1—C1	1.373 (2)	C23—C24	1.389 (2)
N1—C2	1.4151 (19)	C23—H23	0.9500
N1—C21	1.4505 (17)	C24—C25	1.387 (3)
N2—C1	1.320 (2)	C24—H24	0.9500
N2—C4	1.376 (2)	C25—C26	1.396 (2)
C2—C3	1.348 (2)	C25—H25	0.9500
C2—C31	1.476 (2)	C26—H26	0.9500
C3—H3	0.9500	C27—H27A	0.9800
C4—C11	1.497 (2)	C27—H27B	0.9800
C11—C16	1.397 (2)	C27—H27C	0.9800
C11—C12	1.401 (2)	C31—C36	1.402 (2)
C12—C13	1.390 (2)	C31—C32	1.409 (2)
C12—H12	0.9500	C32—C33	1.390 (2)
C13—C14	1.398 (2)	C32—H32	0.9500
C13—H13	0.9500	C33—C34	1.391 (3)
C14—C15	1.398 (2)	C33—H33	0.9500
C14—C17	1.514 (2)	C34—C35	1.392 (2)
C15—C16	1.388 (2)	C34—H34	0.9500
C15—H15	0.9500	C35—C36	1.388 (2)
C16—H16	0.9500	C35—H35	0.9500
C17—H17A	0.9800	C36—H36	0.9500
C3—S1—C1	90.36 (8)	C26—C21—C22	121.34 (13)
C22—O2—C27	117.35 (11)	C26—C21—N1	119.45 (14)
C1—N1—C2	114.55 (12)	C22—C21—N1	118.93 (12)
C1—N1—C21	119.11 (12)	O2—C22—C21	116.16 (12)
C2—N1—C21	125.57 (13)	O2—C22—C23	124.72 (14)
C1—N2—C4	117.12 (13)	C21—C22—C23	119.12 (13)
N2—C1—N1	120.52 (13)	C24—C23—C22	119.43 (15)
N2—C1—S1	129.09 (12)	C24—C23—H23	120.3
N1—C1—S1	110.39 (10)	C22—C23—H23	120.3
C3—C2—N1	111.07 (14)	C25—C24—C23	121.16 (14)
C3—C2—C31	125.28 (14)	C25—C24—H24	119.4
N1—C2—C31	123.35 (13)	C23—C24—H24	119.4
C2—C3—S1	113.61 (12)	C24—C25—C26	119.89 (14)
C2—C3—H3	123.2	C24—C25—H25	120.1
S1—C3—H3	123.2	C26—C25—H25	120.1
O1—C4—N2	124.59 (15)	C21—C26—C25	119.06 (15)

O1—C4—C11	121.19 (15)	C21—C26—H26	120.5
N2—C4—C11	114.19 (13)	C25—C26—H26	120.5
C16—C11—C12	118.75 (15)	O2—C27—H27A	109.5
C16—C11—C4	119.62 (14)	O2—C27—H27B	109.5
C12—C11—C4	121.59 (14)	H27A—C27—H27B	109.5
C13—C12—C11	120.43 (16)	O2—C27—H27C	109.5
C13—C12—H12	119.8	H27A—C27—H27C	109.5
C11—C12—H12	119.8	H27B—C27—H27C	109.5
C12—C13—C14	121.20 (16)	C36—C31—C32	118.12 (15)
C12—C13—H13	119.4	C36—C31—C2	122.50 (13)
C14—C13—H13	119.4	C32—C31—C2	119.00 (14)
C15—C14—C13	117.78 (15)	C33—C32—C31	120.35 (15)
C15—C14—C17	120.57 (16)	C33—C32—H32	119.8
C13—C14—C17	121.64 (16)	C31—C32—H32	119.8
C16—C15—C14	121.64 (16)	C32—C33—C34	120.80 (15)
C16—C15—H15	119.2	C32—C33—H33	119.6
C14—C15—H15	119.2	C34—C33—H33	119.6
C15—C16—C11	120.21 (15)	C33—C34—C35	119.30 (17)
C15—C16—H16	119.9	C33—C34—H34	120.4
C11—C16—H16	119.9	C35—C34—H34	120.4
C14—C17—H17A	109.5	C36—C35—C34	120.24 (16)
C14—C17—H17B	109.5	C36—C35—H35	119.9
H17A—C17—H17B	109.5	C34—C35—H35	119.9
C14—C17—H17C	109.5	C35—C36—C31	121.14 (14)
H17A—C17—H17C	109.5	C35—C36—H36	119.4
H17B—C17—H17C	109.5	C31—C36—H36	119.4

C4—N2—C1—N1	176.95 (12)	C4—C11—C16—C15	−178.16 (15)
C4—N2—C1—S1	−3.0 (2)	C1—N1—C21—C26	−73.97 (18)
C2—N1—C1—N2	179.56 (13)	C2—N1—C21—C26	116.67 (16)
C21—N1—C1—N2	9.1 (2)	C1—N1—C21—C22	99.99 (16)
C2—N1—C1—S1	−0.48 (15)	C2—N1—C21—C22	−69.38 (19)
C21—N1—C1—S1	−170.98 (10)	C27—O2—C22—C21	−171.39 (14)
C3—S1—C1—N2	−178.83 (15)	C27—O2—C22—C23	7.6 (2)
C3—S1—C1—N1	1.21 (12)	C26—C21—C22—O2	178.36 (13)
C1—N1—C2—C3	−0.81 (19)	N1—C21—C22—O2	4.5 (2)
C21—N1—C2—C3	168.98 (15)	C26—C21—C22—C23	−0.7 (2)
C1—N1—C2—C31	173.17 (13)	N1—C21—C22—C23	−174.56 (13)
C21—N1—C2—C31	−17.0 (2)	O2—C22—C23—C24	−178.17 (15)
N1—C2—C3—S1	1.76 (19)	C21—C22—C23—C24	0.8 (2)
C31—C2—C3—S1	−172.09 (12)	C22—C23—C24—C25	−0.6 (2)
C1—S1—C3—C2	−1.74 (15)	C23—C24—C25—C26	0.3 (3)
C1—N2—C4—O1	1.4 (2)	C22—C21—C26—C25	0.4 (2)
C1—N2—C4—C11	−176.94 (12)	N1—C21—C26—C25	174.20 (14)
O1—C4—C11—C16	6.2 (2)	C24—C25—C26—C21	−0.2 (2)
N2—C4—C11—C16	−175.35 (13)	C3—C2—C31—C36	134.02 (18)
O1—C4—C11—C12	−171.36 (15)	N1—C2—C31—C36	−39.1 (2)
N2—C4—C11—C12	7.1 (2)	C3—C2—C31—C32	−38.8 (2)

C16—C11—C12—C13	0.0 (2)	N1—C2—C31—C32	148.05 (15)
C4—C11—C12—C13	177.59 (15)	C36—C31—C32—C33	−1.4 (2)
C11—C12—C13—C14	0.6 (3)	C2—C31—C32—C33	171.72 (14)
C12—C13—C14—C15	−0.6 (3)	C31—C32—C33—C34	−0.6 (3)
C12—C13—C14—C17	177.76 (16)	C32—C33—C34—C35	1.8 (3)
C13—C14—C15—C16	0.1 (3)	C33—C34—C35—C36	−0.8 (2)
C17—C14—C15—C16	−178.30 (16)	C34—C35—C36—C31	−1.3 (2)
C14—C15—C16—C11	0.5 (3)	C32—C31—C36—C35	2.4 (2)
C12—C11—C16—C15	−0.5 (2)	C2—C31—C36—C35	−170.49 (14)