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Methyl 2-((2*Z*,5*Z*)-4-oxo-3-phenyl-2-{2-[(1*E*)-1,2,3,4-tetrahydronaphthalen-1-ylidene]hydrazin-1-ylidene}-1,3-thiazolidin-5-ylidene)acetate

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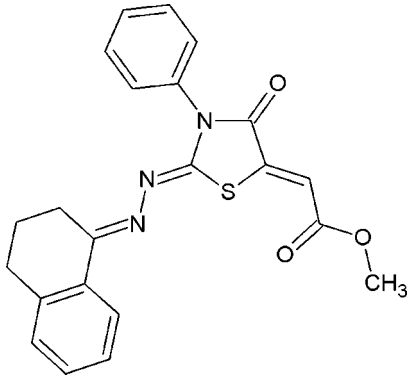
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.104; data-to-parameter ratio = 19.0.

In the title compound, $C_{22}H_{19}N_3O_3S$, the six-membered ring of the 1,2,3,4-tetrahydronaphthalene ring system adopts an envelope conformation with the central CH_2 C atom as the flap. The molecular conformation is stabilized by an S···O contact, forming a pseudo-five-membered ring. In the crystal, molecules are linked *via* C—H···O hydrogen bonds into chains propagating along [102].

Related literature

For the synthesis of thiazolidinediones, see: Patel *et al.* (2010); Aneja *et al.* (2011). For pharmacological properties of thiazolidinedione-containing compounds, see: Gillies & Dunn (2000); Lenhard & Funk (2001); Edelman (2003); Desmet *et al.* (2005). For ring conformation, see: Cremer & Pople (1975). For the synthesis of the title compound, see: Mague *et al.* (2014).



Experimental

Crystal data

$C_{22}H_{19}N_3O_3S$
M_r = 405.47
Triclinic, $P\overline{1}$
a = 9.7078 (6) Å
b = 9.7134 (6) Å
c = 11.1061 (7) Å
α = 67.9810 (9)°
β = 88.8400 (9)°
γ = 85.9840 (9)°
V = 968.47 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 150 K
0.28 × 0.16 × 0.09 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
T_{min} = 0.83, T_{max} = 0.98
17735 measured reflections
4994 independent reflections
4325 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.104
S = 1.05
4994 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O2^{i}	0.95	2.59	3.3704 (18)	140
C11—H11B···N2	0.99	2.38	2.7466 (18)	101
C20—H20···O3^{ii}	0.95	2.56	3.4591 (16)	159
C22—H22C···O1^{ii}	0.98	2.52	3.4397 (18)	157

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+2, -y+2, -z+1$.

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Manchester Metropolitan University, Tulane University and Erciyes University are gratefully acknowledged for supporting this study.

Supporting information for this paper is available from the IUCr electronic archives (Reference: BT6966).

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supporting information

Acta Cryst. (2014). E**70**, o436–o437 [doi:10.1107/S1600536814005285]

Methyl 2-((2*Z*,5*Z*)-4-oxo-3-phenyl-2-{2-[(1*E*)-1,2,3,4-tetrahydronaphthalen-1-ylidene]hydrazin-1-ylidene}-1,3-thiazolidin-5-ylidene)acetate

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S1. Comment

Thiazolidinediones (TZDs) are a pharmacological group of structurally related compounds characterized by a thiazolidinedione ring to which divergent molecular moieties are attached. Many methods have been reoprted for the synthesis of thiazolidinedione-containing compounds and their analogues (Patel *et al.*, 2010; Aneja *et al.*, 2011). The most beneficial effects of TZDs such as rosiglitazone and pioglitazone is the treatment of type II diabetes by lowering blood glucose levels *via* increasing insulin sensitivity with no hepatic side effects (Gillies & Dunn, 2000; Lenhard & Funk, 2001). They were shown also to reduce cardiovascular risk factors associated with this condition (Edelman, 2003). Recently, an anti-inflammatory potential for TZDs has also been suggested (Desmet *et al.*, 2005). In this context we synthesized the title compound as part of our on-going study in synthesis and biological reactivities of thiazolidinedione scaffold compounds.

In the title compound, (Fig. 1), a puckering analysis (Cremer & Pople, 1975) of the six-membered ring C10/C11/C12/C13/C14/C19 indicates it to adopt the "envelope" conformation with puckering parameters Q_T = 0.4855 (17) Å, θ = 126.50 (19)° and φ = 296.6 (2)°. The 1,3-thiazolidine ring (S1/N1/C1—C3) make dihedral angles of 12.22 (7) and 85.72 (6) °, respectively, with the benzene ring (C14–C19) of the 1,2,3,4-tetrahydronaphthalene ring system and the phenyl ring (C4–C9). The C3–N2–N3–C10, C2–C20–C21–O3 and C20–C21–O3–C22 torsion angles are 179.44 (11), 176.24 (12) and -177.15 (11) °, respectively.

The molecular conformation of the title compound is stabilized by a S1···O2 contact forming a pseudo five-membered ring. In the crystal packing, C—H···O hydrogen bonds connect the molecules generating chains running along [1 0 2] (Table 1, Fig. 2).

S2. Experimental

The title compound was synthesized based on our previous reported method (Mague *et al.*, 2014). Orange crystals (m.p.501–503 K) suitable for X-ray analysis were grown from an ethanolic solution at room temperature after two days.

S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.95–0.99 Å, with U_{iso}(H) = 1.2 or 1.5 U_{iso}(C).

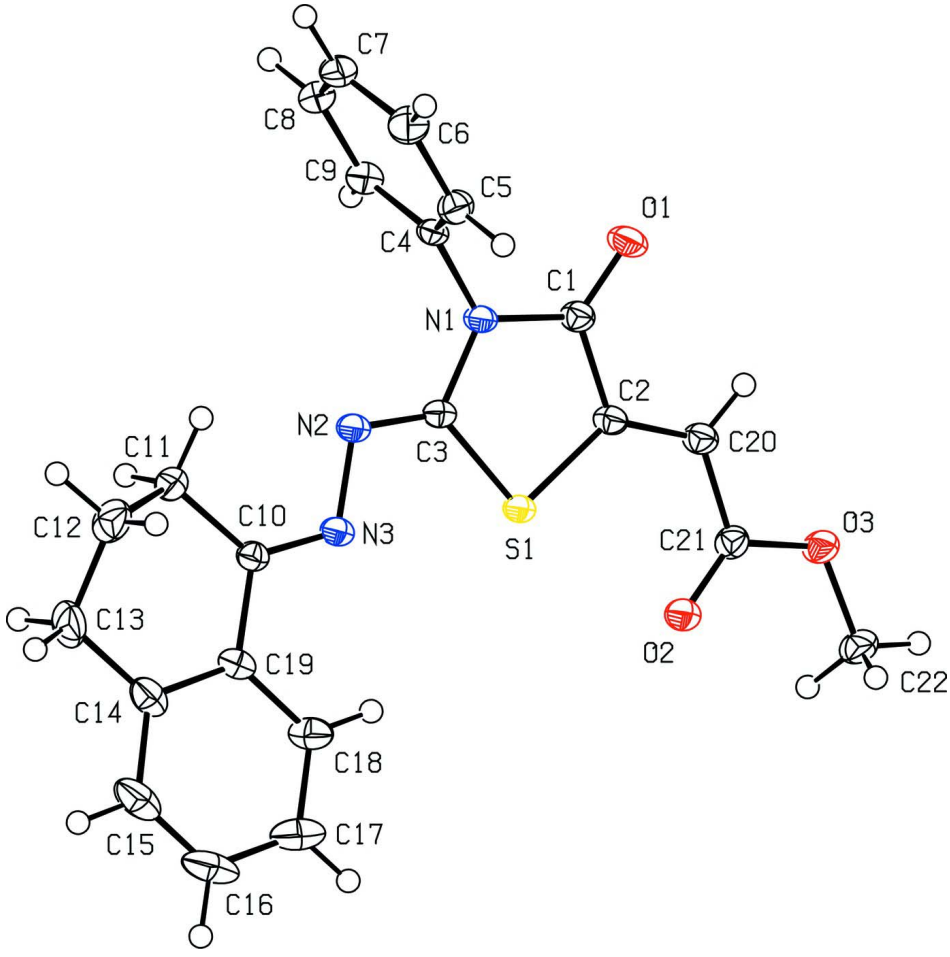

Figure 1

Perspective view of the title molecule with 50% probability ellipsoids.

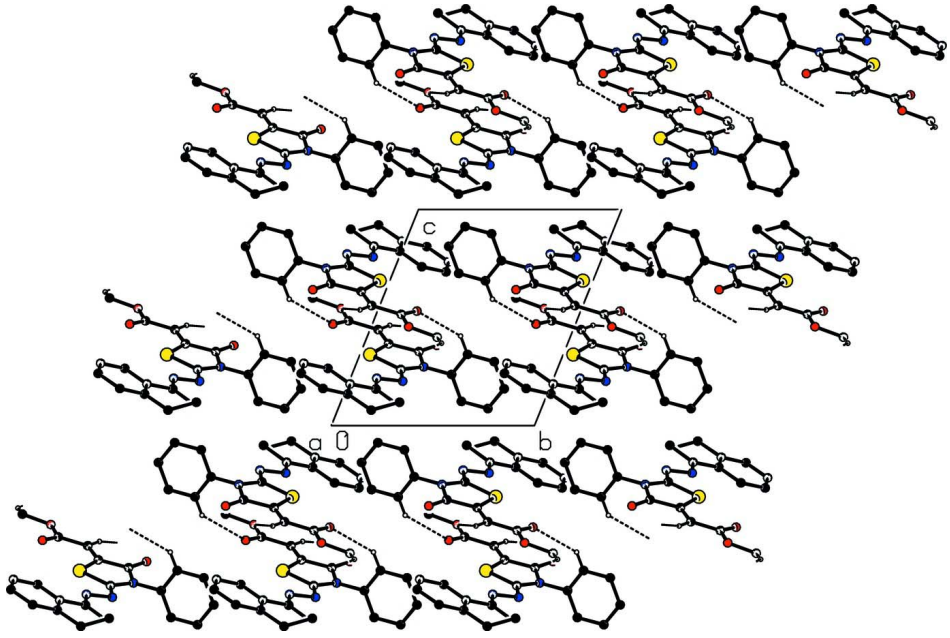

Figure 2

Packing and hydrogen-bonding interactions of the title compound viewed down the *a* axis. H atoms not involved in H bonding are omitted for clarity.

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$c = 11.1061$ (7) Å
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$\beta = 88.8400$ (9)°
$\gamma = 85.9840$ (9)°
$V = 968.47$ (10) Å^3
$Z = 2$
$F(000) = 424$
$D_x = 1.390$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9980 reflections
$\theta = 2.3$–$29.2°$
$\mu = 0.20$ mm^{-1}
$T = 150$ K
Thick plate, orange
0.28 × 0.16 × 0.09 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3660 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min} = 0.83$, $T_{max} = 0.98$
17735 measured reflections
4994 independent reflections
4325 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 29.2°$, $\theta_{min} = 2.0°$
$h = -13 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.104$
$S = 1.05$
4994 reflections
263 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2 + 0.3384P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.52540 (3)	0.95022 (3)	0.67094 (3)	0.0188 (1)
O1	0.76785 (10)	0.63932 (11)	0.62875 (11)	0.0310 (3)
O2	0.66788 (9)	1.19374 (10)	0.53017 (10)	0.0249 (3)
O3	0.88571 (9)	1.18392 (10)	0.45791 (10)	0.0255 (3)
N1	0.56204 (10)	0.66168 (12)	0.72779 (11)	0.0189 (3)
N2	0.34944 (11)	0.73712 (12)	0.79413 (11)	0.0200 (3)
N3	0.27229 (11)	0.87024 (12)	0.78071 (11)	0.0209 (3)
C1	0.67901 (13)	0.71539 (14)	0.65725 (13)	0.0208 (3)
C2	0.67731 (12)	0.88043 (14)	0.62092 (13)	0.0192 (3)
C3	0.46688 (12)	0.76959 (14)	0.74001 (12)	0.0178 (3)
C4	0.52709 (12)	0.50951 (14)	0.76333 (13)	0.0185 (3)
C5	0.46558 (14)	0.47045 (15)	0.67052 (13)	0.0237 (3)
C6	0.42866 (15)	0.32512 (16)	0.70419 (15)	0.0286 (4)
C7	0.45075 (15)	0.22246 (15)	0.82939 (15)	0.0274 (4)
C8	0.51370 (15)	0.26328 (15)	0.92091 (14)	0.0267 (4)
C9	0.55316 (14)	0.40784 (15)	0.88794 (13)	0.0234 (4)
C10	0.15034 (12)	0.85321 (14)	0.83051 (12)	0.0188 (3)
C11	0.09413 (14)	0.70582 (15)	0.90877 (14)	0.0251 (4)
C12	−0.06198 (15)	0.71071 (17)	0.89171 (16)	0.0333 (5)
C13	−0.13270 (15)	0.83434 (19)	0.92826 (16)	0.0363 (5)
C14	−0.07537 (14)	0.98191 (17)	0.85397 (14)	0.0271 (4)
C15	−0.15709 (16)	1.1146 (2)	0.82824 (16)	0.0369 (5)
C16	−0.10746 (18)	1.25107 (19)	0.75859 (17)	0.0400 (5)
C17	0.02647 (18)	1.25928 (18)	0.71144 (17)	0.0379 (5)
C18	0.10916 (15)	1.12992 (16)	0.73521 (15)	0.0289 (4)
C19	0.06062 (13)	0.99048 (15)	0.80716 (13)	0.0216 (3)
C20	0.78083 (13)	0.96017 (14)	0.55569 (13)	0.0219 (4)

C21	0.77041 (13)	1.12321 (14)	0.51469 (13)	0.0210 (3)
C22	0.88037 (15)	1.34487 (15)	0.40941 (15)	0.0282 (4)
H5	0.44880	0.54180	0.58520	0.0280*
H6	0.38810	0.29610	0.64100	0.0340*
H7	0.42280	0.12400	0.85270	0.0330*
H8	0.52990	0.19220	1.00640	0.0320*
H9	0.59720	0.43610	0.94990	0.0280*
H11A	0.11620	0.67920	1.00170	0.0300*
H11B	0.13900	0.62790	0.88110	0.0300*
H12A	−0.08400	0.72830	0.80030	0.0400*
H12B	−0.09670	0.61390	0.94740	0.0400*
H13A	−0.23290	0.84120	0.91030	0.0440*
H13B	−0.12030	0.80970	1.02250	0.0440*
H15	−0.24910	1.11020	0.85960	0.0440*
H16	−0.16480	1.33950	0.74280	0.0480*
H17	0.06110	1.35320	0.66310	0.0450*
H18	0.20050	1.13580	0.70210	0.0350*
H20	0.86120	0.91130	0.53580	0.0260*
H22A	0.84870	1.37910	0.47840	0.0420*
H22B	0.81610	1.38580	0.33560	0.0420*
H22C	0.97260	1.37860	0.38140	0.0420*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0177 (2)	0.0149 (2)	0.0232 (2)	0.0008 (1)	0.0016 (1)	−0.0071 (1)
O1	0.0221 (5)	0.0214 (5)	0.0509 (7)	−0.0001 (4)	0.0105 (4)	−0.0159 (5)
O2	0.0224 (4)	0.0198 (5)	0.0310 (5)	0.0003 (4)	0.0032 (4)	−0.0081 (4)
O3	0.0204 (4)	0.0180 (5)	0.0359 (6)	−0.0037 (4)	0.0039 (4)	−0.0075 (4)
N1	0.0172 (5)	0.0147 (5)	0.0251 (5)	0.0007 (4)	0.0011 (4)	−0.0082 (4)
N2	0.0197 (5)	0.0161 (5)	0.0242 (6)	0.0011 (4)	0.0011 (4)	−0.0080 (4)
N3	0.0198 (5)	0.0170 (5)	0.0258 (6)	0.0012 (4)	0.0021 (4)	−0.0086 (4)
C1	0.0174 (5)	0.0184 (6)	0.0269 (7)	−0.0008 (5)	0.0006 (5)	−0.0090 (5)
C2	0.0173 (5)	0.0175 (6)	0.0232 (6)	0.0013 (4)	−0.0009 (4)	−0.0085 (5)
C3	0.0190 (5)	0.0153 (5)	0.0189 (6)	0.0019 (4)	−0.0021 (4)	−0.0067 (5)
C4	0.0158 (5)	0.0145 (6)	0.0255 (6)	0.0007 (4)	0.0032 (4)	−0.0082 (5)
C5	0.0269 (6)	0.0208 (6)	0.0230 (6)	−0.0017 (5)	0.0002 (5)	−0.0079 (5)
C6	0.0331 (7)	0.0254 (7)	0.0317 (8)	−0.0063 (6)	0.0014 (6)	−0.0150 (6)
C7	0.0312 (7)	0.0177 (6)	0.0351 (8)	−0.0037 (5)	0.0070 (6)	−0.0118 (6)
C8	0.0310 (7)	0.0187 (6)	0.0268 (7)	0.0020 (5)	0.0032 (5)	−0.0051 (5)
C9	0.0238 (6)	0.0210 (6)	0.0255 (7)	0.0015 (5)	−0.0009 (5)	−0.0093 (5)
C10	0.0196 (6)	0.0175 (6)	0.0202 (6)	−0.0001 (5)	0.0006 (4)	−0.0084 (5)
C11	0.0232 (6)	0.0197 (6)	0.0282 (7)	−0.0013 (5)	0.0050 (5)	−0.0046 (5)
C12	0.0234 (7)	0.0295 (8)	0.0400 (9)	−0.0071 (6)	0.0032 (6)	−0.0042 (6)
C13	0.0218 (7)	0.0440 (9)	0.0346 (8)	0.0017 (6)	0.0088 (6)	−0.0061 (7)
C14	0.0227 (6)	0.0355 (8)	0.0237 (7)	0.0064 (6)	−0.0008 (5)	−0.0132 (6)
C15	0.0289 (7)	0.0483 (10)	0.0359 (8)	0.0159 (7)	−0.0031 (6)	−0.0216 (8)
C16	0.0446 (9)	0.0360 (9)	0.0442 (10)	0.0217 (7)	−0.0139 (7)	−0.0239 (8)

C17	0.0476 (9)	0.0214 (7)	0.0460 (10)	0.0071 (7)	−0.0107 (7)	−0.0153 (7)
C18	0.0293 (7)	0.0211 (7)	0.0382 (8)	0.0016 (5)	−0.0029 (6)	−0.0137 (6)
C19	0.0213 (6)	0.0216 (6)	0.0243 (6)	0.0035 (5)	−0.0020 (5)	−0.0120 (5)
C20	0.0185 (6)	0.0193 (6)	0.0276 (7)	0.0005 (5)	0.0003 (5)	−0.0088 (5)
C21	0.0202 (6)	0.0193 (6)	0.0226 (6)	−0.0026 (5)	−0.0001 (5)	−0.0066 (5)
C22	0.0257 (6)	0.0179 (6)	0.0379 (8)	−0.0050 (5)	0.0038 (6)	−0.0066 (6)

Geometric parameters (Å, º)

S1—C2	1.7470 (13)	C14—C19	1.4054 (19)
S1—C3	1.7614 (14)	C15—C16	1.376 (3)
O1—C1	1.2104 (17)	C16—C17	1.388 (2)
O2—C21	1.2147 (16)	C17—C18	1.383 (2)
O3—C21	1.3354 (16)	C18—C19	1.399 (2)
O3—C22	1.4475 (19)	C20—C21	1.471 (2)
N1—C1	1.3841 (17)	C5—H5	0.9500
N1—C3	1.3916 (18)	C6—H6	0.9500
N1—C4	1.4433 (19)	C7—H7	0.9500
N2—N3	1.4069 (17)	C8—H8	0.9500
N2—C3	1.2810 (16)	C9—H9	0.9500
N3—C10	1.2912 (16)	C11—H11A	0.9900
C1—C2	1.498 (2)	C11—H11B	0.9900
C2—C20	1.3392 (18)	C12—H12A	0.9900
C4—C5	1.383 (2)	C12—H12B	0.9900
C4—C9	1.3817 (19)	C13—H13A	0.9900
C5—C6	1.390 (2)	C13—H13B	0.9900
C6—C7	1.384 (2)	C15—H15	0.9500
C7—C8	1.388 (2)	C16—H16	0.9500
C8—C9	1.392 (2)	C17—H17	0.9500
C10—C11	1.503 (2)	C18—H18	0.9500
C10—C19	1.480 (2)	C20—H20	0.9500
C11—C12	1.526 (2)	C22—H22A	0.9800
C12—C13	1.522 (3)	C22—H22B	0.9800
C13—C14	1.501 (2)	C22—H22C	0.9800
C14—C15	1.401 (3)		

C2—S1—C3	90.54 (6)	O3—C21—C20	112.24 (11)
C21—O3—C22	115.22 (11)	C4—C5—H5	121.00
C1—N1—C3	115.28 (12)	C6—C5—H5	121.00
C1—N1—C4	122.38 (11)	C5—C6—H6	120.00
C3—N1—C4	121.19 (10)	C7—C6—H6	120.00
N3—N2—C3	108.54 (11)	C6—C7—H7	120.00
N2—N3—C10	114.88 (12)	C8—C7—H7	120.00
O1—C1—N1	124.49 (13)	C7—C8—H8	120.00
O1—C1—C2	125.72 (12)	C9—C8—H8	120.00
N1—C1—C2	109.78 (11)	C4—C9—H9	121.00
S1—C2—C1	111.61 (9)	C8—C9—H9	121.00
S1—C2—C20	126.19 (12)	C10—C11—H11A	109.00

C1—C2—C20	122.19 (12)	C10—C11—H11B	109.00
S1—C3—N1	112.60 (9)	C12—C11—H11A	109.00
S1—C3—N2	125.31 (11)	C12—C11—H11B	109.00
N1—C3—N2	122.08 (13)	H11A—C11—H11B	108.00
N1—C4—C5	118.25 (12)	C11—C12—H12A	110.00
N1—C4—C9	119.99 (12)	C11—C12—H12B	110.00
C5—C4—C9	121.75 (13)	C13—C12—H12A	110.00
C4—C5—C6	118.88 (13)	C13—C12—H12B	110.00
C5—C6—C7	120.30 (14)	H12A—C12—H12B	108.00
C6—C7—C8	120.01 (14)	C12—C13—H13A	109.00
C7—C8—C9	120.27 (13)	C12—C13—H13B	109.00
C4—C9—C8	118.76 (13)	C14—C13—H13A	109.00
N3—C10—C11	124.91 (13)	C14—C13—H13B	109.00
N3—C10—C19	116.60 (12)	H13A—C13—H13B	108.00
C11—C10—C19	118.49 (11)	C14—C15—H15	119.00
C10—C11—C12	111.39 (12)	C16—C15—H15	119.00
C11—C12—C13	110.22 (13)	C15—C16—H16	120.00
C12—C13—C14	111.71 (13)	C17—C16—H16	120.00
C13—C14—C15	120.61 (13)	C16—C17—H17	120.00
C13—C14—C19	120.99 (14)	C18—C17—H17	120.00
C15—C14—C19	118.40 (15)	C17—C18—H18	119.00
C14—C15—C16	121.64 (15)	C19—C18—H18	119.00
C15—C16—C17	119.89 (17)	C2—C20—H20	120.00
C16—C17—C18	119.62 (17)	C21—C20—H20	120.00
C17—C18—C19	121.12 (14)	O3—C22—H22A	109.00
C10—C19—C14	120.36 (13)	O3—C22—H22B	109.00
C10—C19—C18	120.29 (12)	O3—C22—H22C	109.00
C14—C19—C18	119.32 (14)	H22A—C22—H22B	109.00
C2—C20—C21	120.19 (12)	H22A—C22—H22C	109.00
O2—C21—O3	124.27 (13)	H22B—C22—H22C	110.00
O2—C21—C20	123.49 (12)		

C3—S1—C2—C1	1.03 (10)	C9—C4—C5—C6	0.3 (2)
C3—S1—C2—C20	179.69 (13)	N1—C4—C9—C8	177.63 (12)
C2—S1—C3—N1	1.64 (10)	C5—C4—C9—C8	−1.3 (2)
C2—S1—C3—N2	−177.12 (12)	C4—C5—C6—C7	1.3 (2)
C22—O3—C21—O2	−2.31 (19)	C5—C6—C7—C8	−1.9 (2)
C22—O3—C21—C20	177.15 (11)	C6—C7—C8—C9	0.9 (2)
C3—N1—C1—O1	−174.48 (13)	C7—C8—C9—C4	0.7 (2)
C3—N1—C1—C2	4.83 (15)	N3—C10—C11—C12	−149.23 (14)
C4—N1—C1—O1	−6.7 (2)	C19—C10—C11—C12	30.49 (17)
C4—N1—C1—C2	172.65 (11)	N3—C10—C19—C14	177.77 (13)
C1—N1—C3—S1	−4.18 (14)	N3—C10—C19—C18	−0.49 (19)
C1—N1—C3—N2	174.63 (12)	C11—C10—C19—C14	−1.97 (19)
C4—N1—C3—S1	−172.16 (9)	C11—C10—C19—C18	179.77 (13)
C4—N1—C3—N2	6.65 (19)	C10—C11—C12—C13	−56.61 (16)
C1—N1—C4—C5	−79.47 (16)	C11—C12—C13—C14	54.64 (17)
C1—N1—C4—C9	101.58 (15)	C12—C13—C14—C15	152.42 (15)

C3—N1—C4—C5	87.64 (16)	C12—C13—C14—C19	−26.8 (2)
C3—N1—C4—C9	−91.31 (15)	C13—C14—C15—C16	−178.97 (16)
C3—N2—N3—C10	179.44 (11)	C19—C14—C15—C16	0.2 (2)
N3—N2—C3—S1	4.12 (16)	C13—C14—C19—C10	0.0 (2)
N3—N2—C3—N1	−174.53 (11)	C13—C14—C19—C18	178.25 (14)
N2—N3—C10—C11	5.64 (19)	C15—C14—C19—C10	−179.24 (13)
N2—N3—C10—C19	−174.09 (11)	C15—C14—C19—C18	−1.0 (2)
O1—C1—C2—S1	175.85 (12)	C14—C15—C16—C17	0.3 (3)
O1—C1—C2—C20	−2.9 (2)	C15—C16—C17—C18	−0.2 (3)
N1—C1—C2—S1	−3.45 (14)	C16—C17—C18—C19	−0.6 (3)
N1—C1—C2—C20	177.83 (12)	C17—C18—C19—C10	179.44 (14)
S1—C2—C20—C21	−2.6 (2)	C17—C18—C19—C14	1.2 (2)
C1—C2—C20—C21	175.97 (12)	C2—C20—C21—O2	−4.3 (2)
N1—C4—C5—C6	−178.63 (12)	C2—C20—C21—O3	176.24 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.95	2.59	3.3704 (18)	140
C11—H11*B*···N2	0.99	2.38	2.7466 (18)	101
C20—H20···O3^{ii}	0.95	2.56	3.4591 (16)	159
C22—H22*C*···O1^{ii}	0.98	2.52	3.4397 (18)	157

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