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Crystal structures of *rac*-2,3-diphenyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazine-1,1,4-trione and *N*-[(2*S*,5*R*)-1,1,4-trioxo-2,3-diphenyl-1,3-thiazinan-5-yl]-acetamide

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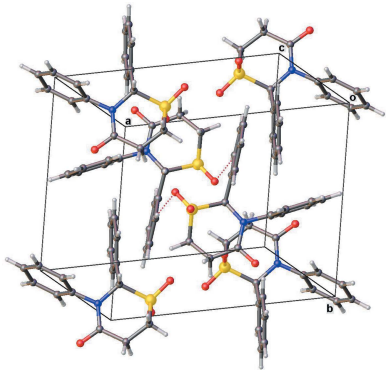
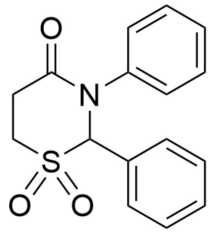
The syntheses and crystal structures of two thiazinone compounds, namely, *rac*-2,3-diphenyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazine-1,1,4-trione, $C_{16}H_{15}NO_3S$, in its racemic form, and *N*-[(2*S*,5*R*)-1,1,4-trioxo-2,3-diphenyl-1,3-thiazinan-5-yl]acetamide, $C_{18}H_{18}N_2O_4S$, in an enantiopure form, are reported. The thiazine rings in the two structures differ in their puckering, as a half-chair in the first and a boat pucker in the second. The extended structures for both compounds have only C—H···O-type interactions between symmetry-related molecules, and exhibit no π–π stacking interactions in spite of each having two phenyl rings.

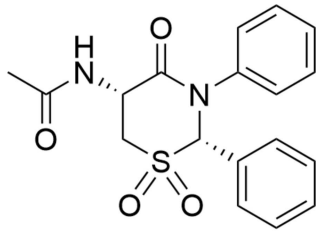
1. Chemical context

The 2,3-dihydro-4*H*-1,3-thiazin-4-ones are a group of six-membered heterocycles with a wide range of biological activity (Ryabukhin *et al.*, 1996; Silverberg & Moyer, 2019). Surrey's research (Surrey *et al.*, 1958; Surrey, 1963*a*,*b*) resulted in the discovery of two drugs, the antianxiety and muscle relaxant chlormezanone, $C_{11}H_{12}ClNO_3S$, [2-(4-chlorophenyl)-3-methyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazin-4-one 1,1-dioxide] (O'Neil, 2006; Tanaka & Horayama, 2005) and the muscle relaxant dichlormezanone, $C_{11}H_{11}Cl_2NO_3S$, [2-(3,4-dichlorophenyl)-3-methyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazin-4-one 1,1-dioxide] (Elks & Ganellin, 1990). These sulfones showed greater activity than the sulfides from which they were synthesized (Surrey *et al.*, 1958).





1



2

We have previously reported the preparation of the sulfones *rac*-2,3-dihydro-2,3-diphenyl-4*H*-1,3-thiazin-4-one 1,1-dioxide and *N*-[(2*S*,5*R*)-1,1-dioxido-4-oxo-2,3-diphenyl-1,3-thiazinan-5-yl]acetamide (Silverberg, 2020). We have also reported X-ray crystal structures of the corresponding sulfides and sulfoxides (Yennawar & Silverberg, 2014, 2015; Yennawar

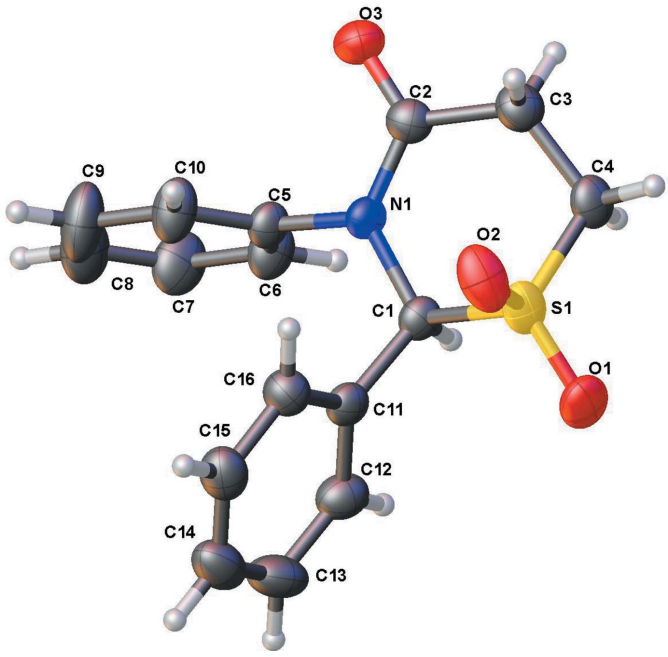


Figure 1
The asymmetric unit of **1** with displacement ellipsoids drawn at 50% probability level.

et al., 2015, 2016, 2017). The crystal structure of chlormezanone has been reported (Tanaka & Horayama, 2005). Herein we report the crystal structures of *rac*-2,3-diphenyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazine-1,1,4-trione, **1**, and *N*-[(2*S*,5*R*)-1,1,4-trioxo-2,3-diphenyl-1,3-thiazinan-5-yl]acetamide, **2**.

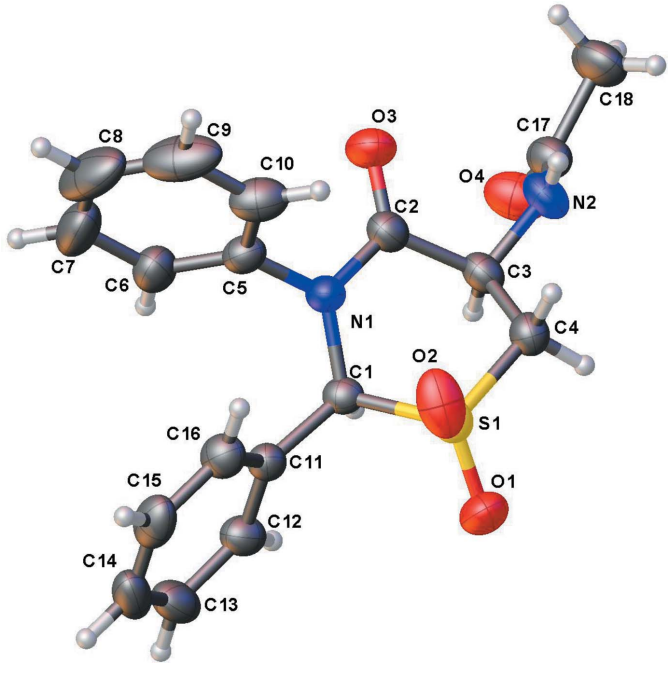


Figure 2
The asymmetric unit of **2** with displacement ellipsoids drawn at 50% probability level.

2. Structural commentary

Compound **1** has one chiral center at C1 with an *S* configuration in the arbitrarily chosen asymmetric unit but crystal symmetry generates a racemic mixture (space group $P2_1/c$). Compound **2** has two chiral centers, at C1 and C3 (*S* and *R* respectively), synthesized as such, and crystallizes in space group $P2_12_12_1$. In **1**, the dihedral angles between the thiazine ring (all atoms) and the pendant C5–C10 and C11–C16 phenyl groups are 84.02 (14) and 79.56 (12)°, respectively; the dihedral angle between the pendant rings is 61.26 (15)°. The equivalent angles in **2** are 81.25 (15), 82.58 (13) and 50.40 (15)°, respectively.

The structure of **1** (Fig. 1) has a half-chair puckering of the thiazine ring with puckering amplitude Q = 0.605 (2) Å, θ = 47.2 (2)°, φ = 346.7 (3)°, while in **2** (Fig. 2) the ring has a boat pucker [Q = 0.770 (2) Å, θ = 85.31 (15)°, φ = 61.89 (17)°]. This change in the puckering of the central ring system of the two molecules leads to differing orientations of one of the phenyl rings, which is clear from the overlay diagram (Fig. 3).

3. Supramolecular features

In both structures, only C—H···O-type hydrogen-bond interactions between symmetry-related molecules are observed (Tables 1 and 2). In **1**, a single hydrogen bond [C12—H12···O1 = 3.454 (4) Å, 157°] and its symmetry-equivalent

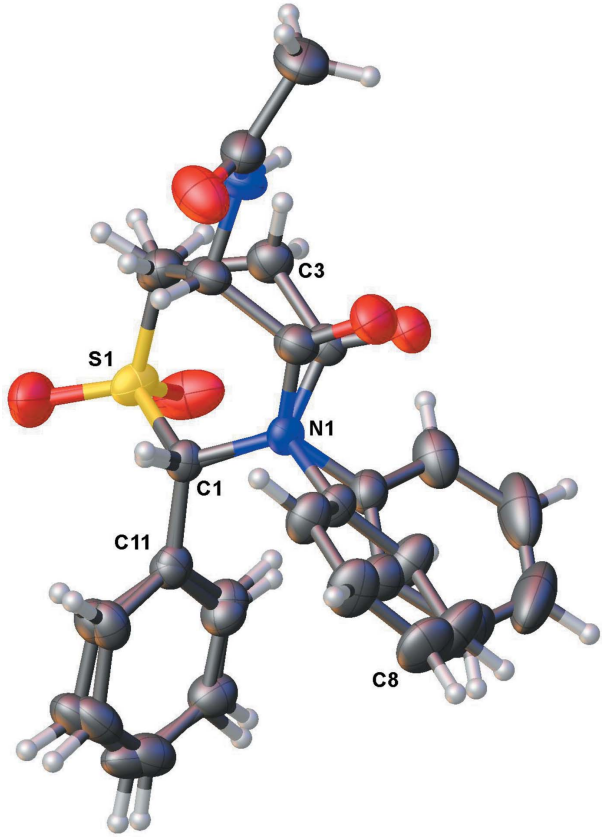


Figure 3
Overlay plot of **1** and **2** where the three atoms S1, N1, and C11 are matched. Atoms C3 and C8 of compound **1** are labeled.

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.95	2.56	3.454 (4)	157

Symmetry code: (i) $-x+1, -y+1, -z+1$.

form a pair of parallel interactions (Fig. 4). In **2** (Fig. 5), the carbon atoms C1 and C4, both of the thiazine ring, as well as C8 of one of the phenyl rings each donate an H atom for three distinct interactions involving three of the four oxygen atoms in the molecule. Although both compounds each have two phenyl rings, neither of the lattices exhibit any π–π stacking interactions.

4. Database survey

Searches undertaken using the American Chemical Society's Chemical Abstract Service (CAS) Scifinder platform did not find crystal structures of any 1,3-thiazin-4-one sulfones other than chlormezanone (CSD refcode KAPNAR; Tanaka & Horayama, 2005).

5. Synthesis and crystallization

General oxidation procedure (Surrey *et al.*, 1958; Silverberg, 2020; Cannon *et al.* 2015): the heterocycle (0.267 mmol) was dissolved in glacial acetic acid (1.2 ml). An aqueous solution of $KMnO_4$ (0.535 mmol in 1.45 ml water) was added dropwise at room temperature with vigorous stirring. The reaction was followed by TLC. Solid sodium bisulfite ($NaHSO_3$/$Na_2S_2O_5$) was added until the mixture remained colorless and then 1.45 ml of water were added and stirred for 10 min. The mixture was extracted with CH_2Cl_2 (3 × 5 ml). The organics were combined and washed once with sat. NaCl. The solution was dried over Na_2SO_4 and filtered. The product was purified by chromatography in a silica gel micro-column.

***rac*-2,3-diphenyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazine-1,1,4-trione, 1:** Eluted with mixtures of ethyl acetate and hexanes. White solid (0.053 g, 70%). m.p.: 418–421 K. Crystals for X-ray diffraction studies were grown by slow evaporation from toluene solution.

***N*-[(2*S*,5*R*)-1,1,4-trioxo-2,3-diphenyl-1,3-thiazinan-5-yl]-acetamide, 2:** Eluted with a mixture of 10% acetone and 90% ethyl acetate. White solid (0.076 g, 80%). m.p.: 443–467 K (decomposition). Crystals were grown by slow evaporation from ethanol solution.

Table 2
Hydrogen-bond geometry (Å, °) for **2**.

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O2^{i}	0.98	2.39	3.365 (3)	173
C4—H4A···O4^{ii}	0.97	2.29	3.185 (4)	153
C8—H8···O3^{iii}	0.93	2.51	3.378 (5)	155

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

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atoms were placed

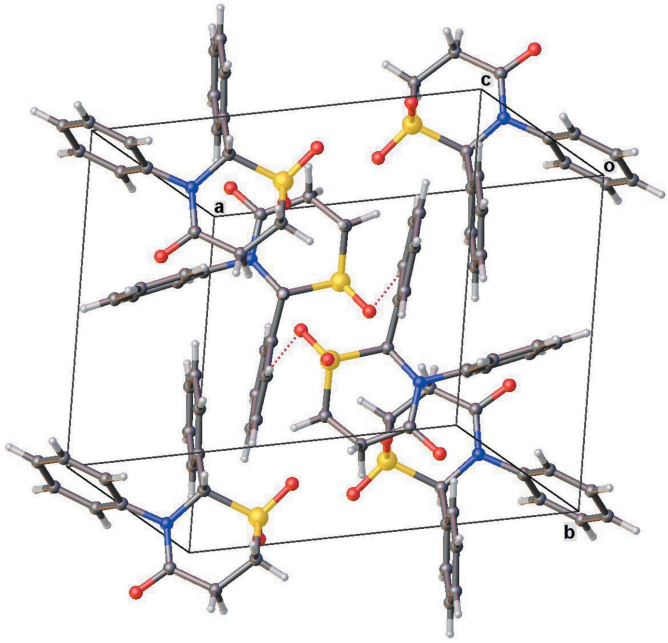


Figure 4
Crystal packing diagram for **1** showing intermolecular pairs of C—H···O hydrogen bonds.

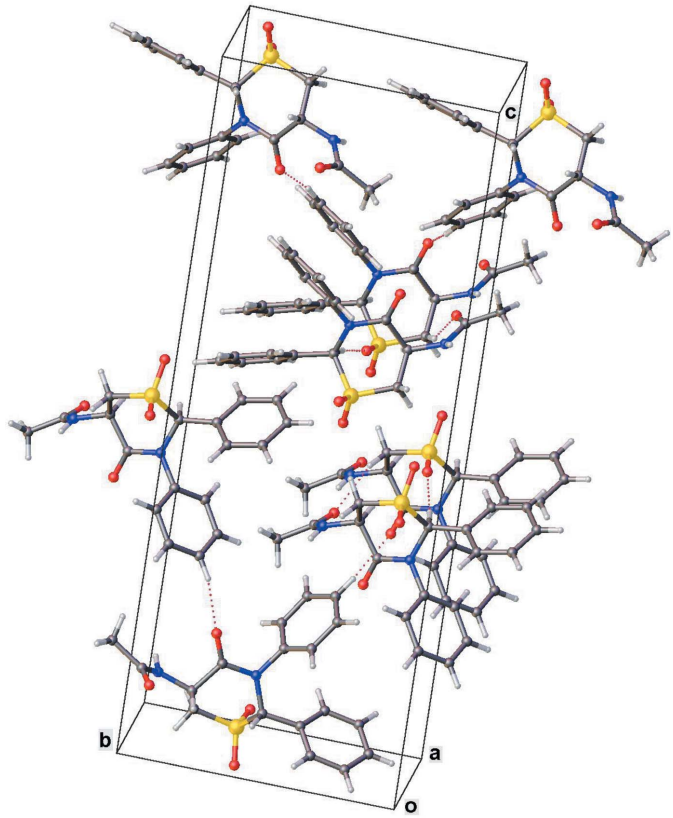


Figure 5
Crystal packing diagram for **2** showing intermolecular C—H···O hydrogen bonds.

Table 3
Experimental details.

	1	**2**
Crystal data		
Chemical formula	$C_{16}H_{15}NO_3S$	$C_{18}H_{18}N_2O_4S$
M_r	301.35	358.40
Crystal system, space group	Monoclinic, $P2_1/c$	Orthorhombic, $P2_12_12_1$
Temperature (K)	173	298
a, b, c (Å)	14.4485 (6), 10.2031 (5), 10.4950 (4)	5.5230 (4), 10.6857 (9), 28.430 (2)
α, β, γ (°)	90, 107.179 (4), 90	90, 90, 90
V (Å^3)	1478.13 (11)	1677.8 (2)
Z	4	4
Radiation type	Cu $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	2.03	0.22
Crystal size (mm)	0.2 × 0.18 × 0.09	0.22 × 0.06 × 0.06
Data collection		
Diffractometer	Rigaku Oxford Diffraction Synergy Custom system, HyPix-Arc 150	Bruker SMART CCD area detector
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.668, 1.000	0.656, 0.900
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7437, 2856, 2139	13301, 4037, 3460
R_{int}	0.056	0.035
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.628	0.667
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.150, 1.10	0.042, 0.103, 1.04
No. of reflections	2856	4037
No. of parameters	191	231
H-atom treatment	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.32, −0.34	0.24, −0.14
Absolute structure	–	Flack x determined using 1213 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	–	0.07 (4)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SMART* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXS* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

in their geometrically calculated positions and their coordinates refined using the riding model with parent-atom—H lengths of 0.93 Å (CH), 0.98 Å (chiral-CH), 0.96 Å (CH_3), 0.97 Å (CH_2). Isotropic displacement parameters for these atoms were set to 1.2 (CH) or 1.5 (CH_3) times U_{eq} of the parent atom.

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supporting information

Acta Cryst. (2023). E**79**, 120-123 [https://doi.org/10.1107/S2056989023000695]

Crystal structures of *rac*-2,3-diphenyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazine-1,1,4-trione and *N*-[(2*S*,5*R*)-1,1,4-trioxo-2,3-diphenyl-1,3-thiazinan-5-yl]acetamide

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2022) for (1); *SMART* (Bruker, 2016) for (2). Cell refinement: *CrysAlis PRO* (Rigaku OD, 2022) for (1); *SAINT* (Bruker, 2016) for (2). Data reduction: *CrysAlis PRO* (Rigaku OD, 2022) for (1); *SAINT* (Bruker, 2016) for (2). Program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a) for (1); *SHELXS* (Sheldrick, 2008) for (2). For both structures, program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

rac-2,3-Diphenyl-2,3,5,6-tetrahydro-4*H*-1,3-thiazine-1,1,4-trione (1)

Crystal data

$C_{16}H_{15}NO_3S$
M_r = 301.35
Monoclinic, $P2_1/c$
a = 14.4485 (6) Å
b = 10.2031 (5) Å
c = 10.4950 (4) Å
β = 107.179 (4)°
V = 1478.13 (11) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.354 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 3416 reflections
θ = 3.2–73.3°
μ = 2.03 mm^{-1}
T = 173 K
Block, clear colourless
0.2 × 0.18 × 0.09 mm

Data collection

Rigaku Oxford Diffraction Synergy Custom system, HyPix-Arc 150 diffractometer
Radiation source: Rotating-anode X-ray tube, Rigaku (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.668, T_{max} = 1.000
7437 measured reflections
2856 independent reflections
2139 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 75.6°, θ_{min} = 3.2°
h = −15→17
k = −11→12
l = −12→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.150
S = 1.10
2856 reflections

191 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2 + 0.268P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Extinction correction: *SHELXL2018/3* (Sheldrick 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0023 (5)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.45082 (4)	0.66477 (7)	0.66401 (5)	0.0380 (2)
O1	0.52700 (12)	0.5704 (2)	0.67907 (19)	0.0514 (6)
O2	0.41925 (14)	0.6961 (2)	0.77812 (16)	0.0519 (6)
O3	0.22170 (13)	0.91599 (19)	0.44575 (18)	0.0455 (5)
N1	0.27444 (13)	0.7076 (2)	0.48536 (18)	0.0306 (5)
C1	0.35000 (16)	0.6063 (3)	0.5290 (2)	0.0310 (5)
H1	0.374440	0.583984	0.451921	0.037*
C4	0.47674 (18)	0.8100 (3)	0.5937 (2)	0.0396 (6)
H4A	0.532525	0.854461	0.656910	0.048*
H4B	0.493981	0.790381	0.511127	0.048*
C3	0.38813 (19)	0.8988 (3)	0.5617 (3)	0.0425 (6)
H3A	0.399282	0.971486	0.505438	0.051*
H3B	0.384838	0.938047	0.646531	0.051*
C2	0.28912 (18)	0.8402 (3)	0.4920 (2)	0.0348 (6)
C5	0.18322 (17)	0.6594 (3)	0.3978 (2)	0.0333 (6)
C6	0.17961 (19)	0.6182 (3)	0.2711 (2)	0.0440 (7)
H6	0.235336	0.625452	0.241121	0.053*
C7	0.0947 (2)	0.5664 (4)	0.1879 (3)	0.0559 (9)
H7	0.091908	0.537900	0.100655	0.067*
C8	0.0141 (2)	0.5563 (4)	0.2324 (3)	0.0633 (10)
H8	−0.044126	0.519958	0.175939	0.076*
C9	0.0179 (2)	0.5990 (4)	0.3588 (3)	0.0682 (11)
H9	−0.038042	0.592964	0.388363	0.082*
C10	0.10296 (19)	0.6506 (3)	0.4427 (3)	0.0496 (8)
H10	0.105807	0.679455	0.529797	0.060*
C11	0.31292 (16)	0.4818 (3)	0.5756 (2)	0.0334 (6)
C12	0.3255 (2)	0.3631 (3)	0.5188 (3)	0.0437 (7)
H12	0.356067	0.360439	0.450153	0.052*
C13	0.2933 (2)	0.2481 (3)	0.5624 (3)	0.0550 (8)
H13	0.301505	0.166705	0.523015	0.066*
C14	0.2495 (2)	0.2515 (3)	0.6624 (3)	0.0541 (8)
H14	0.227909	0.172599	0.692365	0.065*

C15	0.2371 (2)	0.3693 (3)	0.7189 (3)	0.0468 (7)
H15	0.207209	0.371115	0.788272	0.056*
C16	0.26749 (17)	0.4849 (3)	0.6758 (2)	0.0391 (6)
H16	0.257539	0.566039	0.714104	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0329 (4)	0.0492 (5)	0.0252 (3)	−0.0062 (3)	−0.0018 (2)	0.0054 (3)
O1	0.0332 (10)	0.0563 (14)	0.0540 (11)	0.0048 (9)	−0.0038 (8)	0.0172 (10)
O2	0.0568 (12)	0.0699 (15)	0.0249 (9)	−0.0242 (11)	0.0060 (8)	−0.0045 (9)
O3	0.0431 (11)	0.0385 (11)	0.0531 (11)	0.0069 (9)	0.0117 (8)	0.0068 (9)
N1	0.0264 (10)	0.0339 (12)	0.0271 (9)	0.0014 (9)	0.0010 (7)	0.0010 (9)
C1	0.0288 (12)	0.0369 (14)	0.0242 (11)	0.0019 (11)	0.0029 (8)	0.0001 (10)
C4	0.0332 (13)	0.0488 (18)	0.0306 (12)	−0.0078 (12)	−0.0002 (9)	−0.0007 (12)
C3	0.0429 (15)	0.0410 (16)	0.0409 (13)	−0.0035 (13)	0.0085 (11)	−0.0046 (12)
C2	0.0387 (13)	0.0361 (15)	0.0287 (12)	0.0004 (12)	0.0088 (9)	0.0008 (11)
C5	0.0266 (12)	0.0412 (16)	0.0273 (11)	0.0008 (11)	0.0006 (9)	0.0025 (11)
C6	0.0344 (13)	0.061 (2)	0.0318 (13)	0.0004 (13)	0.0024 (10)	−0.0038 (13)
C7	0.0457 (16)	0.075 (2)	0.0375 (14)	−0.0016 (16)	−0.0020 (11)	−0.0111 (15)
C8	0.0393 (16)	0.083 (3)	0.0542 (18)	−0.0118 (17)	−0.0070 (13)	−0.0056 (18)
C9	0.0319 (15)	0.118 (3)	0.0511 (18)	−0.0105 (19)	0.0072 (12)	0.003 (2)
C10	0.0347 (14)	0.079 (2)	0.0340 (13)	−0.0036 (15)	0.0083 (10)	−0.0019 (14)
C11	0.0284 (12)	0.0365 (15)	0.0299 (11)	0.0023 (11)	0.0005 (9)	0.0008 (11)
C12	0.0441 (15)	0.0421 (17)	0.0402 (14)	0.0065 (13)	0.0051 (11)	−0.0036 (13)
C13	0.063 (2)	0.0324 (17)	0.0579 (18)	0.0028 (15)	0.0007 (15)	0.0000 (14)
C14	0.0525 (17)	0.0420 (19)	0.0573 (18)	−0.0064 (15)	−0.0001 (14)	0.0102 (15)
C15	0.0428 (15)	0.0516 (19)	0.0431 (15)	−0.0038 (14)	0.0083 (11)	0.0098 (14)
C16	0.0398 (14)	0.0400 (16)	0.0360 (13)	−0.0006 (12)	0.0089 (10)	0.0013 (12)

Geometric parameters (Å, º)

S1—O1	1.435 (2)	C6—C7	1.383 (4)
S1—O2	1.438 (2)	C7—H7	0.9500
S1—C1	1.807 (2)	C7—C8	1.381 (4)
S1—C4	1.744 (3)	C8—H8	0.9500
O3—C2	1.226 (3)	C8—C9	1.382 (5)
N1—C1	1.475 (3)	C9—H9	0.9500
N1—C2	1.368 (3)	C9—C10	1.387 (4)
N1—C5	1.451 (3)	C10—H10	0.9500
C1—H1	1.0000	C11—C12	1.385 (4)
C1—C11	1.514 (4)	C11—C16	1.394 (3)
C4—H4A	0.9900	C12—H12	0.9500
C4—H4B	0.9900	C12—C13	1.389 (4)
C4—C3	1.523 (4)	C13—H13	0.9500
C3—H3A	0.9900	C13—C14	1.377 (5)
C3—H3B	0.9900	C14—H14	0.9500
C3—C2	1.524 (4)	C14—C15	1.375 (4)

C5—C6	1.381 (3)	C15—H15	0.9500
C5—C10	1.377 (4)	C15—C16	1.381 (4)
C6—H6	0.9500	C16—H16	0.9500

O1—S1—O2	118.62 (12)	C5—C6—H6	120.0
O1—S1—C1	106.20 (12)	C5—C6—C7	119.9 (3)
O1—S1—C4	111.28 (13)	C7—C6—H6	120.0
O2—S1—C1	110.23 (11)	C6—C7—H7	120.2
O2—S1—C4	108.92 (14)	C8—C7—C6	119.6 (3)
C4—S1—C1	99.96 (11)	C8—C7—H7	120.2
C2—N1—C1	126.0 (2)	C7—C8—H8	119.9
C2—N1—C5	117.7 (2)	C7—C8—C9	120.2 (3)
C5—N1—C1	114.2 (2)	C9—C8—H8	119.9
S1—C1—H1	108.3	C8—C9—H9	119.8
N1—C1—S1	111.31 (17)	C8—C9—C10	120.4 (3)
N1—C1—H1	108.3	C10—C9—H9	119.8
N1—C1—C11	112.84 (19)	C5—C10—C9	119.1 (3)
C11—C1—S1	107.70 (15)	C5—C10—H10	120.5
C11—C1—H1	108.3	C9—C10—H10	120.5
S1—C4—H4A	109.9	C12—C11—C1	119.3 (2)
S1—C4—H4B	109.9	C12—C11—C16	119.7 (3)
H4A—C4—H4B	108.3	C16—C11—C1	121.0 (2)
C3—C4—S1	109.11 (19)	C11—C12—H12	120.1
C3—C4—H4A	109.9	C11—C12—C13	119.8 (3)
C3—C4—H4B	109.9	C13—C12—H12	120.1
C4—C3—H3A	107.6	C12—C13—H13	119.9
C4—C3—H3B	107.6	C14—C13—C12	120.2 (3)
C4—C3—C2	118.7 (2)	C14—C13—H13	119.9
H3A—C3—H3B	107.1	C13—C14—H14	120.0
C2—C3—H3A	107.6	C15—C14—C13	119.9 (3)
C2—C3—H3B	107.6	C15—C14—H14	120.0
O3—C2—N1	120.7 (2)	C14—C15—H15	119.7
O3—C2—C3	117.7 (2)	C14—C15—C16	120.7 (3)
N1—C2—C3	121.5 (2)	C16—C15—H15	119.7
C6—C5—N1	118.8 (2)	C11—C16—H16	120.2
C10—C5—N1	120.3 (2)	C15—C16—C11	119.6 (3)
C10—C5—C6	120.9 (2)	C15—C16—H16	120.2

S1—C1—C11—C12	−111.1 (2)	C4—C3—C2—O3	−167.2 (2)
S1—C1—C11—C16	68.1 (2)	C4—C3—C2—N1	15.3 (4)
S1—C4—C3—C2	−45.9 (3)	C2—N1—C1—S1	29.3 (3)
O1—S1—C1—N1	−168.32 (16)	C2—N1—C1—C11	150.5 (2)
O1—S1—C1—C11	67.50 (19)	C2—N1—C5—C6	96.5 (3)
O1—S1—C4—C3	172.01 (17)	C2—N1—C5—C10	−86.0 (3)
O2—S1—C1—N1	62.00 (19)	C5—N1—C1—S1	−167.57 (16)
O2—S1—C1—C11	−62.2 (2)	C5—N1—C1—C11	−46.3 (3)
O2—S1—C4—C3	−55.4 (2)	C5—N1—C2—O3	13.2 (3)
N1—C1—C11—C12	125.6 (2)	C5—N1—C2—C3	−169.4 (2)

N1—C1—C11—C16	−55.2 (3)	C5—C6—C7—C8	0.0 (5)
N1—C5—C6—C7	177.1 (3)	C6—C5—C10—C9	0.3 (5)
N1—C5—C10—C9	−177.2 (3)	C6—C7—C8—C9	0.7 (6)
C1—S1—C4—C3	60.16 (19)	C7—C8—C9—C10	−0.9 (6)
C1—N1—C2—O3	175.8 (2)	C8—C9—C10—C5	0.4 (6)
C1—N1—C2—C3	−6.8 (3)	C10—C5—C6—C7	−0.5 (4)
C1—N1—C5—C6	−68.1 (3)	C11—C12—C13—C14	−0.4 (4)
C1—N1—C5—C10	109.4 (3)	C12—C11—C16—C15	1.1 (4)
C1—C11—C12—C13	178.9 (2)	C12—C13—C14—C15	0.4 (4)
C1—C11—C16—C15	−178.1 (2)	C13—C14—C15—C16	0.4 (4)
C4—S1—C1—N1	−52.56 (18)	C14—C15—C16—C11	−1.2 (4)
C4—S1—C1—C11	−176.73 (18)	C16—C11—C12—C13	−0.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1^{i}	0.95	2.56	3.454 (4)	157

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

N-[(2*S*,5*R*)-1,1,4-Trioxo-2,3-diphenyl-1,3-thiazinan-5-yl]acetamide (2)

Crystal data

$C_{18}H_{18}N_2O_4S$
M_r = 358.40
Orthorhombic, $P2_12_12_1$
a = 5.5230 (4) Å
b = 10.6857 (9) Å
c = 28.430 (2) Å
V = 1677.8 (2) Å^3
Z = 4
$F(000)$ = 752
D_x = 1.419 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4224 reflections
θ = 2.4–25.0°
μ = 0.22 mm^{-1}
T = 298 K
Rod, colorless
0.22 × 0.06 × 0.06 mm

Data collection

Bruker SMART CCD area detector diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.656, T_{max} = 0.900
13301 measured reflections
4037 independent reflections
3460 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 28.3°, θ_{min} = 1.4°
h = −7→5
k = −12→14
l = −36→37

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.103
S = 1.04
4037 reflections
231 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 0.035P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack x determined using 1213 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.07 (4)

Special details

Experimental. The data collection nominally covered a full sphere of reciprocal space by a combination of 4 sets of ω scans each set at different φ and/or 2θ angles and each scan (10 s exposure) covering -0.300° degrees in ω. The crystal to detector distance was 5.82 cm.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.29097 (13)	0.61561 (6)	0.04750 (2)	0.04039 (18)
O1	0.2013 (5)	0.5960 (2)	0.00084 (6)	0.0665 (7)
O2	0.5430 (4)	0.5943 (2)	0.05600 (8)	0.0655 (6)
O3	0.0948 (4)	0.72050 (18)	0.18769 (6)	0.0575 (6)
O4	−0.3983 (4)	0.8940 (2)	0.13514 (8)	0.0659 (6)
N1	0.1594 (4)	0.56459 (18)	0.13538 (6)	0.0394 (5)
N2	0.0062 (5)	0.8977 (2)	0.12438 (9)	0.0485 (6)
C1	0.1124 (4)	0.5198 (2)	0.08754 (7)	0.0333 (5)
H1	−0.058432	0.536713	0.080716	0.040*
C2	0.0930 (5)	0.6841 (2)	0.14753 (8)	0.0409 (6)
C3	0.0251 (5)	0.7713 (2)	0.10656 (8)	0.0398 (6)
H3	−0.132274	0.745690	0.093867	0.048*
C4	0.2134 (6)	0.7692 (2)	0.06686 (8)	0.0424 (6)
H4A	0.359008	0.811013	0.077660	0.051*
H4B	0.150687	0.816206	0.040330	0.051*
C11	0.1560 (4)	0.3832 (2)	0.07738 (7)	0.0350 (5)
C16	0.3688 (5)	0.3203 (3)	0.08898 (9)	0.0448 (6)
H16	0.493371	0.362002	0.104412	0.054*
C15	0.3932 (6)	0.1953 (3)	0.07738 (10)	0.0559 (8)
H15	0.533040	0.152566	0.085968	0.067*
C14	0.2132 (7)	0.1331 (3)	0.05326 (10)	0.0596 (9)
H14	0.232717	0.049213	0.045356	0.072*
C13	0.0065 (7)	0.1949 (3)	0.04104 (10)	0.0565 (8)
H13	−0.114479	0.153289	0.024516	0.068*
C12	−0.0235 (5)	0.3194 (2)	0.05317 (8)	0.0434 (6)
H12	−0.165681	0.360621	0.044990	0.052*
C5	0.2702 (5)	0.4889 (2)	0.17177 (7)	0.0393 (6)
C6	0.1536 (6)	0.3843 (3)	0.18873 (9)	0.0535 (8)
H6	0.004073	0.360301	0.176670	0.064*
C7	0.2639 (10)	0.3152 (3)	0.22429 (10)	0.0815 (13)
H7	0.188747	0.243530	0.235747	0.098*
C8	0.4806 (12)	0.3516 (5)	0.24243 (12)	0.0976 (17)
H8	0.553113	0.304469	0.266063	0.117*
C9	0.5929 (8)	0.4575 (5)	0.22597 (12)	0.0839 (13)
H9	0.738587	0.483351	0.239181	0.101*
C10	0.4902 (6)	0.5261 (3)	0.18983 (10)	0.0560 (8)

H10	0.568552	0.596319	0.177902	0.067*
C17	−0.2027 (7)	0.9434 (3)	0.14185 (9)	0.0490 (7)
C18	−0.1753 (8)	1.0631 (3)	0.16996 (11)	0.0678 (10)
H18A	−0.330040	1.103268	0.172852	0.102*
H18B	−0.064566	1.118103	0.154150	0.102*
H18C	−0.113853	1.043699	0.200700	0.102*
H2	0.139 (5)	0.924 (3)	0.1348 (9)	0.042 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0452 (4)	0.0358 (3)	0.0402 (3)	0.0022 (3)	0.0046 (3)	0.0016 (2)
O1	0.1092 (19)	0.0556 (12)	0.0347 (9)	−0.0001 (14)	0.0030 (11)	−0.0010 (8)
O2	0.0404 (11)	0.0512 (13)	0.1048 (17)	0.0035 (10)	0.0137 (12)	0.0130 (11)
O3	0.0835 (16)	0.0502 (12)	0.0387 (9)	0.0055 (11)	0.0013 (10)	−0.0095 (8)
O4	0.0562 (14)	0.0671 (15)	0.0742 (14)	0.0093 (13)	−0.0051 (11)	−0.0223 (12)
N1	0.0536 (15)	0.0329 (10)	0.0317 (9)	0.0008 (10)	−0.0029 (9)	−0.0018 (8)
N2	0.0530 (16)	0.0315 (12)	0.0611 (14)	−0.0018 (12)	−0.0034 (12)	−0.0078 (10)
C1	0.0321 (12)	0.0353 (12)	0.0324 (10)	0.0017 (10)	−0.0035 (9)	−0.0027 (9)
C2	0.0461 (16)	0.0349 (13)	0.0415 (12)	−0.0033 (12)	0.0008 (12)	−0.0033 (10)
C3	0.0431 (15)	0.0303 (12)	0.0460 (13)	−0.0002 (11)	−0.0029 (11)	−0.0054 (10)
C4	0.0506 (15)	0.0347 (12)	0.0419 (12)	−0.0013 (13)	−0.0016 (12)	0.0019 (9)
C11	0.0406 (14)	0.0327 (11)	0.0317 (10)	−0.0004 (11)	0.0015 (9)	−0.0009 (9)
C16	0.0480 (16)	0.0434 (14)	0.0431 (13)	0.0080 (13)	−0.0010 (11)	0.0002 (11)
C15	0.072 (2)	0.0458 (16)	0.0498 (15)	0.0223 (16)	0.0092 (15)	0.0110 (12)
C14	0.095 (3)	0.0319 (13)	0.0516 (15)	−0.0005 (17)	0.0225 (18)	0.0014 (11)
C13	0.072 (2)	0.0451 (16)	0.0521 (15)	−0.0183 (17)	0.0068 (15)	−0.0108 (12)
C12	0.0463 (15)	0.0445 (15)	0.0394 (12)	−0.0049 (13)	0.0010 (12)	−0.0051 (11)
C5	0.0445 (15)	0.0420 (13)	0.0315 (10)	0.0043 (12)	−0.0011 (11)	−0.0019 (9)
C6	0.071 (2)	0.0473 (15)	0.0422 (13)	−0.0011 (16)	0.0077 (13)	0.0033 (12)
C7	0.138 (4)	0.060 (2)	0.0462 (16)	0.015 (3)	0.012 (2)	0.0154 (14)
C8	0.147 (5)	0.100 (4)	0.0458 (18)	0.058 (3)	−0.020 (2)	0.0019 (19)
C9	0.073 (3)	0.118 (4)	0.060 (2)	0.039 (3)	−0.0289 (19)	−0.029 (2)
C10	0.0483 (18)	0.071 (2)	0.0483 (14)	0.0058 (16)	−0.0050 (13)	−0.0119 (14)
C17	0.065 (2)	0.0384 (14)	0.0435 (13)	0.0077 (15)	−0.0061 (15)	−0.0038 (10)
C18	0.095 (3)	0.0437 (16)	0.0649 (18)	0.0125 (19)	−0.0055 (19)	−0.0156 (13)

Geometric parameters (Å, º)

S1—O1	1.431 (2)	C15—H15	0.9300
S1—O2	1.431 (2)	C15—C14	1.378 (5)
S1—C1	1.821 (2)	C14—H14	0.9300
S1—C4	1.783 (3)	C14—C13	1.364 (5)
O3—C2	1.206 (3)	C13—H13	0.9300
O4—C17	1.218 (4)	C13—C12	1.384 (4)
N1—C1	1.465 (3)	C12—H12	0.9300
N1—C2	1.373 (3)	C5—C6	1.377 (4)
N1—C5	1.449 (3)	C5—C10	1.378 (4)

N2—C3	1.446 (3)	C6—H6	0.9300
N2—C17	1.348 (4)	C6—C7	1.393 (5)
N2—H2	0.84 (3)	C7—H7	0.9300
C1—H1	0.9800	C7—C8	1.360 (7)
C1—C11	1.507 (3)	C8—H8	0.9300
C2—C3	1.538 (3)	C8—C9	1.373 (6)
C3—H3	0.9800	C9—H9	0.9300
C3—C4	1.535 (4)	C9—C10	1.384 (5)
C4—H4A	0.9700	C10—H10	0.9300
C4—H4B	0.9700	C17—C18	1.515 (4)
C11—C16	1.394 (4)	C18—H18A	0.9600
C11—C12	1.386 (3)	C18—H18B	0.9600
C16—H16	0.9300	C18—H18C	0.9600
C16—C15	1.382 (4)		

O1—S1—C1	108.03 (13)	C16—C15—H15	119.5
O1—S1—C4	109.74 (13)	C14—C15—C16	121.0 (3)
O2—S1—O1	118.01 (15)	C14—C15—H15	119.5
O2—S1—C1	109.38 (12)	C15—C14—H14	120.1
O2—S1—C4	109.15 (14)	C13—C14—C15	119.8 (3)
C4—S1—C1	101.20 (11)	C13—C14—H14	120.1
C2—N1—C1	119.34 (19)	C14—C13—H13	119.9
C2—N1—C5	116.91 (18)	C14—C13—C12	120.2 (3)
C5—N1—C1	123.75 (19)	C12—C13—H13	119.9
C3—N2—H2	112 (2)	C11—C12—H12	119.6
C17—N2—C3	122.0 (3)	C13—C12—C11	120.7 (3)
C17—N2—H2	120 (2)	C13—C12—H12	119.6
S1—C1—H1	107.1	C6—C5—N1	120.4 (2)
N1—C1—S1	107.50 (16)	C10—C5—N1	118.5 (3)
N1—C1—H1	107.1	C10—C5—C6	121.1 (3)
N1—C1—C11	117.76 (19)	C5—C6—H6	120.7
C11—C1—S1	109.76 (16)	C5—C6—C7	118.7 (3)
C11—C1—H1	107.1	C7—C6—H6	120.7
O3—C2—N1	122.4 (2)	C6—C7—H7	119.7
O3—C2—C3	121.6 (2)	C8—C7—C6	120.6 (4)
N1—C2—C3	115.99 (19)	C8—C7—H7	119.7
N2—C3—C2	108.5 (2)	C7—C8—H8	119.9
N2—C3—H3	109.0	C7—C8—C9	120.2 (4)
N2—C3—C4	108.7 (2)	C9—C8—H8	119.9
C2—C3—H3	109.0	C8—C9—H9	119.8
C4—C3—C2	112.5 (2)	C8—C9—C10	120.3 (4)
C4—C3—H3	109.0	C10—C9—H9	119.8
S1—C4—H4A	108.8	C5—C10—C9	119.0 (4)
S1—C4—H4B	108.8	C5—C10—H10	120.5
C3—C4—S1	113.79 (17)	C9—C10—H10	120.5
C3—C4—H4A	108.8	O4—C17—N2	123.0 (2)
C3—C4—H4B	108.8	O4—C17—C18	122.5 (3)
H4A—C4—H4B	107.7	N2—C17—C18	114.5 (3)

C16—C11—C1	123.8 (2)	C17—C18—H18A	109.5
C12—C11—C1	117.2 (2)	C17—C18—H18B	109.5
C12—C11—C16	118.9 (2)	C17—C18—H18C	109.5
C11—C16—H16	120.3	H18A—C18—H18B	109.5
C15—C16—C11	119.5 (3)	H18A—C18—H18C	109.5
C15—C16—H16	120.3	H18B—C18—H18C	109.5

S1—C1—C11—C16	73.2 (2)	C2—N1—C5—C6	114.0 (3)
S1—C1—C11—C12	−103.8 (2)	C2—N1—C5—C10	−64.0 (3)
O1—S1—C1—N1	−165.13 (17)	C2—C3—C4—S1	50.6 (3)
O1—S1—C1—C11	65.65 (19)	C3—N2—C17—O4	−15.9 (4)
O1—S1—C4—C3	111.3 (2)	C3—N2—C17—C18	165.1 (2)
O2—S1—C1—N1	65.22 (19)	C4—S1—C1—N1	−49.88 (19)
O2—S1—C1—C11	−64.00 (19)	C4—S1—C1—C11	−179.10 (17)
O2—S1—C4—C3	−117.9 (2)	C11—C16—C15—C14	2.0 (4)
O3—C2—C3—N2	8.7 (4)	C16—C11—C12—C13	0.6 (4)
O3—C2—C3—C4	129.0 (3)	C16—C15—C14—C13	−0.7 (4)
N1—C1—C11—C16	−50.2 (3)	C15—C14—C13—C12	−0.6 (4)
N1—C1—C11—C12	132.9 (2)	C14—C13—C12—C11	0.7 (4)
N1—C2—C3—N2	−169.1 (2)	C12—C11—C16—C15	−1.9 (4)
N1—C2—C3—C4	−48.8 (3)	C5—N1—C1—S1	−117.4 (2)
N1—C5—C6—C7	−178.9 (3)	C5—N1—C1—C11	7.2 (3)
N1—C5—C10—C9	177.3 (3)	C5—N1—C2—O3	−9.9 (4)
N2—C3—C4—S1	170.82 (19)	C5—N1—C2—C3	167.9 (2)
C1—S1—C4—C3	−2.7 (2)	C5—C6—C7—C8	1.1 (5)
C1—N1—C2—O3	169.2 (3)	C6—C5—C10—C9	−0.8 (4)
C1—N1—C2—C3	−13.1 (4)	C6—C7—C8—C9	0.3 (6)
C1—N1—C5—C6	−64.9 (3)	C7—C8—C9—C10	−2.0 (6)
C1—N1—C5—C10	117.0 (3)	C8—C9—C10—C5	2.2 (5)
C1—C11—C16—C15	−178.8 (2)	C10—C5—C6—C7	−0.9 (4)
C1—C11—C12—C13	177.7 (2)	C17—N2—C3—C2	−88.7 (3)
C2—N1—C1—S1	63.7 (3)	C17—N2—C3—C4	148.7 (3)
C2—N1—C1—C11	−171.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O2^{i}	0.98	2.39	3.365 (3)	173
C4—H4*A*···O4^{ii}	0.97	2.29	3.185 (4)	153
C8—H8···O3^{iii}	0.93	2.51	3.378 (5)	155

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