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# *S*,*S*-Diphenyl-*N*-tosyl sulfone diimine

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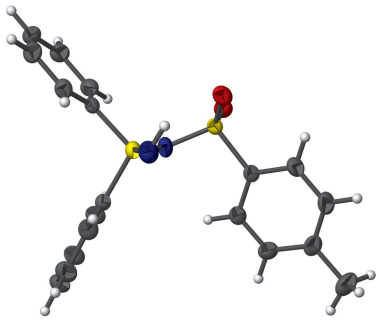
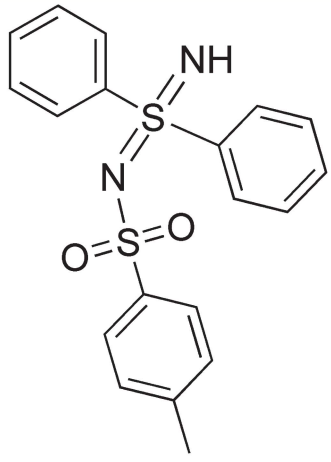
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title compound [systematic name: *N*-(iminodiphenyl-$\lambda^6$-sulfanylidene)-4-methylbenzene-1-sulfonamide], $C_{19}H_{18}N_2O_2S_2$, the configuration around the sulfur atom of the sulfonediimine group is a slightly distorted tetrahedron structure with two S═N bonds and two S—C bonds. The bond lengths of S═N (*p*-toluenesulfonyl) and S═N (NH) are 1.5785 (15) and 1.5158 (18) Å, respectively. The S—N═S plane makes a dihedral angle of 74.24 (14)° with the *p*-toluene ring, while it makes dihedral angles of 73.43 (13) and 41.98 (14)° with the phenyl rings. The two torsion angles of S—N═S—C (phenyl) and the S—N═S═N angle are 105.86 (12), −144.54 (11) and −25.67 (17)°, respectively. In the crystal, molecules are connected by pairs of N—H···O hydrogen bonds, forming inversion dimers with an $R_2^2(12)$ ring motif. The dimers are linked by C—H···O interactions, forming a tape structure along the *a*-axis direction.

**3D view**



**Chemical scheme**




## Structure description

The aza analogues of sulfones such as sulfoximines and sulfonediimines have interesting pharmaceutical properties (Kennewell & Tavlor, 1975; Haake, 1976; Sellinger *et al.*, 1969). However, their chemical reactivities have not been fully explored as yet except for a few scattered utilizations in organic syntheses for example as an alkylidene-transfer reagent (Johnson *et al.*, 1973). To date, some related crystal structures have been reported (Yoshimura *et al.*, 2008). As part of our studies in this area, we report herein on the synthesis and crystal structure of the title compound.

The molecular structure of the title compound is illustrated in Fig. 1. The S2—N1 and S2—N2 bond lengths are 1.5785 (15) and 1.5158 (18) Å, respectively. These bond lengths are significantly longer than the S≡N triple bond of triphenylsulfanenitrile (1.462 Å; Yoshimura *et al.*, 1997), close to the S═N double bond lengths of *S*,*S*-dimethylsulfonediimine (1.533 Å, electron diffraction study; Oberhammer & Zeil, 1970), *S*,*S*-

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H8···O2$^{i}$ | 0.89 (3) | 2.20 (3) | 3.018 (3) | 152 (2) |
| C12—H12···O1$^{ii}$ | 0.95 | 2.34 | 3.283 (2) | 169 |

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

diphenyl-*S*-pyrrolidinoiminosulfonium perchlorate [1.503 (2) Å for S—N (NH), X-ray; Sheikh *et al.*., 2017] and *S,S*-diphenylsulfodiimide-*N*-phenyl [1.526 Å for S—N (NH) and 1.546 (1) Å for S—N (Ph), X-ray; Yoshimura *et al.*, 2008], and shorter than that of *S,S*-diphenyl-*N*-tosylsulfilimine (1.628 Å, X-ray; Kálmán *et al.*, 1971). The N1—S2—N2 bond angle [126.05 (9)°] is larger than 109.5°, while the N—S—C and C—S—C bond angles [102.92 (9)–112.96 (19)°] are close to 109.5°. In the crystal, the molecules are linked through N—H···O and C—H···O hydrogen bonds (Table 1, Fig. 2), forming a tape along the *a*-axis direction (Fig. 3).

## Synthesis and crystallization

The title compound was prepared by the method previously reported (Furukawa *et al.*, 1984) using *S,S*-diphenylsulfilimide mono hydrate with chloramine-T in the presence of excess sodium salt of tosylamide in anhydrous acetonitrile and was crystallized from an ethanol solution (yield 90%; m.p. 153–154°C).

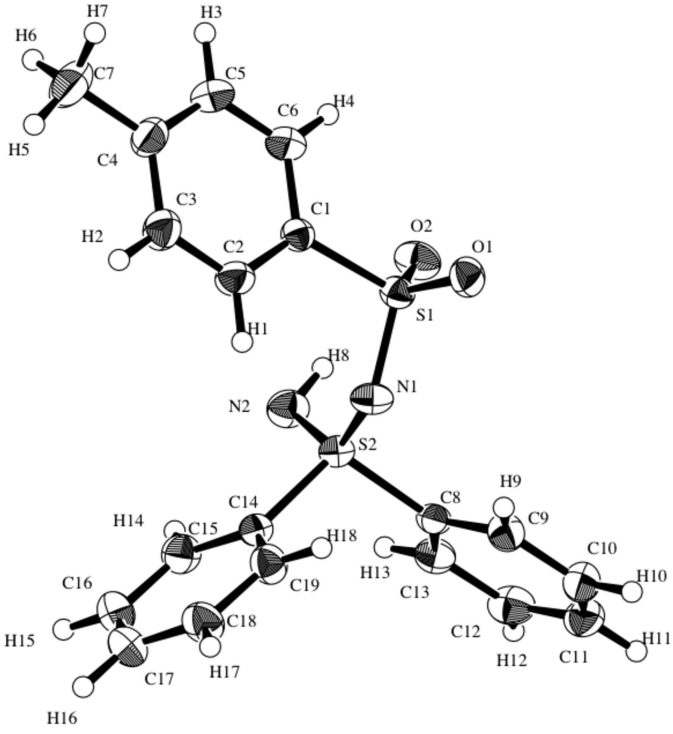



**Figure 1**
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

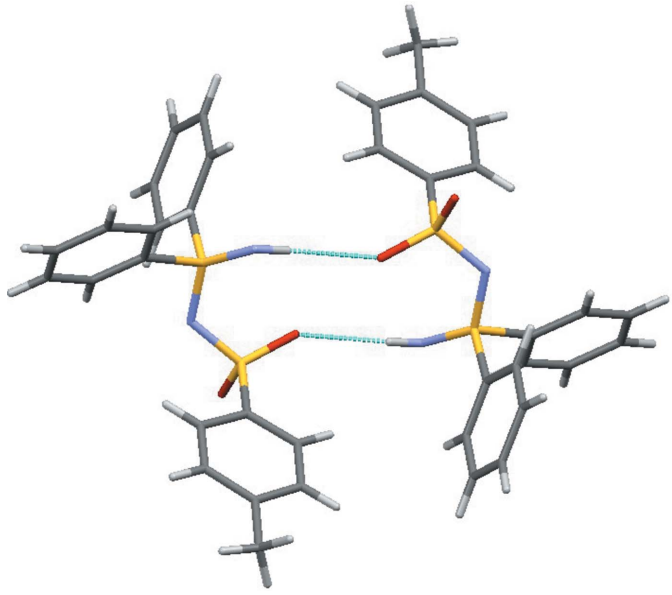


**Figure 2**
A view of the title compound showing a pair of N—H···O hydrogen bonds (blue dashed lines) forming an $R_2^2(12)$ ring motif.

## Refinement

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

## Acknowledgements

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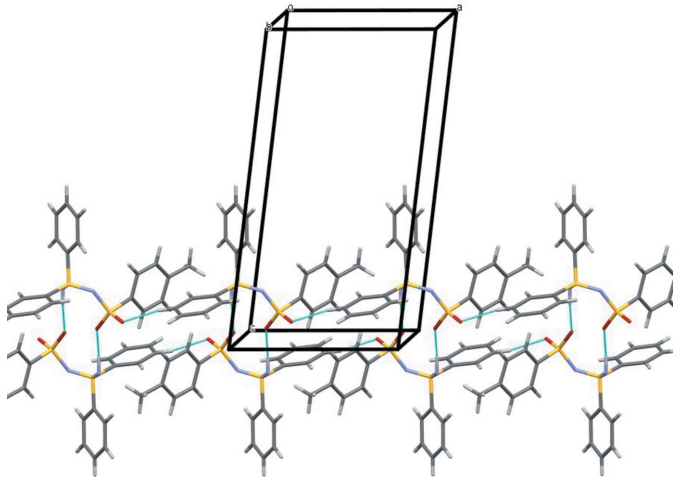

**Figure 3**
A partial packing diagram of the title compound, showing the tape along the *a*-axis direction formed *via* N—H···O and C—H···O hydrogen bonds (blue dashed lines).

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{19}H_{18}N_2O_2S_2$ |
| $M_r$ | 370.48 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 173 |
| $a$, $b$, $c$ (Å) | 9.47865 (17), 10.38462 (19), 18.0852 (4) |
| $\beta$ (°) | 97.4526 (7) |
| $V$ (Å$^3$) | 1765.13 (6) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 2.86 |
| Crystal size (mm) | 0.56 × 0.52 × 0.14 |
| | |
| Data collection | |
| Diffractometer | Rigaku R-AXIS RAPID |
| Absorption correction | Multi-scan (*ABSCOR*; Higashi, 1995) |
| $T_{min}$, $T_{max}$ | 0.500, 0.670 |
| No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections | 19250, 3226, 2893 |
| $R_{int}$ | 0.086 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.602 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.043, 0.127, 1.09 |
| No. of reflections | 3226 |
| No. of parameters | 231 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.83, −0.52 |

Computer programs: *RAPID-AUTO* (Rigaku, 2001), *SIR92* (Altomare *et al.*, 1993), *SHELXL97* (Sheldrick, 2008) and *CrystalStructure* (Rigaku, 2010).


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# full crystallographic data

*IUCrData* (2019). **4**, x190523 [https://doi.org/10.1107/S2414314619005236]

## *S*,*S*-Diphenyl-*N*-tosyl sulfone diimine

**Md. Chanmiya Sheikh, Toshiaki Yoshimura and Ryuta Miyatake**

**N-(Iminodiphenyl-$\lambda^6$-sulfanylidene)-4-methylbenzene-1-sulfonamide**

*Crystal data*

$C_{19}H_{18}N_2O_2S_2$
$M_r$ = 370.48
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 9.47865 (17) Å
$b$ = 10.38462 (19) Å
$c$ = 18.0852 (4) Å
$\beta$ = 97.4526 (7)°
$V$ = 1765.13 (6) Å$^3$
$Z$ = 4
$F(000)$ = 776.00
$D_x$ = 1.394 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.54187 Å
Cell parameters from 18540 reflections
$\theta$ = 4.3–68.2°
$\mu$ = 2.86 mm$^{-1}$
$T$ = 173 K
Platelet, colorless
0.56 × 0.52 × 0.14 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
$T_{min}$ = 0.500, $T_{max}$ = 0.670
19250 measured reflections
3226 independent reflections
2893 reflections with $F^2 > 2.0\sigma(F^2)$
$R_{int}$ = 0.086
$\theta_{max}$ = 68.2°
$h$ = −11→11
$k$ = −12→12
$l$ = −21→21

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
$S$ = 1.09
3226 reflections
231 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0797P)^2 + 0.2545P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.83 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.52 e Å$^{-3}$

*Special details*

**Geometry**. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY
**Refinement**. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on $F^2$. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma($F^2$) is used only for calculating R-factor (gt).

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.17740 (4) | 0.17061 (4) | 0.93189 (2) | 0.02550 (17) |
| S2 | −0.08500 (4) | 0.16500 (4) | 0.84447 (2) | 0.02510 (17) |
| O1 | 0.27017 (14) | 0.27580 (12) | 0.95689 (7) | 0.0345 (4) |
| O2 | 0.10643 (14) | 0.10862 (14) | 0.98795 (7) | 0.0375 (4) |
| N1 | 0.07009 (15) | 0.22168 (15) | 0.86291 (8) | 0.0299 (4) |
| N2 | −0.13277 (18) | 0.03177 (16) | 0.86480 (10) | 0.0349 (4) |
| C1 | 0.28321 (18) | 0.05373 (16) | 0.89394 (10) | 0.0251 (4) |
| C2 | 0.3026 (2) | 0.05765 (18) | 0.81932 (10) | 0.0332 (5) |
| C3 | 0.3949 (3) | −0.02824 (19) | 0.79274 (11) | 0.0375 (5) |
| C4 | 0.4692 (2) | −0.11932 (18) | 0.83931 (11) | 0.0357 (5) |
| C5 | 0.4450 (3) | −0.1227 (2) | 0.91330 (12) | 0.0416 (5) |
| C6 | 0.3530 (3) | −0.03744 (19) | 0.94066 (11) | 0.0362 (5) |
| C7 | 0.5717 (3) | −0.2107 (3) | 0.81015 (14) | 0.0517 (6) |
| C8 | −0.19435 (18) | 0.29055 (17) | 0.87394 (9) | 0.0253 (4) |
| C9 | −0.1404 (2) | 0.41329 (18) | 0.88810 (10) | 0.0311 (4) |
| C10 | −0.2267 (3) | 0.50666 (19) | 0.91370 (11) | 0.0371 (5) |
| C11 | −0.3646 (3) | 0.4763 (2) | 0.92469 (11) | 0.0391 (5) |
| C12 | −0.4183 (2) | 0.3542 (2) | 0.90947 (11) | 0.0387 (5) |
| C13 | −0.33348 (19) | 0.25966 (19) | 0.88366 (10) | 0.0315 (5) |
| C14 | −0.1138 (2) | 0.16802 (16) | 0.74561 (10) | 0.0261 (4) |
| C15 | −0.1989 (2) | 0.07367 (18) | 0.70885 (11) | 0.0344 (5) |
| C16 | −0.2169 (3) | 0.0731 (2) | 0.63126 (12) | 0.0417 (5) |
| C17 | −0.1524 (3) | 0.1666 (2) | 0.59297 (12) | 0.0408 (5) |
| C18 | −0.0697 (3) | 0.2607 (2) | 0.63049 (11) | 0.0387 (5) |
| C19 | −0.0498 (2) | 0.26312 (18) | 0.70765 (10) | 0.0335 (5) |
| H1 | 0.2527 | 0.1189 | 0.7868 | 0.0398* |
| H2 | 0.4083 | −0.0253 | 0.7416 | 0.0450* |
| H3 | 0.4929 | −0.1851 | 0.9458 | 0.0500* |
| H4 | 0.3377 | −0.0415 | 0.9915 | 0.0435* |
| H5 | 0.5742 | −0.1943 | 0.7570 | 0.0620* |
| H6 | 0.5408 | −0.2995 | 0.8170 | 0.0620* |
| H7 | 0.6669 | −0.1981 | 0.8375 | 0.0620* |
| H8 | −0.124 (3) | 0.019 (3) | 0.9139 (14) | 0.046 (7)* |
| H9 | −0.0456 | 0.4332 | 0.8804 | 0.0373* |
| H10 | −0.1913 | 0.5913 | 0.9237 | 0.0445* |
| H11 | −0.4230 | 0.5402 | 0.9429 | 0.0469* |
| H12 | −0.5135 | 0.3349 | 0.9167 | 0.0464* |
| H13 | −0.3698 | 0.1755 | 0.8729 | 0.0378* |
| H14 | −0.2440 | 0.0108 | 0.7359 | 0.0413* |
| H15 | −0.2734 | 0.0084 | 0.6047 | 0.0501* |
| H16 | −0.1654 | 0.1660 | 0.5400 | 0.0489* |
| H17 | −0.0260 | 0.3243 | 0.6033 | 0.0464* |
| H18 | 0.0063 | 0.3283 | 0.7340 | 0.0402* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0227 (3) | 0.0297 (3) | 0.0239 (3) | 0.00039 (16) | 0.0021 (2) | 0.00052 (15) |
| S2 | 0.0231 (3) | 0.0256 (3) | 0.0264 (3) | 0.00086 (15) | 0.0024 (2) | 0.00271 (15) |
| O1 | 0.0313 (7) | 0.0336 (8) | 0.0374 (8) | −0.0019 (6) | −0.0003 (6) | −0.0083 (6) |
| O2 | 0.0347 (8) | 0.0512 (9) | 0.0277 (7) | 0.0014 (7) | 0.0079 (6) | 0.0089 (6) |
| N1 | 0.0219 (8) | 0.0340 (9) | 0.0328 (9) | 0.0008 (7) | 0.0002 (7) | 0.0077 (7) |
| N2 | 0.0360 (9) | 0.0301 (9) | 0.0380 (10) | −0.0026 (7) | 0.0028 (8) | 0.0061 (7) |
| C1 | 0.0233 (9) | 0.0246 (9) | 0.0267 (9) | −0.0021 (7) | 0.0004 (7) | −0.0006 (7) |
| C2 | 0.0386 (11) | 0.0321 (10) | 0.0287 (10) | 0.0064 (9) | 0.0041 (9) | 0.0061 (8) |
| C3 | 0.0440 (12) | 0.0363 (11) | 0.0334 (11) | 0.0061 (9) | 0.0094 (10) | −0.0005 (8) |
| C4 | 0.0336 (11) | 0.0270 (10) | 0.0458 (12) | 0.0029 (8) | 0.0023 (9) | −0.0043 (9) |
| C5 | 0.0459 (12) | 0.0348 (11) | 0.0415 (11) | 0.0123 (10) | −0.0049 (10) | 0.0055 (9) |
| C6 | 0.0416 (12) | 0.0371 (11) | 0.0285 (10) | 0.0066 (9) | −0.0010 (9) | 0.0046 (8) |
| C7 | 0.0517 (14) | 0.0382 (13) | 0.0662 (16) | 0.0148 (11) | 0.0114 (13) | −0.0060 (11) |
| C8 | 0.0233 (9) | 0.0305 (10) | 0.0215 (9) | 0.0032 (8) | 0.0008 (7) | 0.0013 (7) |
| C9 | 0.0281 (9) | 0.0350 (11) | 0.0304 (10) | −0.0016 (8) | 0.0043 (8) | −0.0022 (8) |
| C10 | 0.0439 (12) | 0.0323 (11) | 0.0348 (10) | 0.0032 (9) | 0.0040 (9) | −0.0021 (9) |
| C11 | 0.0411 (12) | 0.0445 (13) | 0.0323 (10) | 0.0139 (10) | 0.0078 (9) | 0.0009 (9) |
| C12 | 0.0268 (10) | 0.0532 (13) | 0.0372 (11) | 0.0054 (9) | 0.0089 (9) | 0.0065 (10) |
| C13 | 0.0265 (9) | 0.0355 (11) | 0.0320 (10) | −0.0013 (8) | 0.0017 (8) | 0.0032 (8) |
| C14 | 0.0265 (9) | 0.0262 (10) | 0.0254 (9) | 0.0036 (7) | 0.0024 (8) | 0.0007 (7) |
| C15 | 0.0354 (11) | 0.0298 (10) | 0.0375 (11) | −0.0027 (8) | 0.0029 (9) | 0.0010 (8) |
| C16 | 0.0449 (12) | 0.0389 (12) | 0.0386 (11) | −0.0024 (10) | −0.0052 (10) | −0.0086 (9) |
| C17 | 0.0487 (13) | 0.0457 (13) | 0.0266 (10) | 0.0035 (10) | −0.0004 (10) | −0.0022 (9) |
| C18 | 0.0468 (12) | 0.0403 (12) | 0.0292 (10) | −0.0018 (9) | 0.0052 (9) | 0.0049 (8) |
| C19 | 0.0391 (11) | 0.0305 (10) | 0.0306 (10) | −0.0045 (8) | 0.0031 (9) | −0.0007 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.4380 (13) | C15—C16 | 1.391 (3) |
| S1—O2 | 1.4394 (15) | C16—C17 | 1.381 (4) |
| S1—N1 | 1.5947 (15) | C17—C18 | 1.375 (3) |
| S1—C1 | 1.7688 (18) | C18—C19 | 1.384 (3) |
| S2—N1 | 1.5785 (15) | N2—H8 | 0.89 (3) |
| S2—N2 | 1.5158 (18) | C2—H1 | 0.950 |
| S2—C8 | 1.7893 (19) | C3—H2 | 0.950 |
| S2—C14 | 1.7735 (19) | C5—H3 | 0.950 |
| C1—C2 | 1.386 (3) | C6—H4 | 0.950 |
| C1—C6 | 1.379 (3) | C7—H5 | 0.980 |
| C2—C3 | 1.379 (3) | C7—H6 | 0.980 |
| C3—C4 | 1.395 (3) | C7—H7 | 0.980 |
| C4—C5 | 1.387 (3) | C9—H9 | 0.950 |
| C4—C7 | 1.502 (4) | C10—H10 | 0.950 |
| C5—C6 | 1.379 (3) | C11—H11 | 0.950 |
| C8—C9 | 1.385 (3) | C12—H12 | 0.950 |
| C8—C13 | 1.390 (3) | C13—H13 | 0.950 |

| | | | |
|---|---|---|---|
| C9—C10 | 1.386 (3) | C15—H14 | 0.950 |
| C10—C11 | 1.384 (3) | C16—H15 | 0.950 |
| C11—C12 | 1.380 (3) | C17—H16 | 0.950 |
| C12—C13 | 1.388 (3) | C18—H17 | 0.950 |
| C14—C15 | 1.384 (3) | C19—H18 | 0.950 |
| C14—C19 | 1.386 (3) | | |

| | | | |
|---|---|---|---|
| S1···N2 | 3.3570 (17) | C12···H2$^{iii}$ | 3.0176 |
| S2···O2 | 3.0244 (13) | C12···H3$^{iv}$ | 3.3035 |
| O1···C2 | 3.408 (3) | C12···H5$^{iii}$ | 3.2164 |
| O1···C6 | 3.368 (3) | C12···H11$^{xiv}$ | 3.4108 |
| O2···N2 | 3.070 (2) | C12···H15$^{xv}$ | 3.3133 |
| O2···C6 | 3.002 (3) | C12···H16$^{v}$ | 3.1456 |
| N1···C2 | 2.972 (3) | C13···H2$^{iii}$ | 3.1945 |
| N1···C9 | 2.896 (3) | C13···H4$^{iv}$ | 3.2026 |
| N1···C19 | 2.921 (3) | C13···H5$^{iii}$ | 3.2245 |
| N2···C13 | 3.083 (3) | C13···H16$^{v}$ | 3.1559 |
| N2···C15 | 2.842 (3) | C15···H6$^{iii}$ | 3.4729 |
| C1···C4 | 2.786 (3) | C15···H9$^{vi}$ | 3.3276 |
| C2···C5 | 2.761 (3) | C15···H18$^{vi}$ | 3.2253 |
| C3···C6 | 2.757 (3) | C16···H6$^{iii}$ | 3.5778 |
| C8···C11 | 2.748 (3) | C16···H9$^{vi}$ | 2.9117 |
| C8···C19 | 3.475 (3) | C16···H11$^{xvi}$ | 3.5185 |
| C9···C12 | 2.780 (3) | C16···H12$^{xvi}$ | 3.5816 |
| C10···C13 | 2.785 (3) | C17···H3$^{iii}$ | 3.5623 |
| C13···C14 | 3.581 (3) | C17···H9$^{vi}$ | 3.0652 |
| C14···C17 | 2.737 (3) | C17···H10$^{vi}$ | 3.4010 |
| C15···C18 | 2.781 (3) | C18···H8$^{iii}$ | 3.40 (3) |
| C16···C19 | 2.783 (3) | C18···H9$^{vi}$ | 3.5850 |
| O1···C10$^{i}$ | 3.317 (3) | C18···H10$^{vi}$ | 3.2861 |
| O1···C11$^{i}$ | 3.394 (3) | H1···C7$^{x}$ | 3.1191 |
| O1···C12$^{ii}$ | 3.283 (3) | H1···H5$^{x}$ | 2.7234 |
| O1···C16$^{iii}$ | 3.481 (3) | H1···H6$^{x}$ | 3.0033 |
| O2···O2$^{iv}$ | 3.095 (2) | H1···H7$^{x}$ | 3.1121 |
| O2···N2$^{iv}$ | 3.018 (3) | H2···C7$^{x}$ | 3.4100 |
| O2···C18$^{v}$ | 3.520 (3) | H2···C8$^{vi}$ | 3.3221 |
| N2···O2$^{iv}$ | 3.018 (3) | H2···C9$^{vi}$ | 3.2879 |
| N2···C18$^{vi}$ | 3.402 (3) | H2···C10$^{vi}$ | 3.1156 |
| C5···C6$^{vii}$ | 3.478 (3) | H2···C11$^{vi}$ | 2.9821 |
| C5···C17$^{vi}$ | 3.523 (4) | H2···C12$^{vi}$ | 3.0176 |
| C6···C5$^{vii}$ | 3.478 (3) | H2···C13$^{vi}$ | 3.1945 |
| C6···C6$^{vii}$ | 3.380 (3) | H2···H5$^{x}$ | 3.4413 |
| C6···C18$^{vi}$ | 3.517 (3) | H2···H6$^{x}$ | 2.6426 |
| C10···O1$^{i}$ | 3.317 (3) | H2···H11$^{vi}$ | 3.4262 |
| C11···O1$^{i}$ | 3.394 (3) | H2···H12$^{vi}$ | 3.4696 |
| C12···O1$^{viii}$ | 3.283 (3) | H2···H14$^{ii}$ | 3.3315 |
| C16···O1$^{vi}$ | 3.481 (3) | H3···S1$^{vii}$ | 3.5901 |
| C17···C5$^{iii}$ | 3.523 (4) | H3···O1$^{vii}$ | 2.8289 |

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|---|---|---|---|
| C18···O2$^{ix}$ | 3.520 (3) | H3···C6$^{vii}$ | 3.3034 |
| C18···N2$^{iii}$ | 3.402 (3) | H3···C12$^{iv}$ | 3.3035 |
| C18···C6$^{iii}$ | 3.517 (3) | H3···C17$^{vi}$ | 3.5623 |
| S1···H1 | 2.8584 | H3···H4$^{vii}$ | 2.9880 |
| S1···H4 | 2.8101 | H3···H11$^{xii}$ | 2.9642 |
| S1···H8 | 3.24 (3) | H3···H12$^{iv}$ | 2.9179 |
| S1···H9 | 3.5019 | H3···H16$^{vi}$ | 3.5068 |
| S2···H1 | 3.5259 | H4···N2$^{iv}$ | 3.4420 |
| S2···H9 | 2.8735 | H4···C5$^{vii}$ | 3.0320 |
| S2···H13 | 2.8142 | H4···C6$^{vii}$ | 3.1367 |
| S2···H14 | 2.8145 | H4···C13$^{iv}$ | 3.2026 |
| S2···H18 | 2.8406 | H4···H3$^{vii}$ | 2.9880 |
| O1···H1 | 3.4659 | H4···H4$^{vii}$ | 3.1712 |
| O1···H4 | 3.3990 | H4···H8$^{iv}$ | 2.8271 |
| O1···H9 | 3.5316 | H4···H13$^{iv}$ | 2.8027 |
| O2···H4 | 2.6838 | H4···H16$^{vi}$ | 3.4609 |
| O2···H8 | 2.58 (3) | H4···H17$^{vi}$ | 3.5072 |
| N1···H1 | 2.5786 | H5···C2$^{xi}$ | 3.2128 |
| N1···H8 | 3.02 (3) | H5···C12$^{vi}$ | 3.2164 |
| N1···H9 | 2.4937 | H5···C13$^{vi}$ | 3.2245 |
| N1···H18 | 2.5815 | H5···H1$^{xi}$ | 2.7234 |
| N2···H13 | 2.7166 | H5···H2$^{xi}$ | 3.4413 |
| N2···H14 | 2.4402 | H5···H12$^{vi}$ | 3.1335 |
| C1···H2 | 3.2430 | H5···H13$^{vi}$ | 3.1487 |
| C1···H3 | 3.2400 | H5···H14$^{ii}$ | 2.7970 |
| C2···H4 | 3.2554 | H6···C2$^{xi}$ | 3.3804 |
| C3···H3 | 3.2424 | H6···C3$^{xi}$ | 3.2034 |
| C3···H5 | 2.5618 | H6···C10$^{xii}$ | 3.3114 |
| C3···H6 | 3.1440 | H6···C11$^{xii}$ | 3.0923 |
| C3···H7 | 3.1412 | H6···C15$^{vi}$ | 3.4729 |
| C4···H1 | 3.2751 | H6···C16$^{vi}$ | 3.5778 |
| C4···H4 | 3.2666 | H6···H1$^{xi}$ | 3.0033 |
| C5···H2 | 3.2414 | H6···H2$^{xi}$ | 2.6426 |
| C5···H5 | 3.3078 | H6···H10$^{xii}$ | 3.1916 |
| C5···H6 | 2.7645 | H6···H11$^{xii}$ | 2.8057 |
| C5···H7 | 2.7686 | H6···H14$^{vi}$ | 3.4652 |
| C6···H1 | 3.2555 | H7···N2$^{ii}$ | 3.0502 |
| C7···H2 | 2.6731 | H7···C10$^{xii}$ | 3.4584 |
| C7···H3 | 2.6691 | H7···H1$^{xi}$ | 3.1121 |
| C8···H8 | 2.97 (3) | H7···H8$^{ii}$ | 3.1947 |
| C8···H10 | 3.2493 | H7···H10$^{xii}$ | 2.9120 |
| C8···H12 | 3.2507 | H7···H11$^{xii}$ | 3.4890 |
| C8···H18 | 3.3808 | H7···H14$^{ii}$ | 3.0321 |
| C9···H11 | 3.2533 | H7···H17$^{xi}$ | 3.4409 |
| C9···H13 | 3.2776 | H7···H18$^{xi}$ | 3.5180 |
| C9···H18 | 3.3896 | H8···S1$^{iv}$ | 3.50 (3) |
| C10···H12 | 3.2577 | H8···O2$^{iv}$ | 2.20 (3) |
| C11···H9 | 3.2581 | H8···C18$^{vi}$ | 3.40 (3) |

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|---|---|---|---|
| C11···H13 | 3.2598 | H8···H4$^{iv}$ | 2.8271 |
| C12···H10 | 3.2581 | H8···H7$^{viii}$ | 3.1947 |
| C13···H8 | 3.20 (3) | H8···H17$^{vi}$ | 2.5120 |
| C13···H9 | 3.2772 | H9···C15$^{iii}$ | 3.3276 |
| C13···H11 | 3.2546 | H9···C16$^{iii}$ | 2.9117 |
| C14···H1 | 3.4944 | H9···C17$^{iii}$ | 3.0652 |
| C14···H8 | 3.43 (3) | H9···C18$^{iii}$ | 3.5850 |
| C14···H13 | 3.5550 | H9···H15$^{iii}$ | 3.1003 |
| C14···H15 | 3.2456 | H9···H16$^{iii}$ | 3.3423 |
| C14···H17 | 3.2413 | H9···H16$^{v}$ | 3.3965 |
| C15···H16 | 3.2554 | H10···S1$^{i}$ | 3.5867 |
| C15···H18 | 3.2797 | H10···O1$^{i}$ | 2.7476 |
| C16···H17 | 3.2519 | H10···O2$^{i}$ | 3.5465 |
| C17···H14 | 3.2617 | H10···C7$^{xiii}$ | 3.5062 |
| C17···H18 | 3.2544 | H10···C17$^{iii}$ | 3.4010 |
| C18···H15 | 3.2523 | H10···C18$^{iii}$ | 3.2861 |
| C19···H1 | 3.3835 | H10···H6$^{xiii}$ | 3.1916 |
| C19···H9 | 3.5843 | H10···H7$^{xiii}$ | 2.9120 |
| C19···H14 | 3.2802 | H10···H16$^{iii}$ | 3.4474 |
| C19···H16 | 3.2478 | H10···H16$^{v}$ | 3.3903 |
| H1···H2 | 2.3234 | H10···H17$^{iii}$ | 3.2546 |
| H1···H18 | 3.2430 | H11···O1$^{i}$ | 2.8900 |
| H2···H5 | 2.3486 | H11···C7$^{xiii}$ | 3.5250 |
| H2···H6 | 3.3322 | H11···C11$^{xiv}$ | 3.3262 |
| H2···H7 | 3.3361 | H11···C12$^{xiv}$ | 3.4108 |
| H3···H4 | 2.3207 | H11···C16$^{xv}$ | 3.5185 |
| H3···H5 | 3.5985 | H11···H2$^{iii}$ | 3.4262 |
| H3···H6 | 2.7061 | H11···H3$^{xiii}$ | 2.9642 |
| H3···H7 | 2.7235 | H11···H6$^{xiii}$ | 2.8057 |
| H8···H13 | 2.8597 | H11···H7$^{xiii}$ | 3.4890 |
| H8···H14 | 3.2723 | H11···H11$^{xiv}$ | 2.8055 |
| H9···H10 | 2.3440 | H11···H12$^{xiv}$ | 2.9812 |
| H9···H18 | 2.9627 | H11···H15$^{xv}$ | 2.9136 |
| H10···H11 | 2.3297 | H11···H15$^{v}$ | 3.1221 |
| H11···H12 | 2.3240 | H11···H16$^{v}$ | 3.5384 |
| H12···H13 | 2.3460 | H12···S1$^{viii}$ | 3.4321 |
| H13···H14 | 3.3530 | H12···O1$^{viii}$ | 2.3445 |
| H14···H15 | 2.3540 | H12···C1$^{viii}$ | 3.4930 |
| H15···H16 | 2.3251 | H12···C16$^{xv}$ | 3.5816 |
| H16···H17 | 2.3167 | H12···H2$^{iii}$ | 3.4696 |
| H17···H18 | 2.3434 | H12···H3$^{iv}$ | 2.9179 |
| S1···H3$^{vii}$ | 3.5901 | H12···H5$^{iii}$ | 3.1335 |
| S1···H8$^{iv}$ | 3.50 (3) | H12···H11$^{xiv}$ | 2.9812 |
| S1···H10$^{i}$ | 3.5867 | H12···H15$^{xv}$ | 2.6972 |
| S1···H12$^{ii}$ | 3.4321 | H13···C1$^{viii}$ | 3.5904 |
| O1···H3$^{vii}$ | 2.8289 | H13···C2$^{viii}$ | 3.3617 |
| O1···H10$^{i}$ | 2.7476 | H13···C3$^{viii}$ | 3.2731 |
| O1···H11$^{i}$ | 2.8900 | H13···C4$^{viii}$ | 3.4401 |

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|---|---|---|---|
| O1···H12$^{ii}$ | 2.3445 | H13···H4$^{iv}$ | 2.8027 |
| O1···H15$^{iii}$ | 2.6614 | H13···H5$^{iii}$ | 3.1487 |
| O2···H8$^{iv}$ | 2.20 (3) | H14···C7$^{viii}$ | 3.2799 |
| O2···H10$^{i}$ | 3.5465 | H14···H2$^{viii}$ | 3.3315 |
| O2···H17$^{vi}$ | 3.4199 | H14···H5$^{viii}$ | 2.7970 |
| O2···H17$^{v}$ | 2.6629 | H14···H6$^{iii}$ | 3.4652 |
| N1···H15$^{iii}$ | 3.5536 | H14···H7$^{viii}$ | 3.0321 |
| N2···H4$^{iv}$ | 3.4420 | H14···H18$^{vi}$ | 2.9405 |
| N2···H7$^{viii}$ | 3.0502 | H15···O1$^{vi}$ | 2.6614 |
| N2···H17$^{vi}$ | 2.6480 | H15···N1$^{vi}$ | 3.5536 |
| N2···H18$^{vi}$ | 3.1056 | H15···C10$^{ix}$ | 3.5418 |
| C1···H12$^{ii}$ | 3.4930 | H15···C11$^{xvi}$ | 3.4196 |
| C1···H13$^{ii}$ | 3.5904 | H15···C11$^{ix}$ | 3.2616 |
| C1···H17$^{vi}$ | 3.4140 | H15···C12$^{xvi}$ | 3.3133 |
| C2···H5$^{x}$ | 3.2128 | H15···H9$^{vi}$ | 3.1003 |
| C2···H6$^{x}$ | 3.3804 | H15···H11$^{xvi}$ | 2.9136 |
| C2···H13$^{ii}$ | 3.3617 | H15···H11$^{ix}$ | 3.1221 |
| C3···H6$^{x}$ | 3.2034 | H15···H12$^{xvi}$ | 2.6972 |
| C3···H13$^{ii}$ | 3.2731 | H16···C6$^{iii}$ | 3.5956 |
| C4···H13$^{ii}$ | 3.4401 | H16···C8$^{ix}$ | 3.0140 |
| C5···H4$^{vii}$ | 3.0320 | H16···C9$^{ix}$ | 2.9069 |
| C6···H3$^{vii}$ | 3.3034 | H16···C10$^{ix}$ | 2.9029 |
| C6···H4$^{vii}$ | 3.1367 | H16···C11$^{ix}$ | 3.0131 |
| C6···H16$^{vi}$ | 3.5956 | H16···C12$^{ix}$ | 3.1456 |
| C6···H17$^{vi}$ | 3.4151 | H16···C13$^{ix}$ | 3.1560 |
| C7···H1$^{xi}$ | 3.1191 | H16···H3$^{iii}$ | 3.5068 |
| C7···H2$^{xi}$ | 3.4100 | H16···H4$^{iii}$ | 3.4609 |
| C7···H10$^{xii}$ | 3.5062 | H16···H9$^{vi}$ | 3.3423 |
| C7···H11$^{xii}$ | 3.5250 | H16···H9$^{ix}$ | 3.3965 |
| C7···H14$^{ii}$ | 3.2799 | H16···H10$^{vi}$ | 3.4474 |
| C8···H2$^{iii}$ | 3.3221 | H16···H10$^{ix}$ | 3.3903 |
| C8···H16$^{v}$ | 3.0140 | H16···H11$^{ix}$ | 3.5384 |
| C9···H2$^{iii}$ | 3.2879 | H17···O2$^{iii}$ | 3.4199 |
| C9···H16$^{v}$ | 2.9069 | H17···O2$^{ix}$ | 2.6629 |
| C10···H2$^{iii}$ | 3.1156 | H17···N2$^{iii}$ | 2.6480 |
| C10···H6$^{xiii}$ | 3.3114 | H17···C1$^{iii}$ | 3.4140 |
| C10···H7$^{xiii}$ | 3.4584 | H17···C6$^{iii}$ | 3.4151 |
| C10···H15$^{v}$ | 3.5418 | H17···H4$^{iii}$ | 3.5072 |
| C10···H16$^{v}$ | 2.9029 | H17···H7$^{x}$ | 3.4409 |
| C11···H2$^{iii}$ | 2.9821 | H17···H8$^{iii}$ | 2.5120 |
| C11···H6$^{xiii}$ | 3.0923 | H17···H10$^{vi}$ | 3.2546 |
| C11···H11$^{xiv}$ | 3.3262 | H18···N2$^{iii}$ | 3.1056 |
| C11···H15$^{xv}$ | 3.4196 | H18···C15$^{iii}$ | 3.2253 |
| C11···H15$^{v}$ | 3.2616 | H18···H7$^{x}$ | 3.5180 |
| C11···H16$^{v}$ | 3.0131 | H18···H14$^{iii}$ | 2.9405 |

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|---|---|---|---|
| O1—S1—O2 | 116.16 (8) | C17—C18—C19 | 120.3 (2) |
| O1—S1—N1 | 107.18 (8) | C14—C19—C18 | 118.38 (18) |

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|---|---|---|---|
| O1—S1—C1 | 106.79 (8) | S2—N2—H8 | 112.7 (15) |
| O2—S1—N1 | 113.01 (8) | C1—C2—H1 | 120.300 |
| O2—S1—C1 | 107.86 (9) | C3—C2—H1 | 120.313 |
| N1—S1—C1 | 105.12 (8) | C2—C3—H2 | 119.289 |
| N1—S2—N2 | 126.05 (9) | C4—C3—H2 | 119.290 |
| N1—S2—C8 | 103.00 (8) | C4—C5—H3 | 119.292 |
| N1—S2—C14 | 102.92 (9) | C6—C5—H3 | 119.301 |
| N2—S2—C8 | 112.96 (10) | C1—C6—H4 | 120.122 |
| N2—S2—C14 | 104.42 (9) | C5—C6—H4 | 120.124 |
| C8—S2—C14 | 105.56 (8) | C4—C7—H5 | 109.473 |
| S1—N1—S2 | 121.56 (10) | C4—C7—H6 | 109.475 |
| S1—C1—C2 | 120.74 (14) | C4—C7—H7 | 109.479 |
| S1—C1—C6 | 118.96 (15) | H5—C7—H6 | 109.468 |
| C2—C1—C6 | 120.20 (18) | H5—C7—H7 | 109.464 |
| C1—C2—C3 | 119.39 (17) | H6—C7—H7 | 109.469 |
| C2—C3—C4 | 121.42 (19) | C8—C9—H9 | 120.460 |
| C3—C4—C5 | 117.80 (19) | C10—C9—H9 | 120.466 |
| C3—C4—C7 | 121.01 (19) | C9—C10—H10 | 120.070 |
| C5—C4—C7 | 121.19 (19) | C11—C10—H10 | 120.067 |
| C4—C5—C6 | 121.41 (19) | C10—C11—H11 | 119.635 |
| C1—C6—C5 | 119.75 (19) | C12—C11—H11 | 119.641 |
| S2—C8—C9 | 120.77 (14) | C11—C12—H12 | 119.913 |
| S2—C8—C13 | 117.72 (14) | C13—C12—H12 | 119.912 |
| C9—C8—C13 | 121.50 (18) | C8—C13—H13 | 120.669 |
| C8—C9—C10 | 119.07 (18) | C12—C13—H13 | 120.677 |
| C9—C10—C11 | 119.86 (19) | C14—C15—H14 | 120.818 |
| C10—C11—C12 | 120.7 (2) | C16—C15—H14 | 120.817 |
| C11—C12—C13 | 120.18 (19) | C15—C16—H15 | 120.052 |
| C8—C13—C12 | 118.65 (18) | C17—C16—H15 | 120.052 |
| S2—C14—C15 | 118.40 (15) | C16—C17—H16 | 119.551 |
| S2—C14—C19 | 119.46 (14) | C18—C17—H16 | 119.556 |
| C15—C14—C19 | 122.13 (17) | C17—C18—H17 | 119.844 |
| C14—C15—C16 | 118.37 (19) | C19—C18—H17 | 119.842 |
| C15—C16—C17 | 119.90 (19) | C14—C19—H18 | 120.805 |
| C16—C17—C18 | 120.9 (2) | C18—C19—H18 | 120.818 |

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|---|---|---|---|
| O1—S1—N1—S2 | −150.69 (11) | S1—C1—C6—C5 | −174.74 (12) |
| O1—S1—C1—C2 | −88.83 (13) | C2—C1—C6—C5 | 1.6 (3) |
| O1—S1—C1—C6 | 87.52 (13) | C6—C1—C2—C3 | −1.6 (3) |
| O2—S1—N1—S2 | −21.45 (14) | C1—C2—C3—C4 | 0.1 (3) |
| O2—S1—C1—C2 | 145.64 (12) | C2—C3—C4—C5 | 1.3 (3) |
| O2—S1—C1—C6 | −38.00 (14) | C2—C3—C4—C7 | −178.79 (16) |
| N1—S1—C1—C2 | 24.81 (14) | C3—C4—C5—C6 | −1.3 (3) |
| N1—S1—C1—C6 | −158.83 (12) | C7—C4—C5—C6 | 178.79 (17) |
| C1—S1—N1—S2 | 95.93 (12) | C4—C5—C6—C1 | −0.2 (3) |
| N2—S2—N1—S1 | −25.67 (17) | S2—C8—C9—C10 | −177.44 (11) |
| N1—S2—C8—C9 | 14.99 (14) | S2—C8—C13—C12 | 177.35 (11) |
| N1—S2—C8—C13 | −163.57 (11) | C9—C8—C13—C12 | −1.2 (3) |

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|---|---|---|---|
| C8—S2—N1—S1 | 105.86 (12) | C13—C8—C9—C10 | 1.1 (3) |
| N1—S2—C14—C15 | 148.19 (13) | C8—C9—C10—C11 | 0.0 (3) |
| N1—S2—C14—C19 | −31.18 (15) | C9—C10—C11—C12 | −0.9 (3) |
| C14—S2—N1—S1 | −144.54 (11) | C10—C11—C12—C13 | 0.7 (3) |
| N2—S2—C8—C9 | 153.90 (12) | C11—C12—C13—C8 | 0.3 (3) |
| N2—S2—C8—C13 | −24.66 (14) | S2—C14—C15—C16 | −177.49 (12) |
| N2—S2—C14—C15 | 15.17 (16) | S2—C14—C19—C18 | 177.70 (12) |
| N2—S2—C14—C19 | −164.20 (13) | C15—C14—C19—C18 | −1.6 (3) |
| C8—S2—C14—C15 | −104.15 (13) | C19—C14—C15—C16 | 1.9 (3) |
| C8—S2—C14—C19 | 76.49 (15) | C14—C15—C16—C17 | −1.2 (3) |
| C14—S2—C8—C9 | −92.61 (13) | C15—C16—C17—C18 | 0.3 (4) |
| C14—S2—C8—C13 | 88.83 (13) | C16—C17—C18—C19 | −0.1 (4) |
| S1—C1—C2—C3 | 174.68 (11) | C17—C18—C19—C14 | 0.7 (3) |

Symmetry codes: (i) −*x*, −*y*+1, −*z*+2; (ii) *x*+1, *y*, *z*; (iii) −*x*, *y*+1/2, −*z*+3/2; (iv) −*x*, −*y*, −*z*+2; (v) *x*, −*y*+1/2, *z*+1/2; (vi) −*x*, *y*−1/2, −*z*+3/2; (vii) −*x*+1, −*y*, −*z*+2; (viii) *x*−1, *y*, *z*; (ix) *x*, −*y*+1/2, *z*−1/2; (x) −*x*+1, *y*+1/2, −*z*+3/2; (xi) −*x*+1, *y*−1/2, −*z*+3/2; (xii) *x*+1, *y*−1, *z*; (xiii) *x*−1, *y*+1, *z*; (xiv) −*x*−1, −*y*+1, −*z*+2; (xv) −*x*−1, *y*+1/2, −*z*+3/2; (xvi) −*x*−1, *y*−1/2, −*z*+3/2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H8···O2$^{iv}$ | 0.89 (3) | 2.20 (3) | 3.018 (3) | 152 (2) |
| C12—H12···O1$^{viii}$ | 0.95 | 2.34 | 3.283 (2) | 169 |

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