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# Dimethyl 3,3′-diphenyl-2,2′-[(*S*)-thiophene-2,5-diylbis(carbonylazanediyl)]-dipropanoate

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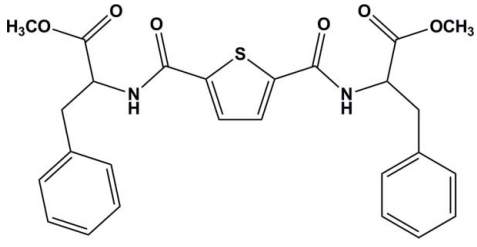
Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.008 Å; disorder in main residue; $R$ factor = 0.068; $wR$ factor = 0.187; data-to-parameter ratio = 14.7.

The asymmetric unit of the title compound, $C_{26}H_{26}N_2O_6S$, contains two independent molecules; each has twofold symmetry with the S atom and the mid-point of the C—C bond of the thiophene ring located on a twofold rotation axis. In the two molecules, the terminal benzene rings are oriented at dihedral angles of 65.8 (3) and 63.5 (3)° with respect to the central thiophene rings. The methoxycarbonyl group of one molecule is disordered over two positions with site-occupancy factors of 0.277 (12) and 0.723 (12). Intermolecular N—H···O hydrogen bonding is present in the crystal structure.

## Related literature

For applications of thiophene derivatives, see: Xia *et al.* (2010).




## Experimental

### Crystal data

$C_{26}H_{26}N_2O_6S$
$M_r$ = 494.56
Orthorhombic, $P2_12_12$
$a$ = 9.0769 (3) Å
$b$ = 29.6371 (7) Å
$c$ = 9.3767 (2) Å
$V$ = 2522.45 (12) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.17 mm$^{-1}$
$T$ = 120 K
0.36 × 0.24 × 0.10 mm

### Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* RED; Oxford Diffraction, 2009)
$T_{min}$ = 0.867, $T_{max}$ = 1.000
6802 measured reflections
4233 independent reflections
3315 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.187
$S$ = 1.10
4233 reflections
288 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.90 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.70 e Å$^{-3}$
Absolute structure: Flack (1983), 1669 Friedel pairs
Flack parameter: 0.00 (18)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O6 | 0.86 | 2.01 | 2.853 (5) | 164 |
| N2—H2···O3$^{i}$ | 0.86 | 2.10 | 2.803 (5) | 139 |

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

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); 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: XU5003).

## References

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Xia, G.-M., Ji, M.-W., Lu, P., Sun, G.-X. & Xu, W.-F. (2010). *Acta Cryst.* E**66**, o148.

# supporting information

*Acta Cryst.* (2010). E**66**, o2385 [https://doi.org/10.1107/S1600536810033210]

## Dimethyl 3,3′-diphenyl-2,2′-[(*S*)-thiophene-2,5-diylbis(carbonylazanediyl)]dipropanoate

**Guang-Ming Xia, Jing Liu, Zhen Li, Mu-Wei Ji and Guo-Xin Sun**

### S1. Comment

The thiophene derivates have been viewed as significant compounds for application in many fields (Xia *et al.*, 2010). The title compound derives from natural amino acids. This makes this kind of compounds promising for biological activities.

In the structure of the title compound, the carboxamide groups are approximately coplanar with thiophene ring, and the dihedral angle between thiophene ring and carboxamide is 3.2 (6)°. Title molecules are connected by intermolecular N—H···O hydrogen-bonding interactions forming a supramolecular frameworks. C3 and C16 are chiral atoms in the structure. And the chiral C atom which derived from *L*-phenylalanine kept its known S configuration for that the synthesis reaction did not befallen on the chiral C atom.

### S2. Experimental

2,5-Thiophenedicarboxylic acid (0.3 mmol), thionyl chloride (3 mmol) and 3–5 drops *N*,*N*-dimethylformamide in a flask was heated to 343 K for 10 h. The resulting solution was evaporated under vacuum, and then pale yellow solution of 2,5-thiophenedicarbonyldichloride was obtained.

To a stirred mixture of *L*-phenylalanine methyl ester hydrochloride (129.4 mg, 0.6 mmol) in 15 ml of dry dichloromethane and triethylamine (0.21 ml, 1.5 mmol), 2,5-thiophenedicarbonyldichloride (62.7 mg, 0.3 mmol) in dichloromethane (3 ml) was added dropwise at 253 K and then 20 h at 293 K. The resulting mixture was diluted with dichloromethane, washed with saturated $NaHCO_3$ solution and brine, and then dried over anhydrous $MgSO_4$. The solvent was condensed *in vacuo*. The title compound was isolated as a white solid by crystallization from 2-propanol (yield: 129.6 mg, 78%). Then the product was recrystallized from THF.

### S3. Refinement

All H atoms were placed in idealized positions and refined using a riding model, with N–H = 0.86 Å, C–H = 0.93–0.98 Å and with $U_{iso}$(H) = 1.2–1.5 $U_{eq}$(C,N).

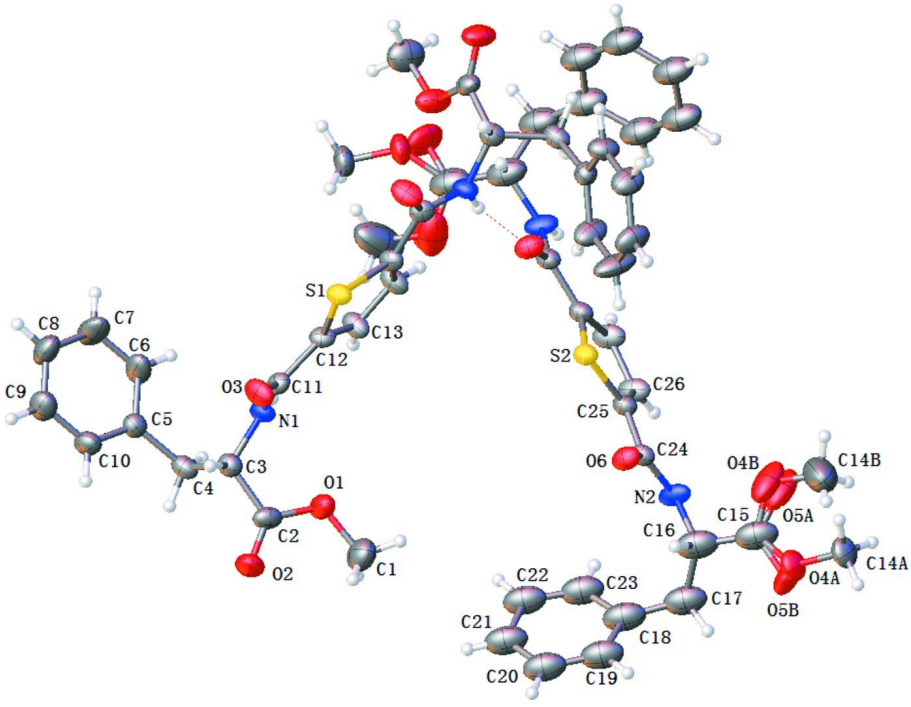


**Figure 1**

Molecular structure with thermal ellipsoids at 30% probability levels.

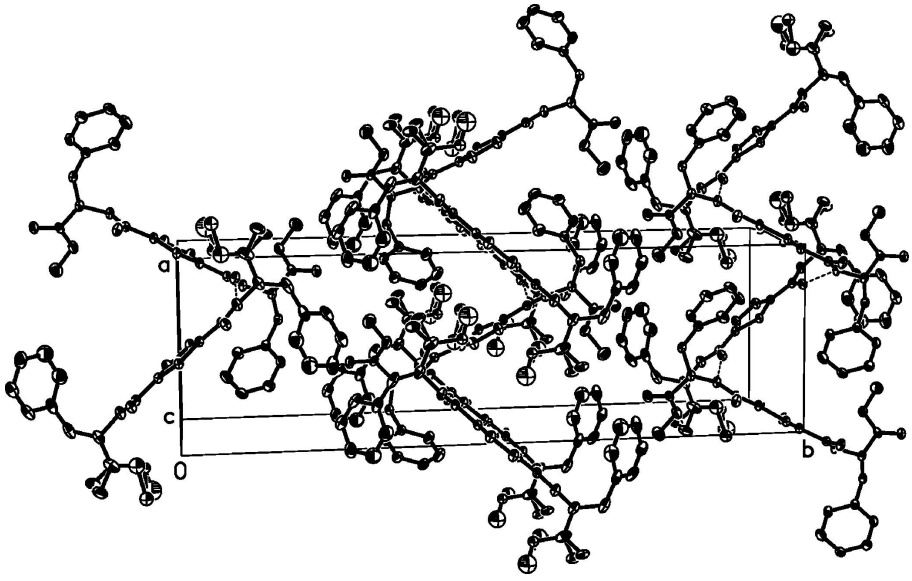


**Figure 2**

A packing diagram of the title compound along *c* axis.

**Dimethyl 3,3′-diphenyl-2,2′-[(*S*)-thiophene-2,5- diylbis(carbonylazanediyl)]dipropanoate**

*Crystal data*

$C_{26}H_{26}N_2O_6S$
$M_r$ = 494.56
Orthorhombic, $P2_12_12$

Hall symbol: P 2 2ab
$a$ = 9.0769 (3) Å
$b$ = 29.6371 (7) Å

$c$ = 9.3767 (2) Å
$V$ = 2522.45 (12) Å$^3$
$Z$ = 4
$F$(000) = 1040
$D_x$ = 1.302 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å

Cell parameters from 4047 reflections
$\theta$ = 3.4–25.3°
$\mu$ = 0.17 mm$^{-1}$
$T$ = 120 K
Block, colourless
0.36 × 0.24 × 0.10 mm

*Data collection*

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.0355 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO* RED; Oxford Diffraction, 2009)
$T_{min}$ = 0.867, $T_{max}$ = 1.000

6802 measured reflections
4233 independent reflections
3315 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 3.4°
$h$ = −6→10
$k$ = −28→35
$l$ = −7→11

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.187
$S$ = 1.10
4233 reflections
288 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.1124P)^2 + 0.8367P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.90 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.70 e Å$^{-3}$
Absolute structure: Flack (1983), 1669 Friedel pairs
Absolute structure parameter: 0.00 (18)

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| C1 | 0.3969 (8) | 0.6948 (2) | 0.3748 (8) | 0.0676 (18) | |
| H1A | 0.3112 | 0.6771 | 0.3529 | 0.101* | |
| H1B | 0.4259 | 0.7117 | 0.2920 | 0.101* | |
| H1C | 0.3745 | 0.7153 | 0.4512 | 0.101* | |
| C2 | 0.6263 (6) | 0.68418 (15) | 0.4908 (5) | 0.0361 (11) | |
| C3 | 0.7416 (5) | 0.65073 (14) | 0.5404 (5) | 0.0336 (11) | |
| H3 | 0.7545 | 0.6551 | 0.6432 | 0.040* | |
| C4 | 0.8884 (6) | 0.66076 (14) | 0.4700 (5) | 0.0338 (11) | |

| | | | | | |
|---|---|---|---|---|---|
| H4B | 0.9036 | 0.6932 | 0.4685 | 0.041* | |
| H4A | 0.8855 | 0.6503 | 0.3720 | 0.041* | |
| C5 | 1.0183 (6) | 0.63839 (14) | 0.5462 (4) | 0.0325 (10) | |
| C6 | 1.0574 (6) | 0.59423 (18) | 0.5155 (7) | 0.0529 (15) | |
| H6 | 1.0076 | 0.5782 | 0.4451 | 0.063* | |
| C7 | 1.1729 (8) | 0.5739 (2) | 0.5915 (8) | 0.069 (2) | |
| H7 | 1.2017 | 0.5446 | 0.5691 | 0.083* | |
| C8 | 1.2438 (6) | 0.59686 (19) | 0.6990 (7) | 0.0549 (15) | |
| H8 | 1.3177 | 0.5828 | 0.7514 | 0.066* | |
| C9 | 1.2052 (7) | 0.64021 (18) | 0.7282 (6) | 0.0521 (14) | |
| H9 | 1.2551 | 0.6562 | 0.7985 | 0.063* | |
| C10 | 1.0909 (6) | 0.66065 (16) | 0.6527 (5) | 0.0433 (13) | |
| H10 | 1.0635 | 0.6900 | 0.6753 | 0.052* | |
| C11 | 0.6350 (5) | 0.57915 (14) | 0.6197 (4) | 0.0281 (10) | |
| C12 | 0.5668 (5) | 0.53566 (13) | 0.5707 (4) | 0.0281 (10) | |
| C13 | 0.5371 (6) | 0.52036 (15) | 0.4374 (4) | 0.0352 (12) | |
| H13 | 0.5639 | 0.5357 | 0.3548 | 0.042* | |
| C14A | 0.207 (2) | 0.6027 (7) | 0.130 (2) | 0.047 (4) | 0.275 (12) |
| H14B | 0.1740 | 0.5900 | 0.0411 | 0.070* | 0.275 (12) |
| H14C | 0.1380 | 0.6250 | 0.1616 | 0.070* | 0.275 (12) |
| H14A | 0.2147 | 0.5792 | 0.1999 | 0.070* | 0.275 (12) |
| C14B | 0.3361 (17) | 0.5483 (4) | 0.091 (2) | 0.123 (6) | 0.725 (12) |
| H14E | 0.2938 | 0.5485 | −0.0026 | 0.184* | 0.725 (12) |
| H14F | 0.2793 | 0.5674 | 0.1529 | 0.184* | 0.725 (12) |
| H14D | 0.3359 | 0.5181 | 0.1280 | 0.184* | 0.725 (12) |
| C15 | 0.4767 (9) | 0.6062 (2) | 0.0647 (6) | 0.0674 (7) | |
| C16 | 0.6251 (9) | 0.6243 (2) | 0.0738 (7) | 0.0674 (7) | |
| H16 | 0.6438 | 0.6299 | 0.1752 | 0.081* | |
| C17 | 0.6498 (9) | 0.6692 (2) | −0.0017 (7) | 0.0674 (7) | |
| H17A | 0.6582 | 0.6638 | −0.1034 | 0.081* | |
| H17B | 0.5646 | 0.6883 | 0.0137 | 0.081* | |
| C18 | 0.7826 (9) | 0.6931 (2) | 0.0477 (6) | 0.0674 (7) | |
| C19 | 0.7774 (9) | 0.7261 (2) | 0.1503 (6) | 0.0674 (7) | |
| H19 | 0.6853 | 0.7354 | 0.1822 | 0.081* | |
| C20 | 0.9003 (9) | 0.7463 (2) | 0.2091 (7) | 0.0674 (7) | |
| H20 | 0.8902 | 0.7686 | 0.2783 | 0.081* | |
| C21 | 1.0373 (9) | 0.7331 (2) | 0.1643 (6) | 0.0674 (7) | |
| H21 | 1.1207 | 0.7472 | 0.2008 | 0.081* | |
| C22 | 1.0519 (9) | 0.6990 (2) | 0.0649 (6) | 0.0674 (7) | |
| H22 | 1.1448 | 0.6886 | 0.0389 | 0.081* | |
| C23 | 0.9280 (9) | 0.6808 (2) | 0.0052 (7) | 0.0674 (7) | |
| H23 | 0.9391 | 0.6594 | −0.0666 | 0.081* | |
| C24 | 0.8109 (6) | 0.56624 (14) | 0.1212 (4) | 0.0287 (10) | |
| C25 | 0.9113 (5) | 0.53145 (14) | 0.0658 (4) | 0.0284 (10) | |
| C26 | 0.9493 (6) | 0.51816 (16) | −0.0702 (4) | 0.0395 (13) | |
| H26 | 0.9124 | 0.5315 | −0.1526 | 0.047* | |
| N1 | 0.6976 (4) | 0.60424 (11) | 0.5186 (4) | 0.0276 (8) | |
| H1 | 0.7127 | 0.5923 | 0.4364 | 0.033* | |

| | | | | | |
|---|---|---|---|---|---|
| N2 | 0.7346 (5) | 0.59066 (12) | 0.0283 (4) | 0.0378 (10) | |
| H2 | 0.7497 | 0.5867 | −0.0614 | 0.045* | |
| O1 | 0.5160 (5) | 0.66529 (11) | 0.4175 (4) | 0.0507 (10) | |
| O2 | 0.6327 (4) | 0.72365 (11) | 0.5165 (5) | 0.0555 (11) | |
| O3 | 0.6321 (4) | 0.59001 (10) | 0.7462 (3) | 0.0403 (9) | |
| O4A | 0.342 (2) | 0.6223 (6) | 0.111 (2) | 0.047 (4) | 0.275 (12) |
| O4B | 0.4741 (16) | 0.5635 (4) | 0.0848 (17) | 0.078 (3) | 0.725 (12) |
| O5A | 0.443 (6) | 0.5668 (8) | 0.057 (5) | 0.078 (3) | 0.275 (12) |
| O5B | 0.3754 (8) | 0.6338 (3) | 0.0463 (11) | 0.070 (2) | 0.725 (12) |
| O6 | 0.8024 (4) | 0.57171 (10) | 0.2509 (3) | 0.0349 (8) | |
| S1 | 0.5000 | 0.5000 | 0.70005 (14) | 0.0268 (4) | |
| S2 | 1.0000 | 0.5000 | 0.19249 (14) | 0.0265 (4) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.063 (4) | 0.068 (4) | 0.072 (4) | 0.008 (3) | −0.025 (4) | −0.005 (3) |
| C2 | 0.042 (3) | 0.030 (2) | 0.037 (2) | 0.007 (2) | 0.012 (2) | 0.0014 (19) |
| C3 | 0.041 (3) | 0.033 (2) | 0.027 (2) | −0.002 (2) | −0.002 (2) | −0.0013 (18) |
| C4 | 0.050 (3) | 0.029 (2) | 0.022 (2) | −0.007 (2) | 0.000 (2) | −0.0004 (17) |
| C5 | 0.033 (3) | 0.034 (2) | 0.030 (2) | −0.001 (2) | 0.004 (2) | −0.0016 (18) |
| C6 | 0.048 (3) | 0.051 (3) | 0.059 (3) | 0.006 (3) | −0.013 (3) | −0.030 (3) |
| C7 | 0.073 (4) | 0.055 (3) | 0.081 (4) | 0.031 (3) | −0.026 (4) | −0.038 (3) |
| C8 | 0.046 (3) | 0.059 (3) | 0.060 (3) | 0.018 (3) | −0.018 (3) | −0.013 (3) |
| C9 | 0.054 (4) | 0.052 (3) | 0.051 (3) | 0.004 (3) | −0.009 (3) | −0.020 (3) |
| C10 | 0.053 (3) | 0.033 (2) | 0.044 (3) | 0.003 (2) | −0.009 (3) | −0.008 (2) |
| C11 | 0.035 (3) | 0.031 (2) | 0.018 (2) | 0.004 (2) | −0.0055 (19) | 0.0008 (16) |
| C12 | 0.041 (3) | 0.027 (2) | 0.0163 (19) | 0.002 (2) | 0.0030 (19) | 0.0048 (16) |
| C13 | 0.056 (4) | 0.035 (2) | 0.015 (2) | −0.012 (2) | −0.005 (2) | 0.0033 (17) |
| C14A | 0.034 (7) | 0.053 (8) | 0.053 (8) | −0.013 (5) | 0.010 (6) | 0.002 (6) |
| C14B | 0.110 (12) | 0.068 (7) | 0.191 (16) | −0.018 (7) | −0.066 (11) | 0.014 (8) |
| C15 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C16 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C17 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C18 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C19 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C20 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C21 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C22 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C23 | 0.0996 (18) | 0.0573 (12) | 0.0455 (11) | 0.0261 (13) | 0.0108 (12) | −0.0013 (9) |
| C24 | 0.040 (3) | 0.026 (2) | 0.020 (2) | −0.002 (2) | 0.000 (2) | −0.0021 (17) |
| C25 | 0.039 (3) | 0.024 (2) | 0.022 (2) | −0.0018 (19) | 0.000 (2) | 0.0001 (16) |
| C26 | 0.069 (4) | 0.036 (2) | 0.013 (2) | 0.008 (2) | −0.002 (2) | 0.0005 (16) |
| N1 | 0.044 (2) | 0.0221 (16) | 0.0167 (16) | −0.0009 (17) | −0.0006 (17) | −0.0027 (14) |
| N2 | 0.065 (3) | 0.0338 (19) | 0.0141 (16) | 0.018 (2) | −0.0050 (19) | −0.0061 (14) |
| O1 | 0.054 (2) | 0.0389 (18) | 0.059 (2) | 0.0089 (18) | −0.026 (2) | −0.0115 (16) |
| O2 | 0.057 (3) | 0.0316 (19) | 0.078 (3) | 0.0055 (18) | −0.012 (2) | −0.0154 (17) |
| O3 | 0.066 (2) | 0.0395 (17) | 0.0156 (15) | −0.0111 (17) | −0.0077 (16) | −0.0038 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O4A | 0.034 (7) | 0.053 (8) | 0.053 (8) | −0.013 (5) | 0.010 (6) | 0.002 (6) |
| O4B | 0.047 (8) | 0.115 (4) | 0.072 (8) | 0.011 (4) | −0.005 (4) | 0.048 (4) |
| O5A | 0.047 (8) | 0.115 (4) | 0.072 (8) | 0.011 (4) | −0.005 (4) | 0.048 (4) |
| O5B | 0.041 (4) | 0.070 (5) | 0.100 (6) | 0.020 (4) | −0.026 (4) | −0.014 (4) |
| O6 | 0.049 (2) | 0.0383 (16) | 0.0170 (15) | 0.0106 (16) | −0.0037 (14) | −0.0017 (12) |
| S1 | 0.0425 (9) | 0.0263 (7) | 0.0118 (6) | 0.0010 (7) | 0.000 | 0.000 |
| S2 | 0.0384 (8) | 0.0268 (7) | 0.0144 (6) | 0.0011 (7) | 0.000 | 0.000 |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O1 | 1.447 (7) | C14B—H14E | 0.9600 |
| C1—H1A | 0.9600 | C14B—H14F | 0.9600 |
| C1—H1B | 0.9600 | C14B—H14D | 0.9600 |
| C1—H1C | 0.9600 | C15—O5A | 1.21 (2) |
| C2—O2 | 1.196 (5) | C15—O5B | 1.243 (9) |
| C2—O1 | 1.337 (6) | C15—O4B | 1.280 (12) |
| C2—C3 | 1.515 (7) | C15—O4A | 1.38 (2) |
| C3—N1 | 1.449 (6) | C15—C16 | 1.453 (11) |
| C3—C4 | 1.516 (7) | C16—N2 | 1.471 (7) |
| C3—H3 | 0.9800 | C16—C17 | 1.523 (9) |
| C4—C5 | 1.530 (7) | C16—H16 | 0.9800 |
| C4—H4B | 0.9700 | C17—C18 | 1.472 (10) |
| C4—H4A | 0.9700 | C17—H17A | 0.9700 |
| C5—C10 | 1.366 (7) | C17—H17B | 0.9700 |
| C5—C6 | 1.386 (7) | C18—C19 | 1.373 (8) |
| C6—C7 | 1.404 (9) | C18—C23 | 1.426 (10) |
| C6—H6 | 0.9300 | C19—C20 | 1.381 (10) |
| C7—C8 | 1.376 (8) | C19—H19 | 0.9300 |
| C7—H7 | 0.9300 | C20—C21 | 1.369 (10) |
| C8—C9 | 1.360 (8) | C20—H20 | 0.9300 |
| C8—H8 | 0.9300 | C21—C22 | 1.381 (9) |
| C9—C10 | 1.395 (8) | C21—H21 | 0.9300 |
| C9—H9 | 0.9300 | C22—C23 | 1.367 (10) |
| C10—H10 | 0.9300 | C22—H22 | 0.9300 |
| C11—O3 | 1.229 (5) | C23—H23 | 0.9300 |
| C11—N1 | 1.332 (6) | C24—O6 | 1.229 (5) |
| C11—C12 | 1.502 (6) | C24—N2 | 1.328 (6) |
| C12—C13 | 1.357 (6) | C24—C25 | 1.471 (6) |
| C12—S1 | 1.719 (4) | C25—C26 | 1.378 (6) |
| C13—C13$^{i}$ | 1.383 (9) | C25—S2 | 1.711 (4) |
| C13—H13 | 0.9300 | C26—C26$^{ii}$ | 1.417 (10) |
| C14A—O4A | 1.37 (3) | C26—H26 | 0.9300 |
| C14A—H14B | 0.9600 | N1—H1 | 0.8600 |
| C14A—H14C | 0.9600 | N2—H2 | 0.8600 |
| C14A—H14A | 0.9600 | S1—C12$^{i}$ | 1.719 (4) |
| C14B—O4B | 1.33 (2) | S2—C25$^{ii}$ | 1.711 (4) |
| | | | |
| O1—C1—H1A | 109.5 | O5A—C15—O4A | 97 (3) |

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|---|---|---|---|
| O1—C1—H1B | 109.5 | O4B—C15—O4A | 106.1 (13) |
| H1A—C1—H1B | 109.5 | O5A—C15—C16 | 126 (3) |
| O1—C1—H1C | 109.5 | O5B—C15—C16 | 116.8 (7) |
| H1A—C1—H1C | 109.5 | O4B—C15—C16 | 112.0 (8) |
| H1B—C1—H1C | 109.5 | O4A—C15—C16 | 132.5 (9) |
| O2—C2—O1 | 123.4 (5) | C15—C16—N2 | 111.0 (5) |
| O2—C2—C3 | 123.0 (5) | C15—C16—C17 | 115.6 (6) |
| O1—C2—C3 | 113.6 (4) | N2—C16—C17 | 110.9 (6) |
| N1—C3—C2 | 112.9 (4) | C15—C16—H16 | 106.2 |
| N1—C3—C4 | 111.6 (4) | N2—C16—H16 | 106.2 |
| C2—C3—C4 | 110.2 (4) | C17—C16—H16 | 106.2 |
| N1—C3—H3 | 107.3 | C18—C17—C16 | 113.2 (6) |
| C2—C3—H3 | 107.3 | C18—C17—H17A | 108.9 |
| C4—C3—H3 | 107.3 | C16—C17—H17A | 108.9 |
| C3—C4—C5 | 112.9 (4) | C18—C17—H17B | 108.9 |
| C3—C4—H4B | 109.0 | C16—C17—H17B | 108.9 |
| C5—C4—H4B | 109.0 | H17A—C17—H17B | 107.7 |
| C3—C4—H4A | 109.0 | C19—C18—C23 | 114.1 (7) |
| C5—C4—H4A | 109.0 | C19—C18—C17 | 122.4 (7) |
| H4B—C4—H4A | 107.8 | C23—C18—C17 | 123.2 (5) |
| C10—C5—C6 | 119.0 (5) | C18—C19—C20 | 124.2 (7) |
| C10—C5—C4 | 120.3 (4) | C18—C19—H19 | 117.9 |
| C6—C5—C4 | 120.6 (4) | C20—C19—H19 | 117.9 |
| C5—C6—C7 | 119.4 (5) | C21—C20—C19 | 119.1 (6) |
| C5—C6—H6 | 120.3 | C21—C20—H20 | 120.4 |
| C7—C6—H6 | 120.3 | C19—C20—H20 | 120.4 |
| C8—C7—C6 | 120.5 (5) | C20—C21—C22 | 120.2 (7) |
| C8—C7—H7 | 119.7 | C20—C21—H21 | 119.9 |
| C6—C7—H7 | 119.7 | C22—C21—H21 | 119.9 |
| C9—C8—C7 | 119.7 (5) | C23—C22—C21 | 119.0 (7) |
| C9—C8—H8 | 120.2 | C23—C22—H22 | 120.5 |
| C7—C8—H8 | 120.2 | C21—C22—H22 | 120.5 |
| C8—C9—C10 | 120.0 (5) | C22—C23—C18 | 123.2 (6) |
| C8—C9—H9 | 120.0 | C22—C23—H23 | 118.4 |
| C10—C9—H9 | 120.0 | C18—C23—H23 | 118.4 |
| C5—C10—C9 | 121.3 (4) | O6—C24—N2 | 123.0 (4) |
| C5—C10—H10 | 119.3 | O6—C24—C25 | 118.7 (4) |
| C9—C10—H10 | 119.3 | N2—C24—C25 | 118.3 (4) |
| O3—C11—N1 | 123.3 (4) | C26—C25—C24 | 133.0 (4) |
| O3—C11—C12 | 120.7 (4) | C26—C25—S2 | 111.7 (3) |
| N1—C11—C12 | 115.9 (4) | C24—C25—S2 | 115.4 (3) |
| C13—C12—C11 | 130.6 (4) | C25—C26—C26$^{ii}$ | 112.3 (3) |
| C13—C12—S1 | 112.0 (3) | C25—C26—H26 | 123.8 |
| C11—C12—S1 | 117.2 (3) | C26$^{ii}$—C26—H26 | 123.8 |
| C12—C13—C13$^{i}$ | 112.9 (3) | C11—N1—C3 | 123.2 (4) |
| C12—C13—H13 | 123.6 | C11—N1—H1 | 118.4 |
| C13$^{i}$—C13—H13 | 123.6 | C3—N1—H1 | 118.4 |
| O4A—C14A—H14B | 109.5 | C24—N2—C16 | 122.1 (4) |

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|---|---|---|---|
| O4A—C14A—H14C | 109.5 | C24—N2—H2 | 119.0 |
| H14B—C14A—H14C | 109.5 | C16—N2—H2 | 119.0 |
| O4A—C14A—H14A | 109.5 | C2—O1—C1 | 116.6 (4) |
| H14B—C14A—H14A | 109.5 | C14A—O4A—C15 | 133.5 (17) |
| H14C—C14A—H14A | 109.5 | C15—O4B—C14B | 111.0 (12) |
| O5A—C15—O5B | 116 (2) | C12$^{i}$—S1—C12 | 90.3 (3) |
| O5B—C15—O4B | 131.1 (11) | C25$^{ii}$—S2—C25 | 92.1 (3) |

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|---|---|---|---|
| O2—C2—C3—N1 | 169.7 (4) | C17—C18—C19—C20 | 173.7 (6) |
| O1—C2—C3—N1 | −9.4 (6) | C18—C19—C20—C21 | −0.1 (10) |
| O2—C2—C3—C4 | −64.8 (6) | C19—C20—C21—C22 | −2.1 (9) |
| O1—C2—C3—C4 | 116.1 (4) | C20—C21—C22—C23 | 4.4 (9) |
| N1—C3—C4—C5 | −71.2 (4) | C21—C22—C23—C18 | −4.6 (10) |
| C2—C3—C4—C5 | 162.7 (4) | C19—C18—C23—C22 | 2.4 (9) |
| C3—C4—C5—C10 | −90.3 (5) | C17—C18—C23—C22 | −171.2 (6) |
| C3—C4—C5—C6 | 85.1 (6) | O6—C24—C25—C26 | −177.5 (5) |
| C10—C5—C6—C7 | −1.7 (9) | N2—C24—C25—C26 | 1.8 (8) |
| C4—C5—C6—C7 | −177.2 (6) | O6—C24—C25—S2 | 3.2 (6) |
| C5—C6—C7—C8 | 2.2 (11) | N2—C24—C25—S2 | −177.5 (4) |
| C6—C7—C8—C9 | −2.4 (11) | C24—C25—C26—C26$^{ii}$ | −179.0 (5) |
| C7—C8—C9—C10 | 2.2 (10) | S2—C25—C26—C26$^{ii}$ | 0.4 (8) |
| C6—C5—C10—C9 | 1.5 (8) | O3—C11—N1—C3 | −13.2 (7) |
| C4—C5—C10—C9 | 177.0 (5) | C12—C11—N1—C3 | 167.1 (4) |
| C8—C9—C10—C5 | −1.8 (9) | C2—C3—N1—C11 | −95.6 (5) |
| O3—C11—C12—C13 | 168.5 (5) | C4—C3—N1—C11 | 139.6 (4) |
| N1—C11—C12—C13 | −11.8 (8) | O6—C24—N2—C16 | −4.5 (8) |
| O3—C11—C12—S1 | −5.5 (6) | C25—C24—N2—C16 | 176.3 (5) |
| N1—C11—C12—S1 | 174.2 (3) | C15—C16—N2—C24 | −99.5 (6) |
| C11—C12—C13—C13$^{i}$ | −175.3 (5) | C17—C16—N2—C24 | 130.5 (6) |
| S1—C12—C13—C13$^{i}$ | −1.0 (8) | O2—C2—O1—C1 | −3.0 (8) |
| O5A—C15—C16—N2 | 18 (3) | C3—C2—O1—C1 | 176.1 (5) |
| O5B—C15—C16—N2 | −153.2 (7) | O5A—C15—O4A—C14A | −6 (3) |
| O4B—C15—C16—N2 | 30.1 (11) | O5B—C15—O4A—C14A | 122 (3) |
| O4A—C15—C16—N2 | 171.0 (12) | O4B—C15—O4A—C14A | −22 (3) |
| O5A—C15—C16—C17 | 145 (3) | C16—C15—O4A—C14A | −164.4 (18) |
| O5B—C15—C16—C17 | −25.7 (9) | O5A—C15—O4B—C14B | −41 (11) |
| O4B—C15—C16—C17 | 157.6 (10) | O5B—C15—O4B—C14B | −3 (2) |
| O4A—C15—C16—C17 | −61.5 (14) | O4A—C15—O4B—C14B | 22.3 (18) |
| C15—C16—C17—C18 | 161.2 (5) | C16—C15—O4B—C14B | 173.4 (12) |
| N2—C16—C17—C18 | −71.2 (7) | C13—C12—S1—C12$^{i}$ | 0.4 (3) |
| C16—C17—C18—C19 | −96.0 (7) | C11—C12—S1—C12$^{i}$ | 175.5 (5) |
| C16—C17—C18—C23 | 77.1 (8) | C26—C25—S2—C25$^{ii}$ | −0.1 (3) |
| C23—C18—C19—C20 | 0.0 (9) | C24—C25—S2—C25$^{ii}$ | 179.3 (5) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O6 | 0.86 | 2.01 | 2.853 (5) | 164 |
| N2—H2···O3$^{iii}$ | 0.86 | 2.10 | 2.803 (5) | 139 |

Symmetry code: (iii) *x*, *y*, *z*−1.