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#### Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
 Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 Disorder in main residue  
 $R$  factor = 0.044  
 $wR$  factor = 0.096  
 Data-to-parameter ratio = 18.0

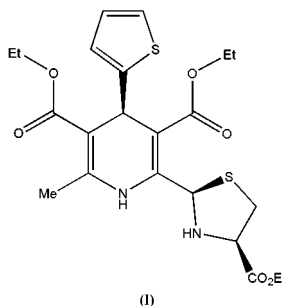
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Diethyl (2'*R*,4*R*,4'*R*)-2-(4'-ethoxycarbonyl-2'-thiazolidinyl)-6-methyl-4-(2''-thienyl)-1,4-dihydropyridine-3,5-dicarboxylate

In the title compound,  $\text{C}_{22}\text{H}_{28}\text{N}_2\text{O}_6\text{S}_2$ , the 1,4-dihydropyridine (DHP) ring has a flat-boat conformation. The 2-thiophene ring is disordered over two orientations and is approximately perpendicular to the DHP ring. For each ester group, at the 3- and 5-positions of the DHP ring, the carbonyl group is *cis* with respect to the conjugated  $\text{C}=\text{C}$  double bond.

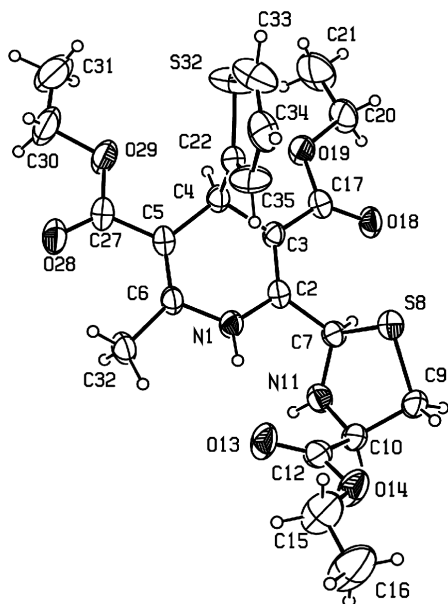
#### Comment

1,4-Dihydropyridine (DHP) derivatives constitute a major class of calcium antagonists and have been a target of structure–activity relationship studies. Stereoselectivity of calcium antagonism has been observed in many DHP compounds whose ester substituents at the C3 and C5 positions are different (Shibanuma *et al.*, 1980; Tamazawa *et al.*, 1986; Rowan & Holt, 1996). Previous studies suggest that ester carbonyl groups which are not involved in hydrogen bonding exist in a synperiplanar (*sp*) conformation, whereas the molecule responds to a hydrogen-bonding opportunity by rotating the carbonyl group to an antiperiplanar (*ap*) conformation (Caignan *et al.*, 2000; Metcalf & Holt, 2000; Caignan & Holt, 2001). We have studied the crystal structure of the title compound, (I), and present its structure here.



The structure of (I) (Fig. 1) consists of discrete molecules, with an *R* configuration at atom C4. The shortest intermolecular contact is 3.283 (4) Å for  $\text{O18}\cdots\text{C15}(x-1, y, z)$ . As in other DHP structures, the DHP ring in (I) exhibits a boat conformation. Atoms N1 and C4 lie 0.128 (2) and 0.289 (3) Å, respectively, from the base of the boat. The nearly planar 2-thiophene ring, which is approximately perpendicular to the DHP ring [dihedral angle 90.6 (3)°], is disordered over two orientations of approximately half-occupancy. The structure shows near coplanarity of the carbonyl  $\text{C}=\text{O}$  bonds with the conjugated double bonds at positions C3 and C5 in the DHP ring. The torsion angles  $\text{C6}-\text{C5}-\text{C27}-\text{O28}$  and  $\text{C2}-\text{C3}-\text{C17}-\text{O18}$  are 9.7 (5) and  $-11.3$  (5)°, respectively. These torsion angles reflect the synperiplanar (*sp*, *sp*) conformations of the carbonyl  $\text{C}=\text{O}$  bonds. The third carbonyl group

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**Figure 1**

The molecular structure of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The thiophene ring shows orientational disorder, and the site occupancy factors of atoms S32 and C33–C35 are 0.469 (6). The other orientation of the thiophene has been omitted for clarity.

(C12=O13) is involved in an intramolecular N–H···O hydrogen bond (Table 2).

## Experimental

The title compound, (I), was prepared by a condensation reaction of diethyl (*R*)-2-formyl-6-methyl-(2-thienyl)-1,4-dihydropyridine-3,5-dicarboxylate (Marchalín *et al.*, 2001) with (*R*)-cysteine ethyl ester. Yellow plate-like single crystals were prepared by recrystallization from an ethanol solution.

### Crystal data

$C_{22}H_{28}N_2O_6S_2$   
 $M_r = 480.58$   
 Monoclinic,  $P2_1$   
 $a = 10.347$  (2) Å  
 $b = 9.3127$  (19) Å  
 $c = 13.160$  (3) Å  
 $\beta = 107.53$  (3)°  
 $V = 1209.1$  (4) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.320$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 7503 reflections  
 $\theta = 3.0$ – $30.3$ °  
 $\mu = 0.26$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Block, yellow  
 $0.4 \times 0.3 \times 0.3$  mm

### Data collection

Oxford Diffraction Xcalibur CCD diffractometer  
 $\omega$  and  $\varphi$  scans  
 Absorption correction: none  
 7507 measured reflections  
 5925 independent reflections

2506 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.022$   
 $\theta_{max} = 30.3$ °  
 $h = -14 \rightarrow 12$   
 $k = -12 \rightarrow 12$   
 $l = -18 \rightarrow 18$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.096$   
 $S = 0.98$   
 5925 reflections  
 330 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.052P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.013$   
 $\Delta\rho_{max} = 0.17$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.19$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 2097 Friedel pairs  
 Flack parameter = 0.01 (8)

**Table 1**

Selected geometric parameters (Å, °).

C2–C3	1.352 (3)	C6–N1	1.385 (3)
C2–N1	1.363 (3)	C6–C32	1.499 (4)
C2–C7	1.520 (3)	C7–N11	1.450 (3)
C3–C4	1.517 (3)	C7–S8	1.829 (3)
C4–C22	1.494 (4)	C9–S8	1.795 (3)
C4–C5	1.524 (3)	C22–S32	1.702 (4)
C5–C6	1.339 (4)	C24–S23	1.700 (5)
C3–C2–N1	119.9 (2)	O28–C27–O29	120.5 (3)
C22–C4–C3	109.9 (2)	C7–N11–C10	114.7 (2)
C3–C4–C5	110.9 (2)	C9–S8–C7	91.01 (15)
O18–C17–O19	121.6 (2)	C33–S32–C22	91.8 (8)
C7–C2–C3–C4	–173.2 (3)	N11–C10–C12–O14	–176.2 (3)
C2–C3–C4–C22	100.4 (3)	C2–C3–C17–O18	–11.3 (5)
C22–C4–C5–C6	–100.7 (3)	C2–C3–C17–O19	169.7 (2)
C3–C2–C7–S8	83.8 (3)	C6–C5–C27–O28	9.7 (5)
N1–C2–C7–S8	–97.2 (2)	C6–C5–C27–O29	–171.6 (3)
N11–C10–C12–O13	7.0 (4)	C7–C2–N1–C6	–166.6 (2)

**Table 2**

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1···O13	0.86	2.12	2.963 (3)	168

Compound (I) has a disordered 2-thiophene ring in which S32, C33, C34 and C35 have the alternative positions S23, C24, C25 and C26, the occupancy factors being 0.469 (6) and 0.531 (6), respectively. All atoms of the thiophene ring were subject to geometrical and displacement parameter restraints. H atoms were positioned geometrically and treated as riding atoms (N–H = 0.86 Å and C–H = 0.93–0.98 Å), with  $U_{iso}$  set at  $1.2U_{eq}$  ( $1.5U_{eq}$  for methyl) of the parent atom.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2002); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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