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Dimethyl [(5-ethoxycarbonyl-4-methyl-1,3-thiazol-2-ylamino)phenylmethyl]-phosphonate

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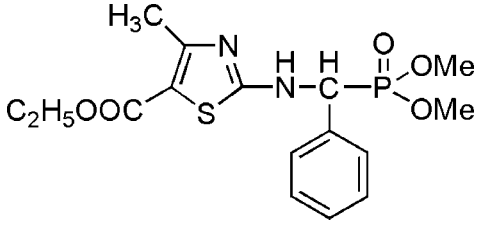
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.045; wR factor = 0.136; data-to-parameter ratio = 15.7.

In the structure of the title compound, $C_{16}H_{21}N_2O_5PS$, the P atom adopts a slightly distorted tetrahedral configuration. The crystal packing is stabilized by intramolecular C—H···N and C—H···O and intermolecular N—H···O hydrogen-bonding interactions.

Related literature

A similar synthetic method is described by Bhagat & Chakraborti (2007) and the bioactivity of substituted aminophosphonates is described by Song & Jiang (2004).

For related literature, see: Garbarczyk *et al.* (1999); Boy & Guernonenneth (2005); Lu & Chen (2000); Vicini *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{21}N_2O_5PS$
M_r = 384.38
Triclinic, $P\overline{1}$
a = 8.1821 (4) Å
b = 9.9884 (5) Å
c = 11.9142 (6) Å
α = 98.249 (1)°
β = 103.299 (1)°
γ = 95.618 (1)°
V = 929.08 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 291 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.945, T_{max} = 0.972
8937 measured reflections
3610 independent reflections
3081 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.136
S = 1.07
3610 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected bond angles (°).

O1—P1—O3	115.59 (10)	O1—P1—C9	113.98 (9)
O1—P1—O2	114.25 (9)	O3—P1—C9	103.11 (10)
O3—P1—O2	102.76 (9)	O2—P1—C9	105.80 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.02	2.791 (2)	148
C13—H13A···O4	0.96	2.36	3.077 (4)	131
C9—H9···N2	0.98	2.47	2.886 (3)	105

Symmetry code: (i) $-x, -y+1, -z+2$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2070).

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supplementary materials

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Dimethyl [(5-ethoxycarbonyl-4-methyl-1,3-thiazol-2-ylamino)phenylmethyl]phosphonate

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Comment

Among many known heterocyclic compounds, the analogues containing a thiazole ring have received much attention since they possess significant biological and pharmacological activity (Vicini *et al.*, 2006). Aminophosphonic acids and their derivatives represent an important class of organophosphorus compounds that continue to attract considerable attention due to their biological importance and extensive application in organic chemistry (Lu & Chen, 2000). The bioactivity of substituted aminophosphonates is described by Song & Jiang (2004). We report here the crystal structure of the title compound (Fig. 1)

The bond lengths of N2—C10 and C10—S1 are longer than those observed in free thiazole [1.286 and 1.728 Å] (Garbarczyk *et al.*, 1999) and the N1—C9 bond is a little longer than the neighbouring N1—C10 bond. The bond angles O1—P1—O3, O1—P1—O2 and O1—P1—C9 are larger than of O3—P1—O2, O2—P1—C9 and O3—P1—C9, indicating the phosphorus atom adopts a slightly distorted tetrahedral configuration.

Some weak intramolecular C—H···N and C—H···O hydrogen-bonding interactions exist in the crystal structure. In additon, the crystal is also stabilized by intermolecular N1—H1···O1 hydrogen-bonding interactions that form dimers (Fig. 2).

Experimental

2-amino-5-carbethoxy-4-methylthiazole was prepared according to the literature method (Boy & Guernonenneth, 2005) in 75% yield. The mixture of benzaldehyde (5 mmol) and $Mg(ClO_4)_2$ (5mol%) was stirred magnetically for 11–15 min, then 2-amino-5-carbethoxy-4-methylthiazole (5 mmol) and dimethylphosphonate(5 mmol) were added and the reaction mixture was stirred at room temperature for 6 h (Bhagat & Chakraborti, 2007). The mixture was extracted with ethanol (3 times 10 ml), the combined ethanol extracts were dried (over $MgSO_4$) and concentrated *in vacuo* to afford a white solid (1.15 g, 61%) which on passing through a column of silica gel elution with acetone-peroleum ether (*v*/*v* 1/4) afford the title compound. The precipitate was recrystallized from ethanol-acetone (*v*/*v* 1/5) to give crystals suitable for X-ray diffraction.

Refinement

All H-atoms were refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq}(C) for aromatic 0.98 Å, U_{iso} = 1.2U_{eq}(C) for CH, 0.96 Å, U_{iso} = 1.5U_{eq}(C) for CH_3 atoms and d(N—H) = 0.86 Å, U_{iso}=1.2U_{eq}(N) for NH.

Figures

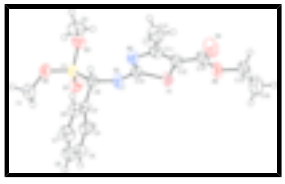

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsolids and the atom-labelling scheme.

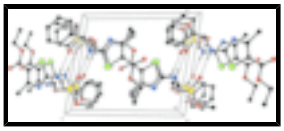

Fig. 2. The crystal structure of (I), showing the formation of N—H···O hydrogen bonds (dashed lines)·H atoms not involved in hydrogen bonding have been omitted.

Dimethyl [(5-ethoxycarbonyl-4-methyl-1,3-thiazol-2-ylamino)phenylmethyl]phosphonate

Crystal data

$C_{16}H_{21}N_2O_5PS$	$Z = 2$
$M_r = 384.38$	$F_{000} = 404$
Triclinic, $P\overline{1}$	$D_x = 1.374$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.1821$ (4) Å	Cell parameters from 4630 reflections
$b = 9.9884$ (5) Å	$\theta = 2.5$–19.2º
$c = 11.9142$ (6) Å	$\mu = 0.29$ mm^{-1}
$\alpha = 98.249$ (1)º	$T = 291$ (2) K
$\beta = 103.299$ (1)º	Block, colorless
$\gamma = 95.618$ (1)º	0.20 × 0.20 × 0.10 mm
$V = 929.08$ (8) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3610 independent reflections
Radiation source: fine-focus sealed tube	3081 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 291$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -10 \rightarrow 9$
$T_{min} = 0.945$, $T_{max} = 0.972$	$k = -12 \rightarrow 12$
8937 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.136$	$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 0.2203P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
3610 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
230 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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}
C1	−0.0145 (4)	0.9080 (3)	1.2151 (2)	0.0730 (8)
H1A	−0.0472	0.8278	1.2449	0.110*
H1B	−0.0555	0.9849	1.2524	0.110*
H1C	0.1069	0.9248	1.2310	0.110*
C2	−0.4101 (3)	0.6895 (3)	0.8875 (3)	0.0758 (8)
H2A	−0.4252	0.5992	0.8430	0.114*
H2B	−0.4895	0.7421	0.8476	0.114*
H2C	−0.4288	0.6842	0.9635	0.114*
C3	0.2526 (3)	0.7897 (2)	1.05538 (19)	0.0411 (5)
C4	0.2955 (3)	0.6954 (2)	1.1295 (2)	0.0550 (6)
H4	0.2265	0.6122	1.1172	0.066*
C5	0.4383 (4)	0.7241 (3)	1.2204 (3)	0.0643 (7)
H5	0.4645	0.6614	1.2702	0.077*
C6	0.5427 (4)	0.8459 (3)	1.2378 (3)	0.0658 (7)
H6	0.6408	0.8644	1.2983	0.079*
C7	0.5023 (3)	0.9404 (3)	1.1659 (2)	0.0634 (7)
H7	0.5726	1.0229	1.1783	0.076*
C8	0.3567 (3)	0.9126 (2)	1.0750 (2)	0.0504 (6)
H8	0.3290	0.9769	1.0271	0.060*
C9	0.0939 (3)	0.7586 (2)	0.95480 (19)	0.0400 (5)
H9	0.0913	0.8335	0.9097	0.048*
C10	0.1302 (3)	0.6288 (2)	0.77337 (18)	0.0388 (5)
C11	0.1807 (3)	0.6978 (2)	0.6147 (2)	0.0490 (5)
C12	0.2079 (3)	0.5648 (2)	0.5898 (2)	0.0479 (5)
C13	0.1884 (4)	0.8039 (3)	0.5388 (3)	0.0727 (8)
H13A	0.2253	0.7672	0.4712	0.109*
H13B	0.2669	0.8820	0.5821	0.109*
H13C	0.0780	0.8306	0.5142	0.109*
C14	0.2556 (3)	0.4942 (3)	0.4884 (2)	0.0563 (6)
C15	0.3114 (4)	0.2811 (4)	0.3995 (2)	0.0750 (9)
H15A	0.4186	0.3233	0.3906	0.090*

H15B	0.2266	0.2748	0.3265	0.090*
C16	0.3282 (5)	0.1417 (4)	0.4301 (3)	0.0942 (11)
H16A	0.4169	0.1487	0.5001	0.141*
H16B	0.3553	0.0842	0.3671	0.141*
H16C	0.2232	0.1031	0.4427	0.141*
N1	0.0889 (3)	0.63109 (17)	0.87592 (16)	0.0444 (4)
H1	0.0584	0.5550	0.8961	0.053*
N2	0.1400 (2)	0.73480 (18)	0.72011 (16)	0.0454 (4)
O1	−0.1179 (2)	0.62813 (15)	1.06639 (15)	0.0521 (4)
O2	−0.0859 (2)	0.88752 (15)	1.09062 (14)	0.0501 (4)
O3	−0.2396 (2)	0.75427 (18)	0.90029 (15)	0.0559 (4)
O4	0.2876 (3)	0.5468 (2)	0.40968 (18)	0.0840 (7)
O5	0.2613 (2)	0.36168 (19)	0.49423 (15)	0.0622 (5)
P1	−0.09523 (7)	0.74679 (5)	1.00991 (5)	0.03896 (18)
S1	0.17583 (8)	0.47814 (5)	0.70125 (5)	0.04578 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.079 (2)	0.0800 (19)	0.0519 (16)	0.0194 (16)	0.0123 (14)	−0.0131 (14)
C2	0.0435 (15)	0.089 (2)	0.087 (2)	0.0010 (14)	0.0043 (14)	0.0139 (17)
C3	0.0396 (12)	0.0400 (10)	0.0473 (12)	0.0088 (9)	0.0171 (9)	0.0071 (9)
C4	0.0541 (14)	0.0451 (12)	0.0663 (16)	0.0076 (10)	0.0115 (12)	0.0156 (11)
C5	0.0588 (16)	0.0698 (16)	0.0649 (17)	0.0145 (13)	0.0064 (13)	0.0241 (14)
C6	0.0490 (15)	0.0834 (19)	0.0589 (16)	0.0050 (13)	0.0054 (12)	0.0079 (14)
C7	0.0562 (16)	0.0632 (15)	0.0633 (16)	−0.0104 (12)	0.0127 (13)	0.0018 (13)
C8	0.0544 (14)	0.0452 (12)	0.0544 (14)	0.0048 (10)	0.0194 (11)	0.0092 (10)
C9	0.0465 (12)	0.0351 (10)	0.0420 (11)	0.0084 (9)	0.0164 (9)	0.0075 (8)
C10	0.0351 (11)	0.0412 (10)	0.0385 (11)	0.0041 (8)	0.0094 (8)	0.0021 (9)
C11	0.0456 (13)	0.0573 (13)	0.0438 (12)	0.0000 (10)	0.0112 (10)	0.0118 (10)
C12	0.0453 (13)	0.0590 (13)	0.0395 (12)	0.0027 (10)	0.0139 (10)	0.0065 (10)
C13	0.093 (2)	0.0731 (18)	0.0582 (17)	0.0049 (16)	0.0270 (15)	0.0216 (14)
C14	0.0462 (14)	0.0843 (18)	0.0375 (12)	0.0042 (12)	0.0150 (10)	0.0035 (12)
C15	0.0663 (18)	0.106 (2)	0.0492 (15)	0.0159 (16)	0.0226 (13)	−0.0144 (15)
C16	0.106 (3)	0.089 (2)	0.084 (2)	0.024 (2)	0.032 (2)	−0.0177 (19)
N1	0.0615 (12)	0.0335 (8)	0.0432 (10)	0.0060 (8)	0.0241 (9)	0.0046 (7)
N2	0.0490 (11)	0.0443 (9)	0.0446 (10)	0.0051 (8)	0.0146 (8)	0.0086 (8)
O1	0.0597 (10)	0.0444 (8)	0.0590 (10)	0.0086 (7)	0.0246 (8)	0.0143 (7)
O2	0.0605 (10)	0.0429 (8)	0.0476 (9)	0.0134 (7)	0.0172 (8)	0.0001 (7)
O3	0.0460 (9)	0.0653 (10)	0.0525 (10)	0.0048 (8)	0.0055 (8)	0.0101 (8)
O4	0.1037 (18)	0.1013 (16)	0.0567 (12)	0.0095 (13)	0.0412 (12)	0.0140 (11)
O5	0.0703 (12)	0.0710 (12)	0.0466 (10)	0.0112 (9)	0.0260 (9)	−0.0058 (8)
P1	0.0423 (3)	0.0363 (3)	0.0398 (3)	0.0079 (2)	0.0128 (2)	0.0050 (2)
S1	0.0526 (4)	0.0450 (3)	0.0425 (3)	0.0096 (2)	0.0189 (3)	0.0030 (2)

Geometric parameters (Å, °)

C1—O2	1.440 (3)	C10—N1	1.338 (3)
C1—H1A	0.9600	C10—S1	1.740 (2)

C1—H1B	0.9600	C11—C12	1.370 (3)
C1—H1C	0.9600	C11—N2	1.382 (3)
C2—O3	1.444 (3)	C11—C13	1.494 (3)
C2—H2A	0.9600	C12—C14	1.462 (3)
C2—H2B	0.9600	C12—S1	1.740 (2)
C2—H2C	0.9600	C13—H13A	0.9600
C3—C8	1.381 (3)	C13—H13B	0.9600
C3—C4	1.397 (3)	C13—H13C	0.9600
C3—C9	1.522 (3)	C14—O4	1.204 (3)
C4—C5	1.372 (4)	C14—O5	1.340 (3)
C4—H4	0.9300	C15—O5	1.451 (3)
C5—C6	1.376 (4)	C15—C16	1.501 (5)
C5—H5	0.9300	C15—H15A	0.9700
C6—C7	1.378 (4)	C15—H15B	0.9700
C6—H6	0.9300	C16—H16A	0.9600
C7—C8	1.387 (4)	C16—H16B	0.9600
C7—H7	0.9300	C16—H16C	0.9600
C8—H8	0.9300	N1—H1	0.8600
C9—N1	1.462 (3)	O1—P1	1.4612 (15)
C9—P1	1.815 (2)	O2—P1	1.5697 (15)
C9—H9	0.9800	O3—P1	1.5625 (17)
C10—N2	1.315 (3)		
O2—C1—H1A	109.5	C12—C11—C13	126.5 (2)
O2—C1—H1B	109.5	N2—C11—C13	117.8 (2)
H1A—C1—H1B	109.5	C11—C12—C14	129.6 (2)
O2—C1—H1C	109.5	C11—C12—S1	109.96 (17)
H1A—C1—H1C	109.5	C14—C12—S1	120.46 (19)
H1B—C1—H1C	109.5	C11—C13—H13A	109.5
O3—C2—H2A	109.5	C11—C13—H13B	109.5
O3—C2—H2B	109.5	H13A—C13—H13B	109.5
H2A—C2—H2B	109.5	C11—C13—H13C	109.5
O3—C2—H2C	109.5	H13A—C13—H13C	109.5
H2A—C2—H2C	109.5	H13B—C13—H13C	109.5
H2B—C2—H2C	109.5	O4—C14—O5	123.6 (2)
C8—C3—C4	118.8 (2)	O4—C14—C12	125.2 (3)
C8—C3—C9	120.25 (19)	O5—C14—C12	111.1 (2)
C4—C3—C9	120.9 (2)	O5—C15—C16	107.4 (3)
C5—C4—C3	120.7 (2)	O5—C15—H15A	110.2
C5—C4—H4	119.6	C16—C15—H15A	110.2
C3—C4—H4	119.6	O5—C15—H15B	110.2
C4—C5—C6	119.9 (2)	C16—C15—H15B	110.2
C4—C5—H5	120.0	H15A—C15—H15B	108.5
C6—C5—H5	120.0	C15—C16—H16A	109.5
C5—C6—C7	120.2 (3)	C15—C16—H16B	109.5
C5—C6—H6	119.9	H16A—C16—H16B	109.5
C7—C6—H6	119.9	C15—C16—H16C	109.5
C6—C7—C8	120.0 (2)	H16A—C16—H16C	109.5
C6—C7—H7	120.0	H16B—C16—H16C	109.5
C8—C7—H7	120.0	C10—N1—C9	122.15 (17)

C3—C8—C7	120.3 (2)	C10—N1—H1	118.9
C3—C8—H8	119.8	C9—N1—H1	118.9
C7—C8—H8	119.8	C10—N2—C11	110.26 (18)
N1—C9—C3	112.70 (17)	C1—O2—P1	121.86 (17)
N1—C9—P1	108.02 (14)	C2—O3—P1	120.73 (17)
C3—C9—P1	110.69 (14)	C14—O5—C15	116.3 (2)
N1—C9—H9	108.4	O1—P1—O3	115.59 (10)
C3—C9—H9	108.4	O1—P1—O2	114.25 (9)
P1—C9—H9	108.4	O3—P1—O2	102.76 (9)
N2—C10—N1	124.56 (19)	O1—P1—C9	113.98 (9)
N2—C10—S1	115.39 (16)	O3—P1—C9	103.11 (10)
N1—C10—S1	120.05 (15)	O2—P1—C9	105.80 (10)
C12—C11—N2	115.7 (2)	C12—S1—C10	88.65 (10)
C8—C3—C4—C5	0.1 (4)	N1—C10—N2—C11	−178.3 (2)
C9—C3—C4—C5	−179.7 (2)	S1—C10—N2—C11	1.8 (2)
C3—C4—C5—C6	−1.3 (4)	C12—C11—N2—C10	−2.3 (3)
C4—C5—C6—C7	1.5 (5)	C13—C11—N2—C10	176.9 (2)
C5—C6—C7—C8	−0.5 (4)	O4—C14—O5—C15	0.8 (4)
C4—C3—C8—C7	0.9 (4)	C12—C14—O5—C15	−178.5 (2)
C9—C3—C8—C7	−179.3 (2)	C16—C15—O5—C14	173.8 (2)
C6—C7—C8—C3	−0.7 (4)	C2—O3—P1—O1	26.7 (2)
C8—C3—C9—N1	124.9 (2)	C2—O3—P1—O2	−98.4 (2)
C4—C3—C9—N1	−55.3 (3)	C2—O3—P1—C9	151.7 (2)
C8—C3—C9—P1	−114.0 (2)	C1—O2—P1—O1	32.1 (2)
C4—C3—C9—P1	65.8 (2)	C1—O2—P1—O3	158.1 (2)
N2—C11—C12—C14	−178.7 (2)	C1—O2—P1—C9	−94.1 (2)
C13—C11—C12—C14	2.2 (4)	N1—C9—P1—O1	55.35 (17)
N2—C11—C12—S1	1.7 (3)	C3—C9—P1—O1	−68.48 (16)
C13—C11—C12—S1	−177.3 (2)	N1—C9—P1—O3	−70.74 (15)
C11—C12—C14—O4	3.9 (4)	C3—C9—P1—O3	165.43 (14)
S1—C12—C14—O4	−176.6 (2)	N1—C9—P1—O2	−178.29 (13)
C11—C12—C14—O5	−176.8 (2)	C3—C9—P1—O2	57.88 (15)
S1—C12—C14—O5	2.7 (3)	C11—C12—S1—C10	−0.55 (18)
N2—C10—N1—C9	−16.7 (3)	C14—C12—S1—C10	179.8 (2)
S1—C10—N1—C9	163.21 (16)	N2—C10—S1—C12	−0.75 (17)
C3—C9—N1—C10	−100.6 (2)	N1—C10—S1—C12	179.34 (19)
P1—C9—N1—C10	136.84 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.02	2.791 (2)	148
C13—H13A···O4	0.96	2.36	3.077 (4)	131
C9—H9···N2	0.98	2.47	2.886 (3)	105

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

Fig. 1

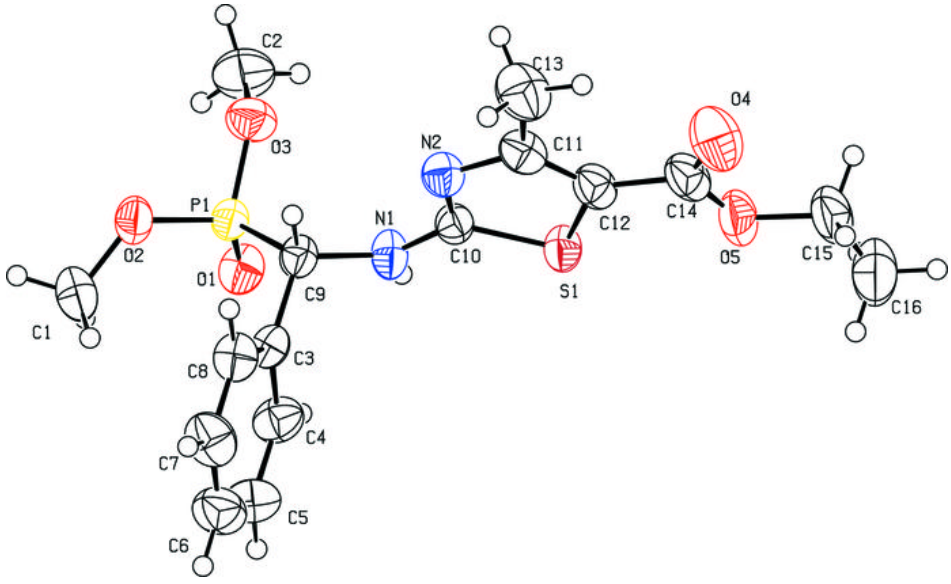
C2
O3
P1
O2
O1
C1
C9
N1
C10
N2
C11
C13
C12
S1
C14
O4
O5
C15
C16
C8
C3
C4
C7
C5
C6

Fig. 2