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Diethyl {2-[(4-chlorophenoxy)methyl]-9-(methylsulfanyl)-7*H*-pyrazolo[4,3-*d*]-[1,2,4]-triazolo[1,5-*d*]pyrimidin-7-yl}-(phenyl)methylphosphonate

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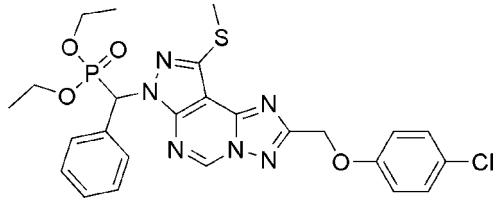
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.059; wR factor = 0.150; data-to-parameter ratio = 15.9.

In the title compound, $C_{25}H_{26}ClN_6O_4PS$, the fused pyrazolotriazolopyrimidine ring system is almost planar. It makes dihedral angles of 78.1 (1) and 17.1 (1)°, respectively, with the attached phenyl ring and 4-chlorophenoxymethyl fragment. The P atom has a distorted tetrahedral configuration. Intra- and intermolecular C—H···O and C—H···N hydrogen bonds, together with strong π–π stacking interactions (interplanar distances 3.312–3.567 Å), stabilize the structure.

Related literature

Many derivatives of pyrazolotriazolopyrimidines have been prepared, and their biological and pharmaceutical activities have been studied by Gatta *et al.* (1993) and Baraldi *et al.* (1996, 1998). For bond-length comparisons, see Sasada (1984) and Wang *et al.* (1998).



Experimental

Crystal data

$C_{25}H_{26}ClN_6O_4PS$
M_r = 573.00
Monoclinic, $P2_1/c$
a = 13.8732 (12) Å
b = 13.5760 (11) Å
c = 16.2034 (14) Å
β = 113.515 (2)°
V = 2798.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 294 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.941, T_{max} = 0.970
26250 measured reflections
5485 independent reflections
3386 reflections with $I > 2\sigma(I)$
R_{int} = 0.108

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.150
S = 0.94
5485 reflections
346 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22A···O2	0.97	2.49	2.948 (4)	109
C17—H17···N6	0.93	2.61	3.238 (4)	125
C15—H15···N4	0.98	2.60	2.991 (3)	104
C7—H7A···O2^{i}	0.97	2.36	3.324 (4)	171
C12—H12···N2^{ii}	0.93	2.53	3.450 (3)	169

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

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: CF2126).

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supplementary materials

Acta Cryst. (2007). E**63**, o3613 [**doi:10.1107/S1600536807035532**]

Diethyl {2-[(4-chlorophenoxy)methyl]-9-(methylsulfanyl)-7*H*-pyrazolo[4,3-*d*][1,2,4]-triazolo[1,5-*d*]pyrimidin-7-yl}(phenyl)methylphosphonate

L.-X. Xiao and D.-Q. Shi

Comment

Pyrazolotriazolopyrimidine derivatives have been reported to retain high affinity for adenosine receptors (Gatta *et al.*, 1993). A series of pyrazolo[4,3-*e*]-1,2,4-triazolo[1,5-*c*]-pyrimidines has been synthesized with the aim of finding potent and selective adenosine A2A antagonists (Baraldi *et al.*, 1996, 1998). Organic phosphorus compounds play an important role in pesticidal science because of their significant biological properties. The title compound, (I), has been prepared as part of our work in the search for novel biologically active heterocyclic compounds. We report here the crystal structure of (I). In the molecule of (I) (Fig. 1), the pyrazolotriazolopyrimidine ring system is almost planar, with a maximum deviation of 0.023 (2) Å, for N2, forming a fully delocalized system. The dihedral angles between the pyrimidine and the triazole and pyrazole rings are 1.31 (1) and 1.1 (1)°, respectively. In the pyrazolotriazolopyrimidine ring system, the the C—N bonds are significantly shorter than a normal single C—N bond (1.47 Å; Sasada, 1984) and close to the value for a C=N bond (1.28 Å; Wang *et al.*, 1998). This indicates significant electron delocalization in the pyrazolotriazolopyrimidine system. The O2—P1—O4, O2—P1—O3 and O2—P1—C15 bond angles are larger than the O4—P1—O3, O4—P1—C15 and O3—P1—C15 bond angles, indicating a distorted tetrahedral configuration for the phosphorus atom.

Intra- and intermolecular C—H···O and C—H···N hydrogen bonds contribute strongly to the stability of the crystal structure (Fig. 2 and Table 1). Strong π—π stacking interactions also occur between C1—C6 and N1—N3/C8/C9, N5/N6/C10/C11/C13, N3/N4/C9—C12 rings of neighboring molecules. Centroid-centroid distances are 3.990 (2), 3.909 (2) and 3.509 (2) Å, dihedral angles are 7.76, 7.35 and 8.26°, and shortest interplanar distances are 3.312, 3.567 and 3.439 Å, respectively.

Experimental

A solution of ethyl *N*-4-cyano-1-((diethoxyphosphoryl)(phenyl)methyl)- 3-(methylthio)-1*H*-pyrazol-5-ylformimidate (0.87 g, 2 mmol) and 2-(4-chlorophenoxy)acetohydrazide (0.41 g, 2 mmol) in ethylene glycol monomethyl ether (20 ml) was refluxed for 4 h, cooled briefly and evaporated. The residue was purified by chromatography on a silica gel column by eluting with petroleum ether/acetone (6:1, *v*/*v*) to give the title compound (yield 61%). Colorless crystals of (I) suitable for X-ray structure analysis were grown from petroleum ether and acetone (6:1, *v*/*v*).

Refinement

H atoms bonded to C were placed at calculated positions, with C—H distances of 0.97 and 0.93Å for H atoms bonded to sp^3 and sp^2 C atoms, respectively. They were refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

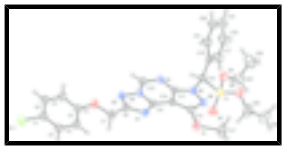

Fig. 1. View of the molecular structure of (I), showing the atom labelling scheme and displacement ellipsoids drawn at the 50% probability level.

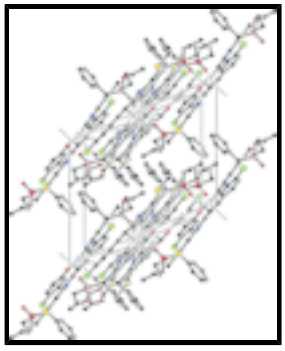

Fig. 2. A partial view of the crystal packing of (I), showing the formation of C—H···O and C—H···N hydrogen bonds and π—π stacking interactions, as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Diethyl {2-[(4-chlorophenoxy)methyl]-9-(methylsulfanyl)-7*H*-pyrazolo[4,3-*d*][1,2,4]triazolo[1,5-*d*]pyrimidin-7-yl}(phenyl)methylphosphonate

Crystal data

$C_{25}H_{26}ClN_6O_4PS$	F_{000} = 1192
M_r = 573.00	D_x = 1.360 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 13.8732 (12) Å	Cell parameters from 4496 reflections
b = 13.5760 (11) Å	θ = 2.2–21.0º
c = 16.2034 (14) Å	μ = 0.31 mm^{-1}
β = 113.515 (2)º	T = 294 (2) K
V = 2798.4 (4) Å^3	Plate, colorless
Z = 4	0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer	5485 independent reflections
Radiation source: fine-focus sealed tube	3386 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.108
T = 294(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	h = −17→17
T_{min} = 0.941, T_{max} = 0.970	k = −15→16
26250 measured reflections	l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H-atom parameters constrained
$wR(F^2) = 0.150$	$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{max} < 0.001$
5485 reflections	$\Delta\rho_{max} = 0.51$ e Å^{-3}
346 parameters	$\Delta\rho_{min} = -0.27$ 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 $F^2 > 2$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	−0.1149 (2)	0.5777 (2)	0.75100 (19)	0.0508 (7)
C2	−0.0868 (2)	0.5265 (2)	0.6910 (2)	0.0557 (8)
H2	−0.0980	0.4589	0.6843	0.067*
C3	−0.0417 (2)	0.57556 (19)	0.64043 (19)	0.0508 (7)
H3	−0.0210	0.5412	0.6006	0.061*
C4	−0.0279 (2)	0.6763 (2)	0.64991 (18)	0.0451 (7)
C5	−0.0550 (2)	0.72648 (19)	0.71144 (19)	0.0518 (7)
H5	−0.0433	0.7940	0.7189	0.062*
C6	−0.0990 (2)	0.6773 (2)	0.7617 (2)	0.0522 (7)
H6	−0.1180	0.7113	0.8028	0.063*
C7	0.0502 (2)	0.68771 (19)	0.5432 (2)	0.0487 (7)
H7A	−0.0041	0.6472	0.5000	0.058*
H7B	0.1097	0.6460	0.5769	0.058*
C8	0.08293 (19)	0.76692 (19)	0.49599 (18)	0.0408 (6)
C9	0.15006 (18)	0.83186 (18)	0.41392 (17)	0.0383 (6)
C10	0.19804 (18)	0.86846 (17)	0.35807 (17)	0.0372 (6)
C11	0.19344 (18)	0.96985 (18)	0.34508 (17)	0.0379 (6)
C12	0.1020 (2)	1.00255 (18)	0.42829 (19)	0.0456 (7)

H12	0.0675	1.0450	0.4526	0.055*
C13	0.2525 (2)	0.83244 (19)	0.30701 (18)	0.0441 (7)
C14	0.3413 (3)	0.7131 (3)	0.2211 (3)	0.0995 (14)
H14A	0.2925	0.7369	0.1639	0.149*
H14B	0.3643	0.6482	0.2140	0.149*
H14C	0.4008	0.7565	0.2441	0.149*
C15	0.2671 (2)	1.08765 (18)	0.26658 (18)	0.0421 (6)
H15	0.2141	1.1318	0.2722	0.051*
C16	0.3721 (2)	1.1259 (2)	0.33355 (19)	0.0453 (7)
C17	0.4588 (3)	1.0674 (2)	0.3706 (2)	0.0709 (10)
H17	0.4548	1.0014	0.3543	0.085*
C18	0.5531 (3)	1.1053 (3)	0.4323 (3)	0.0866 (12)
H18	0.6115	1.0645	0.4573	0.104*
C19	0.5600 (3)	1.2017 (3)	0.4563 (2)	0.0765 (10)
H19	0.6231	1.2273	0.4973	0.092*
C20	0.4743 (3)	1.2605 (3)	0.4199 (3)	0.0808 (11)
H20	0.4788	1.3266	0.4362	0.097*
C21	0.3804 (2)	1.2231 (2)	0.3590 (2)	0.0699 (10)
H21	0.3220	1.2640	0.3350	0.084*
C22	0.3442 (4)	0.9654 (3)	0.0871 (3)	0.0991 (14)
H22A	0.2788	0.9305	0.0742	0.119*
H22B	0.4015	0.9218	0.1218	0.119*
C23	0.3527 (4)	0.9898 (3)	0.0029 (3)	0.1031 (14)
H23A	0.2944	1.0306	−0.0328	0.155*
H23B	0.3520	0.9303	−0.0294	0.155*
H23C	0.4172	1.0246	0.0154	0.155*
C24	0.2595 (3)	1.2565 (3)	0.0636 (2)	0.0849 (11)
H24A	0.1950	1.2935	0.0339	0.102*
H24B	0.2643	1.2079	0.0214	0.102*
C25	0.3491 (4)	1.3229 (4)	0.0895 (3)	0.1304 (18)
H25A	0.3501	1.3646	0.1377	0.196*
H25B	0.3434	1.3628	0.0388	0.196*
H25C	0.4129	1.2853	0.1091	0.196*
Cl1	−0.17098 (9)	0.51602 (7)	0.81553 (7)	0.0888 (4)
N1	0.13835 (16)	0.74467 (15)	0.44512 (15)	0.0419 (5)
N2	0.05817 (17)	0.86038 (15)	0.49857 (15)	0.0461 (6)
N3	0.10306 (16)	0.90381 (14)	0.44590 (14)	0.0401 (5)
N4	0.14721 (16)	1.03871 (15)	0.37903 (15)	0.0430 (5)
N5	0.24196 (17)	0.99000 (14)	0.28979 (15)	0.0423 (5)
N6	0.28024 (17)	0.90563 (15)	0.26614 (16)	0.0482 (6)
O1	0.01191 (16)	0.73385 (14)	0.60181 (14)	0.0632 (6)
O2	0.14870 (16)	1.04858 (16)	0.08870 (14)	0.0684 (6)
O3	0.25682 (18)	1.20711 (13)	0.14157 (14)	0.0650 (6)
O4	0.34735 (17)	1.05220 (16)	0.13979 (15)	0.0686 (6)
P1	0.24715 (6)	1.09311 (5)	0.14878 (5)	0.0484 (2)
S1	0.27892 (8)	0.70881 (5)	0.29756 (6)	0.0705 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0521 (17)	0.0527 (19)	0.0503 (18)	−0.0048 (14)	0.0232 (15)	0.0076 (15)
C2	0.072 (2)	0.0378 (16)	0.061 (2)	−0.0079 (14)	0.0303 (18)	0.0005 (15)
C3	0.0659 (18)	0.0376 (16)	0.0561 (19)	−0.0010 (14)	0.0318 (16)	−0.0004 (14)
C4	0.0496 (16)	0.0401 (16)	0.0487 (18)	0.0053 (13)	0.0228 (14)	0.0107 (13)
C5	0.0699 (19)	0.0324 (15)	0.059 (2)	0.0051 (14)	0.0320 (17)	0.0057 (14)
C6	0.0608 (18)	0.0460 (18)	0.0562 (19)	0.0099 (14)	0.0300 (16)	0.0065 (14)
C7	0.0570 (17)	0.0395 (16)	0.0583 (19)	0.0033 (13)	0.0324 (16)	0.0073 (14)
C8	0.0436 (15)	0.0338 (15)	0.0470 (17)	0.0005 (12)	0.0202 (14)	0.0035 (12)
C9	0.0370 (14)	0.0326 (14)	0.0433 (16)	0.0013 (11)	0.0138 (13)	−0.0004 (12)
C10	0.0395 (14)	0.0273 (14)	0.0450 (16)	−0.0008 (11)	0.0173 (13)	−0.0014 (12)
C11	0.0382 (14)	0.0340 (14)	0.0405 (16)	−0.0038 (11)	0.0146 (13)	0.0010 (12)
C12	0.0528 (16)	0.0316 (15)	0.0586 (19)	0.0044 (12)	0.0286 (15)	0.0002 (13)
C13	0.0521 (16)	0.0343 (15)	0.0495 (17)	−0.0034 (13)	0.0241 (14)	−0.0005 (13)
C14	0.145 (4)	0.067 (2)	0.135 (4)	0.019 (2)	0.108 (3)	0.003 (2)
C15	0.0487 (15)	0.0297 (14)	0.0545 (18)	−0.0009 (12)	0.0275 (14)	0.0027 (13)
C16	0.0493 (16)	0.0399 (16)	0.0519 (18)	−0.0064 (13)	0.0258 (15)	0.0022 (14)
C17	0.065 (2)	0.0445 (19)	0.089 (3)	0.0003 (16)	0.015 (2)	0.0056 (18)
C18	0.060 (2)	0.069 (3)	0.102 (3)	0.0019 (19)	0.003 (2)	0.010 (2)
C19	0.062 (2)	0.081 (3)	0.074 (3)	−0.017 (2)	0.013 (2)	−0.008 (2)
C20	0.065 (2)	0.060 (2)	0.108 (3)	−0.0165 (19)	0.025 (2)	−0.030 (2)
C21	0.058 (2)	0.050 (2)	0.098 (3)	−0.0006 (16)	0.026 (2)	−0.0136 (19)
C22	0.149 (4)	0.060 (2)	0.138 (4)	0.013 (2)	0.109 (3)	0.000 (2)
C23	0.131 (4)	0.100 (3)	0.089 (3)	0.027 (3)	0.055 (3)	−0.007 (2)
C24	0.128 (3)	0.061 (2)	0.073 (3)	−0.011 (2)	0.048 (2)	0.0154 (19)
C25	0.153 (4)	0.118 (4)	0.149 (5)	−0.041 (3)	0.090 (4)	0.015 (3)
Cl1	0.1260 (8)	0.0782 (7)	0.0883 (7)	−0.0364 (6)	0.0703 (7)	−0.0041 (5)
N1	0.0457 (12)	0.0331 (12)	0.0509 (14)	0.0003 (10)	0.0234 (11)	0.0048 (10)
N2	0.0529 (13)	0.0383 (14)	0.0559 (15)	−0.0023 (11)	0.0311 (12)	0.0022 (11)
N3	0.0461 (12)	0.0306 (12)	0.0495 (14)	0.0009 (10)	0.0252 (11)	0.0011 (10)
N4	0.0484 (13)	0.0332 (12)	0.0528 (15)	0.0003 (10)	0.0260 (12)	0.0005 (11)
N5	0.0503 (13)	0.0312 (12)	0.0526 (15)	−0.0011 (10)	0.0281 (12)	0.0025 (10)
N6	0.0592 (14)	0.0358 (13)	0.0593 (16)	0.0009 (11)	0.0338 (13)	−0.0003 (11)
O1	0.0972 (16)	0.0402 (12)	0.0766 (15)	−0.0045 (11)	0.0603 (14)	0.0021 (10)
O2	0.0690 (14)	0.0707 (15)	0.0536 (13)	−0.0144 (12)	0.0119 (12)	0.0025 (11)
O3	0.1016 (16)	0.0395 (12)	0.0639 (14)	−0.0030 (11)	0.0434 (13)	0.0087 (10)
O4	0.0833 (15)	0.0649 (14)	0.0787 (16)	0.0024 (11)	0.0547 (13)	−0.0039 (12)
P1	0.0607 (5)	0.0382 (4)	0.0514 (5)	−0.0034 (4)	0.0277 (4)	0.0035 (4)
S1	0.1130 (7)	0.0354 (4)	0.0902 (7)	0.0041 (4)	0.0692 (6)	−0.0014 (4)

Geometric parameters (Å, °)

C1—C6	1.370 (4)	C15—N5	1.458 (3)
C1—C2	1.372 (4)	C15—C16	1.519 (4)
C1—Cl1	1.745 (3)	C15—P1	1.818 (3)
C2—C3	1.384 (4)	C15—H15	0.980

C2—H2	0.930	C16—C17	1.364 (4)
C3—C4	1.381 (4)	C16—C21	1.373 (4)
C3—H3	0.930	C17—C18	1.389 (4)
C4—O1	1.366 (3)	C17—H17	0.930
C4—C5	1.377 (4)	C18—C19	1.358 (5)
C5—C6	1.371 (4)	C18—H18	0.930
C5—H5	0.930	C19—C20	1.356 (5)
C6—H6	0.930	C19—H19	0.930
C7—O1	1.407 (3)	C20—C21	1.380 (4)
C7—C8	1.492 (3)	C20—H20	0.930
C7—H7A	0.970	C21—H21	0.930
C7—H7B	0.970	C22—O4	1.446 (4)
C8—N2	1.320 (3)	C22—C23	1.453 (5)
C8—N1	1.367 (3)	C22—H22A	0.970
C9—N1	1.322 (3)	C22—H22B	0.970
C9—N3	1.385 (3)	C23—H23A	0.960
C9—C10	1.411 (3)	C23—H23B	0.960
C10—C11	1.390 (3)	C23—H23C	0.960
C10—C13	1.412 (3)	C24—O3	1.444 (4)
C11—N5	1.346 (3)	C24—C25	1.456 (5)
C11—N4	1.367 (3)	C24—H24A	0.970
C12—N4	1.293 (3)	C24—H24B	0.970
C12—N3	1.369 (3)	C25—H25A	0.960
C12—H12	0.930	C25—H25B	0.960
C13—N6	1.333 (3)	C25—H25C	0.960
C13—S1	1.738 (3)	N2—N3	1.374 (3)
C14—S1	1.772 (3)	N5—N6	1.380 (3)
C14—H14A	0.960	O2—P1	1.455 (2)
C14—H14B	0.960	O3—P1	1.5619 (19)
C14—H14C	0.960	O4—P1	1.557 (2)
C6—C1—C2	120.8 (3)	C16—C17—H17	119.6
C6—C1—Cl1	119.0 (2)	C18—C17—H17	119.6
C2—C1—Cl1	120.2 (2)	C19—C18—C17	120.1 (3)
C1—C2—C3	120.0 (3)	C19—C18—H18	120.0
C1—C2—H2	120.0	C17—C18—H18	120.0
C3—C2—H2	120.0	C20—C19—C18	119.6 (3)
C4—C3—C2	119.1 (3)	C20—C19—H19	120.2
C4—C3—H3	120.5	C18—C19—H19	120.2
C2—C3—H3	120.5	C19—C20—C21	120.5 (3)
O1—C4—C5	114.8 (2)	C19—C20—H20	119.8
O1—C4—C3	124.9 (2)	C21—C20—H20	119.8
C5—C4—C3	120.3 (2)	C16—C21—C20	120.7 (3)
C6—C5—C4	120.3 (3)	C16—C21—H21	119.6
C6—C5—H5	119.9	C20—C21—H21	119.6
C4—C5—H5	119.9	O4—C22—C23	111.9 (3)
C1—C6—C5	119.5 (3)	O4—C22—H22A	109.2
C1—C6—H6	120.2	C23—C22—H22A	109.2
C5—C6—H6	120.2	O4—C22—H22B	109.2
O1—C7—C8	107.4 (2)	C23—C22—H22B	109.2

O1—C7—H7A	110.2	H22A—C22—H22B	107.9
C8—C7—H7A	110.2	C22—C23—H23A	109.5
O1—C7—H7B	110.2	C22—C23—H23B	109.5
C8—C7—H7B	110.2	H23A—C23—H23B	109.5
H7A—C7—H7B	108.5	C22—C23—H23C	109.5
N2—C8—N1	116.6 (2)	H23A—C23—H23C	109.5
N2—C8—C7	122.7 (2)	H23B—C23—H23C	109.5
N1—C8—C7	120.6 (2)	O3—C24—C25	110.6 (3)
N1—C9—N3	109.9 (2)	O3—C24—H24A	109.5
N1—C9—C10	136.2 (2)	C25—C24—H24A	109.5
N3—C9—C10	113.9 (2)	O3—C24—H24B	109.5
C11—C10—C9	116.2 (2)	C25—C24—H24B	109.5
C11—C10—C13	104.9 (2)	H24A—C24—H24B	108.1
C9—C10—C13	138.9 (2)	C24—C25—H25A	109.5
N5—C11—N4	124.6 (2)	C24—C25—H25B	109.5
N5—C11—C10	107.3 (2)	H25A—C25—H25B	109.5
N4—C11—C10	128.1 (2)	C24—C25—H25C	109.5
N4—C12—N3	122.2 (2)	H25A—C25—H25C	109.5
N4—C12—H12	118.9	H25B—C25—H25C	109.5
N3—C12—H12	118.9	C9—N1—C8	102.5 (2)
N6—C13—C10	111.2 (2)	C8—N2—N3	101.81 (19)
N6—C13—S1	124.3 (2)	C12—N3—N2	125.4 (2)
C10—C13—S1	124.5 (2)	C12—N3—C9	125.5 (2)
S1—C14—H14A	109.5	N2—N3—C9	109.12 (19)
S1—C14—H14B	109.5	C12—N4—C11	114.2 (2)
H14A—C14—H14B	109.5	C11—N5—N6	111.5 (2)
S1—C14—H14C	109.5	C11—N5—C15	126.2 (2)
H14A—C14—H14C	109.5	N6—N5—C15	121.7 (2)
H14B—C14—H14C	109.5	C13—N6—N5	105.2 (2)
N5—C15—C16	112.8 (2)	C4—O1—C7	118.6 (2)
N5—C15—P1	110.86 (17)	C24—O3—P1	123.9 (2)
C16—C15—P1	115.91 (17)	C22—O4—P1	121.9 (2)
N5—C15—H15	105.4	O2—P1—O4	115.10 (13)
C16—C15—H15	105.4	O2—P1—O3	116.57 (13)
P1—C15—H15	105.4	O4—P1—O3	103.89 (12)
C17—C16—C21	118.3 (3)	O2—P1—C15	113.24 (12)
C17—C16—C15	122.8 (3)	O4—P1—C15	108.43 (12)
C21—C16—C15	119.0 (3)	O3—P1—C15	97.89 (11)
C16—C17—C18	120.8 (3)	C13—S1—C14	102.04 (15)
C6—C1—C2—C3	0.0 (5)	N4—C12—N3—N2	179.0 (2)
Cl1—C1—C2—C3	−179.5 (2)	N4—C12—N3—C9	−0.6 (4)
C1—C2—C3—C4	−1.5 (4)	C8—N2—N3—C12	−178.5 (2)
C2—C3—C4—O1	−177.5 (3)	C8—N2—N3—C9	1.2 (3)
C2—C3—C4—C5	2.5 (4)	N1—C9—N3—C12	178.7 (2)
O1—C4—C5—C6	177.8 (3)	C10—C9—N3—C12	−0.9 (4)
C3—C4—C5—C6	−2.1 (4)	N1—C9—N3—N2	−0.9 (3)
C2—C1—C6—C5	0.4 (4)	C10—C9—N3—N2	179.5 (2)
Cl1—C1—C6—C5	179.9 (2)	N3—C12—N4—C11	1.4 (4)
C4—C5—C6—C1	0.7 (4)	N5—C11—N4—C12	177.7 (3)

O1—C7—C8—N2	−12.1 (4)	C10—C11—N4—C12	−0.7 (4)
O1—C7—C8—N1	169.8 (2)	N4—C11—N5—N6	−179.5 (2)
N1—C9—C10—C11	−178.0 (3)	C10—C11—N5—N6	−0.8 (3)
N3—C9—C10—C11	1.4 (3)	N4—C11—N5—C15	9.3 (4)
N1—C9—C10—C13	2.6 (6)	C10—C11—N5—C15	−172.0 (2)
N3—C9—C10—C13	−178.0 (3)	C16—C15—N5—C11	86.7 (3)
C9—C10—C11—N5	−179.4 (2)	P1—C15—N5—C11	−141.5 (2)
C13—C10—C11—N5	0.2 (3)	C16—C15—N5—N6	−83.7 (3)
C9—C10—C11—N4	−0.7 (4)	P1—C15—N5—N6	48.2 (3)
C13—C10—C11—N4	178.9 (2)	C10—C13—N6—N5	−0.9 (3)
C11—C10—C13—N6	0.4 (3)	S1—C13—N6—N5	178.5 (2)
C9—C10—C13—N6	179.9 (3)	C11—N5—N6—C13	1.1 (3)
C11—C10—C13—S1	−178.9 (2)	C15—N5—N6—C13	172.7 (2)
C9—C10—C13—S1	0.5 (5)	C5—C4—O1—C7	174.5 (3)
N5—C15—C16—C17	40.2 (4)	C3—C4—O1—C7	−5.6 (4)
P1—C15—C16—C17	−89.0 (3)	C8—C7—O1—C4	176.9 (2)
N5—C15—C16—C21	−138.9 (3)	C25—C24—O3—P1	−128.6 (3)
P1—C15—C16—C21	91.8 (3)	C23—C22—O4—P1	106.1 (3)
C21—C16—C17—C18	−0.1 (5)	C22—O4—P1—O2	−10.1 (3)
C15—C16—C17—C18	−179.3 (3)	C22—O4—P1—O3	−138.8 (3)
C16—C17—C18—C19	−0.4 (6)	C22—O4—P1—C15	117.8 (3)
C17—C18—C19—C20	0.4 (6)	C24—O3—P1—O2	−66.4 (3)
C18—C19—C20—C21	0.1 (6)	C24—O3—P1—O4	61.3 (3)
C17—C16—C21—C20	0.6 (5)	C24—O3—P1—C15	172.6 (3)
C15—C16—C21—C20	179.8 (3)	N5—C15—P1—O2	45.4 (2)
C19—C20—C21—C16	−0.5 (6)	C16—C15—P1—O2	175.57 (18)
N3—C9—N1—C8	0.2 (3)	N5—C15—P1—O4	−83.64 (19)
C10—C9—N1—C8	179.7 (3)	C16—C15—P1—O4	46.5 (2)
N2—C8—N1—C9	0.6 (3)	N5—C15—P1—O3	168.81 (17)
C7—C8—N1—C9	178.8 (2)	C16—C15—P1—O3	−61.0 (2)
N1—C8—N2—N3	−1.2 (3)	N6—C13—S1—C14	−2.3 (3)
C7—C8—N2—N3	−179.3 (2)	C10—C13—S1—C14	177.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22A···O2	0.97	2.49	2.948 (4)	109
C17—H17···N6	0.93	2.61	3.238 (4)	125
C15—H15···N4	0.98	2.60	2.991 (3)	104
C7—H7A···O2^{i}	0.97	2.36	3.324 (4)	171
C12—H12···N2^{ii}	0.93	2.53	3.450 (3)	169

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

Fig. 1

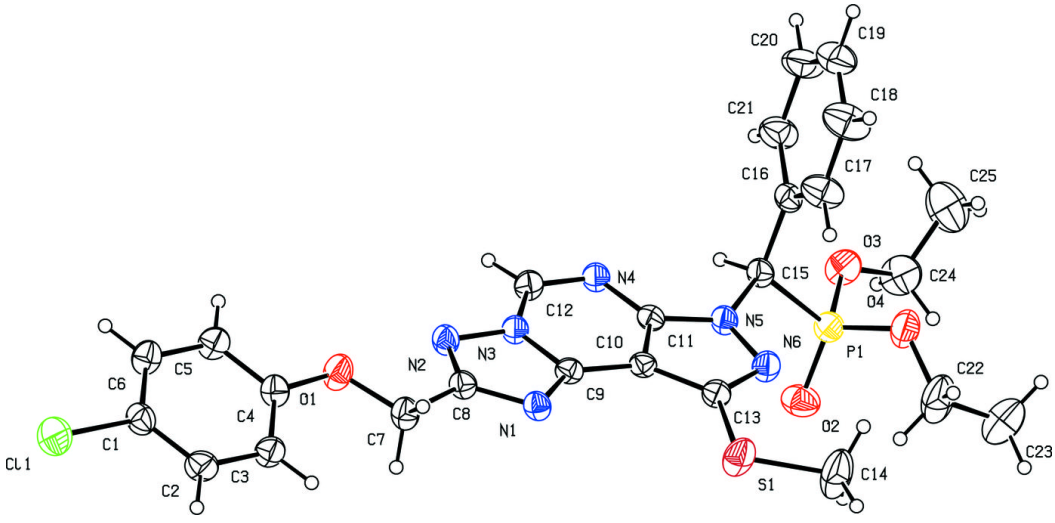
C20
C19
C18
C21
C17
C16
C25
O3
C15
C24
O4
N4
C12
N5
N6
P1
C22
N3
C10
C11
N2
C6
C5
O1
C9
C8
C4
C13
O2
C7
N1
C1
Cl1
C2
C3
S1
C14
C23

Fig. 2