Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

4,6-Dimethyl-2*H*-1,2,3-triazolo[4,5-*d*]-pyrimidine-5,7(4*H*,6*H*)-dione–4,7-phenanthroline (1/1)

Carmen R. Maldonado, Miguel Quirós* and Juan M. Salas

Departamento de Química Inorgánica, Facultad de Ciencias, Universidad de Granada, 18071 Granada, Spain
Correspondence e-mail: mquiros@ugr.es

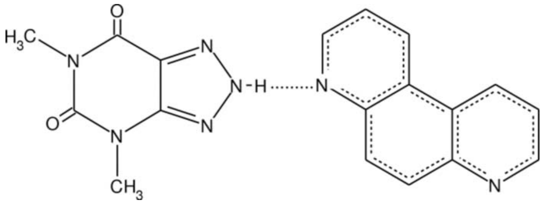
Received 17 April 2007; accepted 24 April 2007

Key indicators: single-crystal X-ray study; *T* = 298 K; mean σ(C–C) = 0.003 Å; disorder in main residue; *R* factor = 0.053; *wR* factor = 0.113; data-to-parameter ratio = 14.8.

The asymmetric unit of the title compound, $C_6H_7N_5\cdot C_{12}H_8N_2$, consists of one molecule of 4,7-phenanthroline (47phen) and one molecule of 4,6-dimethyl-2*H*-1,2,3-triazolo-[4,5-*d*]pyrimidine-5,7(4*H*,6*H*)-dione (Hdmax). The acidic proton of Hdmax (NH acid) is involved in a fairly strong hydrogen bond to one of the 47phen N atoms. Elongation of the N—H bond is in line with the strength of the N—H···N interaction which, in turn, can be related to similar acidity constants of the involved species. Both methyl groups of Hdmax are disordered.

Related literature

Crystal structures of both Hdmax (as the monohydrate; Sánchez *et al.*, 1995) and 47phen (Bond *et al.*, 2001) have been published previously. Geometrical data of both compounds do not significantly differ from those found in the present work. For related literature, see: Colacio *et al.* (1986); Nübel & Pfleiderer (1965); Shan *et al.* (2002).



Experimental

Crystal data

$C_6H_7N_5O_2\cdot C_{12}H_8N_2$
$M_r = 361.37$
Monoclinic, $P2_1/c$
$a = 7.9787$ (9) Å
$b = 11.8174$ (13) Å
$c = 17.7359$ (19) Å
$\beta = 102.674$ (2)°
$V = 1631.5$ (3) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 298$ (2) K
0.65 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEX CCD system diffractometer
Absorption correction: none
10150 measured reflections
3732 independent reflections
2224 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.058$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.113$
$S = 0.94$
3732 reflections
252 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max} = 0.14$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.20$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N4*P*	1.09 (2)	1.66 (2)	2.753 (2)	177.7 (18)

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *Xtal_GX* (Hall & du Boulay, 1997); software used to prepare material for publication: *SHELXL97*.

We acknowledge financial support from the Spanish Ministerio de Ciencia y Tecnología (project CTQ2005–00329/BQU) and from the Junta de Andalucía (research group FQM 0195). C. R. Maldonado is grateful for an FPU grant from the Spanish Ministerio de Educación y Ciencia.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2069).

References

Bond, A. D., Shan, N. & Jones, W. (2001). *Acta Cryst.* E**57**, o145–o146.
Bruker (1999). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Winsconsin, USA.
Colacio, E., Estrella, J. L., Romero, M. A., Nogueras, M. & Sánchez, A. (1986). *An. Quim.* **82B**, 240–245.
Hall, S. R. & du Boulay, D. (1997). *Xtal_GX*. University of Western Australia, Perth, Australia.
Nübel, G. & Pfleiderer, W. (1965). *Chem. Ber.* **98**, 1060–1072.
Sánchez, M. P., Romero, M. A., Salas, J. M., Cárdenas, D. J., Molina, J. & Quirós, M. (1995). *J. Mol. Struct.* **344**, 257–264.
Shan, N., Batchelor, E. & Jones, W. (2002). *Tetrahedron Lett.* **43**, 8721–8725.
Sheldrick, G. M. (1997). *SHELXL97 and SHELXS97*. University of Göttingen, Germany.

doi:10.1107/S1600536807020478

supplementary materials

Acta Cryst. (2007). E**63**, o2727 [**doi:10.1107/S1600536807020478**]

4,6-Dimethyl-2*H*-1,2,3-triazolo[4,5-*d*]pyrimidine-5,7(4*H*,6*H*)-dione-4,7-phenanthroline (1/1)

C. R. Maldonado, M. Quirós and J. M. Salas

Comment

Crystals of the title adduct, (I), were fortuitously obtained when trying to synthesize mixed ligand complexes of different metal ions with these two compounds as ligands. Nevertheless, the crystals are also formed without the presence of such metal ions (see the preparation procedure).

The asymmetric unit of (I) (Figure 1) consists of one molecule of each organic compound: 4,7-phenanthroline (47phen) and 1,3-dimethyl-8-azaxanthine (Hdmax), the systematic IUPAC name for the latter compound being 4,6-dimethyl-2*H*-1,2,3-triazolo-[4,5-*d*]pyrimidine-5,7(4*H*,6*H*)-dione (IUPAC numbering scheme is used in Figure 1 and through this comment). Both molecules are linked by a strong hydrogen bond between N2 of Hdmax and N4P of 47phen (N2···N4P distance, 2.753 (2) Å).

Since Hdmax is an acid and 47phen is a base, the possibility of a proton transfer arises. The ΔF map obtained prior to the introduction of H-atoms displayed a peak close to N2 atom of Hdmax, suggesting that such proton transfer does not occur. Nevertheless, the position of this atom has been freely refined, yielding a final position with a rather long N2—H bond (1.09 (2) Å) and a rather short H···N4P contact [1.66 (2) Å].

The pK_a value of Hdmax is 4.4 (Colacio *et al.*, 1986) and the pH value of a solution 5.10^{-3} *M* in 47phen and 5.10^{-3} *M* in 47phenH$^+$ is 3.8 (this value may be taken as a rough estimate of the pK_a value of 47phenH$^+$). The small difference between the acidity of 47phenH$^+$ and that of Hdmax justifies the strength of the H-bond and the elongation of the N2—H bond towards N4P even if pK_a values in solution are not always a good reference to predict the position of ionizable protons in the solid state. The non-ionic tautomer seems to be also a major form in the adducts of 47phen with carboxylic acids (Shan *et al.*, 2002).

Comparing the geometry of the molecules with the previously published crystal structures of the individual organic compounds (Sánchez *et al.*, 1995 and Bond *et al.*, 2001), the major differences are the bond angles involving the methyl groups of Hdmax, easily attributable to the major flexibility of *N*-methyl bonds.

Experimental

Hdmax was prepared according to a previously published procedure (Nübel & Pfleiderer, 1965) whereas 47phen was obtained from a commercial supplier. Crystals of (I) were obtained by dissolving Hdmax (1 mmol) and 47phen (1 mmol) in 10 ml of DMSO:CH_3CN 1:1, colourless crystals of the adduct appearing after 24 h. Analysis found: C 59.65, H 4.04, N 26.98%; calculated, C 59.83, H 4.18, N 27.13%.

Refinement

The H-atom attached to N2 has been freely refined. The H-atoms of methyl groups have been disordered over two positions, rotated 60° with respect to each other. Occupancy factor of each set was refined, with displacement parameters of the methyl H-atoms fixed at 1.2 U_{eq}(C). The remaining H atoms were positioned geometrically and were treated as riding, with C—H distances of 0.93-0.96 Å and with U_{iso}(H) = 1.2 Ueq(C).

Figures

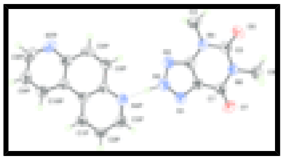


Fig. 1. View of the asymmetric unit of (I) with the displacement ellipsoids shown at the 50% probability level. Hydrogen bond is shown as dashed line.

4,6-Dimethyl-2*H*-1,2,3-triazolo[4,5-d]pyrimidine- 5,7(4*H*,6H)-dione–4,7-phenanthroline (1/1)

Crystal data

$C_6H_7N_5O_2\cdot C_{12}H_8N_2$

$M_r = 361.37$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.9787 (9)$ Å

$b = 11.8174 (13)$ Å

$c = 17.7359 (19)$ Å

$\beta = 102.674 (2)°$

$V = 1631.5 (3)$ Å^3

$Z = 4$

$F_{000} = 752$

$D_x = 1.471$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 1829 reflections

$\theta = 2.4–21.8°$

$\mu = 0.10$ mm^{-1}

$T = 298 (2)$ K

Needle, colourless

0.65 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEX CCD system diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.26 pixels mm^{-1}

$T = 298(2)$ K

φ and ω scans

Absorption correction: none

10150 measured reflections

3732 independent reflections

2224 reflections with $I > 2\sigma(I)$

$R_{int} = 0.058$

$\theta_{max} = 28.2°$

$\theta_{min} = 2.1°$

$h = -10\rightarrow 9$

$k = -13\rightarrow 15$

$l = -23\rightarrow 23$

Refinement

Refinement on F^2

H atoms treated by a mixture of

	independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.053$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.113$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
$S = 0.94$	$\Delta\rho_{min} = -0.20$ e Å^{-3}
3732 reflections	Extinction correction: none
252 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: mixed	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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)
N1	0.9144 (2)	0.58382 (13)	0.62639 (9)	0.0499 (4)	
N2	0.8425 (2)	0.55235 (14)	0.55536 (10)	0.0501 (4)	
H2	0.755 (3)	0.480 (2)	0.5435 (11)	0.083 (7)*	
N3	0.8698 (2)	0.61957 (13)	0.49760 (9)	0.0490 (4)	
C3A	0.9687 (2)	0.69985 (15)	0.53701 (11)	0.0399 (4)	
N4	1.0330 (2)	0.79284 (13)	0.50616 (9)	0.0454 (4)	
C4	0.9980 (3)	0.80945 (19)	0.42245 (10)	0.0609 (6)	
H41	1.0454	0.8805	0.4112	0.073*	0.659 (19)
H42	0.8761	0.8096	0.4021	0.073*	0.659 (19)
H43	1.0495	0.7492	0.3991	0.073*	0.659 (19)
H41'	0.9353	0.7457	0.3971	0.073*	0.341 (19)
H42'	1.1046	0.8166	0.4061	0.073*	0.341 (19)
H43'	0.9312	0.8770	0.4092	0.073*	0.341 (19)
C5	1.1297 (2)	0.87005 (16)	0.55525 (11)	0.0452 (5)	
O5	1.19269 (19)	0.95242 (11)	0.53123 (8)	0.0620 (4)	
N6	1.1525 (2)	0.84981 (12)	0.63502 (9)	0.0449 (4)	
C6	1.2482 (3)	0.93584 (16)	0.68677 (12)	0.0597 (6)	
H61	1.1732	0.9715	0.7151	0.072*	0.707 (19)
H62	1.2922	0.9916	0.6568	0.072*	0.707 (19)
H63	1.3420	0.9007	0.7222	0.072*	0.707 (19)

H61'	1.3650	0.9377	0.6810	0.072*	0.293 (19)
H62'	1.2460	0.9176	0.7393	0.072*	0.293 (19)
H63'	1.1962	1.0086	0.6739	0.072*	0.293 (19)
C7	1.0958 (3)	0.75572 (16)	0.67072 (11)	0.0454 (5)	
O7	1.13016 (19)	0.74539 (12)	0.74070 (8)	0.0633 (4)	
C7A	0.9977 (2)	0.68001 (15)	0.61502 (10)	0.0406 (5)	
C1P	0.4448 (3)	0.16703 (16)	0.51966 (10)	0.0464 (5)	
H1P	0.3864	0.0986	0.5172	0.056*	
C1AP	0.4567 (2)	0.22334 (14)	0.45115 (10)	0.0360 (4)	
C2P	0.5191 (3)	0.21252 (18)	0.58913 (11)	0.0558 (6)	
H2P	0.5099	0.1766	0.6347	0.067*	
C3P	0.6081 (3)	0.31315 (18)	0.59148 (11)	0.0565 (6)	
H3P	0.6588	0.3431	0.6396	0.068*	
N4P	0.6252 (2)	0.36872 (13)	0.52891 (9)	0.0489 (4)	
C4AP	0.5487 (2)	0.32540 (15)	0.45889 (10)	0.0382 (4)	
C5P	0.5651 (3)	0.38752 (16)	0.39178 (11)	0.0468 (5)	
H5P	0.6272	0.4548	0.3971	0.056*	
C6P	0.4909 (3)	0.34933 (17)	0.32115 (11)	0.0504 (5)	
H6P	0.5022	0.3913	0.2782	0.060*	
C6AP	0.3964 (2)	0.24636 (16)	0.31014 (10)	0.0434 (5)	
N7P	0.3279 (2)	0.21427 (16)	0.23622 (9)	0.0590 (5)	
C8P	0.2433 (3)	0.1176 (2)	0.22670 (12)	0.0647 (6)	
H8P	0.1950	0.0949	0.1764	0.078*	
C9P	0.2218 (3)	0.04696 (18)	0.28636 (12)	0.0607 (6)	
H9P	0.1629	−0.0211	0.2756	0.073*	
C10P	0.2895 (3)	0.07916 (16)	0.36057 (11)	0.0489 (5)	
H10P	0.2754	0.0336	0.4015	0.059*	
C0AP	0.3797 (2)	0.18165 (15)	0.37483 (10)	0.0385 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0540 (11)	0.0436 (10)	0.0505 (10)	−0.0005 (9)	0.0080 (9)	0.0010 (8)
N2	0.0499 (11)	0.0418 (10)	0.0566 (12)	−0.0034 (9)	0.0077 (9)	−0.0006 (8)
N3	0.0491 (11)	0.0450 (10)	0.0507 (10)	−0.0001 (8)	0.0059 (8)	−0.0009 (8)
C3A	0.0355 (11)	0.0367 (11)	0.0468 (12)	0.0025 (9)	0.0072 (9)	−0.0018 (9)
N4	0.0491 (10)	0.0452 (10)	0.0410 (9)	−0.0021 (8)	0.0081 (8)	0.0029 (7)
C4	0.0687 (16)	0.0688 (15)	0.0453 (13)	−0.0006 (12)	0.0124 (11)	0.0077 (10)
C5	0.0377 (12)	0.0437 (12)	0.0536 (13)	0.0022 (10)	0.0085 (10)	0.0020 (10)
O5	0.0671 (10)	0.0524 (9)	0.0684 (10)	−0.0153 (8)	0.0187 (8)	0.0079 (7)
N6	0.0460 (10)	0.0413 (10)	0.0441 (10)	−0.0037 (8)	0.0028 (8)	−0.0011 (7)
C6	0.0583 (14)	0.0511 (13)	0.0637 (14)	−0.0069 (11)	0.0001 (11)	−0.0083 (10)
C7	0.0463 (13)	0.0428 (12)	0.0461 (13)	0.0063 (9)	0.0082 (10)	0.0018 (9)
O7	0.0814 (12)	0.0640 (10)	0.0400 (9)	−0.0040 (8)	0.0034 (8)	0.0013 (7)
C7A	0.0420 (12)	0.0355 (11)	0.0435 (12)	0.0009 (9)	0.0075 (9)	0.0012 (8)
C1P	0.0554 (13)	0.0422 (11)	0.0450 (12)	−0.0049 (10)	0.0186 (10)	0.0033 (9)
C1AP	0.0365 (11)	0.0364 (10)	0.0372 (10)	0.0041 (9)	0.0124 (8)	0.0022 (8)
C2P	0.0749 (16)	0.0588 (14)	0.0370 (12)	0.0007 (12)	0.0195 (11)	0.0073 (10)

C3P	0.0707 (16)	0.0570 (14)	0.0393 (12)	0.0002 (12)	0.0065 (11)	−0.0068 (10)
N4P	0.0567 (11)	0.0439 (10)	0.0447 (10)	−0.0042 (8)	0.0078 (8)	−0.0038 (8)
C4AP	0.0385 (11)	0.0378 (11)	0.0390 (11)	0.0024 (9)	0.0100 (9)	0.0008 (8)
C5P	0.0534 (13)	0.0384 (11)	0.0505 (13)	−0.0041 (10)	0.0154 (10)	0.0058 (9)
C6P	0.0602 (14)	0.0517 (13)	0.0431 (12)	0.0050 (11)	0.0196 (11)	0.0151 (9)
C6AP	0.0464 (12)	0.0472 (12)	0.0378 (11)	0.0080 (10)	0.0120 (9)	0.0022 (9)
N7P	0.0694 (13)	0.0682 (13)	0.0386 (10)	0.0087 (11)	0.0099 (9)	−0.0018 (9)
C8P	0.0685 (16)	0.0736 (17)	0.0466 (14)	0.0096 (14)	0.0013 (12)	−0.0173 (12)
C9P	0.0616 (15)	0.0529 (14)	0.0627 (15)	−0.0033 (11)	0.0029 (12)	−0.0156 (11)
C10P	0.0506 (13)	0.0460 (12)	0.0503 (12)	−0.0027 (10)	0.0116 (10)	−0.0034 (9)
C0AP	0.0384 (11)	0.0384 (11)	0.0393 (11)	0.0044 (9)	0.0101 (9)	0.0002 (8)

Geometric parameters (Å, °)

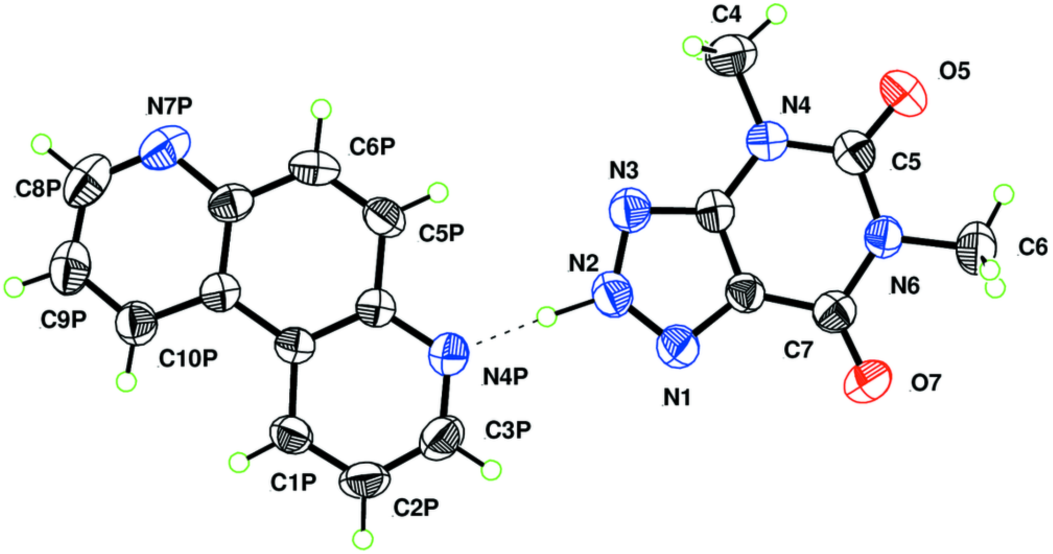
N1—N2	1.318 (2)	C7—C7A	1.432 (3)
N1—C7A	1.354 (2)	C1P—C2P	1.356 (3)
N2—N3	1.351 (2)	C1P—C1AP	1.407 (2)
N2—H2	1.09 (2)	C1P—H1P	0.9300
N3—C3A	1.330 (2)	C1AP—C4AP	1.403 (2)
C3A—C7A	1.372 (2)	C1AP—C0AP	1.445 (2)
C3A—N4	1.376 (2)	C2P—C3P	1.381 (3)
N4—C5	1.375 (2)	C2P—H2P	0.9300
N4—C4	1.462 (2)	C3P—N4P	1.322 (2)
C4—H41	0.9601	C3P—H3P	0.9300
C4—H42	0.9602	N4P—C4AP	1.358 (2)
C4—H43	0.9602	C4AP—C5P	1.429 (2)
C4—H41'	0.9602	C5P—C6P	1.341 (3)
C4—H42'	0.9601	C5P—H5P	0.9300
C4—H43'	0.9601	C6P—C6AP	1.422 (3)
C5—O5	1.215 (2)	C6P—H6P	0.9300
C5—N6	1.407 (2)	C6AP—N7P	1.359 (2)
N6—C7	1.403 (2)	C6AP—C0AP	1.409 (2)
N6—C6	1.467 (2)	N7P—C8P	1.319 (3)
C6—H61	0.9600	C8P—C9P	1.387 (3)
C6—H62	0.9600	C8P—H8P	0.9300
C6—H63	0.9600	C9P—C10P	1.363 (3)
C6—H61'	0.9600	C9P—H9P	0.9300
C6—H62'	0.9600	C10P—C0AP	1.403 (3)
C6—H63'	0.9600	C10P—H10P	0.9300
C7—O7	1.217 (2)		
N2—N1—C7A	102.68 (15)	N6—C7—C7A	111.45 (16)
N1—N2—N3	116.75 (16)	N1—C7A—C3A	108.30 (16)
N1—N2—H2	122.0 (10)	N1—C7A—C7	129.34 (17)
N3—N2—H2	121.0 (11)	C3A—C7A—C7	122.31 (17)
C3A—N3—N2	101.33 (16)	C2P—C1P—C1AP	119.91 (18)
N3—C3A—C7A	110.94 (17)	C2P—C1P—H1P	120.1
N3—C3A—N4	126.19 (17)	C1AP—C1P—H1P	120.0
C7A—C3A—N4	122.85 (17)	C4AP—C1AP—C1P	117.08 (17)
C5—N4—C3A	118.98 (16)	C4AP—C1AP—C0AP	119.39 (16)

C5—N4—C4	120.61 (17)	C1P—C1AP—C0AP	123.54 (17)
C3A—N4—C4	120.41 (16)	C1P—C2P—C3P	119.22 (18)
N4—C4—H41	109.4	C1P—C2P—H2P	120.5
N4—C4—H42	109.5	C3P—C2P—H2P	120.3
H41—C4—H42	109.5	N4P—C3P—C2P	123.34 (19)
N4—C4—H43	109.5	N4P—C3P—H3P	118.4
H41—C4—H43	109.5	C2P—C3P—H3P	118.2
H42—C4—H43	109.5	C3P—N4P—C4AP	118.15 (17)
N4—C4—H41'	109.5	N4P—C4AP—C1AP	122.28 (16)
N4—C4—H42'	109.5	N4P—C4AP—C5P	117.59 (17)
H41'—C4—H42'	109.5	C1AP—C4AP—C5P	120.12 (17)
N4—C4—H43'	109.5	C6P—C5P—C4AP	120.18 (18)
H41'—C4—H43'	109.5	C6P—C5P—H5P	119.9
H42'—C4—H43'	109.5	C4AP—C5P—H5P	119.9
O5—C5—N4	121.84 (18)	C5P—C6P—C6AP	121.91 (17)
O5—C5—N6	121.10 (18)	C5P—C6P—H6P	118.9
N4—C5—N6	117.06 (17)	C6AP—C6P—H6P	119.2
C7—N6—C5	127.24 (16)	N7P—C6AP—C0AP	122.96 (18)
C7—N6—C6	116.24 (16)	N7P—C6AP—C6P	117.40 (17)
C5—N6—C6	116.52 (16)	C0AP—C6AP—C6P	119.63 (17)
N6—C6—H61	109.5	C8P—N7P—C6AP	116.84 (18)
N6—C6—H62	109.4	N7P—C8P—C9P	124.7 (2)
H61—C6—H62	109.5	N7P—C8P—H8P	117.8
N6—C6—H63	109.5	C9P—C8P—H8P	117.6
H61—C6—H63	109.5	C10P—C9P—C8P	118.7 (2)
H62—C6—H63	109.5	C10P—C9P—H9P	121.0
N6—C6—H61'	109.5	C8P—C9P—H9P	120.4
N6—C6—H62'	109.5	C9P—C10P—C0AP	119.60 (18)
H61'—C6—H62'	109.5	C9P—C10P—H10P	120.2
N6—C6—H63'	109.5	C0AP—C10P—H10P	120.2
H61'—C6—H63'	109.5	C10P—C0AP—C6AP	117.26 (17)
H62'—C6—H63'	109.5	C10P—C0AP—C1AP	123.99 (16)
O7—C7—N6	121.13 (18)	C6AP—C0AP—C1AP	118.74 (17)
O7—C7—C7A	127.41 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N4P	1.09 (2)	1.66 (2)	2.753 (2)	177.7 (18)

Fig. 1


C4
O5
N7P
N4
C6P
C5
N3
C8P
C5P
N2
C6
N6
C9P
C10P
N4P
C7
O7
N1
C3P
C1P
C2P