Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Dibenzyl-*N*″-(2,4-difluorobenzoyl)-*N*,*N*′-dimethylphosphoric triamide

Mehrdad Pourayoubi,[a] Samad Shoghpour,[a] Laura Torre-Fernández[b] and Santiago García-Granda[b]*

[a]Department of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, Iran, and [b]Departamento de Química Física y Analítica, Facultad de Química, Universidad de Oviedo – CINN, C/ Julián Clavería, 8, 33006 Oviedo, Asturias, Spain
Correspondence e-mail: sgg@uniovi.es

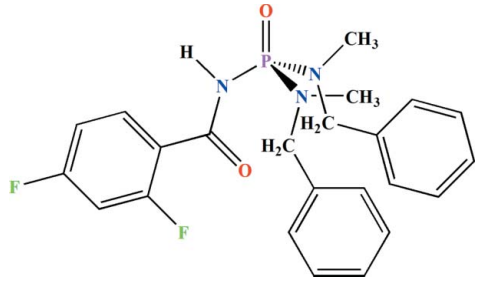
Received 25 November 2011; accepted 21 December 2011

Key indicators: single-crystal X-ray study; T = 300 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.141; data-to-parameter ratio = 15.7.

In the title molecule, $C_{23}H_{24}F_2N_3O_2P$, the P atom is in a distorted tetrahedral P(=O)(N)$(N)_2$ environment, with the bond angles around the P atom in the range 106.78 (11)–114.10 (13)°. The phosphoryl and carbonyl groups, which are separated by an N atom, adopt an *anti* orientation relative to each other. In the C(=O)NHP(=O) fragment, the P—N bond is longer [1.683 (2) Å] and the O—P—N angle is smaller [106.78 (11)°] than the other P—N bonds [1.613 (2) and 1.632 (2) Å] and O—P—N bond angles [114.10 (13) and 110.83 (12)°], respectively. The N atoms have sp^2 character. In the crystal, pairs of P=O···H—N hydrogen bonds form inversion dimers with $R_2^2(8)$ ring motifs.

Related literature

For hydrogen-bond patterns in compounds with formula RC(O)NHP(O)[NR^1R^2]$_2$ and RC(O)NHP(O)[NHR^1]$_2$ and for the discussion of different C(=O) *versus* P(=O) orientations in the C(O)NHP(O) fragment, see: Toghraee *et al.* (2011). For hydrogen-bond strengths in cyclic hydrogen-bond motifs and for bond lengths and angles, see: Pourayoubi *et al.* (2011). For graph-set analysis of hydrogen-bonds motifs, see: Bernstein *et al.* (1995). For the synthesis of the starting phosphorous–chlorine compound, see: Pourayoubi *et al.* (2010).



Experimental

Crystal data

$C_{23}H_{24}F_2N_3O_2P$
M_r = 443.42
Triclinic, $P\overline{1}$
a = 10.3619 (6) Å
b = 10.7721 (10) Å
c = 11.6433 (8) Å
α = 70.523 (7)°
β = 72.495 (5)°
γ = 70.197 (7)°
V = 1126.65 (15) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 1.44 mm^{-1}
T = 300 K
0.17 × 0.14 × 0.03 mm

Data collection

Agilent Xcalibur Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.954, T_{max} = 1.000
10022 measured reflections
4209 independent reflections
2758 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.141
S = 1.01
4209 reflections
268 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 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
N2—H2···O5^{i}	0.86	1.96	2.812 (3)	171

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *enCIFer* (Allen *et al.*, 2004).

Financial support from the Spanish Ministerio de Educacion y Ciencia (MAT2006–01997, MAT2010–15094 and the 'Factoría de Cristalización' Consolider Ingenio 2010) and FEDER funding is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FY2035).

References

Agilent (2011). *CrysAlis PRO*. Agilent Technologies UK Ltd, Yarnton, England.

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.

Pourayoubi, M., Tarahhomi, A., Rheingold, A. L. & Golen, J. A. (2010). *Acta Cryst.* E**66**, o3159.

Pourayoubi, M., Tarahhomi, A., Saneei, A., Rheingold, A. L. & Golen, J. A. (2011). *Acta Cryst.* C**67**, o265–o272.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Toghraee, M., Pourayoubi, M. & Divjakovic, V. (2011). *Polyhedron*, **30**, 1680–1690.

supporting information

Acta Cryst. (2012). E**68**, o270–o271 [doi:10.1107/S1600536811055115]

N,*N*′-Dibenzyl-*N*′′-(2,4-difluorobenzoyl)-*N*,*N*′-dimethylphosphoric triamide

Mehrdad Pourayoubi, Samad Shoghpour, Laura Torre-Fernández and Santiago García-Granda

S1. Comment

In a recently published paper, the collective behavior of hydrogen bonds (HBs) in the crystal packing of phosphoramidates having a C(═O)NHP(═O)$(N)_2$ and C(═O)NHP(═O)$(NH)_2$ skeletons were considered (Toghraee *et al.*, 2011). The authors attempted to arrive at some empirical rules which are useful for predicting hydrogen-bond patterns in systems having "two H-acceptors and one H-donor site" and "two H-acceptors and three H-donor sites". As a continuation, the hydrogen bond strengths in such systems were analyzed based on hydrogen bond motifs (Pourayoubi *et al.*, 2011).

The structure determination of the title molecule, P(O)[NHC(O)C_6H_3(2,4-F_2)][N(CH_3)($CH_2C_6H_5$)]$_2$ (Fig. 1), was performed according to our interest in the collection of structural data related to new compounds having a C(O)NHP(O) skeleton.

The phosphoryl and the carbonyl groups in the title molecule adopt an *anti* orientation relative to each other similarly to most of the carbacylamidophosphates. However, a few examples with a *gauche* orientation of these two groups were also reported (Toghraee *et al.*, 2011). The phosphorus atom has a distorted tetrahedral configuration and the P═O, C═O, P—N bond lengths and P—N—C bond angles are within the expected values. In the crystal structure, pairs of intermolecular P═ O···H—N hydrogen bonds (Table 1) form centrosymmetric dimers, see Figure 2, as $R_2^2(8)$ rings (Bernstein *et al.*, 1995).

S2. Experimental

Synthesis of 2,4-F_2–C_6H_3C(O)NHP(O)Cl_2. 2,4-F_2–C_6H_3C(O)NHP(O)Cl_2 was prepared similarly to the procedure which was used for the preparation of 2,6-F_2–C_6H_3C(O)NHP(O)Cl_2 (Pourayoubi *et al.*, 2010), but by using 2,4–F_2–C_6H_3C(O)NH_2 instead of 2,6–F_2–C_6H_3C(O)NH_2.

Synthesis of title molecule. To a solution of 2,4-F_2–C_6H_3C(O)NHP(O)Cl_2 (2 mmol) in $CHCl_3$ (20 ml), a solution of *N*-methylbenzylamine (8 mmol) in $CHCl_3$ (5 ml) was added dropwise at 273 K. After 4 h stirring, the solvent was evaporated in vacuum and then the resulting solid was washed with distilled water. Single crystals of title compound were obtained from a mixture of $CHCl_3$ and n-C_7H_{16} (5 to 1 v/v) after slow evaporation at room temperature. IR (KBr, cm^{-1}): 3064, 3043, 2872, 1683 (C═O), 1615, 1453, 1343, 1265, 1215, 1175, 1155, 1128, 1088, 1017, 959, 877, 820, 791, 738, 714.

S3. Refinement

All H atoms were placed in geometrically calculated positions with N—H = 0.86 Å and C—H = 0.93 (aromatic C—H), 0.96 (CH_3) or 0.97 Å (CH_2). H atoms were refined in riding mode with U_{iso}(H) = 1.5 U_{eq}(C) for methyl groups and U_{iso}(H) = 1.2 U_{eq}(C/N) for all other H atoms.

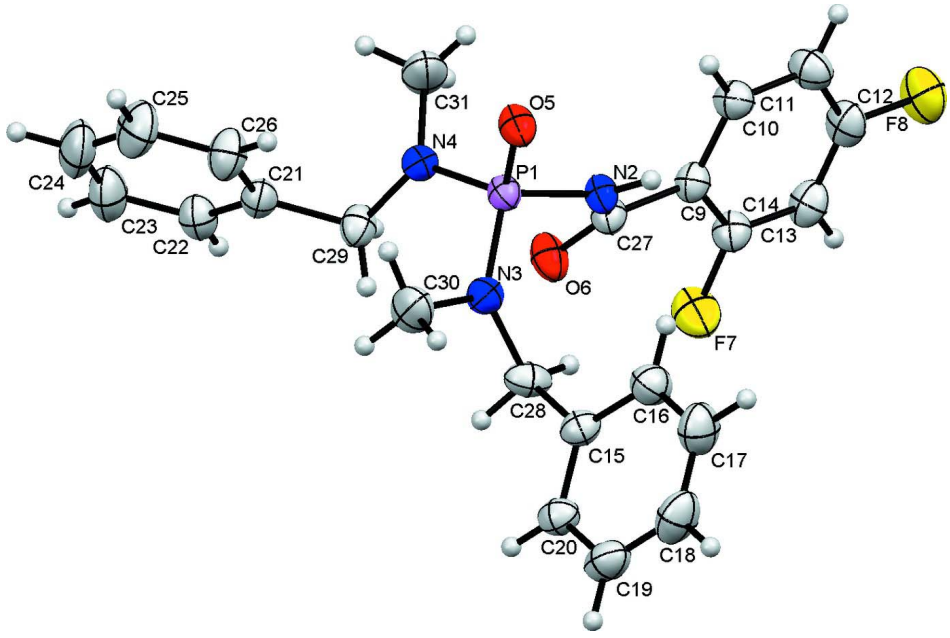


Figure 1

The molecular structure of the title compound with ellipsoids shown at the 30% probability level.

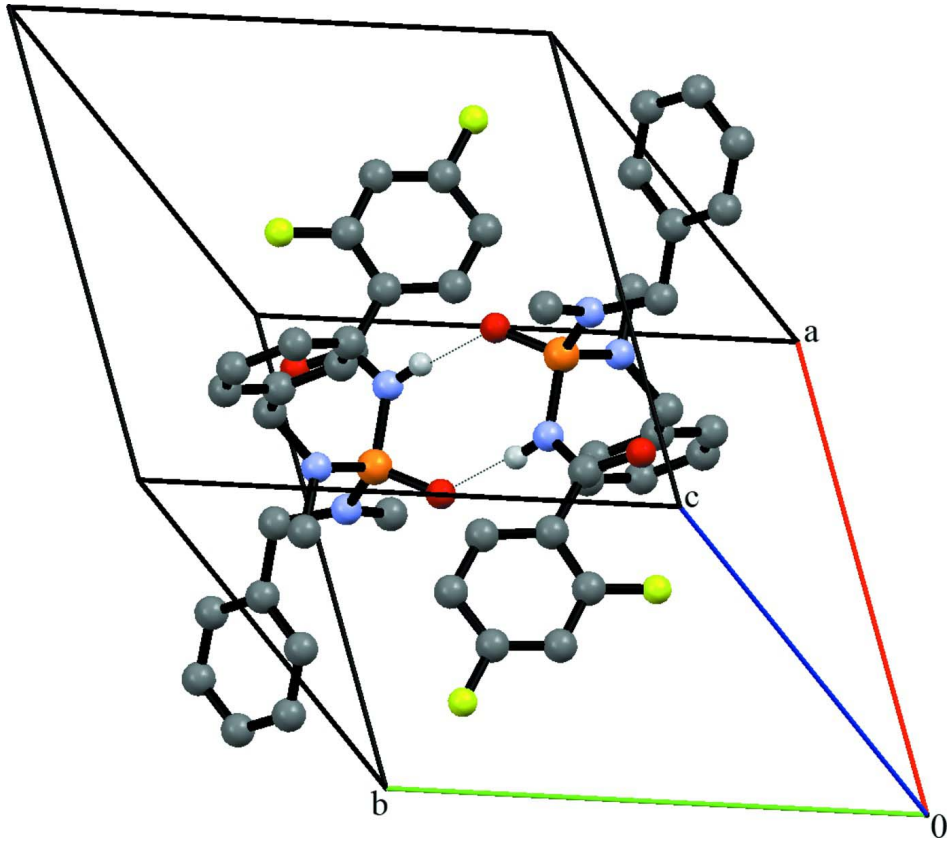


Figure 2

A view of the centrosymmetric dimer formed by H-bonding. The H atoms not involved in the hydrogen bonding interaction have been omitted for clarity.

N,N′-Dibenzyl-N′′-(2,4-difluorobenzoyl)- N,N′-dimethylphosphoric triamide

Crystal data

$C_{23}H_{24}F_2N_3O_2P$
$M_r = 443.42$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 10.3619$ (6) Å
$b = 10.7721$ (10) Å
$c = 11.6433$ (8) Å
$\alpha = 70.523$ (7)°
$\beta = 72.495$ (5)°
$\gamma = 70.197$ (7)°
$V = 1126.65$ (15) Å^3
$Z = 2$
$F(000) = 464$
$D_x = 1.307$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2755 reflections
$\theta = 4.1$–$70.6°$
$\mu = 1.44$ mm^{-1}
$T = 300$ K
Plate, colorless
0.17 × 0.14 × 0.03 mm

Data collection

Agilent Xcalibur Gemini R diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.2673 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.954$, $T_{max} = 1.000$
10022 measured reflections
4209 independent reflections
2758 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 70.7°$, $\theta_{min} = 4.1°$
$h = -8 \rightarrow 12$
$k = -12 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.141$
$S = 1.01$
4209 reflections
268 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0585P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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}
P1	0.58022 (6)	0.27216 (7)	0.57829 (7)	0.0460 (2)
N2	0.4103 (2)	0.3411 (2)	0.5698 (2)	0.0484 (5)
H2	0.3866	0.4255	0.5297	0.058*

N3	0.6579 (2)	0.1967 (3)	0.4676 (2)	0.0586 (6)
N4	0.5904 (2)	0.1570 (2)	0.7108 (2)	0.0528 (6)
O5	0.63610 (18)	0.38484 (19)	0.5704 (2)	0.0595 (5)
O6	0.3324 (2)	0.1512 (2)	0.6516 (2)	0.0684 (6)
F7	0.0748 (2)	0.2082 (2)	0.5985 (2)	0.0946 (7)
F8	−0.24562 (18)	0.6018 (2)	0.6907 (2)	0.0991 (7)
C9	0.1600 (3)	0.3630 (3)	0.6399 (3)	0.0503 (7)
C10	0.1264 (3)	0.4859 (3)	0.6711 (3)	0.0594 (7)
H10	0.1977	0.5144	0.6792	0.071*
C11	−0.0098 (3)	0.5667 (4)	0.6902 (3)	0.0681 (6)
H11	−0.0315	0.6484	0.7115	0.082*
C12	−0.1121 (3)	0.5211 (4)	0.6763 (3)	0.0681 (6)
C13	−0.0871 (3)	0.4028 (3)	0.6477 (3)	0.0604 (5)
H13	−0.1592	0.3749	0.6400	0.072*
C14	0.0492 (3)	0.3252 (3)	0.6305 (3)	0.0604 (5)
C15	0.6261 (3)	0.2312 (3)	0.2566 (3)	0.0548 (7)
C16	0.5939 (3)	0.3719 (3)	0.2161 (3)	0.0689 (9)
H16	0.5505	0.4238	0.2739	0.083*
C17	0.6249 (4)	0.4357 (4)	0.0925 (4)	0.0835 (11)
H17	0.6024	0.5305	0.0666	0.100*
C18	0.6890 (4)	0.3607 (5)	0.0060 (4)	0.0868 (12)
H18	0.7097	0.4047	−0.0783	0.104*
C19	0.7225 (3)	0.2209 (4)	0.0442 (3)	0.0767 (10)
H19	0.7663	0.1699	−0.0142	0.092*
C20	0.6910 (3)	0.1556 (3)	0.1697 (3)	0.0586 (7)
H20	0.7135	0.0607	0.1954	0.070*
C21	0.7259 (3)	−0.0736 (3)	0.8050 (3)	0.0553 (7)
C22	0.7176 (3)	−0.2009 (3)	0.8816 (3)	0.0663 (8)
H22	0.6435	−0.2339	0.8862	0.080*
C23	0.8165 (4)	−0.2796 (4)	0.9508 (4)	0.0905 (12)
H23	0.8101	−0.3658	1.0010	0.109*
C24	0.9252 (4)	−0.2314 (5)	0.9463 (4)	0.1019 (14)
H24	0.9920	−0.2843	0.9940	0.122*
C25	0.9347 (4)	−0.1054 (5)	0.8716 (4)	0.0970 (13)
H25	1.0080	−0.0723	0.8690	0.116*
C26	0.8370 (3)	−0.0268 (4)	0.8002 (4)	0.0770 (10)
H26	0.8456	0.0582	0.7484	0.092*
C27	0.3063 (3)	0.2749 (3)	0.6210 (3)	0.0512 (7)
C28	0.5913 (3)	0.1608 (3)	0.3930 (3)	0.0622 (8)
H28A	0.4903	0.1859	0.4229	0.075*
H28B	0.6220	0.0627	0.4037	0.075*
C29	0.6160 (3)	0.0108 (3)	0.7288 (3)	0.0600 (8)
H29A	0.6461	−0.0092	0.6481	0.072*
H29B	0.5289	−0.0148	0.7704	0.072*
C30	0.8121 (3)	0.1484 (4)	0.4424 (4)	0.0864 (12)
H30A	0.8473	0.1766	0.4943	0.130*
H30B	0.8494	0.1865	0.3563	0.130*
H30C	0.8401	0.0505	0.4600	0.130*

C31	0.5236 (4)	0.2029 (4)	0.8241 (3)	0.0922 (13)
H31A	0.5110	0.2996	0.8052	0.138*
H31B	0.5819	0.1564	0.8842	0.138*
H31C	0.4340	0.1831	0.8575	0.138*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0399 (3)	0.0435 (4)	0.0562 (4)	−0.0113 (3)	−0.0114 (3)	−0.0136 (3)
N2	0.0407 (10)	0.0409 (12)	0.0630 (15)	−0.0116 (9)	−0.0131 (10)	−0.0100 (10)
N3	0.0524 (12)	0.0660 (16)	0.0568 (15)	−0.0061 (11)	−0.0139 (11)	−0.0230 (12)
N4	0.0536 (12)	0.0533 (14)	0.0517 (14)	−0.0087 (10)	−0.0142 (11)	−0.0167 (11)
O5	0.0465 (9)	0.0476 (11)	0.0894 (15)	−0.0148 (8)	−0.0206 (10)	−0.0161 (10)
O6	0.0572 (11)	0.0446 (12)	0.1014 (18)	−0.0157 (9)	−0.0223 (11)	−0.0092 (11)
F7	0.0756 (12)	0.0788 (14)	0.150 (2)	−0.0270 (10)	−0.0354 (13)	−0.0388 (14)
F8	0.0412 (9)	0.1202 (18)	0.1219 (19)	−0.0012 (10)	−0.0078 (10)	−0.0427 (15)
C9	0.0430 (13)	0.0523 (16)	0.0551 (17)	−0.0172 (12)	−0.0112 (12)	−0.0079 (13)
C10	0.0503 (15)	0.0680 (19)	0.065 (2)	−0.0196 (14)	−0.0077 (13)	−0.0238 (16)
C11	0.0461 (10)	0.0789 (16)	0.0738 (16)	−0.0124 (10)	−0.0027 (10)	−0.0261 (13)
C12	0.0461 (10)	0.0789 (16)	0.0738 (16)	−0.0124 (10)	−0.0027 (10)	−0.0261 (13)
C13	0.0479 (9)	0.0677 (13)	0.0672 (14)	−0.0239 (9)	−0.0129 (9)	−0.0101 (11)
C14	0.0479 (9)	0.0677 (13)	0.0672 (14)	−0.0239 (9)	−0.0129 (9)	−0.0101 (11)
C15	0.0556 (15)	0.0624 (18)	0.0538 (18)	−0.0246 (13)	−0.0113 (13)	−0.0154 (14)
C16	0.076 (2)	0.063 (2)	0.067 (2)	−0.0164 (16)	−0.0143 (17)	−0.0183 (17)
C17	0.088 (2)	0.077 (2)	0.070 (2)	−0.018 (2)	−0.022 (2)	0.002 (2)
C18	0.081 (2)	0.110 (3)	0.056 (2)	−0.025 (2)	−0.0169 (18)	−0.002 (2)
C19	0.0647 (19)	0.109 (3)	0.062 (2)	−0.0185 (19)	−0.0110 (16)	−0.036 (2)
C20	0.0537 (15)	0.071 (2)	0.0576 (19)	−0.0199 (14)	−0.0103 (14)	−0.0230 (16)
C21	0.0517 (15)	0.0591 (17)	0.0504 (17)	−0.0104 (13)	−0.0117 (13)	−0.0117 (14)
C22	0.0624 (17)	0.0610 (19)	0.064 (2)	−0.0105 (15)	−0.0121 (15)	−0.0088 (16)
C23	0.085 (3)	0.079 (3)	0.079 (3)	−0.004 (2)	−0.024 (2)	0.003 (2)
C24	0.072 (2)	0.113 (4)	0.095 (3)	0.013 (2)	−0.038 (2)	−0.014 (3)
C25	0.0576 (19)	0.119 (4)	0.112 (3)	−0.012 (2)	−0.036 (2)	−0.022 (3)
C26	0.0608 (18)	0.082 (2)	0.084 (3)	−0.0206 (17)	−0.0262 (17)	−0.005 (2)
C27	0.0479 (14)	0.0464 (16)	0.0629 (18)	−0.0154 (12)	−0.0173 (13)	−0.0107 (13)
C28	0.0791 (19)	0.0574 (18)	0.0570 (19)	−0.0301 (15)	−0.0025 (15)	−0.0216 (15)
C29	0.0641 (17)	0.0502 (17)	0.068 (2)	−0.0211 (14)	−0.0254 (15)	−0.0026 (15)
C30	0.0557 (18)	0.109 (3)	0.083 (3)	0.0049 (18)	−0.0099 (17)	−0.042 (2)
C31	0.098 (3)	0.105 (3)	0.059 (2)	0.006 (2)	−0.019 (2)	−0.034 (2)

Geometric parameters (Å, º)

P1—O5	1.4787 (19)	C17—H17	0.9300
P1—N3	1.613 (2)	C18—C19	1.371 (5)
P1—N4	1.632 (2)	C18—H18	0.9300
P1—N2	1.683 (2)	C19—C20	1.386 (5)
N2—C27	1.370 (3)	C19—H19	0.9300
N2—H2	0.8600	C20—H20	0.9300

N3—C28	1.465 (4)	C21—C22	1.379 (4)
N3—C30	1.472 (4)	C21—C26	1.385 (4)
N4—C31	1.455 (4)	C21—C29	1.510 (4)
N4—C29	1.458 (4)	C22—C23	1.367 (5)
O6—C27	1.213 (3)	C22—H22	0.9300
F7—C14	1.351 (4)	C23—C24	1.372 (6)
F8—C12	1.357 (3)	C23—H23	0.9300
C9—C14	1.385 (4)	C24—C25	1.364 (6)
C9—C10	1.392 (4)	C24—H24	0.9300
C9—C27	1.487 (4)	C25—C26	1.375 (5)
C10—C11	1.381 (4)	C25—H25	0.9300
C10—H10	0.9300	C26—H26	0.9300
C11—C12	1.379 (5)	C28—H28A	0.9700
C11—H11	0.9300	C28—H28B	0.9700
C12—C13	1.345 (4)	C29—H29A	0.9700
C13—C14	1.370 (4)	C29—H29B	0.9700
C13—H13	0.9300	C30—H30A	0.9600
C15—C16	1.381 (4)	C30—H30B	0.9600
C15—C20	1.382 (4)	C30—H30C	0.9600
C15—C28	1.504 (4)	C31—H31A	0.9600
C16—C17	1.363 (5)	C31—H31B	0.9600
C16—H16	0.9300	C31—H31C	0.9600
C17—C18	1.373 (6)		

O5—P1—N3	114.10 (13)	C15—C20—C19	120.1 (3)
O5—P1—N4	110.83 (12)	C15—C20—H20	120.0
N3—P1—N4	108.04 (13)	C19—C20—H20	120.0
O5—P1—N2	106.78 (11)	C22—C21—C26	118.3 (3)
N3—P1—N2	108.02 (12)	C22—C21—C29	120.1 (3)
N4—P1—N2	108.93 (12)	C26—C21—C29	121.7 (3)
C27—N2—P1	125.86 (19)	C23—C22—C21	121.1 (3)
C27—N2—H2	117.1	C23—C22—H22	119.4
P1—N2—H2	117.1	C21—C22—H22	119.4
C28—N3—C30	114.7 (2)	C22—C23—C24	120.1 (4)
C28—N3—P1	127.0 (2)	C22—C23—H23	120.0
C30—N3—P1	118.1 (2)	C24—C23—H23	120.0
C31—N4—C29	114.2 (3)	C25—C24—C23	119.7 (4)
C31—N4—P1	117.2 (2)	C25—C24—H24	120.2
C29—N4—P1	125.2 (2)	C23—C24—H24	120.2
C14—C9—C10	116.4 (3)	C24—C25—C26	120.5 (4)
C14—C9—C27	121.6 (3)	C24—C25—H25	119.7
C10—C9—C27	122.0 (2)	C26—C25—H25	119.7
C11—C10—C9	121.9 (3)	C25—C26—C21	120.4 (4)
C11—C10—H10	119.1	C25—C26—H26	119.8
C9—C10—H10	119.1	C21—C26—H26	119.8
C12—C11—C10	117.2 (3)	O6—C27—N2	121.8 (2)
C12—C11—H11	121.4	O6—C27—C9	122.0 (2)
C10—C11—H11	121.4	N2—C27—C9	116.2 (2)

C13—C12—F8	118.3 (3)	N3—C28—C15	112.2 (2)
C13—C12—C11	124.0 (3)	N3—C28—H28A	109.2
F8—C12—C11	117.7 (3)	C15—C28—H28A	109.2
C12—C13—C14	117.0 (3)	N3—C28—H28B	109.2
C12—C13—H13	121.5	C15—C28—H28B	109.2
C14—C13—H13	121.5	H28A—C28—H28B	107.9
F7—C14—C13	117.0 (3)	N4—C29—C21	112.5 (2)
F7—C14—C9	119.4 (3)	N4—C29—H29A	109.1
C13—C14—C9	123.6 (3)	C21—C29—H29A	109.1
C16—C15—C20	118.9 (3)	N4—C29—H29B	109.1
C16—C15—C28	120.8 (3)	C21—C29—H29B	109.1
C20—C15—C28	120.3 (3)	H29A—C29—H29B	107.8
C17—C16—C15	120.8 (3)	N3—C30—H30A	109.5
C17—C16—H16	119.6	N3—C30—H30B	109.5
C15—C16—H16	119.6	H30A—C30—H30B	109.5
C16—C17—C18	120.4 (4)	N3—C30—H30C	109.5
C16—C17—H17	119.8	H30A—C30—H30C	109.5
C18—C17—H17	119.8	H30B—C30—H30C	109.5
C19—C18—C17	119.8 (4)	N4—C31—H31A	109.5
C19—C18—H18	120.1	N4—C31—H31B	109.5
C17—C18—H18	120.1	H31A—C31—H31B	109.5
C18—C19—C20	120.0 (3)	N4—C31—H31C	109.5
C18—C19—H19	120.0	H31A—C31—H31C	109.5
C20—C19—H19	120.0	H31B—C31—H31C	109.5

O5—P1—N2—C27	−152.1 (2)	C28—C15—C16—C17	−179.7 (3)
N3—P1—N2—C27	84.8 (3)	C15—C16—C17—C18	−0.1 (6)
N4—P1—N2—C27	−32.3 (3)	C16—C17—C18—C19	−0.2 (6)
O5—P1—N3—C28	−133.5 (2)	C17—C18—C19—C20	0.3 (6)
N4—P1—N3—C28	102.7 (3)	C16—C15—C20—C19	−0.1 (4)
N2—P1—N3—C28	−15.0 (3)	C28—C15—C20—C19	179.8 (3)
O5—P1—N3—C30	51.3 (3)	C18—C19—C20—C15	−0.2 (5)
N4—P1—N3—C30	−72.4 (3)	C26—C21—C22—C23	−0.2 (5)
N2—P1—N3—C30	169.9 (2)	C29—C21—C22—C23	179.6 (3)
O5—P1—N4—C31	55.7 (3)	C21—C22—C23—C24	1.0 (6)
N3—P1—N4—C31	−178.6 (2)	C22—C23—C24—C25	−0.7 (7)
N2—P1—N4—C31	−61.5 (3)	C23—C24—C25—C26	−0.5 (7)
O5—P1—N4—C29	−146.5 (2)	C24—C25—C26—C21	1.2 (6)
N3—P1—N4—C29	−20.8 (3)	C22—C21—C26—C25	−0.9 (5)
N2—P1—N4—C29	96.3 (2)	C29—C21—C26—C25	179.3 (3)
C14—C9—C10—C11	−0.7 (5)	P1—N2—C27—O6	−18.5 (4)
C27—C9—C10—C11	−179.1 (3)	P1—N2—C27—C9	159.9 (2)
C9—C10—C11—C12	−0.4 (5)	C14—C9—C27—O6	−34.0 (5)
C10—C11—C12—C13	1.2 (6)	C10—C9—C27—O6	144.4 (3)
C10—C11—C12—F8	−177.8 (3)	C14—C9—C27—N2	147.6 (3)
F8—C12—C13—C14	178.3 (3)	C10—C9—C27—N2	−34.1 (4)
C11—C12—C13—C14	−0.7 (5)	C30—N3—C28—C15	−66.2 (4)
C12—C13—C14—F7	−178.3 (3)	P1—N3—C28—C15	118.5 (3)

C12—C13—C14—C9	−0.6 (5)	C16—C15—C28—N3	−58.5 (4)
C10—C9—C14—F7	178.9 (3)	C20—C15—C28—N3	121.6 (3)
C27—C9—C14—F7	−2.7 (5)	C31—N4—C29—C21	−68.0 (3)
C10—C9—C14—C13	1.2 (5)	P1—N4—C29—C21	133.6 (2)
C27—C9—C14—C13	179.7 (3)	C22—C21—C29—N4	148.0 (3)
C20—C15—C16—C17	0.2 (5)	C26—C21—C29—N4	−32.2 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O5^{i}	0.86	1.96	2.812 (3)	171

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