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N,*N*′-Dibenzyl-*N*″-(2-chloro-2,2-difluoroacetyl)phosphoric triamide

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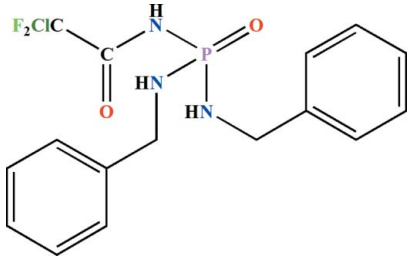
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.051; wR factor = 0.122; data-to-parameter ratio = 20.8.

In the title molecule, $C_{16}H_{17}ClF_2N_3O_2P$, the N—H unit of the C(=O)NHP(=O) fragment adopts a *syn* orientation with respect to the P=O group. The two F atoms and the Cl atom of the ClF_2C group are disordered over two sets of sites with refined occupancies of 0.605 (6) and 0.395 (6). In the crystal, molecules are linked *via* N—H···O=C hydrogen bonds and the (N—H···)(N—H···)O=P group into chains along [010].

Related literature

For related structures with a P(=O)[NHC(=O)$CClF_2$] fragment, and for reference values of P=O, C=O and P—N bond lengths and P—N—C bond angles, see: Pourayoubi *et al.* (2011); Raissi Shabari *et al.* (2011); Pourayoubi & Saneei (2011). For the double hydrogen-bond acceptor capability of the phosphoryl O atom in phosphoramidates, see: Pourayoubi *et al.* (2012). For the synthesis of the starting material, $CClF_2C$(=O)NHP(=O)Cl_2, see: Iriarte *et al.* (2008).



Experimental

Crystal data

$C_{16}H_{17}ClF_2N_3O_2P$
M_r = 387.75
Monoclinic, $P2_1$
a = 12.9734 (5) Å
b = 4.9900 (2) Å
c = 13.7750 (4) Å
β = 96.482 (3)°
V = 886.06 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 173 K
0.35 × 0.22 × 0.12 mm

Data collection

Oxford Xcalibur (Eos, Gemini) diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.890, T_{max} = 0.960
9633 measured reflections
5460 independent reflections
4909 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.122
S = 1.09
5460 reflections
263 parameters
18 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Absolute structure: Flack (1983), with 2216 Friedel pairs
Flack parameter: 0.06 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.88 (2)	2.30 (3)	3.092 (3)	151 (3)
N2—H2N···O1^{i}	0.86 (2)	2.05 (2)	2.867 (3)	158 (3)
N3—H3N···O2^{ii}	0.86 (2)	2.01 (2)	2.854 (3)	166 (3)

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5506).

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supporting information

Acta Cryst. (2012). E**68**, o3009 [https://doi.org/10.1107/S1600536812039712]

N,*N*′-Dibenzyl-*N*′′-(2-chloro-2,2-difluoroacetyl)phosphoric triamide

Mehrdad Pourayoubi, Mojtaba Keikha, Jerry P. Jasinski and Amanda C. Keeley

S1. Comment

In the previous studies, the structures of some compounds with a P(O)[NHC(O)CClF$_2$] fragment have been investigated; for example, [4-CH$_3$-C$_6$H$_4$NH]$_2$P(O)[NHC(O)CClF$_2$] (Pourayoubi, Tarahhomi *et al.*, 2011), [(C$_6$H$_5$CH$_2$)(CH$_3$)N]$_2$P(O)[NHC(O)CClF$_2$] (Raissi Shabari *et al.*, 2011) and [(CH$_3$)$_2$CHNH]$_2$P(O)[NHC(O)CClF$_2$] (Pourayoubi & Saneei, 2011). Here, the structure determination of the title compound (Fig. 1) is reported.

Atoms F1, F2 and Cl1 were refined as disordered over two sets of sites with occupancies of 0.605 (6) and 0.395 (6). The N—H unit of the C(O)NHP(O) fragment adopts a *syn* orientation with respect to the phosphoryl group. The P atom is bonded in a distorted tetrahedral environment as has been noted for other phosphoric triamides. The P═O, C═O and P—N bond lengths and P—N—C bond angles are within the expected values (Pourayoubi, Tarahhomi *et al.*, 2011; Raissi Shabari *et al.*, 2011; Pourayoubi & Saneei, 2011).

In the crystal, the O atom of P═O group acts as a double-hydrogen bond acceptor (Pourayoubi *et al.*, 2012) and molecules are linked by N—H···O═C hydrogen bonds and (N—H···)$_2$O═P group, into a linear arrangement along the *b* axis (Fig. 2).

S2. Experimental

ClF$_2$CC(O)NHP(O)Cl$_2$ was prepared according to the literature method reported by Iriarte *et al.* (2008).

To a solution of ClF$_2$CC(O)NHP(O)Cl$_2$ (0.473 g, 1.92 mmol) in dry chloroform (25 ml), a solution of benzylamine (0.823 g, 7.68 mmol) in the same solvent (5 ml) was added at 273 K. After 6 h stirring, the solvent was removed and the product was washed with distilled water and recrystallized from CH$_3$CN at room temperature.

S3. Refinement

H atoms H1N, H2N and H3N were located in a difference Fourier map and were refined with U_{iso}(H) = 1.2U_{eq}(N), giving N—H distances of 0.88 (2) or 0.86 (2) Å. The other H atoms were placed in calculated positions with 0.95 Å for CH, 0.99 Å for CH$_2$ and with U_{iso}(H) = 1.2U_{eq}(C). F atoms F1 and F2 and chlorine Cl1 are disordered over two sets of sites with occupancies of 0.605 (6) and 0.395 (6).

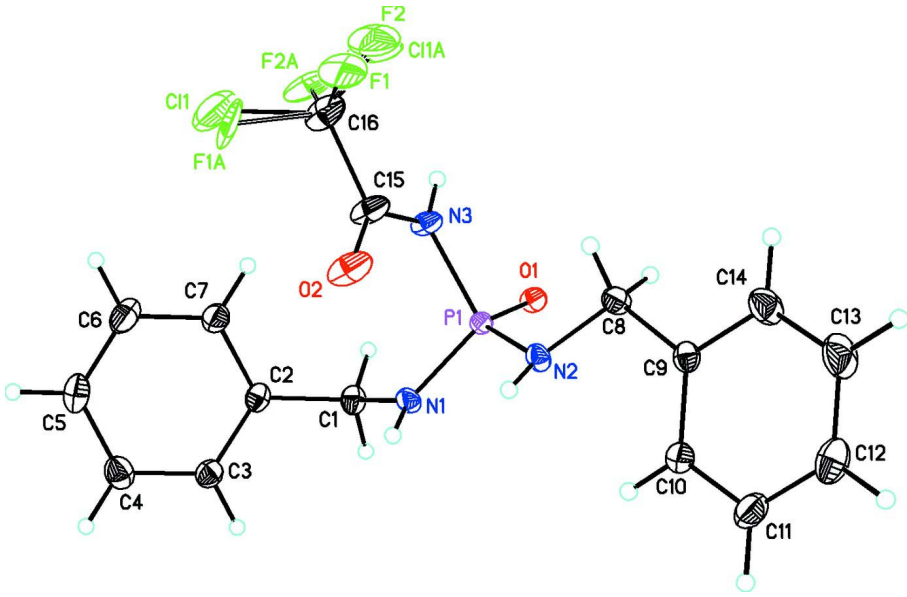

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are given at the 30% probability level and H atoms are drawn as small spheres of arbitrary radii. The atoms of the minor component of disorder are labeled with suffix ′A′.

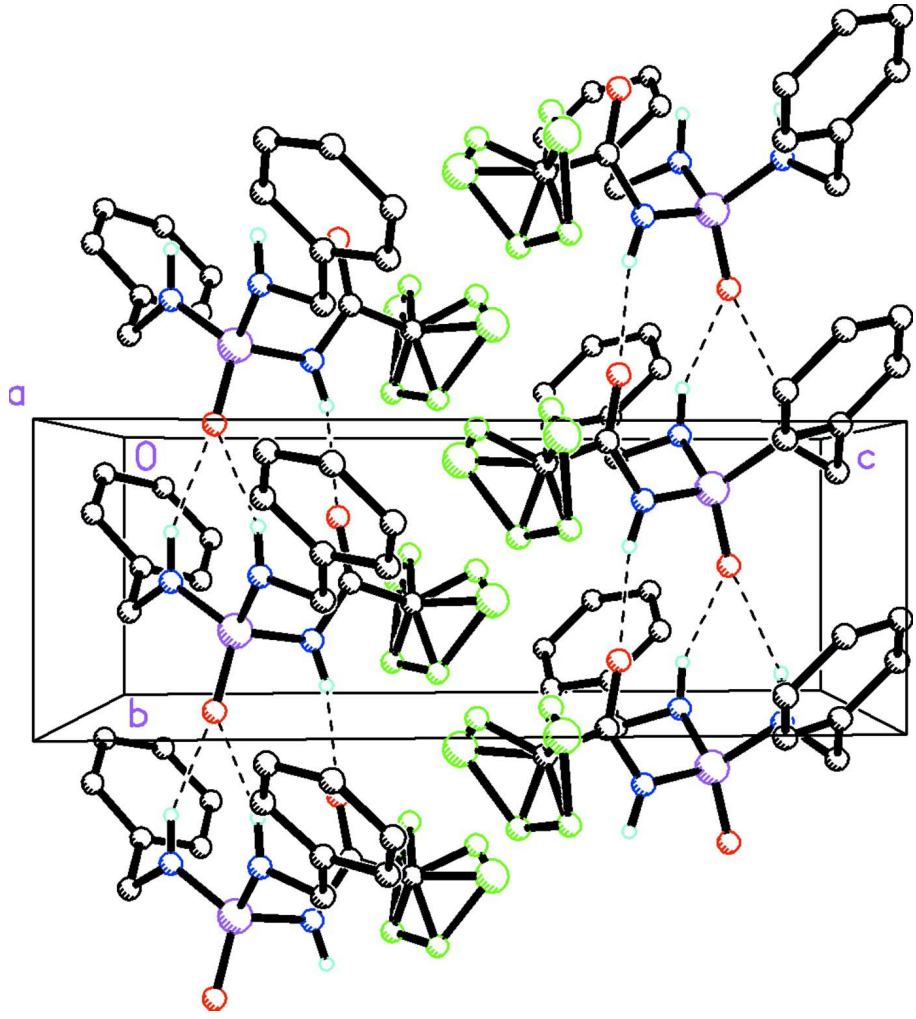

Figure 2

Crystal packing of title compound viewed approximately along the *a* axis. The N—H···O hydrogen bonds are shown by dashed lines. H atoms not involved in hydrogen bonding have been removed for clarity.

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Crystal data

$C_{16}H_{17}ClF_2N_3O_2P$
$M_r = 387.75$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 12.9734\ (5)$ Å
$b = 4.9900\ (2)$ Å
$c = 13.7750\ (4)$ Å
$\beta = 96.482\ (3)°$
$V = 886.06\ (6)$ Å^3
$Z = 2$
$F(000) = 400$
$D_x = 1.453$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3176 reflections
$\theta = 3.3–32.2°$
$\mu = 0.34$ mm^{-1}
$T = 173$ K
Block, colourless
0.35 × 0.22 × 0.12 mm

Data collection

Oxford Xcalibur (Eos, Gemini) diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1500 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.890, T_{max} = 0.960
9633 measured reflections
5460 independent reflections
4909 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 32.2°, θ_{min} = 3.3°
h = −18→19
k = −7→6
l = −9→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.122
S = 1.09
5460 reflections
263 parameters
18 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.3968P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Absolute structure: Flack (1983), with 2216 Friedel pairs
Absolute structure parameter: 0.06 (11)

Special details

Experimental. IR (KBr, v, cm^{-1}): 3253, 1718, 1457, 1419, 1282, 1215, 1139, 1073, 977, 873, 735 and 688.

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}	Occ. (<1)
P1	0.51645 (5)	0.70594 (13)	0.19236 (4)	0.01939 (13)	
Cl1	0.2161 (2)	0.5360 (8)	0.3959 (2)	0.0795 (10)	0.605 (6)
F1	0.3784 (5)	0.5030 (15)	0.4995 (4)	0.086 (2)	0.605 (6)
F2	0.3555 (5)	0.8763 (7)	0.4479 (3)	0.073 (2)	0.605 (6)
Cl1A	0.3973 (4)	0.6102 (13)	0.5203 (3)	0.0829 (18)	0.395 (6)
F1A	0.2518 (6)	0.4471 (17)	0.4089 (7)	0.066 (3)	0.395 (6)
F2A	0.2775 (5)	0.8461 (12)	0.3861 (5)	0.058 (2)	0.395 (6)
O1	0.54403 (15)	0.9827 (4)	0.16821 (14)	0.0261 (4)	
O2	0.4173 (2)	0.3092 (5)	0.3189 (2)	0.0528 (8)	
N1	0.45241 (18)	0.5364 (5)	0.10546 (18)	0.0266 (5)	
H1N	0.460 (3)	0.362 (5)	0.106 (3)	0.032*	
N2	0.61194 (18)	0.5089 (5)	0.22963 (16)	0.0241 (4)	
H2N	0.601 (3)	0.340 (5)	0.226 (2)	0.029*	

N3	0.4401 (2)	0.7487 (5)	0.28612 (18)	0.0288 (5)
H3N	0.428 (3)	0.909 (5)	0.305 (2)	0.035*
C1	0.3635 (2)	0.6492 (6)	0.0436 (2)	0.0294 (6)
H1B	0.3792	0.6516	−0.0251	0.035*
H1A	0.3527	0.8367	0.0637	0.035*
C2	0.2652 (2)	0.4925 (6)	0.04980 (19)	0.0270 (5)
C3	0.2351 (2)	0.2941 (6)	−0.0179 (2)	0.0309 (6)
H3A	0.2759	0.2598	−0.0696	0.037*
C4	0.1463 (3)	0.1456 (7)	−0.0111 (3)	0.0391 (7)
H4A	0.1267	0.0093	−0.0577	0.047*
C5	0.0860 (2)	0.1951 (9)	0.0635 (2)	0.0432 (7)
H5A	0.0247	0.0937	0.0679	0.052*
C6	0.1150 (3)	0.3920 (9)	0.1315 (3)	0.0457 (9)
H6A	0.0742	0.4238	0.1835	0.055*
C7	0.2035 (2)	0.5440 (8)	0.1241 (2)	0.0364 (7)
H7A	0.2219	0.6832	0.1698	0.044*
C8	0.6884 (2)	0.5876 (6)	0.3112 (2)	0.0286 (6)
H8A	0.6577	0.5637	0.3733	0.034*
H8B	0.7050	0.7800	0.3048	0.034*
C9	0.7871 (2)	0.4274 (6)	0.31541 (19)	0.0263 (5)
C10	0.8070 (2)	0.2410 (7)	0.2450 (2)	0.0303 (6)
H10A	0.7574	0.2120	0.1899	0.036*
C11	0.8993 (3)	0.0966 (8)	0.2550 (3)	0.0401 (7)
H11A	0.9121	−0.0311	0.2067	0.048*
C12	0.9720 (3)	0.1367 (8)	0.3341 (3)	0.0453 (9)
H12A	1.0345	0.0358	0.3409	0.054*
C13	0.9537 (3)	0.3244 (9)	0.4035 (3)	0.0505 (10)
H13A	1.0045	0.3561	0.4575	0.061*
C14	0.8624 (3)	0.4658 (8)	0.3949 (2)	0.0403 (7)
H14A	0.8502	0.5920	0.4439	0.048*
C15	0.4032 (3)	0.5428 (6)	0.3344 (3)	0.0405 (8)
C16	0.3359 (2)	0.6241 (6)	0.4143 (2)	0.0490 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0211 (3)	0.0136 (2)	0.0242 (3)	−0.0009 (3)	0.00582 (19)	−0.0014 (2)
Cl1	0.0438 (12)	0.139 (3)	0.0597 (12)	0.0070 (14)	0.0255 (10)	−0.0081 (14)
F1	0.076 (4)	0.169 (7)	0.0121 (19)	−0.017 (4)	0.0062 (19)	−0.016 (3)
F2	0.139 (5)	0.036 (2)	0.056 (3)	−0.013 (3)	0.066 (3)	−0.0126 (18)
Cl1A	0.076 (3)	0.148 (5)	0.0257 (15)	0.005 (3)	0.0091 (13)	−0.0213 (17)
F1A	0.028 (3)	0.079 (6)	0.098 (6)	−0.017 (4)	0.036 (4)	0.007 (5)
F2A	0.081 (5)	0.043 (3)	0.060 (4)	0.032 (3)	0.047 (4)	0.012 (3)
O1	0.0319 (10)	0.0160 (9)	0.0322 (9)	−0.0018 (7)	0.0107 (7)	0.0004 (7)
O2	0.0767 (19)	0.0144 (10)	0.0769 (18)	0.0017 (12)	0.0504 (16)	0.0025 (11)
N1	0.0229 (10)	0.0199 (11)	0.0361 (11)	0.0025 (9)	−0.0006 (8)	−0.0079 (9)
N2	0.0240 (10)	0.0158 (10)	0.0316 (11)	−0.0011 (8)	−0.0008 (8)	−0.0015 (9)
N3	0.0405 (13)	0.0129 (12)	0.0366 (11)	0.0009 (9)	0.0198 (10)	−0.0012 (8)

C1	0.0263 (12)	0.0335 (18)	0.0281 (12)	−0.0024 (10)	0.0009 (9)	0.0050 (10)
C2	0.0218 (12)	0.0308 (14)	0.0281 (12)	0.0024 (10)	0.0014 (9)	0.0067 (10)
C3	0.0275 (13)	0.0332 (16)	0.0321 (13)	0.0026 (11)	0.0033 (11)	0.0008 (11)
C4	0.0366 (16)	0.0320 (19)	0.0477 (17)	−0.0011 (12)	0.0000 (13)	−0.0013 (12)
C5	0.0271 (13)	0.0458 (19)	0.0568 (18)	−0.0050 (17)	0.0047 (12)	0.008 (2)
C6	0.0327 (17)	0.064 (3)	0.0427 (17)	−0.0004 (17)	0.0129 (13)	0.0049 (17)
C7	0.0287 (14)	0.049 (2)	0.0314 (13)	−0.0020 (14)	0.0042 (11)	−0.0040 (13)
C8	0.0296 (13)	0.0269 (14)	0.0284 (12)	0.0019 (11)	−0.0006 (10)	−0.0036 (10)
C9	0.0252 (12)	0.0265 (13)	0.0270 (12)	−0.0032 (10)	0.0025 (9)	0.0035 (10)
C10	0.0260 (12)	0.0340 (17)	0.0309 (12)	−0.0004 (12)	0.0030 (9)	−0.0017 (11)
C11	0.0298 (15)	0.0427 (19)	0.0494 (18)	0.0062 (14)	0.0113 (13)	−0.0021 (15)
C12	0.0297 (15)	0.052 (2)	0.0533 (19)	0.0088 (14)	0.0011 (13)	0.0121 (16)
C13	0.0378 (19)	0.062 (3)	0.0474 (19)	0.0040 (17)	−0.0156 (15)	0.0013 (18)
C14	0.0393 (17)	0.0429 (19)	0.0356 (15)	0.0020 (15)	−0.0096 (12)	−0.0027 (14)
C15	0.060 (2)	0.0165 (13)	0.0516 (18)	0.0013 (13)	0.0366 (16)	0.0015 (12)
C16	0.0641 (16)	0.0245 (15)	0.066 (2)	−0.0012 (15)	0.0394 (15)	0.0048 (15)

Geometric parameters (Å, º)

P1—O1	1.474 (2)	C3—H3A	0.9500
P1—N1	1.617 (2)	C4—C5	1.382 (5)
P1—N2	1.619 (2)	C4—H4A	0.9500
P1—N3	1.728 (2)	C5—C6	1.381 (6)
Cl1—C16	1.607 (3)	C5—H5A	0.9500
F1—C16	1.379 (5)	C6—C7	1.390 (5)
F2—C16	1.355 (4)	C6—H6A	0.9500
Cl1A—C16	1.585 (4)	C7—H7A	0.9500
F1A—C16	1.399 (5)	C8—C9	1.505 (4)
F2A—C16	1.373 (4)	C8—H8A	0.9900
O2—C15	1.203 (4)	C8—H8B	0.9900
N1—C1	1.467 (4)	C9—C10	1.388 (4)
N1—H1N	0.88 (2)	C9—C14	1.396 (4)
N2—C8	1.466 (3)	C10—C11	1.391 (4)
N2—H2N	0.86 (2)	C10—H10A	0.9500
N3—C15	1.341 (4)	C11—C12	1.373 (5)
N3—H3N	0.86 (2)	C11—H11A	0.9500
C1—C2	1.507 (4)	C12—C13	1.378 (6)
C1—H1B	0.9900	C12—H12A	0.9500
C1—H1A	0.9900	C13—C14	1.373 (5)
C2—C3	1.386 (4)	C13—H13A	0.9500
C2—C7	1.393 (4)	C14—H14A	0.9500
C3—C4	1.382 (4)	C15—C16	1.534 (4)
O1—P1—N1	116.13 (13)	C9—C8—H8B	109.0
O1—P1—N2	116.36 (12)	H8A—C8—H8B	107.8
N1—P1—N2	103.17 (12)	C10—C9—C14	118.1 (3)
O1—P1—N3	103.15 (11)	C10—C9—C8	123.6 (2)
N1—P1—N3	109.14 (13)	C14—C9—C8	118.3 (3)

N2—P1—N3	108.72 (12)	C9—C10—C11	120.2 (3)
C1—N1—P1	122.3 (2)	C9—C10—H10A	119.9
C1—N1—H1N	118 (2)	C11—C10—H10A	119.9
P1—N1—H1N	117 (2)	C12—C11—C10	120.7 (3)
C8—N2—P1	120.50 (19)	C12—C11—H11A	119.7
C8—N2—H2N	114 (2)	C10—C11—H11A	119.7
P1—N2—H2N	118 (2)	C11—C12—C13	119.5 (3)
C15—N3—P1	122.91 (19)	C11—C12—H12A	120.2
C15—N3—H3N	119 (2)	C13—C12—H12A	120.2
P1—N3—H3N	118 (2)	C14—C13—C12	120.3 (3)
N1—C1—C2	112.5 (2)	C14—C13—H13A	119.9
N1—C1—H1B	109.1	C12—C13—H13A	119.9
C2—C1—H1B	109.1	C13—C14—C9	121.2 (3)
N1—C1—H1A	109.1	C13—C14—H14A	119.4
C2—C1—H1A	109.1	C9—C14—H14A	119.4
H1B—C1—H1A	107.8	O2—C15—N3	125.7 (3)
C3—C2—C7	118.9 (3)	O2—C15—C16	119.6 (3)
C3—C2—C1	120.6 (2)	N3—C15—C16	114.6 (2)
C7—C2—C1	120.5 (3)	F2—C16—F2A	54.8 (4)
C4—C3—C2	120.8 (3)	F2—C16—F1	94.3 (4)
C4—C3—H3A	119.6	F2A—C16—F1	138.5 (4)
C2—C3—H3A	119.6	F2—C16—F1A	136.0 (5)
C5—C4—C3	120.1 (3)	F2A—C16—F1A	95.3 (5)
C5—C4—H4A	120.0	F1—C16—F1A	90.2 (5)
C3—C4—H4A	120.0	F2—C16—C15	113.0 (3)
C6—C5—C4	119.9 (3)	F2A—C16—C15	110.6 (3)
C6—C5—H5A	120.1	F1—C16—C15	106.8 (4)
C4—C5—H5A	120.1	F1A—C16—C15	107.3 (5)
C5—C6—C7	120.2 (3)	F2—C16—Cl1A	70.7 (4)
C5—C6—H6A	119.9	F2A—C16—Cl1A	120.0 (4)
C7—C6—H6A	119.9	F1A—C16—Cl1A	109.2 (5)
C6—C7—C2	120.1 (3)	C15—C16—Cl1A	112.5 (3)
C6—C7—H7A	119.9	F2—C16—Cl1	116.7 (4)
C2—C7—H7A	119.9	F2A—C16—Cl1	71.6 (4)
N2—C8—C9	112.7 (2)	F1—C16—Cl1	107.5 (4)
N2—C8—H8A	109.0	C15—C16—Cl1	115.7 (3)
C9—C8—H8A	109.0	Cl1A—C16—Cl1	120.6 (3)
N2—C8—H8B	109.0		

O1—P1—N1—C1	−45.6 (3)	C14—C9—C10—C11	0.6 (5)
N2—P1—N1—C1	−174.1 (2)	C8—C9—C10—C11	−178.7 (3)
N3—P1—N1—C1	70.4 (2)	C9—C10—C11—C12	−0.3 (5)
O1—P1—N2—C8	53.1 (2)	C10—C11—C12—C13	−0.8 (6)
N1—P1—N2—C8	−178.5 (2)	C11—C12—C13—C14	1.5 (6)
N3—P1—N2—C8	−62.8 (2)	C12—C13—C14—C9	−1.2 (6)
O1—P1—N3—C15	−175.7 (3)	C10—C9—C14—C13	0.2 (5)
N1—P1—N3—C15	60.2 (3)	C8—C9—C14—C13	179.5 (3)
N2—P1—N3—C15	−51.6 (3)	P1—N3—C15—O2	−0.6 (6)

P1—N1—C1—C2	−120.2 (2)	P1—N3—C15—C16	−179.3 (2)
N1—C1—C2—C3	−94.8 (3)	O2—C15—C16—F2	157.9 (5)
N1—C1—C2—C7	84.9 (3)	N3—C15—C16—F2	−23.3 (5)
C7—C2—C3—C4	−1.2 (4)	O2—C15—C16—F2A	−142.8 (5)
C1—C2—C3—C4	178.4 (3)	N3—C15—C16—F2A	36.0 (6)
C2—C3—C4—C5	0.4 (5)	O2—C15—C16—F1	55.6 (6)
C3—C4—C5—C6	−0.4 (5)	N3—C15—C16—F1	−125.6 (4)
C4—C5—C6—C7	1.2 (6)	O2—C15—C16—F1A	−40.0 (6)
C5—C6—C7—C2	−2.0 (6)	N3—C15—C16—F1A	138.8 (5)
C3—C2—C7—C6	2.0 (5)	O2—C15—C16—Cl1A	80.1 (5)
C1—C2—C7—C6	−177.6 (3)	N3—C15—C16—Cl1A	−101.1 (4)
P1—N2—C8—C9	−162.00 (19)	O2—C15—C16—Cl1	−64.0 (5)
N2—C8—C9—C10	5.0 (4)	N3—C15—C16—Cl1	114.8 (4)
N2—C8—C9—C14	−174.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.88 (2)	2.30 (3)	3.092 (3)	151 (3)
N2—H2*N*···O1^{i}	0.86 (2)	2.05 (2)	2.867 (3)	158 (3)
N3—H3*N*···O2^{ii}	0.86 (2)	2.01 (2)	2.854 (3)	166 (3)

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