

N,N'-Dibenzyl-*N''*-(2,6-difluorobenzoyl)-*N,N'*-dimethylphosphoric triamide

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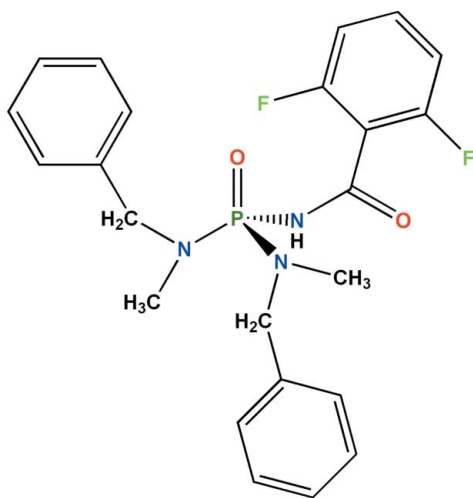
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Key indicators: single-crystal X-ray study; *T* = 200 K; mean $\sigma(\text{C}-\text{C})$ = 0.003 Å; *R* factor = 0.048; *wR* factor = 0.126; data-to-parameter ratio = 18.1.

The phosphoryl and carbonyl groups in the title compound, $\text{C}_{23}\text{H}_{24}\text{F}_2\text{N}_3\text{O}_2\text{P}$, are *anti* to each other. The P atom is in a tetrahedral coordination environment and the environment of each N atom is essentially planar, the average bond angles at the two N atoms being 119.9 and 119.1°. The H atom of the $\text{C}(=\text{O})\text{NHP}(=\text{O})$ group is involved in an intermolecular $\text{P}=\text{O} \cdots \text{H}-\text{N}-$ hydrogen bond, forming centrosymmetric dimers.

Related literature

For related structures, see: Pourayoubi & Sabbaghi (2009); Sabbaghi *et al.* (2010).



Experimental

Crystal data

$\text{C}_{23}\text{H}_{24}\text{F}_2\text{N}_3\text{O}_2\text{P}$
 $M_r = 443.42$
 Triclinic, $P\bar{1}$
 $a = 9.9370$ (11) Å
 $b = 11.1093$ (15) Å
 $c = 11.5902$ (14) Å
 $\alpha = 89.101$ (4)°
 $\beta = 67.826$ (4)°

$\gamma = 71.664$ (4)°
 $V = 1116.9$ (2) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.16$ mm⁻¹
 $T = 200$ K
 $0.30 \times 0.25 \times 0.20$ mm

Data collection

Bruker SMART X2S benchtop
 CCD area-detector
 diffractometer
 Absorption correction: multi-scan
SADABS (Bruker, 2005)
 $T_{\min} = 0.952$, $T_{\max} = 0.968$

13602 measured reflections
 5173 independent reflections
 3851 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.126$
 $S = 1.03$
 5173 reflections
 286 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.37$ e Å⁻³
 $\Delta\rho_{\min} = -0.32$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|---------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N1—H1A \cdots O2 ⁱ | 0.83 (2) | 1.92 (2) | 2.752 (2) | 173 (2) |

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

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5027).

References

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 Pourayoubi, M. & Sabbaghi, F. (2009). *J. Chem. Crystallogr.* **39**, 874–880.
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supplementary materials

Acta Cryst. (2010). E66, o2524 [doi:10.1107/S1600536810035725]

N,N'-Dibenzyl-*N'*-(2,6-difluorobenzoyl)-*N,N'*-dimethylphosphoric triamide

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Comment

Following the previous works about carbacylamidophosphates with a C(=O)NHP(=O) skeleton such as P(O)[NHC(O)C₆H₄(4-NO₂)] [N(CH(CH₃)₂)(CH₂C₆H₅)]₂ (Pourayoubi & Sabbaghi, 2009) and P(O)[NHC(O)C₆H₄(4-NO₂)] [NHC₆H₁₁]₂ (Sabbaghi *et al.*, 2010), here, we report the synthesis and crystal structure of title compound, P(O)[NHC(O)C₆H₃(2,6-F₂)] [N(CH₃)(CH₂C₆H₅)]₂. The phosphoryl and carbonyl groups are *anti* to each other and the phosphorus atom has a slightly distorted tetrahedral configuration (Fig. 1). The bond angles around the P atom are in the range of 107.11 (8)°–114.81 (8)°. The P1–N2 and P1–N3 bond lengths (1.6405 (14) Å and 1.6266 (16) Å) are shorter than the P1–N1 bond (1.6886 (15) Å). The environment of the nitrogen atoms is essentially planar; the angles C23–N3–P1, C16–N3–C23 and C16–N3–P1 are 117.53 (14)°, 116.19 (17)° and 126.13 (14)°, respectively (with average = 119.9°). A similar result was obtained for the bond angles around N2 atom (average = 119.1°). Furthermore, the angle C7–N1–P1 is 126.79 (13)°. The P=O bond length of 1.4796 (13) Å is standard for phosphoramidate compounds. The hydrogen atom of the C(=O)NHP(=O) group is involved in an intermolecular –P=O⋯H–N– hydrogen bond (see Table 1) to form a centrosymmetric dimeric aggregate.

Experimental

The reaction of phosphorus pentachloride (3.478 g, 16.7 mmol) and 2,6-difluorobenzamide (2.624 g, 16.7 mmol) in dry CCl₄ at 358 K (3 h) and then the treatment of formic acid (0.769 g, 16.7 mmol) at ice bath temperature leads to 2,6-F₂–C₆H₃C(O)NHP(O)Cl₂. To a solution of 2,6-F₂–C₆H₃C(O)NHP(O)Cl₂ (0.411 g, 1.5 mmol) in dry CHCl₃, a solution of *N*-methylbenzylamine (0.727 g, 6 mmol) in dry CHCl₃ was added dropwise at 273 K. After 4 h stirring, the solvent was evaporated in vacuum. The solid was washed with distilled water. Single crystals were obtained from a solution of the title compound in CH₃OH and *n*-C₇H₁₄ (5:1) after slow evaporation at room temperature. IR (KBr, cm⁻¹): 3446, 3042, 2867, 1690, 1607, 1465, 1369, 1210, 1150, 1019, 865, 823, 763, 725.

Refinement

APEX2 software was used for preliminary determination of the unit cell. Determination of integral intensities and unit cell refinement were performed using *SAINTE* and data were corrected for absorption using *SADABS*. Structure was solved by direct methods and all non-hydrogen atoms were refined as anisotropic by Fourier full matrix least squares. Hydrogen H1A was found from a Fourier difference map and was allowed to refine and all other hydrogen atoms were placed in calculated positions with appropriate riding factors.

Figures

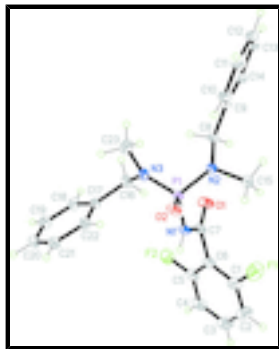


Fig. 1. An ORTEP-style plot of title compound. Ellipsoids are given at the 50% probability level.

N,N'-Dibenzyl-*N''*-(2,6-difluorobenzoyl)-*N,N'*-dimethylphosphoric triamide

Crystal data

| | |
|--------------------------------|---|
| $C_{23}H_{24}F_2N_3O_2P$ | $Z = 2$ |
| $M_r = 443.42$ | $F(000) = 464$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.318 \text{ Mg m}^{-3}$ |
| $a = 9.9370 (11) \text{ \AA}$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $b = 11.1093 (15) \text{ \AA}$ | Cell parameters from 5531 reflections |
| $c = 11.5902 (14) \text{ \AA}$ | $\theta = 2.4\text{--}27.8^\circ$ |
| $\alpha = 89.101 (4)^\circ$ | $\mu = 0.16 \text{ mm}^{-1}$ |
| $\beta = 67.826 (4)^\circ$ | $T = 200 \text{ K}$ |
| $\gamma = 71.664 (4)^\circ$ | BLOCK, colorless |
| $V = 1116.9 (2) \text{ \AA}^3$ | $0.30 \times 0.25 \times 0.20 \text{ mm}$ |

Data collection

| | |
|--|--|
| Bruker SMART X2S benchtop CCD area-detector diffractometer | 5173 independent reflections |
| Radiation source: fine-focus sealed tube | 3851 reflections with $I > 2\sigma(I)$ |
| curved silicon crystal | $R_{\text{int}} = 0.036$ |
| phi and ω scans | $\theta_{\text{max}} = 27.8^\circ$, $\theta_{\text{min}} = 2.4^\circ$ |
| Absorption correction: multi-scan SADABS (Bruker, 2005) | $h = -13 \rightarrow 13$ |
| $T_{\text{min}} = 0.952$, $T_{\text{max}} = 0.968$ | $k = -14 \rightarrow 14$ |
| 13602 measured reflections | $l = -15 \rightarrow 15$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.048$ | Hydrogen site location: inferred from neighbouring sites |

$wR(F^2) = 0.126$

$S = 1.03$

5173 reflections

286 parameters

0 restraints

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.2218P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.37 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.32 \text{ e } \text{Å}^{-3}$$

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)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|--------------|----------------------------------|
| P1 | 0.66485 (5) | 0.42270 (4) | 0.29906 (4) | 0.02461 (13) |
| F1 | 0.41237 (17) | 0.18210 (16) | 0.50507 (15) | 0.0723 (5) |
| F2 | 0.16095 (14) | 0.43844 (12) | 0.27352 (13) | 0.0532 (4) |
| O1 | 0.50833 (16) | 0.27969 (15) | 0.19272 (13) | 0.0445 (4) |
| O2 | 0.68882 (13) | 0.46617 (12) | 0.40757 (12) | 0.0323 (3) |
| N1 | 0.48905 (16) | 0.40601 (15) | 0.35526 (15) | 0.0277 (3) |
| N2 | 0.79630 (15) | 0.28474 (13) | 0.22927 (13) | 0.0246 (3) |
| N3 | 0.66719 (17) | 0.52094 (15) | 0.19333 (15) | 0.0358 (4) |
| C1 | 0.2810 (2) | 0.2390 (2) | 0.4858 (2) | 0.0449 (5) |
| C2 | 0.1464 (3) | 0.2189 (3) | 0.5632 (2) | 0.0583 (7) |
| H2A | 0.1443 | 0.1678 | 0.6299 | 0.070* |
| C3 | 0.0152 (3) | 0.2755 (3) | 0.5402 (2) | 0.0573 (7) |
| H3A | -0.0785 | 0.2634 | 0.5924 | 0.069* |
| C4 | 0.0174 (2) | 0.3490 (2) | 0.4434 (2) | 0.0485 (6) |
| H4A | -0.0733 | 0.3880 | 0.4282 | 0.058* |
| C5 | 0.1560 (2) | 0.3646 (2) | 0.36861 (19) | 0.0370 (5) |
| C6 | 0.2916 (2) | 0.31110 (18) | 0.38644 (17) | 0.0315 (4) |
| C7 | 0.4403 (2) | 0.32953 (18) | 0.30107 (17) | 0.0309 (4) |
| C8 | 0.86123 (19) | 0.24379 (17) | 0.09447 (16) | 0.0280 (4) |
| H8A | 0.8268 | 0.3173 | 0.0509 | 0.034* |
| H8B | 0.8212 | 0.1771 | 0.0792 | 0.034* |
| C9 | 1.03733 (19) | 0.19106 (16) | 0.03916 (16) | 0.0250 (4) |
| C10 | 1.1236 (2) | 0.22336 (17) | 0.09620 (17) | 0.0296 (4) |
| H10A | 1.0727 | 0.2797 | 0.1720 | 0.035* |
| C11 | 1.2842 (2) | 0.17395 (19) | 0.04339 (18) | 0.0341 (4) |

supplementary materials

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|------|------------|--------------|---------------|------------|
| H11A | 1.3419 | 0.1964 | 0.0836 | 0.041* |
| C12 | 1.3599 (2) | 0.09219 (18) | -0.06744 (19) | 0.0358 (5) |
| H12A | 1.4693 | 0.0584 | -0.1033 | 0.043* |
| C13 | 1.2756 (2) | 0.06030 (19) | -0.12524 (19) | 0.0393 (5) |
| H13A | 1.3270 | 0.0049 | -0.2017 | 0.047* |
| C14 | 1.1147 (2) | 0.10908 (18) | -0.07202 (18) | 0.0336 (4) |
| H14A | 1.0575 | 0.0859 | -0.1123 | 0.040* |
| C15 | 0.8149 (2) | 0.18153 (18) | 0.30902 (18) | 0.0351 (4) |
| H15A | 0.9229 | 0.1261 | 0.2767 | 0.053* |
| H15B | 0.7497 | 0.1313 | 0.3084 | 0.053* |
| H15C | 0.7842 | 0.2184 | 0.3951 | 0.053* |
| C16 | 0.5493 (2) | 0.56887 (19) | 0.14191 (18) | 0.0382 (5) |
| H16A | 0.4917 | 0.5083 | 0.1535 | 0.046* |
| H16B | 0.6010 | 0.5705 | 0.0506 | 0.046* |
| C17 | 0.4345 (2) | 0.70157 (17) | 0.20021 (17) | 0.0290 (4) |
| C18 | 0.3442 (2) | 0.76890 (19) | 0.13718 (19) | 0.0360 (5) |
| H18A | 0.3538 | 0.7308 | 0.0604 | 0.043* |
| C19 | 0.2409 (2) | 0.8908 (2) | 0.1858 (2) | 0.0402 (5) |
| H19A | 0.1796 | 0.9355 | 0.1426 | 0.048* |
| C20 | 0.2266 (2) | 0.9478 (2) | 0.2971 (2) | 0.0414 (5) |
| H20A | 0.1568 | 1.0319 | 0.3297 | 0.050* |
| C21 | 0.3144 (2) | 0.88166 (19) | 0.36020 (18) | 0.0399 (5) |
| H21A | 0.3047 | 0.9202 | 0.4368 | 0.048* |
| C22 | 0.4176 (2) | 0.75831 (18) | 0.31215 (18) | 0.0344 (4) |
| H22A | 0.4767 | 0.7130 | 0.3569 | 0.041* |
| C23 | 0.7939 (3) | 0.5743 (2) | 0.1510 (3) | 0.0603 (7) |
| H23A | 0.8498 | 0.5537 | 0.0599 | 0.091* |
| H23B | 0.8646 | 0.5376 | 0.1925 | 0.091* |
| H23C | 0.7516 | 0.6673 | 0.1724 | 0.091* |
| H1A | 0.429 (2) | 0.442 (2) | 0.427 (2) | 0.038 (6)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-------------|-------------|-------------|---------------|---------------|---------------|
| P1 | 0.0173 (2) | 0.0247 (2) | 0.0261 (2) | -0.00350 (17) | -0.00496 (17) | -0.00334 (17) |
| F1 | 0.0611 (9) | 0.0976 (12) | 0.0788 (11) | -0.0319 (9) | -0.0460 (8) | 0.0389 (9) |
| F2 | 0.0449 (7) | 0.0539 (8) | 0.0632 (9) | -0.0087 (6) | -0.0301 (7) | 0.0035 (7) |
| O1 | 0.0354 (8) | 0.0614 (10) | 0.0329 (8) | -0.0183 (7) | -0.0068 (6) | -0.0151 (7) |
| O2 | 0.0208 (6) | 0.0398 (7) | 0.0315 (7) | -0.0084 (5) | -0.0061 (5) | -0.0112 (6) |
| N1 | 0.0182 (7) | 0.0342 (8) | 0.0262 (8) | -0.0076 (6) | -0.0044 (6) | -0.0074 (7) |
| N2 | 0.0206 (7) | 0.0242 (7) | 0.0231 (7) | -0.0022 (6) | -0.0064 (6) | 0.0009 (6) |
| N3 | 0.0259 (8) | 0.0294 (8) | 0.0446 (10) | -0.0035 (7) | -0.0107 (7) | 0.0096 (7) |
| C1 | 0.0398 (12) | 0.0603 (14) | 0.0426 (12) | -0.0222 (11) | -0.0200 (10) | 0.0059 (11) |
| C2 | 0.0607 (16) | 0.0738 (18) | 0.0467 (14) | -0.0402 (14) | -0.0133 (12) | 0.0104 (13) |
| C3 | 0.0415 (13) | 0.0695 (17) | 0.0565 (15) | -0.0329 (13) | -0.0022 (11) | -0.0100 (13) |
| C4 | 0.0249 (10) | 0.0540 (14) | 0.0626 (15) | -0.0107 (10) | -0.0140 (10) | -0.0199 (12) |
| C5 | 0.0305 (10) | 0.0391 (11) | 0.0407 (11) | -0.0086 (8) | -0.0152 (9) | -0.0073 (9) |
| C6 | 0.0242 (9) | 0.0382 (10) | 0.0320 (10) | -0.0110 (8) | -0.0100 (8) | -0.0080 (8) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|-------------|
| C7 | 0.0229 (9) | 0.0361 (10) | 0.0314 (10) | -0.0061 (8) | -0.0110 (8) | -0.0053 (8) |
| C8 | 0.0242 (9) | 0.0297 (9) | 0.0241 (9) | -0.0045 (7) | -0.0065 (7) | -0.0026 (7) |
| C9 | 0.0220 (8) | 0.0247 (9) | 0.0249 (9) | -0.0068 (7) | -0.0062 (7) | 0.0030 (7) |
| C10 | 0.0291 (9) | 0.0305 (9) | 0.0268 (9) | -0.0079 (8) | -0.0100 (8) | 0.0001 (7) |
| C11 | 0.0277 (10) | 0.0394 (11) | 0.0377 (11) | -0.0139 (8) | -0.0135 (8) | 0.0078 (9) |
| C12 | 0.0202 (9) | 0.0349 (10) | 0.0431 (11) | -0.0073 (8) | -0.0042 (8) | 0.0062 (9) |
| C13 | 0.0289 (10) | 0.0364 (11) | 0.0366 (11) | -0.0061 (8) | 0.0008 (8) | -0.0093 (9) |
| C14 | 0.0275 (9) | 0.0347 (10) | 0.0341 (10) | -0.0113 (8) | -0.0063 (8) | -0.0046 (8) |
| C15 | 0.0328 (10) | 0.0314 (10) | 0.0344 (10) | -0.0050 (8) | -0.0106 (8) | 0.0058 (8) |
| C16 | 0.0437 (11) | 0.0322 (10) | 0.0317 (10) | -0.0024 (9) | -0.0158 (9) | 0.0019 (8) |
| C17 | 0.0267 (9) | 0.0288 (9) | 0.0299 (9) | -0.0078 (7) | -0.0107 (8) | 0.0061 (8) |
| C18 | 0.0359 (10) | 0.0403 (11) | 0.0377 (11) | -0.0136 (9) | -0.0202 (9) | 0.0070 (9) |
| C19 | 0.0299 (10) | 0.0413 (12) | 0.0511 (13) | -0.0066 (9) | -0.0222 (9) | 0.0147 (10) |
| C20 | 0.0324 (10) | 0.0326 (11) | 0.0463 (12) | -0.0009 (8) | -0.0100 (9) | 0.0057 (9) |
| C21 | 0.0426 (12) | 0.0362 (11) | 0.0322 (11) | -0.0068 (9) | -0.0103 (9) | 0.0014 (9) |
| C22 | 0.0364 (10) | 0.0304 (10) | 0.0323 (10) | -0.0030 (8) | -0.0158 (8) | 0.0060 (8) |
| C23 | 0.0362 (12) | 0.0495 (14) | 0.0853 (19) | -0.0157 (11) | -0.0129 (12) | 0.0317 (13) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------|-----------|
| P1—O2 | 1.4796 (13) | C10—H10A | 0.9500 |
| P1—N3 | 1.6266 (16) | C11—C12 | 1.385 (3) |
| P1—N2 | 1.6405 (14) | C11—H11A | 0.9500 |
| P1—N1 | 1.6886 (15) | C12—C13 | 1.377 (3) |
| F1—C1 | 1.360 (2) | C12—H12A | 0.9500 |
| F2—C5 | 1.359 (2) | C13—C14 | 1.397 (3) |
| O1—C7 | 1.219 (2) | C13—H13A | 0.9500 |
| N1—C7 | 1.362 (2) | C14—H14A | 0.9500 |
| N1—H1A | 0.83 (2) | C15—H15A | 0.9800 |
| N2—C8 | 1.463 (2) | C15—H15B | 0.9800 |
| N2—C15 | 1.471 (2) | C15—H15C | 0.9800 |
| N3—C16 | 1.462 (2) | C16—C17 | 1.524 (3) |
| N3—C23 | 1.474 (3) | C16—H16A | 0.9900 |
| C1—C6 | 1.383 (3) | C16—H16B | 0.9900 |
| C1—C2 | 1.386 (3) | C17—C22 | 1.380 (3) |
| C2—C3 | 1.380 (4) | C17—C18 | 1.397 (3) |
| C2—H2A | 0.9500 | C18—C19 | 1.385 (3) |
| C3—C4 | 1.375 (3) | C18—H18A | 0.9500 |
| C3—H3A | 0.9500 | C19—C20 | 1.384 (3) |
| C4—C5 | 1.386 (3) | C19—H19A | 0.9500 |
| C4—H4A | 0.9500 | C20—C21 | 1.378 (3) |
| C5—C6 | 1.383 (3) | C20—H20A | 0.9500 |
| C6—C7 | 1.512 (3) | C21—C22 | 1.396 (3) |
| C8—C9 | 1.529 (2) | C21—H21A | 0.9500 |
| C8—H8A | 0.9900 | C22—H22A | 0.9500 |
| C8—H8B | 0.9900 | C23—H23A | 0.9800 |
| C9—C14 | 1.389 (2) | C23—H23B | 0.9800 |
| C9—C10 | 1.389 (2) | C23—H23C | 0.9800 |
| C10—C11 | 1.395 (2) | | |

supplementary materials

| | | | |
|--------------|-------------|---------------|-------------|
| O2—P1—N3 | 114.81 (8) | C12—C11—C10 | 120.19 (18) |
| O2—P1—N2 | 110.54 (7) | C12—C11—H11A | 119.9 |
| N3—P1—N2 | 107.66 (8) | C10—C11—H11A | 119.9 |
| O2—P1—N1 | 107.11 (8) | C13—C12—C11 | 119.55 (17) |
| N3—P1—N1 | 107.24 (8) | C13—C12—H12A | 120.2 |
| N2—P1—N1 | 109.34 (8) | C11—C12—H12A | 120.2 |
| C7—N1—P1 | 126.79 (13) | C12—C13—C14 | 120.31 (18) |
| C7—N1—H1A | 116.4 (14) | C12—C13—H13A | 119.8 |
| P1—N1—H1A | 116.5 (14) | C14—C13—H13A | 119.8 |
| C8—N2—C15 | 115.44 (14) | C9—C14—C13 | 120.73 (18) |
| C8—N2—P1 | 125.15 (12) | C9—C14—H14A | 119.6 |
| C15—N2—P1 | 116.63 (11) | C13—C14—H14A | 119.6 |
| C16—N3—C23 | 116.19 (17) | N2—C15—H15A | 109.5 |
| C16—N3—P1 | 126.13 (14) | N2—C15—H15B | 109.5 |
| C23—N3—P1 | 117.53 (14) | H15A—C15—H15B | 109.5 |
| F1—C1—C6 | 117.31 (18) | N2—C15—H15C | 109.5 |
| F1—C1—C2 | 119.0 (2) | H15A—C15—H15C | 109.5 |
| C6—C1—C2 | 123.7 (2) | H15B—C15—H15C | 109.5 |
| C3—C2—C1 | 117.9 (2) | N3—C16—C17 | 114.79 (16) |
| C3—C2—H2A | 121.1 | N3—C16—H16A | 108.6 |
| C1—C2—H2A | 121.1 | C17—C16—H16A | 108.6 |
| C4—C3—C2 | 121.4 (2) | N3—C16—H16B | 108.6 |
| C4—C3—H3A | 119.3 | C17—C16—H16B | 108.6 |
| C2—C3—H3A | 119.3 | H16A—C16—H16B | 107.5 |
| C3—C4—C5 | 118.0 (2) | C22—C17—C18 | 118.77 (17) |
| C3—C4—H4A | 121.0 | C22—C17—C16 | 122.46 (16) |
| C5—C4—H4A | 121.0 | C18—C17—C16 | 118.76 (17) |
| F2—C5—C6 | 117.05 (18) | C19—C18—C17 | 120.47 (19) |
| F2—C5—C4 | 119.21 (19) | C19—C18—H18A | 119.8 |
| C6—C5—C4 | 123.7 (2) | C17—C18—H18A | 119.8 |
| C5—C6—C1 | 115.30 (18) | C20—C19—C18 | 120.37 (18) |
| C5—C6—C7 | 121.65 (18) | C20—C19—H19A | 119.8 |
| C1—C6—C7 | 123.04 (17) | C18—C19—H19A | 119.8 |
| O1—C7—N1 | 123.93 (17) | C21—C20—C19 | 119.48 (19) |
| O1—C7—C6 | 121.61 (16) | C21—C20—H20A | 120.3 |
| N1—C7—C6 | 114.46 (15) | C19—C20—H20A | 120.3 |
| N2—C8—C9 | 112.58 (14) | C20—C21—C22 | 120.33 (19) |
| N2—C8—H8A | 109.1 | C20—C21—H21A | 119.8 |
| C9—C8—H8A | 109.1 | C22—C21—H21A | 119.8 |
| N2—C8—H8B | 109.1 | C17—C22—C21 | 120.56 (18) |
| C9—C8—H8B | 109.1 | C17—C22—H22A | 119.7 |
| H8A—C8—H8B | 107.8 | C21—C22—H22A | 119.7 |
| C14—C9—C10 | 118.49 (16) | N3—C23—H23A | 109.5 |
| C14—C9—C8 | 119.50 (15) | N3—C23—H23B | 109.5 |
| C10—C9—C8 | 122.01 (15) | H23A—C23—H23B | 109.5 |
| C9—C10—C11 | 120.73 (17) | N3—C23—H23C | 109.5 |
| C9—C10—H10A | 119.6 | H23A—C23—H23C | 109.5 |
| C11—C10—H10A | 119.6 | H23B—C23—H23C | 109.5 |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|--------------------------|-------------|---------------|-----------------------|-------------------------|
| N1—H1A···O2 ⁱ | 0.83 (2) | 1.92 (2) | 2.752 (2) | 173 (2) |

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

Fig. 1

