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# Diethyl (1-benzyl-4-phenyl-3-trifluoromethyl-1*H*-pyrrol-2-yl)phosphonate

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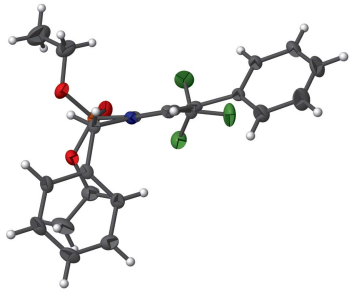
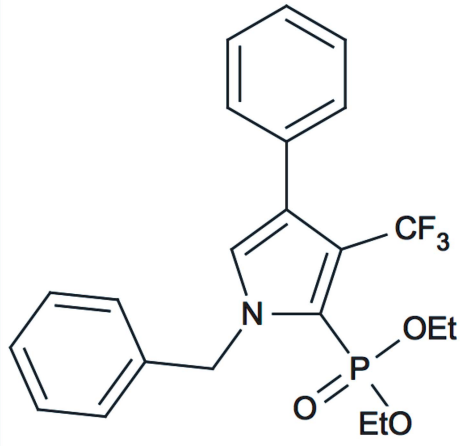
In the title compound, $C_{22}H_{23}F_3NO_3P$, the dihedral angles between the pyrrole ring and the benzyl and phenyl rings are 81.38 (7) and 46.21 (8)°, respectively. The ethyl phosphate groups present with P—O—C—C torsion angles of −178.47 (10) and 106.72 (16)°, and an intramolecular C—H···O hydrogen bond occurs. In the extended structure, molecules are linked by C—H···O and C—H···F hydrogen bonds to generate [001] chains.

**3D view**



**Chemical scheme**




## Structure description

Heterocycles bearing a trifluoromethyl group have attracted much attention in pharmaceutical sciences as the introduction of fluorine atoms into an organic compound can cause enhancement and modification of their original physical, chemical and biological properties (*e.g.*: Gouverneur & Muller, 2012; Zeng *et al.*, 2014). It has been also shown that the presence of a phosphonyl group can influence the biological functions of heterocyclic systems (*e.g.*: Dang *et al.*, 2009; Olszewski & Boduszek, 2010). As part of our studies in this area, we now report the crystal structure of the title compound (Fig. 1).

The dihedral angles between the pyrrole ring and the benzyl (N-bonded) and phenyl (C-bonded) rings are 81.38 (7) and 46.21 (8)°, respectively. The dihedral angle between the benzyl and phenyl aromatic rings amounts to 50.83 (5)°. The ethyl phosphate groups have different conformations: P1—O3—C1—C2 = −178.47 (10) and P1—O2—C3—C4 = 106.72 (16)°. The molecular structure is stabilized by one intramolecular weak hydrogen bond, *i.e.*: C16—H16*A*···O1 (Table 1), which generates an *S*(6) ring.

In the extended structure, the molecules are linked by C—H···O and C—H···F hydrogen bonds to generate [001] chains (Fig. 2) in which O1 acts as a double acceptor.

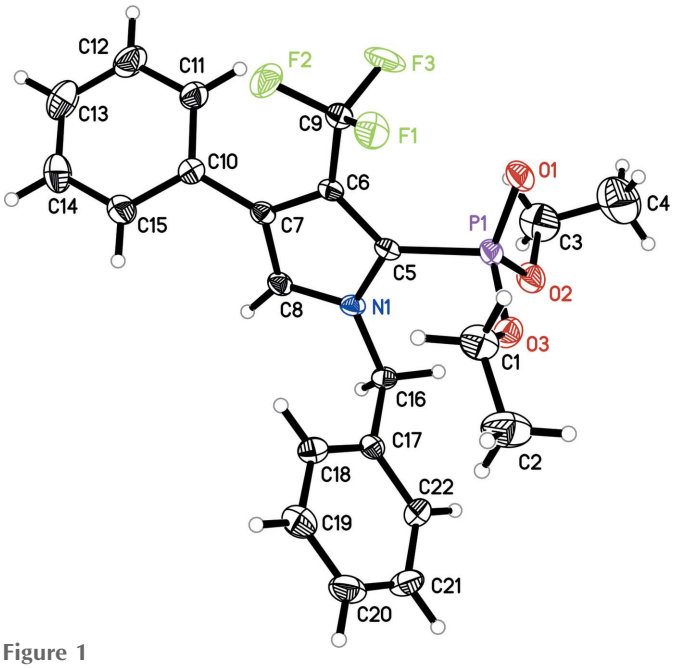



**Figure 1**
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

## Synthesis and crystallization

The title compound was synthesized according to a procedure published previously (Cal & Zagórski, 2011). Irregular colourless chunks of were recrystallized from a petroleum ether/$Et_2O$ 1:4 solution.

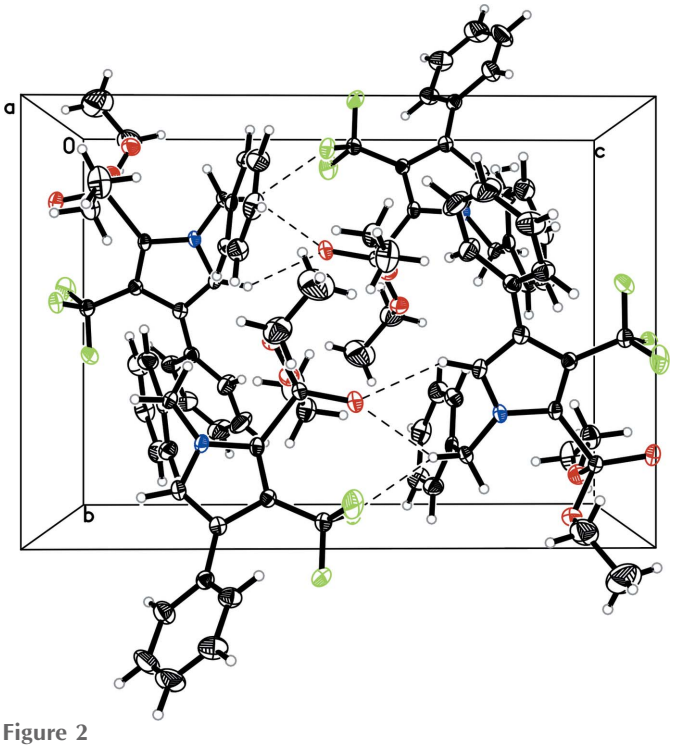



**Figure 2**
The crystal packing of the title compound, viewed along the *a* axis showing C8—H8···O1$^{i}$, C16—H16*B*···O1$^{i}$ and C16—H16*B*···F1$^{i}$ [symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$] intermolecular hydrogen bonds.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C16—H16*A*···O2 | 0.97 | 2.35 | 3.1144 (16) | 135 |
| C8—H8···O1$^{i}$ | 0.93 | 2.43 | 3.2148 (16) | 142 |
| C16—H16*B*···O1$^{i}$ | 0.97 | 2.43 | 3.2178 (17) | 138 |
| C16—H16*B*···F1$^{i}$ | 0.97 | 2.45 | 3.2224 (15) | 136 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{22}H_{23}F_3NO_3P$ |
| $M_r$ | 437.38 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 150 |
| *a*, *b*, *c* (Å) | 13.7056 (3), 10.6494 (2), 14.9163 (3) |
| $\beta$ (°) | 91.744 (2) |
| *V* (Å$^3$) | 2176.12 (8) |
| *Z* | 4 |
| Radiation type | Mo *K*$\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.17 |
| Crystal size (mm) | 0.27 × 0.20 × 0.15 |
| | |
| Data collection | |
| Diffractometer | Oxford Diffraction Xcalibur |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 14420, 4254, 3251 |
| $R_{int}$ | 0.019 |
| $(\sin\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.617 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.031, 0.079, 0.98 |
| No. of reflections | 4254 |
| No. of parameters | 271 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.32, −0.31 |

Computer programs: *CrysAlis CCD* (Oxford Diffraction, 2008), *SHELXS2014* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b) and *SHELXTL* (Sheldrick, 2008).

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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# full crystallographic data

*IUCrData* (2017). **2**, x171122 [https://doi.org/10.1107/S2414314617011221]

## Diethyl (1-benzyl-4-phenyl-3-trifluoromethyl-1*H*-pyrrol-2-yl)phosphonate

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### Diethyl (1-benzyl-4-phenyl-3-trifluoromethyl-1*H*-pyrrol-2-yl)phosphonate

*Crystal data*

$C_{22}H_{23}F_3NO_3P$
$M_r$ = 437.38
Monoclinic, $P2_1/c$
$a$ = 13.7056 (3) Å
$b$ = 10.6494 (2) Å
$c$ = 14.9163 (3) Å
$\beta$ = 91.744 (2)°
$V$ = 2176.12 (8) Å$^3$
$Z$ = 4
$F(000)$ = 912
$D_x$ = 1.335 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 14420 reflections
$\theta$ = 3.0–26.0°
$\mu$ = 0.17 mm$^{-1}$
$T$ = 150 K
Irregular, colourless
0.27 × 0.20 × 0.15 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 1024 x 1024 with blocks 2 x 2 pixels mm$^{-1}$
$\omega$ scan
14420 measured reflections
4254 independent reflections
3251 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 3.0°
$h$ = −16→16
$k$ = −13→13
$l$ = −12→18

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
$S$ = 0.98
4254 reflections
271 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

*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**. All H atoms were found in a difference map but set to idealized positions and treated as riding atoms with $C_{Ar}$—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for C—H, with C—$H_3$ = 0.96 Å and $U_{iso}$(H) = 1.5$U_{eq}$(C) and with C—$H_2$ = 0.97 and $U_{iso}$(H) = 1.2$U_{eq}$(C).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.26227 (8) | 0.28475 (10) | 0.23073 (7) | 0.0171 (2) |
| O1 | 0.25503 (8) | 0.18705 (9) | −0.02572 (6) | 0.0291 (3) |
| O2 | 0.24039 (8) | 0.04337 (9) | 0.11152 (6) | 0.0278 (2) |
| O3 | 0.39528 (7) | 0.13043 (9) | 0.08712 (6) | 0.0263 (2) |
| P1 | 0.28542 (3) | 0.16327 (3) | 0.06738 (2) | 0.02047 (10) |
| F1 | 0.27999 (7) | 0.45000 (8) | −0.02257 (5) | 0.0319 (2) |
| F2 | 0.18429 (7) | 0.58775 (8) | 0.02989 (5) | 0.0386 (3) |
| F3 | 0.12551 (7) | 0.41436 (9) | −0.02136 (6) | 0.0409 (3) |
| C1 | 0.47105 (11) | 0.21634 (16) | 0.05827 (10) | 0.0327 (4) |
| H1A | 0.4640 | 0.2972 | 0.0873 | 0.039* |
| H1B | 0.4656 | 0.2287 | −0.0061 | 0.039* |
| C2 | 0.56792 (12) | 0.1603 (2) | 0.08338 (12) | 0.0469 (5) |
| H2A | 0.6189 | 0.2155 | 0.0650 | 0.070* |
| H2B | 0.5744 | 0.0806 | 0.0541 | 0.070* |
| H2C | 0.5727 | 0.1486 | 0.1472 | 0.070* |
| C3 | 0.13611 (13) | 0.01934 (17) | 0.10071 (12) | 0.0457 (5) |
| H3A | 0.1034 | 0.0943 | 0.0783 | 0.055* |
| H3B | 0.1096 | −0.0014 | 0.1584 | 0.055* |
| C4 | 0.11827 (18) | −0.0846 (2) | 0.03792 (16) | 0.0701 (7) |
| H4A | 0.0493 | −0.0993 | 0.0312 | 0.105* |
| H4B | 0.1497 | −0.1591 | 0.0607 | 0.105* |
| H4C | 0.1441 | −0.0637 | −0.0193 | 0.105* |
| C5 | 0.25575 (10) | 0.29234 (12) | 0.13827 (8) | 0.0172 (3) |
| C6 | 0.21315 (10) | 0.40874 (12) | 0.11826 (8) | 0.0170 (3) |
| C7 | 0.19250 (9) | 0.47038 (13) | 0.20012 (8) | 0.0173 (3) |
| C8 | 0.22526 (10) | 0.39073 (13) | 0.26700 (9) | 0.0188 (3) |
| H8 | 0.2225 | 0.4071 | 0.3281 | 0.023* |
| C9 | 0.20027 (11) | 0.46319 (13) | 0.02681 (9) | 0.0242 (3) |
| C10 | 0.13887 (10) | 0.58735 (13) | 0.21848 (9) | 0.0200 (3) |
| C11 | 0.05005 (11) | 0.61462 (14) | 0.17435 (10) | 0.0267 (3) |
| H11 | 0.0274 | 0.5630 | 0.1279 | 0.032* |
| C12 | −0.00447 (12) | 0.71717 (15) | 0.19877 (12) | 0.0363 (4) |
| H12 | −0.0633 | 0.7345 | 0.1686 | 0.044* |
| C13 | 0.02780 (14) | 0.79382 (17) | 0.26762 (12) | 0.0437 (5) |
| H13 | −0.0096 | 0.8622 | 0.2846 | 0.052* |
| C14 | 0.11546 (14) | 0.76936 (16) | 0.31135 (12) | 0.0433 (5) |
| H14 | 0.1376 | 0.8219 | 0.3574 | 0.052* |
| C15 | 0.17114 (12) | 0.66642 (15) | 0.28696 (10) | 0.0310 (4) |
| H15 | 0.2304 | 0.6505 | 0.3168 | 0.037* |
| C16 | 0.30577 (10) | 0.18449 (13) | 0.28608 (9) | 0.0196 (3) |
| H16A | 0.2948 | 0.1048 | 0.2559 | 0.023* |
| H16B | 0.2726 | 0.1813 | 0.3426 | 0.023* |
| C17 | 0.41387 (10) | 0.19995 (13) | 0.30541 (8) | 0.0197 (3) |
| C18 | 0.46153 (11) | 0.31409 (14) | 0.29963 (9) | 0.0251 (3) |
| H18 | 0.4272 | 0.3847 | 0.2800 | 0.030* |

| | | | | |
|---|---|---|---|---|
| C19 | 0.56011 (12) | 0.32431 (15) | 0.32285 (10) | 0.0315 (4) |
| H19 | 0.5913 | 0.4016 | 0.3187 | 0.038* |
| C20 | 0.61174 (12) | 0.22048 (17) | 0.35194 (10) | 0.0339 (4) |
| H20 | 0.6778 | 0.2273 | 0.3673 | 0.041* |
| C21 | 0.56512 (12) | 0.10625 (16) | 0.35826 (11) | 0.0343 (4) |
| H21 | 0.5998 | 0.0360 | 0.3781 | 0.041* |
| C22 | 0.46686 (11) | 0.09576 (14) | 0.33519 (10) | 0.0271 (3) |
| H22 | 0.4360 | 0.0184 | 0.3396 | 0.033* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0182 (6) | 0.0208 (6) | 0.0122 (5) | 0.0017 (5) | −0.0011 (4) | 0.0016 (5) |
| O1 | 0.0432 (7) | 0.0281 (6) | 0.0156 (5) | 0.0017 (5) | −0.0035 (4) | −0.0029 (4) |
| O2 | 0.0356 (6) | 0.0217 (5) | 0.0259 (5) | −0.0050 (5) | −0.0030 (5) | 0.0010 (4) |
| O3 | 0.0274 (6) | 0.0254 (6) | 0.0262 (5) | 0.0054 (4) | 0.0026 (4) | −0.0006 (4) |
| P1 | 0.0273 (2) | 0.01945 (19) | 0.01456 (18) | 0.00111 (16) | −0.00119 (14) | −0.00163 (14) |
| F1 | 0.0448 (6) | 0.0329 (5) | 0.0183 (4) | −0.0001 (4) | 0.0085 (4) | 0.0028 (4) |
| F2 | 0.0683 (7) | 0.0245 (5) | 0.0230 (4) | 0.0135 (5) | 0.0022 (4) | 0.0064 (4) |
| F3 | 0.0426 (6) | 0.0514 (6) | 0.0273 (5) | −0.0019 (5) | −0.0215 (4) | 0.0024 (4) |
| C1 | 0.0307 (9) | 0.0403 (10) | 0.0272 (8) | −0.0023 (7) | 0.0034 (7) | 0.0030 (7) |
| C2 | 0.0302 (10) | 0.0725 (14) | 0.0380 (10) | 0.0048 (9) | 0.0000 (8) | 0.0055 (9) |
| C3 | 0.0437 (11) | 0.0435 (11) | 0.0497 (11) | −0.0130 (9) | −0.0002 (9) | 0.0068 (9) |
| C4 | 0.0680 (16) | 0.0592 (14) | 0.0819 (16) | −0.0233 (12) | −0.0168 (13) | −0.0115 (12) |
| C5 | 0.0163 (7) | 0.0221 (7) | 0.0130 (6) | −0.0012 (6) | −0.0021 (5) | 0.0003 (5) |
| C6 | 0.0155 (7) | 0.0196 (7) | 0.0158 (6) | −0.0017 (6) | −0.0030 (5) | 0.0005 (5) |
| C7 | 0.0134 (7) | 0.0208 (7) | 0.0177 (7) | −0.0010 (6) | −0.0007 (5) | −0.0009 (5) |
| C8 | 0.0188 (7) | 0.0240 (7) | 0.0135 (6) | 0.0013 (6) | 0.0003 (5) | −0.0024 (5) |
| C9 | 0.0326 (9) | 0.0226 (8) | 0.0172 (7) | 0.0032 (7) | −0.0041 (6) | −0.0004 (6) |
| C10 | 0.0197 (7) | 0.0210 (7) | 0.0196 (7) | 0.0003 (6) | 0.0026 (6) | 0.0016 (6) |
| C11 | 0.0237 (8) | 0.0243 (8) | 0.0320 (8) | 0.0024 (6) | −0.0024 (6) | −0.0007 (6) |
| C12 | 0.0261 (9) | 0.0325 (9) | 0.0502 (10) | 0.0097 (7) | −0.0015 (8) | 0.0004 (8) |
| C13 | 0.0434 (11) | 0.0346 (10) | 0.0537 (11) | 0.0163 (8) | 0.0094 (9) | −0.0074 (8) |
| C14 | 0.0542 (12) | 0.0363 (10) | 0.0393 (10) | 0.0084 (9) | −0.0005 (9) | −0.0182 (8) |
| C15 | 0.0321 (9) | 0.0328 (9) | 0.0278 (8) | 0.0052 (7) | −0.0044 (7) | −0.0072 (7) |
| C16 | 0.0250 (8) | 0.0195 (7) | 0.0141 (6) | 0.0021 (6) | −0.0018 (6) | 0.0033 (5) |
| C17 | 0.0241 (8) | 0.0239 (8) | 0.0110 (6) | 0.0037 (6) | 0.0000 (5) | −0.0019 (5) |
| C18 | 0.0268 (8) | 0.0247 (8) | 0.0235 (7) | 0.0026 (6) | −0.0030 (6) | 0.0034 (6) |
| C19 | 0.0290 (9) | 0.0350 (9) | 0.0303 (8) | −0.0061 (7) | −0.0024 (7) | 0.0000 (7) |
| C20 | 0.0222 (8) | 0.0503 (11) | 0.0290 (9) | 0.0055 (8) | −0.0042 (7) | −0.0063 (7) |
| C21 | 0.0298 (9) | 0.0367 (10) | 0.0359 (9) | 0.0140 (8) | −0.0064 (7) | −0.0003 (8) |
| C22 | 0.0301 (9) | 0.0220 (8) | 0.0290 (8) | 0.0055 (7) | −0.0025 (7) | −0.0008 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C8 | 1.3567 (17) | C7—C10 | 1.4763 (19) |
| N1—C5 | 1.3817 (16) | C8—H8 | 0.9300 |
| N1—C16 | 1.4654 (16) | C10—C15 | 1.386 (2) |

| | | | |
|---|---|---|---|
| O1—P1 | 1.4598 (10) | C10—C11 | 1.3966 (19) |
| O2—C3 | 1.456 (2) | C11—C12 | 1.379 (2) |
| O2—P1 | 1.5715 (10) | C11—H11 | 0.9300 |
| O3—C1 | 1.4586 (18) | C12—C13 | 1.374 (2) |
| O3—P1 | 1.5650 (10) | C12—H12 | 0.9300 |
| P1—C5 | 1.7886 (14) | C13—C14 | 1.374 (2) |
| F1—C9 | 1.3436 (17) | C13—H13 | 0.9300 |
| F2—C9 | 1.3455 (16) | C14—C15 | 1.390 (2) |
| F3—C9 | 1.3385 (16) | C14—H14 | 0.9300 |
| C1—C2 | 1.493 (2) | C15—H15 | 0.9300 |
| C1—H1A | 0.9700 | C16—C17 | 1.5097 (19) |
| C1—H1B | 0.9700 | C16—H16A | 0.9700 |
| C2—H2A | 0.9600 | C16—H16B | 0.9700 |
| C2—H2B | 0.9600 | C17—C18 | 1.384 (2) |
| C2—H2C | 0.9600 | C17—C22 | 1.392 (2) |
| C3—C4 | 1.466 (3) | C18—C19 | 1.389 (2) |
| C3—H3A | 0.9700 | C18—H18 | 0.9300 |
| C3—H3B | 0.9700 | C19—C20 | 1.376 (2) |
| C4—H4A | 0.9600 | C19—H19 | 0.9300 |
| C4—H4B | 0.9600 | C20—C21 | 1.379 (2) |
| C4—H4C | 0.9600 | C20—H20 | 0.9300 |
| C5—C6 | 1.3987 (18) | C21—C22 | 1.384 (2) |
| C6—C7 | 1.4223 (18) | C21—H21 | 0.9300 |
| C6—C9 | 1.4877 (18) | C22—H22 | 0.9300 |
| C7—C8 | 1.3745 (18) | | |

| | | | |
|---|---|---|---|
| C8—N1—C5 | 109.62 (11) | F3—C9—F2 | 106.18 (11) |
| C8—N1—C16 | 122.15 (10) | F1—C9—F2 | 104.94 (11) |
| C5—N1—C16 | 128.16 (11) | F3—C9—C6 | 114.09 (12) |
| C3—O2—P1 | 119.54 (10) | F1—C9—C6 | 112.71 (11) |
| C1—O3—P1 | 119.59 (9) | F2—C9—C6 | 111.58 (11) |
| O1—P1—O3 | 117.57 (6) | C15—C10—C11 | 118.37 (13) |
| O1—P1—O2 | 115.80 (6) | C15—C10—C7 | 120.00 (12) |
| O3—P1—O2 | 97.32 (6) | C11—C10—C7 | 121.31 (12) |
| O1—P1—C5 | 111.45 (6) | C12—C11—C10 | 120.79 (14) |
| O3—P1—C5 | 107.17 (6) | C12—C11—H11 | 119.6 |
| O2—P1—C5 | 106.11 (6) | C10—C11—H11 | 119.6 |
| O3—C1—C2 | 108.10 (13) | C13—C12—C11 | 120.21 (15) |
| O3—C1—H1A | 110.1 | C13—C12—H12 | 119.9 |
| C2—C1—H1A | 110.1 | C11—C12—H12 | 119.9 |
| O3—C1—H1B | 110.1 | C12—C13—C14 | 119.93 (16) |
| C2—C1—H1B | 110.1 | C12—C13—H13 | 120.0 |
| H1A—C1—H1B | 108.4 | C14—C13—H13 | 120.0 |
| C1—C2—H2A | 109.5 | C13—C14—C15 | 120.26 (16) |
| C1—C2—H2B | 109.5 | C13—C14—H14 | 119.9 |
| H2A—C2—H2B | 109.5 | C15—C14—H14 | 119.9 |
| C1—C2—H2C | 109.5 | C10—C15—C14 | 120.43 (15) |
| H2A—C2—H2C | 109.5 | C10—C15—H15 | 119.8 |

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| H2B—C2—H2C | 109.5 | C14—C15—H15 | 119.8 |
| O2—C3—C4 | 110.34 (16) | N1—C16—C17 | 114.09 (11) |
| O2—C3—H3A | 109.6 | N1—C16—H16A | 108.7 |
| C4—C3—H3A | 109.6 | C17—C16—H16A | 108.7 |
| O2—C3—H3B | 109.6 | N1—C16—H16B | 108.7 |
| C4—C3—H3B | 109.6 | C17—C16—H16B | 108.7 |
| H3A—C3—H3B | 108.1 | H16A—C16—H16B | 107.6 |
| C3—C4—H4A | 109.5 | C18—C17—C22 | 118.52 (14) |
| C3—C4—H4B | 109.5 | C18—C17—C16 | 123.11 (12) |
| H4A—C4—H4B | 109.5 | C22—C17—C16 | 118.27 (13) |
| C3—C4—H4C | 109.5 | C17—C18—C19 | 120.72 (14) |
| H4A—C4—H4C | 109.5 | C17—C18—H18 | 119.6 |
| H4B—C4—H4C | 109.5 | C19—C18—H18 | 119.6 |
| N1—C5—C6 | 106.19 (11) | C20—C19—C18 | 120.18 (15) |
| N1—C5—P1 | 122.43 (10) | C20—C19—H19 | 119.9 |
| C6—C5—P1 | 130.99 (10) | C18—C19—H19 | 119.9 |
| C5—C6—C7 | 108.57 (11) | C19—C20—C21 | 119.72 (15) |
| C5—C6—C9 | 125.33 (12) | C19—C20—H20 | 120.1 |
| C7—C6—C9 | 125.88 (12) | C21—C20—H20 | 120.1 |
| C8—C7—C6 | 105.62 (11) | C20—C21—C22 | 120.24 (15) |
| C8—C7—C10 | 122.65 (12) | C20—C21—H21 | 119.9 |
| C6—C7—C10 | 131.45 (12) | C22—C21—H21 | 119.9 |
| N1—C8—C7 | 109.98 (11) | C21—C22—C17 | 120.62 (15) |
| N1—C8—H8 | 125.0 | C21—C22—H22 | 119.7 |
| C7—C8—H8 | 125.0 | C17—C22—H22 | 119.7 |
| F3—C9—F1 | 106.69 (11) | | |

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| C1—O3—P1—O1 | 55.83 (12) | C5—C6—C9—F3 | 77.75 (18) |
| C1—O3—P1—O2 | −179.97 (10) | C7—C6—C9—F3 | −108.26 (15) |
| C1—O3—P1—C5 | −70.55 (11) | C5—C6—C9—F1 | −44.13 (18) |
| C3—O2—P1—O1 | −46.40 (13) | C7—C6—C9—F1 | 129.86 (14) |
| C3—O2—P1—O3 | −171.88 (11) | C5—C6—C9—F2 | −161.91 (13) |
| C3—O2—P1—C5 | 77.82 (12) | C7—C6—C9—F2 | 12.1 (2) |
| P1—O3—C1—C2 | −178.47 (11) | C8—C7—C10—C15 | 44.5 (2) |
| P1—O2—C3—C4 | 106.72 (16) | C6—C7—C10—C15 | −142.47 (15) |
| C8—N1—C5—C6 | 0.25 (14) | C8—C7—C10—C11 | −128.81 (15) |
| C16—N1—C5—C6 | −176.76 (13) | C6—C7—C10—C11 | 44.2 (2) |
| C8—N1—C5—P1 | −173.24 (10) | C15—C10—C11—C12 | −0.5 (2) |
| C16—N1—C5—P1 | 9.75 (19) | C7—C10—C11—C12 | 173.01 (14) |
| O1—P1—C5—N1 | 169.14 (10) | C10—C11—C12—C13 | −0.4 (2) |
| O3—P1—C5—N1 | −60.93 (12) | C11—C12—C13—C14 | 1.0 (3) |
| O2—P1—C5—N1 | 42.25 (12) | C12—C13—C14—C15 | −0.8 (3) |
| O1—P1—C5—C6 | −2.57 (15) | C11—C10—C15—C14 | 0.7 (2) |
| O3—P1—C5—C6 | 127.36 (13) | C7—C10—C15—C14 | −172.85 (14) |
| O2—P1—C5—C6 | −129.45 (13) | C13—C14—C15—C10 | −0.1 (3) |
| N1—C5—C6—C7 | −1.00 (15) | C8—N1—C16—C17 | −89.45 (15) |
| P1—C5—C6—C7 | 171.72 (11) | C5—N1—C16—C17 | 87.23 (16) |
| N1—C5—C6—C9 | 173.87 (12) | N1—C16—C17—C18 | 21.10 (18) |

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| P1—C5—C6—C9 | −13.4 (2) | N1—C16—C17—C22 | −162.55 (12) |
| C5—C6—C7—C8 | 1.35 (15) | C22—C17—C18—C19 | 0.1 (2) |
| C9—C6—C7—C8 | −173.48 (13) | C16—C17—C18—C19 | 176.48 (12) |
| C5—C6—C7—C10 | −172.52 (13) | C17—C18—C19—C20 | 0.1 (2) |
| C9—C6—C7—C10 | 12.7 (2) | C18—C19—C20—C21 | −0.2 (2) |
| C5—N1—C8—C7 | 0.62 (15) | C19—C20—C21—C22 | 0.2 (2) |
| C16—N1—C8—C7 | 177.85 (12) | C20—C21—C22—C17 | 0.0 (2) |
| C6—C7—C8—N1 | −1.20 (15) | C18—C17—C22—C21 | −0.2 (2) |
| C10—C7—C8—N1 | 173.34 (12) | C16—C17—C22—C21 | −176.68 (13) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C16—H16*A*···O2 | 0.97 | 2.35 | 3.1144 (16) | 135 |
| C8—H8···O1$^{i}$ | 0.93 | 2.43 | 3.2148 (16) | 142 |
| C16—H16*B*···O1$^{i}$ | 0.97 | 2.43 | 3.2178 (17) | 138 |
| C16—H16*B*···F1$^{i}$ | 0.97 | 2.45 | 3.2224 (15) | 136 |

Symmetry code: (i) $x$, $-y+1/2$, $z+1/2$.