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# 2-Isopropyl-5-methylcyclohexyl *N*-cyclohexyl-*P*-phenylphosphonamidate

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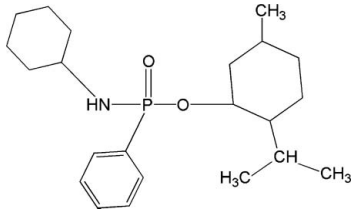
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.044; $wR$ factor = 0.083; data-to-parameter ratio = 17.1.

The title compound, $C_{22}H_{36}NO_2P$, features a P atom bonded to a phenyl ring, a cyclohexylamine unit and the O atom of a menthyl group. In the crystal structure, intermolecular N—H···O hydrogen bonds connect molecules into a one-dimensional chain in the *b* direction.

## Related literature

For the general synthesis of phosphorus–amine compounds, see: Steinberg (1950); Benamer *et al.* (2010). For the structures of related phosphorus–amine compounds, see: Balakrishna *et al.* (2001).




## Experimental

### Crystal data

$C_{22}H_{36}NO_2P$
$M_r$ = 377.49
Orthorhombic, $P2_12_12_1$
$a$ = 10.0205 (10) Å
$b$ = 10.4317 (11) Å
$c$ = 22.101 (2) Å
$V$ = 2310.2 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 298 K
0.40 × 0.14 × 0.07 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.949, $T_{max}$ = 0.991
11780 measured reflections
4064 independent reflections
2537 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.061

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.083
$S$ = 1.00
4064 reflections
238 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$
Absolute structure: Flack (1983), 1727 Friedel pairs
Flack parameter: −0.01 (11)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.86 | 2.15 | 2.969 (3) | 160 |

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: VM2032).

## References

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# supporting information

*Acta Cryst.* (2010). E**66**, o2352 [https://doi.org/10.1107/S1600536810032319]

## 2-Isopropyl-5-methylcyclohexyl *N*-cyclohexyl-*P*-phenylphosphonamidate

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### S1. Comment

The molecular structure of the P-chiral title compound consists of an *O*-menthyl phenylphosphinate core and cyclohexylamine (Steinberg, 1950). The absolute configuration of the central P atom is *S* and the four groups around the central P atom form an irregular tetrahedron (Benamer *et al.*, 2010). In the crystal structure intermolecular N—H···O hydrogen bonds connect molecules into a one-dimensional chain in the b-direction (Table 1, Fig. 2).

### S2. Experimental

Carbon tetrachloride was added to a solution of ($R_p$)-*O*-menthyl-phenyl phosphonothioate dissolved in dry ether and cyclohexylamine. The reaction mixture was stirred for 38 h at room temperature. A single crystal of the title compound suitable for X-ray diffraction was obtained by slow evaporation of an ether solution of the title compound.

### S3. Refinement

The imino H atom was located in a differece Fourier map and refined isotropically, with the N—H distance restrained to 0.86 Å. Other H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93–0.98 Å, with $U_{iso}$(H) = 1.5 $U_{eq}$(methyl) and $U_{iso}$(H) = 1.2 $U_{eq}$(C) for all other H atoms.

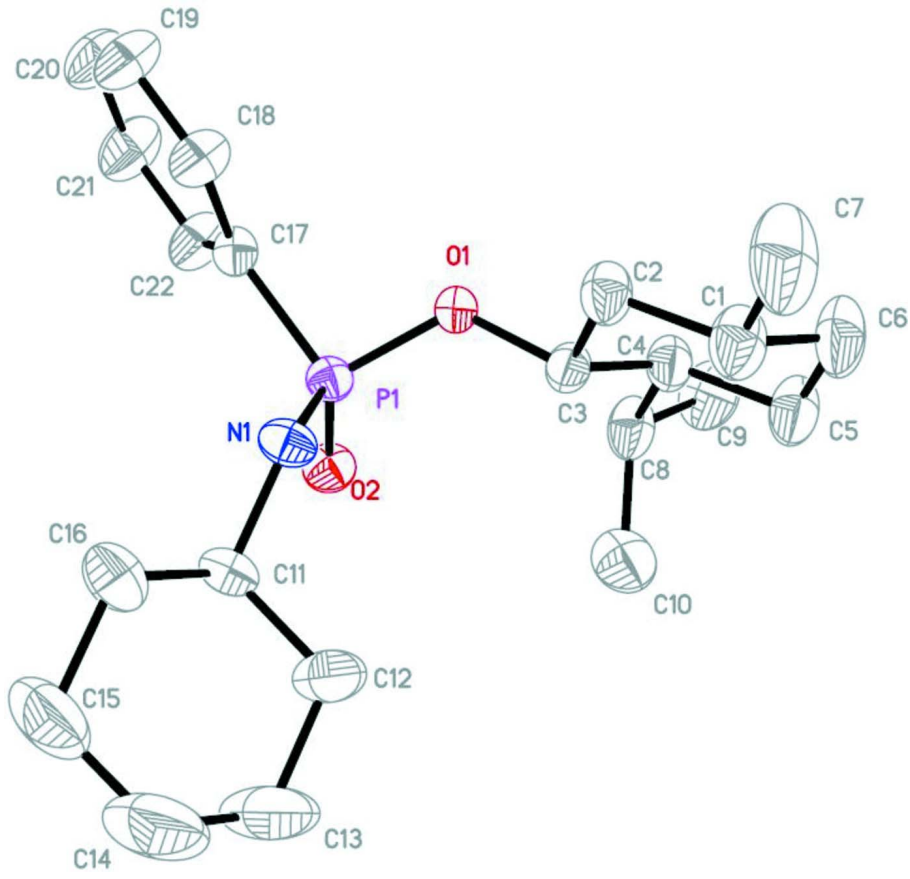


**Figure 1**

The molecular structure of the compound. H atoms have been omitted for clarity.

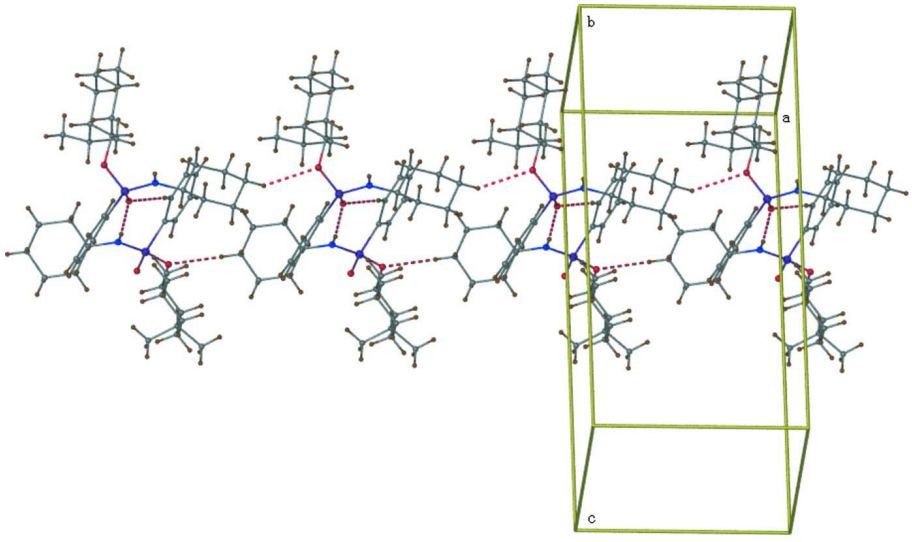


**Figure 2**

A view of the one-dimensional chain structure formed by N—H···O interactions in the title compound.

## 2-Isopropyl-5-methylcyclohexyl *N*-cyclohexyl-*P*-phenylphosphonamidate

*Crystal data*

$C_{22}H_{36}NO_2P$
$M_r = 377.49$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 10.0205$ (10) Å
$b = 10.4317$ (11) Å
$c = 22.101$ (2) Å
$V = 2310.2$ (4) Å$^3$
$Z = 4$
$F(000) = 824$
$D_x = 1.085$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2271 reflections
$\theta = 3.0$–$25.0°$
$\mu = 0.13$ mm$^{-1}$
$T = 298$ K
Block, colourless
0.40 × 0.14 × 0.07 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.949$, $T_{max} = 0.991$
11780 measured reflections
4064 independent reflections
2537 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 12$
$l = -26 \rightarrow 23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.083$
$S = 1.00$
4064 reflections
238 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
$w = 1/[\sigma^2(F_o^2) + (0.0224P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$
Absolute structure: Flack (1983), **with 1727 Friedel pairs [Please check]**
Absolute structure parameter: −0.01 (11)

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 1.06771 (19) | 0.23385 (19) | 0.24171 (9) | 0.0499 (6) |
| H1 | 1.0595 | 0.3159 | 0.2405 | 0.060* |
| O1 | 0.83345 (16) | 0.21330 (17) | 0.19514 (8) | 0.0453 (5) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.96301 (17) | 0.01022 (17) | 0.22946 (8) | 0.0536 (5) |
| P1 | 0.93290 (8) | 0.14723 (7) | 0.24088 (3) | 0.0429 (2) |
| C1 | 0.8879 (4) | 0.4422 (3) | 0.06456 (14) | 0.0768 (11) |
| H1A | 0.9796 | 0.4183 | 0.0541 | 0.092* |
| C2 | 0.8593 (3) | 0.3933 (3) | 0.12811 (12) | 0.0606 (9) |
| H2A | 0.9217 | 0.4326 | 0.1561 | 0.073* |
| H2B | 0.7701 | 0.4193 | 0.1398 | 0.073* |
| C3 | 0.8704 (3) | 0.2485 (3) | 0.13321 (12) | 0.0481 (8) |
| H3 | 0.9629 | 0.2226 | 0.1256 | 0.058* |
| C4 | 0.7777 (3) | 0.1789 (3) | 0.08865 (12) | 0.0592 (9) |
| H4 | 0.6861 | 0.2041 | 0.0987 | 0.071* |
| C5 | 0.8062 (4) | 0.2286 (3) | 0.02431 (12) | 0.0774 (11) |
| H5A | 0.8956 | 0.2033 | 0.0125 | 0.093* |
| H5B | 0.7439 | 0.1894 | −0.0037 | 0.093* |
| C6 | 0.7939 (4) | 0.3748 (3) | 0.02013 (14) | 0.0895 (12) |
| H6A | 0.8147 | 0.4021 | −0.0208 | 0.107* |
| H6B | 0.7026 | 0.3997 | 0.0288 | 0.107* |
| C7 | 0.8768 (4) | 0.5885 (3) | 0.06108 (16) | 0.1226 (17) |
| H7A | 0.7875 | 0.6141 | 0.0712 | 0.184* |
| H7B | 0.8975 | 0.6165 | 0.0208 | 0.184* |
| H7C | 0.9384 | 0.6266 | 0.0891 | 0.184* |
| C8 | 0.7848 (3) | 0.0312 (3) | 0.09409 (14) | 0.0688 (10) |
| H8 | 0.7767 | 0.0105 | 0.1372 | 0.083* |
| C9 | 0.6676 (4) | −0.0338 (3) | 0.06175 (16) | 0.0917 (12) |
| H9A | 0.5853 | 0.0033 | 0.0754 | 0.138* |
| H9B | 0.6680 | −0.1239 | 0.0708 | 0.138* |
| H9C | 0.6762 | −0.0217 | 0.0189 | 0.138* |
| C10 | 0.9165 (3) | −0.0253 (3) | 0.07251 (16) | 0.0912 (12) |
| H10A | 0.9257 | −0.0113 | 0.0298 | 0.137* |
| H10B | 0.9178 | −0.1157 | 0.0807 | 0.137* |
| H10C | 0.9889 | 0.0154 | 0.0934 | 0.137* |
| C11 | 1.2028 (2) | 0.1796 (3) | 0.24442 (13) | 0.0552 (8) |
| H11 | 1.1964 | 0.0928 | 0.2611 | 0.066* |
| C12 | 1.2647 (3) | 0.1704 (4) | 0.18205 (14) | 0.0822 (11) |
| H12A | 1.2098 | 0.1157 | 0.1568 | 0.099* |
| H12B | 1.2665 | 0.2550 | 0.1638 | 0.099* |
| C13 | 1.4051 (4) | 0.1172 (5) | 0.1840 (2) | 0.134 (2) |
| H13A | 1.4426 | 0.1165 | 0.1435 | 0.161* |
| H13B | 1.4032 | 0.0297 | 0.1989 | 0.161* |
| C14 | 1.4916 (4) | 0.1989 (6) | 0.2252 (3) | 0.150 (2) |
| H14A | 1.4984 | 0.2849 | 0.2088 | 0.180* |
| H14B | 1.5807 | 0.1628 | 0.2273 | 0.180* |
| C15 | 1.4315 (4) | 0.2045 (5) | 0.2888 (2) | 0.1302 (18) |
| H15A | 1.4860 | 0.2588 | 0.3144 | 0.156* |
| H15B | 1.4300 | 0.1192 | 0.3062 | 0.156* |
| C16 | 1.2890 (3) | 0.2581 (4) | 0.28578 (16) | 0.0877 (12) |
| H16A | 1.2505 | 0.2584 | 0.3260 | 0.105* |
| H16B | 1.2918 | 0.3459 | 0.2714 | 0.105* |

| | | | | |
|---|---|---|---|---|
| C17 | 0.8400 (3) | 0.1681 (3) | 0.30935 (12) | 0.0452 (7) |
| C18 | 0.8202 (3) | 0.2870 (3) | 0.33534 (14) | 0.0636 (9) |
| H18 | 0.8568 | 0.3594 | 0.3172 | 0.076* |
| C19 | 0.7467 (3) | 0.3002 (3) | 0.38791 (15) | 0.0776 (11) |
| H19 | 0.7345 | 0.3810 | 0.4048 | 0.093* |
| C20 | 0.6920 (4) | 0.1947 (4) | 0.41515 (14) | 0.0763 (11) |
| H20 | 0.6425 | 0.2038 | 0.4505 | 0.092* |
| C21 | 0.7103 (4) | 0.0758 (4) | 0.39042 (15) | 0.0832 (11) |
| H21 | 0.6733 | 0.0039 | 0.4088 | 0.100* |
| C22 | 0.7844 (3) | 0.0634 (3) | 0.33780 (14) | 0.0673 (10) |
| H22 | 0.7969 | −0.0176 | 0.3213 | 0.081* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0427 (11) | 0.0383 (14) | 0.0687 (15) | 0.0012 (12) | −0.0004 (14) | −0.0012 (12) |
| O1 | 0.0465 (11) | 0.0518 (13) | 0.0377 (11) | 0.0046 (10) | −0.0014 (9) | 0.0019 (10) |
| O2 | 0.0624 (12) | 0.0374 (12) | 0.0609 (13) | 0.0023 (10) | 0.0017 (10) | −0.0037 (10) |
| P1 | 0.0461 (4) | 0.0365 (5) | 0.0460 (4) | 0.0015 (4) | −0.0010 (4) | −0.0011 (4) |
| C1 | 0.115 (3) | 0.055 (2) | 0.061 (2) | 0.002 (2) | −0.006 (2) | 0.0105 (17) |
| C2 | 0.084 (2) | 0.048 (2) | 0.050 (2) | 0.0012 (18) | −0.0082 (17) | 0.0013 (15) |
| C3 | 0.0580 (18) | 0.047 (2) | 0.0387 (18) | 0.0040 (16) | 0.0001 (15) | 0.0008 (14) |
| C4 | 0.075 (2) | 0.057 (2) | 0.0455 (19) | 0.006 (2) | −0.0092 (16) | −0.0023 (16) |
| C5 | 0.115 (3) | 0.067 (3) | 0.049 (2) | 0.002 (2) | −0.010 (2) | −0.0007 (17) |
| C6 | 0.144 (3) | 0.071 (3) | 0.053 (2) | 0.004 (3) | −0.016 (2) | 0.0142 (19) |
| C7 | 0.217 (5) | 0.060 (3) | 0.091 (3) | −0.013 (3) | −0.030 (3) | 0.029 (2) |
| C8 | 0.097 (3) | 0.058 (2) | 0.052 (2) | −0.007 (2) | −0.012 (2) | −0.0013 (17) |
| C9 | 0.113 (3) | 0.079 (3) | 0.083 (3) | −0.023 (3) | −0.010 (2) | −0.020 (2) |
| C10 | 0.106 (3) | 0.065 (3) | 0.102 (3) | 0.017 (3) | −0.020 (3) | −0.023 (2) |
| C11 | 0.0372 (15) | 0.055 (2) | 0.074 (2) | 0.0045 (15) | −0.0008 (17) | 0.0021 (18) |
| C12 | 0.063 (2) | 0.093 (3) | 0.091 (3) | 0.007 (2) | 0.0164 (19) | −0.020 (2) |
| C13 | 0.071 (3) | 0.160 (5) | 0.170 (5) | 0.018 (3) | 0.031 (3) | −0.051 (4) |
| C14 | 0.060 (3) | 0.183 (6) | 0.207 (6) | 0.006 (3) | 0.011 (3) | −0.030 (5) |
| C15 | 0.074 (3) | 0.155 (5) | 0.162 (5) | 0.010 (4) | −0.045 (3) | −0.018 (4) |
| C16 | 0.055 (2) | 0.114 (3) | 0.095 (3) | −0.004 (2) | −0.0194 (19) | −0.008 (2) |
| C17 | 0.0514 (17) | 0.040 (2) | 0.0443 (17) | −0.0032 (17) | −0.0040 (14) | 0.0008 (15) |
| C18 | 0.080 (2) | 0.050 (2) | 0.060 (2) | −0.006 (2) | 0.0146 (18) | −0.0004 (17) |
| C19 | 0.106 (3) | 0.064 (3) | 0.063 (2) | −0.002 (2) | 0.024 (2) | −0.013 (2) |
| C20 | 0.105 (3) | 0.073 (3) | 0.051 (2) | −0.002 (3) | 0.026 (2) | 0.005 (2) |
| C21 | 0.124 (3) | 0.064 (3) | 0.061 (2) | −0.012 (3) | 0.027 (2) | 0.010 (2) |
| C22 | 0.098 (3) | 0.049 (2) | 0.055 (2) | −0.008 (2) | 0.015 (2) | −0.0009 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C11 | 1.468 (3) | C9—H9C | 0.9600 |
| N1—P1 | 1.625 (2) | C10—H10A | 0.9600 |
| N1—H1 | 0.8600 | C10—H10B | 0.9600 |
| O1—C3 | 1.465 (3) | C10—H10C | 0.9600 |

| | | | |
|---|---|---|---|
| O1—P1 | 1.5779 (17) | C11—C16 | 1.501 (4) |
| O2—P1 | 1.4823 (19) | C11—C12 | 1.515 (4) |
| P1—C17 | 1.790 (3) | C11—H11 | 0.9800 |
| C1—C2 | 1.522 (4) | C12—C13 | 1.513 (4) |
| C1—C6 | 1.532 (4) | C12—H12A | 0.9700 |
| C1—C7 | 1.532 (4) | C12—H12B | 0.9700 |
| C1—H1A | 0.9800 | C13—C14 | 1.519 (6) |
| C2—C3 | 1.518 (3) | C13—H13A | 0.9700 |
| C2—H2A | 0.9700 | C13—H13B | 0.9700 |
| C2—H2B | 0.9700 | C14—C15 | 1.529 (6) |
| C3—C4 | 1.537 (3) | C14—H14A | 0.9700 |
| C3—H3 | 0.9800 | C14—H14B | 0.9700 |
| C4—C5 | 1.540 (4) | C15—C16 | 1.534 (5) |
| C4—C8 | 1.547 (4) | C15—H15A | 0.9700 |
| C4—H4 | 0.9800 | C15—H15B | 0.9700 |
| C5—C6 | 1.533 (4) | C16—H16A | 0.9700 |
| C5—H5A | 0.9700 | C16—H16B | 0.9700 |
| C5—H5B | 0.9700 | C17—C22 | 1.378 (4) |
| C6—H6A | 0.9700 | C17—C18 | 1.382 (4) |
| C6—H6B | 0.9700 | C18—C19 | 1.382 (4) |
| C7—H7A | 0.9600 | C18—H18 | 0.9300 |
| C7—H7B | 0.9600 | C19—C20 | 1.370 (4) |
| C7—H7C | 0.9600 | C19—H19 | 0.9300 |
| C8—C10 | 1.521 (4) | C20—C21 | 1.367 (4) |
| C8—C9 | 1.533 (4) | C20—H20 | 0.9300 |
| C8—H8 | 0.9800 | C21—C22 | 1.386 (4) |
| C9—H9A | 0.9600 | C21—H21 | 0.9300 |
| C9—H9B | 0.9600 | C22—H22 | 0.9300 |

| | | | |
|---|---|---|---|
| C11—N1—P1 | 123.52 (17) | H9A—C9—H9C | 109.5 |
| C11—N1—H1 | 118.2 | H9B—C9—H9C | 109.5 |
| P1—N1—H1 | 118.2 | C8—C10—H10A | 109.5 |
| C3—O1—P1 | 123.26 (16) | C8—C10—H10B | 109.5 |
| O2—P1—O1 | 116.15 (11) | H10A—C10—H10B | 109.5 |
| O2—P1—N1 | 111.64 (11) | C8—C10—H10C | 109.5 |
| O1—P1—N1 | 106.81 (11) | H10A—C10—H10C | 109.5 |
| O2—P1—C17 | 111.54 (12) | H10B—C10—H10C | 109.5 |
| O1—P1—C17 | 99.19 (11) | N1—C11—C16 | 110.2 (2) |
| N1—P1—C17 | 110.81 (12) | N1—C11—C12 | 111.4 (2) |
| C2—C1—C6 | 108.8 (3) | C16—C11—C12 | 110.7 (2) |
| C2—C1—C7 | 111.5 (3) | N1—C11—H11 | 108.2 |
| C6—C1—C7 | 112.4 (3) | C16—C11—H11 | 108.2 |
| C2—C1—H1A | 108.0 | C12—C11—H11 | 108.2 |
| C6—C1—H1A | 108.0 | C13—C12—C11 | 112.2 (3) |
| C7—C1—H1A | 108.0 | C13—C12—H12A | 109.2 |
| C3—C2—C1 | 112.8 (2) | C11—C12—H12A | 109.2 |
| C3—C2—H2A | 109.0 | C13—C12—H12B | 109.2 |
| C1—C2—H2A | 109.0 | C11—C12—H12B | 109.2 |

| | | | |
|---|---|---|---|
| C3—C2—H2B | 109.0 | H12A—C12—H12B | 107.9 |
| C1—C2—H2B | 109.0 | C12—C13—C14 | 110.0 (4) |
| H2A—C2—H2B | 107.8 | C12—C13—H13A | 109.7 |
| O1—C3—C2 | 107.5 (2) | C14—C13—H13A | 109.7 |
| O1—C3—C4 | 109.1 (2) | C12—C13—H13B | 109.7 |
| C2—C3—C4 | 112.2 (2) | C14—C13—H13B | 109.7 |
| O1—C3—H3 | 109.3 | H13A—C13—H13B | 108.2 |
| C2—C3—H3 | 109.3 | C13—C14—C15 | 110.3 (4) |
| C4—C3—H3 | 109.3 | C13—C14—H14A | 109.6 |
| C3—C4—C5 | 108.7 (2) | C15—C14—H14A | 109.6 |
| C3—C4—C8 | 113.1 (2) | C13—C14—H14B | 109.6 |
| C5—C4—C8 | 113.5 (2) | C15—C14—H14B | 109.6 |
| C3—C4—H4 | 107.1 | H14A—C14—H14B | 108.1 |
| C5—C4—H4 | 107.1 | C14—C15—C16 | 109.9 (4) |
| C8—C4—H4 | 107.1 | C14—C15—H15A | 109.7 |
| C6—C5—C4 | 112.1 (3) | C16—C15—H15A | 109.7 |
| C6—C5—H5A | 109.2 | C14—C15—H15B | 109.7 |
| C4—C5—H5A | 109.2 | C16—C15—H15B | 109.7 |
| C6—C5—H5B | 109.2 | H15A—C15—H15B | 108.2 |
| C4—C5—H5B | 109.2 | C11—C16—C15 | 111.3 (3) |
| H5A—C5—H5B | 107.9 | C11—C16—H16A | 109.4 |
| C1—C6—C5 | 111.6 (3) | C15—C16—H16A | 109.4 |
| C1—C6—H6A | 109.3 | C11—C16—H16B | 109.4 |
| C5—C6—H6A | 109.3 | C15—C16—H16B | 109.4 |
| C1—C6—H6B | 109.3 | H16A—C16—H16B | 108.0 |
| C5—C6—H6B | 109.3 | C22—C17—C18 | 117.6 (3) |
| H6A—C6—H6B | 108.0 | C22—C17—P1 | 120.0 (2) |
| C1—C7—H7A | 109.5 | C18—C17—P1 | 122.4 (2) |
| C1—C7—H7B | 109.5 | C17—C18—C19 | 121.0 (3) |
| H7A—C7—H7B | 109.5 | C17—C18—H18 | 119.5 |
| C1—C7—H7C | 109.5 | C19—C18—H18 | 119.5 |
| H7A—C7—H7C | 109.5 | C20—C19—C18 | 120.2 (3) |
| H7B—C7—H7C | 109.5 | C20—C19—H19 | 119.9 |
| C10—C8—C9 | 110.3 (3) | C18—C19—H19 | 119.9 |
| C10—C8—C4 | 113.7 (3) | C21—C20—C19 | 120.0 (3) |
| C9—C8—C4 | 111.6 (3) | C21—C20—H20 | 120.0 |
| C10—C8—H8 | 106.9 | C19—C20—H20 | 120.0 |
| C9—C8—H8 | 106.9 | C20—C21—C22 | 119.5 (3) |
| C4—C8—H8 | 106.9 | C20—C21—H21 | 120.3 |
| C8—C9—H9A | 109.5 | C22—C21—H21 | 120.3 |
| C8—C9—H9B | 109.5 | C17—C22—C21 | 121.7 (3) |
| H9A—C9—H9B | 109.5 | C17—C22—H22 | 119.1 |
| C8—C9—H9C | 109.5 | C21—C22—H22 | 119.1 |

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|---|---|---|---|
| C3—O1—P1—O2 | −73.7 (2) | P1—N1—C11—C16 | −139.8 (2) |
| C3—O1—P1—N1 | 51.5 (2) | P1—N1—C11—C12 | 96.9 (3) |
| C3—O1—P1—C17 | 166.7 (2) | N1—C11—C12—C13 | 178.8 (3) |
| C11—N1—P1—O2 | −12.7 (2) | C16—C11—C12—C13 | 55.9 (4) |

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|---|---|---|---|
| C11—N1—P1—O1 | −140.6 (2) | C11—C12—C13—C14 | −56.8 (5) |
| C11—N1—P1—C17 | 112.3 (2) | C12—C13—C14—C15 | 57.5 (6) |
| C6—C1—C2—C3 | 55.9 (4) | C13—C14—C15—C16 | −57.7 (6) |
| C7—C1—C2—C3 | −179.6 (3) | N1—C11—C16—C15 | −179.2 (3) |
| P1—O1—C3—C2 | −117.1 (2) | C12—C11—C16—C15 | −55.6 (4) |
| P1—O1—C3—C4 | 121.0 (2) | C14—C15—C16—C11 | 57.0 (5) |
| C1—C2—C3—O1 | −176.8 (2) | O2—P1—C17—C22 | −12.2 (3) |
| C1—C2—C3—C4 | −56.9 (4) | O1—P1—C17—C22 | 110.8 (2) |
| O1—C3—C4—C5 | 173.4 (2) | N1—P1—C17—C22 | −137.2 (2) |
| C2—C3—C4—C5 | 54.4 (3) | O2—P1—C17—C18 | 168.3 (2) |
| O1—C3—C4—C8 | −59.6 (3) | O1—P1—C17—C18 | −68.8 (3) |
| C2—C3—C4—C8 | −178.6 (3) | N1—P1—C17—C18 | 43.3 (3) |
| C3—C4—C5—C6 | −55.0 (4) | C22—C17—C18—C19 | −0.2 (5) |
| C8—C4—C5—C6 | 178.2 (3) | P1—C17—C18—C19 | 179.3 (2) |
| C2—C1—C6—C5 | −55.9 (4) | C17—C18—C19—C20 | −0.1 (5) |
| C7—C1—C6—C5 | −179.9 (3) | C18—C19—C20—C21 | 0.2 (6) |
| C4—C5—C6—C1 | 57.6 (4) | C19—C20—C21—C22 | 0.0 (6) |
| C3—C4—C8—C10 | −69.3 (3) | C18—C17—C22—C21 | 0.4 (4) |
| C5—C4—C8—C10 | 55.2 (4) | P1—C17—C22—C21 | −179.2 (3) |
| C3—C4—C8—C9 | 165.2 (2) | C20—C21—C22—C17 | −0.3 (5) |
| C5—C4—C8—C9 | −70.4 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O2$^{i}$ | 0.86 | 2.15 | 2.969 (3) | 160 |

Symmetry code: (i) −*x*+2, *y*+1/2, −*z*+1/2.