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# *N*-Benzoyl-*N*′,*N*″-dicyclohexylphosphoric triamide

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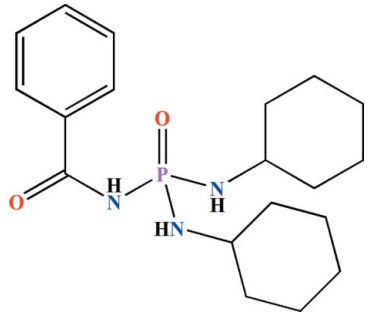
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.008 Å; $R$ factor = 0.051; $wR$ factor = 0.122; data-to-parameter ratio = 11.5.

In the title compound, $C_{19}H_{30}N_3O_2P$, the central P atom has a distorted tetrahedral configuration. The N atoms in both cyclohexylamide moieties exhibit a slight deviation [0.32 (7) and 0.44 (6) Å] from planarity, while the benzoylamide N atom is planar [0.11 (3) Å]. In the crystal, molecules are linked *via* N—H···O(P) and N—H···O(C) hydrogen bonds, forming $R_2^2(10)$ rings within linear arrangements parallel to the *b* axis.

## Related literature

For the synthesis and a spectroscopic study of title compound, see: Gholivand *et al.* (2006). For bond lengths in related structures, see: Sabbaghi *et al.* (2010); Rudd *et al.* (1996). For hydrogen-bond motifs, see: Etter *et al.* (1990); Bernstein *et al.* (1995).



## Experimental

### Crystal data

$C_{19}H_{30}N_3O_2P$
$M_r$ = 363.43
Monoclinic, *Cc*
*a* = 20.9904 (17) Å
*b* = 5.1503 (2) Å
*c* = 21.1125 (18) Å
$\beta$ = 121.955 (11)°
$V$ = 1936.5 (2) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 1.39 mm$^{-1}$
$T$ = 293 K
0.28 × 0.05 × 0.01 mm

### Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
$T_{min}$ = 0.978, $T_{max}$ = 1.000
2758 measured reflections
2758 independent reflections
2294 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.064

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.122
$S$ = 1.05
2758 reflections
239 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Absolute structure: Flack (1983), 908 Friedel pairs
Flack parameter: 0.11 (4)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N4—H4···O3$^{i}$ | 0.90 (4) | 2.16 (4) | 2.988 (4) | 154 (3) |
| N5—H5···O2$^{ii}$ | 0.77 (5) | 2.30 (6) | 3.019 (5) | 156 (6) |

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 PRO*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LD2010).

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# supporting information

*Acta Cryst.* (2011). E**67**, o1360 [doi:10.1107/S1600536811016679]

## *N*-Benzoyl-*N*′,*N*′′-dicyclohexylphosphoric triamide

**Mehrdad Pourayoubi, Mahnaz Rostami Chaijan, Laura Torre-Fernández and Santiago García-Granda**

### S1. Comment

The synthesis of the title compound, $C_6H_5C(O)NHP(O)[NHC_6H_{11}]_2$, was previously published by Gholivand *et al.* (2006). Here, we report its crystal structure (Fig. 1).

The P═O, C═O and P—N bond lengths match those found for other compounds with the [(N)(N)P(O)NHC(O)] skeleton (Sabbaghi *et al.*, 2010). The nitrogen atoms show $sp^2$ character and the environment of N atom in C(O)NHP(O) moiety is practically planar. The tetrahedral configuration of phosphorus atom is significantly distorted (Fig. 1) as it has been noted for other phosphoric triamides and their chalco-derivatives (Rudd *et al.*, 1996): the bond angles at the P atom vary in the range from 102.7 (2)° to 117.2 (2)°, while the P–N bond distances range form 1.615 (4) to 1.730 (4) Å. Cyclohexyl groups are in a chair conformation with the adjacent NH groups oriented equatorially.

The NH unit of the C(O)NHP(O) moiety adopts a *syn* orientation with respect to the phosphoryl group; moreover, the NH units of two $C_6H_{11}NH$ moieties are in a *syn* orientation with respect to each other.

In the crystal structure, the molecules are linked *via* N—H···O═P and N—H···O═C hydrogen bonds, in which carbonyl oxygen interacts with benzamide N—H and P(O) group binds to a cyclohexylamido moiety. This way, $R_2^2(10)$ rings are built (Etter *et al.*, 1990; Bernstein *et al.*, 1995), that are further connected in linear arrangements along *y* axis (Table 1, Fig. 2).

### S2. Experimental

$C_6H_5C(O)NHP(O)[NHC_6H_{11}]_2$ was prepared according to the procedure reported by Gholivand *et al.* (2006). Single crystals of title compound were obtained from $CH_3OH$ after slow evaporation at room temperature.

### S3. Refinement

At the end of the refinement the highest peak in the electron density was 0.460 e Å $^{-3}$, while the deepest hole was -0.180 e Å $^{-3}$.

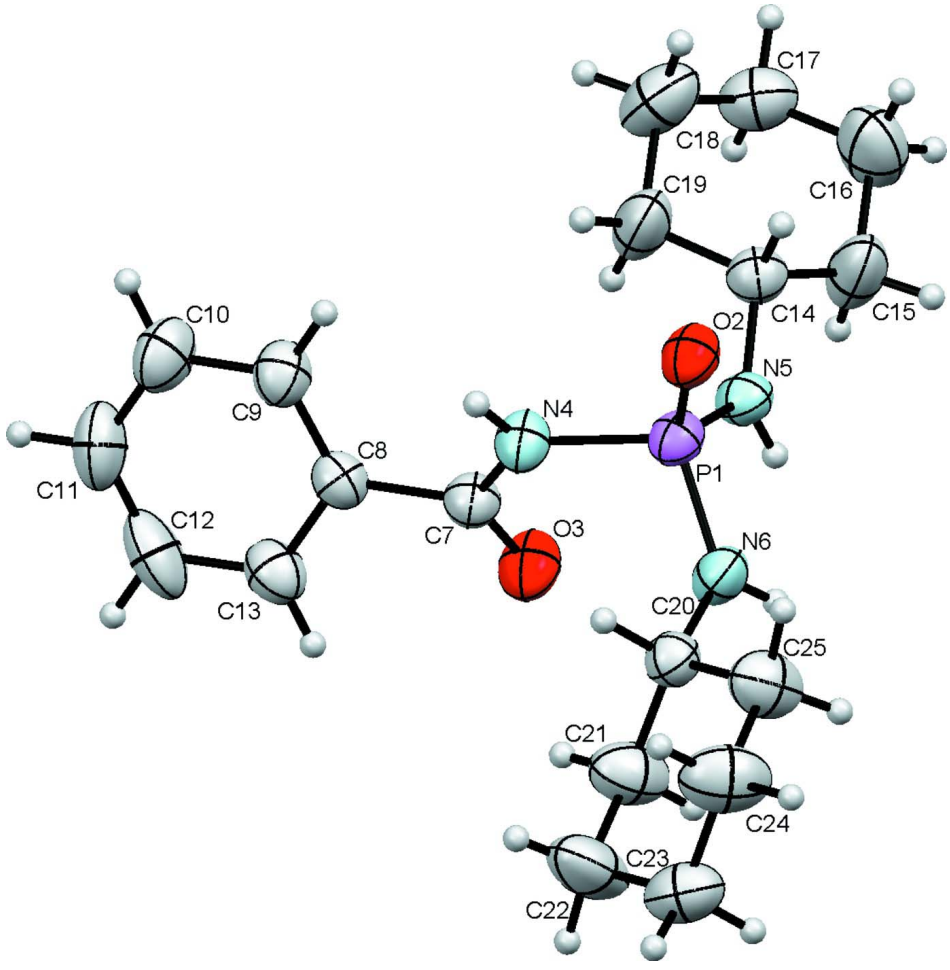


**Figure 1**

An *ORTEP*-style plot of title compound with labeling. Ellipsoids are given at the 50% probability level.

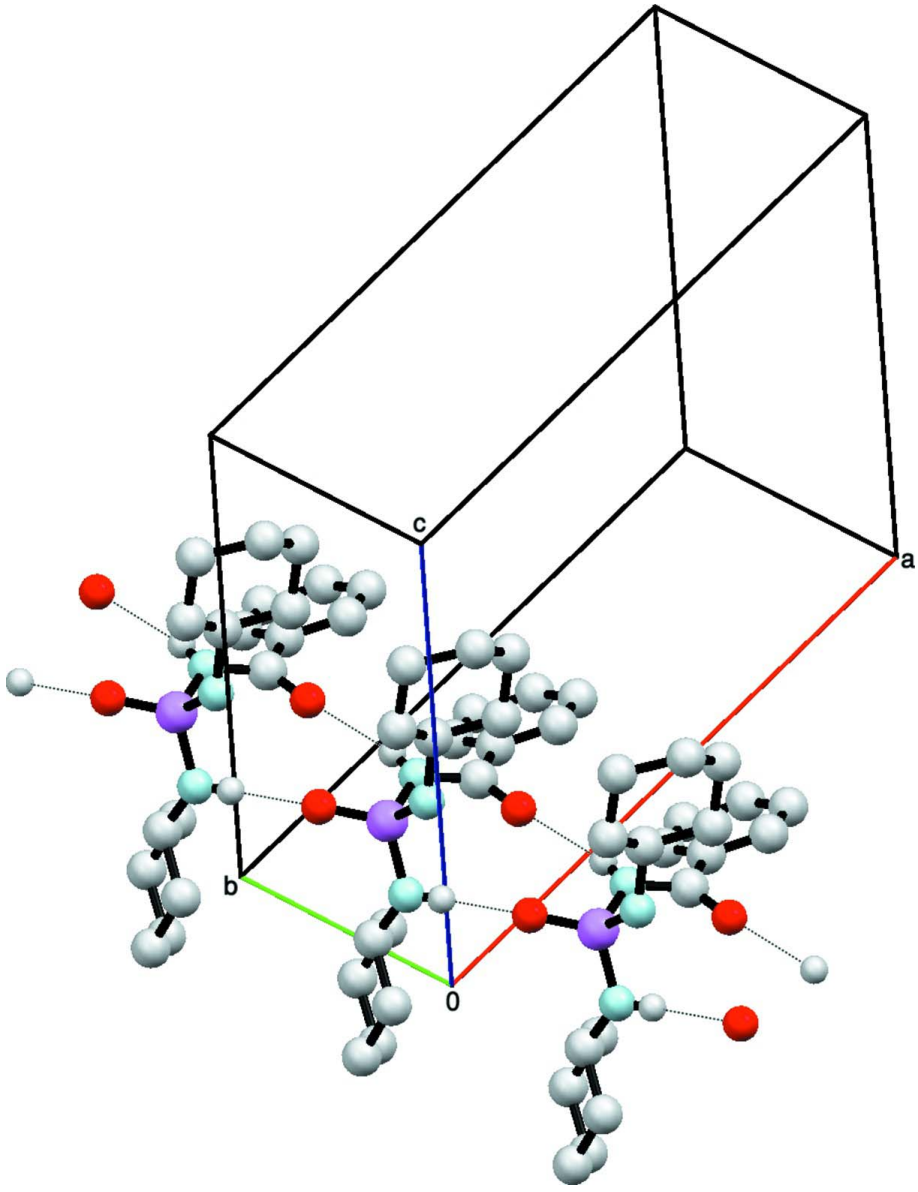


**Figure 2**

Partial packing view showing the formation of the chain through N—H···O hydrogen bonds (along the *b* axis) which are shown as dotted lines. H atoms not involved in the hydrogen bondings are omitted.

### *N*-Benzoyl-*N*′,*N*′′-dicyclohexylphosphoric triamide

*Crystal data*

$C_{19}H_{30}N_3O_2P$
$M_r = 363.43$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 20.9904\ (17)$ Å
$b = 5.1503\ (2)$ Å
$c = 21.1125\ (18)$ Å
$\beta = 121.955\ (11)°$
$V = 1936.5\ (2)$ Å$^3$
$Z = 4$
$F(000) = 784$
$D_x = 1.247$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 1733 reflections
$\theta = 4.2–70.2°$
$\mu = 1.39$ mm$^{-1}$

$T$ = 293 K
Prismatic, colorless

0.28 × 0.05 × 0.01 mm

*Data collection*

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.2673 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
$T_{min}$ = 0.978, $T_{max}$ = 1.000

2758 measured reflections
2758 independent reflections
2294 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.064
$\theta_{max}$ = 70.3°, $\theta_{min}$ = 4.8°
$h$ = −24→24
$k$ = 0→6
$l$ = −25→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.122
$S$ = 1.05
2758 reflections
239 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Absolute structure: Flack (1983), **908 Friedel pairs**
Absolute structure parameter: 0.11 (4)

*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 | 0.00072 (6) | 0.2629 (2) | 0.30701 (6) | 0.0403 (2) |
| O2 | −0.02706 (18) | 0.5292 (5) | 0.30029 (19) | 0.0504 (8) |
| O3 | 0.11281 (18) | −0.1251 (6) | 0.3206 (2) | 0.0578 (9) |
| N4 | 0.0865 (2) | 0.3029 (6) | 0.3150 (2) | 0.0435 (8) |
| N5 | −0.0520 (2) | 0.0724 (7) | 0.2376 (2) | 0.0438 (9) |
| N6 | 0.0150 (2) | 0.0959 (8) | 0.3781 (2) | 0.0458 (9) |
| C7 | 0.1289 (2) | 0.1008 (8) | 0.3169 (2) | 0.0398 (9) |
| C8 | 0.1958 (2) | 0.1615 (7) | 0.3117 (2) | 0.0401 (9) |
| C9 | 0.1990 (3) | 0.3714 (9) | 0.2727 (3) | 0.0490 (11) |
| H9 | 0.1598 | 0.4905 | 0.2518 | 0.059* |
| C10 | 0.2585 (3) | 0.4083 (11) | 0.2640 (3) | 0.0616 (13) |
| H10 | 0.2590 | 0.5492 | 0.2367 | 0.074* |

| | | | | |
|---|---|---|---|---|
| C11 | 0.3180 (3) | 0.2347 (12) | 0.2961 (3) | 0.0677 (14) |
| H11 | 0.3587 | 0.2600 | 0.2907 | 0.081* |
| C12 | 0.3169 (3) | 0.0239 (12) | 0.3362 (3) | 0.0722 (16) |
| H12 | 0.3569 | −0.0923 | 0.3577 | 0.087* |
| C13 | 0.2559 (3) | −0.0130 (10) | 0.3440 (3) | 0.0533 (12) |
| H13 | 0.2549 | −0.1546 | 0.3708 | 0.064* |
| C14 | −0.0945 (2) | 0.1484 (9) | 0.1595 (2) | 0.0451 (10) |
| H14 | −0.1203 | 0.3120 | 0.1554 | 0.054* |
| C15 | −0.1535 (3) | −0.0560 (13) | 0.1154 (3) | 0.0727 (17) |
| H15A | −0.1872 | −0.0665 | 0.1336 | 0.087* |
| H15B | −0.1292 | −0.2234 | 0.1235 | 0.087* |
| C16 | −0.1994 (3) | 0.0014 (16) | 0.0314 (3) | 0.0846 (19) |
| H16A | −0.2337 | −0.1413 | 0.0055 | 0.102* |
| H16B | −0.2290 | 0.1571 | 0.0225 | 0.102* |
| C17 | −0.1502 (3) | 0.0381 (11) | 0.0011 (3) | 0.0638 (13) |
| H17B | −0.1806 | 0.0862 | −0.0511 | 0.077* |
| H17A | −0.1251 | −0.1241 | 0.0045 | 0.077* |
| C18 | −0.0922 (4) | 0.2463 (12) | 0.0436 (4) | 0.0774 (17) |
| H18A | −0.1172 | 0.4125 | 0.0352 | 0.093* |
| H18B | −0.0589 | 0.2579 | 0.0250 | 0.093* |
| C19 | −0.0464 (3) | 0.1896 (13) | 0.1269 (3) | 0.0683 (16) |
| H19A | −0.0162 | 0.0356 | 0.1356 | 0.082* |
| H19B | −0.0124 | 0.3335 | 0.1525 | 0.082* |
| C20 | 0.0677 (2) | 0.1637 (8) | 0.4557 (2) | 0.0426 (9) |
| H20 | 0.0962 | 0.3151 | 0.4562 | 0.051* |
| C21 | 0.1229 (3) | −0.0486 (12) | 0.4978 (3) | 0.0685 (15) |
| H21A | 0.1533 | −0.0758 | 0.4763 | 0.082* |
| H21B | 0.0956 | −0.2081 | 0.4916 | 0.082* |
| C22 | 0.1746 (3) | 0.0067 (15) | 0.5810 (3) | 0.0805 (19) |
| H22A | 0.2054 | −0.1448 | 0.6055 | 0.097* |
| H22B | 0.2077 | 0.1498 | 0.5878 | 0.097* |
| C23 | 0.1303 (3) | 0.0742 (10) | 0.6167 (3) | 0.0650 (14) |
| H23B | 0.1019 | −0.0762 | 0.6155 | 0.078* |
| H23A | 0.1646 | 0.1218 | 0.6685 | 0.078* |
| C24 | 0.0777 (4) | 0.2951 (13) | 0.5762 (3) | 0.0771 (18) |
| H24A | 0.1068 | 0.4505 | 0.5829 | 0.093* |
| H24B | 0.0477 | 0.3271 | 0.5979 | 0.093* |
| C25 | 0.0261 (3) | 0.2433 (12) | 0.4937 (3) | 0.0654 (15) |
| H25A | −0.0029 | 0.3987 | 0.4697 | 0.078* |
| H25B | −0.0088 | 0.1066 | 0.4868 | 0.078* |
| H4 | 0.1046 (19) | 0.457 (7) | 0.3124 (19) | 0.015 (8)* |
| H6 | 0.014 (3) | −0.052 (9) | 0.371 (3) | 0.037 (13)* |
| H5 | −0.038 (3) | −0.067 (11) | 0.248 (3) | 0.062 (17)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P1 | 0.0447 (5) | 0.0336 (4) | 0.0472 (5) | 0.0016 (5) | 0.0276 (4) | 0.0017 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O2 | 0.0546 (17) | 0.0351 (15) | 0.071 (2) | 0.0019 (13) | 0.0401 (17) | 0.0037 (14) |
| O3 | 0.061 (2) | 0.0334 (17) | 0.089 (3) | 0.0009 (14) | 0.047 (2) | 0.0017 (15) |
| N4 | 0.0453 (19) | 0.0326 (18) | 0.060 (2) | 0.0006 (15) | 0.0333 (18) | −0.0008 (15) |
| N5 | 0.048 (2) | 0.035 (2) | 0.047 (2) | 0.0003 (16) | 0.0244 (18) | 0.0047 (16) |
| N6 | 0.054 (2) | 0.044 (2) | 0.046 (2) | −0.0048 (18) | 0.0301 (19) | −0.0002 (17) |
| C7 | 0.0389 (19) | 0.036 (2) | 0.045 (2) | 0.0004 (17) | 0.0228 (18) | 0.0000 (17) |
| C8 | 0.041 (2) | 0.0367 (19) | 0.042 (2) | 0.0018 (17) | 0.0213 (18) | −0.0041 (17) |
| C9 | 0.052 (3) | 0.045 (2) | 0.059 (3) | 0.002 (2) | 0.035 (2) | −0.003 (2) |
| C10 | 0.068 (3) | 0.062 (3) | 0.076 (3) | −0.003 (3) | 0.053 (3) | −0.003 (3) |
| C11 | 0.055 (3) | 0.074 (4) | 0.091 (4) | −0.011 (3) | 0.050 (3) | −0.019 (3) |
| C12 | 0.037 (3) | 0.076 (4) | 0.091 (4) | 0.011 (2) | 0.026 (3) | −0.016 (3) |
| C13 | 0.046 (2) | 0.049 (3) | 0.057 (3) | 0.006 (2) | 0.022 (2) | −0.002 (2) |
| C14 | 0.048 (2) | 0.042 (2) | 0.045 (3) | 0.0027 (19) | 0.024 (2) | 0.0002 (19) |
| C15 | 0.064 (3) | 0.103 (5) | 0.050 (3) | −0.034 (3) | 0.030 (3) | −0.006 (3) |
| C16 | 0.059 (3) | 0.116 (5) | 0.064 (4) | −0.015 (3) | 0.023 (3) | −0.008 (4) |
| C17 | 0.079 (3) | 0.057 (3) | 0.052 (3) | 0.003 (3) | 0.032 (3) | 0.004 (2) |
| C18 | 0.107 (4) | 0.070 (4) | 0.067 (4) | −0.019 (4) | 0.054 (4) | −0.003 (3) |
| C19 | 0.060 (3) | 0.091 (4) | 0.056 (3) | −0.024 (3) | 0.033 (3) | 0.001 (3) |
| C20 | 0.045 (2) | 0.041 (2) | 0.045 (2) | 0.0004 (18) | 0.025 (2) | 0.0032 (18) |
| C21 | 0.074 (3) | 0.077 (4) | 0.057 (3) | 0.027 (3) | 0.037 (3) | 0.010 (3) |
| C22 | 0.065 (3) | 0.114 (5) | 0.051 (4) | 0.028 (4) | 0.022 (3) | 0.018 (3) |
| C23 | 0.083 (4) | 0.055 (3) | 0.053 (3) | −0.001 (3) | 0.034 (3) | 0.004 (2) |
| C24 | 0.102 (5) | 0.075 (4) | 0.056 (3) | 0.017 (4) | 0.043 (3) | 0.000 (3) |
| C25 | 0.071 (3) | 0.078 (4) | 0.057 (3) | 0.023 (3) | 0.040 (3) | 0.006 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| P1—O2 | 1.468 (3) | C16—C17 | 1.487 (8) |
| P1—N6 | 1.615 (4) | C16—H16A | 0.9700 |
| P1—N5 | 1.618 (4) | C16—H16B | 0.9700 |
| P1—N4 | 1.730 (4) | C17—C18 | 1.509 (8) |
| O3—C7 | 1.225 (5) | C17—H17B | 0.9700 |
| N4—C7 | 1.356 (5) | C17—H17A | 0.9700 |
| N4—H4 | 0.90 (4) | C18—C19 | 1.521 (9) |
| N5—C14 | 1.454 (6) | C18—H18A | 0.9700 |
| N5—H5 | 0.77 (5) | C18—H18B | 0.9700 |
| N6—C20 | 1.453 (6) | C19—H19A | 0.9700 |
| N6—H6 | 0.78 (4) | C19—H19B | 0.9700 |
| C7—C8 | 1.499 (6) | C20—C21 | 1.496 (7) |
| C8—C9 | 1.382 (6) | C20—C25 | 1.521 (6) |
| C8—C13 | 1.397 (6) | C20—H20 | 0.9800 |
| C9—C10 | 1.366 (7) | C21—C22 | 1.525 (8) |
| C9—H9 | 0.9300 | C21—H21A | 0.9700 |
| C10—C11 | 1.387 (8) | C21—H21B | 0.9700 |
| C10—H10 | 0.9300 | C22—C23 | 1.514 (8) |
| C11—C12 | 1.383 (9) | C22—H22A | 0.9700 |
| C11—H11 | 0.9300 | C22—H22B | 0.9700 |
| C12—C13 | 1.389 (7) | C23—C24 | 1.498 (8) |

| | | | |
|---|---|---|---|
| C12—H12 | 0.9300 | C23—H23B | 0.9700 |
| C13—H13 | 0.9300 | C23—H23A | 0.9700 |
| C14—C19 | 1.507 (7) | C24—C25 | 1.511 (8) |
| C14—C15 | 1.513 (7) | C24—H24A | 0.9700 |
| C14—H14 | 0.9800 | C24—H24B | 0.9700 |
| C15—C16 | 1.533 (8) | C25—H25A | 0.9700 |
| C15—H15A | 0.9700 | C25—H25B | 0.9700 |
| C15—H15B | 0.9700 | | |

| | | | |
|---|---|---|---|
| O2—P1—N6 | 117.2 (2) | C16—C17—C18 | 111.1 (5) |
| O2—P1—N5 | 115.7 (2) | C16—C17—H17B | 109.4 |
| N6—P1—N5 | 102.73 (19) | C18—C17—H17B | 109.4 |
| O2—P1—N4 | 103.77 (18) | C16—C17—H17A | 109.4 |
| N6—P1—N4 | 107.5 (2) | C18—C17—H17A | 109.4 |
| N5—P1—N4 | 109.79 (19) | H17B—C17—H17A | 108.0 |
| C7—N4—P1 | 123.0 (3) | C17—C18—C19 | 111.6 (5) |
| C7—N4—H4 | 113 (2) | C17—C18—H18A | 109.3 |
| P1—N4—H4 | 124 (2) | C19—C18—H18A | 109.3 |
| C14—N5—P1 | 125.4 (3) | C17—C18—H18B | 109.3 |
| C14—N5—H5 | 120 (4) | C19—C18—H18B | 109.3 |
| P1—N5—H5 | 109 (4) | H18A—C18—H18B | 108.0 |
| C20—N6—P1 | 125.2 (3) | C14—C19—C18 | 112.8 (5) |
| C20—N6—H6 | 113 (4) | C14—C19—H19A | 109.0 |
| P1—N6—H6 | 112 (4) | C18—C19—H19A | 109.0 |
| O3—C7—N4 | 122.2 (4) | C14—C19—H19B | 109.0 |
| O3—C7—C8 | 120.2 (4) | C18—C19—H19B | 109.0 |
| N4—C7—C8 | 117.6 (3) | H19A—C19—H19B | 107.8 |
| C9—C8—C13 | 118.6 (4) | N6—C20—C21 | 112.4 (4) |
| C9—C8—C7 | 123.4 (4) | N6—C20—C25 | 110.6 (4) |
| C13—C8—C7 | 117.9 (4) | C21—C20—C25 | 111.4 (4) |
| C10—C9—C8 | 121.6 (5) | N6—C20—H20 | 107.4 |
| C10—C9—H9 | 119.2 | C21—C20—H20 | 107.4 |
| C8—C9—H9 | 119.2 | C25—C20—H20 | 107.4 |
| C9—C10—C11 | 119.7 (5) | C20—C21—C22 | 113.7 (5) |
| C9—C10—H10 | 120.1 | C20—C21—H21A | 108.8 |
| C11—C10—H10 | 120.1 | C22—C21—H21A | 108.8 |
| C12—C11—C10 | 120.2 (5) | C20—C21—H21B | 108.8 |
| C12—C11—H11 | 119.9 | C22—C21—H21B | 108.8 |
| C10—C11—H11 | 119.9 | H21A—C21—H21B | 107.7 |
| C11—C12—C13 | 119.6 (5) | C23—C22—C21 | 111.5 (5) |
| C11—C12—H12 | 120.2 | C23—C22—H22A | 109.3 |
| C13—C12—H12 | 120.2 | C21—C22—H22A | 109.3 |
| C12—C13—C8 | 120.3 (5) | C23—C22—H22B | 109.3 |
| C12—C13—H13 | 119.9 | C21—C22—H22B | 109.3 |
| C8—C13—H13 | 119.9 | H22A—C22—H22B | 108.0 |
| N5—C14—C19 | 113.5 (4) | C24—C23—C22 | 110.6 (5) |
| N5—C14—C15 | 108.8 (4) | C24—C23—H23B | 109.5 |
| C19—C14—C15 | 110.2 (4) | C22—C23—H23B | 109.5 |

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| N5—C14—H14 | 108.1 | C24—C23—H23A | 109.5 |
| C19—C14—H14 | 108.1 | C22—C23—H23A | 109.5 |
| C15—C14—H14 | 108.1 | H23B—C23—H23A | 108.1 |
| C14—C15—C16 | 112.7 (5) | C23—C24—C25 | 112.7 (5) |
| C14—C15—H15A | 109.1 | C23—C24—H24A | 109.1 |
| C16—C15—H15A | 109.1 | C25—C24—H24A | 109.1 |
| C14—C15—H15B | 109.1 | C23—C24—H24B | 109.1 |
| C16—C15—H15B | 109.1 | C25—C24—H24B | 109.1 |
| H15A—C15—H15B | 107.8 | H24A—C24—H24B | 107.8 |
| C17—C16—C15 | 111.6 (5) | C24—C25—C20 | 113.2 (5) |
| C17—C16—H16A | 109.3 | C24—C25—H25A | 108.9 |
| C15—C16—H16A | 109.3 | C20—C25—H25A | 108.9 |
| C17—C16—H16B | 109.3 | C24—C25—H25B | 108.9 |
| C15—C16—H16B | 109.3 | C20—C25—H25B | 108.9 |
| H16A—C16—H16B | 108.0 | H25A—C25—H25B | 107.8 |

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| O2—P1—N4—C7 | −174.9 (4) | C7—C8—C13—C12 | 175.4 (4) |
| N6—P1—N4—C7 | 60.3 (4) | P1—N5—C14—C19 | 74.0 (5) |
| N5—P1—N4—C7 | −50.7 (4) | P1—N5—C14—C15 | −162.9 (4) |
| O2—P1—N5—C14 | 37.2 (4) | N5—C14—C15—C16 | −177.7 (5) |
| N6—P1—N5—C14 | 166.0 (4) | C19—C14—C15—C16 | −52.6 (7) |
| N4—P1—N5—C14 | −79.8 (4) | C14—C15—C16—C17 | 54.8 (8) |
| O2—P1—N6—C20 | −61.0 (4) | C15—C16—C17—C18 | −55.0 (8) |
| N5—P1—N6—C20 | 171.1 (4) | C16—C17—C18—C19 | 55.1 (8) |
| N4—P1—N6—C20 | 55.2 (4) | N5—C14—C19—C18 | 175.1 (5) |
| P1—N4—C7—O3 | −7.5 (6) | C15—C14—C19—C18 | 52.8 (7) |
| P1—N4—C7—C8 | 170.5 (3) | C17—C18—C19—C14 | −54.7 (8) |
| O3—C7—C8—C9 | 147.1 (4) | P1—N6—C20—C21 | −124.3 (4) |
| N4—C7—C8—C9 | −31.0 (6) | P1—N6—C20—C25 | 110.5 (4) |
| O3—C7—C8—C13 | −28.7 (6) | N6—C20—C21—C22 | −174.9 (5) |
| N4—C7—C8—C13 | 153.3 (4) | C25—C20—C21—C22 | −50.1 (7) |
| C13—C8—C9—C10 | 1.2 (7) | C20—C21—C22—C23 | 53.6 (7) |
| C7—C8—C9—C10 | −174.5 (5) | C21—C22—C23—C24 | −54.7 (7) |
| C8—C9—C10—C11 | −1.2 (8) | C22—C23—C24—C25 | 55.0 (7) |
| C9—C10—C11—C12 | 0.5 (8) | C23—C24—C25—C20 | −52.9 (7) |
| C10—C11—C12—C13 | 0.1 (8) | N6—C20—C25—C24 | 175.3 (5) |
| C11—C12—C13—C8 | −0.1 (8) | C21—C20—C25—C24 | 49.5 (7) |
| C9—C8—C13—C12 | −0.6 (7) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N4—H4···O3$^{i}$ | 0.90 (4) | 2.16 (4) | 2.988 (4) | 154 (3) |
| N5—H5···O2$^{ii}$ | 0.77 (5) | 2.30 (6) | 3.019 (5) | 156 (6) |

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