Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# The Phospha–Michael addition product {(*t*-BuNH)P(*μ*-N-*t*-Bu)$_2$P(=N-*t*-Bu)—C(=CH$_2$)CH(*p*-CH$_3$O—C$_6$H$_4$)-P(O)-[(OCH$_2$C(CH$_3$)$_2$CH$_2$O)]}

**G. Gangadhararao and Srinivas Venu***

School of Chemistry, University of Hyderabad, Hyderabad 500 046, India
Correspondence e-mail: venu.srinivas@gmail.com

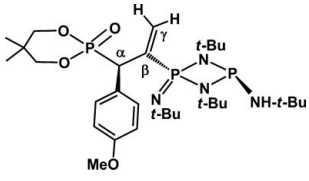
Received 4 February 2011; accepted 14 April 2011

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.049; $wR$ factor = 0.128; data-to-parameter ratio = 15.6.

The title compound, 2-{2-[1,3-di-*tert*-butyl-4-(*tert*-butyl amino)-2-(*tert*-butylimino)-1,3,2$\lambda^5$,4-diazadiphosphetidin-2-yl]-1-(4-methoxyphenyl)prop-2-en-1-yl}-5,5-dimethyl-1,3,2$\lambda^5$-dioxaphosphinan-2-one, C$_{31}$H$_{57}$N$_4$O$_4$P$_3$, was synthesized from the Phospha–Michael addition reaction of cyclodiphosphazane [(*t*-BuNH)P(*μ*-N*t*-Bu)]$_2$ and allenylphosphonate [(OCH$_2$C(CH$_3$)$_2$CH$_2$O)P(O)C(*p*-CH$_3$O—C$_6$H$_4$)=C=CH$_2$]. In the crystal, N—H···O and C—H···O hydrogen bonds link the molecules. The structure exhibits pseudosymmetry but attempts to solve it in a higher (monoclinic) space group were unsuccessful.

## Related literature

For background to cyclodiphosph(III)azanes, see: Rama Suresh *et al.* (2009); Balakrishna (2010); Balakrishna *et al.* (2010). For their use as probes for organic reactions (the P atom reacts readily with activated alkenes/alkynes or azodicarboxylates), see: Satish Kumar *et al.* (2004); Praveen Kumar *et al.* (2004); Balaraman & Kumara Swamy (2004); Bhuvan Kumar & Kumara Swamy (2007, 2008); Kumara Swamy *et al.* (2010, 2011). It has been shown recently that their reactions with allenes generates a chiral carbon center and in some cases spontaneous resolution by crystallization can be effected (Bhuvan Kumar & Kumara Swamy (2008). For related structures, see: Chakravarty *et al.* (2005); Kumara Swamy *et al.* (2010, 2011).




## Experimental

### Crystal data

C$_{31}$H$_{57}$N$_4$O$_4$P$_3$
$M_r$ = 642.72
Triclinic, $P\overline{1}$
$a$ = 13.8603 (9) Å
$b$ = 15.7746 (10) Å
$c$ = 16.2606 (11) Å
$\alpha$ = 88.004 (1)°
$\beta$ = 84.949 (1)°
$\gamma$ = 87.600 (1)°
$V$ = 3536.6 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.21 mm$^{-1}$
$T$ = 100 K
0.22 × 0.18 × 0.14 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.956, $T_{max}$ = 0.972
27730 measured reflections
12397 independent reflections
9894 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.128
$S$ = 1.01
12397 reflections
795 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N8—H8$D$···O1$^{i}$ | 0.82 (2) | 2.61 (3) | 3.394 (2) | 160 (2) |
| N4—H4$D$···O5$^{ii}$ | 0.84 (3) | 2.58 (3) | 3.378 (2) | 158 (2) |
| C26—H26$B$···O5$^{iii}$ | 0.96 | 2.49 | 3.325 (3) | 145 |

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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*.

The National Single Crystal Diffractometer Facility at the School of Chemistry, University of Hyderabad, funded by DST (New Delhi), and the UPE and the CAS programs of the UGC for other equipment are gratefully acknowledged. We thank Professor K. C. Kumara Swamy and Dr Srinivasulu Aitipamula for useful discussions. GG and VS thank the CSIR for fellowships.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2002).

## References

Balakrishna, M. S. (2010). *J. Organomet. Chem.* **695**, 925–936.
Balakrishna, M. S., Venkateswaran, R. & Mague, J. T. (2010). *Dalton Trans.* pp. 11149–11162.
Balaraman, E. & Kumara Swamy, K. C. (2004). *Synthesis*, pp. 3037–3042.
Bhuvan Kumar, N. N. & Kumara Swamy, K. C. (2007). *Polyhedron*, **26**, 883–890.
Bhuvan Kumar, N. N. & Kumara Swamy, K. C. (2008). *Tetrahedron Lett.* **49**, 7135–7138.

Bruker (2002). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Winsonsin, USA.
Chakravarty, M., Kommana, P. & Kumara Swamy, K. C. (2005). *Chem. Commun.* pp. 5396–5398.
Kumara Swamy, K. C., Gangadhararao, G., Rama Suresh, R., Bhuvan Kumar, N. N. & Chakravarty, M. (2010). *J. Organomet. Chem.* **695**, 1042–1051.
Kumara Swamy, K. C., Gangadhararao, G., Srinivas, V., Bhuvan Kumar, N. N., Balaraman, E. & Chakravarty, M. (2011). *Inorg. Chim. Acta*. In the press. doi:10.1016/j.ica.2010.12.072.
Praveen Kumar, K., Chakravarty, M. & Kumara Swamy, K. C. (2004). *Z. Anorg. Allg. Chem.* **630**, 2063-2070.
Rama Suresh, R. & Kumara Swamy, K. C. (2009). *Tetrahedron Lett.* **50**, 6004–6007.
Satish Kumar, N., Praveen Kumar, K., Pavan Kumar, K. V. P., Kommana, P., Vittal, J. J. & Kumara Swamy, K. C. (2004). *J. Org. Chem.* **69**, 1880–1889.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2011). E**67**, o1212–o1213 [doi:10.1107/S1600536811014127]

# The Phospha–Michael addition product {(*t*-BuNH)P($\mu$-N-*t*-Bu)$_2$P(&z-dbnd;N-*t*-Bu)—C(&z-dbnd;CH$_2$)CH(*p*-CH$_3$O—C$_6$H$_4$)-P(O)[(OCH$_2$C(CH$_3$)$_2$CH$_2$O)]}

**G. Gangadhararao and Srinivas Venu**

## S1. Comment

Cyclodiphosph(III)azanes are good phosphorus based ligands (Rama Suresh *et al.*, 2009; Balakrishna *et al.*, 2010). They can also act as probes for organic reactions since the P(III) centre reacts readily with activated alkenes/ alkynes or azodicarboxylates (Satish Kumar *et al.*, 2004; Praveen Kumar *et al.*, 2004; Balaraman *et al.*, 2004; Bhuvan Kumar *et al.*, 2007; 2008; Kumara Swamy *et al.*, 2010; 2011). It has been shown recently that their reactions with allenes generates a chiral carbon center and in some cases spontaneous resolution by crystallization can be effected (Bhuvan Kumar *et al.*, 2008). To probe this aspect further we reacted cyclodiphosph(III)azane [(*t*-BuNH)P($\mu$-N-*t*-Bu)]$_2$ (1a) with allene (OCH$_2$CMe$_2$CH$_2$O)P(O)C(C$_6$H$_4$-*p*-OCH$_3$)═C═CH$_2$ (1b). The reaction afforded compound 1 (Scheme 1) as essentially a single product. The X-ray structure of compound 1 [Figure 1] clearly show the phosphinimine moiety at P(2) and P(5) with P—N distances of 1.546 (4) and 1.546 (1) that are slightly longer than the structures reported earlier (Chakravarty *et al.*, 2005; Kumara Swamy *et al.*, 2010). However, these are still in the range expected for P=N distances; the P—N single bond distances in the cyclophosphazane ring also lie in the same range of the previously reported structures (Kumara Swamy *et al.*, 2011). However, the P—N(ring) distances involving P(III) phosphorus atoms are comparatively longer than that for P(V) phosphorus. The P–C distances are also in line with the structures as written. The P—N—P and N—P—N bond angles are also in the expected range.The crystal packing in compound 1 is mostly governed by classical hydrogen bonds. The two molecules in the asymmetric unit are extended in a one-dimensional fashion through N—H···O interactions [N(4)—H(4D)···O5 and N(8)—H(8D)···O(1)] (Figure 2). But only the first molecule was also having C—H···O(=P) [C26—H(26B)···O(5)] interactions by OC*H*$_3$ hydrogen and with the phosphoryl oxygen (P═*O*) of the second molecule. The crystal structure is showing an alert due to the psuedo symmetry. We have investigated the possibility of solving in higher symmetry space group and also the presence of pseudo-centre of symmetry. All our attempts to solve the structure in a higher symmetry (in Monoclinic) space group were not successful. Therefore, we strongly believe that there is only a pseudo-symmetry.

## S2. Experimental

**Comopound 1:** This compound (**1**) was obtained by the reaction of cyclodiphosphazane **1a** (0.561 g, 1.61 mmol) and allenylphosphonate **1b** (0 474 g, 1.61 mmol) in dry toluene (8 ml) for 20 h. The solution (toluene) was concentrated *in vacuo* (to *ca* 3 ml) and cooled for 1 day at -4°C to obtain the colorless crystals of product. Yield: 0.956 g (92%). mp: 150–154°C. IR (KBr, cm$^{-1}$): 3337, 2967, 2897, 1615, 1584, 1510, 1464, 1364, 1281, 1209, 1063, 1028, 885. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 0.83, 1.08, 1.18, 1.29 and 1.37 (5 s, 42H, C(C*H*$_3$)$_2$+C(C*H*$_3$)$_3$), 2.69 (d, $^2J$(P—H) = 7.6 Hz, 1H, N*H*), 3.78 (s, 3H, Ar—OC*H*$_3$) 3.82–4.36 (m, 4H, OC*H*$_2$), 5.76 (d, $^3J$(P—H) = 28.8 Hz, 1H, =C*H*$_A$H$_B$ *cis* to P), 6.00 (dd, $^3J$(P—H) = 15.2 Hz, $^2J$(P—H) = 18.0 Hz, 1H, P(O)C*H*), 6.76 (d, $^3J$(P—H) = 52.4 Hz, 1H, =CH$_A$*H*$_B$ *trans* to P), 6.81 (d, $^3J$(H—H) = 8.4 Hz, 2H, Ar-*H)*, 7.47 (d, $^3J$(H—H) = 8.0 Hz, 2H, Ar-*H*). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 20.81 and 21.85 (2 s,

C($CH_3$)$_2$), 31.10 (d, $^3J$(P—C) = 23.4 Hz, C($CH_3$)$_3$), 32.31 (d, $^3J$(P—C) = 6.0 Hz, C($CH_3$)$_3$), 32.78 (d, $^3J$(P—C) = 9.2 Hz, C($CH_3$)$_3$), 34.39 (d, $^3J$(P—C) = 11.2 Hz, C($CH_3$)$_3$), 40.72 (d, $^1J$(P—C) = 125.4 Hz, P(O)$C$(Ar)), 51.31 (d, $^2J$(P—C) = 14.5 Hz, $C$($CH_3$)$_3$), 52.25 (d, $^2J$(P—C) = 8.8 Hz, $C$($CH_3$)$_3$), 52.51 (d, $^2J$(P—C) = 7.7 Hz, $C$($CH_3$)$_3$), 55.08 (Ar—O$CH_3$),76.38 and 76.42 (2 s, O$CH_2$), 113.52, 128.06, 131.05, 131.12, 158.67 (d, $^2J$(P—C) = 6.4 Hz, Ar-$C$ + PC=$CH_2$), 143.56 (d, $^1J$(P—C) = 159.0 Hz, P$C$=$CH_2$). $^{31}$P NMR (160 MHz, $CDCl_3$): $\delta$ -18.90 (dd, $^3J$(P—P) = 35.8 Hz, $^2J$(P—P) = 6.7 Hz), 20.91 (d, $^3J$(P—P) = 35.8 Hz), 70.99 (br d, $^2J$(P—P) = 6.7 Hz). LC—MS: m/$z$ 643 [$M$+1]$^+$. Anal. Calc. For $C_{31}H_{57}N_4O_4P_3$: C, 57.93; H, 8.94; N, 8.72. Found: C, 57.79; H, 8.98; N, 8.82. A suitable crystal (Shape: blocks: Size: 0.22 $x$ 0.18 $x$ 0.14 mm$^3$) was mounted on a glass fibre and data was collected on BRUKER *SMART* diffractometer at 100 K.

### S3. Refinement

All H atoms were found on difference maps, with C—H=0.93 Å and included in the final cycles of refinement using a riding model, with $U_{iso}$(H)=1.2Ueq(C)

The structure was solved by direct methods and refined by full-matrix least squares methods using standard procedures. Absorption corrections were done using the *SADABS* program, where applicable. All non-hydrogen atoms were refined anisotropically; hydrogen atoms were fixed by geometry or located by a difference Fourier and refined isotropically.

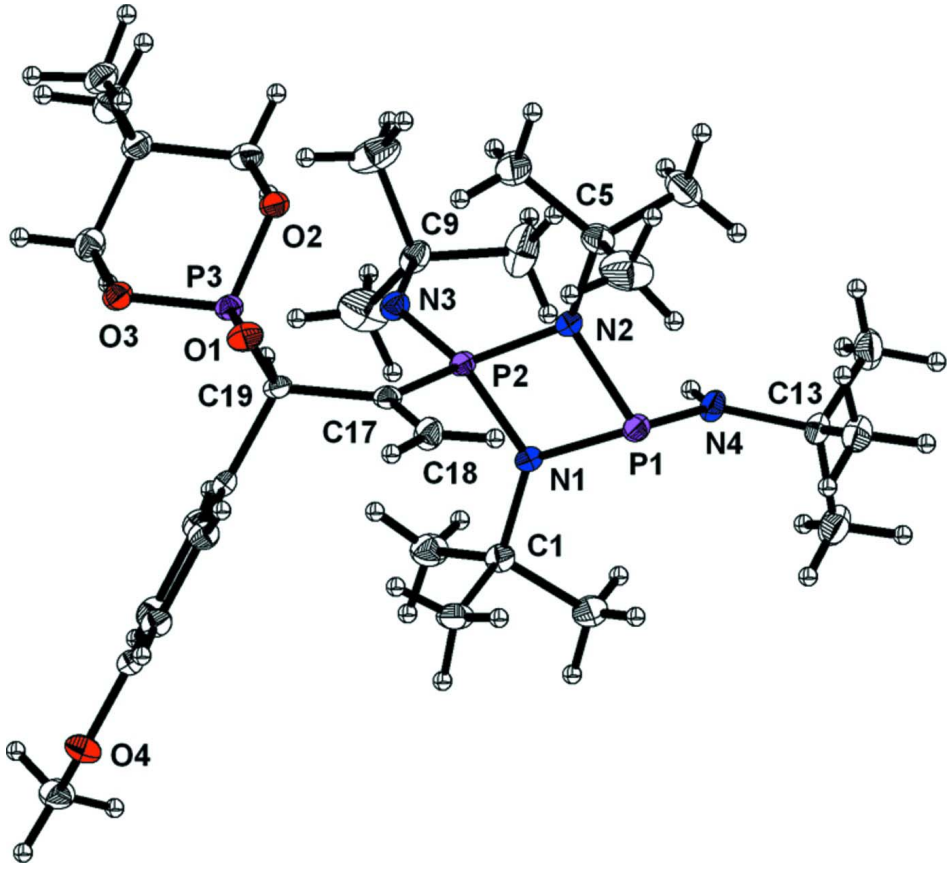



**Figure 1**

An *ORTEP* representation of compound **1** (Thermal ellipsoids are at 50% probability level). Two molecules are present in the asymmetric unit. Second molecule is not shown for clarity.

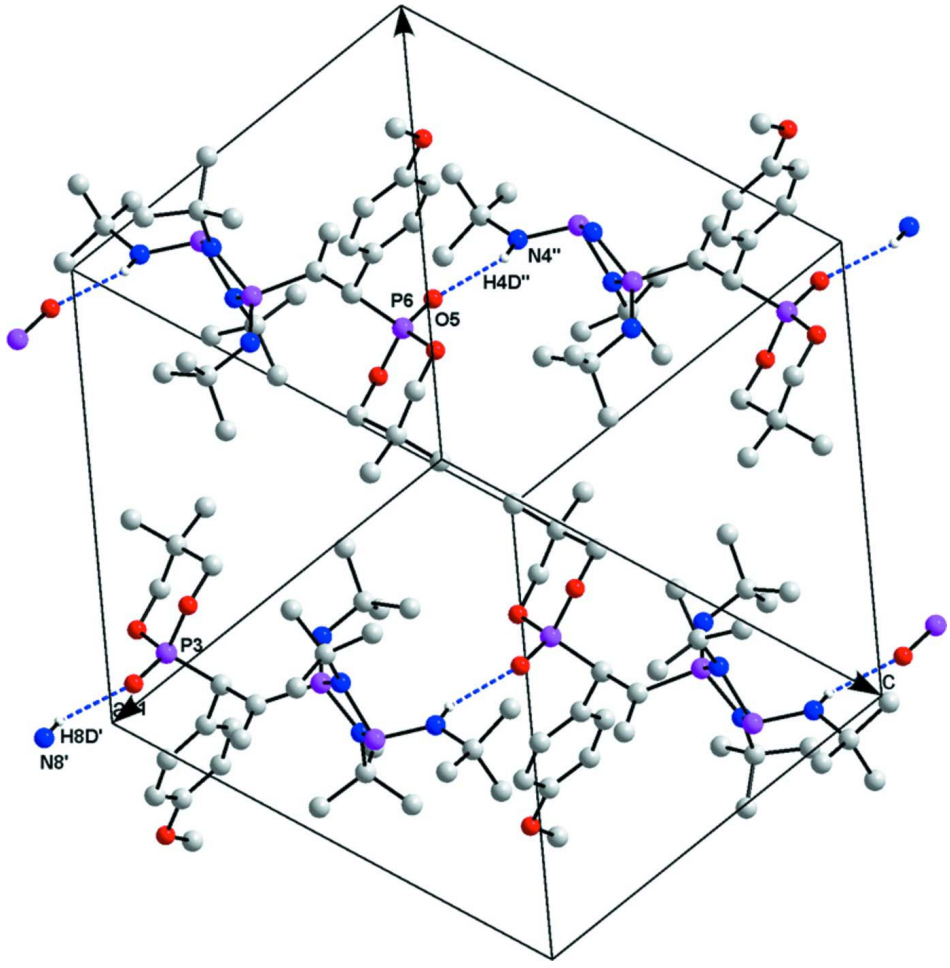



**Figure 2**

1-Dimensional structural unit due to the N—H···O interactions in the crystal structure of compound **1**.

**2-{2-[1,3-di-*tert*-butyl-4-(tert-butylamino)-2-(tert-butylimino)- 1,3,2$\lambda^5$,4-diazadiphosphetidin-2-yl]-1-(4-methoxyphenyl)prop-2-en-1-yl}- 5,5-dimethyl-1,3,2$\lambda^5$-dioxaphosphinan-2-one**

*Crystal data*

$C_{31}H_{57}N_4O_4P_3$
$M_r$ = 642.72
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 13.8603 (9) Å
$b$ = 15.7746 (10) Å
$c$ = 16.2606 (11) Å
$\alpha$ = 88.004 (1)°
$\beta$ = 84.949 (1)°
$\gamma$ = 87.600 (1)°
$V$ = 3536.6 (4) Å$^3$

$Z$ = 4
$F$(000) = 1392
$D_x$ = 1.207 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 6427 reflections
$\theta$ = 2.4–26.0°
$\mu$ = 0.21 mm$^{-1}$
$T$ = 100 K
Blocks, colorless
0.22 × 0.18 × 0.14 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)
$T_{min}$ = 0.956, $T_{max}$ = 0.972
27730 measured reflections
12397 independent reflections
9894 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.3°
$h$ = −16→16
$k$ = −18→18
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.128
$S$ = 1.01
12397 reflections
795 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 1.2977P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.54 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.28 e Å$^{-3}$

*Special details*

**Experimental**. A colorless block with approximate orthogonal dimensions 0.22 *x* 0.18 *x* 0.14 mm3 was placed and optically centered on the Bruker *SMART* CCD system at 100 (2) K.

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| P5 | 0.59309 (4) | 0.74569 (3) | 0.08104 (3) | 0.01270 (13) |
| P6 | 0.40564 (4) | 0.66855 (3) | 0.27677 (3) | 0.01388 (13) |
| P4 | 0.66984 (4) | 0.88814 (3) | 0.03551 (3) | 0.01523 (14) |
| O5 | 0.37256 (11) | 0.74031 (9) | 0.32774 (9) | 0.0187 (3) |
| O8 | 0.03668 (11) | 0.75573 (10) | 0.05412 (9) | 0.0233 (4) |
| O6 | 0.33881 (10) | 0.58979 (9) | 0.29393 (9) | 0.0169 (3) |
| O7 | 0.50990 (10) | 0.63320 (9) | 0.29590 (9) | 0.0157 (3) |
| N6 | 0.67820 (12) | 0.80751 (11) | 0.11155 (10) | 0.0148 (4) |
| C54 | 0.12697 (15) | 0.73681 (13) | 0.07809 (13) | 0.0170 (5) |
| C48 | 0.47736 (15) | 0.76502 (13) | 0.14219 (12) | 0.0137 (4) |
| C55 | 0.14671 (15) | 0.76903 (13) | 0.15315 (13) | 0.0168 (5) |
| H55 | 0.0990 | 0.8006 | 0.1837 | 0.020* |
| N7 | 0.60389 (12) | 0.64798 (11) | 0.07626 (10) | 0.0155 (4) |
| C51 | 0.30881 (15) | 0.70578 (13) | 0.13897 (12) | 0.0143 (4) |

| | | | | |
|---|---|---|---|---|
| N8 | 0.77127 (13) | 0.88560 (12) | −0.02712 (12) | 0.0186 (4) |
| C56 | 0.23648 (15) | 0.75457 (13) | 0.18261 (13) | 0.0173 (5) |
| H56 | 0.2490 | 0.7776 | 0.2323 | 0.021* |
| C58 | 0.54361 (15) | 0.55016 (13) | 0.26565 (13) | 0.0175 (5) |
| H58A | 0.6067 | 0.5355 | 0.2849 | 0.021* |
| H58B | 0.5507 | 0.5526 | 0.2057 | 0.021* |
| C35 | 0.45625 (16) | 0.76226 (15) | −0.06387 (14) | 0.0235 (5) |
| H35A | 0.4821 | 0.7054 | −0.0563 | 0.035* |
| H35B | 0.4217 | 0.7659 | −0.1126 | 0.035* |
| H35C | 0.4128 | 0.7768 | −0.0168 | 0.035* |
| C52 | 0.28674 (15) | 0.67198 (13) | 0.06574 (13) | 0.0151 (5) |
| H52 | 0.3332 | 0.6377 | 0.0367 | 0.018* |
| C36 | 0.72204 (16) | 0.81403 (14) | 0.19125 (13) | 0.0187 (5) |
| C49 | 0.45156 (16) | 0.84466 (13) | 0.16018 (13) | 0.0193 (5) |
| H49A | 0.3916 | 0.8571 | 0.1884 | 0.023* |
| H49B | 0.4934 | 0.8881 | 0.1446 | 0.023* |
| C57 | 0.01704 (17) | 0.72673 (15) | −0.02482 (14) | 0.0245 (5) |
| H57A | 0.0615 | 0.7511 | −0.0668 | 0.037* |
| H57B | −0.0482 | 0.7436 | −0.0355 | 0.037* |
| H57C | 0.0246 | 0.6660 | −0.0252 | 0.037* |
| C53 | 0.19755 (15) | 0.68757 (13) | 0.03410 (13) | 0.0171 (5) |
| H53 | 0.1853 | 0.6653 | −0.0160 | 0.020* |
| C32 | 0.53851 (15) | 0.82327 (13) | −0.07322 (13) | 0.0165 (5) |
| C40 | 0.68215 (16) | 0.59654 (13) | 0.03178 (13) | 0.0176 (5) |
| C59 | 0.47325 (16) | 0.48183 (13) | 0.29526 (13) | 0.0189 (5) |
| N5 | 0.59713 (12) | 0.81344 (11) | −0.00120 (10) | 0.0148 (4) |
| C50 | 0.41072 (15) | 0.69154 (13) | 0.16671 (12) | 0.0140 (4) |
| H50 | 0.4396 | 0.6411 | 0.1392 | 0.017* |
| C34 | 0.49557 (18) | 0.91388 (14) | −0.07822 (15) | 0.0268 (6) |
| H34A | 0.4531 | 0.9245 | −0.0295 | 0.040* |
| H34B | 0.4597 | 0.9209 | −0.1261 | 0.040* |
| H34C | 0.5469 | 0.9532 | −0.0822 | 0.040* |
| C60 | 0.37424 (16) | 0.50669 (13) | 0.26594 (14) | 0.0205 (5) |
| H60A | 0.3786 | 0.5070 | 0.2061 | 0.025* |
| H60B | 0.3283 | 0.4646 | 0.2864 | 0.025* |
| C33 | 0.60321 (17) | 0.80532 (15) | −0.15207 (13) | 0.0237 (5) |
| H33A | 0.6539 | 0.8453 | −0.1586 | 0.036* |
| H33B | 0.5652 | 0.8107 | −0.1987 | 0.036* |
| H33C | 0.6312 | 0.7488 | −0.1485 | 0.036* |
| C61 | 0.50832 (18) | 0.39855 (14) | 0.25481 (15) | 0.0277 (6) |
| H61A | 0.5107 | 0.4061 | 0.1958 | 0.041* |
| H61B | 0.4644 | 0.3548 | 0.2726 | 0.041* |
| H61C | 0.5719 | 0.3826 | 0.2706 | 0.041* |
| C44 | 0.82293 (16) | 0.96108 (13) | −0.06183 (14) | 0.0189 (5) |
| C45 | 0.78670 (18) | 0.98684 (15) | −0.14567 (15) | 0.0296 (6) |
| H45A | 0.7964 | 0.9399 | −0.1819 | 0.044* |
| H45B | 0.8221 | 1.0341 | −0.1692 | 0.044* |
| H45C | 0.7189 | 1.0027 | −0.1385 | 0.044* |

| | | | | |
|---|---|---|---|---|
| C43 | 0.70774 (17) | 0.52019 (14) | 0.08743 (14) | 0.0247 (5) |
| H43A | 0.7288 | 0.5397 | 0.1379 | 0.037* |
| H43B | 0.7589 | 0.4862 | 0.0597 | 0.037* |
| H43C | 0.6517 | 0.4867 | 0.0996 | 0.037* |
| C37 | 0.82582 (18) | 0.84214 (18) | 0.17242 (16) | 0.0358 (7) |
| H37A | 0.8616 | 0.8018 | 0.1375 | 0.054* |
| H37B | 0.8560 | 0.8454 | 0.2231 | 0.054* |
| H37C | 0.8252 | 0.8969 | 0.1448 | 0.054* |
| C39 | 0.72334 (17) | 0.72728 (14) | 0.23515 (14) | 0.0246 (5) |
| H39A | 0.6581 | 0.7093 | 0.2470 | 0.037* |
| H39B | 0.7534 | 0.7308 | 0.2859 | 0.037* |
| H39C | 0.7594 | 0.6870 | 0.2004 | 0.037* |
| C62 | 0.46740 (17) | 0.47035 (14) | 0.38906 (13) | 0.0224 (5) |
| H62A | 0.5285 | 0.4478 | 0.4054 | 0.034* |
| H62B | 0.4175 | 0.4318 | 0.4069 | 0.034* |
| H62C | 0.4526 | 0.5242 | 0.4138 | 0.034* |
| C41 | 0.64407 (17) | 0.56365 (14) | −0.04624 (13) | 0.0225 (5) |
| H41A | 0.5857 | 0.5339 | −0.0315 | 0.034* |
| H41B | 0.6920 | 0.5258 | −0.0730 | 0.034* |
| H41C | 0.6306 | 0.6106 | −0.0832 | 0.034* |
| C38 | 0.6647 (2) | 0.87766 (16) | 0.24708 (15) | 0.0341 (6) |
| H38A | 0.6593 | 0.9315 | 0.2180 | 0.051* |
| H38B | 0.6976 | 0.8843 | 0.2958 | 0.051* |
| H38C | 0.6011 | 0.8573 | 0.2624 | 0.051* |
| C42 | 0.77415 (16) | 0.64415 (14) | 0.00713 (14) | 0.0232 (5) |
| H42A | 0.7601 | 0.6900 | −0.0309 | 0.035* |
| H42B | 0.8225 | 0.6060 | −0.0187 | 0.035* |
| H42C | 0.7978 | 0.6664 | 0.0554 | 0.035* |
| C47 | 0.80763 (18) | 1.03499 (14) | −0.00409 (15) | 0.0288 (6) |
| H47A | 0.7402 | 1.0522 | 0.0015 | 0.043* |
| H47B | 0.8450 | 1.0817 | −0.0264 | 0.043* |
| H47C | 0.8281 | 1.0178 | 0.0491 | 0.043* |
| C46 | 0.93066 (16) | 0.93594 (15) | −0.07427 (15) | 0.0258 (5) |
| H46A | 0.9538 | 0.9188 | −0.0221 | 0.039* |
| H46B | 0.9659 | 0.9835 | −0.0973 | 0.039* |
| H46C | 0.9400 | 0.8896 | −0.1113 | 0.039* |
| P2 | 0.89633 (4) | 0.24677 (3) | 0.41973 (3) | 0.01371 (13) |
| P1 | 0.82093 (4) | 0.10583 (3) | 0.47234 (3) | 0.01574 (14) |
| P3 | 1.09056 (4) | 0.32194 (3) | 0.22058 (3) | 0.01479 (14) |
| O4 | 1.43525 (11) | 0.25060 (10) | 0.47038 (9) | 0.0215 (4) |
| O2 | 0.98715 (10) | 0.35323 (9) | 0.19487 (9) | 0.0164 (3) |
| O1 | 1.13188 (11) | 0.25206 (9) | 0.17058 (9) | 0.0196 (3) |
| O3 | 1.15386 (10) | 0.40346 (9) | 0.20836 (9) | 0.0179 (3) |
| C23 | 1.34641 (15) | 0.26494 (13) | 0.44149 (13) | 0.0164 (5) |
| C21 | 1.18557 (15) | 0.32641 (13) | 0.44112 (13) | 0.0162 (5) |
| H21 | 1.1360 | 0.3610 | 0.4657 | 0.019* |
| N1 | 0.89654 (12) | 0.18141 (11) | 0.50433 (10) | 0.0151 (4) |
| C25 | 1.24771 (15) | 0.23654 (13) | 0.33221 (13) | 0.0167 (5) |

| | | | | |
|---|---|---|---|---|
| H25 | 1.2400 | 0.2092 | 0.2836 | 0.020* |
| C18 | 1.02663 (16) | 0.14940 (13) | 0.32540 (13) | 0.0197 (5) |
| H18A | 1.0838 | 0.1376 | 0.2928 | 0.024* |
| H18B | 0.9835 | 0.1066 | 0.3394 | 0.024* |
| C17 | 1.00657 (15) | 0.22708 (13) | 0.35183 (12) | 0.0143 (4) |
| N3 | 0.88579 (13) | 0.34459 (11) | 0.42252 (11) | 0.0172 (4) |
| C19 | 1.07475 (15) | 0.30000 (13) | 0.33072 (12) | 0.0139 (4) |
| H19 | 1.0426 | 0.3508 | 0.3553 | 0.017* |
| N2 | 0.81034 (12) | 0.18369 (11) | 0.39409 (11) | 0.0157 (4) |
| C28 | 1.01401 (16) | 0.50577 (13) | 0.20302 (13) | 0.0184 (5) |
| C24 | 1.33385 (15) | 0.22616 (13) | 0.36802 (13) | 0.0171 (5) |
| H24 | 1.3842 | 0.1928 | 0.3428 | 0.020* |
| C20 | 1.17163 (15) | 0.28768 (13) | 0.36797 (13) | 0.0148 (4) |
| C26 | 1.45102 (17) | 0.28712 (14) | 0.54678 (13) | 0.0231 (5) |
| H26A | 1.4407 | 0.3476 | 0.5423 | 0.035* |
| H26B | 1.5163 | 0.2739 | 0.5596 | 0.035* |
| H26C | 1.4067 | 0.2644 | 0.5898 | 0.035* |
| N4 | 0.72237 (13) | 0.11378 (12) | 0.53761 (11) | 0.0174 (4) |
| C29 | 0.94605 (16) | 0.43378 (13) | 0.22661 (13) | 0.0182 (5) |
| H29A | 0.9348 | 0.4289 | 0.2863 | 0.022* |
| H29B | 0.8842 | 0.4465 | 0.2043 | 0.022* |
| C5 | 0.75761 (16) | 0.17757 (14) | 0.31903 (14) | 0.0219 (5) |
| C27 | 1.11183 (16) | 0.48426 (13) | 0.23657 (14) | 0.0204 (5) |
| H27A | 1.1561 | 0.5287 | 0.2192 | 0.024* |
| H27B | 1.1036 | 0.4825 | 0.2965 | 0.024* |
| C13 | 0.66233 (16) | 0.04273 (13) | 0.57061 (14) | 0.0189 (5) |
| C4 | 0.98429 (18) | 0.25201 (14) | 0.60522 (14) | 0.0261 (5) |
| H4A | 1.0054 | 0.2922 | 0.5624 | 0.039* |
| H4B | 1.0331 | 0.2441 | 0.6435 | 0.039* |
| H4C | 0.9250 | 0.2730 | 0.6338 | 0.039* |
| C2 | 0.92494 (17) | 0.10746 (15) | 0.63526 (14) | 0.0249 (5) |
| H2A | 0.8647 | 0.1316 | 0.6594 | 0.037* |
| H2B | 0.9695 | 0.0990 | 0.6770 | 0.037* |
| H2C | 0.9138 | 0.0539 | 0.6121 | 0.037* |
| C3 | 1.06421 (16) | 0.12822 (15) | 0.53081 (14) | 0.0237 (5) |
| H3A | 1.0527 | 0.0767 | 0.5042 | 0.036* |
| H3B | 1.1058 | 0.1159 | 0.5742 | 0.036* |
| H3C | 1.0947 | 0.1674 | 0.4912 | 0.036* |
| C7 | 0.64933 (17) | 0.17330 (18) | 0.34434 (16) | 0.0352 (6) |
| H7A | 0.6375 | 0.1238 | 0.3793 | 0.053* |
| H7B | 0.6149 | 0.1702 | 0.2959 | 0.053* |
| H7C | 0.6274 | 0.2232 | 0.3738 | 0.053* |
| C30 | 0.97184 (18) | 0.58638 (14) | 0.24454 (15) | 0.0284 (6) |
| H30A | 0.9085 | 0.5997 | 0.2270 | 0.043* |
| H30B | 1.0133 | 0.6326 | 0.2293 | 0.043* |
| H30C | 0.9673 | 0.5774 | 0.3034 | 0.043* |
| C16 | 0.67254 (17) | −0.03126 (14) | 0.51240 (14) | 0.0237 (5) |
| H16A | 0.6572 | −0.0117 | 0.4583 | 0.036* |

| | | | | |
|---|---|---|---|---|
| H16B | 0.6289 | −0.0745 | 0.5326 | 0.036* |
| H16C | 0.7379 | −0.0542 | 0.5095 | 0.036* |
| C9 | 0.80892 (16) | 0.39872 (13) | 0.46543 (13) | 0.0195 (5) |
| C1 | 0.96760 (16) | 0.16767 (13) | 0.56725 (13) | 0.0177 (5) |
| C31 | 1.02493 (17) | 0.51997 (14) | 0.10952 (13) | 0.0229 (5) |
| H31A | 1.0457 | 0.4676 | 0.0838 | 0.034* |
| H31B | 1.0722 | 0.5619 | 0.0950 | 0.034* |
| H31C | 0.9638 | 0.5393 | 0.0908 | 0.034* |
| C14 | 0.55715 (16) | 0.07624 (15) | 0.57986 (16) | 0.0283 (6) |
| H14A | 0.5510 | 0.1221 | 0.6174 | 0.043* |
| H14B | 0.5161 | 0.0315 | 0.6010 | 0.043* |
| H14C | 0.5382 | 0.0962 | 0.5270 | 0.043* |
| C15 | 0.69229 (18) | 0.01271 (15) | 0.65535 (14) | 0.0283 (6) |
| H15A | 0.7562 | −0.0135 | 0.6493 | 0.042* |
| H15B | 0.6473 | −0.0276 | 0.6796 | 0.042* |
| H15C | 0.6922 | 0.0604 | 0.6904 | 0.042* |
| C12 | 0.7760 (2) | 0.46657 (16) | 0.40394 (16) | 0.0368 (7) |
| H12A | 0.8295 | 0.5010 | 0.3852 | 0.055* |
| H12B | 0.7247 | 0.5015 | 0.4302 | 0.055* |
| H12C | 0.7529 | 0.4399 | 0.3576 | 0.055* |
| C6 | 0.77596 (19) | 0.25584 (16) | 0.26283 (15) | 0.0331 (6) |
| H6A | 0.7556 | 0.3060 | 0.2924 | 0.050* |
| H6B | 0.7399 | 0.2530 | 0.2153 | 0.050* |
| H6C | 0.8439 | 0.2577 | 0.2454 | 0.050* |
| C11 | 0.8506 (2) | 0.44271 (16) | 0.53541 (17) | 0.0392 (7) |
| H11A | 0.8656 | 0.4014 | 0.5777 | 0.059* |
| H11B | 0.8039 | 0.4841 | 0.5582 | 0.059* |
| H11C | 0.9085 | 0.4703 | 0.5146 | 0.059* |
| C10 | 0.72105 (18) | 0.35083 (15) | 0.49979 (17) | 0.0358 (7) |
| H10A | 0.6933 | 0.3244 | 0.4556 | 0.054* |
| H10B | 0.6740 | 0.3896 | 0.5263 | 0.054* |
| H10C | 0.7402 | 0.3081 | 0.5393 | 0.054* |
| C8 | 0.7922 (2) | 0.09845 (17) | 0.27171 (17) | 0.0404 (7) |
| H8A | 0.8581 | 0.1045 | 0.2494 | 0.061* |
| H8B | 0.7519 | 0.0916 | 0.2275 | 0.061* |
| H8C | 0.7883 | 0.0495 | 0.3085 | 0.061* |
| C22 | 1.27127 (16) | 0.31485 (13) | 0.47850 (13) | 0.0182 (5) |
| H22 | 1.2784 | 0.3404 | 0.5282 | 0.022* |
| H4D | 0.7089 (18) | 0.1594 (17) | 0.5623 (16) | 0.032 (7)* |
| H8D | 0.7859 (18) | 0.8433 (16) | −0.0543 (15) | 0.026 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P5 | 0.0127 (3) | 0.0133 (3) | 0.0118 (3) | 0.0010 (2) | −0.0003 (2) | 0.0008 (2) |
| P6 | 0.0142 (3) | 0.0154 (3) | 0.0120 (3) | −0.0005 (2) | −0.0021 (2) | 0.0019 (2) |
| P4 | 0.0160 (3) | 0.0137 (3) | 0.0158 (3) | 0.0000 (2) | −0.0008 (2) | 0.0016 (2) |
| O5 | 0.0221 (8) | 0.0195 (8) | 0.0140 (8) | 0.0026 (6) | −0.0009 (6) | −0.0003 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O8 | 0.0168 (8) | 0.0291 (9) | 0.0250 (9) | 0.0032 (7) | −0.0088 (7) | −0.0021 (7) |
| O6 | 0.0161 (8) | 0.0170 (8) | 0.0171 (8) | −0.0010 (6) | −0.0005 (6) | 0.0034 (6) |
| O7 | 0.0162 (8) | 0.0151 (8) | 0.0162 (8) | −0.0006 (6) | −0.0040 (6) | 0.0021 (6) |
| N6 | 0.0150 (9) | 0.0154 (9) | 0.0140 (9) | −0.0006 (7) | −0.0026 (7) | 0.0019 (7) |
| C54 | 0.0142 (11) | 0.0157 (11) | 0.0216 (12) | −0.0008 (9) | −0.0067 (9) | 0.0056 (9) |
| C48 | 0.0144 (11) | 0.0163 (11) | 0.0106 (10) | 0.0003 (9) | −0.0031 (9) | 0.0021 (8) |
| C55 | 0.0170 (11) | 0.0143 (11) | 0.0186 (11) | 0.0015 (9) | 0.0004 (9) | −0.0002 (9) |
| N7 | 0.0150 (9) | 0.0159 (9) | 0.0149 (9) | 0.0027 (7) | 0.0000 (7) | −0.0002 (7) |
| C51 | 0.0157 (11) | 0.0124 (10) | 0.0147 (11) | −0.0011 (8) | −0.0017 (9) | 0.0024 (8) |
| N8 | 0.0208 (10) | 0.0127 (10) | 0.0215 (10) | −0.0016 (8) | 0.0022 (8) | 0.0007 (8) |
| C56 | 0.0183 (12) | 0.0174 (11) | 0.0163 (11) | −0.0002 (9) | −0.0034 (9) | −0.0009 (9) |
| C58 | 0.0170 (11) | 0.0166 (11) | 0.0185 (11) | 0.0034 (9) | −0.0023 (9) | 0.0014 (9) |
| C35 | 0.0223 (13) | 0.0314 (13) | 0.0176 (12) | −0.0053 (10) | −0.0072 (10) | 0.0041 (10) |
| C52 | 0.0161 (11) | 0.0127 (10) | 0.0161 (11) | 0.0000 (9) | 0.0010 (9) | 0.0003 (8) |
| C36 | 0.0176 (12) | 0.0229 (12) | 0.0167 (11) | −0.0027 (9) | −0.0058 (9) | −0.0003 (9) |
| C49 | 0.0176 (12) | 0.0172 (11) | 0.0219 (12) | −0.0003 (9) | 0.0042 (10) | 0.0016 (9) |
| C57 | 0.0242 (13) | 0.0259 (13) | 0.0254 (13) | −0.0018 (10) | −0.0137 (10) | 0.0034 (10) |
| C53 | 0.0217 (12) | 0.0165 (11) | 0.0138 (11) | −0.0030 (9) | −0.0047 (9) | 0.0001 (9) |
| C32 | 0.0180 (11) | 0.0177 (11) | 0.0144 (11) | 0.0013 (9) | −0.0062 (9) | 0.0017 (9) |
| C40 | 0.0190 (12) | 0.0145 (11) | 0.0186 (11) | 0.0038 (9) | 0.0014 (9) | −0.0014 (9) |
| C59 | 0.0209 (12) | 0.0165 (11) | 0.0190 (12) | 0.0010 (9) | −0.0017 (10) | 0.0014 (9) |
| N5 | 0.0155 (9) | 0.0150 (9) | 0.0137 (9) | 0.0004 (7) | −0.0012 (7) | 0.0023 (7) |
| C50 | 0.0155 (11) | 0.0132 (10) | 0.0129 (10) | 0.0019 (8) | −0.0010 (9) | 0.0011 (8) |
| C34 | 0.0314 (14) | 0.0239 (13) | 0.0262 (13) | 0.0060 (11) | −0.0131 (11) | 0.0020 (10) |
| C60 | 0.0228 (12) | 0.0167 (11) | 0.0222 (12) | −0.0023 (9) | −0.0024 (10) | 0.0002 (9) |
| C33 | 0.0254 (13) | 0.0301 (13) | 0.0157 (12) | −0.0033 (10) | −0.0021 (10) | 0.0006 (10) |
| C61 | 0.0319 (14) | 0.0208 (12) | 0.0295 (14) | 0.0028 (11) | 0.0000 (11) | −0.0009 (10) |
| C44 | 0.0197 (12) | 0.0152 (11) | 0.0212 (12) | −0.0033 (9) | 0.0005 (10) | 0.0036 (9) |
| C45 | 0.0341 (15) | 0.0248 (13) | 0.0300 (14) | −0.0074 (11) | −0.0055 (11) | 0.0116 (11) |
| C43 | 0.0268 (13) | 0.0214 (12) | 0.0235 (13) | 0.0098 (10) | 0.0044 (10) | 0.0031 (10) |
| C37 | 0.0285 (14) | 0.0532 (17) | 0.0280 (14) | −0.0183 (13) | −0.0114 (12) | 0.0102 (12) |
| C39 | 0.0281 (13) | 0.0275 (13) | 0.0192 (12) | −0.0042 (10) | −0.0080 (10) | 0.0042 (10) |
| C62 | 0.0241 (13) | 0.0230 (12) | 0.0192 (12) | 0.0004 (10) | −0.0014 (10) | 0.0083 (9) |
| C41 | 0.0273 (13) | 0.0201 (12) | 0.0198 (12) | 0.0034 (10) | −0.0017 (10) | −0.0036 (9) |
| C38 | 0.0461 (17) | 0.0356 (15) | 0.0225 (13) | 0.0088 (12) | −0.0141 (12) | −0.0109 (11) |
| C42 | 0.0222 (12) | 0.0216 (12) | 0.0245 (13) | 0.0015 (10) | 0.0052 (10) | −0.0027 (10) |
| C47 | 0.0368 (15) | 0.0197 (12) | 0.0289 (14) | −0.0062 (11) | 0.0047 (11) | 0.0005 (10) |
| C46 | 0.0207 (13) | 0.0245 (13) | 0.0317 (14) | −0.0057 (10) | 0.0022 (11) | 0.0020 (10) |
| P2 | 0.0136 (3) | 0.0131 (3) | 0.0141 (3) | 0.0003 (2) | −0.0009 (2) | 0.0017 (2) |
| P1 | 0.0163 (3) | 0.0140 (3) | 0.0167 (3) | −0.0004 (2) | −0.0009 (2) | 0.0017 (2) |
| P3 | 0.0148 (3) | 0.0160 (3) | 0.0133 (3) | 0.0004 (2) | −0.0014 (2) | 0.0017 (2) |
| O4 | 0.0194 (8) | 0.0262 (9) | 0.0199 (8) | 0.0012 (7) | −0.0079 (7) | −0.0022 (7) |
| O2 | 0.0166 (8) | 0.0162 (8) | 0.0162 (8) | 0.0009 (6) | −0.0021 (6) | 0.0020 (6) |
| O1 | 0.0233 (9) | 0.0194 (8) | 0.0155 (8) | 0.0040 (7) | −0.0010 (7) | −0.0004 (6) |
| O3 | 0.0169 (8) | 0.0181 (8) | 0.0182 (8) | 0.0005 (6) | −0.0002 (6) | 0.0029 (6) |
| C23 | 0.0167 (11) | 0.0148 (11) | 0.0181 (11) | −0.0024 (9) | −0.0047 (9) | 0.0042 (9) |
| C21 | 0.0183 (11) | 0.0140 (11) | 0.0159 (11) | 0.0009 (9) | 0.0004 (9) | −0.0001 (8) |
| N1 | 0.0159 (9) | 0.0147 (9) | 0.0146 (9) | −0.0004 (7) | −0.0026 (7) | 0.0027 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C25 | 0.0210 (12) | 0.0180 (11) | 0.0113 (10) | −0.0003 (9) | −0.0023 (9) | −0.0005 (8) |
| C18 | 0.0176 (12) | 0.0190 (12) | 0.0215 (12) | 0.0000 (9) | 0.0028 (10) | 0.0010 (9) |
| C17 | 0.0142 (11) | 0.0170 (11) | 0.0119 (10) | 0.0008 (9) | −0.0032 (9) | 0.0021 (8) |
| N3 | 0.0176 (10) | 0.0143 (9) | 0.0192 (10) | 0.0010 (7) | 0.0000 (8) | 0.0007 (7) |
| C19 | 0.0145 (11) | 0.0140 (10) | 0.0130 (10) | 0.0019 (8) | −0.0019 (9) | 0.0026 (8) |
| N2 | 0.0163 (9) | 0.0153 (9) | 0.0156 (9) | −0.0018 (7) | −0.0031 (8) | 0.0035 (7) |
| C28 | 0.0192 (12) | 0.0163 (11) | 0.0194 (12) | 0.0006 (9) | −0.0012 (9) | 0.0022 (9) |
| C24 | 0.0176 (12) | 0.0169 (11) | 0.0159 (11) | 0.0026 (9) | 0.0013 (9) | 0.0009 (9) |
| C20 | 0.0162 (11) | 0.0128 (10) | 0.0155 (11) | −0.0024 (9) | −0.0017 (9) | 0.0044 (8) |
| C26 | 0.0261 (13) | 0.0248 (12) | 0.0197 (12) | −0.0017 (10) | −0.0091 (10) | 0.0001 (10) |
| N4 | 0.0189 (10) | 0.0123 (9) | 0.0205 (10) | −0.0023 (8) | 0.0008 (8) | 0.0015 (8) |
| C29 | 0.0183 (12) | 0.0174 (11) | 0.0185 (11) | 0.0037 (9) | −0.0019 (9) | 0.0010 (9) |
| C5 | 0.0219 (12) | 0.0259 (13) | 0.0189 (12) | −0.0036 (10) | −0.0074 (10) | 0.0005 (10) |
| C27 | 0.0231 (12) | 0.0176 (11) | 0.0206 (12) | −0.0025 (9) | −0.0021 (10) | −0.0011 (9) |
| C13 | 0.0182 (12) | 0.0160 (11) | 0.0221 (12) | −0.0039 (9) | −0.0002 (10) | 0.0039 (9) |
| C4 | 0.0311 (14) | 0.0244 (13) | 0.0240 (13) | −0.0004 (11) | −0.0097 (11) | −0.0013 (10) |
| C2 | 0.0265 (13) | 0.0285 (13) | 0.0200 (12) | −0.0027 (10) | −0.0053 (10) | 0.0057 (10) |
| C3 | 0.0222 (13) | 0.0265 (13) | 0.0227 (12) | 0.0033 (10) | −0.0073 (10) | 0.0050 (10) |
| C7 | 0.0218 (14) | 0.0541 (18) | 0.0310 (14) | −0.0112 (12) | −0.0094 (11) | 0.0103 (13) |
| C30 | 0.0319 (14) | 0.0211 (13) | 0.0310 (14) | 0.0023 (11) | 0.0025 (11) | 0.0002 (10) |
| C16 | 0.0268 (13) | 0.0197 (12) | 0.0246 (13) | −0.0052 (10) | −0.0008 (10) | 0.0012 (10) |
| C9 | 0.0209 (12) | 0.0143 (11) | 0.0217 (12) | 0.0032 (9) | 0.0043 (10) | 0.0009 (9) |
| C1 | 0.0185 (12) | 0.0177 (11) | 0.0170 (11) | −0.0011 (9) | −0.0029 (9) | 0.0013 (9) |
| C31 | 0.0246 (13) | 0.0218 (12) | 0.0213 (12) | 0.0010 (10) | 0.0004 (10) | 0.0063 (9) |
| C14 | 0.0190 (13) | 0.0215 (12) | 0.0431 (16) | −0.0029 (10) | 0.0051 (11) | 0.0025 (11) |
| C15 | 0.0369 (15) | 0.0260 (13) | 0.0222 (13) | −0.0107 (11) | −0.0018 (11) | 0.0051 (10) |
| C12 | 0.0398 (16) | 0.0348 (15) | 0.0306 (14) | 0.0201 (12) | 0.0108 (12) | 0.0092 (12) |
| C6 | 0.0351 (15) | 0.0410 (16) | 0.0249 (14) | −0.0128 (12) | −0.0129 (12) | 0.0138 (11) |
| C11 | 0.0410 (17) | 0.0277 (14) | 0.0497 (18) | 0.0137 (12) | −0.0085 (14) | −0.0171 (13) |
| C10 | 0.0315 (15) | 0.0234 (13) | 0.0474 (17) | 0.0010 (11) | 0.0251 (13) | −0.0052 (12) |
| C8 | 0.0513 (18) | 0.0394 (16) | 0.0336 (15) | 0.0051 (13) | −0.0202 (14) | −0.0126 (12) |
| C22 | 0.0257 (12) | 0.0148 (11) | 0.0145 (11) | −0.0028 (9) | −0.0024 (10) | −0.0015 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| P5—N7 | 1.5463 (17) | P2—N3 | 1.5457 (17) |
| P5—N6 | 1.6798 (18) | P2—N2 | 1.6735 (18) |
| P5—N5 | 1.6810 (17) | P2—N1 | 1.6904 (17) |
| P5—C48 | 1.831 (2) | P2—C17 | 1.827 (2) |
| P6—O5 | 1.4606 (15) | P1—N4 | 1.6577 (19) |
| P6—O7 | 1.5799 (15) | P1—N1 | 1.7419 (18) |
| P6—O6 | 1.5832 (15) | P1—N2 | 1.7486 (17) |
| P6—C50 | 1.809 (2) | P3—O1 | 1.4601 (15) |
| P4—N8 | 1.6616 (19) | P3—O2 | 1.5826 (15) |
| P4—N5 | 1.7362 (18) | P3—O3 | 1.5840 (15) |
| P4—N6 | 1.7503 (17) | P3—C19 | 1.808 (2) |
| O8—C54 | 1.361 (2) | O4—C23 | 1.364 (2) |
| O8—C57 | 1.430 (3) | O4—C26 | 1.425 (3) |

| | | | |
|---|---|---|---|
| O6—C60 | 1.454 (2) | O2—C29 | 1.462 (2) |
| O7—C58 | 1.459 (2) | O3—C27 | 1.451 (2) |
| N6—C36 | 1.488 (3) | C23—C22 | 1.386 (3) |
| C54—C53 | 1.387 (3) | C23—C24 | 1.389 (3) |
| C54—C55 | 1.392 (3) | C21—C22 | 1.384 (3) |
| C48—C49 | 1.327 (3) | C21—C20 | 1.388 (3) |
| C48—C50 | 1.532 (3) | C21—H21 | 0.9300 |
| C55—C56 | 1.380 (3) | N1—C1 | 1.486 (3) |
| C55—H55 | 0.9300 | C25—C24 | 1.375 (3) |
| N7—C40 | 1.479 (3) | C25—C20 | 1.398 (3) |
| C51—C52 | 1.385 (3) | C25—H25 | 0.9300 |
| C51—C56 | 1.396 (3) | C18—C17 | 1.323 (3) |
| C51—C50 | 1.526 (3) | C18—H18A | 0.9300 |
| N8—C44 | 1.484 (3) | C18—H18B | 0.9300 |
| N8—H8D | 0.82 (2) | C17—C19 | 1.530 (3) |
| C56—H56 | 0.9300 | N3—C9 | 1.478 (3) |
| C58—C59 | 1.521 (3) | C19—C20 | 1.523 (3) |
| C58—H58A | 0.9700 | C19—H19 | 0.9800 |
| C58—H58B | 0.9700 | N2—C5 | 1.485 (3) |
| C35—C32 | 1.517 (3) | C28—C29 | 1.523 (3) |
| C35—H35A | 0.9600 | C28—C31 | 1.524 (3) |
| C35—H35B | 0.9600 | C28—C27 | 1.526 (3) |
| C35—H35C | 0.9600 | C28—C30 | 1.531 (3) |
| C52—C53 | 1.390 (3) | C24—H24 | 0.9300 |
| C52—H52 | 0.9300 | C26—H26A | 0.9600 |
| C36—C39 | 1.521 (3) | C26—H26B | 0.9600 |
| C36—C37 | 1.525 (3) | C26—H26C | 0.9600 |
| C36—C38 | 1.528 (3) | N4—C13 | 1.481 (3) |
| C49—H49A | 0.9300 | N4—H4D | 0.84 (3) |
| C49—H49B | 0.9300 | C29—H29A | 0.9700 |
| C57—H57A | 0.9600 | C29—H29B | 0.9700 |
| C57—H57B | 0.9600 | C5—C7 | 1.524 (3) |
| C57—H57C | 0.9600 | C5—C6 | 1.527 (3) |
| C53—H53 | 0.9300 | C5—C8 | 1.527 (3) |
| C32—N5 | 1.483 (3) | C27—H27A | 0.9700 |
| C32—C33 | 1.526 (3) | C27—H27B | 0.9700 |
| C32—C34 | 1.527 (3) | C13—C16 | 1.522 (3) |
| C40—C42 | 1.523 (3) | C13—C14 | 1.526 (3) |
| C40—C43 | 1.530 (3) | C13—C15 | 1.528 (3) |
| C40—C41 | 1.531 (3) | C4—C1 | 1.521 (3) |
| C59—C60 | 1.524 (3) | C4—H4A | 0.9600 |
| C59—C62 | 1.525 (3) | C4—H4B | 0.9600 |
| C59—C61 | 1.532 (3) | C4—H4C | 0.9600 |
| C50—H50 | 0.9800 | C2—C1 | 1.528 (3) |
| C34—H34A | 0.9600 | C2—H2A | 0.9600 |
| C34—H34B | 0.9600 | C2—H2B | 0.9600 |
| C34—H34C | 0.9600 | C2—H2C | 0.9600 |
| C60—H60A | 0.9700 | C3—C1 | 1.532 (3) |

| | | | |
|---|---|---|---|
| C60—H60B | 0.9700 | C3—H3A | 0.9600 |
| C33—H33A | 0.9600 | C3—H3B | 0.9600 |
| C33—H33B | 0.9600 | C3—H3C | 0.9600 |
| C33—H33C | 0.9600 | C7—H7A | 0.9600 |
| C61—H61A | 0.9600 | C7—H7B | 0.9600 |
| C61—H61B | 0.9600 | C7—H7C | 0.9600 |
| C61—H61C | 0.9600 | C30—H30A | 0.9600 |
| C44—C47 | 1.519 (3) | C30—H30B | 0.9600 |
| C44—C46 | 1.527 (3) | C30—H30C | 0.9600 |
| C44—C45 | 1.530 (3) | C16—H16A | 0.9600 |
| C45—H45A | 0.9600 | C16—H16B | 0.9600 |
| C45—H45B | 0.9600 | C16—H16C | 0.9600 |
| C45—H45C | 0.9600 | C9—C10 | 1.515 (3) |
| C43—H43A | 0.9600 | C9—C11 | 1.521 (3) |
| C43—H43B | 0.9600 | C9—C12 | 1.523 (3) |
| C43—H43C | 0.9600 | C31—H31A | 0.9600 |
| C37—H37A | 0.9600 | C31—H31B | 0.9600 |
| C37—H37B | 0.9600 | C31—H31C | 0.9600 |
| C37—H37C | 0.9600 | C14—H14A | 0.9600 |
| C39—H39A | 0.9600 | C14—H14B | 0.9600 |
| C39—H39B | 0.9600 | C14—H14C | 0.9600 |
| C39—H39C | 0.9600 | C15—H15A | 0.9600 |
| C62—H62A | 0.9600 | C15—H15B | 0.9600 |
| C62—H62B | 0.9600 | C15—H15C | 0.9600 |
| C62—H62C | 0.9600 | C12—H12A | 0.9600 |
| C41—H41A | 0.9600 | C12—H12B | 0.9600 |
| C41—H41B | 0.9600 | C12—H12C | 0.9600 |
| C41—H41C | 0.9600 | C6—H6A | 0.9600 |
| C38—H38A | 0.9600 | C6—H6B | 0.9600 |
| C38—H38B | 0.9600 | C6—H6C | 0.9600 |
| C38—H38C | 0.9600 | C11—H11A | 0.9600 |
| C42—H42A | 0.9600 | C11—H11B | 0.9600 |
| C42—H42B | 0.9600 | C11—H11C | 0.9600 |
| C42—H42C | 0.9600 | C10—H10A | 0.9600 |
| C47—H47A | 0.9600 | C10—H10B | 0.9600 |
| C47—H47B | 0.9600 | C10—H10C | 0.9600 |
| C47—H47C | 0.9600 | C8—H8A | 0.9600 |
| C46—H46A | 0.9600 | C8—H8B | 0.9600 |
| C46—H46B | 0.9600 | C8—H8C | 0.9600 |
| C46—H46C | 0.9600 | C22—H22 | 0.9300 |

| | | | |
|---|---|---|---|
| N7—P5—N6 | 124.35 (9) | N3—P2—N2 | 124.76 (9) |
| N7—P5—N5 | 124.74 (9) | N3—P2—N1 | 124.18 (9) |
| N6—P5—N5 | 83.15 (9) | N2—P2—N1 | 83.44 (9) |
| N7—P5—C48 | 104.57 (9) | N3—P2—C17 | 104.18 (9) |
| N6—P5—C48 | 110.55 (9) | N2—P2—C17 | 109.04 (9) |
| N5—P5—C48 | 107.94 (9) | N1—P2—C17 | 109.89 (9) |
| O5—P6—O7 | 112.08 (8) | N4—P1—N1 | 104.25 (9) |

| | | | |
|---|---|---|---|
| O5—P6—O6 | 112.22 (8) | N4—P1—N2 | 107.84 (9) |
| O7—P6—O6 | 104.38 (8) | N1—P1—N2 | 79.78 (8) |
| O5—P6—C50 | 114.40 (9) | O1—P3—O2 | 111.94 (8) |
| O7—P6—C50 | 106.75 (9) | O1—P3—O3 | 111.96 (8) |
| O6—P6—C50 | 106.31 (9) | O2—P3—O3 | 104.51 (8) |
| N8—P4—N5 | 105.48 (9) | O1—P3—C19 | 115.86 (9) |
| N8—P4—N6 | 108.74 (9) | O2—P3—C19 | 105.64 (9) |
| N5—P4—N6 | 79.54 (8) | O3—P3—C19 | 106.07 (9) |
| C54—O8—C57 | 116.51 (17) | C23—O4—C26 | 117.37 (17) |
| C60—O6—P6 | 119.34 (13) | C29—O2—P3 | 117.98 (13) |
| C58—O7—P6 | 118.72 (13) | C27—O3—P3 | 118.86 (13) |
| C36—N6—P5 | 132.78 (14) | O4—C23—C22 | 125.48 (19) |
| C36—N6—P4 | 126.17 (14) | O4—C23—C24 | 115.15 (18) |
| P5—N6—P4 | 97.72 (9) | C22—C23—C24 | 119.4 (2) |
| O8—C54—C53 | 124.7 (2) | C22—C21—C20 | 121.72 (19) |
| O8—C54—C55 | 115.91 (19) | C22—C21—H21 | 119.1 |
| C53—C54—C55 | 119.35 (19) | C20—C21—H21 | 119.1 |
| C49—C48—C50 | 121.78 (19) | C1—N1—P2 | 131.48 (14) |
| C49—C48—P5 | 117.78 (16) | C1—N1—P1 | 126.07 (14) |
| C50—C48—P5 | 120.34 (14) | P2—N1—P1 | 97.61 (9) |
| C56—C55—C54 | 120.59 (19) | C24—C25—C20 | 120.8 (2) |
| C56—C55—H55 | 119.7 | C24—C25—H25 | 119.6 |
| C54—C55—H55 | 119.7 | C20—C25—H25 | 119.6 |
| C40—N7—P5 | 128.33 (15) | C17—C18—H18A | 120.0 |
| C52—C51—C56 | 117.58 (19) | C17—C18—H18B | 120.0 |
| C52—C51—C50 | 119.41 (18) | H18A—C18—H18B | 120.0 |
| C56—C51—C50 | 122.96 (19) | C18—C17—C19 | 122.28 (19) |
| C44—N8—P4 | 125.36 (15) | C18—C17—P2 | 118.82 (17) |
| C44—N8—H8D | 111.8 (17) | C19—C17—P2 | 118.84 (14) |
| P4—N8—H8D | 119.6 (17) | C9—N3—P2 | 129.59 (15) |
| C55—C56—C51 | 121.0 (2) | C20—C19—C17 | 113.54 (16) |
| C55—C56—H56 | 119.5 | C20—C19—P3 | 111.75 (14) |
| C51—C56—H56 | 119.5 | C17—C19—P3 | 111.47 (14) |
| O7—C58—C59 | 111.41 (16) | C20—C19—H19 | 106.5 |
| O7—C58—H58A | 109.3 | C17—C19—H19 | 106.5 |
| C59—C58—H58A | 109.3 | P3—C19—H19 | 106.5 |
| O7—C58—H58B | 109.3 | C5—N2—P2 | 133.49 (14) |
| C59—C58—H58B | 109.3 | C5—N2—P1 | 126.78 (14) |
| H58A—C58—H58B | 108.0 | P2—N2—P1 | 97.99 (9) |
| C32—C35—H35A | 109.5 | C29—C28—C31 | 110.21 (18) |
| C32—C35—H35B | 109.5 | C29—C28—C27 | 109.06 (17) |
| H35A—C35—H35B | 109.5 | C31—C28—C27 | 111.21 (18) |
| C32—C35—H35C | 109.5 | C29—C28—C30 | 108.57 (18) |
| H35A—C35—H35C | 109.5 | C31—C28—C30 | 110.11 (18) |
| H35B—C35—H35C | 109.5 | C27—C28—C30 | 107.60 (18) |
| C51—C52—C53 | 122.26 (19) | C25—C24—C23 | 120.63 (19) |
| C51—C52—H52 | 118.9 | C25—C24—H24 | 119.7 |
| C53—C52—H52 | 118.9 | C23—C24—H24 | 119.7 |

| | | | |
|---|---|---|---|
| N6—C36—C39 | 109.13 (17) | C21—C20—C25 | 117.83 (19) |
| N6—C36—C37 | 108.16 (18) | C21—C20—C19 | 119.76 (18) |
| C39—C36—C37 | 109.28 (19) | C25—C20—C19 | 122.39 (19) |
| N6—C36—C38 | 111.29 (18) | O4—C26—H26A | 109.5 |
| C39—C36—C38 | 109.10 (19) | O4—C26—H26B | 109.5 |
| C37—C36—C38 | 109.9 (2) | H26A—C26—H26B | 109.5 |
| C48—C49—H49A | 120.0 | O4—C26—H26C | 109.5 |
| C48—C49—H49B | 120.0 | H26A—C26—H26C | 109.5 |
| H49A—C49—H49B | 120.0 | H26B—C26—H26C | 109.5 |
| O8—C57—H57A | 109.5 | C13—N4—P1 | 126.02 (15) |
| O8—C57—H57B | 109.5 | C13—N4—H4D | 113.2 (18) |
| H57A—C57—H57B | 109.5 | P1—N4—H4D | 119.7 (18) |
| O8—C57—H57C | 109.5 | O2—C29—C28 | 110.96 (16) |
| H57A—C57—H57C | 109.5 | O2—C29—H29A | 109.4 |
| H57B—C57—H57C | 109.5 | C28—C29—H29A | 109.4 |
| C54—C53—C52 | 119.2 (2) | O2—C29—H29B | 109.4 |
| C54—C53—H53 | 120.4 | C28—C29—H29B | 109.4 |
| C52—C53—H53 | 120.4 | H29A—C29—H29B | 108.0 |
| N5—C32—C35 | 110.04 (17) | N2—C5—C7 | 109.23 (18) |
| N5—C32—C33 | 109.30 (17) | N2—C5—C6 | 109.41 (18) |
| C35—C32—C33 | 109.83 (18) | C7—C5—C6 | 109.3 (2) |
| N5—C32—C34 | 109.50 (17) | N2—C5—C8 | 110.65 (18) |
| C35—C32—C34 | 108.71 (18) | C7—C5—C8 | 109.4 (2) |
| C33—C32—C34 | 109.44 (18) | C6—C5—C8 | 108.9 (2) |
| N7—C40—C42 | 114.31 (17) | O3—C27—C28 | 112.45 (17) |
| N7—C40—C43 | 108.27 (17) | O3—C27—H27A | 109.1 |
| C42—C40—C43 | 108.48 (19) | C28—C27—H27A | 109.1 |
| N7—C40—C41 | 108.59 (17) | O3—C27—H27B | 109.1 |
| C42—C40—C41 | 108.72 (18) | C28—C27—H27B | 109.1 |
| C43—C40—C41 | 108.32 (18) | H27A—C27—H27B | 107.8 |
| C58—C59—C60 | 108.60 (17) | N4—C13—C16 | 110.99 (18) |
| C58—C59—C62 | 110.83 (18) | N4—C13—C14 | 107.38 (17) |
| C60—C59—C62 | 111.06 (18) | C16—C13—C14 | 109.91 (19) |
| C58—C59—C61 | 108.43 (18) | N4—C13—C15 | 110.10 (18) |
| C60—C59—C61 | 107.80 (18) | C16—C13—C15 | 109.44 (18) |
| C62—C59—C61 | 110.02 (18) | C14—C13—C15 | 108.99 (19) |
| C32—N5—P5 | 132.65 (14) | C1—C4—H4A | 109.5 |
| C32—N5—P4 | 127.28 (14) | C1—C4—H4B | 109.5 |
| P5—N5—P4 | 98.22 (9) | H4A—C4—H4B | 109.5 |
| C51—C50—C48 | 113.51 (16) | C1—C4—H4C | 109.5 |
| C51—C50—P6 | 110.54 (14) | H4A—C4—H4C | 109.5 |
| C48—C50—P6 | 110.95 (14) | H4B—C4—H4C | 109.5 |
| C51—C50—H50 | 107.2 | C1—C2—H2A | 109.5 |
| C48—C50—H50 | 107.2 | C1—C2—H2B | 109.5 |
| P6—C50—H50 | 107.2 | H2A—C2—H2B | 109.5 |
| C32—C34—H34A | 109.5 | C1—C2—H2C | 109.5 |
| C32—C34—H34B | 109.5 | H2A—C2—H2C | 109.5 |
| H34A—C34—H34B | 109.5 | H2B—C2—H2C | 109.5 |

| | | | |
|---|---|---|---|
| C32—C34—H34C | 109.5 | C1—C3—H3A | 109.5 |
| H34A—C34—H34C | 109.5 | C1—C3—H3B | 109.5 |
| H34B—C34—H34C | 109.5 | H3A—C3—H3B | 109.5 |
| O6—C60—C59 | 112.22 (17) | C1—C3—H3C | 109.5 |
| O6—C60—H60A | 109.2 | H3A—C3—H3C | 109.5 |
| C59—C60—H60A | 109.2 | H3B—C3—H3C | 109.5 |
| O6—C60—H60B | 109.2 | C5—C7—H7A | 109.5 |
| C59—C60—H60B | 109.2 | C5—C7—H7B | 109.5 |
| H60A—C60—H60B | 107.9 | H7A—C7—H7B | 109.5 |
| C32—C33—H33A | 109.5 | C5—C7—H7C | 109.5 |
| C32—C33—H33B | 109.5 | H7A—C7—H7C | 109.5 |
| H33A—C33—H33B | 109.5 | H7B—C7—H7C | 109.5 |
| C32—C33—H33C | 109.5 | C28—C30—H30A | 109.5 |
| H33A—C33—H33C | 109.5 | C28—C30—H30B | 109.5 |
| H33B—C33—H33C | 109.5 | H30A—C30—H30B | 109.5 |
| C59—C61—H61A | 109.5 | C28—C30—H30C | 109.5 |
| C59—C61—H61B | 109.5 | H30A—C30—H30C | 109.5 |
| H61A—C61—H61B | 109.5 | H30B—C30—H30C | 109.5 |
| C59—C61—H61C | 109.5 | C13—C16—H16A | 109.5 |
| H61A—C61—H61C | 109.5 | C13—C16—H16B | 109.5 |
| H61B—C61—H61C | 109.5 | H16A—C16—H16B | 109.5 |
| N8—C44—C47 | 111.24 (18) | C13—C16—H16C | 109.5 |
| N8—C44—C46 | 107.63 (17) | H16A—C16—H16C | 109.5 |
| C47—C44—C46 | 109.83 (19) | H16B—C16—H16C | 109.5 |
| N8—C44—C45 | 109.44 (18) | N3—C9—C10 | 113.80 (18) |
| C47—C44—C45 | 109.77 (19) | N3—C9—C11 | 109.23 (19) |
| C46—C44—C45 | 108.88 (19) | C10—C9—C11 | 109.1 (2) |
| C44—C45—H45A | 109.5 | N3—C9—C12 | 108.13 (17) |
| C44—C45—H45B | 109.5 | C10—C9—C12 | 108.2 (2) |
| H45A—C45—H45B | 109.5 | C11—C9—C12 | 108.2 (2) |
| C44—C45—H45C | 109.5 | N1—C1—C4 | 109.14 (17) |
| H45A—C45—H45C | 109.5 | N1—C1—C2 | 108.54 (17) |
| H45B—C45—H45C | 109.5 | C4—C1—C2 | 108.54 (18) |
| C40—C43—H43A | 109.5 | N1—C1—C3 | 112.22 (17) |
| C40—C43—H43B | 109.5 | C4—C1—C3 | 109.96 (19) |
| H43A—C43—H43B | 109.5 | C2—C1—C3 | 108.35 (18) |
| C40—C43—H43C | 109.5 | C28—C31—H31A | 109.5 |
| H43A—C43—H43C | 109.5 | C28—C31—H31B | 109.5 |
| H43B—C43—H43C | 109.5 | H31A—C31—H31B | 109.5 |
| C36—C37—H37A | 109.5 | C28—C31—H31C | 109.5 |
| C36—C37—H37B | 109.5 | H31A—C31—H31C | 109.5 |
| H37A—C37—H37B | 109.5 | H31B—C31—H31C | 109.5 |
| C36—C37—H37C | 109.5 | C13—C14—H14A | 109.5 |
| H37A—C37—H37C | 109.5 | C13—C14—H14B | 109.5 |
| H37B—C37—H37C | 109.5 | H14A—C14—H14B | 109.5 |
| C36—C39—H39A | 109.5 | C13—C14—H14C | 109.5 |
| C36—C39—H39B | 109.5 | H14A—C14—H14C | 109.5 |
| H39A—C39—H39B | 109.5 | H14B—C14—H14C | 109.5 |

| | | | |
|---|---|---|---|
| C36—C39—H39C | 109.5 | C13—C15—H15A | 109.5 |
| H39A—C39—H39C | 109.5 | C13—C15—H15B | 109.5 |
| H39B—C39—H39C | 109.5 | H15A—C15—H15B | 109.5 |
| C59—C62—H62A | 109.5 | C13—C15—H15C | 109.5 |
| C59—C62—H62B | 109.5 | H15A—C15—H15C | 109.5 |
| H62A—C62—H62B | 109.5 | H15B—C15—H15C | 109.5 |
| C59—C62—H62C | 109.5 | C9—C12—H12A | 109.5 |
| H62A—C62—H62C | 109.5 | C9—C12—H12B | 109.5 |
| H62B—C62—H62C | 109.5 | H12A—C12—H12B | 109.5 |
| C40—C41—H41A | 109.5 | C9—C12—H12C | 109.5 |
| C40—C41—H41B | 109.5 | H12A—C12—H12C | 109.5 |
| H41A—C41—H41B | 109.5 | H12B—C12—H12C | 109.5 |
| C40—C41—H41C | 109.5 | C5—C6—H6A | 109.5 |
| H41A—C41—H41C | 109.5 | C5—C6—H6B | 109.5 |
| H41B—C41—H41C | 109.5 | H6A—C6—H6B | 109.5 |
| C36—C38—H38A | 109.5 | C5—C6—H6C | 109.5 |
| C36—C38—H38B | 109.5 | H6A—C6—H6C | 109.5 |
| H38A—C38—H38B | 109.5 | H6B—C6—H6C | 109.5 |
| C36—C38—H38C | 109.5 | C9—C11—H11A | 109.5 |
| H38A—C38—H38C | 109.5 | C9—C11—H11B | 109.5 |
| H38B—C38—H38C | 109.5 | H11A—C11—H11B | 109.5 |
| C40—C42—H42A | 109.5 | C9—C11—H11C | 109.5 |
| C40—C42—H42B | 109.5 | H11A—C11—H11C | 109.5 |
| H42A—C42—H42B | 109.5 | H11B—C11—H11C | 109.5 |
| C40—C42—H42C | 109.5 | C9—C10—H10A | 109.5 |
| H42A—C42—H42C | 109.5 | C9—C10—H10B | 109.5 |
| H42B—C42—H42C | 109.5 | H10A—C10—H10B | 109.5 |
| C44—C47—H47A | 109.5 | C9—C10—H10C | 109.5 |
| C44—C47—H47B | 109.5 | H10A—C10—H10C | 109.5 |
| H47A—C47—H47B | 109.5 | H10B—C10—H10C | 109.5 |
| C44—C47—H47C | 109.5 | C5—C8—H8A | 109.5 |
| H47A—C47—H47C | 109.5 | C5—C8—H8B | 109.5 |
| H47B—C47—H47C | 109.5 | H8A—C8—H8B | 109.5 |
| C44—C46—H46A | 109.5 | C5—C8—H8C | 109.5 |
| C44—C46—H46B | 109.5 | H8A—C8—H8C | 109.5 |
| H46A—C46—H46B | 109.5 | H8B—C8—H8C | 109.5 |
| C44—C46—H46C | 109.5 | C21—C22—C23 | 119.6 (2) |
| H46A—C46—H46C | 109.5 | C21—C22—H22 | 120.2 |
| H46B—C46—H46C | 109.5 | C23—C22—H22 | 120.2 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N8—H8*D*···O1$^{i}$ | 0.82 (2) | 2.61 (3) | 3.394 (2) | 160 (2) |
| N4—H4*D*···O5$^{ii}$ | 0.84 (3) | 2.58 (3) | 3.378 (2) | 158 (2) |
| C26—H26*B*···O5$^{iii}$ | 0.96 | 2.49 | 3.325 (3) | 145 |

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+2, −*y*+1, −*z*+1.