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# Low-temperature superstructure of [(*N,N*-diisobutylcarbamoyl)methyl]-octyl(phenyl)phosphine oxide (CMPO)

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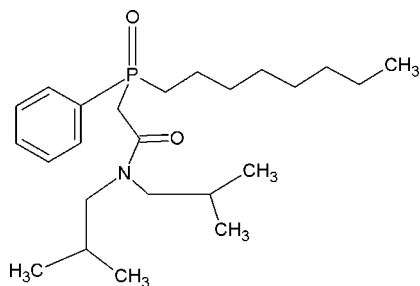
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Key indicators: single-crystal X-ray study;  $T = 120$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å; disorder in main residue;  $R$  factor = 0.050;  $wR$  factor = 0.135; data-to-parameter ratio = 14.7.

At 120 K, the title compound,  $\text{C}_{24}\text{H}_{42}\text{NO}_2\text{P}$ , crystallizes in a unit cell with a doubled  $a$  parameter compared with the room-temperature structure. There are four molecules in the asymmetric unit, one of which shows extensive disorder in a 0.588 (3):0.412 (3) ratio. In the crystal, numerous  $\text{C}-\text{H}\cdots\text{O}$  interactions link the molecules.

## Related literature

For the room-temperature structure, see: Rogers *et al.* (1995). For the use of the title compound as a ligand, see: Cherfa *et al.* (1999).



## Experimental

### Crystal data

$\text{C}_{24}\text{H}_{42}\text{NO}_2\text{P}$   $V = 9808.7$  (2) Å<sup>3</sup>  
 $M_r = 407.56$   $Z = 16$   
 Monoclinic,  $P2_1/c$   $\text{Cu K}\alpha$  radiation  
 $a = 26.1649$  (3) Å  $\mu = 1.12$  mm<sup>-1</sup>  
 $b = 22.0926$  (3) Å  $T = 120$  K  
 $c = 16.9697$  (2) Å  $0.23 \times 0.17 \times 0.13$  mm  
 $\beta = 90.662$  (1)°

### Data collection

Oxford Diffraction Gemini diffractometer with an Atlas CCD detector and mirror-collimated  $\text{Cu K}\alpha$  radiation  
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2009)  
 $T_{\min} = 0.705$ ,  $T_{\max} = 1.000$   
 79104 measured reflections  
 15383 independent reflections  
 11781 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.045$   
 $\theta_{\max} = 62.3^\circ$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$   
 $wR(F^2) = 0.135$   
 $S = 1.03$   
 15383 reflections  
 1043 parameters  
 148 restraints  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.80$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.56$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$                                  | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{C9A}-\text{H9A1}\cdots\text{O2A}^i$            | 0.99         | 2.37               | 3.339 (3)   | 165                  |
| $\text{C9A}-\text{H9A2}\cdots\text{O2D}$              | 0.99         | 2.31               | 3.238 (5)   | 156                  |
| $\text{C9B}-\text{H9B2}\cdots\text{O2C}$              | 0.99         | 2.49               | 3.442 (3)   | 160                  |
| $\text{C9B}-\text{H9B1}\cdots\text{O2B}^{\text{ii}}$  | 0.99         | 2.50               | 3.483 (3)   | 175                  |
| $\text{C9C}-\text{H9C2}\cdots\text{O2B}$              | 0.99         | 2.36               | 3.305 (3)   | 158                  |
| $\text{C5A}-\text{H5A}\cdots\text{O11D}^{\text{iii}}$ | 0.95         | 2.48               | 3.379 (14)  | 157                  |
| $\text{C6C}-\text{H6C}\cdots\text{O11C}^{\text{iv}}$  | 0.95         | 2.51               | 3.453 (3)   | 170                  |
| $\text{C6D}-\text{H6D}\cdots\text{O11D}^{\text{iv}}$  | 0.95         | 2.47               | 3.37 (2)    | 159                  |
| $\text{C9D}-\text{H9D1}\cdots\text{O11A}^i$           | 0.99         | 2.56               | 3.265 (7)   | 128                  |
| $\text{C7B}-\text{H7B}\cdots\text{O11C}^{\text{v}}$   | 0.95         | 2.59               | 3.477 (3)   | 156                  |
| $\text{C9D}-\text{H9D2}\cdots\text{O2A}$              | 0.99         | 2.36               | 3.265 (11)  | 151                  |
| $\text{C13B}-\text{H13D}\cdots\text{O2C}$             | 0.99         | 2.52               | 3.431 (3)   | 154                  |
| $\text{C13C}-\text{H13E}\cdots\text{O2B}$             | 0.99         | 2.49               | 3.448 (3)   | 162                  |
| $\text{C15D}-\text{H15L}\cdots\text{O2A}$             | 0.98         | 2.55               | 3.332 (10)  | 137                  |
| $\text{C17A}-\text{H17B}\cdots\text{O2D}$             | 0.99         | 2.52               | 3.375 (7)   | 145                  |
| $\text{C21A}-\text{H21B}\cdots\text{O11A}$            | 0.99         | 2.52               | 3.139 (3)   | 120                  |
| $\text{C4D}-\text{H4D}\cdots\text{O11D}$              | 0.95         | 2.58               | 3.36 (2)    | 140                  |
| $\text{C8C}-\text{H8C}\cdots\text{O11C}$              | 0.95         | 2.52               | 3.239 (3)   | 132                  |
| $\text{C21B}-\text{H21D}\cdots\text{O11B}$            | 0.99         | 2.51               | 3.175 (3)   | 124                  |
| $\text{C21C}-\text{H21F}\cdots\text{O11C}$            | 0.99         | 2.43               | 3.093 (3)   | 124                  |
| $\text{C21D}-\text{H21H}\cdots\text{O11D}$            | 0.99         | 2.53               | 3.224 (19)  | 127                  |

Symmetry codes: (i)  $-x, -y + 1, -z$ ; (ii)  $-x + 1, -y + 1, -z$ ; (iii)  $-x, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (iv)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (v)  $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$ .

Data collection: *CrysAlis PRO* (Agilent, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6481).

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## supporting information

*Acta Cryst.* (2011). E67, o3272–o3273 [https://doi.org/10.1107/S1600536811046939]

## Low-temperature superstructure of [(*N,N*-diisobutylcarbamoyl)methyl]-octyl(phenyl)phosphine oxide (CMPO)

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### S1. Comment

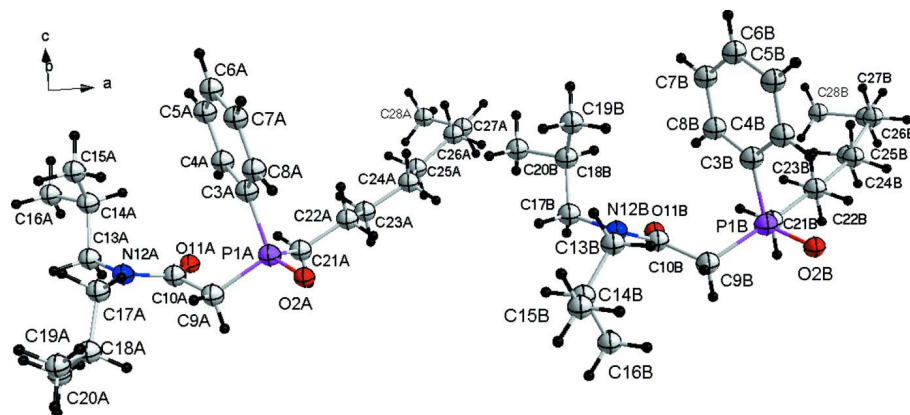
The ligand octyl(phenyl)-*N,N*-diisobutylcarbamoyl-methylphosphine oxide, C<sub>24</sub>H<sub>42</sub>N<sub>1</sub>O<sub>2</sub>P<sub>1</sub>, is used in extraction of transuranium elements (Cherfa *et al.*, 1999). The crystal structure of titled compound determined at room temperature (20°C) was already reported (Rogers *et al.*, 1995). The newly determined crystal structure at 120 K has also monoclinic *P*2<sub>1</sub>/*c* space group with a twofold length of *a* parameter which leads to four molecules (A–D) in asymmetric unit (Fig 1 and 2). The molecule D is disordered over two positions with partial occupancies 0.588 (3) and 0.412 (3). The four molecules differ in the orientation of the octyl chain. Due to the arrangement in crystal, the molecules form several types of noncovalent interactions (Table 1). They are connected *via* hydrogen bonds between the P=O group and methylene group (C9) in amide residues. There are weak intra- and intermolecular interactions between the aromatic C–H group with the amide oxygen and also intramolecular interaction between the first methylene group in octyl chain and oxygen atom in amide group.

### S2. Experimental

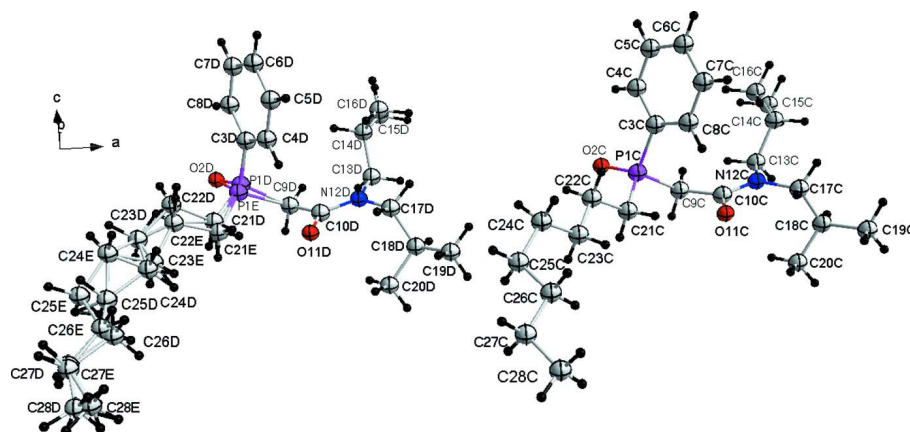
Octyl(phenyl)-*N,N*-diisobutylcarbamoyl-methylphosphine oxide was used as received as colourless prisms from Elf-Atochem (USA).

### S3. Refinement

The positions of disorder atoms were found from the electron density maps. Disordered fragments were then placed in appropriate positions, and all distances between neighbouring atoms were restrained as well as angles. Site occupancies were refined for the different parts with the same thermal parameters for the same atoms in various fragments. The final partial occupancies were found 0.588 (3). At the end of refinement, hydrogen atoms were placed in calculated positions with the thermal parameters  $U_{\text{iso}}(\text{H})$  (in the range 1.2–1.5 times  $U_{\text{eq}}$  of the parent atom). The electron density of terminal carbon atoms (C27 and C28) in the octyl chain was checked from maps of electron density. Based on the maps and the considerations given in details in the description of refinement, the last two terminal atoms were refined isotropically.

**Figure 1**

A view of first two molecules of CMPO (A,B) with atom's numbering. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

A view of second two molecules of CMPO (C,D) with atom's numbering. Displacement ellipsoids are drawn at the 50% probability level. The disordered atoms of octyl chain in molecule D were omitted for better clarity.

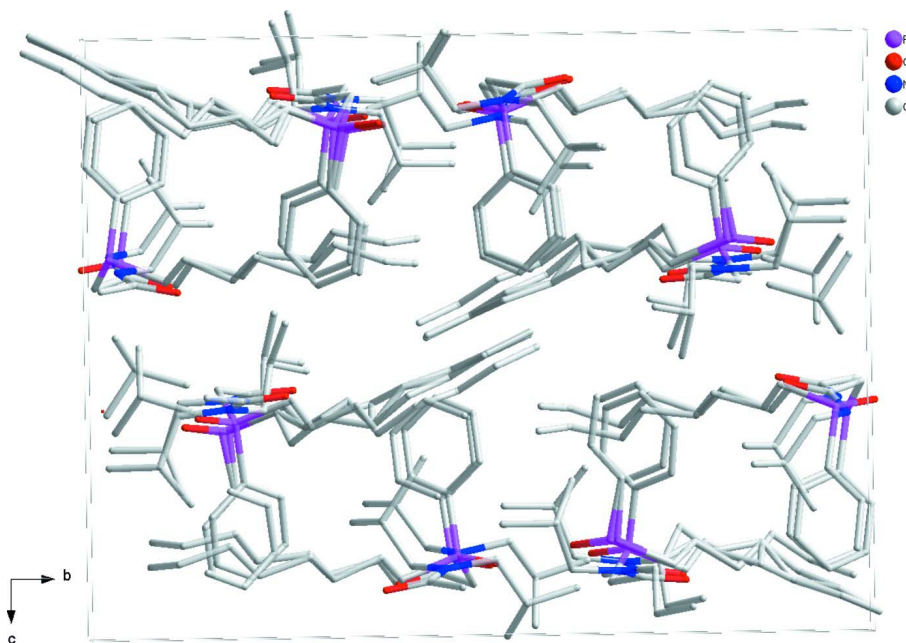


Figure 3

Packaging of molecules in direction of *a* axis.

### [[*N,N*-diisobutylcarbamoyl)methyl]octyl(phenyl)phosphine oxide

#### Crystal data

$C_{24}H_{42}NO_2P$

$M_r = 407.56$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P\ 2_1/c$

$a = 26.1649\ (3)\ \text{\AA}$

$b = 22.0926\ (3)\ \text{\AA}$

$c = 16.9697\ (2)\ \text{\AA}$

$\beta = 90.662\ (1)^\circ$

$V = 9808.7\ (2)\ \text{\AA}^3$

$Z = 16$

$F(000) = 3584$

$D_x = 1.104\ \text{Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.54180\ \text{\AA}$

Cell parameters from 37947 reflections

$\theta = 3.1\text{--}62.2^\circ$

$\mu = 1.12\ \text{mm}^{-1}$

$T = 120\ \text{K}$

Prism, colourless

$0.23 \times 0.17 \times 0.13\ \text{mm}$

#### Data collection

Oxford Diffraction Gemini  
diffractometer with an Atlas CCD detector and  
mirror-collimated Cu  $K\alpha$  radiation

Radiation source: X-ray tube

Mirror (Gemini ultra Cu) monochromator

Rotation method data acquisition using  $\omega$  scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2009)

$T_{\min} = 0.705$ ,  $T_{\max} = 1.000$

79104 measured reflections

15383 independent reflections

11781 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\max} = 62.3^\circ$ ,  $\theta_{\min} = 3.3^\circ$

$h = -30 \rightarrow 28$

$k = -24 \rightarrow 25$

$l = -19 \rightarrow 19$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.135$

$S = 1.03$

15383 reflections

1043 parameters

148 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 8.3042P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.80 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.56 \text{ e } \text{\AA}^{-3}$

### Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger. The positions of disorder atoms were found from the electron density maps. Disordered fragments were then placed in appropriate positions, and all distances between neighbouring atoms were restrained as well as angles. Site occupancies were refined for the different parts with the same thermal parameters for the same atoms in various fragments. The final partial occupancies were found 0.588 (3). At the end of refinement, hydrogen atoms were placed in calculated positions with the thermal parameters  $U_{\text{iso}}(\text{H})$  (in the range 1.2–1.5 times  $U_{\text{eq}}$  of the parent atom). The electron density of terminal carbon atoms (C27 and C28) in the octyl chain was checked from maps of electron density. Based on the maps and the considerations given in details in the description of refinement, the last two terminal atoms were refined isotropically. If refined anisotropically, the thermal ellipsoids pointed out into the C—C bonds. The difference in the  $R$ -factors of isotropic and anisotropic refinement was very small indicating that the wrongly oriented thermal ellipsoids did not improve the fit with experimental data. We did not find any systematic error in frame scaling or absorption correction and we also ensured the instrument stability by checking structures measured before and after this case. We finally concluded that our data set did not contain information about thermal ellipsoids of C27 and C28.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

|      | <i>x</i>      | <i>y</i>     | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|------|---------------|--------------|--------------|----------------------------------|-----------|
| P1A  | 0.01080 (2)   | 0.54030 (3)  | 0.12821 (3)  | 0.02449 (14)                     |           |
| O2A  | 0.04911 (6)   | 0.49138 (7)  | 0.11735 (9)  | 0.0290 (4)                       |           |
| O11A | −0.08727 (6)  | 0.61924 (7)  | 0.07558 (9)  | 0.0308 (4)                       |           |
| N12A | −0.13898 (7)  | 0.54231 (8)  | 0.11059 (11) | 0.0278 (4)                       |           |
| C3A  | −0.00385 (9)  | 0.55190 (10) | 0.23106 (13) | 0.0265 (5)                       |           |
| C4A  | −0.03206 (10) | 0.60107 (11) | 0.25772 (14) | 0.0344 (6)                       |           |
| H4A  | −0.0440       | 0.6305       | 0.2211       | 0.041*                           |           |
| C5A  | −0.04292 (10) | 0.60770 (12) | 0.33718 (15) | 0.0386 (6)                       |           |
| H5A  | −0.0623       | 0.6413       | 0.3549       | 0.046*                           |           |
| C6A  | −0.02516 (11) | 0.56485 (12) | 0.39031 (15) | 0.0403 (6)                       |           |
| H6A  | −0.0322       | 0.5693       | 0.4448       | 0.048*                           |           |
| C7A  | 0.00257 (11)  | 0.51601 (12) | 0.36482 (15) | 0.0436 (7)                       |           |
| H7A  | 0.0144        | 0.4866       | 0.4017       | 0.052*                           |           |
| C8A  | 0.01343 (10)  | 0.50941 (11) | 0.28555 (14) | 0.0351 (6)                       |           |
| H8A  | 0.0328        | 0.4756       | 0.2684       | 0.042*                           |           |
| C9A  | −0.04880 (8)  | 0.52124 (10) | 0.07875 (13) | 0.0250 (5)                       |           |
| H9A1 | −0.0421       | 0.5175       | 0.0217       | 0.030*                           |           |
| H9A2 | −0.0598       | 0.4809       | 0.0976       | 0.030*                           |           |
| C10A | −0.09302 (9)  | 0.56482 (10) | 0.08903 (13) | 0.0256 (5)                       |           |

|      |               |              |               |              |
|------|---------------|--------------|---------------|--------------|
| C13A | -0.18165 (9)  | 0.58545 (11) | 0.11553 (15)  | 0.0330 (6)   |
| H13A | -0.2141       | 0.5626       | 0.1118        | 0.040*       |
| H13B | -0.1803       | 0.6130       | 0.0695        | 0.040*       |
| C14A | -0.18226 (10) | 0.62381 (12) | 0.19074 (15)  | 0.0375 (6)   |
| H14A | -0.1522       | 0.6517       | 0.1902        | 0.045*       |
| C15A | -0.17900 (12) | 0.58523 (13) | 0.26482 (16)  | 0.0464 (7)   |
| H15A | -0.2084       | 0.5579       | 0.2665        | 0.056*       |
| H15B | -0.1791       | 0.6115       | 0.3113        | 0.056*       |
| H15C | -0.1474       | 0.5614       | 0.2644        | 0.056*       |
| C16A | -0.23083 (11) | 0.66192 (14) | 0.18990 (18)  | 0.0515 (8)   |
| H16A | -0.2328       | 0.6852       | 0.1408        | 0.062*       |
| H16B | -0.2302       | 0.6898       | 0.2348        | 0.062*       |
| H16C | -0.2607       | 0.6353       | 0.1935        | 0.062*       |
| C17A | -0.14954 (9)  | 0.47810 (10) | 0.12517 (14)  | 0.0293 (5)   |
| H17A | -0.1800       | 0.4750       | 0.1591        | 0.035*       |
| H17B | -0.1203       | 0.4605       | 0.1547        | 0.035*       |
| C18A | -0.15897 (10) | 0.43999 (12) | 0.05064 (15)  | 0.0354 (6)   |
| H18A | -0.1264       | 0.4389       | 0.0203        | 0.042*       |
| C19A | -0.17116 (11) | 0.37578 (12) | 0.07612 (19)  | 0.0481 (7)   |
| H19A | -0.2025       | 0.3758       | 0.1072        | 0.058*       |
| H19B | -0.1428       | 0.3599       | 0.1082        | 0.058*       |
| H19C | -0.1760       | 0.3502       | 0.0294        | 0.058*       |
| C20A | -0.20040 (11) | 0.46545 (14) | -0.00288 (16) | 0.0473 (7)   |
| H20A | -0.2034       | 0.4404       | -0.0504       | 0.057*       |
| H20B | -0.1916       | 0.5070       | -0.0177       | 0.057*       |
| H20C | -0.2330       | 0.4654       | 0.0249        | 0.057*       |
| C21A | 0.03224 (9)   | 0.61198 (10) | 0.09086 (13)  | 0.0269 (5)   |
| H21A | 0.0365        | 0.6088       | 0.0331        | 0.032*       |
| H21B | 0.0057        | 0.6429       | 0.1009        | 0.032*       |
| C22A | 0.08282 (9)   | 0.63280 (10) | 0.12820 (14)  | 0.0282 (5)   |
| H22A | 0.0803        | 0.6305       | 0.1863        | 0.034*       |
| H22B | 0.1105        | 0.6053       | 0.1116        | 0.034*       |
| C23A | 0.09604 (9)   | 0.69722 (11) | 0.10437 (14)  | 0.0316 (6)   |
| H23A | 0.0983        | 0.6991       | 0.0462        | 0.038*       |
| H23B | 0.0679        | 0.7243       | 0.1205        | 0.038*       |
| C24A | 0.14580 (9)   | 0.72052 (11) | 0.13988 (15)  | 0.0314 (6)   |
| H24A | 0.1748        | 0.6996       | 0.1146        | 0.038*       |
| H24B | 0.1469        | 0.7107       | 0.1968        | 0.038*       |
| C25A | 0.15209 (10)  | 0.78869 (11) | 0.12953 (15)  | 0.0355 (6)   |
| H25A | 0.1568        | 0.7975       | 0.0729        | 0.043*       |
| H25B | 0.1202        | 0.8089       | 0.1462        | 0.043*       |
| C26A | 0.19661 (11)  | 0.81547 (13) | 0.17551 (17)  | 0.0457 (7)   |
| H26A | 0.2279        | 0.7920       | 0.1639        | 0.055*       |
| H26B | 0.1899        | 0.8116       | 0.2326        | 0.055*       |
| C27A | 0.20618 (13)  | 0.88229 (15) | 0.1562 (2)    | 0.0631 (9)*  |
| H27A | 0.2331        | 0.8980       | 0.1922        | 0.076*       |
| H27B | 0.2193        | 0.8852       | 0.1018        | 0.076*       |
| C28A | 0.15983 (15)  | 0.92178 (18) | 0.1628 (2)    | 0.0764 (11)* |

|      |              |              |              |              |
|------|--------------|--------------|--------------|--------------|
| H28A | 0.1347       | 0.9103       | 0.1222       | 0.092*       |
| H28B | 0.1697       | 0.9642       | 0.1554       | 0.092*       |
| H28C | 0.1448       | 0.9167       | 0.2150       | 0.092*       |
| P1B  | 0.50464 (2)  | 0.52944 (3)  | 0.13204 (3)  | 0.02519 (14) |
| O2B  | 0.54306 (6)  | 0.48119 (7)  | 0.11856 (10) | 0.0312 (4)   |
| O11B | 0.40211 (6)  | 0.60593 (7)  | 0.08700 (9)  | 0.0322 (4)   |
| N12B | 0.35704 (7)  | 0.52836 (9)  | 0.13750 (12) | 0.0311 (5)   |
| C3B  | 0.49258 (9)  | 0.54066 (10) | 0.23595 (13) | 0.0262 (5)   |
| C4B  | 0.51457 (10) | 0.50018 (11) | 0.28938 (14) | 0.0336 (6)   |
| H4B  | 0.5345       | 0.4673       | 0.2709       | 0.040*       |
| C5B  | 0.50736 (11) | 0.50791 (13) | 0.36968 (15) | 0.0426 (7)   |
| H5B  | 0.5226       | 0.4804       | 0.4060       | 0.051*       |
| C6B  | 0.47839 (10) | 0.55507 (12) | 0.39685 (15) | 0.0389 (6)   |
| H6B  | 0.4734       | 0.5598       | 0.4519       | 0.047*       |
| C7B  | 0.45637 (10) | 0.59593 (12) | 0.34453 (14) | 0.0356 (6)   |
| H7B  | 0.4365       | 0.6287       | 0.3635       | 0.043*       |
| C8B  | 0.46360 (9)  | 0.58847 (11) | 0.26407 (14) | 0.0305 (5)   |
| H8B  | 0.4486       | 0.6163       | 0.2280       | 0.037*       |
| C9B  | 0.44415 (9)  | 0.51036 (10) | 0.08521 (13) | 0.0271 (5)   |
| H9B1 | 0.4490       | 0.5103       | 0.0274       | 0.032*       |
| H9B2 | 0.4349       | 0.4686       | 0.1009       | 0.032*       |
| C10B | 0.39946 (9)  | 0.55158 (11) | 0.10363 (13) | 0.0275 (5)   |
| C13B | 0.34851 (10) | 0.46423 (11) | 0.15607 (15) | 0.0336 (6)   |
| H13C | 0.3316       | 0.4614       | 0.2078       | 0.057 (9)*   |
| H13D | 0.3820       | 0.4437       | 0.1609       | 0.038 (7)*   |
| C14B | 0.31632 (12) | 0.43117 (13) | 0.09542 (18) | 0.0484 (7)   |
| H14B | 0.2819       | 0.4507       | 0.0928       | 0.058*       |
| C15B | 0.30975 (13) | 0.36567 (14) | 0.1228 (2)   | 0.0647 (10)  |
| H15D | 0.2870       | 0.3442       | 0.0859       | 0.078*       |
| H15E | 0.2949       | 0.3652       | 0.1755       | 0.078*       |
| H15F | 0.3431       | 0.3456       | 0.1244       | 0.078*       |
| C16B | 0.33887 (14) | 0.43268 (15) | 0.01548 (19) | 0.0617 (9)   |
| H16D | 0.3449       | 0.4748       | 0.0000       | 0.074*       |
| H16E | 0.3152       | 0.4137       | -0.0223      | 0.074*       |
| H16F | 0.3713       | 0.4106       | 0.0160       | 0.074*       |
| C17B | 0.31320 (10) | 0.56925 (12) | 0.14730 (16) | 0.0362 (6)   |
| H17C | 0.2817       | 0.5446       | 0.1491       | 0.043*       |
| H17D | 0.3106       | 0.5957       | 0.1003       | 0.043*       |
| C18B | 0.31535 (11) | 0.60941 (13) | 0.22088 (16) | 0.0425 (7)   |
| H18B | 0.3454       | 0.6372       | 0.2166       | 0.051*       |
| C19B | 0.32103 (13) | 0.57310 (15) | 0.29629 (17) | 0.0542 (8)   |
| H19D | 0.3229       | 0.6007       | 0.3414       | 0.065*       |
| H19E | 0.3524       | 0.5489       | 0.2943       | 0.065*       |
| H19F | 0.2915       | 0.5462       | 0.3019       | 0.065*       |
| C20B | 0.26669 (12) | 0.64766 (15) | 0.2222 (2)   | 0.0581 (8)   |
| H20D | 0.2369       | 0.6211       | 0.2279       | 0.070*       |
| H20E | 0.2635       | 0.6704       | 0.1728       | 0.070*       |
| H20F | 0.2684       | 0.6759       | 0.2667       | 0.070*       |



|      |              |              |              |              |
|------|--------------|--------------|--------------|--------------|
| C21B | 0.52336 (9)  | 0.60184 (10) | 0.09378 (13) | 0.0267 (5)   |
| H21C | 0.5284       | 0.5981       | 0.0362       | 0.032*       |
| H21D | 0.4953       | 0.6311       | 0.1022       | 0.032*       |
| C22B | 0.57236 (9)  | 0.62703 (10) | 0.13147 (14) | 0.0301 (5)   |
| H22C | 0.5676       | 0.6315       | 0.1890       | 0.036*       |
| H22D | 0.6008       | 0.5982       | 0.1231       | 0.036*       |
| C23B | 0.58611 (10) | 0.68828 (11) | 0.09612 (15) | 0.0323 (6)   |
| H23C | 0.5923       | 0.6829       | 0.0391       | 0.039*       |
| H23D | 0.5565       | 0.7158       | 0.1016       | 0.039*       |
| C24B | 0.63263 (11) | 0.71789 (12) | 0.13350 (16) | 0.0399 (6)   |
| H24C | 0.6633       | 0.6935       | 0.1216       | 0.048*       |
| H24D | 0.6286       | 0.7186       | 0.1914       | 0.048*       |
| C25B | 0.64055 (11) | 0.78268 (12) | 0.10373 (16) | 0.0416 (7)   |
| H25C | 0.6534       | 0.7809       | 0.0491       | 0.050*       |
| H25D | 0.6071       | 0.8035       | 0.1022       | 0.050*       |
| C26B | 0.67734 (13) | 0.81975 (13) | 0.15320 (18) | 0.0534 (8)   |
| H26C | 0.7110       | 0.7993       | 0.1540       | 0.064*       |
| H26D | 0.6648       | 0.8210       | 0.2080       | 0.064*       |
| C27B | 0.68431 (12) | 0.88457 (14) | 0.12384 (19) | 0.0537 (8)*  |
| H27C | 0.7090       | 0.9055       | 0.1591       | 0.064*       |
| H27D | 0.6994       | 0.8832       | 0.0706       | 0.064*       |
| C28B | 0.63552 (12) | 0.92151 (15) | 0.11984 (19) | 0.0573 (8)*  |
| H28D | 0.6121       | 0.9036       | 0.0809       | 0.069*       |
| H28E | 0.6436       | 0.9631       | 0.1043       | 0.069*       |
| H28F | 0.6194       | 0.9217       | 0.1717       | 0.069*       |
| P1C  | 0.48393 (2)  | 0.31171 (3)  | 0.14073 (4)  | 0.02857 (15) |
| O2C  | 0.44377 (6)  | 0.35912 (7)  | 0.13383 (10) | 0.0357 (4)   |
| O11C | 0.58035 (7)  | 0.23781 (7)  | 0.08795 (10) | 0.0349 (4)   |
| N12C | 0.63308 (8)  | 0.31775 (9)  | 0.10350 (11) | 0.0305 (5)   |
| C3C  | 0.50522 (9)  | 0.30133 (10) | 0.24182 (14) | 0.0289 (5)   |
| C4C  | 0.48844 (10) | 0.34266 (11) | 0.29777 (15) | 0.0358 (6)   |
| H4C  | 0.4658       | 0.3743       | 0.2827       | 0.043*       |
| C5C  | 0.50478 (11) | 0.33764 (13) | 0.37570 (16) | 0.0428 (7)   |
| H5C  | 0.4931       | 0.3659       | 0.4137       | 0.051*       |
| C6C  | 0.53789 (11) | 0.29179 (12) | 0.39841 (15) | 0.0405 (7)   |
| H6C  | 0.5494       | 0.2890       | 0.4516       | 0.049*       |
| C7C  | 0.55427 (10) | 0.24977 (12) | 0.34312 (15) | 0.0374 (6)   |
| H7C  | 0.5765       | 0.2178       | 0.3586       | 0.045*       |
| C8C  | 0.53805 (10) | 0.25472 (11) | 0.26523 (14) | 0.0331 (6)   |
| H8C  | 0.5494       | 0.2261       | 0.2275       | 0.040*       |
| C9C  | 0.53970 (9)  | 0.33385 (11) | 0.08537 (14) | 0.0303 (5)   |
| H9C1 | 0.5298       | 0.3359       | 0.0289       | 0.036*       |
| H9C2 | 0.5496       | 0.3752       | 0.1020       | 0.036*       |
| C10C | 0.58629 (9)  | 0.29334 (11) | 0.09318 (13) | 0.0279 (5)   |
| C13C | 0.64498 (10) | 0.38276 (11) | 0.10708 (15) | 0.0335 (6)   |
| H13E | 0.6129       | 0.4060       | 0.1002       | 0.040*       |
| H13F | 0.6676       | 0.3931       | 0.0627       | 0.040*       |
| C14C | 0.67081 (10) | 0.40213 (12) | 0.18392 (15) | 0.0374 (6)   |

|      |              |               |               |             |           |
|------|--------------|---------------|---------------|-------------|-----------|
| H14C | 0.7055       | 0.3833        | 0.1861        | 0.045*      |           |
| C15C | 0.67757 (12) | 0.47057 (12)  | 0.18362 (17)  | 0.0473 (7)  |           |
| H15G | 0.6439       | 0.4901        | 0.1819        | 0.057*      |           |
| H15H | 0.6971       | 0.4826        | 0.1373        | 0.057*      |           |
| H15I | 0.6960       | 0.4831        | 0.2315        | 0.057*      |           |
| C16C | 0.64203 (13) | 0.38139 (15)  | 0.25495 (17)  | 0.0561 (8)  |           |
| H16G | 0.6072       | 0.3978        | 0.2529        | 0.067*      |           |
| H16H | 0.6595       | 0.3958        | 0.3028        | 0.067*      |           |
| H16I | 0.6406       | 0.3371        | 0.2555        | 0.067*      |           |
| C17C | 0.67684 (10) | 0.27641 (11)  | 0.10617 (15)  | 0.0347 (6)  |           |
| H17E | 0.6644       | 0.2351        | 0.1182        | 0.042*      |           |
| H17F | 0.7001       | 0.2889        | 0.1496        | 0.042*      |           |
| C18C | 0.70634 (11) | 0.27449 (15)  | 0.03107 (19)  | 0.0533 (8)  |           |
| H18C | 0.7224       | 0.3151        | 0.0238        | 0.064*      |           |
| C19C | 0.74963 (13) | 0.22836 (18)  | 0.0419 (2)    | 0.0687 (10) |           |
| H19G | 0.7351       | 0.1876        | 0.0460        | 0.082*      |           |
| H19H | 0.7690       | 0.2378        | 0.0901        | 0.082*      |           |
| H19I | 0.7724       | 0.2302        | -0.0034       | 0.082*      |           |
| C20C | 0.67531 (13) | 0.26156 (16)  | -0.03997 (18) | 0.0617 (9)  |           |
| H20G | 0.6582       | 0.2224        | -0.0339       | 0.074*      |           |
| H20H | 0.6975       | 0.2603        | -0.0861       | 0.074*      |           |
| H20I | 0.6496       | 0.2934        | -0.0472       | 0.074*      |           |
| C21C | 0.46282 (10) | 0.23899 (11)  | 0.10529 (14)  | 0.0314 (6)  |           |
| H21E | 0.4529       | 0.2427        | 0.0490        | 0.038*      |           |
| H21F | 0.4917       | 0.2101        | 0.1089        | 0.038*      |           |
| C22C | 0.41774 (10) | 0.21348 (11)  | 0.15081 (15)  | 0.0343 (6)  |           |
| H22E | 0.4289       | 0.2052        | 0.2057        | 0.041*      |           |
| H22F | 0.3904       | 0.2444        | 0.1526        | 0.041*      |           |
| C23C | 0.39600 (10) | 0.15571 (11)  | 0.11521 (15)  | 0.0339 (6)  |           |
| H23E | 0.4238       | 0.1255        | 0.1110        | 0.041*      |           |
| H23F | 0.3833       | 0.1645        | 0.0612        | 0.041*      |           |
| C24C | 0.35265 (10) | 0.12820 (11)  | 0.16242 (15)  | 0.0353 (6)  |           |
| H24E | 0.3289       | 0.1609        | 0.1779        | 0.042*      |           |
| H24F | 0.3671       | 0.1104        | 0.2114        | 0.042*      |           |
| C25C | 0.32236 (10) | 0.07946 (11)  | 0.11835 (15)  | 0.0362 (6)  |           |
| H25E | 0.2945       | 0.0651        | 0.1527        | 0.043*      |           |
| H25F | 0.3063       | 0.0980        | 0.0711        | 0.043*      |           |
| C26C | 0.35367 (10) | 0.02525 (11)  | 0.09268 (15)  | 0.0340 (6)  |           |
| H26E | 0.3803       | 0.0391        | 0.0559        | 0.041*      |           |
| H26F | 0.3712       | 0.0078        | 0.1395        | 0.041*      |           |
| C27C | 0.32204 (10) | -0.02377 (12) | 0.05281 (16)  | 0.0398 (6)* |           |
| H27E | 0.3025       | -0.0056       | 0.0084        | 0.048*      |           |
| H27F | 0.2971       | -0.0399       | 0.0910        | 0.048*      |           |
| C28C | 0.35400 (12) | -0.07582 (13) | 0.02177 (18)  | 0.0495 (7)* |           |
| H28G | 0.3770       | -0.0608       | -0.0190       | 0.059*      |           |
| H28H | 0.3314       | -0.1069       | -0.0008       | 0.059*      |           |
| H28I | 0.3742       | -0.0934       | 0.0651        | 0.059*      |           |
| PID  | -0.0132 (2)  | 0.3322 (2)    | 0.1553 (2)    | 0.0261 (4)  | 0.588 (3) |

|      |               |              |              |             |           |
|------|---------------|--------------|--------------|-------------|-----------|
| O2D  | -0.0483 (3)   | 0.3850 (2)   | 0.1491 (4)   | 0.0272 (11) | 0.588 (3) |
| O11D | 0.0778 (7)    | 0.2446 (5)   | 0.0928 (13)  | 0.028 (3)   | 0.588 (3) |
| N12D | 0.1349 (4)    | 0.3187 (8)   | 0.1196 (16)  | 0.0264 (5)  | 0.588 (3) |
| C3D  | 0.0067 (2)    | 0.3186 (2)   | 0.25637 (19) | 0.0302 (8)  | 0.588 (3) |
| C4D  | 0.0390 (2)    | 0.2705 (2)   | 0.2779 (2)   | 0.0302 (8)  | 0.588 (3) |
| H4D  | 0.0514        | 0.2437       | 0.2388       | 0.036*      | 0.588 (3) |
| C5D  | 0.05270 (15)  | 0.26211 (17) | 0.3567 (3)   | 0.0302 (8)  | 0.588 (3) |
| H5D  | 0.0749        | 0.2298       | 0.3711       | 0.036*      | 0.588 (3) |
| C6D  | 0.03407 (13)  | 0.30070 (17) | 0.4146 (2)   | 0.0302 (8)  | 0.588 (3) |
| H6D  | 0.0477        | 0.2991       | 0.4667       | 0.036*      | 0.588 (3) |
| C7D  | -0.00539 (13) | 0.34242 (15) | 0.3951 (2)   | 0.0302 (8)  | 0.588 (3) |
| H7D  | -0.0262       | 0.3598       | 0.4346       | 0.036*      | 0.588 (3) |
| C8D  | -0.01251 (14) | 0.35727 (15) | 0.3137 (2)   | 0.0302 (8)  | 0.588 (3) |
| H8D  | -0.0301       | 0.3932       | 0.2988       | 0.036*      | 0.588 (3) |
| C9D  | 0.0440 (3)    | 0.3445 (5)   | 0.0978 (4)   | 0.0265 (6)  | 0.588 (3) |
| H9D1 | 0.0340        | 0.3451       | 0.0413       | 0.032*      | 0.588 (3) |
| H9D2 | 0.0577        | 0.3851       | 0.1110       | 0.032*      | 0.588 (3) |
| C10D | 0.0866 (4)    | 0.2986 (5)   | 0.1088 (13)  | 0.0254 (9)  | 0.588 (3) |
| C13D | 0.1491 (5)    | 0.3824 (9)   | 0.1321 (10)  | 0.0275 (7)  | 0.588 (3) |
| H13G | 0.1278        | 0.4079       | 0.0967       | 0.033*      | 0.588 (3) |
| H13H | 0.1852        | 0.3878       | 0.1167       | 0.033*      | 0.588 (3) |
| C14D | 0.1429 (5)    | 0.4049 (6)   | 0.2168 (8)   | 0.0364 (11) | 0.588 (3) |
| H14D | 0.1058        | 0.4020       | 0.2300       | 0.044*      | 0.588 (3) |
| C15D | 0.1576 (3)    | 0.4723 (5)   | 0.2191 (8)   | 0.0362 (18) | 0.588 (3) |
| H15J | 0.1944        | 0.4764       | 0.2101       | 0.043*      | 0.588 (3) |
| H15K | 0.1492        | 0.4892       | 0.2707       | 0.043*      | 0.588 (3) |
| H15L | 0.1386        | 0.4941       | 0.1778       | 0.043*      | 0.588 (3) |
| C16D | 0.1724 (9)    | 0.3678 (8)   | 0.2773 (12)  | 0.048 (3)   | 0.588 (3) |
| H16J | 0.1598        | 0.3260       | 0.2767       | 0.057*      | 0.588 (3) |
| H16K | 0.1676        | 0.3852       | 0.3298       | 0.057*      | 0.588 (3) |
| H16L | 0.2088        | 0.3682       | 0.2645       | 0.057*      | 0.588 (3) |
| C17D | 0.1761 (6)    | 0.2736 (10)  | 0.1250 (10)  | 0.0305 (9)  | 0.588 (3) |
| H17G | 0.1615        | 0.2349       | 0.1438       | 0.037*      | 0.588 (3) |
| H17H | 0.2015        | 0.2873       | 0.1649       | 0.037*      | 0.588 (3) |
| C18D | 0.2034 (6)    | 0.2622 (7)   | 0.0476 (10)  | 0.0307 (13) | 0.588 (3) |
| H18D | 0.2194        | 0.3011       | 0.0306       | 0.037*      | 0.588 (3) |
| C19D | 0.2460 (8)    | 0.2166 (13)  | 0.0631 (12)  | 0.040 (3)   | 0.588 (3) |
| H19J | 0.2693        | 0.2324       | 0.1038       | 0.048*      | 0.588 (3) |
| H19K | 0.2650        | 0.2097       | 0.0144       | 0.048*      | 0.588 (3) |
| H19L | 0.2312        | 0.1783       | 0.0810       | 0.048*      | 0.588 (3) |
| C20D | 0.1675 (9)    | 0.2410 (10)  | -0.0183 (10) | 0.037 (2)   | 0.588 (3) |
| H20J | 0.1491        | 0.2047       | -0.0011      | 0.044*      | 0.588 (3) |
| H20K | 0.1874        | 0.2315       | -0.0653      | 0.044*      | 0.588 (3) |
| H20L | 0.1428        | 0.2731       | -0.0307      | 0.044*      | 0.588 (3) |
| C21D | -0.0428 (2)   | 0.2629 (3)   | 0.1215 (4)   | 0.0257 (12) | 0.588 (3) |
| H21G | -0.0566       | 0.2690       | 0.0675       | 0.031*      | 0.588 (3) |
| H21H | -0.0166       | 0.2306       | 0.1192       | 0.031*      | 0.588 (3) |
| C22D | -0.0860 (2)   | 0.2427 (2)   | 0.1755 (3)   | 0.0288 (11) | 0.588 (3) |

|      |               |              |              |             |           |
|------|---------------|--------------|--------------|-------------|-----------|
| H22G | -0.0712       | 0.2206       | 0.2212       | 0.035*      | 0.588 (3) |
| H22H | -0.1038       | 0.2789       | 0.1959       | 0.035*      | 0.588 (3) |
| C23D | -0.12469 (15) | 0.20207 (18) | 0.1340 (2)   | 0.0312 (8)  | 0.588 (3) |
| H23G | -0.1369       | 0.2229       | 0.0857       | 0.037*      | 0.588 (3) |
| H23H | -0.1545       | 0.1968       | 0.1688       | 0.037*      | 0.588 (3) |
| C24D | -0.10496 (16) | 0.13974 (19) | 0.1111 (3)   | 0.0322 (8)  | 0.588 (3) |
| H24G | -0.0873       | 0.1212       | 0.1571       | 0.039*      | 0.588 (3) |
| H24H | -0.0798       | 0.1441       | 0.0684       | 0.039*      | 0.588 (3) |
| C25D | -0.14814 (18) | 0.09821 (19) | 0.0835 (3)   | 0.0353 (10) | 0.588 (3) |
| H25G | -0.1724       | 0.0933       | 0.1273       | 0.042*      | 0.588 (3) |
| H25H | -0.1667       | 0.1185       | 0.0397       | 0.042*      | 0.588 (3) |
| C26D | -0.1322 (3)   | 0.0359 (4)   | 0.0559 (9)   | 0.0372 (18) | 0.588 (3) |
| H26G | -0.1120       | 0.0161       | 0.0983       | 0.045*      | 0.588 (3) |
| H26H | -0.1098       | 0.0403       | 0.0096       | 0.045*      | 0.588 (3) |
| C27D | -0.1772 (4)   | -0.0046 (11) | 0.034 (3)    | 0.0427 (7)  | 0.588 (3) |
| H27G | -0.1970       | -0.0135      | 0.0817       | 0.051*      | 0.588 (3) |
| H27H | -0.1999       | 0.0175       | -0.0034      | 0.051*      | 0.588 (3) |
| C28D | -0.1614 (4)   | -0.0640 (6)  | -0.0041 (14) | 0.054 (3)   | 0.588 (3) |
| H28J | -0.1420       | -0.0557      | -0.0519      | 0.065*      | 0.588 (3) |
| H28K | -0.1920       | -0.0875      | -0.0178      | 0.065*      | 0.588 (3) |
| H28L | -0.1401       | -0.0871      | 0.0330       | 0.065*      | 0.588 (3) |
| P1E  | -0.0150 (3)   | 0.3228 (3)   | 0.1529 (3)   | 0.0261 (4)  | 0.412 (3) |
| O2E  | -0.0548 (4)   | 0.3703 (4)   | 0.1425 (7)   | 0.0272 (11) | 0.412 (3) |
| O11E | 0.0751 (10)   | 0.2442 (7)   | 0.107 (2)    | 0.028 (3)   | 0.412 (3) |
| N12E | 0.1344 (6)    | 0.3177 (11)  | 0.121 (2)    | 0.0264 (5)  | 0.412 (3) |
| C3E  | 0.0011 (3)    | 0.3118 (3)   | 0.2561 (3)   | 0.0326 (12) | 0.412 (3) |
| C4E  | 0.0334 (3)    | 0.2651 (3)   | 0.2820 (4)   | 0.0326 (12) | 0.412 (3) |
| H4E  | 0.0486        | 0.2386       | 0.2449       | 0.039*      | 0.412 (3) |
| C5E  | 0.0434 (2)    | 0.2573 (3)   | 0.3625 (4)   | 0.0326 (12) | 0.412 (3) |
| H5E  | 0.0639        | 0.2245       | 0.3803       | 0.039*      | 0.412 (3) |
| C6E  | 0.02312 (18)  | 0.2980 (3)   | 0.4167 (3)   | 0.0326 (12) | 0.412 (3) |
| H6E  | 0.0241        | 0.2892       | 0.4715       | 0.039*      | 0.412 (3) |
| C7E  | 0.00095 (19)  | 0.3530 (2)   | 0.3890 (3)   | 0.0326 (12) | 0.412 (3) |
| H7E  | 0.0001        | 0.3885       | 0.4205       | 0.039*      | 0.412 (3) |
| C8E  | -0.0201 (2)   | 0.3516 (2)   | 0.3105 (3)   | 0.0326 (12) | 0.412 (3) |
| H8E  | -0.0478       | 0.3772       | 0.2960       | 0.039*      | 0.412 (3) |
| C9E  | 0.0434 (4)    | 0.3452 (7)   | 0.1035 (6)   | 0.0265 (6)  | 0.412 (3) |
| H9E1 | 0.0348        | 0.3548       | 0.0479       | 0.032*      | 0.412 (3) |
| H9E2 | 0.0563        | 0.3828       | 0.1284       | 0.032*      | 0.412 (3) |
| C10E | 0.0863 (5)    | 0.2990 (7)   | 0.1044 (19)  | 0.0254 (9)  | 0.412 (3) |
| C13E | 0.1499 (7)    | 0.3815 (12)  | 0.1271 (15)  | 0.0275 (7)  | 0.412 (3) |
| H13I | 0.1293        | 0.4056       | 0.0893       | 0.033*      | 0.412 (3) |
| H13J | 0.1861        | 0.3850       | 0.1116       | 0.033*      | 0.412 (3) |
| C14E | 0.1439 (7)    | 0.4090 (9)   | 0.2095 (12)  | 0.0364 (11) | 0.412 (3) |
| H14E | 0.1067        | 0.4165       | 0.2177       | 0.044*      | 0.412 (3) |
| C15E | 0.1711 (6)    | 0.4707 (9)   | 0.2103 (13)  | 0.0362 (18) | 0.412 (3) |
| H15M | 0.2068        | 0.4654       | 0.1951       | 0.043*      | 0.412 (3) |
| H15N | 0.1697        | 0.4880       | 0.2633       | 0.043*      | 0.412 (3) |

|      |             |              |              |             |           |
|------|-------------|--------------|--------------|-------------|-----------|
| H15O | 0.1540      | 0.4980       | 0.1729       | 0.043*      | 0.412 (3) |
| C16E | 0.1626 (14) | 0.3678 (12)  | 0.2755 (17)  | 0.048 (3)   | 0.412 (3) |
| H16M | 0.1470      | 0.3277       | 0.2694       | 0.057*      | 0.412 (3) |
| H16N | 0.1529      | 0.3851       | 0.3264       | 0.057*      | 0.412 (3) |
| H16O | 0.1998      | 0.3641       | 0.2733       | 0.057*      | 0.412 (3) |
| C17E | 0.1756 (8)  | 0.2724 (15)  | 0.1187 (14)  | 0.0305 (9)  | 0.412 (3) |
| H17I | 0.1612      | 0.2325       | 0.1330       | 0.037*      | 0.412 (3) |
| H17J | 0.2016      | 0.2830       | 0.1591       | 0.037*      | 0.412 (3) |
| C18E | 0.2016 (8)  | 0.2668 (11)  | 0.0392 (15)  | 0.0307 (13) | 0.412 (3) |
| H18E | 0.2167      | 0.3071       | 0.0259       | 0.037*      | 0.412 (3) |
| C19E | 0.2453 (12) | 0.222 (2)    | 0.0478 (18)  | 0.040 (3)   | 0.412 (3) |
| H19M | 0.2693      | 0.2357       | 0.0885       | 0.048*      | 0.412 (3) |
| H19N | 0.2630      | 0.2179       | -0.0025      | 0.048*      | 0.412 (3) |
| H19O | 0.2315      | 0.1820       | 0.0629       | 0.048*      | 0.412 (3) |
| C20E | 0.1649 (13) | 0.2491 (16)  | -0.0273 (14) | 0.037 (2)   | 0.412 (3) |
| H20M | 0.1500      | 0.2093       | -0.0160      | 0.044*      | 0.412 (3) |
| H20N | 0.1834      | 0.2472       | -0.0771      | 0.044*      | 0.412 (3) |
| H20O | 0.1375      | 0.2792       | -0.0316      | 0.044*      | 0.412 (3) |
| C21E | -0.0339 (3) | 0.2503 (4)   | 0.1138 (5)   | 0.0257 (12) | 0.412 (3) |
| H21I | -0.0390     | 0.2541       | 0.0561       | 0.031*      | 0.412 (3) |
| H21J | -0.0058     | 0.2211       | 0.1230       | 0.031*      | 0.412 (3) |
| C22E | -0.0827 (3) | 0.2248 (3)   | 0.1494 (4)   | 0.0288 (11) | 0.412 (3) |
| H22I | -0.0757     | 0.2137       | 0.2050       | 0.035*      | 0.412 (3) |
| H22J | -0.1092     | 0.2569       | 0.1490       | 0.035*      | 0.412 (3) |
| C23E | -0.1036 (2) | 0.1696 (3)   | 0.1061 (4)   | 0.0312 (8)  | 0.412 (3) |
| H23I | -0.1157     | 0.1822       | 0.0531       | 0.037*      | 0.412 (3) |
| H23J | -0.0755     | 0.1402       | 0.0991       | 0.037*      | 0.412 (3) |
| C24E | -0.1474 (2) | 0.1383 (2)   | 0.1481 (3)   | 0.0322 (8)  | 0.412 (3) |
| H24I | -0.1335     | 0.1177       | 0.1956       | 0.039*      | 0.412 (3) |
| H24J | -0.1718     | 0.1694       | 0.1660       | 0.039*      | 0.412 (3) |
| C25E | -0.1762 (3) | 0.0921 (3)   | 0.0983 (4)   | 0.0353 (10) | 0.412 (3) |
| H25I | -0.2046     | 0.0756       | 0.1299       | 0.042*      | 0.412 (3) |
| H25J | -0.1916     | 0.1132       | 0.0523       | 0.042*      | 0.412 (3) |
| C26E | -0.1447 (4) | 0.0395 (6)   | 0.0683 (14)  | 0.0372 (18) | 0.412 (3) |
| H26I | -0.1250     | 0.0220       | 0.1129       | 0.045*      | 0.412 (3) |
| H26J | -0.1199     | 0.0549       | 0.0294       | 0.045*      | 0.412 (3) |
| C27E | -0.1767 (5) | -0.0102 (15) | 0.030 (4)    | 0.0427 (7)  | 0.412 (3) |
| H27I | -0.2013     | -0.0257      | 0.0691       | 0.051*      | 0.412 (3) |
| H27J | -0.1966     | 0.0074       | -0.0143      | 0.051*      | 0.412 (3) |
| C28E | -0.1452 (7) | -0.0627 (8)  | -0.001 (2)   | 0.054 (3)   | 0.412 (3) |
| H28M | -0.1241     | -0.0489      | -0.0444      | 0.065*      | 0.412 (3) |
| H28N | -0.1681     | -0.0950      | -0.0190      | 0.065*      | 0.412 (3) |
| H28O | -0.1231     | -0.0782      | 0.0418       | 0.065*      | 0.412 (3) |

Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$   | $U^{13}$    | $U^{23}$    |
|-----|------------|------------|------------|------------|-------------|-------------|
| P1A | 0.0258 (3) | 0.0229 (3) | 0.0247 (3) | 0.0009 (2) | -0.0012 (2) | -0.0019 (2) |

|      |             |             |             |              |              |              |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| O2A  | 0.0275 (9)  | 0.0260 (8)  | 0.0336 (9)  | 0.0040 (7)   | -0.0010 (7)  | -0.0040 (7)  |
| O11A | 0.0327 (10) | 0.0265 (9)  | 0.0330 (9)  | 0.0028 (7)   | 0.0011 (7)   | 0.0011 (7)   |
| N12A | 0.0271 (11) | 0.0258 (10) | 0.0305 (10) | 0.0028 (8)   | 0.0001 (8)   | -0.0015 (8)  |
| C3A  | 0.0258 (13) | 0.0257 (12) | 0.0281 (12) | -0.0029 (10) | -0.0018 (10) | -0.0031 (10) |
| C4A  | 0.0407 (15) | 0.0318 (13) | 0.0307 (13) | 0.0040 (12)  | -0.0030 (11) | -0.0026 (11) |
| C5A  | 0.0459 (16) | 0.0373 (15) | 0.0326 (14) | 0.0029 (12)  | 0.0011 (12)  | -0.0095 (11) |
| C6A  | 0.0502 (17) | 0.0444 (16) | 0.0264 (13) | -0.0103 (13) | 0.0013 (12)  | -0.0047 (12) |
| C7A  | 0.0598 (19) | 0.0385 (15) | 0.0324 (14) | 0.0010 (14)  | -0.0022 (13) | 0.0058 (12)  |
| C8A  | 0.0443 (16) | 0.0297 (13) | 0.0312 (13) | 0.0022 (12)  | -0.0006 (11) | 0.0015 (10)  |
| C9A  | 0.0260 (12) | 0.0246 (12) | 0.0244 (12) | 0.0003 (10)  | 0.0011 (10)  | -0.0024 (9)  |
| C10A | 0.0284 (13) | 0.0285 (13) | 0.0199 (11) | 0.0001 (10)  | -0.0016 (9)  | -0.0032 (9)  |
| C13A | 0.0271 (13) | 0.0342 (14) | 0.0378 (14) | 0.0051 (11)  | 0.0008 (11)  | 0.0004 (11)  |
| C14A | 0.0363 (15) | 0.0356 (14) | 0.0408 (15) | 0.0067 (12)  | 0.0069 (12)  | -0.0028 (11) |
| C15A | 0.0517 (18) | 0.0506 (17) | 0.0370 (15) | 0.0082 (14)  | 0.0067 (13)  | -0.0057 (13) |
| C16A | 0.0494 (18) | 0.0503 (18) | 0.0552 (18) | 0.0203 (15)  | 0.0129 (15)  | -0.0001 (14) |
| C17A | 0.0275 (13) | 0.0295 (13) | 0.0309 (13) | -0.0012 (10) | 0.0018 (10)  | -0.0006 (10) |
| C18A | 0.0293 (14) | 0.0383 (14) | 0.0386 (14) | -0.0045 (11) | -0.0007 (11) | -0.0068 (11) |
| C19A | 0.0409 (17) | 0.0383 (16) | 0.0649 (19) | -0.0053 (13) | -0.0072 (14) | -0.0110 (14) |
| C20A | 0.0462 (17) | 0.0553 (18) | 0.0401 (15) | -0.0056 (14) | -0.0079 (13) | -0.0055 (13) |
| C21A | 0.0272 (13) | 0.0268 (12) | 0.0267 (12) | 0.0023 (10)  | -0.0013 (10) | -0.0007 (9)  |
| C22A | 0.0287 (13) | 0.0256 (12) | 0.0303 (12) | 0.0012 (10)  | -0.0022 (10) | 0.0001 (10)  |
| C23A | 0.0306 (14) | 0.0297 (13) | 0.0344 (13) | -0.0005 (11) | -0.0009 (11) | 0.0039 (10)  |
| C24A | 0.0302 (14) | 0.0300 (13) | 0.0340 (13) | -0.0012 (11) | 0.0001 (11)  | 0.0003 (10)  |
| C25A | 0.0360 (15) | 0.0316 (14) | 0.0391 (14) | -0.0026 (11) | 0.0042 (12)  | -0.0003 (11) |
| C26A | 0.0516 (18) | 0.0434 (16) | 0.0420 (15) | -0.0174 (14) | -0.0036 (13) | 0.0011 (13)  |
| P1B  | 0.0280 (3)  | 0.0217 (3)  | 0.0259 (3)  | 0.0019 (2)   | -0.0002 (2)  | -0.0004 (2)  |
| O2B  | 0.0300 (9)  | 0.0249 (8)  | 0.0387 (9)  | 0.0043 (7)   | 0.0032 (7)   | -0.0015 (7)  |
| O11B | 0.0348 (10) | 0.0281 (9)  | 0.0334 (9)  | 0.0028 (7)   | -0.0039 (7)  | 0.0000 (7)   |
| N12B | 0.0270 (11) | 0.0298 (11) | 0.0363 (11) | 0.0023 (9)   | -0.0039 (9)  | -0.0010 (9)  |
| C3B  | 0.0245 (12) | 0.0252 (12) | 0.0289 (12) | -0.0035 (10) | -0.0002 (10) | 0.0014 (10)  |
| C4B  | 0.0342 (14) | 0.0306 (13) | 0.0360 (14) | 0.0007 (11)  | -0.0002 (11) | 0.0081 (11)  |
| C5B  | 0.0473 (17) | 0.0472 (16) | 0.0332 (14) | -0.0002 (14) | -0.0071 (12) | 0.0153 (12)  |
| C6B  | 0.0443 (16) | 0.0474 (16) | 0.0250 (13) | -0.0105 (13) | -0.0003 (11) | 0.0020 (12)  |
| C7B  | 0.0413 (15) | 0.0347 (14) | 0.0308 (13) | -0.0035 (12) | 0.0012 (11)  | -0.0050 (11) |
| C8B  | 0.0351 (14) | 0.0289 (13) | 0.0274 (12) | 0.0009 (11)  | -0.0041 (11) | -0.0006 (10) |
| C9B  | 0.0289 (13) | 0.0267 (12) | 0.0256 (12) | -0.0011 (10) | -0.0002 (10) | -0.0030 (9)  |
| C10B | 0.0302 (13) | 0.0291 (13) | 0.0231 (12) | 0.0002 (10)  | -0.0056 (10) | -0.0028 (10) |
| C13B | 0.0297 (14) | 0.0337 (14) | 0.0374 (14) | -0.0003 (11) | -0.0033 (11) | 0.0040 (11)  |
| C14B | 0.0489 (18) | 0.0399 (16) | 0.0562 (18) | -0.0067 (13) | -0.0136 (14) | 0.0017 (13)  |
| C15B | 0.060 (2)   | 0.0466 (19) | 0.087 (3)   | -0.0192 (16) | -0.0245 (19) | 0.0122 (17)  |
| C16B | 0.075 (2)   | 0.055 (2)   | 0.0545 (19) | -0.0099 (17) | -0.0059 (17) | -0.0169 (16) |
| C17B | 0.0263 (13) | 0.0384 (15) | 0.0438 (15) | 0.0070 (11)  | -0.0033 (11) | 0.0003 (12)  |
| C18B | 0.0368 (16) | 0.0461 (16) | 0.0445 (16) | 0.0100 (13)  | -0.0008 (12) | -0.0039 (13) |
| C19B | 0.058 (2)   | 0.064 (2)   | 0.0412 (16) | 0.0154 (16)  | 0.0020 (14)  | -0.0033 (14) |
| C20B | 0.0512 (19) | 0.062 (2)   | 0.061 (2)   | 0.0220 (16)  | 0.0067 (16)  | -0.0052 (16) |
| C21B | 0.0314 (13) | 0.0238 (12) | 0.0250 (12) | 0.0027 (10)  | 0.0000 (10)  | 0.0026 (9)   |
| C22B | 0.0308 (14) | 0.0278 (13) | 0.0315 (13) | -0.0008 (10) | -0.0017 (11) | 0.0031 (10)  |
| C23B | 0.0339 (14) | 0.0277 (13) | 0.0355 (13) | 0.0010 (11)  | 0.0017 (11)  | 0.0023 (10)  |

|      |             |             |             |              |              |              |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C24B | 0.0427 (16) | 0.0386 (15) | 0.0382 (15) | -0.0105 (12) | -0.0021 (12) | 0.0069 (12)  |
| C25B | 0.0485 (17) | 0.0381 (15) | 0.0383 (15) | -0.0106 (13) | 0.0028 (13)  | 0.0057 (12)  |
| C26B | 0.066 (2)   | 0.0454 (17) | 0.0491 (17) | -0.0166 (15) | -0.0059 (15) | 0.0053 (14)  |
| P1C  | 0.0314 (4)  | 0.0241 (3)  | 0.0302 (3)  | 0.0007 (3)   | 0.0001 (3)   | 0.0031 (2)   |
| O2C  | 0.0329 (10) | 0.0280 (9)  | 0.0461 (10) | 0.0044 (7)   | 0.0006 (8)   | 0.0039 (8)   |
| O11C | 0.0393 (10) | 0.0246 (9)  | 0.0411 (10) | 0.0008 (7)   | 0.0065 (8)   | 0.0014 (7)   |
| N12C | 0.0343 (12) | 0.0254 (10) | 0.0318 (11) | 0.0037 (9)   | -0.0069 (9)  | -0.0014 (8)  |
| C3C  | 0.0305 (13) | 0.0253 (12) | 0.0309 (13) | -0.0038 (10) | 0.0032 (10)  | 0.0023 (10)  |
| C4C  | 0.0399 (15) | 0.0311 (14) | 0.0366 (14) | -0.0015 (12) | 0.0048 (12)  | -0.0032 (11) |
| C5C  | 0.0513 (18) | 0.0418 (16) | 0.0354 (15) | -0.0061 (14) | 0.0059 (13)  | -0.0087 (12) |
| C6C  | 0.0498 (17) | 0.0426 (16) | 0.0291 (13) | -0.0153 (13) | -0.0011 (12) | 0.0011 (11)  |
| C7C  | 0.0415 (16) | 0.0334 (14) | 0.0373 (14) | -0.0040 (12) | -0.0036 (12) | 0.0067 (11)  |
| C8C  | 0.0408 (15) | 0.0273 (13) | 0.0311 (13) | -0.0022 (11) | 0.0018 (11)  | 0.0023 (10)  |
| C9C  | 0.0355 (14) | 0.0265 (12) | 0.0288 (12) | 0.0025 (11)  | 0.0006 (11)  | 0.0050 (10)  |
| C10C | 0.0350 (14) | 0.0288 (13) | 0.0200 (11) | 0.0024 (11)  | 0.0037 (10)  | 0.0021 (9)   |
| C13C | 0.0402 (15) | 0.0248 (13) | 0.0355 (14) | 0.0032 (11)  | -0.0050 (11) | -0.0035 (10) |
| C14C | 0.0403 (15) | 0.0360 (14) | 0.0358 (14) | -0.0022 (12) | -0.0040 (12) | -0.0037 (11) |
| C15C | 0.0522 (18) | 0.0408 (16) | 0.0488 (17) | -0.0055 (14) | -0.0060 (14) | -0.0098 (13) |
| C16C | 0.073 (2)   | 0.0545 (19) | 0.0408 (17) | -0.0176 (17) | 0.0087 (15)  | -0.0133 (14) |
| C17C | 0.0337 (14) | 0.0305 (13) | 0.0399 (14) | 0.0063 (11)  | -0.0076 (12) | -0.0012 (11) |
| C18C | 0.0425 (18) | 0.0567 (19) | 0.061 (2)   | 0.0146 (15)  | 0.0013 (15)  | 0.0061 (15)  |
| C19C | 0.0469 (19) | 0.091 (3)   | 0.069 (2)   | 0.0307 (19)  | 0.0080 (17)  | 0.0094 (19)  |
| C20C | 0.072 (2)   | 0.070 (2)   | 0.0439 (17) | 0.0290 (18)  | 0.0048 (16)  | -0.0046 (16) |
| C21C | 0.0350 (14) | 0.0297 (13) | 0.0294 (13) | 0.0005 (11)  | -0.0038 (11) | 0.0025 (10)  |
| C22C | 0.0384 (15) | 0.0288 (13) | 0.0358 (14) | -0.0016 (11) | 0.0005 (11)  | 0.0016 (11)  |
| C23C | 0.0361 (15) | 0.0304 (13) | 0.0351 (14) | -0.0021 (11) | -0.0018 (11) | -0.0001 (11) |
| C24C | 0.0353 (15) | 0.0334 (14) | 0.0371 (14) | -0.0023 (11) | 0.0000 (11)  | -0.0001 (11) |
| C25C | 0.0345 (15) | 0.0366 (14) | 0.0375 (14) | -0.0035 (12) | -0.0021 (11) | 0.0034 (11)  |
| C26C | 0.0331 (14) | 0.0334 (13) | 0.0356 (14) | -0.0047 (11) | -0.0028 (11) | 0.0035 (11)  |
| P1D  | 0.0243 (5)  | 0.0230 (13) | 0.0308 (4)  | -0.0019 (7)  | -0.0011 (3)  | 0.0095 (6)   |
| O2D  | 0.020 (2)   | 0.014 (3)   | 0.0468 (16) | -0.009 (2)   | -0.0027 (12) | 0.009 (2)    |
| O11D | 0.0328 (19) | 0.0241 (9)  | 0.026 (8)   | -0.0047 (9)  | 0.009 (3)    | 0.0022 (17)  |
| N12D | 0.0258 (11) | 0.0243 (11) | 0.0290 (11) | 0.0007 (8)   | -0.0015 (9)  | 0.0002 (9)   |
| C3D  | 0.0290 (14) | 0.0292 (14) | 0.0323 (17) | -0.0111 (12) | -0.0013 (11) | 0.0066 (11)  |
| C4D  | 0.0290 (14) | 0.0292 (14) | 0.0323 (17) | -0.0111 (12) | -0.0013 (11) | 0.0066 (11)  |
| C5D  | 0.0290 (14) | 0.0292 (14) | 0.0323 (17) | -0.0111 (12) | -0.0013 (11) | 0.0066 (11)  |
| C6D  | 0.0290 (14) | 0.0292 (14) | 0.0323 (17) | -0.0111 (12) | -0.0013 (11) | 0.0066 (11)  |
| C7D  | 0.0290 (14) | 0.0292 (14) | 0.0323 (17) | -0.0111 (12) | -0.0013 (11) | 0.0066 (11)  |
| C8D  | 0.0290 (14) | 0.0292 (14) | 0.0323 (17) | -0.0111 (12) | -0.0013 (11) | 0.0066 (11)  |
| C9D  | 0.0276 (13) | 0.0273 (12) | 0.0245 (14) | -0.0007 (10) | -0.0015 (11) | 0.0053 (11)  |
| C10D | 0.0274 (13) | 0.0266 (13) | 0.022 (2)   | -0.0015 (10) | 0.0020 (11)  | 0.0046 (11)  |
| C13D | 0.0279 (13) | 0.0230 (12) | 0.032 (2)   | -0.0011 (10) | 0.0001 (12)  | -0.0006 (13) |
| C14D | 0.0422 (16) | 0.034 (2)   | 0.032 (3)   | -0.0003 (13) | -0.0023 (15) | -0.0046 (18) |
| C15D | 0.023 (5)   | 0.0400 (17) | 0.046 (3)   | 0.000 (3)    | 0.006 (3)    | -0.0156 (17) |
| C16D | 0.050 (9)   | 0.0585 (19) | 0.0343 (17) | 0.000 (3)    | -0.009 (3)   | -0.0041 (14) |
| C17D | 0.0290 (14) | 0.0266 (14) | 0.036 (3)   | 0.0034 (11)  | -0.0049 (14) | 0.0033 (17)  |
| C18D | 0.0306 (16) | 0.023 (2)   | 0.038 (3)   | 0.0027 (14)  | 0.0003 (18)  | 0.002 (2)    |
| C19D | 0.0341 (17) | 0.032 (5)   | 0.054 (7)   | 0.0067 (17)  | 0.002 (4)    | 0.005 (5)    |

|      |             |             |             |              |              |              |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| C20D | 0.040 (2)   | 0.032 (5)   | 0.038 (3)   | 0.003 (3)    | 0.001 (2)    | -0.002 (3)   |
| C21D | 0.019 (2)   | 0.025 (3)   | 0.0329 (17) | 0.004 (2)    | -0.0017 (14) | 0.0064 (15)  |
| C22D | 0.0321 (18) | 0.031 (3)   | 0.024 (3)   | -0.006 (2)   | 0.001 (2)    | -0.0004 (19) |
| C23D | 0.030 (2)   | 0.031 (2)   | 0.032 (2)   | -0.0058 (17) | -0.0021 (16) | 0.0001 (16)  |
| C24D | 0.0311 (19) | 0.032 (2)   | 0.033 (2)   | -0.0052 (18) | -0.0023 (15) | -0.0023 (16) |
| C25D | 0.034 (3)   | 0.0340 (19) | 0.038 (2)   | -0.006 (2)   | -0.004 (2)   | -0.0004 (16) |
| C26D | 0.039 (4)   | 0.0332 (18) | 0.039 (5)   | 0.000 (2)    | -0.008 (4)   | -0.0030 (14) |
| C27D | 0.0447 (17) | 0.040 (4)   | 0.043 (4)   | -0.0077 (15) | -0.0010 (14) | -0.006 (3)   |
| C28D | 0.062 (8)   | 0.0411 (18) | 0.058 (3)   | -0.012 (4)   | -0.002 (7)   | -0.0152 (16) |
| PIE  | 0.0243 (5)  | 0.0230 (13) | 0.0308 (4)  | -0.0019 (7)  | -0.0011 (3)  | 0.0095 (6)   |
| O2E  | 0.020 (2)   | 0.014 (3)   | 0.0468 (16) | -0.009 (2)   | -0.0027 (12) | 0.009 (2)    |
| O11E | 0.0328 (19) | 0.0241 (9)  | 0.026 (8)   | -0.0047 (9)  | 0.009 (3)    | 0.0022 (17)  |
| N12E | 0.0258 (11) | 0.0243 (11) | 0.0290 (11) | 0.0007 (8)   | -0.0015 (9)  | 0.0002 (9)   |
| C3E  | 0.025 (2)   | 0.035 (2)   | 0.037 (3)   | -0.0100 (17) | 0.0054 (16)  | 0.0070 (17)  |
| C4E  | 0.025 (2)   | 0.035 (2)   | 0.037 (3)   | -0.0100 (17) | 0.0054 (16)  | 0.0070 (17)  |
| C5E  | 0.025 (2)   | 0.035 (2)   | 0.037 (3)   | -0.0100 (17) | 0.0054 (16)  | 0.0070 (17)  |
| C6E  | 0.025 (2)   | 0.035 (2)   | 0.037 (3)   | -0.0100 (17) | 0.0054 (16)  | 0.0070 (17)  |
| C7E  | 0.025 (2)   | 0.035 (2)   | 0.037 (3)   | -0.0100 (17) | 0.0054 (16)  | 0.0070 (17)  |
| C8E  | 0.025 (2)   | 0.035 (2)   | 0.037 (3)   | -0.0100 (17) | 0.0054 (16)  | 0.0070 (17)  |
| C9E  | 0.0276 (13) | 0.0273 (12) | 0.0245 (14) | -0.0007 (10) | -0.0015 (11) | 0.0053 (11)  |
| C10E | 0.0274 (13) | 0.0266 (13) | 0.022 (2)   | -0.0015 (10) | 0.0020 (11)  | 0.0046 (11)  |
| C13E | 0.0279 (13) | 0.0230 (12) | 0.032 (2)   | -0.0011 (10) | 0.0001 (12)  | -0.0006 (13) |
| C14E | 0.0422 (16) | 0.034 (2)   | 0.032 (3)   | -0.0003 (13) | -0.0023 (15) | -0.0046 (18) |
| C15E | 0.023 (5)   | 0.0400 (17) | 0.046 (3)   | 0.000 (3)    | 0.006 (3)    | -0.0156 (17) |
| C16E | 0.050 (9)   | 0.0585 (19) | 0.0343 (17) | 0.000 (3)    | -0.009 (3)   | -0.0041 (14) |
| C17E | 0.0290 (14) | 0.0266 (14) | 0.036 (3)   | 0.0034 (11)  | -0.0049 (14) | 0.0033 (17)  |
| C18E | 0.0306 (16) | 0.023 (2)   | 0.038 (3)   | 0.0027 (14)  | 0.0003 (18)  | 0.002 (2)    |
| C19E | 0.0341 (17) | 0.032 (5)   | 0.054 (7)   | 0.0067 (17)  | 0.002 (4)    | 0.005 (5)    |
| C20E | 0.040 (2)   | 0.032 (5)   | 0.038 (3)   | 0.003 (3)    | 0.001 (2)    | -0.002 (3)   |
| C21E | 0.019 (2)   | 0.025 (3)   | 0.0329 (17) | 0.004 (2)    | -0.0017 (14) | 0.0064 (15)  |
| C22E | 0.0321 (18) | 0.031 (3)   | 0.024 (3)   | -0.006 (2)   | 0.001 (2)    | -0.0004 (19) |
| C23E | 0.030 (2)   | 0.031 (2)   | 0.032 (2)   | -0.0058 (17) | -0.0021 (16) | 0.0001 (16)  |
| C24E | 0.0311 (19) | 0.032 (2)   | 0.033 (2)   | -0.0052 (18) | -0.0023 (15) | -0.0023 (16) |
| C25E | 0.034 (3)   | 0.0340 (19) | 0.038 (2)   | -0.006 (2)   | -0.004 (2)   | -0.0004 (16) |
| C26E | 0.039 (4)   | 0.0332 (18) | 0.039 (5)   | 0.000 (2)    | -0.008 (4)   | -0.0030 (14) |
| C27E | 0.0447 (17) | 0.040 (4)   | 0.043 (4)   | -0.0077 (15) | -0.0010 (14) | -0.006 (3)   |
| C28E | 0.062 (8)   | 0.0411 (18) | 0.058 (3)   | -0.012 (4)   | -0.002 (7)   | -0.0152 (16) |

*Geometric parameters (Å, °)*

|           |             |           |           |
|-----------|-------------|-----------|-----------|
| PIA—O2A   | 1.4869 (16) | C17C—H17E | 0.9900    |
| PIA—C21A  | 1.798 (2)   | C17C—H17F | 0.9900    |
| PIA—C3A   | 1.809 (2)   | C18C—C20C | 1.474 (4) |
| PIA—C9A   | 1.812 (2)   | C18C—C19C | 1.533 (4) |
| O11A—C10A | 1.233 (3)   | C18C—H18C | 1.0000    |
| N12A—C10A | 1.356 (3)   | C19C—H19G | 0.9800    |
| N12A—C17A | 1.467 (3)   | C19C—H19H | 0.9800    |
| N12A—C13A | 1.471 (3)   | C19C—H19I | 0.9800    |



|           |           |           |           |
|-----------|-----------|-----------|-----------|
| C3A—C8A   | 1.390 (3) | C20C—H20G | 0.9800    |
| C3A—C4A   | 1.392 (3) | C20C—H20H | 0.9800    |
| C4A—C5A   | 1.389 (3) | C20C—H20I | 0.9800    |
| C4A—H4A   | 0.9500    | C21C—C22C | 1.525 (3) |
| C5A—C6A   | 1.384 (4) | C21C—H21E | 0.9900    |
| C5A—H5A   | 0.9500    | C21C—H21F | 0.9900    |
| C6A—C7A   | 1.373 (4) | C22C—C23C | 1.520 (3) |
| C6A—H6A   | 0.9500    | C22C—H22E | 0.9900    |
| C7A—C8A   | 1.386 (4) | C22C—H22F | 0.9900    |
| C7A—H7A   | 0.9500    | C23C—C24C | 1.523 (3) |
| C8A—H8A   | 0.9500    | C23C—H23E | 0.9900    |
| C9A—C10A  | 1.517 (3) | C23C—H23F | 0.9900    |
| C9A—H9A1  | 0.9900    | C24C—C25C | 1.527 (3) |
| C9A—H9A2  | 0.9900    | C24C—H24E | 0.9900    |
| C13A—C14A | 1.532 (3) | C24C—H24F | 0.9900    |
| C13A—H13A | 0.9900    | C25C—C26C | 1.518 (4) |
| C13A—H13B | 0.9900    | C25C—H25E | 0.9900    |
| C14A—C15A | 1.520 (4) | C25C—H25F | 0.9900    |
| C14A—C16A | 1.524 (4) | C26C—C27C | 1.518 (3) |
| C14A—H14A | 1.0000    | C26C—H26E | 0.9900    |
| C15A—H15A | 0.9800    | C26C—H26F | 0.9900    |
| C15A—H15B | 0.9800    | C27C—C28C | 1.520 (4) |
| C15A—H15C | 0.9800    | C27C—H27E | 0.9900    |
| C16A—H16A | 0.9800    | C27C—H27F | 0.9900    |
| C16A—H16B | 0.9800    | C28C—H28G | 0.9800    |
| C16A—H16C | 0.9800    | C28C—H28H | 0.9800    |
| C17A—C18A | 1.537 (3) | C28C—H28I | 0.9800    |
| C17A—H17A | 0.9900    | P1D—O2D   | 1.488 (3) |
| C17A—H17B | 0.9900    | P1D—C21D  | 1.806 (3) |
| C18A—C20A | 1.515 (4) | P1D—C3D   | 1.812 (2) |
| C18A—C19A | 1.518 (4) | P1D—C9D   | 1.815 (3) |
| C18A—H18A | 1.0000    | O11D—C10D | 1.245 (6) |
| C19A—H19A | 0.9800    | N12D—C10D | 1.349 (4) |
| C19A—H19B | 0.9800    | N12D—C13D | 1.470 (3) |
| C19A—H19C | 0.9800    | N12D—C17D | 1.471 (4) |
| C20A—H20A | 0.9800    | C3D—C8D   | 1.3931    |
| C20A—H20B | 0.9800    | C3D—C4D   | 1.4030    |
| C20A—H20C | 0.9800    | C4D—C5D   | 1.3939    |
| C21A—C22A | 1.531 (3) | C4D—H4D   | 0.9500    |
| C21A—H21A | 0.9900    | C5D—C6D   | 1.3924    |
| C21A—H21B | 0.9900    | C5D—H5D   | 0.9500    |
| C22A—C23A | 1.520 (3) | C6D—C7D   | 1.4204    |
| C22A—H22A | 0.9900    | C6D—H6D   | 0.9500    |
| C22A—H22B | 0.9900    | C7D—C8D   | 1.4299    |
| C23A—C24A | 1.518 (3) | C7D—H7D   | 0.9500    |
| C23A—H23A | 0.9900    | C8D—H8D   | 0.9500    |
| C23A—H23B | 0.9900    | C9D—C10D  | 1.517 (4) |
| C24A—C25A | 1.525 (3) | C9D—H9D1  | 0.9900    |

|           |             |           |           |
|-----------|-------------|-----------|-----------|
| C24A—H24A | 0.9900      | C9D—H9D2  | 0.9900    |
| C24A—H24B | 0.9900      | C13D—C14D | 1.532 (4) |
| C25A—C26A | 1.515 (4)   | C13D—H13G | 0.9900    |
| C25A—H25A | 0.9900      | C13D—H13H | 0.9900    |
| C25A—H25B | 0.9900      | C14D—C16D | 1.518 (5) |
| C26A—C27A | 1.534 (4)   | C14D—C15D | 1.537 (5) |
| C26A—H26A | 0.9900      | C14D—H14D | 1.0000    |
| C26A—H26B | 0.9900      | C15D—H15J | 0.9800    |
| C27A—C28A | 1.499 (5)   | C15D—H15K | 0.9800    |
| C27A—H27A | 0.9900      | C15D—H15L | 0.9800    |
| C27A—H27B | 0.9900      | C16D—H16J | 0.9800    |
| C28A—H28A | 0.9800      | C16D—H16K | 0.9800    |
| C28A—H28B | 0.9800      | C16D—H16L | 0.9800    |
| C28A—H28C | 0.9800      | C17D—C18D | 1.524 (4) |
| P1B—O2B   | 1.4848 (16) | C17D—H17G | 0.9900    |
| P1B—C21B  | 1.796 (2)   | C17D—H17H | 0.9900    |
| P1B—C3B   | 1.812 (2)   | C18D—C19D | 1.524 (4) |
| P1B—C9B   | 1.812 (2)   | C18D—C20D | 1.525 (4) |
| O11B—C10B | 1.236 (3)   | C18D—H18D | 1.0000    |
| N12B—C10B | 1.356 (3)   | C19D—H19J | 0.9800    |
| N12B—C13B | 1.469 (3)   | C19D—H19K | 0.9800    |
| N12B—C17B | 1.471 (3)   | C19D—H19L | 0.9800    |
| C3B—C8B   | 1.388 (3)   | C20D—H20J | 0.9800    |
| C3B—C4B   | 1.393 (3)   | C20D—H20K | 0.9800    |
| C4B—C5B   | 1.388 (4)   | C20D—H20L | 0.9800    |
| C4B—H4B   | 0.9500      | C21D—C22D | 1.532 (4) |
| C5B—C6B   | 1.371 (4)   | C21D—H21G | 0.9900    |
| C5B—H5B   | 0.9500      | C21D—H21H | 0.9900    |
| C6B—C7B   | 1.387 (4)   | C22D—C23D | 1.520 (5) |
| C6B—H6B   | 0.9500      | C22D—H22G | 0.9900    |
| C7B—C8B   | 1.390 (3)   | C22D—H22H | 0.9900    |
| C7B—H7B   | 0.9500      | C23D—C24D | 1.522 (5) |
| C8B—H8B   | 0.9500      | C23D—H23G | 0.9900    |
| C9B—C10B  | 1.518 (3)   | C23D—H23H | 0.9900    |
| C9B—H9B1  | 0.9900      | C24D—C25D | 1.525 (5) |
| C9B—H9B2  | 0.9900      | C24D—H24G | 0.9900    |
| C13B—C14B | 1.511 (4)   | C24D—H24H | 0.9900    |
| C13B—H13C | 0.9900      | C25D—C26D | 1.513 (5) |
| C13B—H13D | 0.9900      | C25D—H25G | 0.9900    |
| C14B—C16B | 1.486 (4)   | C25D—H25H | 0.9900    |
| C14B—C15B | 1.530 (4)   | C26D—C27D | 1.523 (6) |
| C14B—H14B | 1.0000      | C26D—H26G | 0.9900    |
| C15B—H15D | 0.9800      | C26D—H26H | 0.9900    |
| C15B—H15E | 0.9800      | C27D—C28D | 1.520 (5) |
| C15B—H15F | 0.9800      | C27D—H27G | 0.9900    |
| C16B—H16D | 0.9800      | C27D—H27H | 0.9900    |
| C16B—H16E | 0.9800      | C28D—H28J | 0.9800    |
| C16B—H16F | 0.9800      | C28D—H28K | 0.9800    |

|           |             |           |           |
|-----------|-------------|-----------|-----------|
| C17B—C18B | 1.532 (4)   | C28D—H28L | 0.9800    |
| C17B—H17C | 0.9900      | P1E—O2E   | 1.488 (3) |
| C17B—H17D | 0.9900      | P1E—C21E  | 1.801 (4) |
| C18B—C19B | 1.516 (4)   | P1E—C3E   | 1.813 (3) |
| C18B—C20B | 1.529 (4)   | P1E—C9E   | 1.820 (4) |
| C18B—H18B | 1.0000      | O11E—C10E | 1.245 (6) |
| C19B—H19D | 0.9800      | N12E—C10E | 1.350 (5) |
| C19B—H19E | 0.9800      | N12E—C13E | 1.470 (4) |
| C19B—H19F | 0.9800      | N12E—C17E | 1.471 (4) |
| C20B—H20D | 0.9800      | C3E—C8E   | 1.3951    |
| C20B—H20E | 0.9800      | C3E—C4E   | 1.4033    |
| C20B—H20F | 0.9800      | C4E—C5E   | 1.3983    |
| C21B—C22B | 1.531 (3)   | C4E—H4E   | 0.9500    |
| C21B—H21C | 0.9900      | C5E—C6E   | 1.3958    |
| C21B—H21D | 0.9900      | C5E—H5E   | 0.9500    |
| C22B—C23B | 1.525 (3)   | C6E—C7E   | 1.4237    |
| C22B—H22C | 0.9900      | C6E—H6E   | 0.9500    |
| C22B—H22D | 0.9900      | C7E—C8E   | 1.4350    |
| C23B—C24B | 1.515 (3)   | C7E—H7E   | 0.9500    |
| C23B—H23C | 0.9900      | C8E—H8E   | 0.9500    |
| C23B—H23D | 0.9900      | C9E—C10E  | 1.517 (4) |
| C24B—C25B | 1.533 (4)   | C9E—H9E1  | 0.9900    |
| C24B—H24C | 0.9900      | C9E—H9E2  | 0.9900    |
| C24B—H24D | 0.9900      | C13E—C14E | 1.532 (5) |
| C25B—C26B | 1.511 (4)   | C13E—H13I | 0.9900    |
| C25B—H25C | 0.9900      | C13E—H13J | 0.9900    |
| C25B—H25D | 0.9900      | C14E—C16E | 1.518 (5) |
| C26B—C27B | 1.528 (4)   | C14E—C15E | 1.538 (5) |
| C26B—H26C | 0.9900      | C14E—H14E | 1.0000    |
| C26B—H26D | 0.9900      | C15E—H15M | 0.9800    |
| C27B—C28B | 1.516 (4)   | C15E—H15N | 0.9800    |
| C27B—H27C | 0.9900      | C15E—H15O | 0.9800    |
| C27B—H27D | 0.9900      | C16E—H16M | 0.9800    |
| C28B—H28D | 0.9800      | C16E—H16N | 0.9800    |
| C28B—H28E | 0.9800      | C16E—H16O | 0.9800    |
| C28B—H28F | 0.9800      | C17E—C18E | 1.524 (5) |
| P1C—O2C   | 1.4873 (17) | C17E—H17I | 0.9900    |
| P1C—C21C  | 1.800 (2)   | C17E—H17J | 0.9900    |
| P1C—C9C   | 1.812 (2)   | C18E—C19E | 1.524 (5) |
| P1C—C3C   | 1.812 (2)   | C18E—C20E | 1.525 (5) |
| O11C—C10C | 1.240 (3)   | C18E—H18E | 1.0000    |
| N12C—C10C | 1.347 (3)   | C19E—H19M | 0.9800    |
| N12C—C17C | 1.465 (3)   | C19E—H19N | 0.9800    |
| N12C—C13C | 1.471 (3)   | C19E—H19O | 0.9800    |
| C3C—C4C   | 1.392 (3)   | C20E—H20M | 0.9800    |
| C3C—C8C   | 1.396 (3)   | C20E—H20N | 0.9800    |
| C4C—C5C   | 1.389 (4)   | C20E—H20O | 0.9800    |
| C4C—H4C   | 0.9500      | C21E—C22E | 1.525 (5) |

|                |             |                |           |
|----------------|-------------|----------------|-----------|
| C5C—C6C        | 1.385 (4)   | C21E—H21I      | 0.9900    |
| C5C—H5C        | 0.9500      | C21E—H21J      | 0.9900    |
| C6C—C7C        | 1.391 (4)   | C22E—C23E      | 1.522 (6) |
| C6C—H6C        | 0.9500      | C22E—H22I      | 0.9900    |
| C7C—C8C        | 1.388 (3)   | C22E—H22J      | 0.9900    |
| C7C—H7C        | 0.9500      | C23E—C24E      | 1.521 (5) |
| C8C—H8C        | 0.9500      | C23E—H23I      | 0.9900    |
| C9C—C10C       | 1.517 (3)   | C23E—H23J      | 0.9900    |
| C9C—H9C1       | 0.9900      | C24E—C25E      | 1.521 (6) |
| C9C—H9C2       | 0.9900      | C24E—H24I      | 0.9900    |
| C13C—C14C      | 1.523 (3)   | C24E—H24J      | 0.9900    |
| C13C—H13E      | 0.9900      | C25E—C26E      | 1.515 (6) |
| C13C—H13F      | 0.9900      | C25E—H25I      | 0.9900    |
| C14C—C16C      | 1.500 (4)   | C25E—H25J      | 0.9900    |
| C14C—C15C      | 1.522 (4)   | C26E—C27E      | 1.522 (6) |
| C14C—H14C      | 1.0000      | C26E—H26I      | 0.9900    |
| C15C—H15G      | 0.9800      | C26E—H26J      | 0.9900    |
| C15C—H15H      | 0.9800      | C27E—C28E      | 1.520 (6) |
| C15C—H15I      | 0.9800      | C27E—H27I      | 0.9900    |
| C16C—H16G      | 0.9800      | C27E—H27J      | 0.9900    |
| C16C—H16H      | 0.9800      | C28E—H28M      | 0.9800    |
| C16C—H16I      | 0.9800      | C28E—H28N      | 0.9800    |
| C17C—C18C      | 1.498 (4)   | C28E—H28O      | 0.9800    |
|                |             |                |           |
| O2A—P1A—C21A   | 112.52 (10) | C23C—C22C—C21C | 113.4 (2) |
| O2A—P1A—C3A    | 111.92 (10) | C23C—C22C—H22E | 108.9     |
| C21A—P1A—C3A   | 106.61 (11) | C21C—C22C—H22E | 108.9     |
| O2A—P1A—C9A    | 110.57 (10) | C23C—C22C—H22F | 108.9     |
| C21A—P1A—C9A   | 108.17 (11) | C21C—C22C—H22F | 108.9     |
| C3A—P1A—C9A    | 106.78 (11) | H22E—C22C—H22F | 107.7     |
| C10A—N12A—C17A | 124.72 (19) | C22C—C23C—C24C | 113.8 (2) |
| C10A—N12A—C13A | 117.00 (19) | C22C—C23C—H23E | 108.8     |
| C17A—N12A—C13A | 118.20 (19) | C24C—C23C—H23E | 108.8     |
| C8A—C3A—C4A    | 118.7 (2)   | C22C—C23C—H23F | 108.8     |
| C8A—C3A—P1A    | 118.37 (18) | C24C—C23C—H23F | 108.8     |
| C4A—C3A—P1A    | 122.90 (18) | H23E—C23C—H23F | 107.7     |
| C5A—C4A—C3A    | 120.9 (2)   | C23C—C24C—C25C | 114.2 (2) |
| C5A—C4A—H4A    | 119.6       | C23C—C24C—H24E | 108.7     |
| C3A—C4A—H4A    | 119.6       | C25C—C24C—H24E | 108.7     |
| C6A—C5A—C4A    | 119.3 (2)   | C23C—C24C—H24F | 108.7     |
| C6A—C5A—H5A    | 120.3       | C25C—C24C—H24F | 108.7     |
| C4A—C5A—H5A    | 120.3       | H24E—C24C—H24F | 107.6     |
| C7A—C6A—C5A    | 120.5 (2)   | C26C—C25C—C24C | 114.7 (2) |
| C7A—C6A—H6A    | 119.8       | C26C—C25C—H25E | 108.6     |
| C5A—C6A—H6A    | 119.8       | C24C—C25C—H25E | 108.6     |
| C6A—C7A—C8A    | 120.2 (3)   | C26C—C25C—H25F | 108.6     |
| C6A—C7A—H7A    | 119.9       | C24C—C25C—H25F | 108.6     |
| C8A—C7A—H7A    | 119.9       | H25E—C25C—H25F | 107.6     |

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| C7A—C8A—C3A    | 120.4 (2)   | C27C—C26C—C25C | 113.4 (2) |
| C7A—C8A—H8A    | 119.8       | C27C—C26C—H26E | 108.9     |
| C3A—C8A—H8A    | 119.8       | C25C—C26C—H26E | 108.9     |
| C10A—C9A—P1A   | 116.92 (16) | C27C—C26C—H26F | 108.9     |
| C10A—C9A—H9A1  | 108.1       | C25C—C26C—H26F | 108.9     |
| P1A—C9A—H9A1   | 108.1       | H26E—C26C—H26F | 107.7     |
| C10A—C9A—H9A2  | 108.1       | C26C—C27C—C28C | 113.3 (2) |
| P1A—C9A—H9A2   | 108.1       | C26C—C27C—H27E | 108.9     |
| H9A1—C9A—H9A2  | 107.3       | C28C—C27C—H27E | 108.9     |
| O11A—C10A—N12A | 121.2 (2)   | C26C—C27C—H27F | 108.9     |
| O11A—C10A—C9A  | 120.2 (2)   | C28C—C27C—H27F | 108.9     |
| N12A—C10A—C9A  | 118.6 (2)   | H27E—C27C—H27F | 107.7     |
| N12A—C13A—C14A | 114.9 (2)   | O2D—P1D—C21D   | 112.3 (2) |
| N12A—C13A—H13A | 108.5       | O2D—P1D—C3D    | 111.6 (2) |
| C14A—C13A—H13A | 108.5       | C21D—P1D—C3D   | 106.0 (2) |
| N12A—C13A—H13B | 108.5       | O2D—P1D—C9D    | 110.9 (3) |
| C14A—C13A—H13B | 108.5       | C21D—P1D—C9D   | 108.0 (3) |
| H13A—C13A—H13B | 107.5       | C3D—P1D—C9D    | 107.8 (2) |
| C15A—C14A—C16A | 110.9 (2)   | C10D—N12D—C13D | 124.7 (4) |
| C15A—C14A—C13A | 112.2 (2)   | C10D—N12D—C17D | 118.1 (4) |
| C16A—C14A—C13A | 108.3 (2)   | C13D—N12D—C17D | 117.1 (3) |
| C15A—C14A—H14A | 108.5       | C8D—C3D—C4D    | 120.2     |
| C16A—C14A—H14A | 108.5       | C8D—C3D—P1D    | 117.2 (2) |
| C13A—C14A—H14A | 108.5       | C4D—C3D—P1D    | 122.5 (2) |
| N12A—C17A—C18A | 114.8 (2)   | C5D—C4D—C3D    | 119.9     |
| N12A—C17A—H17A | 108.6       | C5D—C4D—H4D    | 120.1     |
| C18A—C17A—H17A | 108.6       | C3D—C4D—H4D    | 120.1     |
| N12A—C17A—H17B | 108.6       | C6D—C5D—C4D    | 120.5     |
| C18A—C17A—H17B | 108.6       | C6D—C5D—H5D    | 119.8     |
| H17A—C17A—H17B | 107.5       | C4D—C5D—H5D    | 119.8     |
| C20A—C18A—C19A | 111.5 (2)   | C5D—C6D—C7D    | 119.5     |
| C20A—C18A—C17A | 113.4 (2)   | C5D—C6D—H6D    | 120.2     |
| C19A—C18A—C17A | 108.1 (2)   | C7D—C6D—H6D    | 120.2     |
| C20A—C18A—H18A | 107.9       | C6D—C7D—C8D    | 117.4     |
| C19A—C18A—H18A | 107.9       | C6D—C7D—H7D    | 121.3     |
| C17A—C18A—H18A | 107.9       | C8D—C7D—H7D    | 121.3     |
| C22A—C21A—P1A  | 112.98 (16) | C3D—C8D—C7D    | 119.3     |
| C22A—C21A—H21A | 109.0       | C3D—C8D—H8D    | 120.3     |
| P1A—C21A—H21A  | 109.0       | C7D—C8D—H8D    | 120.3     |
| C22A—C21A—H21B | 109.0       | C10D—C9D—P1D   | 116.2 (4) |
| P1A—C21A—H21B  | 109.0       | C10D—C9D—H9D1  | 108.2     |
| H21A—C21A—H21B | 107.8       | P1D—C9D—H9D1   | 108.2     |
| C23A—C22A—C21A | 111.67 (19) | C10D—C9D—H9D2  | 108.2     |
| C23A—C22A—H22A | 109.3       | P1D—C9D—H9D2   | 108.2     |
| C21A—C22A—H22A | 109.3       | H9D1—C9D—H9D2  | 107.4     |
| C23A—C22A—H22B | 109.3       | O11D—C10D—N12D | 121.0 (5) |
| C21A—C22A—H22B | 109.3       | O11D—C10D—C9D  | 118.7 (5) |
| H22A—C22A—H22B | 107.9       | N12D—C10D—C9D  | 118.9 (4) |

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| C24A—C23A—C22A | 114.1 (2)   | N12D—C13D—C14D | 114.6 (4) |
| C24A—C23A—H23A | 108.7       | N12D—C13D—H13G | 108.6     |
| C22A—C23A—H23A | 108.7       | C14D—C13D—H13G | 108.6     |
| C24A—C23A—H23B | 108.7       | N12D—C13D—H13H | 108.6     |
| C22A—C23A—H23B | 108.7       | C14D—C13D—H13H | 108.6     |
| H23A—C23A—H23B | 107.6       | H13G—C13D—H13H | 107.6     |
| C23A—C24A—C25A | 112.5 (2)   | C16D—C14D—C13D | 113.6 (4) |
| C23A—C24A—H24A | 109.1       | C16D—C14D—C15D | 112.4 (4) |
| C25A—C24A—H24A | 109.1       | C13D—C14D—C15D | 108.0 (4) |
| C23A—C24A—H24B | 109.1       | C16D—C14D—H14D | 107.5     |
| C25A—C24A—H24B | 109.1       | C13D—C14D—H14D | 107.5     |
| H24A—C24A—H24B | 107.8       | C15D—C14D—H14D | 107.5     |
| C26A—C25A—C24A | 114.2 (2)   | N12D—C17D—C18D | 114.1 (4) |
| C26A—C25A—H25A | 108.7       | N12D—C17D—H17G | 108.7     |
| C24A—C25A—H25A | 108.7       | C18D—C17D—H17G | 108.7     |
| C26A—C25A—H25B | 108.7       | N12D—C17D—H17H | 108.7     |
| C24A—C25A—H25B | 108.7       | C18D—C17D—H17H | 108.7     |
| H25A—C25A—H25B | 107.6       | H17G—C17D—H17H | 107.6     |
| C25A—C26A—C27A | 113.1 (2)   | C19D—C18D—C17D | 108.0 (4) |
| C25A—C26A—H26A | 109.0       | C19D—C18D—C20D | 111.6 (4) |
| C27A—C26A—H26A | 109.0       | C17D—C18D—C20D | 113.0 (4) |
| C25A—C26A—H26B | 109.0       | C19D—C18D—H18D | 108.0     |
| C27A—C26A—H26B | 109.0       | C17D—C18D—H18D | 108.0     |
| H26A—C26A—H26B | 107.8       | C20D—C18D—H18D | 108.0     |
| C28A—C27A—C26A | 114.2 (3)   | C22D—C21D—P1D  | 112.0 (3) |
| C28A—C27A—H27A | 108.7       | C22D—C21D—H21G | 109.2     |
| C26A—C27A—H27A | 108.7       | P1D—C21D—H21G  | 109.2     |
| C28A—C27A—H27B | 108.7       | C22D—C21D—H21H | 109.2     |
| C26A—C27A—H27B | 108.7       | P1D—C21D—H21H  | 109.2     |
| H27A—C27A—H27B | 107.6       | H21G—C21D—H21H | 107.9     |
| O2B—P1B—C21B   | 113.30 (10) | C23D—C22D—C21D | 112.8 (4) |
| O2B—P1B—C3B    | 111.95 (10) | C23D—C22D—H22G | 109.0     |
| C21B—P1B—C3B   | 106.33 (11) | C21D—C22D—H22G | 109.0     |
| O2B—P1B—C9B    | 110.78 (10) | C23D—C22D—H22H | 109.0     |
| C21B—P1B—C9B   | 106.80 (11) | C21D—C22D—H22H | 109.0     |
| C3B—P1B—C9B    | 107.31 (11) | H22G—C22D—H22H | 107.8     |
| C10B—N12B—C13B | 125.6 (2)   | C22D—C23D—C24D | 115.2 (3) |
| C10B—N12B—C17B | 117.3 (2)   | C22D—C23D—H23G | 108.5     |
| C13B—N12B—C17B | 116.6 (2)   | C24D—C23D—H23G | 108.5     |
| C8B—C3B—C4B    | 119.2 (2)   | C22D—C23D—H23H | 108.5     |
| C8B—C3B—P1B    | 122.73 (18) | C24D—C23D—H23H | 108.5     |
| C4B—C3B—P1B    | 118.06 (18) | H23G—C23D—H23H | 107.5     |
| C5B—C4B—C3B    | 120.0 (2)   | C23D—C24D—C25D | 111.7 (3) |
| C5B—C4B—H4B    | 120.0       | C23D—C24D—H24G | 109.3     |
| C3B—C4B—H4B    | 120.0       | C25D—C24D—H24G | 109.3     |
| C6B—C5B—C4B    | 120.3 (2)   | C23D—C24D—H24H | 109.3     |
| C6B—C5B—H5B    | 119.8       | C25D—C24D—H24H | 109.3     |
| C4B—C5B—H5B    | 119.8       | H24G—C24D—H24H | 107.9     |

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| C5B—C6B—C7B    | 120.4 (2)   | C26D—C25D—C24D | 115.8 (4) |
| C5B—C6B—H6B    | 119.8       | C26D—C25D—H25G | 108.3     |
| C7B—C6B—H6B    | 119.8       | C24D—C25D—H25G | 108.3     |
| C6B—C7B—C8B    | 119.4 (2)   | C26D—C25D—H25H | 108.3     |
| C6B—C7B—H7B    | 120.3       | C24D—C25D—H25H | 108.3     |
| C8B—C7B—H7B    | 120.3       | H25G—C25D—H25H | 107.4     |
| C3B—C8B—C7B    | 120.6 (2)   | C25D—C26D—C27D | 113.3 (4) |
| C3B—C8B—H8B    | 119.7       | C25D—C26D—H26G | 108.9     |
| C7B—C8B—H8B    | 119.7       | C27D—C26D—H26G | 108.9     |
| C10B—C9B—P1B   | 116.17 (16) | C25D—C26D—H26H | 108.9     |
| C10B—C9B—H9B1  | 108.2       | C27D—C26D—H26H | 108.9     |
| P1B—C9B—H9B1   | 108.2       | H26G—C26D—H26H | 107.7     |
| C10B—C9B—H9B2  | 108.2       | C28D—C27D—C26D | 113.6 (5) |
| P1B—C9B—H9B2   | 108.2       | C28D—C27D—H27G | 108.8     |
| H9B1—C9B—H9B2  | 107.4       | C26D—C27D—H27G | 108.8     |
| O11B—C10B—N12B | 120.8 (2)   | C28D—C27D—H27H | 108.8     |
| O11B—C10B—C9B  | 119.4 (2)   | C26D—C27D—H27H | 108.8     |
| N12B—C10B—C9B  | 119.8 (2)   | H27G—C27D—H27H | 107.7     |
| N12B—C13B—C14B | 113.9 (2)   | O2E—P1E—C21E   | 113.2 (4) |
| N12B—C13B—H13C | 108.8       | O2E—P1E—C3E    | 111.3 (4) |
| C14B—C13B—H13C | 108.8       | C21E—P1E—C3E   | 107.3 (3) |
| N12B—C13B—H13D | 108.8       | O2E—P1E—C9E    | 110.1 (4) |
| C14B—C13B—H13D | 108.8       | C21E—P1E—C9E   | 107.6 (3) |
| H13C—C13B—H13D | 107.7       | C3E—P1E—C9E    | 107.1 (3) |
| C16B—C14B—C13B | 112.8 (2)   | C10E—N12E—C13E | 124.4 (6) |
| C16B—C14B—C15B | 110.2 (3)   | C10E—N12E—C17E | 117.8 (5) |
| C13B—C14B—C15B | 108.3 (2)   | C13E—N12E—C17E | 117.0 (5) |
| C16B—C14B—H14B | 108.5       | C8E—C3E—C4E    | 119.9     |
| C13B—C14B—H14B | 108.5       | C8E—C3E—P1E    | 117.8 (3) |
| C15B—C14B—H14B | 108.5       | C4E—C3E—P1E    | 122.3 (3) |
| N12B—C17B—C18B | 115.2 (2)   | C5E—C4E—C3E    | 120.1     |
| N12B—C17B—H17C | 108.5       | C5E—C4E—H4E    | 119.9     |
| C18B—C17B—H17C | 108.5       | C3E—C4E—H4E    | 119.9     |
| N12B—C17B—H17D | 108.5       | C6E—C5E—C4E    | 119.8     |
| C18B—C17B—H17D | 108.5       | C6E—C5E—H5E    | 120.1     |
| H17C—C17B—H17D | 107.5       | C4E—C5E—H5E    | 120.1     |
| C19B—C18B—C20B | 110.7 (2)   | C5E—C6E—C7E    | 119.2     |
| C19B—C18B—C17B | 112.6 (2)   | C5E—C6E—H6E    | 120.4     |
| C20B—C18B—C17B | 108.0 (2)   | C7E—C6E—H6E    | 120.4     |
| C19B—C18B—H18B | 108.5       | C6E—C7E—C8E    | 116.1     |
| C20B—C18B—H18B | 108.5       | C6E—C7E—H7E    | 122.0     |
| C17B—C18B—H18B | 108.5       | C8E—C7E—H7E    | 122.0     |
| C22B—C21B—P1B  | 113.78 (16) | C3E—C8E—C7E    | 118.5     |
| C22B—C21B—H21C | 108.8       | C3E—C8E—H8E    | 120.8     |
| P1B—C21B—H21C  | 108.8       | C7E—C8E—H8E    | 120.8     |
| C22B—C21B—H21D | 108.8       | C10E—C9E—P1E   | 115.9 (4) |
| P1B—C21B—H21D  | 108.8       | C10E—C9E—H9E1  | 108.3     |
| H21C—C21B—H21D | 107.7       | P1E—C9E—H9E1   | 108.3     |

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|----------------|-------------|----------------|-----------|
| C23B—C22B—C21B | 111.00 (19) | C10E—C9E—H9E2  | 108.3     |
| C23B—C22B—H22C | 109.4       | P1E—C9E—H9E2   | 108.3     |
| C21B—C22B—H22C | 109.4       | H9E1—C9E—H9E2  | 107.4     |
| C23B—C22B—H22D | 109.4       | O11E—C10E—N12E | 120.7 (8) |
| C21B—C22B—H22D | 109.4       | O11E—C10E—C9E  | 118.6 (6) |
| H22C—C22B—H22D | 108.0       | N12E—C10E—C9E  | 118.9 (6) |
| C24B—C23B—C22B | 114.2 (2)   | N12E—C13E—C14E | 114.7 (5) |
| C24B—C23B—H23C | 108.7       | N12E—C13E—H13I | 108.6     |
| C22B—C23B—H23C | 108.7       | C14E—C13E—H13I | 108.6     |
| C24B—C23B—H23D | 108.7       | N12E—C13E—H13J | 108.6     |
| C22B—C23B—H23D | 108.7       | C14E—C13E—H13J | 108.6     |
| H23C—C23B—H23D | 107.6       | H13I—C13E—H13J | 107.6     |
| C23B—C24B—C25B | 112.1 (2)   | C16E—C14E—C13E | 113.6 (5) |
| C23B—C24B—H24C | 109.2       | C16E—C14E—C15E | 112.3 (5) |
| C25B—C24B—H24C | 109.2       | C13E—C14E—C15E | 107.9 (5) |
| C23B—C24B—H24D | 109.2       | C16E—C14E—H14E | 107.6     |
| C25B—C24B—H24D | 109.2       | C13E—C14E—H14E | 107.6     |
| H24C—C24B—H24D | 107.9       | C15E—C14E—H14E | 107.6     |
| C26B—C25B—C24B | 114.2 (2)   | C14E—C15E—H15M | 109.5     |
| C26B—C25B—H25C | 108.7       | C14E—C15E—H15N | 109.5     |
| C24B—C25B—H25C | 108.7       | H15M—C15E—H15N | 109.5     |
| C26B—C25B—H25D | 108.7       | C14E—C15E—H15O | 109.5     |
| C24B—C25B—H25D | 108.7       | H15M—C15E—H15O | 109.5     |
| H25C—C25B—H25D | 107.6       | H15N—C15E—H15O | 109.5     |
| C25B—C26B—C27B | 113.9 (3)   | C14E—C16E—H16M | 109.5     |
| C25B—C26B—H26C | 108.8       | C14E—C16E—H16N | 109.5     |
| C27B—C26B—H26C | 108.8       | H16M—C16E—H16N | 109.5     |
| C25B—C26B—H26D | 108.8       | C14E—C16E—H16O | 109.5     |
| C27B—C26B—H26D | 108.8       | H16M—C16E—H16O | 109.5     |
| H26C—C26B—H26D | 107.7       | H16N—C16E—H16O | 109.5     |
| C28B—C27B—C26B | 114.5 (3)   | N12E—C17E—C18E | 114.1 (5) |
| C28B—C27B—H27C | 108.6       | N12E—C17E—H17I | 108.7     |
| C26B—C27B—H27C | 108.6       | C18E—C17E—H17I | 108.7     |
| C28B—C27B—H27D | 108.6       | N12E—C17E—H17J | 108.7     |
| C26B—C27B—H27D | 108.6       | C18E—C17E—H17J | 108.7     |
| H27C—C27B—H27D | 107.6       | H17I—C17E—H17J | 107.6     |
| O2C—P1C—C21C   | 112.86 (11) | C19E—C18E—C17E | 108.1 (5) |
| O2C—P1C—C9C    | 109.98 (10) | C19E—C18E—C20E | 111.5 (5) |
| C21C—P1C—C9C   | 108.27 (11) | C17E—C18E—C20E | 113.0 (5) |
| O2C—P1C—C3C    | 111.90 (11) | C19E—C18E—H18E | 108.0     |
| C21C—P1C—C3C   | 107.04 (11) | C17E—C18E—H18E | 108.0     |
| C9C—P1C—C3C    | 106.52 (11) | C20E—C18E—H18E | 108.0     |
| C10C—N12C—C17C | 117.6 (2)   | C18E—C19E—H19M | 109.5     |
| C10C—N12C—C13C | 126.0 (2)   | C18E—C19E—H19N | 109.5     |
| C17C—N12C—C13C | 116.3 (2)   | H19M—C19E—H19N | 109.5     |
| C4C—C3C—C8C    | 119.2 (2)   | C18E—C19E—H19O | 109.5     |
| C4C—C3C—P1C    | 117.82 (19) | H19M—C19E—H19O | 109.5     |
| C8C—C3C—P1C    | 122.99 (18) | H19N—C19E—H19O | 109.5     |



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|----------------|-------------|----------------|-----------|
| C5C—C4C—C3C    | 120.1 (2)   | C18E—C20E—H20M | 109.5     |
| C5C—C4C—H4C    | 120.0       | C18E—C20E—H20N | 109.5     |
| C3C—C4C—H4C    | 120.0       | H20M—C20E—H20N | 109.5     |
| C6C—C5C—C4C    | 120.5 (2)   | C18E—C20E—H20O | 109.5     |
| C6C—C5C—H5C    | 119.7       | H20M—C20E—H20O | 109.5     |
| C4C—C5C—H5C    | 119.7       | H20N—C20E—H20O | 109.5     |
| C5C—C6C—C7C    | 119.8 (2)   | C22E—C21E—P1E  | 114.2 (4) |
| C5C—C6C—H6C    | 120.1       | C22E—C21E—H21I | 108.7     |
| C7C—C6C—H6C    | 120.1       | P1E—C21E—H21I  | 108.7     |
| C8C—C7C—C6C    | 119.8 (2)   | C22E—C21E—H21J | 108.7     |
| C8C—C7C—H7C    | 120.1       | P1E—C21E—H21J  | 108.7     |
| C6C—C7C—H7C    | 120.1       | H21I—C21E—H21J | 107.6     |
| C7C—C8C—C3C    | 120.7 (2)   | C23E—C22E—C21E | 113.8 (5) |
| C7C—C8C—H8C    | 119.7       | C23E—C22E—H22I | 108.8     |
| C3C—C8C—H8C    | 119.7       | C21E—C22E—H22I | 108.8     |
| C10C—C9C—P1C   | 116.54 (16) | C23E—C22E—H22J | 108.8     |
| C10C—C9C—H9C1  | 108.2       | C21E—C22E—H22J | 108.8     |
| P1C—C9C—H9C1   | 108.2       | H22I—C22E—H22J | 107.7     |
| C10C—C9C—H9C2  | 108.2       | C24E—C23E—C22E | 114.0 (5) |
| P1C—C9C—H9C2   | 108.2       | C24E—C23E—H23I | 108.7     |
| H9C1—C9C—H9C2  | 107.3       | C22E—C23E—H23I | 108.7     |
| O11C—C10C—N12C | 121.2 (2)   | C24E—C23E—H23J | 108.7     |
| O11C—C10C—C9C  | 118.5 (2)   | C22E—C23E—H23J | 108.7     |
| N12C—C10C—C9C  | 120.2 (2)   | H23I—C23E—H23J | 107.6     |
| N12C—C13C—C14C | 113.7 (2)   | C25E—C24E—C23E | 114.5 (4) |
| N12C—C13C—H13E | 108.8       | C25E—C24E—H24I | 108.6     |
| C14C—C13C—H13E | 108.8       | C23E—C24E—H24I | 108.6     |
| N12C—C13C—H13F | 108.8       | C25E—C24E—H24J | 108.6     |
| C14C—C13C—H13F | 108.8       | C23E—C24E—H24J | 108.6     |
| H13E—C13C—H13F | 107.7       | H24I—C24E—H24J | 107.6     |
| C16C—C14C—C15C | 111.4 (2)   | C26E—C25E—C24E | 115.6 (5) |
| C16C—C14C—C13C | 112.3 (2)   | C26E—C25E—H25I | 108.4     |
| C15C—C14C—C13C | 109.1 (2)   | C24E—C25E—H25I | 108.4     |
| C16C—C14C—H14C | 107.9       | C26E—C25E—H25J | 108.4     |
| C15C—C14C—H14C | 107.9       | C24E—C25E—H25J | 108.4     |
| C13C—C14C—H14C | 107.9       | H25I—C25E—H25J | 107.4     |
| N12C—C17C—C18C | 113.7 (2)   | C25E—C26E—C27E | 113.4 (5) |
| N12C—C17C—H17E | 108.8       | C25E—C26E—H26I | 108.9     |
| C18C—C17C—H17E | 108.8       | C27E—C26E—H26I | 108.9     |
| N12C—C17C—H17F | 108.8       | C25E—C26E—H26J | 108.9     |
| C18C—C17C—H17F | 108.8       | C27E—C26E—H26J | 108.9     |
| H17E—C17C—H17F | 107.7       | H26I—C26E—H26J | 107.7     |
| C20C—C18C—C17C | 114.7 (3)   | C28E—C27E—C26E | 113.5 (6) |
| C20C—C18C—C19C | 111.6 (3)   | C28E—C27E—H27I | 108.9     |
| C17C—C18C—C19C | 107.7 (2)   | C26E—C27E—H27I | 108.9     |
| C20C—C18C—H18C | 107.5       | C28E—C27E—H27J | 108.9     |
| C17C—C18C—H18C | 107.5       | C26E—C27E—H27J | 108.9     |
| C19C—C18C—H18C | 107.5       | H27I—C27E—H27J | 107.7     |

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| C22C—C21C—P1C       | 113.37 (17)  | C27E—C28E—H28M      | 109.5        |
| C22C—C21C—H21E      | 108.9        | C27E—C28E—H28N      | 109.5        |
| P1C—C21C—H21E       | 108.9        | H28M—C28E—H28N      | 109.5        |
| C22C—C21C—H21F      | 108.9        | C27E—C28E—H28O      | 109.5        |
| P1C—C21C—H21F       | 108.9        | H28M—C28E—H28O      | 109.5        |
| H21E—C21C—H21F      | 107.7        | H28N—C28E—H28O      | 109.5        |
|                     |              |                     |              |
| O2A—P1A—C3A—C8A     | -11.3 (2)    | C13C—N12C—C10C—C9C  | -1.0 (3)     |
| C21A—P1A—C3A—C8A    | -134.72 (19) | P1C—C9C—C10C—O11C   | 46.2 (3)     |
| C9A—P1A—C3A—C8A     | 109.8 (2)    | P1C—C9C—C10C—N12C   | -135.55 (19) |
| O2A—P1A—C3A—C4A     | 169.38 (19)  | C10C—N12C—C13C—C14C | 121.0 (3)    |
| C21A—P1A—C3A—C4A    | 46.0 (2)     | C17C—N12C—C13C—C14C | -63.4 (3)    |
| C9A—P1A—C3A—C4A     | -69.5 (2)    | N12C—C13C—C14C—C16C | -51.6 (3)    |
| C8A—C3A—C4A—C5A     | -0.1 (4)     | N12C—C13C—C14C—C15C | -175.7 (2)   |
| P1A—C3A—C4A—C5A     | 179.2 (2)    | C10C—N12C—C17C—C18C | 102.0 (3)    |
| C3A—C4A—C5A—C6A     | 0.3 (4)      | C13C—N12C—C17C—C18C | -74.1 (3)    |
| C4A—C5A—C6A—C7A     | -0.5 (4)     | N12C—C17C—C18C—C20C | -53.5 (3)    |
| C5A—C6A—C7A—C8A     | 0.5 (4)      | N12C—C17C—C18C—C19C | -178.4 (3)   |
| C6A—C7A—C8A—C3A     | -0.4 (4)     | O2C—P1C—C21C—C22C   | -61.5 (2)    |
| C4A—C3A—C8A—C7A     | 0.2 (4)      | C9C—P1C—C21C—C22C   | 176.53 (17)  |
| P1A—C3A—C8A—C7A     | -179.2 (2)   | C3C—P1C—C21C—C22C   | 62.1 (2)     |
| O2A—P1A—C9A—C10A    | 175.96 (16)  | P1C—C21C—C22C—C23C  | 173.37 (17)  |
| C21A—P1A—C9A—C10A   | -60.4 (2)    | C21C—C22C—C23C—C24C | 177.2 (2)    |
| C3A—P1A—C9A—C10A    | 53.98 (19)   | C22C—C23C—C24C—C25C | 166.3 (2)    |
| C17A—N12A—C10A—O11A | 177.9 (2)    | C23C—C24C—C25C—C26C | 60.0 (3)     |
| C13A—N12A—C10A—O11A | 1.2 (3)      | C24C—C25C—C26C—C27C | 177.0 (2)    |
| C17A—N12A—C10A—C9A  | 0.1 (3)      | C25C—C26C—C27C—C28C | 175.7 (2)    |
| C13A—N12A—C10A—C9A  | -176.58 (19) | O2D—P1D—C3D—C8D     | 0.1 (4)      |
| P1A—C9A—C10A—O11A   | 52.0 (3)     | C21D—P1D—C3D—C8D    | -122.5 (3)   |
| P1A—C9A—C10A—N12A   | -130.17 (19) | C9D—P1D—C3D—C8D     | 122.0 (3)    |
| C10A—N12A—C13A—C14A | -79.2 (3)    | O2D—P1D—C3D—C4D     | 178.6 (3)    |
| C17A—N12A—C13A—C14A | 103.9 (2)    | C21D—P1D—C3D—C4D    | 56.0 (3)     |
| N12A—C13A—C14A—C15A | -52.6 (3)    | C9D—P1D—C3D—C4D     | -59.4 (4)    |
| N12A—C13A—C14A—C16A | -175.3 (2)   | C8D—C3D—C4D—C5D     | -1.2         |
| C10A—N12A—C17A—C18A | -80.3 (3)    | P1D—C3D—C4D—C5D     | -179.7 (3)   |
| C13A—N12A—C17A—C18A | 96.4 (2)     | C3D—C4D—C5D—C6D     | 0.8          |
| N12A—C17A—C18A—C20A | -53.8 (3)    | C4D—C5D—C6D—C7D     | 10.2         |
| N12A—C17A—C18A—C19A | -177.9 (2)   | C5D—C6D—C7D—C8D     | -20.4        |
| O2A—P1A—C21A—C22A   | -57.23 (19)  | C4D—C3D—C8D—C7D     | -9.3         |
| C3A—P1A—C21A—C22A   | 65.82 (19)   | P1D—C3D—C8D—C7D     | 169.2 (3)    |
| C9A—P1A—C21A—C22A   | -179.66 (16) | C6D—C7D—C8D—C3D     | 19.9         |
| P1A—C21A—C22A—C23A  | -171.83 (17) | O2D—P1D—C9D—C10D    | 170.9 (9)    |
| C21A—C22A—C23A—C24A | 179.8 (2)    | C21D—P1D—C9D—C10D   | -65.6 (9)    |
| C22A—C23A—C24A—C25A | -167.6 (2)   | C3D—P1D—C9D—C10D    | 48.5 (9)     |
| C23A—C24A—C25A—C26A | 170.4 (2)    | C13D—N12D—C10D—O11D | 174.7 (17)   |
| C24A—C25A—C26A—C27A | 172.8 (2)    | C17D—N12D—C10D—O11D | -10 (3)      |
| C25A—C26A—C27A—C28A | 52.3 (4)     | C13D—N12D—C10D—C9D  | 9 (3)        |
| O2B—P1B—C3B—C8B     | 171.00 (19)  | C17D—N12D—C10D—C9D  | -176.1 (11)  |

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| C21B—P1B—C3B—C8B    | 46.8 (2)     | P1D—C9D—C10D—O11D   | 60 (2)      |
| C9B—P1B—C3B—C8B     | -67.2 (2)    | P1D—C9D—C10D—N12D   | -133.3 (19) |
| O2B—P1B—C3B—C4B     | -7.4 (2)     | C10D—N12D—C13D—C14D | 81 (2)      |
| C21B—P1B—C3B—C4B    | -131.59 (19) | C17D—N12D—C13D—C14D | -94.0 (14)  |
| C9B—P1B—C3B—C4B     | 114.40 (19)  | N12D—C13D—C14D—C16D | 56.4 (10)   |
| C8B—C3B—C4B—C5B     | 0.0 (4)      | N12D—C13D—C14D—C15D | -178.2 (9)  |
| P1B—C3B—C4B—C5B     | 178.5 (2)    | C10D—N12D—C17D—C18D | 96.0 (17)   |
| C3B—C4B—C5B—C6B     | 0.4 (4)      | C13D—N12D—C17D—C18D | -88.2 (17)  |
| C4B—C5B—C6B—C7B     | -0.6 (4)     | N12D—C17D—C18D—C19D | 177.8 (13)  |
| C5B—C6B—C7B—C8B     | 0.4 (4)      | N12D—C17D—C18D—C20D | -58.2 (13)  |
| C4B—C3B—C8B—C7B     | -0.2 (4)     | O2D—P1D—C21D—C22D   | -67.3 (6)   |
| P1B—C3B—C8B—C7B     | -178.55 (19) | C3D—P1D—C21D—C22D   | 54.8 (5)    |
| C6B—C7B—C8B—C3B     | 0.0 (4)      | C9D—P1D—C21D—C22D   | 170.1 (5)   |
| O2B—P1B—C9B—C10B    | 171.94 (16)  | P1D—C21D—C22D—C23D  | 156.4 (4)   |
| C21B—P1B—C9B—C10B   | -64.2 (2)    | C21D—C22D—C23D—C24D | 68.3 (6)    |
| C3B—P1B—C9B—C10B    | 49.5 (2)     | C22D—C23D—C24D—C25D | 169.8 (4)   |
| C13B—N12B—C10B—O11B | 176.6 (2)    | C23D—C24D—C25D—C26D | 177.4 (7)   |
| C17B—N12B—C10B—O11B | 5.0 (3)      | C24D—C25D—C26D—C27D | 177 (2)     |
| C13B—N12B—C10B—C9B  | -2.8 (3)     | C25D—C26D—C27D—C28D | 172 (3)     |
| C17B—N12B—C10B—C9B  | -174.5 (2)   | O2E—P1E—C3E—C8E     | -6.8 (5)    |
| P1B—C9B—C10B—O11B   | 59.8 (3)     | C21E—P1E—C3E—C8E    | -131.1 (4)  |
| P1B—C9B—C10B—N12B   | -120.7 (2)   | C9E—P1E—C3E—C8E     | 113.6 (5)   |
| C10B—N12B—C13B—C14B | -98.6 (3)    | O2E—P1E—C3E—C4E     | 172.8 (5)   |
| C17B—N12B—C13B—C14B | 73.2 (3)     | C21E—P1E—C3E—C4E    | 48.4 (5)    |
| N12B—C13B—C14B—C16B | 58.8 (3)     | C9E—P1E—C3E—C4E     | -66.8 (5)   |
| N12B—C13B—C14B—C15B | -179.0 (2)   | C8E—C3E—C4E—C5E     | 1.6         |
| C10B—N12B—C17B—C18B | -83.4 (3)    | P1E—C3E—C4E—C5E     | -178.0 (5)  |
| C13B—N12B—C17B—C18B | 104.1 (3)    | C3E—C4E—C5E—C6E     | -3.1        |
| N12B—C17B—C18B—C19B | -56.4 (3)    | C4E—C5E—C6E—C7E     | -12.0       |
| N12B—C17B—C18B—C20B | -179.0 (2)   | C5E—C6E—C7E—C8E     | 27.6        |
| O2B—P1B—C21B—C22B   | -61.62 (19)  | C4E—C3E—C8E—C7E     | 14.7        |
| C3B—P1B—C21B—C22B   | 61.78 (19)   | P1E—C3E—C8E—C7E     | -165.7 (4)  |
| C9B—P1B—C21B—C22B   | 176.13 (17)  | C6E—C7E—C8E—C3E     | -28.9       |
| P1B—C21B—C22B—C23B  | 179.78 (17)  | O2E—P1E—C9E—C10E    | -176.0 (13) |
| C21B—C22B—C23B—C24B | 176.8 (2)    | C21E—P1E—C9E—C10E   | -52.2 (14)  |
| C22B—C23B—C24B—C25B | -172.3 (2)   | C3E—P1E—C9E—C10E    | 62.9 (14)   |
| C23B—C24B—C25B—C26B | 165.0 (3)    | C13E—N12E—C10E—O11E | -173 (3)    |
| C24B—C25B—C26B—C27B | -179.1 (3)   | C17E—N12E—C10E—O11E | 17 (5)      |
| C25B—C26B—C27B—C28B | 58.7 (4)     | C13E—N12E—C10E—C9E  | -9 (5)      |
| O2C—P1C—C3C—C4C     | -9.0 (2)     | C17E—N12E—C10E—C9E  | -178.1 (15) |
| C21C—P1C—C3C—C4C    | -133.2 (2)   | P1E—C9E—C10E—O11E   | 29 (3)      |
| C9C—P1C—C3C—C4C     | 111.2 (2)    | P1E—C9E—C10E—N12E   | -136 (3)    |
| O2C—P1C—C3C—C8C     | 172.05 (19)  | C10E—N12E—C13E—C14E | 87 (3)      |
| C21C—P1C—C3C—C8C    | 47.9 (2)     | C17E—N12E—C13E—C14E | -103 (2)    |
| C9C—P1C—C3C—C8C     | -67.7 (2)    | N12E—C13E—C14E—C16E | 44.0 (15)   |
| C8C—C3C—C4C—C5C     | 0.7 (4)      | N12E—C13E—C14E—C15E | 169.2 (13)  |
| P1C—C3C—C4C—C5C     | -178.3 (2)   | C10E—N12E—C17E—C18E | 92 (3)      |
| C3C—C4C—C5C—C6C     | 0.2 (4)      | C13E—N12E—C17E—C18E | -78 (2)     |

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| C4C—C5C—C6C—C7C     | -1.1 (4)    | N12E—C17E—C18E—C19E | 176 (2)   |
| C5C—C6C—C7C—C8C     | 1.2 (4)     | N12E—C17E—C18E—C20E | -60 (2)   |
| C6C—C7C—C8C—C3C     | -0.3 (4)    | O2E—P1E—C21E—C22E   | -58.1 (9) |
| C4C—C3C—C8C—C7C     | -0.6 (4)    | C3E—P1E—C21E—C22E   | 65.1 (8)  |
| P1C—C3C—C8C—C7C     | 178.28 (19) | C9E—P1E—C21E—C22E   | 180.0 (8) |
| O2C—P1C—C9C—C10C    | 173.92 (17) | P1E—C21E—C22E—C23E  | 169.6 (7) |
| C21C—P1C—C9C—C10C   | -62.3 (2)   | C21E—C22E—C23E—C24E | 171.2 (7) |
| C3C—P1C—C9C—C10C    | 52.5 (2)    | C22E—C23E—C24E—C25E | 167.3 (7) |
| C17C—N12C—C10C—O11C | 1.6 (3)     | C23E—C24E—C25E—C26E | 60.5 (13) |
| C13C—N12C—C10C—O11C | 177.2 (2)   | C24E—C25E—C26E—C27E | 171 (3)   |
| C17C—N12C—C10C—C9C  | -176.6 (2)  | C25E—C26E—C27E—C28E | 180 (4)   |

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

| $D-H\cdots A$                        | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------------|-------|-------------|-------------|---------------|
| C9A—H9A1 $\cdots$ O2A <sup>i</sup>   | 0.99  | 2.37        | 3.339 (3)   | 165           |
| C9A—H9A2 $\cdots$ O2D                | 0.99  | 2.31        | 3.238 (5)   | 156           |
| C9B—H9B2 $\cdots$ O2C                | 0.99  | 2.49        | 3.442 (3)   | 160           |
| C9B—H9B1 $\cdots$ O2B <sup>ii</sup>  | 0.99  | 2.50        | 3.483 (3)   | 175           |
| C9C—H9C2 $\cdots$ O2B                | 0.99  | 2.36        | 3.305 (3)   | 158           |
| C5A—H5A $\cdots$ O11D <sup>iii</sup> | 0.95  | 2.48        | 3.379 (14)  | 157           |
| C6C—H6C $\cdots$ O11C <sup>iv</sup>  | 0.95  | 2.51        | 3.453 (3)   | 170           |
| C6D—H6D $\cdots$ O11D <sup>iv</sup>  | 0.95  | 2.47        | 3.37 (2)    | 159           |
| C9D—H9D1 $\cdots$ O11A <sup>i</sup>  | 0.99  | 2.56        | 3.265 (7)   | 128           |
| C7B—H7B $\cdots$ O11C <sup>v</sup>   | 0.95  | 2.59        | 3.477 (3)   | 156           |
| C9D—H9D2 $\cdots$ O2A                | 0.99  | 2.36        | 3.265 (11)  | 151           |
| C13B—H13D $\cdots$ O2C               | 0.99  | 2.52        | 3.431 (3)   | 154           |
| C13C—H13E $\cdots$ O2B               | 0.99  | 2.49        | 3.448 (3)   | 162           |
| C15D—H15L $\cdots$ O2A               | 0.98  | 2.55        | 3.332 (10)  | 137           |
| C17A—H17B $\cdots$ O2D               | 0.99  | 2.52        | 3.375 (7)   | 145           |
| C21A—H21B $\cdots$ O11A              | 0.99  | 2.52        | 3.139 (3)   | 120           |
| C4D—H4D $\cdots$ O11D                | 0.95  | 2.58        | 3.36 (2)    | 140           |
| C8C—H8C $\cdots$ O11C                | 0.95  | 2.52        | 3.239 (3)   | 132           |
| C21B—H21D $\cdots$ O11B              | 0.99  | 2.51        | 3.175 (3)   | 124           |
| C21C—H21F $\cdots$ O11C              | 0.99  | 2.43        | 3.093 (3)   | 124           |
| C21D—H21H $\cdots$ O11D              | 0.99  | 2.53        | 3.224 (19)  | 127           |

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