

# Naphthalen-2-yl 1-(benzamido(diethoxyphosphoryl)methyl)-1H-1,2,3-triazole-4-carboxylate

Datablock I - ellipsoid plot

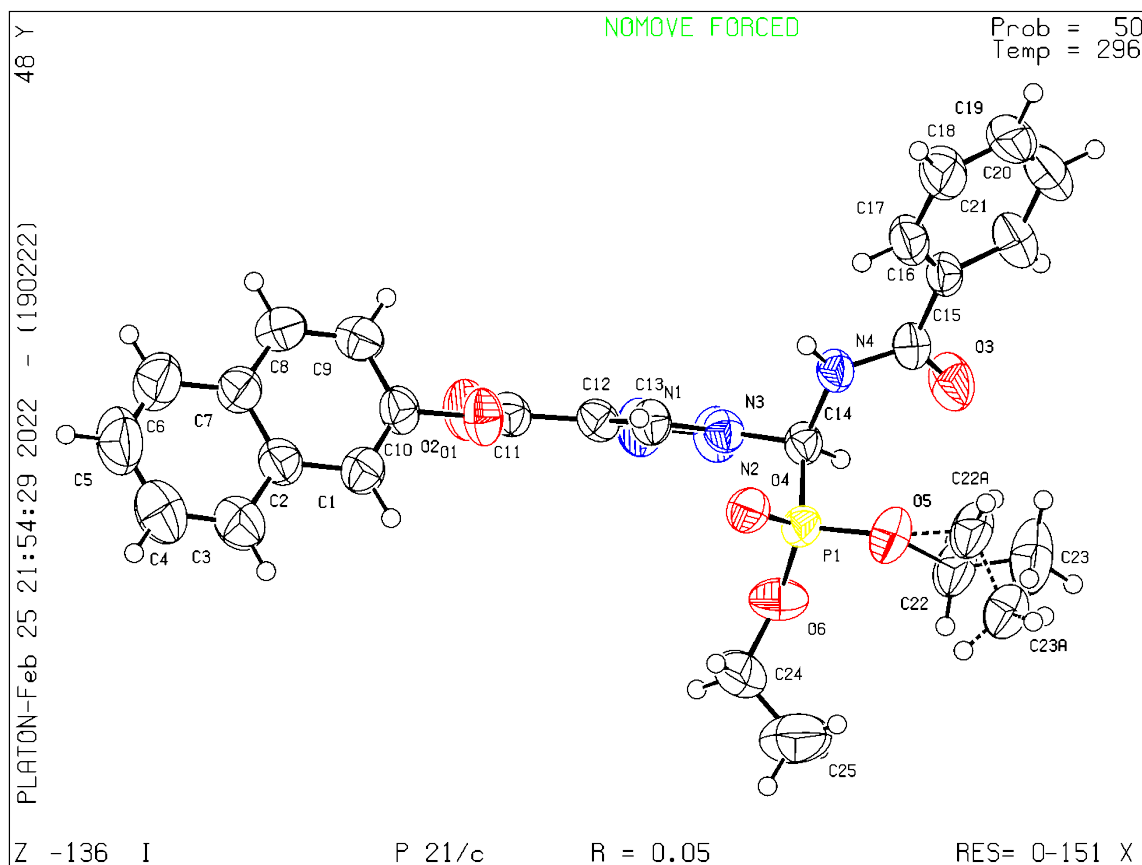


Figure S1. Crystallography data for title compound.

Table S1. Crystal data, data collection and structure refinement details are summarized.

| Crystal data                       |                                                                 |
|------------------------------------|-----------------------------------------------------------------|
| Chemical formula                   | C <sub>25</sub> H <sub>25</sub> N <sub>4</sub> O <sub>6</sub> P |
| <i>M</i> <sub>r</sub>              | 508.46                                                          |
| Crystal system, space group        | Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>                  |
| Temperature (K)                    | 296                                                             |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 10.6281 (8), 14.2828 (10), 16.5913 (12)                         |
| (°)                                | 91.946 (3)                                                      |
| <i>V</i> (Å <sup>3</sup> )         | 2517.1 (3)                                                      |
| <i>Z</i>                           | 4                                                               |
| Radiation type                     | Mo <i>K</i>                                                     |
| (mm <sup>-1</sup> )                | 0.16                                                            |
| Crystal size (mm)                  | 0.32 × 0.28 × 0.19                                              |
| Data collection                    |                                                                 |
| Diffractometer                     | Bruker D8 VENTURE Super DUO                                     |

|                                                                               |                                                                        |
|-------------------------------------------------------------------------------|------------------------------------------------------------------------|
| Absorption correction                                                         | Multi-scan<br>SADABS(Krause <i>et al.</i> , 2015)                      |
| $T_{\min}, T_{\max}$                                                          | 0.617, 0.746                                                           |
| No. of measured, independent and<br>observed [ $I > 2\sigma(I)$ ] reflections | 61924, 5559, 3723                                                      |
| $R_{\text{int}}$                                                              | 0.062                                                                  |
| $(\sin \theta / \lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )                  | 0.641                                                                  |
| Refinement                                                                    |                                                                        |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$                                           | 0.052, 0.142, 1.04                                                     |
| No. of reflections                                                            | 5559                                                                   |
| No. of parameters                                                             | 345                                                                    |
| No. of restraints                                                             | 306                                                                    |
| H-atom treatment                                                              | H atoms treated by a mixture of independent and constrained refinement |
| $\text{max}, \text{min}$ ( $\text{e \AA}^{-3}$ )                              | 0.30, -0.26                                                            |

**Table S2.** Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ) for (shelx).

| $D-H\cdots A$                     | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|----------|-------------|-------------|---------------|
| C25—H25A $\cdots$ O3 <sup>i</sup> | 0.96     | 2.59        | 3.471 (5)   | 153           |
| C17—H17 $\cdots$ O4 <sup>ii</sup> | 0.93     | 2.56        | 3.433 (3)   | 157           |
| N4—H4A $\cdots$ O4 <sup>ii</sup>  | 0.84 (2) | 2.06 (2)    | 2.870 (2)   | 163 (3)       |
| C14—H14 $\cdots$ O3               | 0.98     | 2.23        | 2.702 (3)   | 108           |

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

**Table S3.** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for (shelx).

|     | $x$          | $y$          | $z$          | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. ( $<1$ ) |
|-----|--------------|--------------|--------------|----------------------------------|---------------|
| C1  | 0.6472 (2)   | 0.07678 (17) | 0.54397 (15) | 0.0620 (6)                       |               |
| H1  | 0.602569     | 0.088686     | 0.495860     | 0.074*                           |               |
| O1  | 0.53612 (17) | 0.19984 (11) | 0.60382 (10) | 0.0663 (5)                       |               |
| P1  | 0.27908 (5)  | 0.49313 (4)  | 0.44200 (4)  | 0.04962 (18)                     |               |
| N1  | 0.2441 (2)   | 0.29687 (15) | 0.66278 (14) | 0.0705 (6)                       |               |
| N2  | 0.19957 (19) | 0.37677 (15) | 0.63784 (14) | 0.0656 (6)                       |               |
| O2  | 0.40346 (18) | 0.13547 (12) | 0.69067 (12) | 0.0767 (5)                       |               |
| C2  | 0.7429 (2)   | 0.00708 (17) | 0.54727 (15) | 0.0619 (6)                       |               |
| C3  | 0.7738 (3)   | -0.0448 (2)  | 0.4790 (2)   | 0.0896 (9)                       |               |
| H3  | 0.731263     | -0.034189    | 0.429901     | 0.107*                           |               |
| O3  | 0.15767 (16) | 0.66613 (13) | 0.60075 (13) | 0.0805 (6)                       |               |
| N3  | 0.28788 (16) | 0.41578 (12) | 0.59148 (11) | 0.0481 (4)                       |               |
| C4  | 0.8661 (4)   | -0.1105 (3)  | 0.4848 (2)   | 0.1088 (12)                      |               |
| H4  | 0.886053     | -0.144691    | 0.439234     | 0.131*                           |               |
| O4  | 0.40794 (14) | 0.47238 (11) | 0.42139 (10) | 0.0586 (4)                       |               |
| N4  | 0.33209 (16) | 0.58104 (12) | 0.58309 (11) | 0.0493 (4)                       |               |
| H4A | 0.4106 (16)  | 0.5757 (19)  | 0.5871 (16)  | 0.074*                           |               |
| O5  | 0.23719 (15) | 0.58914 (13) | 0.40700 (11) | 0.0707 (5)                       |               |
| C5  | 0.9312 (3)   | -0.1279 (2)  | 0.5574 (3)   | 0.1067 (11)                      |               |
| H5  | 0.994423     | -0.172951    | 0.559980     | 0.128*                           |               |
| O6  | 0.17852 (16) | 0.41822 (14) | 0.41900 (11) | 0.0755 (5)                       |               |
| C6  | 0.9028 (3)   | -0.0796 (2)  | 0.6236 (2)   | 0.0917 (9)                       |               |
| H6  | 0.946428     | -0.091936    | 0.671941     | 0.110*                           |               |

|      |              |               |              |             |           |
|------|--------------|---------------|--------------|-------------|-----------|
| C7   | 0.8074 (2)   | -0.00997 (17) | 0.62132 (16) | 0.0635 (6)  |           |
| C8   | 0.7750 (3)   | 0.0419 (2)    | 0.68921 (17) | 0.0755 (8)  |           |
| H8   | 0.816237     | 0.030246      | 0.738534     | 0.091*      |           |
| C9   | 0.6849 (3)   | 0.10845 (18)  | 0.68420 (16) | 0.0690 (7)  |           |
| H9   | 0.665100     | 0.143021      | 0.729546     | 0.083*      |           |
| C10  | 0.6218 (2)   | 0.12498 (15)  | 0.61054 (14) | 0.0570 (6)  |           |
| C11  | 0.4320 (2)   | 0.19821 (16)  | 0.64770 (14) | 0.0558 (6)  |           |
| C12  | 0.3593 (2)   | 0.28411 (15)  | 0.63257 (13) | 0.0508 (5)  |           |
| C13  | 0.3881 (2)   | 0.35985 (15)  | 0.58761 (14) | 0.0505 (5)  |           |
| H13  | 0.461557     | 0.370523      | 0.560106     | 0.061*      |           |
| C14  | 0.25973 (19) | 0.50396 (14)  | 0.55048 (14) | 0.0481 (5)  |           |
| H14  | 0.170843     | 0.518058      | 0.558698     | 0.058*      |           |
| C15  | 0.2727 (2)   | 0.66123 (15)  | 0.60387 (14) | 0.0519 (5)  |           |
| C16  | 0.3518 (2)   | 0.74156 (14)  | 0.63139 (13) | 0.0503 (5)  |           |
| C17  | 0.4793 (2)   | 0.74593 (16)  | 0.62389 (17) | 0.0672 (7)  |           |
| H17  | 0.521161     | 0.696616      | 0.599847     | 0.081*      |           |
| C18  | 0.5466 (3)   | 0.82262 (19)  | 0.6516 (2)   | 0.0863 (9)  |           |
| H18  | 0.633165     | 0.825304      | 0.645304     | 0.104*      |           |
| C19  | 0.4865 (4)   | 0.89439 (19)  | 0.68799 (19) | 0.0864 (9)  |           |
| H19  | 0.532332     | 0.945363      | 0.707869     | 0.104*      |           |
| C20  | 0.3603 (4)   | 0.8917 (2)    | 0.69532 (19) | 0.0901 (9)  |           |
| H20  | 0.319342     | 0.941136      | 0.719736     | 0.108*      |           |
| C21  | 0.2920 (3)   | 0.81588 (18)  | 0.66677 (17) | 0.0733 (7)  |           |
| H21  | 0.205087     | 0.814881      | 0.671413     | 0.088*      |           |
| C24  | 0.1837 (3)   | 0.3582 (2)    | 0.3471 (2)   | 0.0984 (11) |           |
| H24A | 0.268719     | 0.358431      | 0.327655     | 0.118*      |           |
| H24B | 0.163196     | 0.294384      | 0.361843     | 0.118*      |           |
| C25  | 0.0999 (3)   | 0.3881 (3)    | 0.2849 (2)   | 0.1184 (14) |           |
| H25A | 0.015606     | 0.388085      | 0.303899     | 0.178*      |           |
| H25B | 0.104907     | 0.346315      | 0.239763     | 0.178*      |           |
| H25C | 0.122051     | 0.450230      | 0.268508     | 0.178*      |           |
| C22  | 0.1071 (3)   | 0.6202 (2)    | 0.4017 (2)   | 0.0748 (10) | 0.893 (4) |
| H22A | 0.060304     | 0.582604      | 0.362246     | 0.090*      | 0.893 (4) |
| H22B | 0.068836     | 0.612345      | 0.453476     | 0.090*      | 0.893 (4) |
| C23  | 0.1025 (4)   | 0.7169 (3)    | 0.3783 (4)   | 0.1087 (16) | 0.893 (4) |
| H23A | 0.147692     | 0.725328      | 0.329729     | 0.163*      | 0.893 (4) |
| H23B | 0.140207     | 0.754607      | 0.420503     | 0.163*      | 0.893 (4) |
| H23C | 0.016375     | 0.735514      | 0.369100     | 0.163*      | 0.893 (4) |
| C22A | 0.188 (2)    | 0.6755 (13)   | 0.3964 (16)  | 0.0748 (10) | 0.107 (4) |
| H22C | 0.254342     | 0.720161      | 0.386773     | 0.090*      | 0.107 (4) |
| H22D | 0.145283     | 0.694589      | 0.444552     | 0.090*      | 0.107 (4) |
| C23A | 0.099 (2)    | 0.674 (2)     | 0.3279 (15)  | 0.063 (6)   | 0.107 (4) |
| H23D | 0.092520     | 0.611840      | 0.306575     | 0.095*      | 0.107 (4) |
| H23E | 0.127164     | 0.715849      | 0.286856     | 0.095*      | 0.107 (4) |
| H23F | 0.017505     | 0.694186      | 0.344897     | 0.095*      | 0.107 (4) |

**Table S4.** Atomic displacement parameters ( $\text{\AA}^2$ ) for (shelx).

|    | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$     | $U^{23}$    |
|----|-------------|-------------|-------------|-------------|--------------|-------------|
| C1 | 0.0737 (16) | 0.0557 (14) | 0.0565 (14) | 0.0048 (12) | -0.0010 (12) | 0.0060 (11) |
| O1 | 0.0791 (11) | 0.0477 (9)  | 0.0732 (11) | 0.0125 (8)  | 0.0174 (9)   | 0.0148 (8)  |

|      |             |             |             |              |              |              |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| P1   | 0.0397 (3)  | 0.0486 (3)  | 0.0600 (4)  | 0.0019 (2)   | -0.0064 (2)  | -0.0002 (3)  |
| N1   | 0.0658 (13) | 0.0575 (13) | 0.0892 (16) | -0.0043 (10) | 0.0184 (11)  | 0.0162 (11)  |
| N2   | 0.0528 (11) | 0.0606 (13) | 0.0845 (15) | -0.0029 (10) | 0.0174 (10)  | 0.0093 (11)  |
| O2   | 0.0885 (13) | 0.0520 (10) | 0.0905 (13) | -0.0011 (9)  | 0.0172 (10)  | 0.0220 (10)  |
| C2   | 0.0707 (16) | 0.0505 (14) | 0.0645 (15) | 0.0000 (11)  | 0.0022 (12)  | -0.0018 (11) |
| C3   | 0.109 (2)   | 0.080 (2)   | 0.0792 (19) | 0.0185 (18)  | 0.0032 (17)  | -0.0162 (16) |
| O3   | 0.0471 (10) | 0.0685 (12) | 0.1264 (17) | 0.0114 (8)   | 0.0109 (10)  | -0.0194 (11) |
| N3   | 0.0428 (9)  | 0.0423 (9)  | 0.0592 (11) | -0.0044 (7)  | 0.0027 (8)   | -0.0004 (8)  |
| C4   | 0.119 (3)   | 0.092 (2)   | 0.116 (3)   | 0.031 (2)    | 0.012 (2)    | -0.025 (2)   |
| O4   | 0.0448 (8)  | 0.0646 (10) | 0.0662 (10) | 0.0082 (7)   | -0.0020 (7)  | -0.0058 (8)  |
| N4   | 0.0396 (9)  | 0.0414 (9)  | 0.0667 (12) | 0.0036 (8)   | -0.0014 (9)  | -0.0041 (8)  |
| O5   | 0.0561 (10) | 0.0713 (11) | 0.0846 (12) | 0.0164 (8)   | 0.0008 (8)   | 0.0178 (9)   |
| C5   | 0.094 (2)   | 0.082 (2)   | 0.144 (3)   | 0.0322 (19)  | 0.007 (2)    | -0.008 (2)   |
| O6   | 0.0665 (11) | 0.0862 (13) | 0.0730 (11) | -0.0227 (10) | -0.0094 (9)  | -0.0107 (10) |
| C6   | 0.0758 (19) | 0.083 (2)   | 0.115 (3)   | 0.0146 (16)  | -0.0137 (18) | 0.0057 (19)  |
| C7   | 0.0612 (14) | 0.0538 (14) | 0.0748 (16) | -0.0032 (11) | -0.0078 (12) | 0.0028 (12)  |
| C8   | 0.0816 (18) | 0.0753 (18) | 0.0682 (17) | -0.0006 (15) | -0.0180 (14) | -0.0015 (14) |
| C9   | 0.0830 (18) | 0.0623 (16) | 0.0611 (15) | 0.0005 (13)  | -0.0046 (13) | -0.0078 (12) |
| C10  | 0.0687 (15) | 0.0413 (12) | 0.0610 (14) | 0.0024 (10)  | 0.0053 (11)  | 0.0060 (10)  |
| C11  | 0.0669 (15) | 0.0438 (12) | 0.0567 (13) | -0.0052 (11) | 0.0018 (11)  | 0.0021 (10)  |
| C12  | 0.0556 (13) | 0.0425 (12) | 0.0544 (13) | -0.0056 (10) | 0.0036 (10)  | -0.0011 (10) |
| C13  | 0.0455 (11) | 0.0459 (12) | 0.0605 (13) | 0.0009 (9)   | 0.0063 (10)  | 0.0029 (10)  |
| C14  | 0.0362 (10) | 0.0435 (11) | 0.0645 (13) | 0.0026 (9)   | 0.0000 (9)   | -0.0024 (10) |
| C15  | 0.0510 (13) | 0.0462 (12) | 0.0588 (13) | 0.0080 (10)  | 0.0068 (10)  | 0.0010 (10)  |
| C16  | 0.0634 (14) | 0.0379 (11) | 0.0496 (12) | 0.0071 (10)  | 0.0013 (10)  | 0.0039 (9)   |
| C17  | 0.0661 (15) | 0.0411 (12) | 0.0939 (19) | 0.0039 (11)  | -0.0038 (14) | -0.0052 (12) |
| C18  | 0.0794 (19) | 0.0510 (15) | 0.127 (3)   | -0.0093 (13) | -0.0202 (18) | -0.0015 (16) |
| C19  | 0.121 (3)   | 0.0449 (15) | 0.091 (2)   | -0.0129 (16) | -0.0232 (19) | -0.0019 (14) |
| C20  | 0.134 (3)   | 0.0497 (16) | 0.088 (2)   | 0.0045 (17)  | 0.016 (2)    | -0.0200 (14) |
| C21  | 0.0875 (19) | 0.0521 (14) | 0.0814 (18) | 0.0073 (13)  | 0.0187 (15)  | -0.0096 (13) |
| C24  | 0.095 (2)   | 0.0732 (19) | 0.124 (3)   | 0.0040 (17)  | -0.032 (2)   | -0.0348 (19) |
| C25  | 0.094 (2)   | 0.171 (4)   | 0.089 (2)   | 0.012 (2)    | -0.0121 (19) | -0.043 (2)   |
| C22  | 0.0502 (16) | 0.075 (2)   | 0.099 (2)   | 0.0154 (14)  | -0.0050 (15) | 0.0122 (17)  |
| C23  | 0.070 (2)   | 0.072 (2)   | 0.184 (5)   | 0.0186 (19)  | 0.006 (3)    | 0.030 (3)    |
| C22A | 0.0502 (16) | 0.075 (2)   | 0.099 (2)   | 0.0154 (14)  | -0.0050 (15) | 0.0122 (17)  |
| C23A | 0.053 (10)  | 0.058 (13)  | 0.079 (11)  | -0.008 (9)   | 0.004 (8)    | 0.026 (10)   |

**Table S5.** Geometric parameters (Å, °) for (shelx).

|               |                  |              |               |
|---------------|------------------|--------------|---------------|
| <b>C1—C10</b> | <b>1.337 (3)</b> | <b>C9—H9</b> | <b>0.9300</b> |
| C1—C2         | 1.423 (3)        | C11—C12      | 1.466 (3)     |
| C1—H1         | 0.9300           | C12—C13      | 1.355 (3)     |
| O1—C11        | 1.346 (3)        | C13—H13      | 0.9300        |
| O1—C10        | 1.407 (3)        | C14—H14      | 0.9800        |
| P1—O4         | 1.4534 (16)      | C15—C16      | 1.485 (3)     |
| P1—O5         | 1.5485 (17)      | C16—C17      | 1.367 (3)     |
| P1—O6         | 1.5508 (17)      | C16—C21      | 1.378 (3)     |
| P1—C14        | 1.825 (2)        | C17—C18      | 1.378 (3)     |
| N1—N2         | 1.298 (3)        | C17—H17      | 0.9300        |
| N1—C12        | 1.352 (3)        | C18—C19      | 1.360 (4)     |
| N2—N3         | 1.353 (3)        | C18—H18      | 0.9300        |

|            |             |             |             |
|------------|-------------|-------------|-------------|
| O2—C11     | 1.191 (3)   | C19—C20     | 1.352 (5)   |
| C2—C3      | 1.402 (4)   | C19—H19     | 0.9300      |
| C2—C7      | 1.408 (3)   | C20—C21     | 1.378 (4)   |
| C3—C4      | 1.359 (4)   | C20—H20     | 0.9300      |
| C3—H3      | 0.9300      | C21—H21     | 0.9300      |
| O3—C15     | 1.224 (3)   | C24—C25     | 1.407 (4)   |
| N3—C13     | 1.335 (3)   | C24—H24A    | 0.9700      |
| N3—C14     | 1.458 (3)   | C24—H24B    | 0.9700      |
| C4—C5      | 1.391 (5)   | C25—H25A    | 0.9600      |
| C4—H4      | 0.9300      | C25—H25B    | 0.9600      |
| N4—C15     | 1.358 (3)   | C25—H25C    | 0.9600      |
| N4—C14     | 1.438 (3)   | C22—C23     | 1.436 (4)   |
| N4—H4A     | 0.838 (16)  | C22—H22A    | 0.9700      |
| O5—C22A    | 1.350 (16)  | C22—H22B    | 0.9700      |
| O5—C22     | 1.451 (3)   | C23—H23A    | 0.9600      |
| C5—C6      | 1.340 (5)   | C23—H23B    | 0.9600      |
| C5—H5      | 0.9300      | C23—H23C    | 0.9600      |
| O6—C24     | 1.472 (3)   | C22A—C23A   | 1.455 (18)  |
| C6—C7      | 1.420 (4)   | C22A—H22C   | 0.9700      |
| C6—H6      | 0.9300      | C22A—H22D   | 0.9700      |
| C7—C8      | 1.401 (4)   | C23A—H23D   | 0.9600      |
| C8—C9      | 1.350 (4)   | C23A—H23E   | 0.9600      |
| C8—H8      | 0.9300      | C23A—H23F   | 0.9600      |
| C9—C10     | 1.394 (3)   |             |             |
| C10—C1—C2  | 119.5 (2)   | N4—C14—H14  | 107.2       |
| C10—C1—H1  | 120.3       | N3—C14—H14  | 107.2       |
| C2—C1—H1   | 120.3       | P1—C14—H14  | 107.2       |
| C11—O1—C10 | 119.11 (18) | O3—C15—N4   | 120.6 (2)   |
| O4—P1—O5   | 110.71 (10) | O3—C15—C16  | 121.5 (2)   |
| O4—P1—O6   | 116.64 (10) | N4—C15—C16  | 117.84 (19) |
| O5—P1—O6   | 109.38 (10) | C17—C16—C21 | 118.4 (2)   |
| O4—P1—C14  | 112.82 (9)  | C17—C16—C15 | 124.0 (2)   |
| O5—P1—C14  | 104.72 (10) | C21—C16—C15 | 117.5 (2)   |
| O6—P1—C14  | 101.62 (10) | C16—C17—C18 | 120.7 (3)   |
| N2—N1—C12  | 108.99 (19) | C16—C17—H17 | 119.6       |
| N1—N2—N3   | 106.93 (19) | C18—C17—H17 | 119.6       |
| C3—C2—C7   | 119.6 (3)   | C19—C18—C17 | 120.1 (3)   |
| C3—C2—C1   | 121.7 (2)   | C19—C18—H18 | 120.0       |
| C7—C2—C1   | 118.8 (2)   | C17—C18—H18 | 120.0       |
| C4—C3—C2   | 119.7 (3)   | C20—C19—C18 | 120.0 (3)   |
| C4—C3—H3   | 120.1       | C20—C19—H19 | 120.0       |
| C2—C3—H3   | 120.1       | C18—C19—H19 | 120.0       |
| C13—N3—N2  | 110.54 (18) | C19—C20—C21 | 120.3 (3)   |
| C13—N3—C14 | 130.25 (19) | C19—C20—H20 | 119.9       |
| N2—N3—C14  | 119.06 (18) | C21—C20—H20 | 119.9       |
| C3—C4—C5   | 121.4 (3)   | C20—C21—C16 | 120.4 (3)   |
| C3—C4—H4   | 119.3       | C20—C21—H21 | 119.8       |
| C5—C4—H4   | 119.3       | C16—C21—H21 | 119.8       |
| C15—N4—C14 | 119.62 (18) | C25—C24—O6  | 112.2 (3)   |

|                |             |                |              |
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| C15—N4—H4A     | 121.7 (19)  | C25—C24—H24A   | 109.2        |
| C14—N4—H4A     | 118.6 (19)  | O6—C24—H24A    | 109.2        |
| C22A—O5—P1     | 164.5 (12)  | C25—C24—H24B   | 109.2        |
| C22—O5—P1      | 123.66 (18) | O6—C24—H24B    | 109.2        |
| C6—C5—C4       | 119.9 (3)   | H24A—C24—H24B  | 107.9        |
| C6—C5—H5       | 120.1       | C24—C25—H25A   | 109.5        |
| C4—C5—H5       | 120.1       | C24—C25—H25B   | 109.5        |
| C24—O6—P1      | 123.9 (2)   | H25A—C25—H25B  | 109.5        |
| C5—C6—C7       | 121.3 (3)   | C24—C25—H25C   | 109.5        |
| C5—C6—H6       | 119.3       | H25A—C25—H25C  | 109.5        |
| C7—C6—H6       | 119.3       | H25B—C25—H25C  | 109.5        |
| C8—C7—C2       | 119.0 (2)   | C23—C22—O5     | 109.5 (3)    |
| C8—C7—C6       | 123.0 (3)   | C23—C22—H22A   | 109.8        |
| C2—C7—C6       | 118.1 (3)   | O5—C22—H22A    | 109.8        |
| C9—C8—C7       | 121.1 (2)   | C23—C22—H22B   | 109.8        |
| C9—C8—H8       | 119.5       | O5—C22—H22B    | 109.8        |
| C7—C8—H8       | 119.5       | H22A—C22—H22B  | 108.2        |
| C8—C9—C10      | 119.5 (2)   | C22—C23—H23A   | 109.5        |
| C8—C9—H9       | 120.3       | C22—C23—H23B   | 109.5        |
| C10—C9—H9      | 120.3       | H23A—C23—H23B  | 109.5        |
| C1—C10—C9      | 122.2 (2)   | C22—C23—H23C   | 109.5        |
| C1—C10—O1      | 118.3 (2)   | H23A—C23—H23C  | 109.5        |
| C9—C10—O1      | 119.3 (2)   | H23B—C23—H23C  | 109.5        |
| O2—C11—O1      | 124.6 (2)   | O5—C22A—C23A   | 109.3 (18)   |
| O2—C11—C12     | 126.1 (2)   | O5—C22A—H22C   | 109.8        |
| O1—C11—C12     | 109.32 (19) | C23A—C22A—H22C | 109.8        |
| N1—C12—C13     | 108.7 (2)   | O5—C22A—H22D   | 109.8        |
| N1—C12—C11     | 121.9 (2)   | C23A—C22A—H22D | 109.8        |
| C13—C12—C11    | 129.4 (2)   | H22C—C22A—H22D | 108.3        |
| N3—C13—C12     | 104.8 (2)   | C22A—C23A—H23D | 109.5        |
| N3—C13—H13     | 127.6       | C22A—C23A—H23E | 109.5        |
| C12—C13—H13    | 127.6       | H23D—C23A—H23E | 109.5        |
| N4—C14—N3      | 112.78 (16) | C22A—C23A—H23F | 109.5        |
| N4—C14—P1      | 111.05 (15) | H23D—C23A—H23F | 109.5        |
| N3—C14—P1      | 111.03 (14) | H23E—C23A—H23F | 109.5        |
| C12—N1—N2—N3   | -0.3 (3)    | O2—C11—C12—N1  | -5.3 (4)     |
| C10—C1—C2—C3   | -179.4 (3)  | O1—C11—C12—N1  | 173.4 (2)    |
| C10—C1—C2—C7   | 0.8 (4)     | O2—C11—C12—C13 | 176.8 (2)    |
| C7—C2—C3—C4    | -0.4 (5)    | O1—C11—C12—C13 | -4.5 (3)     |
| C1—C2—C3—C4    | 179.9 (3)   | N2—N3—C13—C12  | 0.5 (2)      |
| N1—N2—N3—C13   | -0.1 (3)    | C14—N3—C13—C12 | -174.9 (2)   |
| N1—N2—N3—C14   | 175.87 (19) | N1—C12—C13—N3  | -0.7 (3)     |
| C2—C3—C4—C5    | 0.0 (6)     | C11—C12—C13—N3 | 177.5 (2)    |
| O4—P1—O5—C22A  | -136 (4)    | C15—N4—C14—N3  | -129.4 (2)   |
| O6—P1—O5—C22A  | 94 (4)      | C15—N4—C14—P1  | 105.2 (2)    |
| C14—P1—O5—C22A | -14 (4)     | C13—N3—C14—N4  | -74.2 (3)    |
| O4—P1—O5—C22   | 165.9 (2)   | N2—N3—C14—N4   | 110.8 (2)    |
| O6—P1—O5—C22   | 36.0 (3)    | C13—N3—C14—P1  | 51.2 (3)     |
| C14—P1—O5—C22  | -72.2 (2)   | N2—N3—C14—P1   | -123.87 (18) |

|                |             |                 |              |
|----------------|-------------|-----------------|--------------|
| C3—C4—C5—C6    | 0.4 (6)     | O4—P1—C14—N4    | 62.98 (16)   |
| O4—P1—O6—C24   | -33.2 (2)   | O5—P1—C14—N4    | -57.50 (16)  |
| O5—P1—O6—C24   | 93.3 (2)    | O6—P1—C14—N4    | -171.35 (14) |
| C14—P1—O6—C24  | -156.4 (2)  | O4—P1—C14—N3    | -63.36 (16)  |
| C4—C5—C6—C7    | -0.4 (6)    | O5—P1—C14—N3    | 176.16 (13)  |
| C3—C2—C7—C8    | -179.5 (3)  | O6—P1—C14—N3    | 62.31 (16)   |
| C1—C2—C7—C8    | 0.2 (4)     | C14—N4—C15—O3   | 5.4 (3)      |
| C3—C2—C7—C6    | 0.3 (4)     | C14—N4—C15—C16  | -175.41 (19) |
| C1—C2—C7—C6    | -179.9 (2)  | O3—C15—C16—C17  | -168.9 (2)   |
| C5—C6—C7—C8    | 179.9 (3)   | N4—C15—C16—C17  | 12.0 (3)     |
| C5—C6—C7—C2    | 0.1 (5)     | O3—C15—C16—C21  | 11.3 (3)     |
| C2—C7—C8—C9    | -1.1 (4)    | N4—C15—C16—C21  | -167.9 (2)   |
| C6—C7—C8—C9    | 179.0 (3)   | C21—C16—C17—C18 | 0.4 (4)      |
| C7—C8—C9—C10   | 0.9 (4)     | C15—C16—C17—C18 | -179.4 (2)   |
| C2—C1—C10—C9   | -1.0 (4)    | C16—C17—C18—C19 | 1.1 (5)      |
| C2—C1—C10—O1   | 173.6 (2)   | C17—C18—C19—C20 | -1.6 (5)     |
| C8—C9—C10—C1   | 0.2 (4)     | C18—C19—C20—C21 | 0.7 (5)      |
| C8—C9—C10—O1   | -174.4 (2)  | C19—C20—C21—C16 | 0.8 (5)      |
| C11—O1—C10—C1  | 121.3 (3)   | C17—C16—C21—C20 | -1.4 (4)     |
| C11—O1—C10—C9  | -63.9 (3)   | C15—C16—C21—C20 | 178.5 (2)    |
| C10—O1—C11—O2  | -2.9 (4)    | P1—O6—C24—C25   | -103.1 (3)   |
| C10—O1—C11—C12 | 178.40 (19) | P1—O5—C22—C23   | 171.1 (3)    |
| N2—N1—C12—C13  | 0.6 (3)     | P1—O5—C22A—C23A | -122 (3)     |
| N2—N1—C12—C11  | -177.7 (2)  |                 |              |