# Structure Tables

## Table 1. Crystal data and structure refinement for p-1.cif

|  |  |
| --- | --- |
| CCDC number |  |
| Empirical formula | C86.60H90N3O9.70P3S2Sn |
| Formula weight | 1603.73 |
| Temperature/K | 100(2) |
| Crystal system | triclinic |
| Space group (number) | *P-*1 (2) |
| *a*/Å | 10.9564(18) |
| *b*/Å | 14.820(2) |
| *c*/Å | 24.610(4) |
| α/Å | 76.204(3) |
| β/Å | 88.086(2) |
| γ/Å | 80.175(2) |
| Volume/Å3 | 3823.6(11) |
| *Z* | 2 |
| *ρ*calc g/cm3 | 1.393 |
| μ/mm-1 | 0.514 |
| *F*(000) | 1670 |
| Crystal size/mm3 | ?×?×? |
| Crystal colour | ? |
| Crystal shape | ? |
| Radiation | Mo*Kα* (λ=0.71073) |
| 2ϴ range/° | 4.34 to 52.79 |
| Index ranges | -13 ≤ h ≤ 13 -18 ≤ k ≤ 18 -30 ≤ l ≤ 30 |
| Reflections collected | 109559 |
| Independent reflections | 15644 *R*int = 0.0708 *R*sigma = 0.0377 |
| Completeness to θ = ° | 99.90 |
| Data / Restraints / Param. | 15644/2968/1404 |
| Goodness-of-fit on *F*2 | 1.118 |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = 0.0495 w*R*2 = 0.1212 |
| Final *R* indexes  [all data] | *R*1 = 0.0624 w*R*2 = 0.1275 |
| Largest peak/hole /eÅ3 | 1.43/-1.23 |

## Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å2) for p-1.cif. Ueq is defined as 1/3 of the trace of the orthogonalized U*ij* tensor.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atom** | ***x*** | ***y*** | ***z*** | ***U*eq** |
| N1 | 0.4218(2) | 0.4838(2) | 0.18543(11) | 0.0190(6) |
| N2 | 0.2703(2) | 0.4550(2) | 0.28662(11) | 0.0192(6) |
| N3 | 0.3479(2) | 0.6416(2) | 0.24014(11) | 0.0194(6) |
| P2 | 0.46254(7) | 0.48452(6) | 0.12206(3) | 0.01847(17) |
| P3 | 0.18150(7) | 0.37767(7) | 0.30910(4) | 0.02135(18) |
| P4 | 0.28570(7) | 0.74715(6) | 0.24338(4) | 0.02064(18) |
| Sn1 | 0.24101(2) | 0.55622(2) | 0.20542(2) | 0.01760(7) |
| C1 | 0.6095(3) | 0.4560(3) | 0.31905(14) | 0.0261(7) |
| H1A | 0.674268 | 0.490549 | 0.300889 | 0.039 |
| H1B | 0.637314 | 0.388231 | 0.323061 | 0.039 |
| H1D | 0.592501 | 0.468727 | 0.356096 | 0.039 |
| C2 | 0.4901(3) | 0.4881(2) | 0.28294(13) | 0.0200(7) |
| C3 | 0.5206(3) | 0.4524(2) | 0.22948(13) | 0.0205(7) |
| H3A | 0.597596 | 0.473994 | 0.213388 | 0.025 |
| H3B | 0.537230 | 0.382633 | 0.239828 | 0.025 |
| C4 | 0.3896(3) | 0.4408(2) | 0.31756(13) | 0.0201(7) |
| H4A | 0.420683 | 0.372389 | 0.330076 | 0.024 |
| H4B | 0.373843 | 0.466169 | 0.351372 | 0.024 |
| C5 | 0.4639(3) | 0.5955(2) | 0.27177(14) | 0.0212(7) |
| H5A | 0.460169 | 0.613497 | 0.308119 | 0.025 |
| H5B | 0.534323 | 0.620531 | 0.250701 | 0.025 |
| C6 | 0.1432(3) | 0.3657(3) | 0.38207(15) | 0.0268(7) |
| C7 | 0.0318(4) | 0.4110(3) | 0.39982(16) | 0.0361(9) |
| H7 | -0.029971 | 0.445047 | 0.373035 | 0.043 |
| C8 | 0.0109(4) | 0.4066(4) | 0.45607(17) | 0.0467(11) |
| H8 | -0.065336 | 0.436914 | 0.467883 | 0.056 |
| C9 | 0.1018(4) | 0.3576(4) | 0.49525(17) | 0.0430(10) |
| H9 | 0.088429 | 0.356058 | 0.533778 | 0.052 |
| C10 | 0.2120(4) | 0.3110(4) | 0.47840(17) | 0.0443(11) |
| H10 | 0.272861 | 0.275821 | 0.505353 | 0.053 |
| C11 | 0.2326(3) | 0.3162(3) | 0.42175(16) | 0.0348(9) |
| H11 | 0.308796 | 0.285549 | 0.410059 | 0.042 |
| C12 | 0.2543(3) | 0.2612(3) | 0.30315(15) | 0.0264(7) |
| C13 | 0.3393(3) | 0.2551(3) | 0.25996(16) | 0.0313(8) |
| H13 | 0.359101 | 0.310734 | 0.235668 | 0.038 |
| C14 | 0.3945(4) | 0.1674(3) | 0.2528(2) | 0.0438(10) |
| H14 | 0.452133 | 0.162730 | 0.223489 | 0.053 |
| C15 | 0.3654(5) | 0.0863(3) | 0.2885(2) | 0.0529(12) |
| H15 | 0.404338 | 0.026103 | 0.284125 | 0.063 |
| C16 | 0.2794(5) | 0.0933(3) | 0.3305(2) | 0.0508(11) |
| H16 | 0.258612 | 0.037679 | 0.354463 | 0.061 |
| C17 | 0.2243(4) | 0.1795(3) | 0.33775(18) | 0.0381(9) |
| H17 | 0.165180 | 0.183489 | 0.366589 | 0.046 |
| C18 | 0.0487(3) | 0.4140(3) | 0.26348(14) | 0.0249(7) |
| C19 | -0.0311(3) | 0.4988(3) | 0.26265(15) | 0.0267(7) |
| H19 | -0.023906 | 0.532602 | 0.290377 | 0.032 |
| C20 | -0.1213(3) | 0.5333(3) | 0.22081(16) | 0.0315(8) |
| H20 | -0.177527 | 0.589899 | 0.220451 | 0.038 |
| C21 | -0.1285(3) | 0.4846(3) | 0.17973(16) | 0.0356(9) |
| H21 | -0.188647 | 0.509471 | 0.150713 | 0.043 |
| C22 | -0.0507(3) | 0.4011(3) | 0.18000(16) | 0.0359(9) |
| H22 | -0.057103 | 0.368597 | 0.151579 | 0.043 |
| C23 | 0.0375(3) | 0.3651(3) | 0.22236(15) | 0.0292(8) |
| H23 | 0.090452 | 0.306837 | 0.223377 | 0.035 |
| C24 | 0.2358(3) | 0.7522(3) | 0.31340(15) | 0.0271(7) |
| C25 | 0.2062(3) | 0.6711(3) | 0.34934(16) | 0.0302(8) |
| H25 | 0.217787 | 0.613373 | 0.337866 | 0.036 |
| C26 | 0.1597(4) | 0.6751(3) | 0.40206(17) | 0.0393(9) |
| H26 | 0.140167 | 0.619931 | 0.427035 | 0.047 |
| C27 | 0.1422(4) | 0.7591(4) | 0.41789(19) | 0.0474(11) |
| H27 | 0.109949 | 0.761712 | 0.453898 | 0.057 |
| C28 | 0.1706(5) | 0.8394(4) | 0.3826(2) | 0.0561(13) |
| H28 | 0.157590 | 0.896960 | 0.394213 | 0.067 |
| C29 | 0.2182(4) | 0.8365(3) | 0.32994(19) | 0.0450(11) |
| H29 | 0.238591 | 0.891854 | 0.305482 | 0.054 |
| C30 | 0.1520(3) | 0.7761(3) | 0.19890(16) | 0.0261(7) |
| C31 | 0.1681(3) | 0.7976(3) | 0.14083(16) | 0.0307(8) |
| H31 | 0.247639 | 0.804165 | 0.125349 | 0.037 |
| C32 | 0.0661(4) | 0.8092(3) | 0.10610(19) | 0.0403(10) |
| H32 | 0.075028 | 0.824988 | 0.066593 | 0.048 |
| C33 | -0.0494(4) | 0.7976(3) | 0.1299(2) | 0.0452(10) |
| H33 | -0.119149 | 0.805920 | 0.106134 | 0.054 |
| C34 | -0.0641(3) | 0.7742(3) | 0.1868(2) | 0.0401(10) |
| H34 | -0.143111 | 0.765352 | 0.202198 | 0.048 |
| C35 | 0.0365(3) | 0.7635(3) | 0.22206(18) | 0.0315(8) |
| H35 | 0.026613 | 0.747858 | 0.261516 | 0.038 |
| C36 | 0.3832(3) | 0.8357(3) | 0.22126(15) | 0.0246(7) |
| C37 | 0.3414(4) | 0.9225(3) | 0.18524(17) | 0.0329(8) |
| H37 | 0.258439 | 0.936620 | 0.171694 | 0.039 |
| C38 | 0.4187(4) | 0.9885(3) | 0.1689(2) | 0.0448(10) |
| H38 | 0.389583 | 1.047382 | 0.143936 | 0.054 |
| C39 | 0.5393(4) | 0.9678(3) | 0.1892(2) | 0.0431(10) |
| H39 | 0.593004 | 1.012799 | 0.177825 | 0.052 |
| C40 | 0.5823(4) | 0.8831(3) | 0.22566(19) | 0.0388(9) |
| H40 | 0.665093 | 0.869974 | 0.239347 | 0.047 |
| C41 | 0.5045(3) | 0.8169(3) | 0.24242(17) | 0.0302(8) |
| H41 | 0.533485 | 0.758878 | 0.268205 | 0.036 |
| C42 | 0.5701(3) | 0.5644(3) | 0.09807(13) | 0.0214(7) |
| C43 | 0.5655(3) | 0.6401(3) | 0.12286(15) | 0.0282(8) |
| H43 | 0.508608 | 0.647172 | 0.152121 | 0.034 |
| C44 | 0.6440(4) | 0.7049(3) | 0.10481(17) | 0.0392(10) |
| H44 | 0.642222 | 0.755914 | 0.122160 | 0.047 |
| C45 | 0.7256(4) | 0.6953(3) | 0.06122(17) | 0.0404(10) |
| H45 | 0.778680 | 0.740384 | 0.048498 | 0.049 |
| C46 | 0.7296(3) | 0.6210(3) | 0.03649(15) | 0.0318(8) |
| H46 | 0.785596 | 0.614917 | 0.006750 | 0.038 |
| C47 | 0.6527(3) | 0.5549(3) | 0.05461(14) | 0.0238(7) |
| H47 | 0.656208 | 0.503353 | 0.037566 | 0.029 |
| C48 | 0.5372(3) | 0.3702(2) | 0.11359(14) | 0.0225(7) |
| C49 | 0.6578(3) | 0.3360(3) | 0.13515(16) | 0.0305(8) |
| H49 | 0.698677 | 0.373951 | 0.152163 | 0.037 |
| C50 | 0.7169(3) | 0.2480(3) | 0.13171(18) | 0.0367(9) |
| H50 | 0.798312 | 0.225309 | 0.146493 | 0.044 |
| C51 | 0.6584(4) | 0.1923(3) | 0.10683(18) | 0.0363(9) |
| H51 | 0.699828 | 0.131679 | 0.104250 | 0.044 |
| C52 | 0.5388(4) | 0.2253(3) | 0.08563(19) | 0.0381(9) |
| H52 | 0.498432 | 0.187244 | 0.068514 | 0.046 |
| C53 | 0.4785(3) | 0.3136(3) | 0.08943(16) | 0.0288(8) |
| H53 | 0.396359 | 0.335453 | 0.075381 | 0.035 |
| C54 | 0.3245(3) | 0.5275(2) | 0.08004(13) | 0.0200(6) |
| C55 | 0.3105(3) | 0.6161(2) | 0.04326(14) | 0.0227(7) |
| H55 | 0.377012 | 0.650865 | 0.037645 | 0.027 |
| C56 | 0.1986(3) | 0.6536(3) | 0.01471(15) | 0.0282(8) |
| H56 | 0.188654 | 0.714127 | -0.010287 | 0.034 |
| C57 | 0.1020(3) | 0.6026(3) | 0.02279(15) | 0.0295(8) |
| H57 | 0.025613 | 0.628653 | 0.003537 | 0.035 |
| C58 | 0.1159(3) | 0.5144(3) | 0.05861(15) | 0.0268(7) |
| H58 | 0.049652 | 0.479438 | 0.063256 | 0.032 |
| C59 | 0.2261(3) | 0.4762(3) | 0.08795(14) | 0.0230(7) |
| H59 | 0.234907 | 0.415898 | 0.113139 | 0.028 |
| S1L | 0.13717(11) | 0.19770(10) | 0.07475(7) | 0.0411(4) |
| O1L | 0.1060(5) | 0.2917(3) | 0.08296(19) | 0.0669(14) |
| O2L | 0.2699(4) | 0.1620(4) | 0.0781(2) | 0.088(2) |
| O3L | 0.0810(3) | 0.1869(2) | 0.02478(13) | 0.0414(9) |
| C1L | -0.0418(5) | 0.0204(4) | 0.2239(2) | 0.0331(12) |
| C2L | 0.0462(5) | 0.0737(4) | 0.2314(2) | 0.0344(10) |
| H2L | 0.068548 | 0.074523 | 0.268229 | 0.041 |
| C3L | 0.1020(4) | 0.1260(3) | 0.1858(2) | 0.0308(10) |
| H3L | 0.161997 | 0.162106 | 0.191625 | 0.037 |
| C4L | 0.0705(4) | 0.1255(3) | 0.13191(19) | 0.0262(9) |
| C5L | -0.0149(4) | 0.0703(3) | 0.1241(2) | 0.0279(10) |
| H5L | -0.035460 | 0.067887 | 0.087309 | 0.034 |
| C6L | -0.0703(5) | 0.0188(4) | 0.1699(2) | 0.0308(11) |
| H6L | -0.128933 | -0.018423 | 0.164046 | 0.037 |
| C7L | -0.1072(6) | -0.0356(6) | 0.2750(3) | 0.0485(15) |
| H7L1 | -0.075576 | -0.026136 | 0.309646 | 0.073 |
| H7L2 | -0.196750 | -0.012978 | 0.272123 | 0.073 |
| H7L3 | -0.090478 | -0.102802 | 0.275327 | 0.073 |
| S1K | 0.1530(11) | 0.2009(9) | 0.1068(6) | 0.053(4) |
| O1K | 0.057(2) | 0.2720(19) | 0.0766(16) | 0.070(9) |
| O2K | 0.236(2) | 0.240(2) | 0.1360(11) | 0.061(7) |
| O3K | 0.225(2) | 0.138(2) | 0.0743(12) | 0.048(7) |
| C1K | -0.034(4) | 0.012(3) | 0.2406(14) | 0.030(5) |
| C2K | 0.050(3) | 0.061(2) | 0.2542(13) | 0.033(5) |
| H2K | 0.069085 | 0.056140 | 0.292334 | 0.039 |
| C3K | 0.106(3) | 0.118(2) | 0.2128(11) | 0.031(5) |
| H3K | 0.163080 | 0.153271 | 0.222231 | 0.037 |
| C4K | 0.082(3) | 0.124(2) | 0.1579(10) | 0.029(5) |
| C5K | -0.003(3) | 0.077(3) | 0.1442(12) | 0.028(5) |
| H5K | -0.024489 | 0.083417 | 0.106190 | 0.033 |
| C6K | -0.058(5) | 0.019(3) | 0.1859(13) | 0.032(5) |
| H6K | -0.114547 | -0.016774 | 0.176391 | 0.038 |
| C7K | -0.079(5) | -0.028(5) | 0.272(3) | 0.0485(15) |
| H7K1 | -0.049495 | -0.025054 | 0.308360 | 0.073 |
| H7K2 | -0.168525 | -0.004427 | 0.268538 | 0.073 |
| H7K3 | -0.063654 | -0.094053 | 0.268724 | 0.073 |
| S1E | 0.2077(6) | 0.3213(4) | 0.6541(3) | 0.0359(10) |
| O1E | 0.1972(13) | 0.4126(7) | 0.6174(5) | 0.121(5) |
| O2E | 0.2564(10) | 0.3200(10) | 0.7081(3) | 0.044(3) |
| O3E | 0.0914(6) | 0.2935(10) | 0.6575(4) | 0.092(3) |
| C1E | 0.4848(9) | 0.1225(6) | 0.5773(3) | 0.063(2) |
| C2E | 0.3671(11) | 0.0978(7) | 0.5961(4) | 0.066(3) |
| H2E | 0.345870 | 0.039701 | 0.593017 | 0.079 |
| C3E | 0.2843(9) | 0.1609(6) | 0.6192(3) | 0.050(2) |
| H3E | 0.205676 | 0.145352 | 0.631420 | 0.060 |
| C4E | 0.3134(8) | 0.2451(6) | 0.6246(4) | 0.0392(18) |
| C5E | 0.4279(7) | 0.2707(7) | 0.6062(4) | 0.038(2) |
| H5E | 0.447308 | 0.329319 | 0.609446 | 0.045 |
| C6E | 0.5133(8) | 0.2088(7) | 0.5830(4) | 0.053(2) |
| H6E | 0.591434 | 0.225464 | 0.570907 | 0.064 |
| C7E | 0.5768(13) | 0.0569(9) | 0.5506(4) | 0.096(4) |
| H7E1 | 0.541886 | 0.000446 | 0.550086 | 0.143 |
| H7E2 | 0.593410 | 0.089441 | 0.512159 | 0.143 |
| H7E3 | 0.654189 | 0.038619 | 0.572250 | 0.143 |
| S1F | 0.2071(9) | 0.3490(8) | 0.6521(5) | 0.0348(18) |
| O1F | 0.2224(11) | 0.4360(9) | 0.6120(5) | 0.046(3) |
| O2F | 0.266(2) | 0.340(2) | 0.7048(7) | 0.053(5) |
| O3F | 0.0784(9) | 0.3639(15) | 0.6476(7) | 0.084(5) |
| C1F | 0.409(2) | 0.1057(11) | 0.5872(6) | 0.079(5) |
| C2F | 0.284(2) | 0.1099(11) | 0.6001(7) | 0.087(5) |
| H2F | 0.241118 | 0.061802 | 0.594971 | 0.104 |
| C3F | 0.2198(18) | 0.1867(10) | 0.6209(7) | 0.072(4) |
| H3F | 0.134682 | 0.189975 | 0.630422 | 0.086 |
| C4F | 0.2840(15) | 0.2560(10) | 0.6270(7) | 0.058(4) |
| C5F | 0.4109(16) | 0.2512(13) | 0.6144(9) | 0.065(5) |
| H5F | 0.453009 | 0.299121 | 0.620231 | 0.078 |
| C6F | 0.4766(18) | 0.1765(12) | 0.5934(8) | 0.073(4) |
| H6F | 0.561662 | 0.173677 | 0.583902 | 0.088 |
| C7F | 0.478(3) | 0.0226(15) | 0.5651(9) | 0.146(10) |
| H7F1 | 0.564964 | 0.030167 | 0.558089 | 0.219 |
| H7F2 | 0.474555 | -0.036409 | 0.592858 | 0.219 |
| H7F3 | 0.439196 | 0.021136 | 0.530110 | 0.219 |
| O1G | 0.4952(16) | 0.4690(12) | 0.4514(8) | 0.072(4) |
| C2G | 0.3870(18) | 0.470(3) | 0.4829(11) | 0.057(2) |
| H2G1 | 0.378309 | 0.405060 | 0.502425 | 0.068 |
| H2G2 | 0.314289 | 0.497267 | 0.457841 | 0.068 |
| C3G | 0.391(2) | 0.527(3) | 0.5238(11) | 0.069(4) |
| H3G1 | 0.395065 | 0.592886 | 0.504248 | 0.082 |
| H3G2 | 0.315897 | 0.526061 | 0.546996 | 0.082 |
| O4G | 0.4992(15) | 0.4884(10) | 0.5587(7) | 0.055(3) |
| C5G | 0.5882(19) | 0.524(3) | 0.5207(10) | 0.057(2) |
| H5G1 | 0.666093 | 0.521596 | 0.540750 | 0.068 |
| H5G2 | 0.557386 | 0.590672 | 0.501650 | 0.068 |
| C6G | 0.610(2) | 0.465(3) | 0.4792(11) | 0.075(5) |
| H6G1 | 0.672112 | 0.487948 | 0.451472 | 0.090 |
| H6G2 | 0.642977 | 0.398747 | 0.498430 | 0.090 |
| C1C | 0.8143(8) | 0.2128(7) | 0.3043(5) | 0.086(3) |
| H1C | 0.864583 | 0.215230 | 0.271907 | 0.103 |
| C2C | 0.7011(8) | 0.1844(6) | 0.3070(5) | 0.081(3) |
| H2C | 0.671433 | 0.164641 | 0.276639 | 0.098 |
| C3C | 0.6300(8) | 0.1849(7) | 0.3551(4) | 0.076(2) |
| H3C | 0.550142 | 0.167710 | 0.355953 | 0.092 |
| C4C | 0.6687(9) | 0.2085(7) | 0.4004(4) | 0.086(3) |
| C5C | 0.7813(10) | 0.2398(10) | 0.4007(5) | 0.086(3) |
| H5C | 0.807820 | 0.260530 | 0.431285 | 0.104 |
| C6C | 0.8528(10) | 0.2385(8) | 0.3526(5) | 0.091(3) |
| H6C | 0.932458 | 0.256002 | 0.352044 | 0.110 |
| C7C | 0.5873(15) | 0.2097(15) | 0.4518(6) | 0.171(7) |
| H7C1 | 0.631669 | 0.228499 | 0.480130 | 0.257 |
| H7C2 | 0.510569 | 0.254655 | 0.441195 | 0.257 |
| H7C3 | 0.567401 | 0.146566 | 0.467243 | 0.257 |
| C1B | 0.778(2) | 0.2110(15) | 0.3568(9) | 0.095(4) |
| C2B | 0.794(2) | 0.2406(19) | 0.4034(10) | 0.103(6) |
| H2B | 0.869859 | 0.259694 | 0.410219 | 0.124 |
| C3B | 0.701(2) | 0.2419(17) | 0.4394(9) | 0.093(5) |
| H3B1 | 0.706984 | 0.261069 | 0.473215 | 0.112 |
| C4B | 0.598(2) | 0.215(2) | 0.4257(11) | 0.102(5) |
| H4B1 | 0.529931 | 0.219279 | 0.450358 | 0.122 |
| C5B | 0.582(2) | 0.1823(18) | 0.3807(10) | 0.095(5) |
| H5B1 | 0.507093 | 0.161693 | 0.374443 | 0.114 |
| C6B | 0.678(2) | 0.180(2) | 0.3448(11) | 0.100(5) |
| H6B | 0.673365 | 0.157654 | 0.312007 | 0.120 |
| C7B | 0.869(3) | 0.213(3) | 0.3252(16) | 0.128(10) |
| H7B1 | 0.933487 | 0.237780 | 0.341201 | 0.192 |
| H7B2 | 0.902045 | 0.148963 | 0.321385 | 0.192 |
| H7B3 | 0.844452 | 0.253542 | 0.288332 | 0.192 |
| O1I | -0.0546(12) | -0.0189(9) | 0.5531(6) | 0.062(3) |
| C1I | 0.0601(16) | 0.0258(16) | 0.5460(7) | 0.065(4) |
| H1I1 | 0.134003 | -0.021762 | 0.559995 | 0.078 |
| H1I2 | 0.052606 | 0.076106 | 0.566697 | 0.078 |
| C2I | 0.0705(18) | 0.0668(15) | 0.4835(8) | 0.062(4) |
| H2I1 | -0.003783 | 0.114021 | 0.469593 | 0.075 |
| H2I2 | 0.144483 | 0.097802 | 0.475676 | 0.075 |
| O2I | 0.0811(16) | -0.0126(12) | 0.4561(8) | 0.108(6) |
| C3I | -0.057(2) | -0.0043(18) | 0.4531(7) | 0.081(5) |
| H3I1 | -0.080406 | -0.030797 | 0.422459 | 0.097 |
| H3I2 | -0.096600 | 0.062718 | 0.446103 | 0.097 |
| C4I | -0.097(2) | -0.0586(15) | 0.5086(8) | 0.072(5) |
| H4I1 | -0.188858 | -0.052887 | 0.509435 | 0.086 |
| H4I2 | -0.061170 | -0.126155 | 0.514612 | 0.086 |
| C1O | 0.5017(17) | 0.4338(14) | 0.5284(9) | 0.057(5) |
| H1O | 0.564597 | 0.456260 | 0.503928 | 0.068 |
| C2O | 0.5247(17) | 0.3460(14) | 0.5634(8) | 0.064(6) |
| H2O | 0.602757 | 0.306864 | 0.562693 | 0.076 |
| C3O | 0.4351(17) | 0.3146(13) | 0.5997(9) | 0.051(4) |
| H3O | 0.451610 | 0.253983 | 0.624539 | 0.061 |
| C4O | 0.3216(17) | 0.3702(14) | 0.6003(8) | 0.053(5) |
| H4O | 0.259004 | 0.347951 | 0.625000 | 0.064 |
| C5O | 0.2990(17) | 0.4581(14) | 0.5650(9) | 0.055(5) |
| H5O | 0.221291 | 0.497530 | 0.565927 | 0.066 |
| C6O | 0.3881(19) | 0.4895(13) | 0.5283(10) | 0.051(4) |
| H6O | 0.371201 | 0.549630 | 0.502979 | 0.061 |
| O1N | 0.387(3) | -0.032(2) | -0.0227(17) | 0.078(5) |
| C1N | 0.409(3) | -0.066(3) | 0.0352(17) | 0.096(6) |
| H1NA | 0.393791 | -0.131631 | 0.047871 | 0.115 |
| H1NB | 0.353407 | -0.026124 | 0.056113 | 0.115 |
| C2N | 0.551(3) | -0.060(3) | 0.0446(17) | 0.085(7) |
| H2NA | 0.567547 | -0.075369 | 0.085358 | 0.101 |
| H2NB | 0.603579 | -0.109499 | 0.029334 | 0.101 |
| O2N | 0.595(3) | 0.033(2) | 0.0189(12) | 0.060(5) |
| C3N | 0.5519(17) | 0.0643(19) | -0.0365(11) | 0.041(4) |
| H3NA | 0.599533 | 0.024240 | -0.059553 | 0.049 |
| H3NB | 0.565453 | 0.129889 | -0.051754 | 0.049 |
| C4N | 0.4098(17) | 0.0597(19) | -0.0403(11) | 0.041(4) |
| H4NA | 0.362403 | 0.098869 | -0.016761 | 0.050 |
| H4NB | 0.380789 | 0.086068 | -0.079483 | 0.050 |
| O1P | 0.4651(19) | 0.0312(15) | 0.0172(9) | 0.106(4) |
| C1P | 0.351(2) | 0.0628(17) | -0.0122(12) | 0.108(5) |
| H1PA | 0.363635 | 0.068155 | -0.052798 | 0.130 |
| H1PB | 0.311907 | 0.125003 | -0.006337 | 0.130 |
| C2P | 0.268(2) | -0.0148(16) | 0.0129(14) | 0.105(5) |
| H2PA | 0.238429 | -0.004447 | 0.049792 | 0.126 |
| H2PB | 0.193332 | -0.000554 | -0.011504 | 0.126 |
| O2P | 0.3159(13) | -0.1195(11) | 0.0214(7) | 0.084(4) |
| C3P | 0.4397(17) | -0.1330(15) | 0.0291(11) | 0.095(5) |
| H3PA | 0.475424 | -0.189409 | 0.015340 | 0.114 |
| H3PB | 0.455078 | -0.149264 | 0.069967 | 0.114 |
| C4P | 0.516(2) | -0.0539(18) | 0.0026(13) | 0.090(4) |
| H4PA | 0.602966 | -0.073447 | 0.015920 | 0.108 |
| H4PB | 0.515858 | -0.044067 | -0.038654 | 0.108 |
| O1' | 0.1247(6) | 0.0152(5) | -0.0085(3) | 0.081(2) |
| H1 | 0.127(11) | 0.077(4) | 0.000(5) | 0.121 |
| H2 | 0.206(5) | -0.026(7) | -0.006(5) | 0.121 |
| O2' | 0.292(2) | 0.0375(18) | -0.0877(10) | 0.143(10) |
| H1' | 0.32(4) | -0.015(14) | -0.106(12) | 0.214 |
| H2' | 0.26(4) | 0.02(2) | -0.050(8) | 0.214 |

## Table 3. Bond lengths and angles for p-1.cif.

|  |  |
| --- | --- |
| **Atom - Atom** | **Length [Å]** |
| N1 - C3 | 1.493(4) |
| N1 - P2 | 1.606(3) |
| N1 - Sn1 | 2.186(3) |
| N2 - C4 | 1.493(4) |
| N2 - P3 | 1.615(3) |
| N2 - Sn1 | 2.189(3) |
| N3 - C5 | 1.484(4) |
| N3 - P4 | 1.616(3) |
| N3 - Sn1 | 2.189(3) |
| P2 - C54 | 1.796(3) |
| P2 - C42 | 1.799(3) |
| P2 - C48 | 1.808(3) |
| P3 - C18 | 1.794(3) |
| P3 - C6 | 1.804(4) |
| P3 - C12 | 1.812(4) |
| P4 - C30 | 1.788(3) |
| P4 - C24 | 1.805(4) |
| P4 - C36 | 1.805(3) |
| C1 - C2 | 1.546(4) |
| C1 - H1A | 0.9800 |
| C1 - H1B | 0.9800 |
| C1 - H1D | 0.9800 |
| C2 - C5 | 1.528(5) |
| C2 - C4 | 1.531(4) |
| C2 - C3 | 1.538(4) |
| C3 - H3A | 0.9900 |
| C3 - H3B | 0.9900 |
| C4 - H4A | 0.9900 |
| C4 - H4B | 0.9900 |
| C5 - H5A | 0.9900 |
| C5 - H5B | 0.9900 |
| C6 - C11 | 1.389(5) |
| C6 - C7 | 1.398(5) |
| C7 - C8 | 1.384(6) |
| C7 - H7 | 0.9500 |
| C8 - C9 | 1.390(6) |
| C8 - H8 | 0.9500 |
| C9 - C10 | 1.387(7) |
| C9 - H9 | 0.9500 |
| C10 - C11 | 1.391(6) |
| C10 - H10 | 0.9500 |
| C11 - H11 | 0.9500 |
| C12 - C17 | 1.387(5) |
| C12 - C13 | 1.399(5) |
| C13 - C14 | 1.386(6) |
| C13 - H13 | 0.9500 |
| C14 - C15 | 1.387(7) |
| C14 - H14 | 0.9500 |
| C15 - C16 | 1.385(7) |
| C15 - H15 | 0.9500 |
| C16 - C17 | 1.366(6) |
| C16 - H16 | 0.9500 |
| C17 - H17 | 0.9500 |
| C18 - C23 | 1.397(5) |
| C18 - C19 | 1.400(5) |
| C19 - C20 | 1.394(5) |
| C19 - H19 | 0.9500 |
| C20 - C21 | 1.386(6) |
| C20 - H20 | 0.9500 |
| C21 - C22 | 1.377(6) |
| C21 - H21 | 0.9500 |
| C22 - C23 | 1.390(5) |
| C22 - H22 | 0.9500 |
| C23 - H23 | 0.9500 |
| C24 - C29 | 1.386(6) |
| C24 - C25 | 1.393(5) |
| C25 - C26 | 1.389(5) |
| C25 - H25 | 0.9500 |
| C26 - C27 | 1.373(6) |
| C26 - H26 | 0.9500 |
| C27 - C28 | 1.371(7) |
| C27 - H27 | 0.9500 |
| C28 - C29 | 1.388(6) |
| C28 - H28 | 0.9500 |
| C29 - H29 | 0.9500 |
| C30 - C35 | 1.394(5) |
| C30 - C31 | 1.400(5) |
| C31 - C32 | 1.392(5) |
| C31 - H31 | 0.9500 |
| C32 - C33 | 1.397(7) |
| C32 - H32 | 0.9500 |
| C33 - C34 | 1.373(7) |
| C33 - H33 | 0.9500 |
| C34 - C35 | 1.389(5) |
| C34 - H34 | 0.9500 |
| C35 - H35 | 0.9500 |
| C36 - C37 | 1.390(5) |
| C36 - C41 | 1.402(5) |
| C37 - C38 | 1.382(6) |
| C37 - H37 | 0.9500 |
| C38 - C39 | 1.387(6) |
| C38 - H38 | 0.9500 |
| C39 - C40 | 1.375(6) |
| C39 - H39 | 0.9500 |
| C40 - C41 | 1.389(5) |
| C40 - H40 | 0.9500 |
| C41 - H41 | 0.9500 |
| C42 - C43 | 1.392(5) |
| C42 - C47 | 1.395(4) |
| C43 - C44 | 1.383(5) |
| C43 - H43 | 0.9500 |
| C44 - C45 | 1.391(6) |
| C44 - H44 | 0.9500 |
| C45 - C46 | 1.374(6) |
| C45 - H45 | 0.9500 |
| C46 - C47 | 1.385(5) |
| C46 - H46 | 0.9500 |
| C47 - H47 | 0.9500 |
| C48 - C53 | 1.385(5) |
| C48 - C49 | 1.405(5) |
| C49 - C50 | 1.374(5) |
| C49 - H49 | 0.9500 |
| C50 - C51 | 1.384(6) |
| C50 - H50 | 0.9500 |
| C51 - C52 | 1.391(6) |
| C51 - H51 | 0.9500 |
| C52 - C53 | 1.384(5) |
| C52 - H52 | 0.9500 |
| C53 - H53 | 0.9500 |
| C54 - C55 | 1.393(5) |
| C54 - C59 | 1.404(5) |
| C55 - C56 | 1.394(5) |
| C55 - H55 | 0.9500 |
| C56 - C57 | 1.385(5) |
| C56 - H56 | 0.9500 |
| C57 - C58 | 1.379(6) |
| C57 - H57 | 0.9500 |
| C58 - C59 | 1.389(5) |
| C58 - H58 | 0.9500 |
| C59 - H59 | 0.9500 |
| S1L - O1L | 1.438(5) |
| S1L - O3L | 1.447(4) |
| S1L - O2L | 1.458(4) |
| S1L - C4L | 1.772(4) |
| C1L - C6L | 1.382(6) |
| C1L - C2L | 1.389(6) |
| C1L - C7L | 1.558(9) |
| C2L - C3L | 1.392(6) |
| C2L - H2L | 0.9500 |
| C3L - C4L | 1.383(6) |
| C3L - H3L | 0.9500 |
| C4L - C5L | 1.389(5) |
| C5L - C6L | 1.387(6) |
| C5L - H5L | 0.9500 |
| C6L - H6L | 0.9500 |
| C7L - H7L1 | 0.9800 |
| C7L - H7L2 | 0.9800 |
| C7L - H7L3 | 0.9800 |
| S1K - O1K | 1.438(14) |
| S1K - O2K | 1.451(14) |
| S1K - O3K | 1.476(14) |
| S1K - C4K | 1.740(16) |
| C1K - C7K | 1.03(8) |
| C1K - C6K | 1.36(2) |
| C1K - C2K | 1.36(2) |
| C2K - C3K | 1.36(2) |
| C2K - H2K | 0.9500 |
| C3K - C4K | 1.36(2) |
| C3K - H3K | 0.9500 |
| C4K - C5K | 1.36(2) |
| C5K - C6K | 1.36(2) |
| C5K - H5K | 0.9500 |
| C6K - H6K | 0.9500 |
| C7K - H7K1 | 0.9800 |
| C7K - H7K2 | 0.9800 |
| C7K - H7K3 | 0.9800 |
| S1E - O3E | 1.400(7) |
| S1E - O1E | 1.425(8) |
| S1E - O2E | 1.443(7) |
| S1E - C4E | 1.740(8) |
| C1E - C6E | 1.407(10) |
| C1E - C2E | 1.433(10) |
| C1E - C7E | 1.523(12) |
| C2E - C3E | 1.396(10) |
| C2E - H2E | 0.9500 |
| C3E - C4E | 1.377(9) |
| C3E - H3E | 0.9500 |
| C4E - C5E | 1.402(8) |
| C5E - C6E | 1.402(9) |
| C5E - H5E | 0.9500 |
| C6E - H6E | 0.9500 |
| C7E - H7E1 | 0.9800 |
| C7E - H7E2 | 0.9800 |
| C7E - H7E3 | 0.9800 |
| S1F - O3F | 1.394(10) |
| S1F - O2F | 1.433(11) |
| S1F - O1F | 1.455(11) |
| S1F - C4F | 1.721(11) |
| C1F - C2F | 1.397(13) |
| C1F - C6F | 1.418(13) |
| C1F - C7F | 1.535(18) |
| C2F - C3F | 1.425(13) |
| C2F - H2F | 0.9500 |
| C3F - C4F | 1.379(12) |
| C3F - H3F | 0.9500 |
| C4F - C5F | 1.408(12) |
| C5F - C6F | 1.410(13) |
| C5F - H5F | 0.9500 |
| C6F - H6F | 0.9500 |
| C7F - H7F1 | 0.9800 |
| C7F - H7F2 | 0.9800 |
| C7F - H7F3 | 0.9800 |
| O1G - C2G | 1.394(15) |
| O1G - C6G | 1.440(16) |
| C2G - C3G | 1.463(15) |
| C2G - H2G1 | 0.9900 |
| C2G - H2G2 | 0.9900 |
| C3G - O4G | 1.435(15) |
| C3G - H3G1 | 0.9900 |
| C3G - H3G2 | 0.9900 |
| O4G - C5G | 1.409(15) |
| C5G - C6G | 1.491(15) |
| C5G - H5G1 | 0.9900 |
| C5G - H5G2 | 0.9900 |
| C6G - H6G1 | 0.9900 |
| C6G - H6G2 | 0.9900 |
| C1C - C2C | 1.371(10) |
| C1C - C6C | 1.430(10) |
| C1C - H1C | 0.9500 |
| C2C - C3C | 1.396(10) |
| C2C - H2C | 0.9500 |
| C3C - C4C | 1.346(11) |
| C3C - H3C | 0.9500 |
| C4C - C5C | 1.391(11) |
| C4C - C7C | 1.525(13) |
| C5C - C6C | 1.399(11) |
| C5C - H5C | 0.9500 |
| C6C - H6C | 0.9500 |
| C7C - H7C1 | 0.9800 |
| C7C - H7C2 | 0.9800 |
| C7C - H7C3 | 0.9800 |
| C1B - C7B | 1.25(4) |
| C1B - C6B | 1.322(17) |
| C1B - C2B | 1.351(18) |
| C2B - C3B | 1.333(17) |
| C2B - H2B | 0.9500 |
| C3B - C4B | 1.335(17) |
| C3B - H3B1 | 0.9500 |
| C4B - C5B | 1.337(17) |
| C4B - H4B1 | 0.9500 |
| C5B - C6B | 1.352(17) |
| C5B - H5B1 | 0.9500 |
| C6B - H6B | 0.9500 |
| C7B - H7B1 | 0.9800 |
| C7B - H7B2 | 0.9800 |
| C7B - H7B3 | 0.9800 |
| O1I - C4I | 1.483(15) |
| O1I - C1I | 1.505(15) |
| C1I - C2I | 1.519(15) |
| C1I - H1I1 | 0.9900 |
| C1I - H1I2 | 0.9900 |
| C2I - O2I | 1.477(17) |
| C2I - H2I1 | 0.9900 |
| C2I - H2I2 | 0.9900 |
| O2I - C3I | 1.498(17) |
| C3I - C4I | 1.507(15) |
| C3I - H3I1 | 0.9900 |
| C3I - H3I2 | 0.9900 |
| C4I - H4I1 | 0.9900 |
| C4I - H4I2 | 0.9900 |
| C1O - C2O | 1.367(16) |
| C1O - C6O | 1.371(16) |
| C1O - H1O | 0.9500 |
| C2O - C3O | 1.370(16) |
| C2O - H2O | 0.9500 |
| C3O - C4O | 1.372(16) |
| C3O - H3O | 0.9500 |
| C4O - C5O | 1.371(16) |
| C4O - H4O | 0.9500 |
| C5O - C6O | 1.371(16) |
| C5O - H5O | 0.9500 |
| C6O - H6O | 0.9500 |
| O1N - C4N | 1.394(18) |
| O1N - C1N | 1.405(18) |
| C1N - C2N | 1.61(2) |
| C1N - H1NA | 0.9900 |
| C1N - H1NB | 0.9900 |
| C2N - O2N | 1.52(3) |
| C2N - H2NA | 0.9900 |
| C2N - H2NB | 0.9900 |
| O2N - C3N | 1.402(16) |
| C3N - C4N | 1.58(2) |
| C3N - H3NA | 0.9900 |
| C3N - H3NB | 0.9900 |
| C4N - H4NA | 0.9900 |
| C4N - H4NB | 0.9900 |
| O1P - C1P | 1.414(18) |
| O1P - C4P | 1.411(16) |
| C1P - C2P | 1.59(2) |
| C1P - H1PA | 0.9900 |
| C1P - H1PB | 0.9900 |
| C2P - O2P | 1.52(3) |
| C2P - H2PA | 0.9900 |
| C2P - H2PB | 0.9900 |
| O2P - C3P | 1.350(16) |
| C3P - C4P | 1.56(2) |
| C3P - H3PA | 0.9900 |
| C3P - H3PB | 0.9900 |
| C4P - H4PA | 0.9900 |
| C4P - H4PB | 0.9900 |
| O1' - H1 | 0.99(2) |
| O1' - H2 | 0.99(2) |
| O2' - H1' | 0.98(2) |
| O2' - H2' | 0.98(2) |
|  |  |
| **Atom - Atom - Atom** | **Angle [°]** |
| C3 - N1 - P2 | 117.6(2) |
| C3 - N1 - Sn1 | 119.10(19) |
| P2 - N1 - Sn1 | 121.80(14) |
| C4 - N2 - P3 | 116.2(2) |
| C4 - N2 - Sn1 | 119.97(19) |
| P3 - N2 - Sn1 | 122.42(14) |
| C5 - N3 - P4 | 119.7(2) |
| C5 - N3 - Sn1 | 119.3(2) |
| P4 - N3 - Sn1 | 119.49(14) |
| N1 - P2 - C54 | 106.38(14) |
| N1 - P2 - C42 | 111.08(15) |
| C54 - P2 - C42 | 107.81(15) |
| N1 - P2 - C48 | 112.89(15) |
| C54 - P2 - C48 | 111.81(15) |
| C42 - P2 - C48 | 106.80(16) |
| N2 - P3 - C18 | 105.20(15) |
| N2 - P3 - C6 | 112.94(15) |
| C18 - P3 - C6 | 113.48(16) |
| N2 - P3 - C12 | 111.77(15) |
| C18 - P3 - C12 | 107.96(17) |
| C6 - P3 - C12 | 105.53(18) |
| N3 - P4 - C30 | 105.29(15) |
| N3 - P4 - C24 | 111.66(16) |
| C30 - P4 - C24 | 108.40(16) |
| N3 - P4 - C36 | 115.40(15) |
| C30 - P4 - C36 | 109.30(17) |
| C24 - P4 - C36 | 106.62(16) |
| N1 - Sn1 - N3 | 84.89(10) |
| N1 - Sn1 - N2 | 84.17(10) |
| N3 - Sn1 - N2 | 85.93(10) |
| C2 - C1 - H1A | 109.5 |
| C2 - C1 - H1B | 109.5 |
| H1A - C1 - H1B | 109.5 |
| C2 - C1 - H1D | 109.5 |
| H1A - C1 - H1D | 109.5 |
| H1B - C1 - H1D | 109.5 |
| C5 - C2 - C4 | 113.4(3) |
| C5 - C2 - C3 | 112.9(3) |
| C4 - C2 - C3 | 112.2(3) |
| C5 - C2 - C1 | 106.0(3) |
| C4 - C2 - C1 | 106.1(3) |
| C3 - C2 - C1 | 105.5(3) |
| N1 - C3 - C2 | 114.9(3) |
| N1 - C3 - H3A | 108.5 |
| C2 - C3 - H3A | 108.5 |
| N1 - C3 - H3B | 108.5 |
| C2 - C3 - H3B | 108.5 |
| H3A - C3 - H3B | 107.5 |
| N2 - C4 - C2 | 113.7(3) |
| N2 - C4 - H4A | 108.8 |
| C2 - C4 - H4A | 108.8 |
| N2 - C4 - H4B | 108.8 |
| C2 - C4 - H4B | 108.8 |
| H4A - C4 - H4B | 107.7 |
| N3 - C5 - C2 | 115.2(3) |
| N3 - C5 - H5A | 108.5 |
| C2 - C5 - H5A | 108.5 |
| N3 - C5 - H5B | 108.5 |
| C2 - C5 - H5B | 108.5 |
| H5A - C5 - H5B | 107.5 |
| C11 - C6 - C7 | 119.0(3) |
| C11 - C6 - P3 | 118.2(3) |
| C7 - C6 - P3 | 122.5(3) |
| C8 - C7 - C6 | 120.5(4) |
| C8 - C7 - H7 | 119.7 |
| C6 - C7 - H7 | 119.7 |
| C7 - C8 - C9 | 119.8(4) |
| C7 - C8 - H8 | 120.1 |
| C9 - C8 - H8 | 120.1 |
| C10 - C9 - C8 | 120.4(4) |
| C10 - C9 - H9 | 119.8 |
| C8 - C9 - H9 | 119.8 |
| C9 - C10 - C11 | 119.5(4) |
| C9 - C10 - H10 | 120.3 |
| C11 - C10 - H10 | 120.3 |
| C6 - C11 - C10 | 120.8(4) |
| C6 - C11 - H11 | 119.6 |
| C10 - C11 - H11 | 119.6 |
| C17 - C12 - C13 | 119.7(4) |
| C17 - C12 - P3 | 122.5(3) |
| C13 - C12 - P3 | 117.7(3) |
| C14 - C13 - C12 | 119.6(4) |
| C14 - C13 - H13 | 120.2 |
| C12 - C13 - H13 | 120.2 |
| C13 - C14 - C15 | 119.9(4) |
| C13 - C14 - H14 | 120.0 |
| C15 - C14 - H14 | 120.0 |
| C16 - C15 - C14 | 119.9(4) |
| C16 - C15 - H15 | 120.0 |
| C14 - C15 - H15 | 120.0 |
| C17 - C16 - C15 | 120.6(4) |
| C17 - C16 - H16 | 119.7 |
| C15 - C16 - H16 | 119.7 |
| C16 - C17 - C12 | 120.2(4) |
| C16 - C17 - H17 | 119.9 |
| C12 - C17 - H17 | 119.9 |
| C23 - C18 - C19 | 119.7(3) |
| C23 - C18 - P3 | 118.9(3) |
| C19 - C18 - P3 | 120.5(3) |
| C20 - C19 - C18 | 119.5(3) |
| C20 - C19 - H19 | 120.3 |
| C18 - C19 - H19 | 120.3 |
| C21 - C20 - C19 | 119.6(4) |
| C21 - C20 - H20 | 120.2 |
| C19 - C20 - H20 | 120.2 |
| C22 - C21 - C20 | 121.6(4) |
| C22 - C21 - H21 | 119.2 |
| C20 - C21 - H21 | 119.2 |
| C21 - C22 - C23 | 119.1(4) |
| C21 - C22 - H22 | 120.4 |
| C23 - C22 - H22 | 120.4 |
| C22 - C23 - C18 | 120.4(4) |
| C22 - C23 - H23 | 119.8 |
| C18 - C23 - H23 | 119.8 |
| C29 - C24 - C25 | 120.3(3) |
| C29 - C24 - P4 | 120.9(3) |
| C25 - C24 - P4 | 118.7(3) |
| C26 - C25 - C24 | 119.6(4) |
| C26 - C25 - H25 | 120.2 |
| C24 - C25 - H25 | 120.2 |
| C27 - C26 - C25 | 119.6(4) |
| C27 - C26 - H26 | 120.2 |
| C25 - C26 - H26 | 120.2 |
| C28 - C27 - C26 | 121.1(4) |
| C28 - C27 - H27 | 119.4 |
| C26 - C27 - H27 | 119.4 |
| C27 - C28 - C29 | 120.1(4) |
| C27 - C28 - H28 | 120.0 |
| C29 - C28 - H28 | 120.0 |
| C24 - C29 - C28 | 119.3(4) |
| C24 - C29 - H29 | 120.3 |
| C28 - C29 - H29 | 120.3 |
| C35 - C30 - C31 | 120.9(3) |
| C35 - C30 - P4 | 119.6(3) |
| C31 - C30 - P4 | 118.9(3) |
| C32 - C31 - C30 | 119.1(4) |
| C32 - C31 - H31 | 120.4 |
| C30 - C31 - H31 | 120.4 |
| C31 - C32 - C33 | 119.4(4) |
| C31 - C32 - H32 | 120.3 |
| C33 - C32 - H32 | 120.3 |
| C34 - C33 - C32 | 121.2(4) |
| C34 - C33 - H33 | 119.4 |
| C32 - C33 - H33 | 119.4 |
| C33 - C34 - C35 | 120.0(4) |
| C33 - C34 - H34 | 120.0 |
| C35 - C34 - H34 | 120.0 |
| C34 - C35 - C30 | 119.3(4) |
| C34 - C35 - H35 | 120.3 |
| C30 - C35 - H35 | 120.3 |
| C37 - C36 - C41 | 119.0(3) |
| C37 - C36 - P4 | 122.4(3) |
| C41 - C36 - P4 | 118.6(3) |
| C38 - C37 - C36 | 120.9(4) |
| C38 - C37 - H37 | 119.5 |
| C36 - C37 - H37 | 119.5 |
| C37 - C38 - C39 | 119.3(4) |
| C37 - C38 - H38 | 120.4 |
| C39 - C38 - H38 | 120.4 |
| C40 - C39 - C38 | 120.9(4) |
| C40 - C39 - H39 | 119.5 |
| C38 - C39 - H39 | 119.5 |
| C39 - C40 - C41 | 119.9(4) |
| C39 - C40 - H40 | 120.1 |
| C41 - C40 - H40 | 120.1 |
| C40 - C41 - C36 | 119.9(4) |
| C40 - C41 - H41 | 120.0 |
| C36 - C41 - H41 | 120.0 |
| C43 - C42 - C47 | 119.9(3) |
| C43 - C42 - P2 | 117.7(2) |
| C47 - C42 - P2 | 122.4(3) |
| C44 - C43 - C42 | 119.9(3) |
| C44 - C43 - H43 | 120.1 |
| C42 - C43 - H43 | 120.1 |
| C43 - C44 - C45 | 119.9(4) |
| C43 - C44 - H44 | 120.0 |
| C45 - C44 - H44 | 120.0 |
| C46 - C45 - C44 | 120.2(4) |
| C46 - C45 - H45 | 119.9 |
| C44 - C45 - H45 | 119.9 |
| C45 - C46 - C47 | 120.5(3) |
| C45 - C46 - H46 | 119.8 |
| C47 - C46 - H46 | 119.8 |
| C46 - C47 - C42 | 119.6(3) |
| C46 - C47 - H47 | 120.2 |
| C42 - C47 - H47 | 120.2 |
| C53 - C48 - C49 | 119.1(3) |
| C53 - C48 - P2 | 122.9(3) |
| C49 - C48 - P2 | 118.0(3) |
| C50 - C49 - C48 | 120.3(4) |
| C50 - C49 - H49 | 119.9 |
| C48 - C49 - H49 | 119.9 |
| C49 - C50 - C51 | 120.4(4) |
| C49 - C50 - H50 | 119.8 |
| C51 - C50 - H50 | 119.8 |
| C50 - C51 - C52 | 119.7(4) |
| C50 - C51 - H51 | 120.1 |
| C52 - C51 - H51 | 120.1 |
| C53 - C52 - C51 | 120.1(4) |
| C53 - C52 - H52 | 119.9 |
| C51 - C52 - H52 | 119.9 |
| C52 - C53 - C48 | 120.4(3) |
| C52 - C53 - H53 | 119.8 |
| C48 - C53 - H53 | 119.8 |
| C55 - C54 - C59 | 119.9(3) |
| C55 - C54 - P2 | 119.7(2) |
| C59 - C54 - P2 | 120.2(3) |
| C54 - C55 - C56 | 119.8(3) |
| C54 - C55 - H55 | 120.1 |
| C56 - C55 - H55 | 120.1 |
| C57 - C56 - C55 | 120.0(4) |
| C57 - C56 - H56 | 120.0 |
| C55 - C56 - H56 | 120.0 |
| C58 - C57 - C56 | 120.4(3) |
| C58 - C57 - H57 | 119.8 |
| C56 - C57 - H57 | 119.8 |
| C57 - C58 - C59 | 120.5(3) |
| C57 - C58 - H58 | 119.8 |
| C59 - C58 - H58 | 119.8 |
| C58 - C59 - C54 | 119.4(3) |
| C58 - C59 - H59 | 120.3 |
| C54 - C59 - H59 | 120.3 |
| O1L - S1L - O3L | 112.8(2) |
| O1L - S1L - O2L | 113.4(4) |
| O3L - S1L - O2L | 112.4(3) |
| O1L - S1L - C4L | 105.4(2) |
| O3L - S1L - C4L | 106.2(2) |
| O2L - S1L - C4L | 106.0(2) |
| C6L - C1L - C2L | 118.2(4) |
| C6L - C1L - C7L | 120.9(4) |
| C2L - C1L - C7L | 120.9(5) |
| C1L - C2L - C3L | 121.0(4) |
| C1L - C2L - H2L | 119.5 |
| C3L - C2L - H2L | 119.5 |
| C4L - C3L - C2L | 120.2(4) |
| C4L - C3L - H3L | 119.9 |
| C2L - C3L - H3L | 119.9 |
| C3L - C4L - C5L | 119.2(4) |
| C3L - C4L - S1L | 119.0(3) |
| C5L - C4L - S1L | 121.8(3) |
| C6L - C5L - C4L | 120.0(4) |
| C6L - C5L - H5L | 120.0 |
| C4L - C5L - H5L | 120.0 |
| C1L - C6L - C5L | 121.3(4) |
| C1L - C6L - H6L | 119.3 |
| C5L - C6L - H6L | 119.3 |
| C1L - C7L - H7L1 | 109.5 |
| C1L - C7L - H7L2 | 109.5 |
| H7L1 - C7L - H7L2 | 109.5 |
| C1L - C7L - H7L3 | 109.5 |
| H7L1 - C7L - H7L3 | 109.5 |
| H7L2 - C7L - H7L3 | 109.5 |
| O1K - S1K - O2K | 112.4(16) |
| O1K - S1K - O3K | 116.0(18) |
| O2K - S1K - O3K | 110.0(15) |
| O1K - S1K - C4K | 107.8(19) |
| O2K - S1K - C4K | 106.4(16) |
| O3K - S1K - C4K | 103.4(19) |
| C7K - C1K - C6K | 121(2) |
| C7K - C1K - C2K | 119(2) |
| C6K - C1K - C2K | 119.2(17) |
| C3K - C2K - C1K | 119.3(16) |
| C3K - C2K - H2K | 120.3 |
| C1K - C2K - H2K | 120.4 |
| C2K - C3K - C4K | 121.3(16) |
| C2K - C3K - H3K | 119.4 |
| C4K - C3K - H3K | 119.4 |
| C5K - C4K - C3K | 119.5(16) |
| C5K - C4K - S1K | 121.2(16) |
| C3K - C4K - S1K | 119.1(15) |
| C4K - C5K - C6K | 119.0(16) |
| C4K - C5K - H5K | 120.5 |
| C6K - C5K - H5K | 120.5 |
| C1K - C6K - C5K | 121.6(17) |
| C1K - C6K - H6K | 119.2 |
| C5K - C6K - H6K | 119.2 |
| C1K - C7K - H7K1 | 109.5 |
| C1K - C7K - H7K2 | 109.5 |
| H7K1 - C7K - H7K2 | 109.5 |
| C1K - C7K - H7K3 | 109.5 |
| H7K1 - C7K - H7K3 | 109.5 |
| H7K2 - C7K - H7K3 | 109.5 |
| O3E - S1E - O1E | 108.1(7) |
| O3E - S1E - O2E | 112.7(6) |
| O1E - S1E - O2E | 111.5(7) |
| O3E - S1E - C4E | 109.8(5) |
| O1E - S1E - C4E | 107.4(6) |
| O2E - S1E - C4E | 107.3(6) |
| C6E - C1E - C2E | 119.0(8) |
| C6E - C1E - C7E | 120.6(9) |
| C2E - C1E - C7E | 120.4(9) |
| C3E - C2E - C1E | 118.6(9) |
| C3E - C2E - H2E | 120.7 |
| C1E - C2E - H2E | 120.7 |
| C4E - C3E - C2E | 121.8(8) |
| C4E - C3E - H3E | 119.1 |
| C2E - C3E - H3E | 119.1 |
| C3E - C4E - C5E | 120.5(7) |
| C3E - C4E - S1E | 120.2(6) |
| C5E - C4E - S1E | 119.3(6) |
| C6E - C5E - C4E | 119.2(8) |
| C6E - C5E - H5E | 120.4 |
| C4E - C5E - H5E | 120.4 |
| C5E - C6E - C1E | 120.9(8) |
| C5E - C6E - H6E | 119.5 |
| C1E - C6E - H6E | 119.5 |
| C1E - C7E - H7E1 | 109.5 |
| C1E - C7E - H7E2 | 109.5 |
| H7E1 - C7E - H7E2 | 109.5 |
| C1E - C7E - H7E3 | 109.5 |
| H7E1 - C7E - H7E3 | 109.5 |
| H7E2 - C7E - H7E3 | 109.5 |
| O3F - S1F - O2F | 120.5(12) |
| O3F - S1F - O1F | 95.3(10) |
| O2F - S1F - O1F | 112.1(12) |
| O3F - S1F - C4F | 115.4(9) |
| O2F - S1F - C4F | 104.9(11) |
| O1F - S1F - C4F | 108.1(8) |
| C2F - C1F - C6F | 122.2(13) |
| C2F - C1F - C7F | 119.6(15) |
| C6F - C1F - C7F | 118.3(15) |
| C1F - C2F - C3F | 119.7(13) |
| C1F - C2F - H2F | 120.2 |
| C3F - C2F - H2F | 120.1 |
| C4F - C3F - C2F | 118.7(12) |
| C4F - C3F - H3F | 120.6 |
| C2F - C3F - H3F | 120.7 |
| C3F - C4F - C5F | 121.5(12) |
| C3F - C4F - S1F | 118.9(10) |
| C5F - C4F - S1F | 119.6(9) |
| C4F - C5F - C6F | 121.2(13) |
| C4F - C5F - H5F | 119.4 |
| C6F - C5F - H5F | 119.4 |
| C5F - C6F - C1F | 116.8(13) |
| C5F - C6F - H6F | 121.6 |
| C1F - C6F - H6F | 121.6 |
| C1F - C7F - H7F1 | 109.5 |
| C1F - C7F - H7F2 | 109.5 |
| H7F1 - C7F - H7F2 | 109.5 |
| C1F - C7F - H7F3 | 109.4 |
| H7F1 - C7F - H7F3 | 109.5 |
| H7F2 - C7F - H7F3 | 109.5 |
| C2G - O1G - C6G | 118.3(12) |
| O1G - C2G - C3G | 109.8(10) |
| O1G - C2G - H2G1 | 109.9 |
| C3G - C2G - H2G1 | 109.7 |
| O1G - C2G - H2G2 | 109.6 |
| C3G - C2G - H2G2 | 109.7 |
| H2G1 - C2G - H2G2 | 108.2 |
| O4G - C3G - C2G | 109.1(10) |
| O4G - C3G - H3G1 | 109.6 |
| C2G - C3G - H3G1 | 109.8 |
| O4G - C3G - H3G2 | 110.0 |
| C2G - C3G - H3G2 | 110.0 |
| H3G1 - C3G - H3G2 | 108.3 |
| C5G - O4G - C3G | 98(3) |
| O4G - C5G - C6G | 107.3(9) |
| O4G - C5G - H5G1 | 110.3 |
| C6G - C5G - H5G1 | 110.4 |
| O4G - C5G - H5G2 | 110.1 |
| C6G - C5G - H5G2 | 110.3 |
| H5G1 - C5G - H5G2 | 108.5 |
| O1G - C6G - C5G | 109.0(10) |
| O1G - C6G - H6G1 | 109.7 |
| C5G - C6G - H6G1 | 109.8 |
| O1G - C6G - H6G2 | 110.1 |
| C5G - C6G - H6G2 | 109.9 |
| H6G1 - C6G - H6G2 | 108.3 |
| C2C - C1C - C6C | 116.6(9) |
| C2C - C1C - H1C | 121.7 |
| C6C - C1C - H1C | 121.7 |
| C1C - C2C - C3C | 119.0(9) |
| C1C - C2C - H2C | 120.5 |
| C3C - C2C - H2C | 120.5 |
| C4C - C3C - C2C | 123.4(9) |
| C4C - C3C - H3C | 118.3 |
| C2C - C3C - H3C | 118.3 |
| C3C - C4C - C5C | 121.1(9) |
| C3C - C4C - C7C | 121.8(9) |
| C5C - C4C - C7C | 116.9(9) |
| C4C - C5C - C6C | 115.3(10) |
| C4C - C5C - H5C | 122.4 |
| C6C - C5C - H5C | 122.4 |
| C5C - C6C - C1C | 124.5(9) |
| C5C - C6C - H6C | 117.8 |
| C1C - C6C - H6C | 117.8 |
| C4C - C7C - H7C1 | 109.5 |
| C4C - C7C - H7C2 | 109.5 |
| H7C1 - C7C - H7C2 | 109.5 |
| C4C - C7C - H7C3 | 109.5 |
| H7C1 - C7C - H7C3 | 109.5 |
| H7C2 - C7C - H7C3 | 109.5 |
| C7B - C1B - C6B | 121.7(19) |
| C7B - C1B - C2B | 112.8(18) |
| C6B - C1B - C2B | 125.5(17) |
| C3B - C2B - C1B | 117.1(17) |
| C3B - C2B - H2B | 121.4 |
| C1B - C2B - H2B | 121.4 |
| C2B - C3B - C4B | 117.0(16) |
| C2B - C3B - H3B1 | 121.5 |
| C4B - C3B - H3B1 | 121.5 |
| C3B - C4B - C5B | 126.4(17) |
| C3B - C4B - H4B1 | 116.8 |
| C5B - C4B - H4B1 | 116.8 |
| C4B - C5B - C6B | 116.1(16) |
| C4B - C5B - H5B1 | 122.0 |
| C6B - C5B - H5B1 | 121.9 |
| C1B - C6B - C5B | 117.7(17) |
| C1B - C6B - H6B | 121.1 |
| C5B - C6B - H6B | 121.1 |
| C1B - C7B - H7B1 | 109.5 |
| C1B - C7B - H7B2 | 109.4 |
| H7B1 - C7B - H7B2 | 109.5 |
| C1B - C7B - H7B3 | 109.5 |
| H7B1 - C7B - H7B3 | 109.5 |
| H7B2 - C7B - H7B3 | 109.5 |
| C4I - O1I - C1I | 121.3(8) |
| O1I - C1I - C2I | 105.9(10) |
| O1I - C1I - H1I1 | 110.5 |
| C2I - C1I - H1I1 | 110.6 |
| O1I - C1I - H1I2 | 110.6 |
| C2I - C1I - H1I2 | 110.6 |
| H1I1 - C1I - H1I2 | 108.7 |
| O2I - C2I - C1I | 106.8(12) |
| O2I - C2I - H2I1 | 110.4 |
| C1I - C2I - H2I1 | 110.4 |
| O2I - C2I - H2I2 | 110.3 |
| C1I - C2I - H2I2 | 110.4 |
| H2I1 - C2I - H2I2 | 108.6 |
| C2I - O2I - C3I | 91.8(13) |
| O2I - C3I - C4I | 106.9(13) |
| O2I - C3I - H3I1 | 110.3 |
| C4I - C3I - H3I1 | 110.3 |
| O2I - C3I - H3I2 | 110.3 |
| C4I - C3I - H3I2 | 110.3 |
| H3I1 - C3I - H3I2 | 108.6 |
| O1I - C4I - C3I | 108.0(10) |
| O1I - C4I - H4I1 | 110.1 |
| C3I - C4I - H4I1 | 110.1 |
| O1I - C4I - H4I2 | 110.1 |
| C3I - C4I - H4I2 | 110.1 |
| H4I1 - C4I - H4I2 | 108.4 |
| C2O - C1O - C6O | 120.2(8) |
| C2O - C1O - H1O | 119.9 |
| C6O - C1O - H1O | 119.9 |
| C1O - C2O - C3O | 119.9(8) |
| C1O - C2O - H2O | 120.1 |
| C3O - C2O - H2O | 120.1 |
| C2O - C3O - C4O | 120.3(8) |
| C2O - C3O - H3O | 119.9 |
| C4O - C3O - H3O | 119.9 |
| C5O - C4O - C3O | 119.6(8) |
| C5O - C4O - H4O | 120.2 |
| C3O - C4O - H4O | 120.2 |
| C4O - C5O - C6O | 120.3(8) |
| C4O - C5O - H5O | 119.8 |
| C6O - C5O - H5O | 119.8 |
| C1O - C6O - C5O | 119.7(8) |
| C1O - C6O - H6O | 120.2 |
| C5O - C6O - H6O | 120.2 |
| C4N - O1N - C1N | 110(3) |
| O1N - C1N - C2N | 105.5(19) |
| O1N - C1N - H1NA | 110.6 |
| C2N - C1N - H1NA | 110.7 |
| O1N - C1N - H1NB | 110.6 |
| C2N - C1N - H1NB | 110.7 |
| H1NA - C1N - H1NB | 108.8 |
| O2N - C2N - C1N | 117(2) |
| O2N - C2N - H2NA | 108.0 |
| C1N - C2N - H2NA | 107.9 |
| O2N - C2N - H2NB | 108.0 |
| C1N - C2N - H2NB | 108.0 |
| H2NA - C2N - H2NB | 107.2 |
| C3N - O2N - C2N | 108.2(18) |
| O2N - C3N - C4N | 111.1(15) |
| O2N - C3N - H3NA | 109.4 |
| C4N - C3N - H3NA | 109.4 |
| O2N - C3N - H3NB | 109.4 |
| C4N - C3N - H3NB | 109.4 |
| H3NA - C3N - H3NB | 108.0 |
| O1N - C4N - C3N | 111.5(16) |
| O1N - C4N - H4NA | 109.3 |
| C3N - C4N - H4NA | 109.3 |
| O1N - C4N - H4NB | 109.4 |
| C3N - C4N - H4NB | 109.3 |
| H4NA - C4N - H4NB | 108.0 |
| C1P - O1P - C4P | 105.6(19) |
| O1P - C1P - C2P | 105.3(17) |
| O1P - C1P - H1PA | 110.6 |
| C2P - C1P - H1PA | 110.6 |
| O1P - C1P - H1PB | 110.7 |
| C2P - C1P - H1PB | 110.7 |
| H1PA - C1P - H1PB | 108.8 |
| O2P - C2P - C1P | 122.2(18) |
| O2P - C2P - H2PA | 106.8 |
| C1P - C2P - H2PA | 106.7 |
| O2P - C2P - H2PB | 106.8 |
| C1P - C2P - H2PB | 106.8 |
| H2PA - C2P - H2PB | 106.6 |
| C3P - O2P - C2P | 107.8(15) |
| O2P - C3P - C4P | 120.8(17) |
| O2P - C3P - H3PA | 107.2 |
| C4P - C3P - H3PA | 107.2 |
| O2P - C3P - H3PB | 107.1 |
| C4P - C3P - H3PB | 107.1 |
| H3PA - C3P - H3PB | 106.8 |
| O1P - C4P - C3P | 110.5(17) |
| O1P - C4P - H4PA | 109.6 |
| C3P - C4P - H4PA | 109.6 |
| O1P - C4P - H4PB | 109.5 |
| C3P - C4P - H4PB | 109.5 |
| H4PA - C4P - H4PB | 108.1 |
| H1 - O1' - H2 | 114(10) |
| H1' - O2' - H2' | 115(10) |

## Table 4. Torsion angles for p-1.cif.

|  |  |
| --- | --- |
| **Atom - Atom - Atom - Atom** | **Torsion Angle [°]** |
| C3 - N1 - P2 - C54 | -178.9(2) |
| Sn1 - N1 - P2 - C54 | -13.2(2) |
| C3 - N1 - P2 - C42 | -61.8(3) |
| Sn1 - N1 - P2 - C42 | 103.88(18) |
| C3 - N1 - P2 - C48 | 58.1(3) |
| Sn1 - N1 - P2 - C48 | -136.18(17) |
| C4 - N2 - P3 - C18 | -179.6(2) |
| Sn1 - N2 - P3 - C18 | -13.0(2) |
| C4 - N2 - P3 - C6 | 56.1(3) |
| Sn1 - N2 - P3 - C6 | -137.30(18) |
| C4 - N2 - P3 - C12 | -62.7(3) |
| Sn1 - N2 - P3 - C12 | 103.88(19) |
| C5 - N3 - P4 - C30 | 178.9(2) |
| Sn1 - N3 - P4 - C30 | -14.9(2) |
| C5 - N3 - P4 - C24 | -63.7(3) |
| Sn1 - N3 - P4 - C24 | 102.50(18) |
| C5 - N3 - P4 - C36 | 58.3(3) |
| Sn1 - N3 - P4 - C36 | -135.54(17) |
| P2 - N1 - C3 - C2 | 157.3(2) |
| Sn1 - N1 - C3 - C2 | -8.8(4) |
| C5 - C2 - C3 - N1 | -58.8(4) |
| C4 - C2 - C3 - N1 | 70.8(4) |
| C1 - C2 - C3 - N1 | -174.1(3) |
| P3 - N2 - C4 - C2 | 156.6(2) |
| Sn1 - N2 - C4 - C2 | -10.4(4) |
| C5 - C2 - C4 - N2 | 70.7(3) |
| C3 - C2 - C4 - N2 | -58.7(4) |
| C1 - C2 - C4 - N2 | -173.4(3) |
| P4 - N3 - C5 - C2 | 159.4(2) |
| Sn1 - N3 - C5 - C2 | -6.9(3) |
| C4 - C2 - C5 - N3 | -60.6(4) |
| C3 - C2 - C5 - N3 | 68.4(3) |
| C1 - C2 - C5 - N3 | -176.6(3) |
| N2 - P3 - C6 - C11 | -76.2(3) |
| C18 - P3 - C6 - C11 | 164.1(3) |
| C12 - P3 - C6 - C11 | 46.1(3) |
| N2 - P3 - C6 - C7 | 98.1(3) |
| C18 - P3 - C6 - C7 | -21.6(4) |
| C12 - P3 - C6 - C7 | -139.6(3) |
| C11 - C6 - C7 - C8 | 0.0(6) |
| P3 - C6 - C7 - C8 | -174.3(3) |
| C6 - C7 - C8 - C9 | 0.7(7) |
| C7 - C8 - C9 - C10 | -1.8(7) |
| C8 - C9 - C10 - C11 | 2.1(7) |
| C7 - C6 - C11 - C10 | 0.4(6) |
| P3 - C6 - C11 - C10 | 174.9(3) |
| C9 - C10 - C11 - C6 | -1.4(7) |
| N2 - P3 - C12 - C17 | 153.6(3) |
| C18 - P3 - C12 - C17 | -91.2(3) |
| C6 - P3 - C12 - C17 | 30.5(3) |
| N2 - P3 - C12 - C13 | -29.6(3) |
| C18 - P3 - C12 - C13 | 85.6(3) |
| C6 - P3 - C12 - C13 | -152.7(3) |
| C17 - C12 - C13 - C14 | -1.2(5) |
| P3 - C12 - C13 - C14 | -178.1(3) |
| C12 - C13 - C14 - C15 | -0.1(6) |
| C13 - C14 - C15 - C16 | 1.3(7) |
| C14 - C15 - C16 - C17 | -1.1(7) |
| C15 - C16 - C17 - C12 | -0.3(7) |
| C13 - C12 - C17 - C16 | 1.4(6) |
| P3 - C12 - C17 - C16 | 178.1(3) |
| N2 - P3 - C18 - C23 | 104.0(3) |
| C6 - P3 - C18 - C23 | -132.1(3) |
| C12 - P3 - C18 - C23 | -15.5(3) |
| N2 - P3 - C18 - C19 | -65.4(3) |
| C6 - P3 - C18 - C19 | 58.6(3) |
| C12 - P3 - C18 - C19 | 175.2(3) |
| C23 - C18 - C19 - C20 | 0.2(5) |
| P3 - C18 - C19 - C20 | 169.5(3) |
| C18 - C19 - C20 - C21 | -1.8(5) |
| C19 - C20 - C21 - C22 | 1.8(6) |
| C20 - C21 - C22 - C23 | -0.2(6) |
| C21 - C22 - C23 - C18 | -1.4(5) |
| C19 - C18 - C23 - C22 | 1.4(5) |
| P3 - C18 - C23 - C22 | -168.0(3) |
| N3 - P4 - C24 - C29 | 158.7(3) |
| C30 - P4 - C24 - C29 | -85.8(4) |
| C36 - P4 - C24 - C29 | 31.8(4) |
| N3 - P4 - C24 - C25 | -26.0(3) |
| C30 - P4 - C24 - C25 | 89.5(3) |
| C36 - P4 - C24 - C25 | -152.9(3) |
| C29 - C24 - C25 - C26 | -0.4(6) |
| P4 - C24 - C25 - C26 | -175.7(3) |
| C24 - C25 - C26 - C27 | 0.7(6) |
| C25 - C26 - C27 - C28 | -0.4(7) |
| C26 - C27 - C28 - C29 | -0.2(8) |
| C25 - C24 - C29 - C28 | -0.2(7) |
| P4 - C24 - C29 - C28 | 175.0(4) |
| C27 - C28 - C29 - C24 | 0.5(8) |
| N3 - P4 - C30 - C35 | 96.1(3) |
| C24 - P4 - C30 - C35 | -23.5(3) |
| C36 - P4 - C30 - C35 | -139.4(3) |
| N3 - P4 - C30 - C31 | -74.6(3) |
| C24 - P4 - C30 - C31 | 165.8(3) |
| C36 - P4 - C30 - C31 | 49.9(3) |
| C35 - C30 - C31 - C32 | 1.9(6) |
| P4 - C30 - C31 - C32 | 172.5(3) |
| C30 - C31 - C32 - C33 | -1.1(6) |
| C31 - C32 - C33 - C34 | -0.4(6) |
| C32 - C33 - C34 - C35 | 1.2(6) |
| C33 - C34 - C35 - C30 | -0.5(6) |
| C31 - C30 - C35 - C34 | -1.1(6) |
| P4 - C30 - C35 - C34 | -171.6(3) |
| N3 - P4 - C36 - C37 | 133.5(3) |
| C30 - P4 - C36 - C37 | 15.1(4) |
| C24 - P4 - C36 - C37 | -101.9(3) |
| N3 - P4 - C36 - C41 | -48.2(3) |
| C30 - P4 - C36 - C41 | -166.6(3) |
| C24 - P4 - C36 - C41 | 76.4(3) |
| C41 - C36 - C37 - C38 | 2.1(6) |
| P4 - C36 - C37 - C38 | -179.6(3) |
| C36 - C37 - C38 - C39 | -0.6(7) |
| C37 - C38 - C39 - C40 | -0.5(7) |
| C38 - C39 - C40 - C41 | 0.2(7) |
| C39 - C40 - C41 - C36 | 1.3(6) |
| C37 - C36 - C41 - C40 | -2.4(6) |
| P4 - C36 - C41 - C40 | 179.2(3) |
| N1 - P2 - C42 - C43 | -26.4(3) |
| C54 - P2 - C42 - C43 | 89.8(3) |
| C48 - P2 - C42 - C43 | -149.9(3) |
| N1 - P2 - C42 - C47 | 156.3(3) |
| C54 - P2 - C42 - C47 | -87.5(3) |
| C48 - P2 - C42 - C47 | 32.8(3) |
| C47 - C42 - C43 - C44 | -0.8(5) |
| P2 - C42 - C43 - C44 | -178.2(3) |
| C42 - C43 - C44 - C45 | 1.3(6) |
| C43 - C44 - C45 - C46 | -0.9(7) |
| C44 - C45 - C46 - C47 | 0.0(6) |
| C45 - C46 - C47 - C42 | 0.4(6) |
| C43 - C42 - C47 - C46 | 0.0(5) |
| P2 - C42 - C47 - C46 | 177.3(3) |
| N1 - P2 - C48 - C53 | 104.6(3) |
| C54 - P2 - C48 - C53 | -15.4(4) |
| C42 - P2 - C48 - C53 | -133.1(3) |
| N1 - P2 - C48 - C49 | -72.2(3) |
| C54 - P2 - C48 - C49 | 167.9(3) |
| C42 - P2 - C48 - C49 | 50.2(3) |
| C53 - C48 - C49 - C50 | 0.6(5) |
| P2 - C48 - C49 - C50 | 177.5(3) |
| C48 - C49 - C50 - C51 | 0.2(6) |
| C49 - C50 - C51 - C52 | -0.5(6) |
| C50 - C51 - C52 - C53 | 0.0(6) |
| C51 - C52 - C53 - C48 | 0.9(6) |
| C49 - C48 - C53 - C52 | -1.2(5) |
| P2 - C48 - C53 - C52 | -177.9(3) |
| N1 - P2 - C54 - C55 | 110.3(3) |
| C42 - P2 - C54 - C55 | -8.9(3) |
| C48 - P2 - C54 - C55 | -126.0(3) |
| N1 - P2 - C54 - C59 | -63.7(3) |
| C42 - P2 - C54 - C59 | 177.1(3) |
| C48 - P2 - C54 - C59 | 60.0(3) |
| C59 - C54 - C55 - C56 | 0.4(5) |
| P2 - C54 - C55 - C56 | -173.7(3) |
| C54 - C55 - C56 - C57 | -0.3(5) |
| C55 - C56 - C57 - C58 | -0.6(5) |
| C56 - C57 - C58 - C59 | 1.3(5) |
| C57 - C58 - C59 - C54 | -1.2(5) |
| C55 - C54 - C59 - C58 | 0.4(5) |
| P2 - C54 - C59 - C58 | 174.4(2) |
| C6L - C1L - C2L - C3L | 1.6(6) |
| C7L - C1L - C2L - C3L | -178.1(5) |
| C1L - C2L - C3L - C4L | -0.1(6) |
| C2L - C3L - C4L - C5L | -1.7(6) |
| C2L - C3L - C4L - S1L | 176.6(3) |
| O1L - S1L - C4L - C3L | -56.5(4) |
| O3L - S1L - C4L - C3L | -176.4(3) |
| O2L - S1L - C4L - C3L | 63.9(5) |
| O1L - S1L - C4L - C5L | 121.8(4) |
| O3L - S1L - C4L - C5L | 1.9(4) |
| O2L - S1L - C4L - C5L | -117.8(5) |
| C3L - C4L - C5L - C6L | 1.9(7) |
| S1L - C4L - C5L - C6L | -176.4(4) |
| C2L - C1L - C6L - C5L | -1.4(8) |
| C7L - C1L - C6L - C5L | 178.3(5) |
| C4L - C5L - C6L - C1L | -0.4(8) |
| C7K - C1K - C2K - C3K | -177(4) |
| C6K - C1K - C2K - C3K | 1(3) |
| C1K - C2K - C3K - C4K | -2(2) |
| C2K - C3K - C4K - C5K | 3(4) |
| C2K - C3K - C4K - S1K | 177.7(19) |
| O1K - S1K - C4K - C5K | 58(4) |
| O2K - S1K - C4K - C5K | 179(3) |
| O3K - S1K - C4K - C5K | -65(4) |
| O1K - S1K - C4K - C3K | -116(3) |
| O2K - S1K - C4K - C3K | 4(4) |
| O3K - S1K - C4K - C3K | 120(3) |
| C3K - C4K - C5K - C6K | -4(6) |
| S1K - C4K - C5K - C6K | -178(3) |
| C7K - C1K - C6K - C5K | 176(5) |
| C2K - C1K - C6K - C5K | -2(5) |
| C4K - C5K - C6K - C1K | 3(6) |
| C6E - C1E - C2E - C3E | 0.4(9) |
| C7E - C1E - C2E - C3E | -178.4(7) |
| C1E - C2E - C3E - C4E | -0.6(11) |
| C2E - C3E - C4E - C5E | 0.9(13) |
| C2E - C3E - C4E - S1E | -179.5(6) |
| O3E - S1E - C4E - C3E | -13.1(9) |
| O1E - S1E - C4E - C3E | -130.4(9) |
| O2E - S1E - C4E - C3E | 109.6(9) |
| O3E - S1E - C4E - C5E | 166.4(8) |
| O1E - S1E - C4E - C5E | 49.2(10) |
| O2E - S1E - C4E - C5E | -70.8(9) |
| C3E - C4E - C5E - C6E | -1.0(13) |
| S1E - C4E - C5E - C6E | 179.4(7) |
| C4E - C5E - C6E - C1E | 0.8(12) |
| C2E - C1E - C6E - C5E | -0.6(10) |
| C7E - C1E - C6E - C5E | 178.3(7) |
| C6F - C1F - C2F - C3F | -0.8(11) |
| C7F - C1F - C2F - C3F | 179.6(10) |
| C1F - C2F - C3F - C4F | 1.0(16) |
| C2F - C3F - C4F - C5F | -2(2) |
| C2F - C3F - C4F - S1F | 179.9(9) |
| O3F - S1F - C4F - C3F | -19.9(17) |
| O2F - S1F - C4F - C3F | 115.1(17) |
| O1F - S1F - C4F - C3F | -125.0(14) |
| O3F - S1F - C4F - C5F | 161.6(16) |
| O2F - S1F - C4F - C5F | -63.5(18) |
| O1F - S1F - C4F - C5F | 56.4(16) |
| C3F - C4F - C5F - C6F | 2(2) |
| S1F - C4F - C5F - C6F | -179.5(12) |
| C4F - C5F - C6F - C1F | -2(2) |
| C2F - C1F - C6F - C5F | 1.2(16) |
| C7F - C1F - C6F - C5F | -179.3(12) |
| C6G - O1G - C2G - C3G | 38(4) |
| O1G - C2G - C3G - O4G | -57.7(16) |
| C2G - C3G - O4G - C5G | 77(3) |
| C3G - O4G - C5G - C6G | -77(3) |
| C2G - O1G - C6G - C5G | -38(4) |
| O4G - C5G - C6G - O1G | 59.2(16) |
| C6C - C1C - C2C - C3C | 1.8(11) |
| C1C - C2C - C3C - C4C | -2.7(11) |
| C2C - C3C - C4C - C5C | 3.9(16) |
| C2C - C3C - C4C - C7C | 179.0(11) |
| C3C - C4C - C5C - C6C | -4.1(17) |
| C7C - C4C - C5C - C6C | -179.4(12) |
| C4C - C5C - C6C - C1C | 3.5(18) |
| C2C - C1C - C6C - C5C | -2.5(16) |
| C7B - C1B - C2B - C3B | 179(2) |
| C6B - C1B - C2B - C3B | -2(2) |
| C1B - C2B - C3B - C4B | -1(2) |
| C2B - C3B - C4B - C5B | 4(4) |
| C3B - C4B - C5B - C6B | -3(5) |
| C7B - C1B - C6B - C5B | -179(3) |
| C2B - C1B - C6B - C5B | 3(4) |
| C4B - C5B - C6B - C1B | 0(4) |
| C4I - O1I - C1I - C2I | 30(2) |
| O1I - C1I - C2I - O2I | -60.2(17) |
| C1I - C2I - O2I - C3I | 86.4(15) |
| C2I - O2I - C3I - C4I | -84.3(16) |
| C1I - O1I - C4I - C3I | -29(2) |
| O2I - C3I - C4I - O1I | 57(2) |
| C6O - C1O - C2O - C3O | -2(2) |
| C1O - C2O - C3O - C4O | 1.1(19) |
| C2O - C3O - C4O - C5O | -1(3) |
| C3O - C4O - C5O - C6O | 2(4) |
| C2O - C1O - C6O - C5O | 2(3) |
| C4O - C5O - C6O - C1O | -2(4) |
| C4N - O1N - C1N - C2N | -60(4) |
| O1N - C1N - C2N - O2N | 51(4) |
| C1N - C2N - O2N - C3N | -47(4) |
| C2N - O2N - C3N - C4N | 49(3) |
| C1N - O1N - C4N - C3N | 69(4) |
| O2N - C3N - C4N - O1N | -63(3) |
| C4P - O1P - C1P - C2P | 64(2) |
| O1P - C1P - C2P - O2P | -47(3) |
| C1P - C2P - O2P - C3P | 27(3) |
| C2P - O2P - C3P - C4P | -28(3) |
| C1P - O1P - C4P - C3P | -70(3) |
| O2P - C3P - C4P - O1P | 53(3) |