**18srv020**

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| Table 1 Crystal data and structure refinement for 18srv020. | |
| Identification code | 18srv020 |
| Empirical formula | C12H12B2O5 |
| Formula weight | 257.84 |
| Temperature/K | 120.0 |
| Crystal system | orthorhombic |
| Space group | Pbca |
| a/Å | 12.4294(6) |
| b/Å | 12.3804(6) |
| c/Å | 15.3932(7) |
| α/° | 90 |
| β/° | 90 |
| γ/° | 90 |
| Volume/Å3 | 2368.72(19) |
| Z | 8 |
| ρcalcg/cm3 | 1.446 |
| μ/mm‑1 | 0.108 |
| F(000) | 1072.0 |
| Crystal size/mm3 | 0.12 × 0.11 × 0.05 |
| Radiation | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 5.346 to 57.996 |
| Index ranges | -16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -21 ≤ l ≤ 21 |
| Reflections collected | 46156 |
| Independent reflections | 3142 [Rint = 0.0562, Rsigma = 0.0263] |
| Data/restraints/parameters | 3142/0/220 |
| Goodness-of-fit on F2 | 1.034 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0419, wR2 = 0.1011 |
| Final R indexes [all data] | R1 = 0.0648, wR2 = 0.1122 |
| Largest diff. peak/hole / e Å-3 | 0.39/-0.23 |

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| Table 2 Fractional Atomic Coordinates (×104) and Equivalent Isotropic Displacement Parameters (Å2×103) for 18srv020. Ueq is defined as 1/3 of of the trace of the orthogonalised UIJ tensor. | | | | |
| **Atom** | ***x*** | ***y*** | ***z*** | **U(eq)** |
| O1 | 10237.8(8) | 6127.1(7) | 6982.0(5) | 20.1(2) |
| O2 | 9590.7(9) | 4616.2(8) | 7680.4(6) | 26.4(3) |
| O3 | 11084.2(8) | 7633.4(8) | 6418.0(6) | 20.6(2) |
| O4 | 8130.7(8) | 3477.2(8) | 6750.6(6) | 23.0(2) |
| O5 | 10524.5(8) | 8130.9(7) | 4783.1(6) | 22.4(2) |
| C1 | 8891.3(10) | 5017(1) | 6122.6(7) | 15.3(3) |
| C2 | 8187.5(10) | 4152.1(11) | 6047.7(8) | 17.6(3) |
| C3 | 7586.3(11) | 3955.5(12) | 5284.8(8) | 21.1(3) |
| C4 | 7695.1(10) | 4646.4(12) | 4595.5(8) | 20.9(3) |
| C5 | 8387.4(10) | 5546.5(11) | 4629.8(8) | 17.3(3) |
| C6 | 8510.4(11) | 6263.1(12) | 3921.8(8) | 20.4(3) |
| C7 | 9197.3(11) | 7120.8(11) | 3955.7(8) | 20.0(3) |
| C8 | 9806.9(10) | 7294.8(10) | 4721.0(8) | 17.0(3) |
| C9 | 9725.2(10) | 6625.8(10) | 5439.2(8) | 15.1(3) |
| C10 | 9001.3(10) | 5730.3(10) | 5398.8(7) | 14.3(3) |
| C11 | 7336.7(14) | 2648.1(13) | 6766.1(10) | 29.3(3) |
| C12 | 10497.7(15) | 8961.7(13) | 4131.9(10) | 29.2(3) |
| B1 | 9581.1(12) | 5227.6(12) | 6954.2(9) | 18.1(3) |
| B2 | 10382.6(12) | 6812.8(12) | 6291.1(9) | 15.7(3) |

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| Table 3 Anisotropic Displacement Parameters (Å2×103) for 18srv020. The Anisotropic displacement factor exponent takes the form: -2π2[h2a\*2U11+2hka\*b\*U12+…]. | | | | | | |
| **Atom** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| O1 | 27.9(5) | 20.5(5) | 11.9(4) | -0.2(3) | -5.7(4) | -6.8(4) |
| O2 | 41.2(6) | 22.7(5) | 15.2(5) | 1.3(4) | -6.8(4) | -13.5(5) |
| O3 | 28.3(5) | 19.8(5) | 13.7(4) | 0.3(4) | -3.7(4) | -5.8(4) |
| O4 | 25.5(5) | 24.6(5) | 18.9(5) | 1.4(4) | -3.4(4) | -10.7(4) |
| O5 | 30.7(5) | 21.3(5) | 15.2(4) | 4.9(4) | -5.5(4) | -4.8(4) |
| C1 | 14.9(6) | 18.5(6) | 12.5(5) | -4.2(5) | 0.1(4) | 2.1(5) |
| C2 | 16.3(6) | 20.7(7) | 15.7(6) | -3.3(5) | 1.3(5) | 0.2(5) |
| C3 | 16.0(6) | 26.0(7) | 21.3(6) | -6.8(5) | -2.1(5) | -2.9(6) |
| C4 | 14.8(6) | 30.6(7) | 17.4(6) | -5.7(5) | -4.4(5) | 1.1(5) |
| C5 | 13.5(6) | 23.7(7) | 14.7(6) | -4.0(5) | -2.1(5) | 4.1(5) |
| C6 | 18.0(6) | 29.2(8) | 14.0(6) | -3.5(5) | -4.8(5) | 6.4(6) |
| C7 | 22.5(7) | 23.7(7) | 13.9(6) | 1.3(5) | -2.7(5) | 5.9(5) |
| C8 | 17.5(6) | 18.3(6) | 15.0(6) | -2.6(5) | -0.7(5) | 3.5(5) |
| C9 | 15.2(6) | 17.7(6) | 12.3(5) | -3.3(5) | -0.9(4) | 4.0(5) |
| C10 | 12.5(6) | 18.1(6) | 12.4(5) | -4.2(4) | -0.1(4) | 4.5(5) |
| C11 | 31.1(8) | 31.9(8) | 24.9(7) | -1.5(7) | -1.1(6) | -16.0(7) |
| C12 | 42.5(9) | 26.3(8) | 18.8(7) | 8.5(6) | -5.8(6) | -7.0(7) |
| B1 | 22.2(7) | 19.0(7) | 13.1(6) | -3.0(5) | -0.9(5) | -1.3(6) |
| B2 | 18.5(7) | 16.0(7) | 12.6(6) | -2.5(5) | -1.8(5) | 0.9(6) |

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| Table 4 Bond Lengths for 18srv020. | | | | | | |
| **Atom** | **Atom** | **Length/Å** |  | **Atom** | **Atom** | **Length/Å** |
| O1 | B1 | 1.3814(17) |  | C2 | C3 | 1.4131(17) |
| O1 | B2 | 1.3727(17) |  | C3 | C4 | 1.369(2) |
| O2 | B1 | 1.3502(17) |  | C4 | C5 | 1.4090(19) |
| O3 | B2 | 1.3531(17) |  | C5 | C6 | 1.4135(19) |
| O4 | C2 | 1.3689(16) |  | C5 | C10 | 1.4266(16) |
| O4 | C11 | 1.4242(17) |  | C6 | C7 | 1.364(2) |
| O5 | C8 | 1.3697(16) |  | C7 | C8 | 1.4171(17) |
| O5 | C12 | 1.4367(16) |  | C8 | C9 | 1.3851(17) |
| C1 | C2 | 1.3875(18) |  | C9 | C10 | 1.4292(17) |
| C1 | C10 | 1.4283(17) |  | C9 | B2 | 1.5623(18) |
| C1 | B1 | 1.5625(18) |  |  |  |  |

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| Table 5 Bond Angles for 18srv020. | | | | | | | | |
| **Atom** | **Atom** | **Atom** | **Angle/˚** |  | **Atom** | **Atom** | **Atom** | **Angle/˚** |
| B2 | O1 | B1 | 123.50(10) |  | O5 | C8 | C7 | 121.41(11) |
| C2 | O4 | C11 | 119.27(11) |  | O5 | C8 | C9 | 116.35(11) |
| C8 | O5 | C12 | 118.50(11) |  | C9 | C8 | C7 | 122.23(12) |
| C2 | C1 | C10 | 118.21(11) |  | C8 | C9 | C10 | 118.38(11) |
| C2 | C1 | B1 | 122.88(11) |  | C8 | C9 | B2 | 122.89(11) |
| C10 | C1 | B1 | 118.90(11) |  | C10 | C9 | B2 | 118.74(11) |
| O4 | C2 | C1 | 115.97(11) |  | C1 | C10 | C9 | 120.39(11) |
| O4 | C2 | C3 | 121.64(12) |  | C5 | C10 | C1 | 119.83(11) |
| C1 | C2 | C3 | 122.37(12) |  | C5 | C10 | C9 | 119.78(11) |
| C4 | C3 | C2 | 118.95(13) |  | O1 | B1 | C1 | 118.96(11) |
| C3 | C4 | C5 | 121.69(12) |  | O2 | B1 | O1 | 114.90(11) |
| C4 | C5 | C6 | 122.25(11) |  | O2 | B1 | C1 | 126.13(12) |
| C4 | C5 | C10 | 118.94(12) |  | O1 | B2 | C9 | 119.35(11) |
| C6 | C5 | C10 | 118.80(12) |  | O3 | B2 | O1 | 115.91(11) |
| C7 | C6 | C5 | 121.80(12) |  | O3 | B2 | C9 | 124.72(12) |
| C6 | C7 | C8 | 119.01(12) |  |  |  |  |  |

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| Table 6 Hydrogen Bonds for 18srv020. | | | | | | |
| **D** | **H** | **A** | **d(D-H)/Å** | **d(H-A)/Å** | **d(D-A)/Å** | **D-H-A/°** |
| O2 | H2 | O4 | 0.85(2) | 2.06(2) | 2.7074(14) | 132.9(17) |
| O3 | H3 | O5 | 0.85(2) | 1.97(2) | 2.6826(13) | 141.0(18) |

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| Table 7 selected Torsion Angles for 18srv020. | | | | | | | | | | |
| **A** | **B** | **C** | **D** | **Angle/˚** |  | **A** | **B** | **C** | **D** | **Angle/˚** |
| C1 | C2 | O4 | C11 | 172.58(12) |  | C10 | C1 | B1 | O1 | 3.15(18) |
| C2 | C1 | B1 | O1 | -178.12(12) |  | C10 | C1 | B1 | O2 | -178.23(13) |
| C2 | C1 | B1 | O2 | 0.5(2) |  | C10 | C9 | B2 | O1 | -1.03(18) |
| C3 | C2 | O4 | C11 | -9.22(19) |  | C10 | C9 | B2 | O3 | -179.26(12) |
| C7 | C8 | O5 | C12 | 12.50(18) |  | B1 | O1 | B2 | O3 | -177.66(12) |
| C8 | C9 | B2 | O1 | 178.51(12) |  | B1 | O1 | B2 | C9 | 3.96(19) |
| C8 | C9 | B2 | O3 | 0.3(2) |  | B2 | O1 | B1 | O2 | 176.24(12) |
| C9 | C8 | O5 | C12 | -168.45(12) |  | B2 | O1 | B1 | C1 | -4.98(19) |

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| Table 8 Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103) for 18srv020. | | | | |
| **Atom** | ***x*** | ***y*** | ***z*** | **U(eq)** |
| H2 | 9202(16) | 4051(16) | 7657(13) | 45(6) |
| H3 | 11143(16) | 8005(16) | 5954(13) | 49(6) |
| H3A | 7121(14) | 3345(13) | 5240(11) | 33(5) |
| H4 | 7283(14) | 4531(13) | 4062(11) | 32(5) |
| H6 | 8097(13) | 6122(12) | 3391(10) | 24(4) |
| H7 | 9294(13) | 7593(13) | 3481(11) | 27(4) |
| H11A | 7450(14) | 2135(13) | 6281(11) | 31(4) |
| H11B | 6617(15) | 2960(14) | 6728(11) | 36(5) |
| H11C | 7457(14) | 2266(14) | 7314(12) | 38(5) |
| H12A | 10686(14) | 8667(14) | 3571(12) | 34(4) |
| H12B | 11014(15) | 9500(14) | 4332(12) | 38(5) |
| H12C | 9751(16) | 9305(14) | 4104(12) | 42(5) |