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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  $F^2 > 2\sigma(F^2)$  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.
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# SQUEEZE RESULTS (APPEND TO CIF)
# Note: Data are Listed for all Voids in the P1 Unit Cell
# i.e. Centre of Gravity, Solvent Accessible Volume,
# Recovered number of Electrons in the Void and
# Details about the Squeezed Material
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C42A C -0.1016(8) 0.4241(7) 1.537(3) 0.151(9) Uani 0.495(5) 1 d PDU A 2
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C40B 0.123(7) 0.118(7) 0.075(5) 0.004(5) 0.005(5) -0.035(5)
C41B 0.132(14) 0.132(16) 0.059(10) 0.013(11) -0.017(10) -0.073(13)
C42B 0.144(16) 0.152(19) 0.099(12) 0.043(13) 0.003(12) -0.072(14)
C43B 0.129(15) 0.20(2) 0.126(14) -0.047(16) 0.016(14) -0.071(14)
C44B 0.173(18) 0.159(17) 0.158(17) -0.031(16) 0.031(16) -0.108(15)
C45B 0.148(18) 0.20(2) 0.083(11) 0.013(15) 0.016(12) -0.080(17)
C46B 0.139(18) 0.18(2) 0.098(14) -0.014(15) -0.005(13) -0.089(16)
C31B 0.22(3) 0.20(2) 0.32(3) -0.04(2) 0.10(3) -0.13(2)
C32B 0.27(3) 0.23(2) 0.45(3) 0.00(2) 0.16(3) -0.12(3)
O21A 0.113(10) 0.138(11) 0.149(10) 0.017(10) 0.046(8) -0.027(9)
O22A 0.020(4) 0.061(5) 0.069(5) 0.038(4) -0.010(3) -0.018(3)
C21A 0.106(13) 0.105(13) 0.157(15) 0.105(12) -0.067(11) -0.064(12)
C22A 0.101(13) 0.203(17) 0.34(2) 0.207(18) -0.039(14) -0.081(14)
C23A 0.24(2) 0.33(3) 0.34(3) 0.20(2) 0.02(2) -0.14(2)
C24A 0.24(2) 0.34(3) 0.42(3) 0.17(3) 0.01(2) -0.16(2)
C25A 0.22(2) 0.29(2) 0.42(3) 0.27(2) -0.05(2) -0.13(2)
C26A 0.17(2) 0.27(2) 0.50(3) 0.27(2) -0.08(2) -0.07(2)
C27A 0.106(14) 0.24(2) 0.46(3) 0.26(2) -0.065(17) -0.096(15)
O41A 0.159(12) 0.090(13) 0.048(6) 0.011(8) -0.010(7) -0.086(12)
O42A 0.132(5) 0.150(5) 0.114(4) 0.020(4) 0.020(4) -0.054(4)
C40A 0.123(7) 0.118(7) 0.075(5) 0.004(5) 0.005(5) -0.035(5)
C41A 0.163(19) 0.125(17) 0.085(14) 0.042(12) -0.001(14) -0.069(15)
C42A 0.20(2) 0.099(15) 0.155(17) 0.037(14) -0.043(17) -0.087(15)
C43A 0.24(2) 0.104(14) 0.166(18) 0.032(15) -0.064(19) -0.092(15)
C44A 0.188(19) 0.168(19) 0.19(2) 0.061(18) -0.010(18) -0.128(16)
C45A 0.27(3) 0.18(2) 0.20(2) 0.07(2) 0.01(2) -0.09(2)
C46A 0.21(3) 0.17(2) 0.17(2) 0.052(19) -0.01(2) -0.10(2)
C31A 0.23(2) 0.29(3) 0.41(3) 0.18(3) -0.03(2) -0.14(2)
C32A 0.19(2) 0.24(3) 0.35(3) 0.06(3) -0.02(2) -0.15(2)

_geom_special_details

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

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Zn1 N3A 1.883(15) . ?
Zn1 O1 1.9479(6) . ?
Zn1 O41A 2.08(2) 4_554 ?
Zn1 N2A 2.215(16) 2_565 ?
Zn1 N2 2.245(18) . ?
Zn1 Zn1 3.0599(13) 2_565 ?
Zn2 O22A 1.937(7) 8_667 ?
Zn2 O21B 1.940(7) . ?
Zn2 N4 2.01(2) 8_667 ?
Zn2 N1 2.09(2) . ?
Zn2 N4A 2.124(15) . ?
Zn2 N1A 2.18(2) 8_667 ?
Zn2 O22B 2.446(12) . ?
Zn2 C21A 2.455(13) 8_667 ?
Zn2 O21A 2.473(12) 8_667 ?
Zn2 C21B 2.492(13) . ?
O1 Zn1 1.9479(6) 2_565 ?
O1 Zn1 1.9479(6) 8_666 ?
O1 Zn1 1.9479(6) 7_566 ?
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C1 N5 1.37(4) . ?
C1 C4 1.44(2) . ?
N1 C2 1.36(5) . ?
C2 N2 1.32(4) . ?
C2 H2A 0.9300 . ?
N2 C3 1.38(2) . ?
C3 C4 1.28(3) . ?
C3 N3 1.36(3) . ?
C3 C5 1.99(4) . ?
C4 N4 1.28(3) . ?
C4 C5 2.03(3) . ?
C5 N3 1.34(4) . ?
C5 N4 1.63(5) . ?
C5 H5A 0.9300 . ?
N3 Zn1 1.84(2) 2_565 ?
N4 Zn2 2.01(2) 7_567 ?
C1A C4A 1.33(2) . ?

C1A N5A 1.38(3) . ?
C1A N1A 1.63(3) . ?
N1A C2A 1.04(4) . ?
N1A Zn2 2.18(2) 7_567 ?
N2A C2A 1.33(4) . ?
N2A C3A 1.34(2) . ?
N2A Zn1 2.215(16) 2_565 ?
C2A H2AA 0.9300 . ?
C3A C4A 1.36(2) . ?
C3A N3A 1.369(19) . ?
C4A N4A 1.43(2) . ?
C5A N4A 1.29(4) . ?
C5A N3A 1.33(3) . ?
C5A H5AA 0.9300 . ?
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O22B C21B 1.118(12) . ?
C21B C22B 1.608(15) . ?
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C22B C27B 1.3900 . ?
C23B C24B 1.3900 . ?
C23B H23A 0.9300 . ?
C24B C25B 1.3900 . ?
C24B H24A 0.9300 . ?
C25B C26B 1.3900 . ?
C25B C32B 1.56(2) . ?
C26B C27B 1.3900 . ?
C26B H26A 0.9300 . ?
C27B H27A 0.9300 . ?
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C41B C42B 1.337(16) . ?
C42B C43B 1.314(15) . ?
C42B H42A 0.9300 . ?
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C44B C45B 1.295(16) . ?
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C45B C46B 1.351(15) . ?
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C46B H46A 0.9300 . ?
C31B C32B 1.26(3) . ?
C31B H31A 0.9300 . ?
C32B H32A 0.9300 . ?
O21A C21A 1.128(12) . ?
O21A Zn2 2.473(12) 7_567 ?
O22A C21A 1.059(13) . ?
O22A Zn2 1.937(7) 7_567 ?
C21A C22A 1.624(15) . ?
C21A Zn2 2.455(13) 7_567 ?
C22A C23A 1.3900 . ?
C22A C27A 1.3900 . ?

C23A C24A 1.3900 . ?
C23A H23B 0.9300 . ?
C24A C25A 1.3900 . ?
C24A H24B 0.9300 . ?
C25A C26A 1.3900 . ?
C25A C31A 1.56(2) . ?
C26A C27A 1.3900 . ?
C26A H26B 0.9300 . ?
C27A H27B 0.9300 . ?
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C41A C42A 1.278(17) . ?
C42A C43A 1.259(17) . ?
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C43A C44A 1.266(17) . ?
C43A H43B 0.9300 . ?
C44A C45A 1.258(18) . ?
C44A C32A 1.55(2) . ?
C45A C46A 1.298(17) . ?
C45A H45B 0.9300 . ?
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loop_

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N3 Zn1 N3A 98.3(7) 2_565 . ?
O41B Zn1 O1 104.7(9) 4_554 . ?
N3 Zn1 O1 109.5(8) 2_565 . ?
N3A Zn1 O1 109.8(5) . . ?
O41B Zn1 O41A 14.4(18) 4_554 4_554 ?
N3 Zn1 O41A 112.6(11) 2_565 4_554 ?
N3A Zn1 O41A 121.1(10) . 4_554 ?
O1 Zn1 O41A 105.2(6) . 4_554 ?
O41B Zn1 N2A 131.8(11) 4_554 2_565 ?
N3 Zn1 N2A 7.8(13) 2_565 2_565 ?
N3A Zn1 N2A 98.0(6) . 2_565 ?
O1 Zn1 N2A 102.5(4) . 2_565 ?
O41A Zn1 N2A 118.8(9) 4_554 2_565 ?
O41B Zn1 N2 117.0(12) 4_554 . ?
N3 Zn1 N2 96.9(8) 2_565 . ?
N3A Zn1 N2 9.8(9) . . ?
O1 Zn1 N2 101.4(4) . . ?
O41A Zn1 N2 129.9(10) 4_554 . ?
N2A Zn1 N2 95.3(5) 2_565 . ?

O41B Zn1 Zn1 142.2(9) 4_554 2_565 ?
N3 Zn1 Zn1 85.0(9) 2_565 2_565 ?
N3A Zn1 Zn1 85.5(6) . 2_565 ?
O1 Zn1 Zn1 38.238(18) . 2_565 ?
O41A Zn1 Zn1 143.2(6) 4_554 2_565 ?
N2A Zn1 Zn1 77.3(5) 2_565 2_565 ?
N2 Zn1 Zn1 75.6(4) . 2_565 ?
O22A Zn2 O21B 144.5(3) 8_667 . ?
O22A Zn2 N4 98.3(9) 8_667 8_667 ?
O21B Zn2 N4 106.2(9) . 8_667 ?
O22A Zn2 N1 109.6(7) 8_667 . ?
O21B Zn2 N1 95.0(7) . . ?
N4 Zn2 N1 92.2(8) 8_667 . ?
O22A Zn2 N4A 97.7(7) 8_667 . ?
O21B Zn2 N4A 106.5(7) . . ?
N4 Zn2 N4A 92.1(8) 8_667 . ?
N1 Zn2 N4A 12.0(11) . . ?
O22A Zn2 N1A 102.1(8) 8_667 8_667 ?
O21B Zn2 N1A 100.8(8) . 8_667 ?
N4 Zn2 N1A 5.9(15) 8_667 8_667 ?
N1 Zn2 N1A 95.2(9) . 8_667 ?
N4A Zn2 N1A 96.0(6) . 8_667 ?
O22A Zn2 O22B 101.1(4) 8_667 . ?
O21B Zn2 O22B 50.0(4) . . ?
N4 Zn2 O22B 100.0(8) 8_667 . ?
N1 Zn2 O22B 144.9(8) . . ?
N4A Zn2 O22B 155.8(7) . . ?
N1A Zn2 O22B 94.7(7) 8_667 . ?
O22A Zn2 C21A 24.4(4) 8_667 8_667 ?
O21B Zn2 C21A 124.3(4) . 8_667 ?
N4 Zn2 C21A 122.7(10) 8_667 8_667 ?
N1 Zn2 C21A 107.1(8) . 8_667 ?
N4A Zn2 C21A 97.2(7) . 8_667 ?
N1A Zn2 C21A 126.2(9) 8_667 8_667 ?
O22B Zn2 C21A 93.8(5) . 8_667 ?
O22A Zn2 O21A 50.9(4) 8_667 8_667 ?
O21B Zn2 O21A 100.9(4) . 8_667 ?
N4 Zn2 O21A 149.1(10) 8_667 8_667 ?
N1 Zn2 O21A 99.9(7) . 8_667 ?
N4A Zn2 O21A 94.2(6) . 8_667 ?
N1A Zn2 O21A 152.3(8) 8_667 8_667 ?
O22B Zn2 O21A 86.2(5) . 8_667 ?
C21A Zn2 O21A 26.5(3) 8_667 8_667 ?
O22A Zn2 C21B 124.0(4) 8_667 . ?
O21B Zn2 C21B 23.9(4) . . ?
N4 Zn2 C21B 106.0(10) 8_667 . ?
N1 Zn2 C21B 118.7(8) . . ?
N4A Zn2 C21B 130.0(7) . . ?
N1A Zn2 C21B 100.1(8) 8_667 . ?
O22B Zn2 C21B 26.2(3) . . ?
C21A Zn2 C21B 109.9(5) 8_667 . ?
O21A Zn2 C21B 92.9(5) 8_667 . ?
Zn1 O1 Zn1 112.524(19) 2_565 8_666 ?
Zn1 O1 Zn1 112.524(19) 2_565 7_566 ?

Zn1 O1 Zn1 103.52(4) 8_666 7_566 ?
Zn1 O1 Zn1 103.52(4) 2_565 . ?
Zn1 O1 Zn1 112.524(19) 8_666 . ?
Zn1 O1 Zn1 112.524(19) 7_566 . ?
N1 C1 N5 118.4(17) . . ?
N1 C1 C4 117.4(18) . . ?
N5 C1 C4 124.2(17) . . ?
C1 N1 C2 121(2) . . ?
C1 N1 Zn2 123.6(17) . . ?
C2 N1 Zn2 113.9(18) . . ?
N2 C2 N1 123(2) . . ?
N2 C2 H2A 118.5 . . ?
N1 C2 H2A 118.5 . . ?
C2 N2 C3 115(2) . . ?
C2 N2 Zn1 118.1(17) . . ?
C3 N2 Zn1 125.6(14) . . ?
C4 C3 N3 115.0(17) . . ?
C4 C3 N2 125.9(18) . . ?
N3 C3 N2 119(2) . . ?
C4 C3 C5 73.1(13) . . ?
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N2 C3 C5 161(2) . . ?
C3 C4 N4 123.0(19) . . ?
C3 C4 C1 117.7(14) . . ?
N4 C4 C1 118.6(19) . . ?
C3 C4 C5 70.0(14) . . ?
N4 C4 C5 53(2) . . ?
C1 C4 C5 171.0(15) . . ?
N3 C5 N4 119(2) . . ?
N3 C5 C3 42.9(13) . . ?
N4 C5 C3 76.0(15) . . ?
N3 C5 C4 79.8(16) . . ?
N4 C5 C4 39.1(11) . . ?
C3 C5 C4 36.9(10) . . ?
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N4 C5 H5A 120.5 . . ?
C3 C5 H5A 163.5 . . ?
C4 C5 H5A 159.5 . . ?
C5 N3 C3 95.1(19) . . ?
C5 N3 Zn1 129.7(18) . 2_565 ?
C3 N3 Zn1 133(2) . 2_565 ?
C4 N4 C5 88(2) . . ?
C4 N4 Zn2 161(2) . 7_567 ?
C5 N4 Zn2 110.0(19) . 7_567 ?
C4A C1A N5A 128.9(18) . . ?
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N5A C1A N1A 124.4(14) . . ?
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C2A N1A Zn2 124(2) . 7_567 ?
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C2A N2A C3A 116.2(18) . . ?
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N2A C3A N3A 128.7(16) .. ?
C4A C3A N3A 108.7(13) .. ?
C1A C4A C3A 122.2(16) .. ?
C1A C4A N4A 129.8(17) .. ?
C3A C4A N4A 107.9(12) .. ?
N4A C5A N3A 117(2) .. ?
N4A C5A H5AA 121.3 .. ?
N3A C5A H5AA 121.3 .. ?
C5A N3A C3A 103.7(15) .. ?
C5A N3A Zn1 128.9(14) .. ?
C3A N3A Zn1 126.1(14) .. ?
C5A N4A C4A 102.3(18) .. ?
C5A N4A Zn2 118.4(14) .. ?
C4A N4A Zn2 137.8(15) .. ?
C21B O21B Zn2 108.5(10) .. ?
C21B O22B Zn2 79.2(10) .. ?
O21B C21B O22B 121.9(16) .. ?
O21B C21B C22B 117.7(15) .. ?
O22B C21B C22B 120.3(16) .. ?
O21B C21B Zn2 47.6(7) .. ?
O22B C21B Zn2 74.6(10) .. ?
C22B C21B Zn2 162.9(13) .. ?
C23B C22B C27B 120.0 .. ?
C23B C22B C21B 118.7(15) .. ?
C27B C22B C21B 121.2(15) .. ?
C22B C23B C24B 120.0 .. ?
C22B C23B H23A 120.0 .. ?
C24B C23B H23A 120.0 .. ?
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C25B C24B H24A 120.0 .. ?
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C24B C25B C26B 120.0 .. ?
C24B C25B C32B 97(2) .. ?
C26B C25B C32B 142(2) .. ?
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C27B C26B H26A 120.0 .. ?
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O42B C40B O41B 118.0(14) .. ?
O42B C40B C41B 116.0(11) .. ?
O41B C40B C41B 120.4(18) .. ?
C46B C41B C42B 105.7(19) .. ?
C46B C41B C40B 128.4(17) .. ?
C42B C41B C40B 125.8(16) .. ?
C43B C42B C41B 124.0(19) .. ?
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C41B C42B H42A 118.0 .. ?
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C43B C44B C45B 117(2) .. ?
C43B C44B C31B 123(2) .. ?
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C44B C45B C46B 114(2) .. ?
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C46B C45B H45A 123.0 .. ?
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C41B C46B H46A 114.1 .. ?
C45B C46B H46A 114.1 .. ?
C32B C31B C44B 124(4) .. ?
C32B C31B H31A 118.0 .. ?
C44B C31B H31A 118.0 .. ?
C31B C32B C25B 147(4) .. ?
C31B C32B H32A 106.5 .. ?
C25B C32B H32A 106.5 .. ?
C21A O21A Zn2 75.9(10) . 7_567 ?
C21A O22A Zn2 106.4(10) . 7_567 ?
O22A C21A O21A 126.8(16) .. ?
O22A C21A C22A 117.0(15) .. ?
O21A C21A C22A 115.8(16) .. ?
O22A C21A Zn2 49.2(7) . 7_567 ?
O21A C21A Zn2 77.7(10) . 7_567 ?
C22A C21A Zn2 163.8(13) . 7_567 ?
C23A C22A C27A 120.0 .. ?
C23A C22A C21A 122.0(14) .. ?
C27A C22A C21A 117.8(14) .. ?
C24A C23A C22A 120.0 .. ?
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C23A C24A C25A 120.0 .. ?
C23A C24A H24B 120.0 .. ?
C25A C24A H24B 120.0 .. ?
C26A C25A C24A 120.0 .. ?
C26A C25A C31A 97(2) .. ?
C24A C25A C31A 143(2) .. ?
C27A C26A C25A 120.0 .. ?
C27A C26A H26B 120.0 .. ?
C25A C26A H26B 120.0 .. ?
C26A C27A C22A 120.0 .. ?
C26A C27A H27B 120.0 .. ?
C22A C27A H27B 120.0 .. ?
C46A C41A C42A 115(2) .. ?
C43A C42A C41A 119(2) .. ?
C43A C42A H42B 120.4 .. ?
C41A C42A H42B 120.4 .. ?
C42A C43A C44A 129(2) .. ?
C42A C43A H43B 115.5 .. ?
C44A C43A H43B 115.5 .. ?
C45A C44A C43A 108(2) .. ?
C45A C44A C32A 119(2) .. ?
C43A C44A C32A 133(3) .. ?
C44A C45A C46A 127(3) .. ?

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C46A C45A H45B 116.5 . . ?
C41A C46A C45A 119(3) . . ?
C41A C46A H46B 120.3 . . ?
C45A C46A H46B 120.3 . . ?
C32A C31A C25A 146(4) . . ?
C32A C31A H31B 106.9 . . ?
C25A C31A H31B 106.9 . . ?
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C31A C32A H32B 122.8 . . ?
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