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C7 C 0.4752(9) 0.3887(6) 0.2637(3) 0.051(2) Uani 0.804(8) 1 d PDU A 1
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F3A 0.137(5) 0.058(3) 0.066(3) 0.003(2) -0.023(3) 0.014(3)
F4A 0.149(6) 0.067(3) 0.070(3) -0.007(3) -0.037(3) -0.005(3)
F1B 0.058(9) 0.081(10) 0.111(11) 0.006(8) 0.017(8) 0.000(8)
F2B 0.071(10) 0.090(11) 0.121(11) -0.011(8) 0.029(8) 0.008(8)
F3B 0.107(11) 0.082(10) 0.051(8) 0.009(7) 0.024(7) -0.001(8)
F4B 0.109(11) 0.099(11) 0.070(9) 0.007(8) 0.012(8) 0.005(9)

_geom_special_details
;
 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.
;

loop_
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Co N11_b 1.935(16) . ?
Co N1_b 1.954(16) . ?
Co N8 1.964(4) . Y
Co N16 1.974(4) . Y
Co N1 1.976(5) . Y
Co N4 1.978(5) . Y
Co N15 1.989(4) . Y
Co N11 1.989(5) . Y
Co N8_b 1.998(16) . ?
Co N4_b 2.025(15) . ?
N1 C14 1.470(8) . ?
N1 C2 1.484(9) . ?
N1 H1 0.9100 . ?
C2 C3 1.515(9) . ?
C2 H2A 0.9700 . ?
C2 H2B 0.9700 . ?
C3 N4 1.479(9) . ?
C3 H3A 0.9700 . ?
C3 H3B 0.9700 . ?
N4 C5 1.487(9) . ?
N4 H4 0.9100 . ?
C5 C6 1.458(13) . ?
C5 H5A 0.9700 . ?
C5 H5B 0.9700 . ?
C6 C7 1.539(11) . ?
C6 H6A 0.9700 . ?
C6 H6B 0.9700 . ?
C7 N8 1.485(8) . ?
C7 H7A 0.9700 . ?
C7 H7B 0.9700 . ?
N8 C9 1.467(9) . ?
N8 H8 0.9100 . ?
C9 C10 1.531(9) . ?
C9 H9A 0.9700 . ?
C9 H9B 0.9700 . ?
C10 N11 1.490(8) . ?
C10 H10A 0.9700 . ?
C10 H10B 0.9700 . ?
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N11 C12 1.470(8) . ?
N11 H11 0.9100 . ?
C12 C13 1.518(12) . ?
C12 H12A 0.9700 . ?
C12 H12B 0.9700 . ?
C13 C14 1.535(11) . ?
C13 H13A 0.9700 . ?
C13 H13B 0.9700 . ?
C14 H14A 0.9700 . ?
C14 H14B 0.9700 . ?
N1_b C14_b 1.481(18) . ?
N1_b C2_b 1.495(19) . ?
N1_b H1_b 0.9100 . ?
C2_b C3_b 1.526(18) . ?
C2_b H2A_b 0.9700 . ?
C2_b H2B_b 0.9700 . ?
C3_b N4_b 1.452(18) . ?
C3_b H3A_b 0.9700 . ?
C3_b H3B_b 0.9700 . ?
N4_b C5_b 1.492(18) . ?
N4_b H4_b 0.9100 . ?
C5_b C6_b 1.47(2) . ?
C5_b H5A_b 0.9700 . ?
C5_b H5B_b 0.9700 . ?
C6_b C7_b 1.54(2) . ?
C6_b H6A_b 0.9700 . ?
C6_b H6B_b 0.9700 . ?
C7_b N8_b 1.469(19) . ?
C7_b H7A_b 0.9700 . ?
C7_b H7B_b 0.9700 . ?
N8_b C9_b 1.465(19) . ?
N8_b H8_b 0.9100 . ?
C9_b C10_b 1.539(18) . ?
C9_b H9A_b 0.9700 . ?
C9_b H9B_b 0.9700 . ?
C10_b N11_b 1.465(18) . ?
C10_b H10A_b 0.9700 . ?
C10_b H10B_b 0.9700 . ?
N11_b C12_b 1.474(19) . ?
N11_b H11_b 0.9100 . ?
C12_b C13_b 1.52(2) . ?
C12_b H12A_b 0.9700 . ?
C12_b H12B_b 0.9700 . ?
C13_b C14_b 1.51(2) . ?
C13_b H13A_b 0.9700 . ?
C13_b H13B_b 0.9700 . ?
C14_b H14A_b 0.9700 . ?
C14_b H14B_b 0.9700 . ?
N15 H15A 0.8900 . ?
N15 H15B 0.8900 . ?
N15 H15C 0.8900 . ?
N16 H16A 0.8900 . ?
N16 H16B 0.8900 . ?
N16 H16C 0.8900 . ?
B F2B 1.33(2) . ?
B F1B 1.34(2) . ?
B F4A 1.367(7) . ?
B F1A 1.369(8) . ?
B F2A 1.371(8) . ?
B F3A 1.378(7) . ?
B F4B 1.38(2) . ?
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B F3B 1.421(18) . ?

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N11_b Co N8 68.7(6) . . ?
N1_b Co N8 164.2(5) . . ?
N11_b Co N16 85.9(8) . . ?
N1_b Co N16 91.0(9) . . ?
N8 Co N16 91.64(19) . . Y
N11_b Co N1 110.6(6) . . ?
N1_b Co N1 15.0(5) . . ?
N8 Co N1 179.0(3) . . Y
N16 Co N1 88.9(2) . . Y
N11_b Co N4 162.2(5) . . ?
N1_b Co N4 101.6(5) . . ?
N8 Co N4 93.9(3) . . Y
N16 Co N4 90.6(2) . . Y
N1 Co N4 86.8(3) . . Y
N11_b Co N15 93.9(8) . . ?
N1_b Co N15 89.1(9) . . ?
N8 Co N15 88.24(19) . . Y
N16 Co N15 179.83(16) . . Y
N1 Co N15 91.2(2) . . Y
N4 Co N15 89.5(2) . . Y
N11_b Co N11 18.1(5) . . ?
N1_b Co N11 78.2(5) . . ?
N8 Co N11 86.3(2) . . Y
N16 Co N11 89.76(18) . . Y
N1 Co N11 93.0(3) . . Y
N4 Co N11 179.6(3) . . Y
N15 Co N11 90.11(18) . . Y
N11_b Co N8_b 87.0(7) . . ?
N1_b Co N8_b 176.9(8) . . ?
N8 Co N8_b 18.9(5) . . ?
N16 Co N8_b 88.4(8) . . ?
N1 Co N8_b 162.0(6) . . ?
N4 Co N8_b 75.4(6) . . ?
N15 Co N8_b 91.5(8) . . ?
N11 Co N8_b 104.9(5) . . ?
N11_b Co N4_b 178.2(8) . . ?
N1_b Co N4_b 85.7(6) . . ?
N8 Co N4_b 109.7(5) . . ?
N16 Co N4_b 93.3(8) . . ?
N1 Co N4_b 71.0(5) . . ?
N4 Co N4_b 16.1(4) . . ?
N15 Co N4_b 86.9(8) . . ?
N11 Co N4_b 163.6(5) . . ?
N8_b Co N4_b 91.3(6) . . ?
C14 N1 C2 111.8(5) . . ?
C14 N1 Co 120.0(5) . . ?
C2 N1 Co 108.0(4) . . ?
C14 N1 H1 105.3 . . ?
C2 N1 H1 105.3 . . ?
Co N1 H1 105.3 . . ?
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N1 C2 C3 107.9(5) . . ?
N1 C2 H2A 110.1 . . ?
C3 C2 H2A 110.1 . . ?
N1 C2 H2B 110.1 . . ?
C3 C2 H2B 110.1 . . ?
H2A C2 H2B 108.4 . . ?
N4 C3 C2 107.6(5) . . ?
N4 C3 H3A 110.2 . . ?
C2 C3 H3A 110.2 . . ?
N4 C3 H3B 110.2 . . ?
C2 C3 H3B 110.2 . . ?
H3A C3 H3B 108.5 . . ?
C3 N4 C5 111.7(6) . . ?
C3 N4 Co 107.4(4) . . ?
C5 N4 Co 120.3(5) . . ?
C3 N4 H4 105.4 . . ?
C5 N4 H4 105.4 . . ?
Co N4 H4 105.4 . . ?
C6 C5 N4 112.4(6) . . ?
C6 C5 H5A 109.1 . . ?
N4 C5 H5A 109.1 . . ?
C6 C5 H5B 109.1 . . ?
N4 C5 H5B 109.1 . . ?
H5A C5 H5B 107.9 . . ?
C5 C6 C7 117.0(6) . . ?
C5 C6 H6A 108.1 . . ?
C7 C6 H6A 108.1 . . ?
C5 C6 H6B 108.1 . . ?
C7 C6 H6B 108.1 . . ?
H6A C6 H6B 107.3 . . ?
N8 C7 C6 110.4(5) . . ?
N8 C7 H7A 109.6 . . ?
C6 C7 H7A 109.6 . . ?
N8 C7 H7B 109.6 . . ?
C6 C7 H7B 109.6 . . ?
H7A C7 H7B 108.1 . . ?
C9 N8 C7 111.1(5) . . ?
C9 N8 Co 109.2(4) . . ?
C7 N8 Co 119.6(4) . . ?
C9 N8 H8 105.2 . . ?
C7 N8 H8 105.2 . . ?
Co N8 H8 105.2 . . ?
N8 C9 C10 107.8(5) . . ?
N8 C9 H9A 110.1 . . ?
C10 C9 H9A 110.1 . . ?
N8 C9 H9B 110.1 . . ?
C10 C9 H9B 110.1 . . ?
H9A C9 H9B 108.5 . . ?
N11 C10 C9 106.6(5) . . ?
N11 C10 H10A 110.4 . . ?
C9 C10 H10A 110.4 . . ?
N11 C10 H10B 110.4 . . ?
C9 C10 H10B 110.4 . . ?
H10A C10 H10B 108.6 . . ?
C12 N11 C10 109.7(5) . . ?
C12 N11 Co 122.1(5) . . ?
C10 N11 Co 107.8(4) . . ?
C12 N11 H11 105.3 . . ?
C10 N11 H11 105.3 . . ?
Co N11 H11 105.3 . . ?
N11 C12 C13 111.0(5) . . ?
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N11 C12 H12A 109.4 . . ?
C13 C12 H12A 109.4 . . ?
N11 C12 H12B 109.4 . . ?
C13 C12 H12B 109.4 . . ?
H12A C12 H12B 108.0 . . ?
C12 C13 C14 115.8(5) . . ?
C12 C13 H13A 108.3 . . ?
C14 C13 H13A 108.3 . . ?
C12 C13 H13B 108.3 . . ?
C14 C13 H13B 108.3 . . ?
H13A C13 H13B 107.4 . . ?
N1 C14 C13 110.5(6) . . ?
N1 C14 H14A 109.6 . . ?
C13 C14 H14A 109.6 . . ?
N1 C14 H14B 109.6 . . ?
C13 C14 H14B 109.6 . . ?
H14A C14 H14B 108.1 . . ?
C14_b N1_b C2_b 108.8(16) . . ?
C14_b N1_b Co 121.8(16) . . ?
C2_b N1_b Co 108.9(12) . . ?
C14_b N1_b H1_b 105.4 . . ?
C2_b N1_b H1_b 105.4 . . ?
Co N1_b H1_b 105.4 . . ?
N1_b C2_b C3_b 107.4(14) . . ?
N1_b C2_b H2A_b 110.2 . . ?
C3_b C2_b H2A_b 110.2 . . ?
N1_b C2_b H2B_b 110.2 . . ?
C3_b C2_b H2B_b 110.2 . . ?
H2A_b C2_b H2B_b 108.5 . . ?
N4_b C3_b C2_b 108.4(15) . . ?
N4_b C3_b H3A_b 110.0 . . ?
C2_b C3_b H3A_b 110.0 . . ?
N4_b C3_b H3B_b 110.0 . . ?
C2_b C3_b H3B_b 110.0 . . ?
H3A_b C3_b H3B_b 108.4 . . ?
C3_b N4_b C5_b 112.8(15) . . ?
C3_b N4_b Co 108.7(10) . . ?
C5_b N4_b Co 118.4(16) . . ?
C3_b N4_b H4_b 105.2 . . ?
C5_b N4_b H4_b 105.2 . . ?
Co N4_b H4_b 105.2 . . ?
C6_b C5_b N4_b 111.0(18) . . ?
C6_b C5_b H5A_b 109.4 . . ?
N4_b C5_b H5A_b 109.4 . . ?
C6_b C5_b H5B_b 109.4 . . ?
N4_b C5_b H5B_b 109.4 . . ?
H5A_b C5_b H5B_b 108.0 . . ?
C5_b C6_b C7_b 117.3(19) . . ?
C5_b C6_b H6A_b 108.0 . . ?
C7_b C6_b H6A_b 108.0 . . ?
C5_b C6_b H6B_b 108.0 . . ?
C7_b C6_b H6B_b 108.0 . . ?
H6A_b C6_b H6B_b 107.2 . . ?
N8_b C7_b C6_b 111.3(17) . . ?
N8_b C7_b H7A_b 109.4 . . ?
C6_b C7_b H7A_b 109.4 . . ?
N8_b C7_b H7B_b 109.4 . . ?
C6_b C7_b H7B_b 109.4 . . ?
H7A_b C7_b H7B_b 108.0 . . ?
C9_b N8_b C7_b 111.8(15) . . ?
C9_b N8_b Co 107.5(12) . . ?
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C7_b N8_b Co 125.3(15) . . ?
C9_b N8_b H8_b 103.2 . . ?
C7_b N8_b H8_b 103.2 . . ?
Co N8_b H8_b 103.2 . . ?
N8_b C9_b C10_b 107.6(15) . . ?
N8_b C9_b H9A_b 110.2 . . ?
C10_b C9_b H9A_b 110.2 . . ?
N8_b C9_b H9B_b 110.2 . . ?
C10_b C9_b H9B_b 110.2 . . ?
H9A_b C9_b H9B_b 108.5 . . ?
N11_b C10_b C9_b 107.6(15) . . ?
N11_b C10_b H10A_b 110.2 . . ?
C9_b C10_b H10A_b 110.2 . . ?
N11_b C10_b H10B_b 110.2 . . ?
C9_b C10_b H10B_b 110.2 . . ?
H10A_b C10_b H10B_b 108.5 . . ?
C10_b N11_b C12_b 110.1(16) . . ?
C10_b N11_b Co 108.7(11) . . ?
C12_b N11_b Co 115.9(17) . . ?
C10_b N11_b H11_b 107.3 . . ?
C12_b N11_b H11_b 107.3 . . ?
Co N11_b H11_b 107.3 . . ?
N11_b C12_b C13_b 111.2(18) . . ?
N11_b C12_b H12A_b 109.4 . . ?
C13_b C12_b H12A_b 109.4 . . ?
N11_b C12_b H12B_b 109.4 . . ?
C13_b C12_b H12B_b 109.4 . . ?
H12A_b C12_b H12B_b 108.0 . . ?
C14_b C13_b C12_b 117.8(18) . . ?
C14_b C13_b H13A_b 107.9 . . ?
C12_b C13_b H13A_b 107.9 . . ?
C14_b C13_b H13B_b 107.9 . . ?
C12_b C13_b H13B_b 107.9 . . ?
H13A_b C13_b H13B_b 107.2 . . ?
N1_b C14_b C13_b 110.0(15) . . ?
N1_b C14_b H14A_b 109.7 . . ?
C13_b C14_b H14A_b 109.7 . . ?
N1_b C14_b H14B_b 109.7 . . ?
C13_b C14_b H14B_b 109.7 . . ?
H14A_b C14_b H14B_b 108.2 . . ?
Co N15 H15A 109.5 . . ?
Co N15 H15B 109.5 . . ?
H15A N15 H15B 109.5 . . ?
Co N15 H15C 109.5 . . ?
H15A N15 H15C 109.5 . . ?
H15B N15 H15C 109.5 . . ?
Co N16 H16A 109.5 . . ?
Co N16 H16B 109.5 . . ?
H16A N16 H16B 109.5 . . ?
Co N16 H16C 109.5 . . ?
H16A N16 H16C 109.5 . . ?
H16B N16 H16C 109.5 . . ?
F2B B F1B 108.7(13) . . ?
F4A B F1A 107.0(6) . . ?
F4A B F2A 113.9(7) . . ?
F1A B F2A 107.7(5) . . ?
F4A B F3A 109.5(5) . . ?
F1A B F3A 112.3(7) . . ?
F2A B F3A 106.5(6) . . ?
F2B B F4B 108.3(15) . . ?
F1B B F4B 116.9(16) . . ?
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F2B B F3B 109.9(15) . . ?
F1B B F3B 111.4(14) . . ?
F4B B F3B 101.2(12) . . ?

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N8 Co N1 C14 0(16) . . . . ?
N16 Co N1 C14 127.7(5) . . . . ?
N4 Co N1 C14 -141.6(6) . . . . ?
N15 Co N1 C14 -52.2(5) . . . . ?
N11 Co N1 C14 38.0(6) . . . . ?
N8 Co N1 C2 130(16) . . . . ?
N16 Co N1 C2 -102.7(5) . . . . ?
N4 Co N1 C2 -12.0(5) . . . . ?
N15 Co N1 C2 77.4(5) . . . . ?
N11 Co N1 C2 167.6(5) . . . . ?
C14 N1 C2 C3 171.4(6) . . . . ?
Co N1 C2 C3 37.3(7) . . . . ?
N1 C2 C3 N4 -52.0(7) . . . . ?
C2 C3 N4 C5 174.6(6) . . . . ?
C2 C3 N4 Co 40.6(6) . . . . ?
N16 Co N4 C3 72.7(5) . . . . ?
N1 Co N4 C3 -16.2(5) . . . . ?
N15 Co N4 C3 -107.4(5) . . . . ?
N11 Co N4 C3 -76(40) . . . . ?
N8 Co N4 C5 35.2(6) . . . . ?
N16 Co N4 C5 -56.5(6) . . . . ?
N1 Co N4 C5 -145.4(6) . . . . ?
N15 Co N4 C5 123.4(6) . . . . ?
N11 Co N4 C5 155(40) . . . . ?
C3 N4 C5 C6 -178.4(7) . . . . ?
Co N4 C5 C6 -51.1(8) . . . . ?
N4 C5 C6 C7 64.7(9) . . . . ?
C5 C6 C7 N8 -66.6(8) . . . . ?
C6 C7 N8 C9 -176.9(6) . . . . ?
C6 C7 N8 Co 54.3(7) . . . . ?
N16 Co N8 C9 -76.7(5) . . . . ?
N1 Co N8 C9 51(16) . . . . ?
N4 Co N8 C9 -167.4(5) . . . . ?
N15 Co N8 C9 103.2(5) . . . . ?
N11 Co N8 C9 13.0(5) . . . . ?
N16 Co N8 C7 52.9(5) . . . . ?
N1 Co N8 C7 -180(100) . . . . ?
N4 Co N8 C7 -37.8(5) . . . . ?
N15 Co N8 C7 -127.2(5) . . . . ?
N11 Co N8 C7 142.6(5) . . . . ?
C7 N8 C9 C10 -172.5(5) . . . . ?
Co N8 C9 C10 -38.4(7) . . . . ?
N8 C9 C10 N11 51.7(7) . . . . ?
C9 C10 N11 C12 -174.9(5) . . . . ?
C9 C10 N11 Co -39.8(6) . . . . ?
N16 Co N11 C12 -124.3(5) . . . . ?
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N1 Co N11 C12 -35.3(6) . . . . ?
N4 Co N11 C12 24(40) . . . . ?
N15 Co N11 C12 55.9(5) . . . . ?
N8 Co N11 C10 15.8(4) . . . . ?
N16 Co N11 C10 107.4(4) . . . . ?
N1 Co N11 C10 -163.6(4) . . . . ?
N4 Co N11 C10 -104(40) . . . . ?
N15 Co N11 C10 -72.5(4) . . . . ?
C10 N11 C12 C13 178.1(6) . . . . ?
Co N11 C12 C13 50.6(8) . . . . ?
N11 C12 C13 C14 -64.1(8) . . . . ?
C2 N1 C14 C13 175.6(6) . . . . ?
Co N1 C14 C13 -56.5(7) . . . . ?
C12 C13 C14 N1 67.9(8) . . . . ?
N11_b Co N1_b C14_b 36(2) . . . . ?
N8 Co N1_b C14_b 23(5) . . . . ?
N8_b Co N1_b C14_b -160(22) . . . . ?
N4_b Co N1_b C14_b -145(2) . . . . ?
N11_b Co N1_b C2_b 164.0(18) . . . . ?
N8_b Co N1_b C2_b -32(24) . . . . ?
N4_b Co N1_b C2_b -16.7(19) . . . . ?
C14_b N1_b C2_b C3_b 175(2) . . . . ?
Co N1_b C2_b C3_b 40(3) . . . . ?
N1_b C2_b C3_b N4_b -50(3) . . . . ?
C2_b C3_b N4_b C5_b 169(2) . . . . ?
C2_b C3_b N4_b Co 36(3) . . . . ?
N11_b Co N4_b C3_b 144(35) . . . . ?
N1_b Co N4_b C3_b -11.0(19) . . . . ?
N8_b Co N4_b C3_b 168.2(18) . . . . ?
N11_b Co N4_b C5_b 14(37) . . . . ?
N1_b Co N4_b C5_b -141(2) . . . . ?
N8_b Co N4_b C5_b 38(2) . . . . ?
C3_b N4_b C5_b C6_b 172(2) . . . . ?
Co N4_b C5_b C6_b -60(3) . . . . ?
N4_b C5_b C6_b C7_b 70(3) . . . . ?
C5_b C6_b C7_b N8_b -60(4) . . . . ?
C6_b C7_b N8_b C9_b 177(3) . . . . ?
C6_b C7_b N8_b Co 44(4) . . . . ?
N11_b Co N8_b C9_b 13(2) . . . . ?
N1_b Co N8_b C9_b -152(23) . . . . ?
N4_b Co N8_b C9_b -166.6(19) . . . . ?
N11_b Co N8_b C7_b 147(2) . . . . ?
N1_b Co N8_b C7_b -17(24) . . . . ?
N4_b Co N8_b C7_b -32(2) . . . . ?
C7_b N8_b C9_b C10_b -178(2) . . . . ?
Co N8_b C9_b C10_b -37(3) . . . . ?
N8_b C9_b C10_b N11_b 51(3) . . . . ?
C9_b C10_b N11_b C12_b -168(2) . . . . ?
C9_b C10_b N11_b Co -40(2) . . . . ?
N1_b Co N11_b C10_b -165.0(18) . . . . ?
N8 Co N11_b C10_b 11.1(15) . . . . ?
N8_b Co N11_b C10_b 15.9(18) . . . . ?
N4_b Co N11_b C10_b 40(37) . . . . ?
N1_b Co N11_b C12_b -40(2) . . . . ?
N8_b Co N11_b C12_b 140(2) . . . . ?
N4_b Co N11_b C12_b 165(35) . . . . ?
C10_b N11_b C12_b C13_b -178(2) . . . . ?
Co N11_b C12_b C13_b 59(3) . . . . ?
N11_b C12_b C13_b C14_b -69(3) . . . . ?
C2_b N1_b C14_b C13_b -175(2) . . . . ?
Co N1_b C14_b C13_b -47(3) . . . . ?
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C12_b C13_b C14_b N1_b 61(3) . . . . ?

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N4 H4 Cl1  0.91 2.38 3.256(7) 161.7 .
N8 H8 Cl2  0.91 2.28 3.179(5) 167.8 2_545
N11 H11 Cl2  0.91 2.40 3.275(6) 161.4 2_645
N1_b H1_b Cl1  0.91 2.37 3.26(3) 164.7 1_655
N4_b H4_b Cl1  0.91 2.25 3.15(3) 168.5 .
N8_b H8_b Cl2  0.91 2.41 3.28(3) 161.3 2_545
N11_b H11_b Cl2  0.91 2.28 3.18(3) 169.1 2_645
N15 H15A F3B  0.89 2.17 2.817(17) 129.4 4_566
N15 H15A F1A  0.89 2.39 3.227(6) 155.8 4_566
N15 H15A F4A  0.89 2.61 3.159(7) 120.5 4_566
N15 H15A F2B  0.89 2.99 3.82(3) 155.5 4_566
N15 H15B Cl1  0.89 2.43 3.271(4) 157.4 .
N15 H15C Cl2  0.89 2.47 3.345(4) 168.7 2_545
N16 H16A F4B  0.89 2.26 2.91(2) 129.0 .
N16 H16A F2A  0.89 2.36 3.196(6) 157.3 .
N16 H16A F3A  0.89 2.64 3.154(7) 117.7 .
N16 H16A F1B  0.89 3.04 3.84(2) 150.7 .
N16 H16B Cl1  0.89 2.47 3.335(4) 164.5 1_655
N16 H16C Cl2  0.89 2.43 3.288(4) 162.0 2_645

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_refine_diff_density_rms    0.073
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 'H'  'H'   0.0000   0.0000
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 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Co'  'Co'   0.3494   0.9721
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    P1-

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-x, -y, -z'

_cell_length_a                    7.3988(14)
_cell_length_b                    8.5682(16)
_cell_length_c                    9.209(3)
_cell_angle_alpha                 89.02(2)
_cell_angle_beta                  76.64(3)
_cell_angle_gamma                 82.340(16)
_cell_volume                      562.9(2)
_cell_formula_units_Z             1
_cell_measurement_temperature     293(1)
_cell_measurement_reflns_used     25
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 'bis-(nitrato)(1,4,8,11-tetraazacyclotetradecane)cobalt(III) nitrate'
;

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_diffrn_reflns_number             3170
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_computing_cell_refinement        'CAD-4 Software'
_computing_data_reduction         'PROCESS_DATA (Gable et al., 1993)'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
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_computing_molecular_graphics     'ORTEP3 for WINDOWS (Farrugia, 1997)'
_computing_publication_material   SHELXL

_refine_special_details
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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^ > 2sigma(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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_refine_ls_weighting_details
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_atom_sites_solution_secondary    difmap
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Co Co 0.0000 0.0000 0.0000 0.02612(16) Uani 1 2 d S . .
N1 N 0.1565(3) -0.1415(2) 0.1075(2) 0.0337(4) Uani 1 1 d . . .
H1 H 0.2748 -0.1158 0.0773 0.042(8) Uiso 1 1 calc R . .
C2 C 0.0943(4) -0.1000(4) 0.2687(3) 0.0451(6) Uani 1 1 d . . .
H2A H 0.1927 -0.1371 0.3196 0.065(11) Uiso 1 1 calc R . .
H2B H -0.0161 -0.1486 0.3137 0.050(9) Uiso 1 1 calc R . .
C3 C 0.0507(4) 0.0752(4) 0.2816(3) 0.0472(7) Uani 1 1 d . . .
H3A H -0.0046 0.1067 0.3846 0.054(10) Uiso 1 1 calc R . .
H3B H 0.1644 0.1232 0.2481 0.053(9) Uiso 1 1 calc R . .
N4 N 0.0832(3) -0.1264(3) -0.1867(2) 0.0362(5) Uani 1 1 d . . .
H4A H 0.1954 -0.0973 -0.2348 0.040(8) Uiso 1 1 calc R . .
C5 C 0.1126(5) -0.3016(3) -0.1764(4) 0.0513(7) Uani 1 1 d . . .
H5A H 0.1606 -0.3467 -0.2760 0.062(11) Uiso 1 1 calc R . .
H5B H -0.0071 -0.3383 -0.1355 0.045(9) Uiso 1 1 calc R . .
C6 C 0.2466(5) -0.3593(4) -0.0807(4) 0.0543(8) Uani 1 1 d . . .
H6A H 0.3633 -0.3164 -0.1176 0.054(10) Uiso 1 1 calc R . .
H6B H 0.2738 -0.4731 -0.0898 0.094(15) Uiso 1 1 calc R . .
C7 C 0.1726(4) -0.3144(3) 0.0831(4) 0.0456(6) Uani 1 1 d . . .
H7A H 0.0504 -0.3487 0.1185 0.040(8) Uiso 1 1 calc R . .
H7B H 0.2563 -0.3681 0.1405 0.057(10) Uiso 1 1 calc R . .
O15 O 0.1816(2) 0.1425(2) -0.0607(2) 0.0381(4) Uani 1 1 d . . .
N16 N 0.3616(3) 0.1129(3) -0.1140(2) 0.0378(5) Uani 1 1 d . . .
O17 O 0.4380(3) -0.0235(3) -0.1392(3) 0.0490(5) Uani 1 1 d . . .
O18 O 0.4454(3) 0.2270(3) -0.1357(3) 0.0631(7) Uani 1 1 d . . .
N19A N 0.2270(11) -0.5521(7) -0.5548(7) 0.0659(17) Uiso 0.50 1 d PD A 1
O20A O 0.1269(12) -0.4317(8) -0.5392(8) 0.097(2) Uiso 0.50 1 d PD A 1
O21A O 0.2971(12) -0.6224(9) -0.6730(7) 0.076(2) Uiso 0.50 1 d PD A 1
```

```
O22A O 0.2593(11) -0.6201(8) -0.4334(7) 0.0843(18) Uiso 0.50 1 d PD A 1
H22A H 0.3478 -0.6906 -0.4556 0.093 Uiso 0.50 1 calc PR A 1
N19B N 0.3154(12) -0.5502(8) -0.5637(8) 0.0740(19) Uiso 0.50 1 d PD B 2
O20B O 0.2618(13) -0.4153(9) -0.5647(9) 0.107(2) Uiso 0.50 1 d PD B 2
O21B O 0.3482(18) -0.6505(13) -0.6620(10) 0.134(5) Uiso 0.50 1 d PD B 2
O22B O 0.3535(11) -0.6030(8) -0.4383(7) 0.0846(18) Uiso 0.50 1 d PD B 2
H22B H 0.3871 -0.6982 -0.4460 0.093 Uiso 0.50 1 calc PR B 2
N23 N 0.478(3) -0.021(2) -0.4870(19) 0.054(3) Uani 0.50 1 d P . .
O24 O 0.3475(12) 0.0849(9) -0.4413(11) 0.082(2) Uani 0.50 1 d P . .
O26 O 0.6394(11) 0.0050(12) -0.5382(8) 0.0725(18) Uani 0.50 1 d P . .
O25 O 0.4398(9) -0.1586(8) -0.4729(9) 0.0869(19) Uani 0.50 1 d P . .

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N1 0.0258(9) 0.0392(11) 0.0363(10) 0.0058(8) -0.0075(8) -0.0044(8)
C2 0.0410(14) 0.0616(18) 0.0339(12) 0.0092(12) -0.0114(11) -0.0069(12)
C3 0.0477(15) 0.0634(18) 0.0333(12) -0.0057(12) -0.0136(11) -0.0090(13)
N4 0.0327(10) 0.0408(11) 0.0332(10) -0.0052(8) -0.0035(8) -0.0048(8)
C5 0.0563(18) 0.0393(14) 0.0548(17) -0.0153(12) -0.0065(14) -0.0028(12)
C6 0.0493(17) 0.0350(14) 0.072(2) -0.0074(13) -0.0061(15) 0.0063(12)
C7 0.0375(13) 0.0373(13) 0.0613(17) 0.0108(12) -0.0121(12) -0.0025(11)
O15 0.0243(8) 0.0386(9) 0.0496(10) 0.0037(8) -0.0041(7) -0.0060(7)
N16 0.0260(9) 0.0466(12) 0.0416(11) 0.0097(9) -0.0084(8) -0.0084(9)
O17 0.0296(9) 0.0514(12) 0.0594(12) 0.0027(9) 0.0000(8) 0.0002(8)
O18 0.0338(10) 0.0546(13) 0.103(2) 0.0209(13) -0.0142(11) -0.0179(9)
N23 0.047(10) 0.067(11) 0.041(6) 0.005(5) -0.002(6) 0.001(6)
O24 0.054(3) 0.067(4) 0.108(6) 0.016(4) 0.010(3) 0.005(4)
O26 0.040(3) 0.105(6) 0.065(4) 0.006(4) 0.004(3) -0.011(5)
O25 0.068(4) 0.070(4) 0.113(5) -0.010(4) -0.003(3) -0.005(3)

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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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Co O15 1.9173(17) . Y
Co N1 1.976(2) . Y
Co N1 1.976(2) 2 Y
Co N4 1.976(2) . Y
Co N4 1.976(2) 2 Y
N1 C2 1.484(3) . ?
N1 C7 1.488(3) . ?
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N1 H1 0.9100 . ?
C2 C3 1.494(5) . ?
C2 H2A 0.9700 . ?
C2 H2B 0.9700 . ?
C3 N4 1.486(4) 2 ?
C3 H3A 0.9700 . ?
C3 H3B 0.9700 . ?
N4 C3 1.486(4) 2 ?
N4 C5 1.493(4) . ?
N4 H4A 0.9100 . ?
C5 C6 1.505(5) . ?
C5 H5A 0.9700 . ?
C5 H5B 0.9700 . ?
C6 C7 1.518(5) . ?
C6 H6A 0.9700 . ?
C6 H6B 0.9700 . ?
C7 H7A 0.9700 . ?
C7 H7B 0.9700 . ?
O15 N16 1.300(3) . ?
N16 O18 1.216(3) . ?
N16 O17 1.229(3) . ?
N19A O20A 1.177(8) . ?
N19A O21A 1.223(7) . ?
N19A O22A 1.308(7) . ?
O22A H22A 0.8200 . ?
N19B O20B 1.172(8) . ?
N19B O21B 1.220(8) . ?
N19B O22B 1.309(7) . ?
O22B H22B 0.8200 . ?
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N23 O26 0.84(2) 2_654 ?
N23 O26 1.224(19) . ?
N23 O24 1.24(3) . ?
N23 O25 1.246(18) . ?
N23 O24 1.35(2) 2_654 ?
N23 O25 1.732(13) 2_654 ?
O24 O26 0.785(9) 2_654 ?
O24 N23 1.35(2) 2_654 ?
O24 O25 1.781(11) 2_654 ?
O26 O24 0.785(9) 2_654 ?
O26 N23 0.84(2) 2_654 ?
O26 O25 1.362(12) 2_654 ?
O25 O26 1.362(12) 2_654 ?
O25 N23 1.732(13) 2_654 ?
O25 O24 1.781(11) 2_654 ?

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O15 Co N1 85.22(8) 2 . Y
O15 Co N1 94.78(8) . . Y
O15 Co N1 94.78(8) 2 2 Y
O15 Co N1 85.22(8) . 2 Y
N1 Co N1 180.00(10) . 2 Y
O15 Co N4 85.96(9) 2 . Y
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```
O15 Co N4 94.04(9) . . Y
N1 Co N4 93.60(9) . . Y
N1 Co N4 86.40(9) 2 . Y
O15 Co N4 94.04(9) 2 2 Y
O15 Co N4 85.96(9) . 2 Y
N1 Co N4 86.40(9) . 2 Y
N1 Co N4 93.60(9) 2 2 Y
N4 Co N4 180.0(2) . 2 Y
C2 N1 C7 111.0(2) . . ?
C2 N1 Co 107.94(16) . . ?
C7 N1 Co 118.68(17) . . ?
C2 N1 H1 106.1 . . ?
C7 N1 H1 106.1 . . ?
Co N1 H1 106.1 . . ?
N1 C2 C3 107.5(2) . . ?
N1 C2 H2A 110.2 . . ?
C3 C2 H2A 110.2 . . ?
N1 C2 H2B 110.2 . . ?
C3 C2 H2B 110.2 . . ?
H2A C2 H2B 108.5 . . ?
N4 C3 C2 107.7(2) 2 . ?
N4 C3 H3A 110.2 2 . ?
C2 C3 H3A 110.2 . . ?
N4 C3 H3B 110.2 2 . ?
C2 C3 H3B 110.2 . . ?
H3A C3 H3B 108.5 . . ?
C3 N4 C5 110.8(2) 2 . ?
C3 N4 Co 107.22(17) 2 . ?
C5 N4 Co 118.59(18) . . ?
C3 N4 H4A 106.5 2 . ?
C5 N4 H4A 106.5 . . ?
Co N4 H4A 106.5 . . ?
N4 C5 C6 112.8(2) . . ?
N4 C5 H5A 109.0 . . ?
C6 C5 H5A 109.0 . . ?
N4 C5 H5B 109.0 . . ?
C6 C5 H5B 109.0 . . ?
H5A C5 H5B 107.8 . . ?
C5 C6 C7 113.5(2) . . ?
C5 C6 H6A 108.9 . . ?
C7 C6 H6A 108.9 . . ?
C5 C6 H6B 108.9 . . ?
C7 C6 H6B 108.9 . . ?
H6A C6 H6B 107.7 . . ?
N1 C7 C6 111.6(2) . . ?
N1 C7 H7A 109.3 . . ?
C6 C7 H7A 109.3 . . ?
N1 C7 H7B 109.3 . . ?
C6 C7 H7B 109.3 . . ?
H7A C7 H7B 108.0 . . ?
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Co N4 C5 C6 -55.1(3) . . . . ?
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C2 N1 C7 C6 -176.8(2) . . . . ?
Co N1 C7 C6 57.3(3) . . . . ?
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Co O15 N16 O18 -176.1(2) . . . . ?
Co O15 N16 O17 3.7(4) . . . . ?
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N1 H1 N16  0.91 2.65 3.242(3) 123.0 .
N1 H1 O17  0.91 2.74 3.555(3) 149.0 2_655
N1 H1 N16  0.91 2.79 3.621(3) 152.1 2_655
N4 H4A O17  0.91 2.33 3.003(3) 130.2 .
N4 H4A O26  0.91 2.35 3.128(8) 143.8 2_654
N4 H4A O25  0.91 2.51 3.256(7) 139.3 .
N4 H4A O24  0.91 2.59 3.358(8) 142.7 .
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O22A H22A O25  0.82 1.89 2.710(10) 173.6 2_644
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