cif data

Complex **1**

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_chemical_formula_sum
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_chemical_formula_weight                591.98

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 'H'   'H'    0.0000    0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Cu'   'Cu'    0.3201    1.2651
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'   'N'    0.0061    0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'   'O'    0.0106    0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M          P-1

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 'x, y, z'
 '-x, -y, -z'

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_cell_length_b                          8.9006(4)
_cell_length_c                          10.3196(5)
_cell_angle_alpha                       86.613(4)
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_cell_angle_beta                    71.990(4)
_cell_angle_gamma                   76.660(4)
_cell_volume                        594.14(5)
_cell_formula_units_Z               1
_cell_measurement_temperature       293(2)
_cell_measurement_reflns_used       ?
_cell_measurement_theta_min         ?
_cell_measurement_theta_max         ?

_exptl_crystal_description          block
_exptl_crystal_colour               green
_exptl_crystal_size_max             0.18
_exptl_crystal_size_mid             0.15
_exptl_crystal_size_min             0.12
_exptl_crystal_density_meas         ?
_exptl_crystal_density_diffrn       1.654
_exptl_crystal_density_method       'not measured'
_exptl_crystal_F_000                303
_exptl_absorpt_coefficient_mu       0.991
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_exptl_absorpt_process_details      ?

_exptl_special_details
;
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_diffrn_ambient_temperature         293(2)
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_diffrn_measurement_method          ?
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_diffrn_reflns_number               3742
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_reflns_number_gt                      1994
_reflns_threshold_expression           >2sigma(I)

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_computing_cell_refinement             ?
_computing_data_reduction              ?
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_computing_molecular_graphics          ?
_computing_publication_material        ?

_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
 'calc w=1/[\s^2^(Fo^2^)+(0.0497P)^2^+0.2932P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary         difmap
_atom_sites_solution_hydrogens         geom
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_refine_ls_extinction_method           none
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_refine_ls_wR_factor_ref              0.1021
_refine_ls_wR_factor_gt               0.0986
_refine_ls_goodness_of_fit_ref        1.057
_refine_ls_restrained_S_all           1.057
_refine_ls_shift/su_max               0.014
_refine_ls_shift/su_mean              0.000

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  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_symmetry_multiplicity
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  _atom_site_refinement_flags
  _atom_site_disorder_assembly
  _atom_site_disorder_group
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N1 N 0.4161(3) 0.4244(3) 0.2344(2) 0.0244(5) Uani 1 1 d . . .
N2 N 0.3001(4) 0.2672(3) 0.4736(2) 0.0290(6) Uani 1 1 d . . .
N3 N 0.7999(3) 0.5007(3) -0.0009(2) 0.0258(5) Uani 1 1 d . . .
O1 O 0.6435(4) 0.0575(2) 0.0913(2) 0.0426(6) Uani 1 1 d . . .
O2 O 0.5706(3) 0.2783(2) -0.00974(18) 0.0252(4) Uani 1 1 d . . .
O3 O 0.3802(4) 0.0451(2) 0.3542(2) 0.0444(6) Uani 1 1 d . . .
O4 O 0.1742(4) 0.1275(3) 0.7204(2) 0.0464(6) Uani 1 1 d . . .
H1W H 0.1785 0.2178 0.7383 0.74(17) Uiso 1 1 d R . .
H2W H 0.2851 0.0714 0.7300 0.067(14) Uiso 1 1 d R . .
O5 O 0.1367(4) 0.0364(3) 0.1808(2) 0.0535(7) Uani 1 1 d . . .
H4W H 0.1994 0.0105 0.0980 0.059(12) Uiso 1 1 d R . .
H3W H 0.0763 -0.0361 0.1878 0.34(7) Uiso 1 1 d R . .
C1 C 0.5609(4) 0.1944(3) 0.0956(3) 0.0251(6) Uani 1 1 d . . .
C2 C 0.4461(4) 0.2751(3) 0.2325(3) 0.0251(6) Uani 1 1 d . . .
C3 C 0.3764(4) 0.1835(3) 0.3556(3) 0.0287(6) Uani 1 1 d . . .
C4 C 0.3281(4) 0.5046(3) 0.3571(3) 0.0257(6) Uani 1 1 d . . .
C5 C 0.2733(4) 0.4246(3) 0.4791(3) 0.0256(6) Uani 1 1 d . . .
C6 C 0.1896(5) 0.5067(4) 0.6037(3) 0.0337(7) Uani 1 1 d . . .
H6 H 0.1537 0.4545 0.6853 0.040 Uiso 1 1 calc R . .
```

C7 C 0.1618(5) 0.6632(4) 0.6037(3) 0.0365(7) Uani 1 1 d . . .
H7 H 0.1056 0.7175 0.6861 0.044 Uiso 1 1 calc R . .
C8 C 0.2156(5) 0.7438(4) 0.4828(3) 0.0367(7) Uani 1 1 d . . .
H8 H 0.1964 0.8506 0.4850 0.044 Uiso 1 1 calc R . .
C9 C 0.2968(5) 0.6656(3) 0.3611(3) 0.0330(7) Uani 1 1 d . . .
H9 H 0.3314 0.7196 0.2804 0.040 Uiso 1 1 calc R . .
C10 C 0.9540(5) 0.3756(4) -0.0357(3) 0.0337(7) Uani 1 1 d . . .
H10 H 0.9271 0.2857 -0.0606 0.040 Uiso 1 1 calc R . .
C11 C 0.8488(5) 0.6250(4) 0.0359(3) 0.0335(7) Uani 1 1 d . . .
H11 H 0.7464 0.7146 0.0624 0.040 Uiso 1 1 calc R . .

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 _atom_site_aniso_U_22
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 _atom_site_aniso_U_13
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N1 0.0252(12) 0.0238(12) 0.0239(12) 0.0037(9) -0.0061(10) -0.0073(9)
N2 0.0338(14) 0.0279(13) 0.0244(12) 0.0038(10) -0.0065(11) -0.0091(11)
N3 0.0247(12) 0.0282(13) 0.0246(12) 0.0029(9) -0.0064(10) -0.0079(10)
O1 0.0600(15) 0.0275(12) 0.0305(12) 0.0005(9) -0.0091(11) 0.0031(10)
O2 0.0273(10) 0.0269(10) 0.0218(10) 0.0033(8) -0.0078(8) -0.0070(8)
O3 0.0691(16) 0.0267(12) 0.0359(12) 0.0064(9) -0.0090(12) -0.0189(11)
O4 0.0509(15) 0.0430(14) 0.0382(13) 0.0125(10) -0.0122(11) -0.0016(11)
O5 0.0562(16) 0.0523(15) 0.0418(15) -0.0134(11) 0.0008(12) -0.0102(12)
C1 0.0245(14) 0.0244(15) 0.0285(15) 0.0029(11) -0.0100(12) -0.0076(11)
C2 0.0259(14) 0.0272(15) 0.0239(14) 0.0044(11) -0.0094(12) -0.0078(11)
C3 0.0347(16) 0.0273(16) 0.0257(15) 0.0066(12) -0.0094(13) -0.0115(12)
C4 0.0237(14) 0.0291(15) 0.0248(14) 0.0025(11) -0.0077(12) -0.0067(11)
C5 0.0246(14) 0.0275(15) 0.0242(14) 0.0026(11) -0.0070(12) -0.0063(11)
C6 0.0360(17) 0.0398(18) 0.0240(15) 0.0018(12) -0.0064(13) -0.0101(14)
C7 0.0389(18) 0.0400(18) 0.0286(16) -0.0061(13) -0.0076(14) -0.0067(14)
C8 0.0372(17) 0.0261(16) 0.0438(18) -0.0038(13) -0.0085(15) -0.0053(13)
C9 0.0346(16) 0.0273(16) 0.0337(16) 0.0059(12) -0.0056(14) -0.0081(13)
C10 0.0297(16) 0.0327(17) 0.0389(17) -0.0061(13) -0.0079(14) -0.0093(13)
C11 0.0269(15) 0.0333(17) 0.0384(17) -0.0048(13) -0.0099(14) -0.0019(12)

_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.
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Cu1 O2 1.9214(18) . ?
Cu1 N3 2.095(2) 2_665 ?
Cu1 N3 2.095(2) . ?
Cu1 N1 2.400(2) . ?
Cu1 N1 2.400(2) 2_665 ?
N1 C2 1.296(3) . ?
N1 C4 1.383(3) . ?
N2 C3 1.358(4) . ?
N2 C5 1.372(4) . ?
N3 C10 1.336(4) . ?
N3 C11 1.338(4) . ?
O1 C1 1.219(3) . ?
O2 C1 1.275(3) . ?
O3 C3 1.226(3) . ?
O4 H1W 0.8445 . ?
O4 H2W 0.8499 . ?
O5 H4W 0.8490 . ?
O5 H3W 0.8376 . ?
C1 C2 1.520(4) . ?
C2 C3 1.482(4) . ?
C4 C5 1.400(4) . ?
C4 C9 1.400(4) . ?
C5 C6 1.406(4) . ?
C6 C7 1.362(4) . ?
C6 H6 0.9300 . ?
C7 C8 1.393(4) . ?
C7 H7 0.9300 . ?
C8 C9 1.366(4) . ?
C8 H8 0.9300 . ?
C9 H9 0.9300 . ?
C10 C11 1.377(4) 2_765 ?
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C11 C10 1.377(4) 2_765 ?
C11 H11 0.9300 . ?

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O2 Cu1 N3 89.95(8) 2_665 2_665 ?
O2 Cu1 N3 90.05(8) . 2_665 ?
O2 Cu1 N3 90.05(8) 2_665 . ?
O2 Cu1 N3 89.95(8) . . ?
N3 Cu1 N3 180.00(12) 2_665 . ?
O2 Cu1 N1 103.74(7) 2_665 . ?
O2 Cu1 N1 76.26(7) . . ?
N3 Cu1 N1 89.86(8) 2_665 . ?
N3 Cu1 N1 90.14(8) . . ?
O2 Cu1 N1 76.26(7) 2_665 2_665 ?
O2 Cu1 N1 103.74(7) . 2_665 ?
N3 Cu1 N1 90.14(8) 2_665 2_665 ?
N3 Cu1 N1 89.86(8) . 2_665 ?
N1 Cu1 N1 180.00(10) . 2_665 ?
C2 N1 C4 119.9(2) . . ?
C2 N1 Cu1 105.69(17) . . ?
C4 N1 Cu1 133.94(18) . . ?
C3 N2 C5 123.6(2) . . ?
C10 N3 C11 115.6(2) . . ?
C10 N3 Cu1 122.0(2) . . ?
C11 N3 Cu1 122.38(19) . . ?
C1 O2 Cu1 122.67(17) . . ?
H1W O4 H2W 104.1 . . ?
H4W O5 H3W 89.0 . . ?
O1 C1 O2 123.6(3) . . ?
O1 C1 C2 119.8(2) . . ?
O2 C1 C2 116.5(2) . . ?
N1 C2 C3 123.2(2) . . ?
N1 C2 C1 116.7(2) . . ?
C3 C2 C1 120.0(2) . . ?
O3 C3 N2 121.5(2) . . ?

O3 C3 C2 124.4(3) . . ?
N2 C3 C2 114.0(2) . . ?
N1 C4 C5 120.1(3) . . ?
N1 C4 C9 120.6(2) . . ?
C5 C4 C9 119.3(3) . . ?
N2 C5 C4 118.8(2) . . ?
N2 C5 C6 121.6(2) . . ?
C4 C5 C6 119.7(3) . . ?
C7 C6 C5 119.4(3) . . ?
C7 C6 H6 120.3 . . ?
C5 C6 H6 120.3 . . ?
C6 C7 C8 121.3(3) . . ?
C6 C7 H7 119.3 . . ?
C8 C7 H7 119.3 . . ?
C9 C8 C7 119.9(3) . . ?
C9 C8 H8 120.1 . . ?
C7 C8 H8 120.1 . . ?
C8 C9 C4 120.4(3) . . ?
C8 C9 H9 119.8 . . ?
C4 C9 H9 119.8 . . ?
N3 C10 C11 122.3(3) . 2_765 ?
N3 C10 H10 118.8 . . ?
C11 C10 H10 118.8 2_765 . ?
N3 C11 C10 122.1(3) . 2_765 ?
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C10 C11 H11 119.0 2_765 . ?

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O2 Cu1 N1 C2 -4.97(17) . . . . ?
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N3 Cu1 N1 C2 -94.89(18) . . . . ?
N1 Cu1 N1 C2 -57(100) 2_665 . . . ?
O2 Cu1 N1 C4 3.4(3) 2_665 . . . ?

O2 Cu1 N1 C4 -176.6(3) . . . . ?
N3 Cu1 N1 C4 -86.6(3) 2_665 . . . ?
N3 Cu1 N1 C4 93.4(3) . . . . ?
N1 Cu1 N1 C4 131(100) 2_665 . . . ?
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O2 Cu1 N3 C10 14.5(2) . . . . ?
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N1 Cu1 N3 C10 90.8(2) . . . . ?
N1 Cu1 N3 C10 -89.2(2) 2_665 . . . ?
O2 Cu1 N3 C11 15.9(2) 2_665 . . . ?
O2 Cu1 N3 C11 -164.1(2) . . . . ?
N3 Cu1 N3 C11 110(6) 2_665 . . . ?
N1 Cu1 N3 C11 -87.8(2) . . . . ?
N1 Cu1 N3 C11 92.2(2) 2_665 . . . ?
O2 Cu1 O2 C1 -119(100) 2_665 . . . ?
N3 Cu1 O2 C1 -94.7(2) 2_665 . . . ?
N3 Cu1 O2 C1 85.3(2) . . . . ?
N1 Cu1 O2 C1 -4.9(2) . . . . ?
N1 Cu1 O2 C1 175.1(2) 2_665 . . . ?
Cu1 O2 C1 O1 -164.2(2) . . . . ?
Cu1 O2 C1 C2 13.2(3) . . . . ?
C4 N1 C2 C3 4.7(4) . . . . ?
Cu1 N1 C2 C3 -168.4(2) . . . . ?
C4 N1 C2 C1 -174.6(2) . . . . ?
Cu1 N1 C2 C1 12.3(3) . . . . ?
O1 C1 C2 N1 159.8(3) . . . . ?
O2 C1 C2 N1 -17.7(4) . . . . ?
O1 C1 C2 C3 -19.5(4) . . . . ?
O2 C1 C2 C3 163.0(2) . . . . ?
C5 N2 C3 O3 -173.2(3) . . . . ?
C5 N2 C3 C2 5.0(4) . . . . ?
N1 C2 C3 O3 170.7(3) . . . . ?
C1 C2 C3 O3 -10.0(4) . . . . ?
N1 C2 C3 N2 -7.4(4) . . . . ?
C1 C2 C3 N2 171.9(2) . . . . ?
C2 N1 C4 C5 0.6(4) . . . . ?
Cu1 N1 C4 C5 171.37(19) . . . . ?
C2 N1 C4 C9 179.3(3) . . . . ?
Cu1 N1 C4 C9 -9.9(4) . . . . ?
C3 N2 C5 C4 -0.3(4) . . . . ?
C3 N2 C5 C6 178.7(3) . . . . ?
N1 C4 C5 N2 -2.9(4) . . . . ?
C9 C4 C5 N2 178.4(3) . . . . ?
N1 C4 C5 C6 178.1(3) . . . . ?

C9 C4 C5 C6 -0.6(4) . . . . ?
N2 C5 C6 C7 -178.5(3) . . . . ?
C4 C5 C6 C7 0.5(5) . . . . ?
C5 C6 C7 C8 -0.4(5) . . . . ?
C6 C7 C8 C9 0.5(5) . . . . ?
C7 C8 C9 C4 -0.6(5) . . . . ?
N1 C4 C9 C8 -178.0(3) . . . . ?
C5 C4 C9 C8 0.7(4) . . . . ?
C11 N3 C10 C11 -1.0(5) . . . 2_765 ?
Cu1 N3 C10 C11 -179.7(2) . . . 2_765 ?
C10 N3 C11 C10 1.0(5) . . . 2_765 ?
Cu1 N3 C11 C10 179.7(2) . . . 2_765 ?

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Complex **2**

data_20111124b

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_chemical_melting_point ?
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'C28 H16 Cu N6 O6'
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  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'N'    'N'      0.0061      0.0033
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'O'    'O'      0.0106      0.0060
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Cu'    'Cu'      0.3201      1.2651
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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  'x+1/4, -y+1/4, z+1/4'
  'x, y+1/2, z+1/2'
  'x, -y+1/2, -z+1/2'
  'x+1/4, y+3/4, -z+3/4'
  'x+1/4, -y+3/4, z+3/4'
  'x+1/2, y, z+1/2'
  'x+1/2, -y, -z+1/2'
  'x+3/4, y+1/4, -z+3/4'
  'x+3/4, -y+1/4, z+3/4'
  'x+1/2, y+1/2, z'
  'x+1/2, -y+1/2, -z'
  'x+3/4, y+3/4, -z+1/4'
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_cell_length_a                        11.1387(4)
_cell_length_b                        12.2921(4)
_cell_length_c                        35.3173(16)
_cell_angle_alpha                     90.00
_cell_angle_beta                      90.00
_cell_angle_gamma                       90.00
_cell_volume                          4835.6(3)
_cell_formula_units_Z                 8
_cell_measurement_temperature         293(2)
_cell_measurement_reflns_used         ?
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_exptl_crystal_density_meas            ?
_exptl_crystal_density_diffrn          1.637
_exptl_crystal_density_method          'not measured'
_exptl_crystal_F_000                   2424
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_exptl_absorpt_correction_T_max        0.8689
_exptl_absorpt_process_details         ?

_exptl_special_details
;
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;

_diffrn_ambient_temperature            293(2)
_diffrn_radiation_wavelength           0.71073
_diffrn_radiation_type                 MoK\a
_diffrn_radiation_source               'fine-focus sealed tube'
_diffrn_radiation_monochromator        graphite
_diffrn_measurement_device_type        ?
_diffrn_measurement_method             ?
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_diffrn_standards_number               ?
_diffrn_standards_interval_count       ?
_diffrn_standards_interval_time        ?
_diffrn_standards_decay_%              ?
_diffrn_reflns_number                  9997
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_diffrn_reflns_av_sigmaI/netI          0.0272
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_diffrn_reflns_limit_k_min             -14
_diffrn_reflns_limit_k_max             14
_diffrn_reflns_limit_l_min             -38
_diffrn_reflns_limit_l_max             42
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_reflns_number_gt                 2070
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_computing_cell_refinement        ?
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_computing_molecular_graphics     ?
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_refine_special_details
;
 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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 'calc w=1/[\s^2^(Fo^2^)+(0.0308P)^2^+4.4631P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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 'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack    0.000(18)
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_atom_site_adp_type
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N1 N 1.1599(2) 0.03677(14) 0.06559(5) 0.0213(4) Uani 1 1 d . . .
N3 N 0.9830(3) 0.0000 0.0000 0.0209(9) Uani 1 2 d S . .
N4 N 0.3485(3) 0.0000 0.0000 0.0196(9) Uani 1 2 d S . .
O1 O 1.2044(3) -0.24533(14) 0.07455(7) 0.0407(7) Uani 1 1 d . . .
O2 O 1.17074(16) -0.14777(12) 0.02302(4) 0.0225(3) Uani 1 1 d . . .
O3 O 1.1960(2) -0.16145(17) 0.13960(6) 0.0468(6) Uani 1 1 d . . .
C1 C 1.1850(2) -0.15725(18) 0.05825(7) 0.0236(5) Uani 1 1 d . . .
C2 C 1.1740(3) -0.05725(19) 0.08267(7) 0.0233(5) Uani 1 1 d . . .
C3 C 1.1780(3) -0.0647(2) 0.12325(7) 0.0298(6) Uani 1 1 d . . .
N2 N 1.1619(3) 0.01999(16) 0.14520(6) 0.0325(5) Uani 1 1 d . . .
C5 C 1.1425(2) 0.1174(2) 0.12756(7) 0.0274(6) Uani 1 1 d . . .
C6 C 1.1430(2) 0.12692(19) 0.08761(7) 0.0235(5) Uani 1 1 d . . .
C7 C 1.1220(3) 0.2284(2) 0.07050(10) 0.0314(7) Uani 1 1 d . . .
H7 H 1.1232 0.2350 0.0443 0.038 Uiso 1 1 calc R . .
C8 C 1.1000(3) 0.3169(2) 0.09254(9) 0.0404(7) Uani 1 1 d . . .
H8 H 1.0855 0.3840 0.0813 0.048 Uiso 1 1 calc R . .
C9 C 1.0991(3) 0.3077(2) 0.13194(10) 0.0447(8) Uani 1 1 d . . .
H9 H 1.0833 0.3688 0.1466 0.054 Uiso 1 1 calc R . .
C10 C 1.1209(3) 0.2109(2) 0.14912(9) 0.0389(7) Uani 1 1 d . . .
H10 H 1.1214 0.2066 0.1754 0.047 Uiso 1 1 calc R . .
C11 C 0.9194(2) 0.09230(19) 0.00419(6) 0.0228(5) Uani 1 1 d . . .
H11 H 0.9611 0.1574 0.0069 0.027 Uiso 1 1 calc R . .

C12 C 0.7963(2) 0.0955(2) 0.00470(7) 0.0234(6) Uani 1 1 d . . .
H12 H 0.7568 0.1614 0.0082 0.028 Uiso 1 1 calc R . .
C13 C 0.7303(4) 0.0000 0.0000 0.0177(11) Uani 1 2 d S . .
C14 C 0.5975(4) 0.0000 0.0000 0.0235(12) Uani 1 2 d S . .
C15 C 0.5332(2) 0.07703(19) 0.02043(8) 0.0248(6) Uani 1 1 d . . .
H15 H 0.5731 0.1296 0.0346 0.030 Uiso 1 1 calc R . .
C16 C 0.4099(3) 0.07455(18) 0.01949(7) 0.0251(5) Uani 1 1 d . . .
H16 H 0.3674 0.1270 0.0330 0.030 Uiso 1 1 calc R . .

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N1 0.0182(9) 0.0239(9) 0.0219(10) -0.0022(7) -0.0010(11) -0.0009(11)
N3 0.017(2) 0.028(2) 0.019(2) -0.0019(12) 0.000 0.000
N4 0.012(2) 0.024(2) 0.023(2) -0.0015(12) 0.000 0.000
O1 0.0622(18) 0.0256(11) 0.0342(14) 0.0027(8) -0.0041(12) 0.0107(8)
O2 0.0247(8) 0.0223(8) 0.0206(9) -0.0021(6) -0.0010(8) 0.0028(7)
O3 0.0725(19) 0.0406(11) 0.0273(11) 0.0123(9) -0.0053(11) 0.0087(11)
C1 0.0190(13) 0.0242(12) 0.0274(14) 0.0020(10) 0.0002(10) 0.0028(10)
C2 0.0188(12) 0.0288(12) 0.0223(12) 0.0006(10) -0.0005(12) -0.0012(12)
C3 0.0301(15) 0.0377(14) 0.0214(14) 0.0048(11) -0.0011(12) 0.0011(13)
N2 0.0358(11) 0.0406(13) 0.0212(10) -0.0025(8) -0.0004(14) 0.0041(13)
C5 0.0220(15) 0.0370(14) 0.0231(14) -0.0066(11) 0.0017(11) -0.0020(11)
C6 0.0191(13) 0.0284(12) 0.0229(13) -0.0042(10) 0.0009(10) -0.0015(10)
C7 0.0366(19) 0.0291(14) 0.0284(17) -0.0015(12) -0.0006(14) 0.0003(13)
C8 0.0442(19) 0.0291(15) 0.048(2) -0.0073(13) -0.0041(14) 0.0065(12)
C9 0.0468(19) 0.0391(18) 0.048(2) -0.0197(14) 0.0019(14) 0.0077(14)
C10 0.0426(17) 0.0488(17) 0.0254(16) -0.0134(13) 0.0025(13) 0.0006(14)
C11 0.0195(12) 0.0216(12) 0.0273(14) -0.0021(9) -0.0005(13) -0.0031(10)
C12 0.0205(13) 0.0211(13) 0.0287(15) -0.0035(10) -0.0006(10) 0.0024(9)
C13 0.019(3) 0.025(2) 0.009(2) -0.0027(13) 0.000 0.000
C14 0.014(3) 0.027(2) 0.029(3) -0.0012(15) 0.000 0.000
C15 0.0190(14) 0.0281(13) 0.0272(15) -0.0081(11) -0.0018(11) -0.0019(10)
C16 0.0214(12) 0.0297(12) 0.0241(14) -0.0078(10) 0.0041(13) 0.0020(12)

_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.
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Cu1 O2 1.9909(14) . ?
Cu1 O2 1.9909(14) 2 ?
Cu1 N3 2.031(4) . ?
Cu1 N4 2.040(4) 1_655 ?
Cu1 N1 2.3611(18) 2 ?
Cu1 N1 2.3611(18) . ?
N1 C2 1.313(3) . ?
N1 C6 1.367(3) . ?
N3 C11 1.346(3) 2 ?
N3 C11 1.346(3) . ?
N4 C16 1.334(3) 2 ?
N4 C16 1.334(3) . ?
N4 Cu1 2.040(4) 1_455 ?
O1 C1 1.245(3) . ?
O2 C1 1.260(3) . ?
O3 C3 1.337(3) . ?
C1 C2 1.507(3) . ?
C2 C3 1.437(3) . ?
C3 N2 1.310(3) . ?
N2 C5 1.366(3) . ?
C5 C10 1.400(4) . ?
C5 C6 1.416(3) . ?
C6 C7 1.406(4) . ?
C7 C8 1.360(4) . ?
C7 H7 0.9300 . ?
C8 C9 1.396(4) . ?
C8 H8 0.9300 . ?
C9 C10 1.358(5) . ?
C9 H9 0.9300 . ?
C10 H10 0.9300 . ?
C11 C12 1.371(4) . ?
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C11 H11 0.9300 . ?
C12 C13 1.395(3) . ?
C12 H12 0.9300 . ?
C13 C12 1.395(3) 2 ?
C13 C14 1.479(3) . ?
C14 C15 1.390(3) 2 ?
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C16 H16 0.9300 . ?

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O2 Cu1 N3 91.71(5) . . ?
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O2 Cu1 N4 88.29(5) 2 1_655 ?
N3 Cu1 N4 180.0 . 1_655 ?
O2 Cu1 N1 103.11(6) . 2 ?
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N4 Cu1 N1 91.50(6) 1_655 2 ?
O2 Cu1 N1 76.98(6) . . ?
O2 Cu1 N1 103.11(6) 2 . ?
N3 Cu1 N1 88.50(6) . . ?
N4 Cu1 N1 91.50(6) 1_655 . ?
N1 Cu1 N1 177.01(12) 2 . ?
C2 N1 C6 118.0(2) . . ?
C2 N1 Cu1 106.20(13) . . ?
C6 N1 Cu1 135.81(15) . . ?
C11 N3 C11 116.4(4) 2 . ?
C11 N3 Cu1 121.79(19) 2 . ?
C11 N3 Cu1 121.79(19) . . ?
C16 N4 C16 118.4(4) 2 . ?
C16 N4 Cu1 120.80(19) 2 1_455 ?
C16 N4 Cu1 120.80(19) . 1_455 ?
C1 O2 Cu1 119.44(14) . . ?

O1 C1 O2 124.0(2) . . ?
O1 C1 C2 117.3(2) . . ?
O2 C1 C2 118.7(2) . . ?
N1 C2 C3 121.2(2) . . ?
N1 C2 C1 117.71(19) . . ?
C3 C2 C1 121.1(2) . . ?
N2 C3 O3 118.1(2) . . ?
N2 C3 C2 122.4(2) . . ?
O3 C3 C2 119.5(2) . . ?
C3 N2 C5 116.6(2) . . ?
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N2 C5 C6 121.8(2) . . ?
C10 C5 C6 118.3(3) . . ?
N1 C6 C7 119.8(2) . . ?
N1 C6 C5 120.0(2) . . ?
C7 C6 C5 120.1(2) . . ?
C8 C7 C6 119.6(3) . . ?
C8 C7 H7 120.2 . . ?
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C7 C8 C9 120.5(3) . . ?
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C15 C16 H16 118.7 . . ?

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O2 Cu1 N1 C2 -170.99(16) 2 . . . ?
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N4 Cu1 N1 C2 -82.41(16) 1_655 . . . ?
N1 Cu1 N1 C2 97.59(16) 2 . . . ?
O2 Cu1 N1 C6 -172.3(3) . . . . ?
O2 Cu1 N1 C6 11.3(3) 2 . . . ?
N3 Cu1 N1 C6 -80.2(3) . . . . ?
N4 Cu1 N1 C6 99.8(3) 1_655 . . . ?
N1 Cu1 N1 C6 -80.2(3) 2 . . . ?
O2 Cu1 N3 C11 -31.55(12) . . . 2 ?
O2 Cu1 N3 C11 148.45(12) 2 . . 2 ?
N4 Cu1 N3 C11 172.56(11) 1_655 . . 2 ?
N1 Cu1 N3 C11 71.52(11) 2 . . 2 ?
N1 Cu1 N3 C11 -108.48(11) . . . 2 ?
O2 Cu1 N3 C11 148.45(12) . . . . ?
O2 Cu1 N3 C11 -31.55(12) 2 . . . ?
N4 Cu1 N3 C11 -7.44(11) 1_655 . . . ?
N1 Cu1 N3 C11 -108.48(11) 2 . . . ?
N1 Cu1 N3 C11 71.52(11) . . . . ?
O2 Cu1 O2 C1 82.64(17) 2 . . . ?
N3 Cu1 O2 C1 -97.36(17) . . . . ?
N4 Cu1 O2 C1 82.64(17) 1_655 . . . ?
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Cu1 O2 C1 O1 -170.7(2) . . . . ?
Cu1 O2 C1 C2 11.5(3) . . . . ?
C6 N1 C2 C3 -3.3(4) . . . . ?
Cu1 N1 C2 C3 178.5(2) . . . . ?
C6 N1 C2 C1 176.4(2) . . . . ?

Cu1 N1 C2 C1 -1.9(3) . . . . ?
O1 C1 C2 N1 176.5(3) . . . . ?
O2 C1 C2 N1 -5.6(3) . . . . ?
O1 C1 C2 C3 -3.8(4) . . . . ?
O2 C1 C2 C3 174.1(3) . . . . ?
N1 C2 C3 N2 3.6(5) . . . . ?
C1 C2 C3 N2 -176.0(3) . . . . ?
N1 C2 C3 O3 -178.1(3) . . . . ?
C1 C2 C3 O3 2.3(4) . . . . ?
O3 C3 N2 C5 -179.3(3) . . . . ?
C2 C3 N2 C5 -1.0(5) . . . . ?
C3 N2 C5 C10 178.1(3) . . . . ?
C3 N2 C5 C6 -1.5(5) . . . . ?
C2 N1 C6 C7 -177.1(3) . . . . ?
Cu1 N1 C6 C7 0.5(4) . . . . ?
C2 N1 C6 C5 0.8(4) . . . . ?
Cu1 N1 C6 C5 178.34(19) . . . . ?
N2 C5 C6 N1 1.7(4) . . . . ?
C10 C5 C6 N1 -177.9(3) . . . . ?
N2 C5 C6 C7 179.6(3) . . . . ?
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N1 C6 C7 C8 177.1(3) . . . . ?
C5 C6 C7 C8 -0.7(4) . . . . ?
C6 C7 C8 C9 0.5(5) . . . . ?
C7 C8 C9 C10 0.5(5) . . . . ?
C8 C9 C10 C5 -1.2(5) . . . . ?
N2 C5 C10 C9 -178.6(3) . . . . ?
C6 C5 C10 C9 1.0(4) . . . . ?
C11 N3 C11 C12 0.64(17) 2 . . . ?
Cu1 N3 C11 C12 -179.36(17) . . . . ?
N3 C11 C12 C13 -1.3(3) . . . . ?
C11 C12 C13 C12 0.59(16) . . . 2 ?
C11 C12 C13 C14 -179.41(16) . . . . ?
C12 C13 C14 C15 -29.26(18) 2 . . 2 ?
C12 C13 C14 C15 150.74(18) . . . 2 ?
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C12 C13 C14 C15 -29.26(18) . . . . ?
C15 C14 C15 C16 -0.39(16) 2 . . . ?
C13 C14 C15 C16 179.61(16) . . . . ?
C16 N4 C16 C15 -0.42(18) 2 . . . ?
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Complex **3**

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2012-06-17 # Formatted by publCIF
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'-x, -y, -z'
'x-1/2, y-1/2, -z-1/2'
'x, -y, z-1/2'
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_cell_length_b 11.1914(8)
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_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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_atom_sites_solution_hydrogens        geom
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O1 O 0.54705(11) 0.3979(2) 0.16599(15) 0.0274(6) Uani 1 1 d . A .
O2 O 0.58210(10) 0.3342(2) 0.29581(16) 0.0284(6) Uani 1 1 d . . .
O3 O 0.63728(12) 0.4813(3) 0.44763(17) 0.0409(7) Uani 1 1 d . . .
O4 O 0.70896(12) 0.3580(3) 0.38714(19) 0.0438(8) Uani 1 1 d . . .
O6 O 0.45099(11) 0.3000(2) 0.02271(16) 0.0349(7) Uani 1 1 d . . .
H1W H 0.4790 0.3376 -0.0073 0.052 Uiso 1 1 d R . .
H2W H 0.4185 0.3467 0.0188 0.052 Uiso 1 1 d R . .
O7 O 0.52683(12) 0.6010(2) 0.40107(18) 0.0481(8) Uani 1 1 d . . .
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H4W H 0.5083 0.5403 0.3790 0.072 Uiso 1 1 d R . .
N1 N 0.56524(13) 0.1620(3) 0.09839(19) 0.0306(8) Uani 1 1 d . . .
N2 N 0.45355(13) 0.0939(3) 0.16070(19) 0.0271(8) Uani 1 1 d . . .
C1 C 0.63468(15) 0.5001(3) 0.2320(2) 0.0228(9) Uani 1 1 d . A .
C2 C 0.67338(15) 0.5236(3) 0.3051(2) 0.0218(8) Uani 1 1 d . . .
C3 C 0.71593(16) 0.6200(3) 0.3038(2) 0.0291(9) Uani 1 1 d . A .
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C4 C 0.72248(17) 0.6902(4) 0.2306(3) 0.0331(10) Uani 1 1 d . . .
H4 H 0.7516 0.7573 0.2306 0.040 Uiso 0.120(6) 1 d PR A 2
O5' O 0.6969(10) 0.727(2) 0.0745(17) 0.047(8) Uani 0.120(6) 1 d P A 2
H5' H 0.6700 0.7035 0.0365 0.070 Uiso 0.120(6) 1 d PR A 2
C5 C 0.68656(18) 0.6637(4) 0.1569(3) 0.0350(10) Uani 1 1 d . A .
H5A H 0.6923 0.7104 0.1053 0.042 Uiso 0.880(6) 1 d PR A 1
O5 O 0.76265(14) 0.7858(3) 0.2296(2) 0.0464(11) Uani 0.880(6) 1 d P A 1
H5 H 0.7721 0.8053 0.2813 0.070 Uiso 0.880(6) 1 d PR A 1
C6 C 0.64329(17) 0.5712(4) 0.1578(2) 0.0314(10) Uani 1 1 d . . .
H6A H 0.6190 0.5548 0.1084 0.038 Uiso 1 1 calc R A .
C7 C 0.58494(16) 0.4046(3) 0.2316(2) 0.0245(9) Uani 1 1 d . . .
C8 C 0.67261(17) 0.4467(4) 0.3860(2) 0.0302(9) Uani 1 1 d . . .
C9 C 0.61996(18) 0.2064(4) 0.0649(3) 0.0438(12) Uani 1 1 d . . .
H9 H 0.6266 0.2885 0.0665 0.053 Uiso 1 1 calc R . .
C10 C 0.6671(2) 0.1347(5) 0.0281(3) 0.0564(14) Uani 1 1 d . . .
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H10 H 0.7048 0.1675 0.0048 0.068 Uiso 1 1 calc R . .
C11 C 0.6569(2) 0.0141(5) 0.0270(3) 0.0602(15) Uani 1 1 d . . .
H11 H 0.6884 -0.0362 0.0036 0.072 Uiso 1 1 calc R . .
C12 C 0.6007(2) -0.0333(4) 0.0599(3) 0.0471(12) Uani 1 1 d . . .
H12 H 0.5933 -0.1153 0.0583 0.057 Uiso 1 1 calc R . .
C13 C 0.55488(17) 0.0429(4) 0.0956(2) 0.0287(9) Uani 1 1 d . . .
C14 C 0.49222(17) 0.0034(4) 0.1333(2) 0.0295(9) Uani 1 1 d . . .
C15 C 0.4729(2) -0.1131(4) 0.1401(3) 0.0409(11) Uani 1 1 d . . .
H15 H 0.5000 -0.1742 0.1209 0.049 Uiso 1 1 calc R . .
C16 C 0.4132(2) -0.1396(4) 0.1754(3) 0.0513(13) Uani 1 1 d . . .
H16 H 0.3999 -0.2186 0.1811 0.062 Uiso 1 1 calc R . .
C17 C 0.3733(2) -0.0483(4) 0.2024(3) 0.0453(12) Uani 1 1 d . . .
H17 H 0.3325 -0.0645 0.2258 0.054 Uiso 1 1 calc R . .
C18 C 0.39504(17) 0.0678(4) 0.1941(3) 0.0343(10) Uani 1 1 d . . .
H18 H 0.3682 0.1299 0.2122 0.041 Uiso 1 1 calc R . .

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O1 0.0309(14) 0.0264(17) 0.0248(15) 0.0007(12) -0.0056(10) -0.0060(12)
O2 0.0239(14) 0.0307(17) 0.0305(16) 0.0057(13) -0.0029(11) -0.0024(12)
O3 0.0514(18) 0.047(2) 0.0238(16) -0.0039(14) 0.0056(12) -0.0033(14)
O4 0.0373(17) 0.046(2) 0.049(2) 0.0129(16) -0.0056(13) 0.0108(15)
O6 0.0368(15) 0.0394(18) 0.0285(15) 0.0017(13) -0.0004(11) 0.0025(13)
O7 0.0454(17) 0.034(2) 0.065(2) -0.0129(16) 0.0074(15) -0.0001(14)
N1 0.0267(17) 0.037(2) 0.0282(19) -0.0037(16) 0.0039(14) -0.0011(16)
N2 0.0247(17) 0.029(2) 0.0271(19) -0.0023(15) -0.0023(13) -0.0004(15)
C1 0.0195(18) 0.021(2) 0.028(2) -0.0026(17) 0.0032(14) -0.0010(16)
C2 0.0173(18) 0.021(2) 0.028(2) -0.0007(17) 0.0002(14) 0.0008(16)
C3 0.025(2) 0.033(3) 0.028(2) -0.0057(19) -0.0020(15) -0.0017(18)
C4 0.022(2) 0.031(3) 0.046(3) -0.002(2) 0.0029(17) -0.0060(19)
O5' 0.042(14) 0.028(16) 0.07(2) 0.010(13) 0.005(12) -0.009(11)
C5 0.039(2) 0.033(3) 0.033(2) 0.011(2) 0.0015(17) -0.009(2)
O5 0.045(2) 0.044(2) 0.050(2) 0.0034(17) -0.0002(15) -0.0270(17)
C6 0.030(2) 0.038(3) 0.026(2) 0.0023(19) -0.0022(15) -0.005(2)
C7 0.0208(19) 0.028(2) 0.025(2) -0.0005(18) -0.0001(15) 0.0060(17)
C8 0.024(2) 0.037(3) 0.030(2) -0.005(2) -0.0079(17) -0.0066(19)

C9 0.037(2) 0.056(3) 0.038(3) -0.013(2) 0.007(2) -0.009(2)
C10 0.031(3) 0.083(4) 0.055(3) -0.017(3) 0.011(2) -0.002(3)
C11 0.047(3) 0.071(4) 0.062(3) -0.019(3) 0.010(2) 0.021(3)
C12 0.049(3) 0.045(3) 0.047(3) -0.010(2) 0.005(2) 0.014(2)
C13 0.031(2) 0.028(3) 0.027(2) -0.0053(19) -0.0070(16) 0.0025(19)
C14 0.034(2) 0.025(3) 0.029(2) -0.0043(18) -0.0046(16) 0.0012(19)
C15 0.047(3) 0.021(3) 0.055(3) -0.008(2) -0.002(2) 0.003(2)
C16 0.064(3) 0.027(3) 0.063(3) -0.001(2) -0.002(3) -0.013(2)
C17 0.040(3) 0.037(3) 0.059(3) 0.000(2) -0.002(2) -0.011(2)
C18 0.029(2) 0.033(3) 0.040(3) -0.004(2) 0.0035(17) -0.0021(19)

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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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Cu1 O1 1.960(2) . ?
Cu1 N2 1.992(3) . ?
Cu1 N1 1.994(3) . ?
Cu1 O6 2.186(2) . ?
O1 C7 1.280(4) . ?
O2 C7 1.268(4) . ?
O2 Cu1 1.952(2) 3_655 ?
O3 C8 1.259(4) . ?
O4 C8 1.242(4) . ?
O6 H1W 0.8500 . ?
O6 H2W 0.8501 . ?
O7 H3W 0.8500 . ?
O7 H4W 0.8500 . ?
N1 C9 1.333(4) . ?

N1 C13 1.351(5) . ?
N2 C18 1.340(4) . ?
N2 C14 1.355(4) . ?
C1 C2 1.405(5) . ?
C1 C6 1.407(5) . ?
C1 C7 1.478(5) . ?
C2 C3 1.388(5) . ?
C2 C8 1.517(5) . ?
C3 C4 1.384(5) . ?
C3 H3 0.9300 . ?
C4 O5 1.350(5) . ?
C4 C5 1.389(5) . ?
C4 H4 0.9600 . ?
O5' C5 1.47(2) . ?
O5' H5' 0.8500 . ?
O5' H5A 0.5208 . ?
C5 C6 1.364(5) . ?
C5 H5A 0.9599 . ?
O5 H4 0.3911 . ?
O5 H5 0.8501 . ?
C6 H6A 0.9300 . ?
C9 C10 1.380(5) . ?
C9 H9 0.9300 . ?
C10 C11 1.366(6) . ?
C10 H10 0.9300 . ?
C11 C12 1.369(6) . ?
C11 H11 0.9300 . ?
C12 C13 1.383(5) . ?
C12 H12 0.9300 . ?
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N1 Cu1 O6 93.30(11) . . ?
C7 O1 Cu1 120.0(2) . . ?
C7 O2 Cu1 130.8(2) . 3_655 ?
Cu1 O6 H1W 109.6 . . ?
Cu1 O6 H2W 120.4 . . ?
H1W O6 H2W 100.9 . . ?
H3W O7 H4W 113.9 . . ?
C9 N1 C13 119.2(3) . . ?
C9 N1 Cu1 126.1(3) . . ?
C13 N1 Cu1 114.6(2) . . ?
C18 N2 C14 118.8(3) . . ?
C18 N2 Cu1 126.3(3) . . ?
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C2 C1 C6 118.6(3) . . ?
C2 C1 C7 121.9(3) . . ?
C6 C1 C7 119.5(3) . . ?
C3 C2 C1 119.3(3) . . ?
C3 C2 C8 117.4(3) . . ?
C1 C2 C8 123.3(3) . . ?
C4 C3 C2 121.0(3) . . ?
C4 C3 H3 119.5 . . ?
C2 C3 H3 119.5 . . ?
O5 C4 C3 121.2(4) . . ?
O5 C4 C5 119.0(4) . . ?
C3 C4 C5 119.8(4) . . ?
O5 C4 H4 1.2 . . ?
C3 C4 H4 120.3 . . ?
C5 C4 H4 119.9 . . ?
C5 O5' H5' 110.5 . . ?
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C6 C5 C4 120.0(4) . . ?
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H4 O5 H5 107.6 . . ?
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O2 C7 C1 118.6(3) . . ?
O1 C7 C1 117.8(3) . . ?
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O4 C8 C2 117.4(3) . . ?
O3 C8 C2 117.0(4) . . ?
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N1 C9 H9 118.8 . . ?
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C11 C12 C13 118.8(4) . . ?
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O6 Cu1 O1 C7 -174.6(2) . . . . ?
O2 Cu1 N1 C9 -163.8(10) 3_655 . . . ?
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O1 Cu1 N1 C13 163.8(3) . . . . ?
N2 Cu1 N1 C13 0.2(3) . . . . ?
O6 Cu1 N1 C13 -96.8(3) . . . . ?
O2 Cu1 N2 C18 1.8(3) 3_655 . . . ?
O1 Cu1 N2 C18 108.4(4) . . . . ?
N1 Cu1 N2 C18 180.0(3) . . . . ?
O6 Cu1 N2 C18 -87.8(3) . . . . ?
O2 Cu1 N2 C14 -176.5(3) 3_655 . . . ?
O1 Cu1 N2 C14 -70.0(5) . . . . ?
N1 Cu1 N2 C14 1.7(3) . . . . ?
O6 Cu1 N2 C14 93.9(3) . . . . ?
C6 C1 C2 C3 3.8(5) . . . . ?
C7 C1 C2 C3 -175.3(3) . . . . ?
C6 C1 C2 C8 -174.6(3) . . . . ?
C7 C1 C2 C8 6.3(5) . . . . ?
C1 C2 C3 C4 -2.4(5) . . . . ?
C8 C2 C3 C4 176.1(3) . . . . ?
C2 C3 C4 O5 178.4(3) . . . . ?

C2 C3 C4 C5 -0.6(6) . . . . ?
O5 C4 C5 C6 -176.8(4) . . . . ?
C3 C4 C5 C6 2.3(6) . . . . ?
O5 C4 C5 O5' 7.6(12) . . . . ?
C3 C4 C5 O5' -173.3(11) . . . . ?
C4 C5 C6 C1 -0.9(6) . . . . ?
O5' C5 C6 C1 174.9(10) . . . . ?
C2 C1 C6 C5 -2.1(6) . . . . ?
C7 C1 C6 C5 177.0(3) . . . . ?
Cu1 O2 C7 O1 -34.4(5) 3_655 . . . ?
Cu1 O2 C7 C1 145.7(3) 3_655 . . . ?
Cu1 O1 C7 O2 -12.4(5) . . . . ?
Cu1 O1 C7 C1 167.6(2) . . . . ?
C2 C1 C7 O2 -7.6(5) . . . . ?
C6 C1 C7 O2 173.3(3) . . . . ?
C2 C1 C7 O1 172.5(3) . . . . ?
C6 C1 C7 O1 -6.6(5) . . . . ?
C3 C2 C8 O4 -92.3(4) . . . . ?
C1 C2 C8 O4 86.1(4) . . . . ?
C3 C2 C8 O3 84.6(4) . . . . ?
C1 C2 C8 O3 -97.0(4) . . . . ?
C13 N1 C9 C10 -0.7(6) . . . . ?
Cu1 N1 C9 C10 -177.6(3) . . . . ?
N1 C9 C10 C11 -0.5(7) . . . . ?
C9 C10 C11 C12 1.4(7) . . . . ?
C10 C11 C12 C13 -1.0(7) . . . . ?
C9 N1 C13 C12 1.1(6) . . . . ?
Cu1 N1 C13 C12 178.3(3) . . . . ?
C9 N1 C13 C14 -179.1(3) . . . . ?
Cu1 N1 C13 C14 -1.8(4) . . . . ?
C11 C12 C13 N1 -0.2(6) . . . . ?
C11 C12 C13 C14 180.0(4) . . . . ?
C18 N2 C14 C15 -0.8(5) . . . . ?
Cu1 N2 C14 C15 177.7(3) . . . . ?
C18 N2 C14 C13 178.5(3) . . . . ?
Cu1 N2 C14 C13 -3.0(4) . . . . ?
N1 C13 C14 N2 3.2(5) . . . . ?
C12 C13 C14 N2 -176.9(4) . . . . ?
N1 C13 C14 C15 -177.5(4) . . . . ?
C12 C13 C14 C15 2.3(6) . . . . ?
N2 C14 C15 C16 -0.1(6) . . . . ?
C13 C14 C15 C16 -179.3(4) . . . . ?
C14 C15 C16 C17 0.9(7) . . . . ?
C15 C16 C17 C18 -0.8(7) . . . . ?

C14 N2 C18 C17 0.8(6) . . . . ?
Cu1 N2 C18 C17 -177.4(3) . . . . ?
C16 C17 C18 N2 0.0(6) . . . . ?

loop_
  _geom_hbond_atom_site_label_D
  _geom_hbond_atom_site_label_H
  _geom_hbond_atom_site_label_A
  _geom_hbond_distance_DH
  _geom_hbond_distance_HA
  _geom_hbond_distance_DA
  _geom_hbond_angle_DHA
  _geom_hbond_site_symmetry_A
O6 H1W O7 0.85 1.85 2.680(4) 163.3 7_565
O6 H2W O3 0.85 1.96 2.759(4) 155.7 3_655
O7 H3W O3 0.85 1.96 2.730(4) 149.4 .
O7 H4W O1 0.85 2.08 2.922(4) 173.0 3_655
O5' H5' O4 0.85 2.54 3.06(3) 120.6 7_565
O5' H5' O3 0.85 2.57 3.29(3) 142.5 7_565
O5' H5' O6 0.85 2.65 3.40(2) 148.5 5_665
O5 H5 O4 0.85 1.78 2.630(4) 175.5 8_765

_diffrn_measured_fraction_theta_max 0.998
_diffrn_reflns_theta_full 25.49
_diffrn_measured_fraction_theta_full 0.998
_refine_diff_density_max 0.627
_refine_diff_density_min -0.903
_refine_diff_density_rms 0.102
===end