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 'C40 H33 Cu N2 P2 S'
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 'x, y, z'
 '-x, -y, -z'

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_cell_length_c                    18.860(6)
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_cell_angle_beta                  92.208(12)
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correction'

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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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_refine_ls_extinction_method      SHELXL
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 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          7178
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C2 C 0.5557(4) 0.7013(3) 0.09677(15) 0.0598(7) Uani 1 1 d . . .
H2 H 0.6140 0.6548 0.0822 0.072 Uiso 1 1 calc R . .
C3 C 0.5967(4) 0.8291(3) 0.07766(18) 0.0772(10) Uani 1 1 d . . .
H3 H 0.6819 0.8675 0.0502 0.093 Uiso 1 1 calc R . .
C4 C 0.5121(6) 0.8994(3) 0.0992(2) 0.0886(12) Uani 1 1 d . . .
H4 H 0.5403 0.9851 0.0864 0.106 Uiso 1 1 calc R . .
C5 C 0.3851(6) 0.8422(4) 0.1397(2) 0.0886(12) Uani 1 1 d . . .
H5 H 0.3276 0.8894 0.1541 0.106 Uiso 1 1 calc R . .
C6 C 0.3429(4) 0.7137(3) 0.15919(17) 0.0674(8) Uani 1 1 d . . .
H6 H 0.2577 0.6757 0.1867 0.081 Uiso 1 1 calc R . .
C7 C 0.2206(3) 0.3701(2) 0.09796(13) 0.0425(5) Uani 1 1 d . . .
C8 C 0.1827(3) 0.4169(3) 0.03678(15) 0.0581(7) Uani 1 1 d . . .
H8 H 0.2352 0.5053 0.0285 0.070 Uiso 1 1 calc R . .
C9 C 0.0666(4) 0.3324(4) -0.01212(18) 0.0753(9) Uani 1 1 d . . .
H9 H 0.0415 0.3648 -0.0530 0.090 Uiso 1 1 calc R . .
C10 C -0.0119(4) 0.2017(4) -0.00103(19) 0.0790(10) Uani 1 1 d . . .
H10 H -0.0898 0.1457 -0.0341 0.095 Uiso 1 1 calc R . .
C11 C 0.0256(4) 0.1540(3) 0.0593(2) 0.0765(9) Uani 1 1 d . . .
H11 H -0.0266 0.0652 0.0669 0.092 Uiso 1 1 calc R . .
C12 C 0.1406(3) 0.2374(3) 0.10891(16) 0.0579(7) Uani 1 1 d . . .
H12 H 0.1646 0.2045 0.1499 0.069 Uiso 1 1 calc R . .
C13 C 0.5405(3) 0.4374(2) 0.14914(13) 0.0443(5) Uani 1 1 d . . .
C14 C 0.6730(3) 0.5002(3) 0.19440(17) 0.0641(8) Uani 1 1 d . . .
H14 H 0.6736 0.5598 0.2310 0.077 Uiso 1 1 calc R . .
C15 C 0.8056(4) 0.4751(4) 0.1856(2) 0.0818(11) Uani 1 1 d . . .
H15 H 0.8957 0.5206 0.2152 0.098 Uiso 1 1 calc R . .
C16 C 0.8043(4) 0.3832(4) 0.1334(2) 0.0829(11) Uani 1 1 d . . .
H16 H 0.8923 0.3650 0.1285 0.099 Uiso 1 1 calc R . .
C17 C 0.6740(4) 0.3193(4) 0.0890(2) 0.0753(9) Uani 1 1 d . . .
H17 H 0.6729 0.2573 0.0537 0.090 Uiso 1 1 calc R . .
C18 C 0.5418(3) 0.3465(3) 0.09620(15) 0.0571(7) Uani 1 1 d . . .
H18 H 0.4536 0.3031 0.0652 0.069 Uiso 1 1 calc R . .
C19 C 0.3158(3) 0.6791(2) 0.34021(13) 0.0472(6) Uani 1 1 d . . .
C20 C 0.4794(5) 0.8866(3) 0.3815(2) 0.0893(12) Uani 1 1 d . . .
H20 H 0.4956 0.9720 0.3971 0.107 Uiso 1 1 calc R . .
C21 C 0.6082(5) 0.8569(3) 0.3790(2) 0.0844(11) Uani 1 1 d . . .
H21 H 0.7085 0.9192 0.3929 0.101 Uiso 1 1 calc R . .
C22 C 0.5810(4) 0.7294(3) 0.35471(16) 0.0650(8) Uani 1 1 d . . .
H22 H 0.6653 0.7056 0.3519 0.078 Uiso 1 1 calc R . .
C23 C 0.1359(3) 0.1167(2) 0.29953(13) 0.0416(5) Uani 1 1 d . . .
C24 C 0.1620(4) 0.0020(3) 0.29776(16) 0.0586(7) Uani 1 1 d . . .
H24 H 0.2532 0.0031 0.3199 0.070 Uiso 1 1 calc R . .
C25 C 0.0524(5) -0.1143(3) 0.2632(2) 0.0781(10) Uani 1 1 d . . .
H25 H 0.0704 -0.1905 0.2623 0.094 Uiso 1 1 calc R . .
C26 C -0.0815(5) -0.1165(4) 0.2305(2) 0.0848(11) Uani 1 1 d . . .
H26 H -0.1533 -0.1938 0.2064 0.102 Uiso 1 1 calc R . .
C27 C -0.1107(4) -0.0044(4) 0.23303(19) 0.0774(10) Uani 1 1 d . . .
H27 H -0.2036 -0.0071 0.2119 0.093 Uiso 1 1 calc R . .
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C28 C -0.0022(3) 0.1119(3) 0.26687(16) 0.0582(7) Uani 1 1 d . . .
H28 H -0.0218 0.1874 0.2678 0.070 Uiso 1 1 calc R . .
C29 C 0.4509(3) 0.2536(2) 0.36433(13) 0.0428(5) Uani 1 1 d . . .
C30 C 0.5074(3) 0.2500(3) 0.43250(15) 0.0567(7) Uani 1 1 d . . .
H30 H 0.4480 0.2506 0.4709 0.068 Uiso 1 1 calc R . .
C31 C 0.6525(4) 0.2453(3) 0.44402(19) 0.0704(9) Uani 1 1 d . . .
H31 H 0.6895 0.2431 0.4902 0.084 Uiso 1 1 calc R . .
C32 C 0.7415(4) 0.2438(4) 0.3890(2) 0.0748(10) Uani 1 1 d . . .
H32 H 0.8394 0.2422 0.3975 0.090 Uiso 1 1 calc R . .
C33 C 0.6865(4) 0.2446(4) 0.3216(2) 0.0891(12) Uani 1 1 d . . .
H33 H 0.7457 0.2413 0.2837 0.107 Uiso 1 1 calc R . .
C34 C 0.5426(4) 0.2504(4) 0.30879(17) 0.0724(9) Uani 1 1 d . . .
H34 H 0.5070 0.2522 0.2623 0.087 Uiso 1 1 calc R . .
C35 C 0.1851(3) 0.2773(2) 0.42931(13) 0.0421(5) Uani 1 1 d . . .
C36 C 0.0698(4) 0.1662(3) 0.45348(16) 0.0623(7) Uani 1 1 d . . .
H36 H 0.0375 0.0857 0.4271 0.075 Uiso 1 1 calc R . .
C37 C 0.0017(4) 0.1741(4) 0.51704(18) 0.0755(9) Uani 1 1 d . . .
H37 H -0.0762 0.0989 0.5325 0.091 Uiso 1 1 calc R . .
C38 C 0.0480(4) 0.2904(4) 0.55652(17) 0.0730(10) Uani 1 1 d . . .
H38 H 0.0047 0.2948 0.5996 0.088 Uiso 1 1 calc R . .
C39 C 0.1580(6) 0.4001(4) 0.53252(19) 0.0988(14) Uani 1 1 d . . .
H39 H 0.1883 0.4803 0.5590 0.119 Uiso 1 1 calc R . .
C40 C 0.2267(5) 0.3948(3) 0.46873(17) 0.0793(11) Uani 1 1 d . . .
H40 H 0.3012 0.4715 0.4529 0.095 Uiso 1 1 calc R . .
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N2 N 0.4368(2) 0.6400(2) 0.33522(11) 0.0452(5) Uani 1 1 d . . .
P1 P 0.36947(7) 0.47408(6) 0.16675(3) 0.03967(15) Uani 1 1 d . . .
P2 P 0.27036(7) 0.27539(6) 0.34334(3) 0.03775(15) Uani 1 1 d . . .
S1 S 0.13511(8) 0.55879(7) 0.31354(4) 0.05321(18) Uani 1 1 d . . .
Cu1 Cu 0.30362(3) 0.45051(3) 0.280955(15) 0.04115(11) Uani 1 1 d . . .

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C3 0.083(2) 0.0566(19) 0.065(2) 0.0129(15) -0.0018(17) -0.0004(17)
C4 0.127(3) 0.0486(18) 0.074(2) 0.0144(17) -0.010(2) 0.019(2)
C5 0.135(4) 0.068(2) 0.081(2) 0.0148(19) 0.007(2) 0.059(2)
C6 0.089(2) 0.0623(18) 0.0630(19) 0.0157(15) 0.0124(16) 0.0414(18)
C7 0.0350(12) 0.0514(14) 0.0403(13) -0.0002(10) 0.0040(10) 0.0170(11)
C8 0.0527(16) 0.0666(18) 0.0494(16) 0.0087(13) -0.0008(12) 0.0185(14)
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C11 0.069(2) 0.0586(19) 0.081(2) -0.0081(17) -0.0070(18) 0.0070(16)
C12 0.0570(17) 0.0519(16) 0.0551(16) 0.0028(13) -0.0005(13) 0.0128(13)
C13 0.0374(13) 0.0506(14) 0.0448(13) 0.0084(11) 0.0047(10) 0.0170(11)
C14 0.0443(16) 0.072(2) 0.0671(19) 0.0001(15) -0.0052(13) 0.0164(14)
C15 0.0376(16) 0.107(3) 0.091(3) 0.022(2) -0.0062(16) 0.0190(17)
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C19 0.0662(17) 0.0449(13) 0.0381(13) 0.0007(10) 0.0010(11) 0.0311(13)
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C29 0.0420(13) 0.0416(13) 0.0493(14) 0.0064(10) 0.0037(10) 0.0211(11)
C30 0.0542(16) 0.0673(18) 0.0513(16) -0.0036(13) -0.0042(12) 0.0293(14)
C31 0.0622(19) 0.079(2) 0.072(2) -0.0030(17) -0.0219(16) 0.0344(17)
C32 0.0513(18) 0.084(2) 0.101(3) 0.021(2) 0.0001(18) 0.0389(17)
C33 0.073(2) 0.138(4) 0.094(3) 0.049(2) 0.037(2) 0.074(2)
C34 0.074(2) 0.116(3) 0.0592(18) 0.0299(18) 0.0184(15) 0.067(2)
C35 0.0459(13) 0.0440(13) 0.0436(13) 0.0055(10) 0.0089(10) 0.0251(11)
C36 0.074(2) 0.0596(17) 0.0574(17) 0.0111(14) 0.0175(15) 0.0295(16)
C37 0.081(2) 0.085(2) 0.069(2) 0.0288(18) 0.0328(18) 0.038(2)
C38 0.104(3) 0.093(3) 0.0534(17) 0.0203(17) 0.0326(17) 0.068(2)
C39 0.178(4) 0.066(2) 0.065(2) 0.0007(17) 0.044(3) 0.059(3)
C40 0.127(3) 0.0465(16) 0.0607(19) 0.0037(14) 0.035(2) 0.0294(19)
N1 0.087(2) 0.0431(13) 0.0821(19) -0.0046(12) 0.0007(15) 0.0297(14)
N2 0.0422(11) 0.0433(11) 0.0458(11) 0.0003(9) -0.0039(9) 0.0140(9)
P1 0.0412(3) 0.0413(3) 0.0370(3) 0.0020(2) 0.0033(2) 0.0174(3)
P2 0.0411(3) 0.0383(3) 0.0392(3) 0.0031(2) 0.0054(2) 0.0215(3)
S1 0.0486(4) 0.0578(4) 0.0613(4) -0.0057(3) 0.0005(3) 0.0315(3)
Cu1 0.04882(19) 0.03979(17) 0.03994(17) 0.00226(12) 0.00518(12)
0.02321(14)

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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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C2 C3 1.389(4) . ?
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C3 C4 1.377(6) . ?
C3 H3 0.9300 . ?
C4 C5 1.382(6) . ?
C4 H4 0.9300 . ?
C5 C6 1.396(5) . ?
C5 H5 0.9300 . ?
C6 H6 0.9300 . ?
C7 C8 1.383(4) . ?
C7 C12 1.391(4) . ?
C7 P1 1.832(2) . ?
C8 C9 1.385(4) . ?
C8 H8 0.9300 . ?
C9 C10 1.372(5) . ?
C9 H9 0.9300 . ?
C10 C11 1.373(5) . ?
C10 H10 0.9300 . ?
C11 C12 1.384(4) . ?
C11 H11 0.9300 . ?
C12 H12 0.9300 . ?
C13 C14 1.380(4) . ?
C13 C18 1.388(4) . ?
C13 P1 1.841(3) . ?
C14 C15 1.390(5) . ?
C14 H14 0.9300 . ?
C15 C16 1.379(6) . ?
C15 H15 0.9300 . ?
C16 C17 1.359(5) . ?
C16 H16 0.9300 . ?
C17 C18 1.396(4) . ?
C17 H17 0.9300 . ?
C18 H18 0.9300 . ?
C19 N1 1.354(3) . ?
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C19 S1 1.712(3) . ?
C20 N1 1.319(5) . ?
C20 C21 1.373(6) . ?
C20 H20 0.9300 . ?
C21 C22 1.387(5) . ?
C21 H21 0.9300 . ?
C22 N2 1.334(4) . ?
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C23 C28 1.389(4) . ?
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C23 P2 1.830(2) . ?
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CrysAlisRED; Oxford Diffraction, 2010.
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conventional
<i>R</i>-factors <i>R</i> are based on <i>F</i>, with <i>F</i> set to zero
for
negative <i>F</i>^2^. The threshold expression of <i>F</i>^2^ >
\s(<i>F</i>^2^) is used only for calculating <i>R</i>-factors(gt)
<i>etc</i>.
and is not relevant to the choice of reflections for refinement.
<i>R</i>-factors based on <i>F</i>^2^ are statistically about twice as
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be
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S1 S 0.44479(6) 0.72577(2) 0.19131(3) 0.03907(12) Uani 1 1 d . . .
P1 P 0.17513(5) 0.599546(18) 0.12905(3) 0.02816(10) Uani 1 1 d . . .
P2 P 0.33486(5) 0.652641(19) 0.35578(3) 0.02917(10) Uani 1 1 d . . .
O1 O 0.6684(2) 0.85004(7) 0.16436(13) 0.0580(4) Uani 1 1 d D . .
H1O H 0.579(2) 0.8400(12) 0.1613(19) 0.070 Uiso 1 1 d D . .
N1 N 0.09785(19) 0.72722(7) 0.19992(11) 0.0405(4) Uani 1 1 d . . .
N2 N -0.0571(2) 0.79677(8) 0.18606(14) 0.0529(5) Uani 1 1 d D . .
H2N H -0.141(2) 0.8154(11) 0.1843(17) 0.064 Uiso 1 1 d D . .
N3 N 0.1150(3) 0.86434(8) 0.15407(14) 0.0570(5) Uani 1 1 d . . .
N4 N 0.3642(2) 0.82789(7) 0.15929(12) 0.0477(4) Uani 1 1 d . . .
C1 C -0.0368(3) 0.74398(10) 0.20270(16) 0.0498(5) Uani 1 1 d . . .
H1A H -0.1132 0.7217 0.2151 0.060 Uiso 1 1 calc R . .
C2 C 0.0763(3) 0.81511(9) 0.17129(13) 0.0447(5) Uani 1 1 d . . .
C3 C 0.2585(3) 0.86653(10) 0.14953(17) 0.0589(7) Uani 1 1 d . . .
H3A H 0.2928 0.9006 0.1375 0.071 Uiso 1 1 calc R . .
C4 C 0.3214(2) 0.77809(8) 0.17511(11) 0.0363(4) Uani 1 1 d . . .
C5 C 0.1715(2) 0.77169(8) 0.18036(12) 0.0365(4) Uani 1 1 d . . .
C6 C 0.2792(2) 0.53707(7) 0.13442(11) 0.0320(4) Uani 1 1 d . . .
C7 C 0.3322(2) 0.51485(9) 0.21015(13) 0.0403(4) Uani 1 1 d . . .
H7A H 0.3171 0.5330 0.2568 0.048 Uiso 1 1 calc R . .
C8 C 0.4069(3) 0.46647(10) 0.21823(17) 0.0523(6) Uani 1 1 d . . .
H8A H 0.4405 0.4512 0.2701 0.063 Uiso 1 1 calc R . .
C9 C 0.4321(3) 0.44067(10) 0.1512(2) 0.0621(7) Uani 1 1 d . . .
H9A H 0.4841 0.4077 0.1567 0.075 Uiso 1 1 calc R . .
C10 C 0.3825(3) 0.46228(11) 0.07608(18) 0.0628(7) Uani 1 1 d . . .
H10A H 0.4009 0.4443 0.0299 0.075 Uiso 1 1 calc R . .
C11 C 0.3055(3) 0.51034(9) 0.06720(14) 0.0468(5) Uani 1 1 d . . .
H11A H 0.2709 0.5249 0.0150 0.056 Uiso 1 1 calc R . .
C12 C -0.0136(2) 0.57759(7) 0.13645(11) 0.0312(4) Uani 1 1 d . . .
C13 C -0.0493(2) 0.52585(9) 0.15150(14) 0.0443(5) Uani 1 1 d . . .
H13A H 0.0252 0.4989 0.1554 0.053 Uiso 1 1 calc R . .
C14 C -0.1936(3) 0.51289(10) 0.16097(17) 0.0544(6) Uani 1 1 d . . .
H14A H -0.2175 0.4771 0.1706 0.065 Uiso 1 1 calc R . .
C15 C -0.3014(3) 0.55164(11) 0.15636(15) 0.0519(6) Uani 1 1 d . . .
H15A H -0.3991 0.5429 0.1640 0.062 Uiso 1 1 calc R . .
C16 C -0.2673(3) 0.60322(11) 0.14063(16) 0.0517(6) Uani 1 1 d . . .
H16A H -0.3418 0.6301 0.1372 0.062 Uiso 1 1 calc R . .
C17 C -0.1250(2) 0.61609(9) 0.12977(14) 0.0436(5) Uani 1 1 d . . .
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H17A H -0.1031 0.6516 0.1176 0.052 Uiso 1 1 calc R . .
C18 C 0.1511(2) 0.61951(8) 0.02378(11) 0.0360(4) Uani 1 1 d . . .
C19 C 0.0354(3) 0.60105(10) -0.03641(13) 0.0486(5) Uani 1 1 d . . .
H19A H -0.0359 0.5766 -0.0238 0.058 Uiso 1 1 calc R . .
C20 C 0.0233(3) 0.61815(12) -0.11533(14) 0.0605(7) Uani 1 1 d . . .
H20A H -0.0563 0.6052 -0.1564 0.073 Uiso 1 1 calc R . .
C21 C 0.1242(4) 0.65316(12) -0.13440(16) 0.0694(8) Uani 1 1 d . . .
H21A H 0.1137 0.6652 -0.1883 0.083 Uiso 1 1 calc R . .
C22 C 0.2415(5) 0.67121(14) -0.07537(18) 0.0802(10) Uani 1 1 d . . .
H22A H 0.3141 0.6948 -0.0888 0.096 Uiso 1 1 calc R . .
C23 C 0.2536(3) 0.65488(11) 0.00395(15) 0.0598(7) Uani 1 1 d . . .
H23A H 0.3330 0.6682 0.0448 0.072 Uiso 1 1 calc R . .
C24 C 0.2824(2) 0.59281(7) 0.40428(12) 0.0335(4) Uani 1 1 d . . .
C25 C 0.3690(3) 0.57139(10) 0.47426(15) 0.0517(6) Uani 1 1 d . . .
H25A H 0.4597 0.5884 0.5003 0.062 Uiso 1 1 calc R . .
C26 C 0.3225(4) 0.52497(11) 0.50617(19) 0.0667(8) Uani 1 1 d . . .
H26A H 0.3821 0.5102 0.5538 0.080 Uiso 1 1 calc R . .
C27 C 0.1910(4) 0.50043(11) 0.4692(2) 0.0692(8) Uani 1 1 d . . .
H27A H 0.1600 0.4687 0.4912 0.083 Uiso 1 1 calc R . .
C28 C 0.1048(3) 0.52174(11) 0.4009(2) 0.0644(7) Uani 1 1 d . . .
H28A H 0.0131 0.5050 0.3758 0.077 Uiso 1 1 calc R . .
C29 C 0.1505(2) 0.56757(9) 0.36788(14) 0.0447(5) Uani 1 1 d . . .
H29A H 0.0906 0.5818 0.3198 0.054 Uiso 1 1 calc R . .
C30 C 0.5397(2) 0.65195(8) 0.38379(12) 0.0357(4) Uani 1 1 d . . .
C31 C 0.6129(3) 0.61752(12) 0.34183(17) 0.0603(7) Uani 1 1 d . . .
H31A H 0.5557 0.5954 0.3013 0.072 Uiso 1 1 calc R . .
C32 C 0.7678(3) 0.61486(15) 0.3579(2) 0.0800(10) Uani 1 1 d . . .
H32A H 0.8171 0.5903 0.3297 0.096 Uiso 1 1 calc R . .
C33 C 0.8508(3) 0.64775(16) 0.4148(2) 0.0762(9) Uani 1 1 d . . .
H33A H 0.9578 0.6463 0.4254 0.091 Uiso 1 1 calc R . .
C34 C 0.7802(3) 0.68257(14) 0.45641(18) 0.0704(8) Uani 1 1 d . . .
H34A H 0.8382 0.7053 0.4957 0.084 Uiso 1 1 calc R . .
C35 C 0.6237(3) 0.68481(11) 0.44123(15) 0.0530(6) Uani 1 1 d . . .
H35A H 0.5748 0.7089 0.4703 0.064 Uiso 1 1 calc R . .
C36 C 0.2775(2) 0.70686(8) 0.41369(11) 0.0329(4) Uani 1 1 d . . .
C37 C 0.2190(2) 0.69965(9) 0.48225(13) 0.0418(4) Uani 1 1 d . . .
H37A H 0.2179 0.6652 0.5049 0.050 Uiso 1 1 calc R . .
C38 C 0.1620(3) 0.74251(11) 0.51791(15) 0.0539(6) Uani 1 1 d . . .
H38A H 0.1219 0.7374 0.5647 0.065 Uiso 1 1 calc R . .
C39 C 0.1638(3) 0.79237(11) 0.48526(17) 0.0582(7) Uani 1 1 d . . .
H39A H 0.1217 0.8214 0.5086 0.070 Uiso 1 1 calc R . .
C40 C 0.2266(3) 0.80058(10) 0.41881(18) 0.0612(7) Uani 1 1 d . . .
H40A H 0.2303 0.8353 0.3975 0.073 Uiso 1 1 calc R . .
C41 C 0.2841(3) 0.75786(9) 0.38350(14) 0.0489(5) Uani 1 1 d . . .
H41A H 0.3283 0.7635 0.3382 0.059 Uiso 1 1 calc R . .
C42 C 0.6723(4) 0.90430(12) 0.1600(3) 0.0907(11) Uani 1 1 d . . .
H42C H 0.7597 0.9152 0.1385 0.136 Uiso 1 1 calc R . .
H42B H 0.6803 0.9193 0.2140 0.136 Uiso 1 1 calc R . .
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P1 0.0260(2) 0.0285(2) 0.0294(2) -0.00047(16) 0.00441(16) -0.00175(16)
P2 0.0265(2) 0.0312(2) 0.0301(2) -0.00232(17) 0.00673(17) -0.00299(17)
O1 0.0459(9) 0.0476(10) 0.0843(13) 0.0009(9) 0.0221(9) 0.0073(8)
N1 0.0354(9) 0.0318(8) 0.0539(10) -0.0013(7) 0.0085(8) -0.0004(7)
N2 0.0383(10) 0.0456(11) 0.0704(13) -0.0072(9) 0.0014(9) 0.0134(8)
N3 0.0627(13) 0.0358(10) 0.0663(13) 0.0039(9) 0.0000(11) 0.0098(9)
N4 0.0546(12) 0.0353(9) 0.0525(11) 0.0065(8) 0.0099(9) -0.0059(8)
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C2 0.0459(12) 0.0370(11) 0.0453(11) -0.0050(9) -0.0038(9) 0.0087(9)
C3 0.0740(18) 0.0320(11) 0.0664(16) 0.0101(10) 0.0048(13) -0.0020(11)
C4 0.0415(10) 0.0329(9) 0.0326(9) 0.0016(7) 0.0037(8) -0.0022(8)
C5 0.0361(10) 0.0296(9) 0.0404(10) -0.0008(7) 0.0005(8) 0.0025(7)
C6 0.0270(8) 0.0301(9) 0.0390(9) -0.0020(7) 0.0071(7) -0.0026(7)
C7 0.0342(10) 0.0415(11) 0.0460(11) 0.0063(9) 0.0098(8) 0.0019(8)
C8 0.0444(12) 0.0418(12) 0.0699(15) 0.0184(11) 0.0104(11) 0.0028(9)
C9 0.0547(14) 0.0318(11) 0.096(2) -0.0035(12) 0.0072(14) 0.0045(10)
C10 0.0647(16) 0.0468(14) 0.0737(17) -0.0252(13) 0.0075(13) 0.0074(12)
C11 0.0469(12) 0.0440(12) 0.0468(12) -0.0122(9) 0.0036(9) 0.0038(9)
C12 0.0283(8) 0.0327(9) 0.0319(8) -0.0015(7) 0.0047(7) -0.0035(7)
C13 0.0336(10) 0.0368(11) 0.0620(13) 0.0055(9) 0.0090(9) -0.0022(8)
C14 0.0414(12) 0.0497(14) 0.0723(16) 0.0105(12) 0.0124(11) -0.0149(10)
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C17 0.0340(10) 0.0387(11) 0.0581(13) -0.0010(9) 0.0100(9) -0.0007(8)
C18 0.0417(10) 0.0347(10) 0.0318(9) 0.0003(7) 0.0083(8) 0.0015(8)
C19 0.0496(13) 0.0573(14) 0.0361(10) -0.0011(9) 0.0028(9) -0.0031(10)
C20 0.0702(17) 0.0720(18) 0.0330(11) -0.0043(11) -0.0035(11) 0.0099(14)
C21 0.107(3) 0.0678(18) 0.0346(12) 0.0086(11) 0.0170(14) 0.0106(17)
C22 0.113(3) 0.084(2) 0.0482(15) 0.0097(14) 0.0274(17) -0.0325(19)
C23 0.0694(17) 0.0708(17) 0.0394(12) 0.0031(11) 0.0121(11) -0.0266(14)
C24 0.0331(9) 0.0315(9) 0.0385(9) -0.0016(7) 0.0129(8) 0.0003(7)
C25 0.0508(13) 0.0513(14) 0.0523(13) 0.0129(10) 0.0095(10) 0.0022(10)
C26 0.081(2) 0.0551(16) 0.0704(17) 0.0276(13) 0.0311(15) 0.0207(14)
C27 0.091(2) 0.0363(13) 0.096(2) 0.0107(13) 0.0568(19) 0.0005(13)
C28 0.0665(17) 0.0487(14) 0.086(2) -0.0064(14) 0.0335(15) -0.0217(12)
C29 0.0390(11) 0.0445(12) 0.0536(12) -0.0026(9) 0.0166(9) -0.0084(9)
C30 0.0272(9) 0.0455(11) 0.0342(9) 0.0006(8) 0.0060(7) -0.0026(7)
C31 0.0310(11) 0.0811(19) 0.0653(16) -0.0284(14) 0.0026(10) 0.0003(11)
C32 0.0348(13) 0.113(3) 0.091(2) -0.036(2) 0.0101(13) 0.0114(14)
C33 0.0272(11) 0.118(3) 0.079(2) -0.0137(19) 0.0017(12) -0.0036(14)
C34 0.0394(13) 0.099(2) 0.0672(17) -0.0211(16) -0.0024(12) -0.0183(14)
C35 0.0369(11) 0.0695(16) 0.0517(13) -0.0158(12) 0.0072(10) -0.0093(11)
C36 0.0308(9) 0.0339(9) 0.0333(9) -0.0063(7) 0.0053(7) -0.0038(7)
C37 0.0415(11) 0.0455(12) 0.0406(10) -0.0060(9) 0.0138(9) -0.0029(9)
C38 0.0495(13) 0.0651(16) 0.0520(13) -0.0199(11) 0.0217(11) -0.0052(11)
C39 0.0532(14) 0.0526(15) 0.0686(16) -0.0271(12) 0.0127(12) 0.0036(11)
C40 0.0772(18) 0.0349(12) 0.0709(17) -0.0086(11) 0.0146(14) 0.0001(11)
C41 0.0650(15) 0.0364(11) 0.0480(12) -0.0036(9) 0.0181(11) -0.0054(10)
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C42 0.089(2) 0.0463(17) 0.142(3) 0.0075(19) 0.038(2) 0.0000(15)

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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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S1 C4 1.715(2) . ?
P1 C18 1.825(2) . ?
P1 C6 1.8286(19) . ?
P1 C12 1.8298(18) . ?
P2 C30 1.820(2) . ?
P2 C36 1.8223(19) . ?
P2 C24 1.829(2) . ?
O1 C42 1.370(3) . ?
O1 H1O 0.839(17) . ?
N1 C1 1.304(3) . ?
N1 C5 1.381(3) . ?
N2 C1 1.364(3) . ?
N2 C2 1.368(3) . ?
N2 H2N 0.887(17) . ?
N3 C3 1.322(4) . ?
N3 C2 1.339(3) . ?
N4 C3 1.353(3) . ?
N4 C4 1.358(3) . ?
C1 H1A 0.9500 . ?
C2 C5 1.383(3) . ?
C3 H3A 0.9500 . ?
C4 C5 1.391(3) . ?
C6 C11 1.389(3) . ?
C6 C7 1.392(3) . ?
C7 C8 1.388(3) . ?
C7 H7A 0.9500 . ?
C8 C9 1.372(4) . ?
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C10 C11 1.391(3) . ?
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C10 H10A 0.9500 . ?
C11 H11A 0.9500 . ?
C12 C13 1.381(3) . ?
C12 C17 1.389(3) . ?
C13 C14 1.392(3) . ?
C13 H13A 0.9500 . ?
C14 C15 1.373(4) . ?
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C16 C17 1.382(3) . ?
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C19 C20 1.390(3) . ?
C19 H19A 0.9500 . ?
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P1 Cu1 S1 117.66(2) . . ?
P2 Cu1 S1 101.816(19) . . ?
C4 S1 Cu1 93.60(7) . . ?
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C36 P2 Cu1 112.81(6) . . ?
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C42 O1 H1O 109(2) . . ?
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C1 N1 Cu1 147.80(17) . . ?
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C1 N2 C2 106.38(19) . . ?
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N1 C1 H1A 123.4 . . ?
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N3 C2 N2 129.6(2) . . ?
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C5 C4 S1 121.02(15) . . ?
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C11 C6 C7 118.57(19) . . ?
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Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET)
(compiled Aug 27 2010,11:50:40)
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 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
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R-
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H1AA H 0.8104 -0.2168 0.0797 0.062(12) Uiso 1 1 calc R . .
C2A C 0.7738(4) -0.0612(3) 0.2271(2) 0.0520(8) Uani 1 1 d . . .
C3A C 0.7654(5) 0.0737(4) 0.3128(3) 0.0669(11) Uani 1 1 d . . .
H3AA H 0.7500 0.1053 0.3663 0.080 Uiso 1 1 calc R . .
C4A C 0.8314(3) 0.0903(3) 0.1651(2) 0.0447(7) Uani 1 1 d . . .
C5A C 0.8105(3) -0.0070(3) 0.1567(2) 0.0444(7) Uani 1 1 d . . .
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C11A C 0.8543(4) 0.0483(3) -0.2115(2) 0.0530(8) Uani 1 1 d . . .
C12A C 0.8329(6) 0.1212(5) -0.2716(3) 0.0899(17) Uani 1 1 d . . .
H12A H 0.7898 0.2017 -0.2556 0.108 Uiso 1 1 calc R . .
C13A C 0.8746(8) 0.0762(6) -0.3555(3) 0.113(2) Uani 1 1 d . . .
H13A H 0.8600 0.1266 -0.3953 0.136 Uiso 1 1 calc R . .
C14A C 0.9366(6) -0.0407(6) -0.3796(3) 0.0947(17) Uani 1 1 d . . .
H14A H 0.9628 -0.0707 -0.4357 0.114 Uiso 1 1 calc R . .
C15A C 0.9608(5) -0.1150(5) -0.3214(3) 0.0801(14) Uani 1 1 d . . .
H15A H 1.0055 -0.1952 -0.3382 0.096 Uiso 1 1 calc R . .
C16A C 0.9183(4) -0.0700(4) -0.2371(3) 0.0640(10) Uani 1 1 d . . .
H16A H 0.9334 -0.1208 -0.1976 0.077 Uiso 1 1 calc R . .
C21A C 0.7884(3) 0.2525(3) -0.1021(2) 0.0465(7) Uani 1 1 d . . .
C22A C 0.6779(4) 0.3523(3) -0.0898(3) 0.0576(9) Uani 1 1 d . . .
H22A H 0.6042 0.3455 -0.0814 0.069 Uiso 1 1 calc R . .
C23A C 0.6781(5) 0.4618(4) -0.0902(3) 0.0696(12) Uani 1 1 d . . .
H23A H 0.6040 0.5285 -0.0810 0.084 Uiso 1 1 calc R . .
C24A C 0.7861(5) 0.4723(4) -0.1039(3) 0.0739(12) Uani 1 1 d . . .
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C35A C 0.4578(5) 0.1144(6) -0.0721(4) 0.0923(17) Uani 1 1 d . . .
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C36A C 0.5809(4) 0.0981(4) -0.1070(3) 0.0691(11) Uani 1 1 d . . .
H36A H 0.6274 0.0667 -0.1634 0.083 Uiso 1 1 calc R . .
Cu2 Cu 0.55924(6) 0.55330(5) 0.52478(3) 0.06095(19) Uani 1 1 d . . .
S1B S 0.65896(10) 0.35592(7) 0.43602(5) 0.0549(2) Uani 1 1 d . . .
P1B P 0.63794(11) 0.54436(10) 0.62390(6) 0.0578(3) Uani 1 1 d . . .
N1B N 0.6294(3) 0.6176(3) 0.41630(19) 0.0571(8) Uani 1 1 d . . .
N2B N 0.7261(4) 0.6831(3) 0.3028(2) 0.0619(9) Uani 1 1 d . . .
H2BA H 0.7474 0.7308 0.2715 0.070(14) Uiso 1 1 calc R . .
N3B N 0.8504(3) 0.4995(3) 0.2078(2) 0.0609(8) Uani 1 1 d . . .
N4B N 0.8098(3) 0.3418(3) 0.27418(19) 0.0558(7) Uani 1 1 d . . .
C1B C 0.6442(5) 0.7091(3) 0.3842(3) 0.0651(11) Uani 1 1 d . . .
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C2B C 0.7678(4) 0.5662(3) 0.2809(2) 0.0515(8) Uani 1 1 d . . .
C3B C 0.8643(4) 0.3898(4) 0.2104(3) 0.0634(10) Uani 1 1 d . . .
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C5B C 0.7064(4) 0.5273(3) 0.3514(2) 0.0475(8) Uani 1 1 d . . .
C11B C 0.8009(5) 0.4421(4) 0.6008(3) 0.0701(11) Uani 1 1 d . . .
C12B C 0.8822(6) 0.4167(6) 0.5166(3) 0.0922(17) Uani 1 1 d . . .
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C14B C 1.0543(7) 0.2953(8) 0.5559(7) 0.131(3) Uani 1 1 d . . .
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C16B C 0.8494(6) 0.3911(6) 0.6612(4) 0.0988(18) Uani 1 1 d . . .
H16B H 0.7962 0.4059 0.7174 0.119 Uiso 1 1 calc R . .
C21B C 0.5498(4) 0.5038(4) 0.7194(2) 0.0594(9) Uani 1 1 d . . .
C22B C 0.5569(5) 0.3919(4) 0.7157(3) 0.0706(11) Uani 1 1 d . . .
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C23B C 0.4824(6) 0.3594(6) 0.7833(4) 0.0861(15) Uani 1 1 d . . .
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C24B C 0.4002(5) 0.4384(6) 0.8542(3) 0.0921(19) Uani 1 1 d . . .
H24B H 0.3505 0.4162 0.8995 0.111 Uiso 1 1 calc R . .
C25B C 0.3910(5) 0.5495(6) 0.8586(3) 0.0886(17) Uani 1 1 d . . .
H25B H 0.3349 0.6028 0.9067 0.106 Uiso 1 1 calc R . .
C26B C 0.4654(4) 0.5832(5) 0.7912(3) 0.0715(12) Uani 1 1 d . . .
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C31B C 0.6350(5) 0.6828(4) 0.6553(3) 0.0698(12) Uani 1 1 d . . .
C32B C 0.7074(7) 0.6903(7) 0.6979(3) 0.0964(18) Uani 1 1 d . . .
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C33B C 0.7043(9) 0.8001(10) 0.7146(4) 0.124(3) Uani 1 1 d . . .
H33B H 0.7512 0.8068 0.7443 0.149 Uiso 1 1 calc R . .
C34B C 0.6340(10) 0.8954(8) 0.6879(6) 0.132(3) Uani 1 1 d . . .
H34B H 0.6346 0.9669 0.6981 0.158 Uiso 1 1 calc R . .
C35B C 0.5620(9) 0.8884(6) 0.6463(6) 0.134(3) Uani 1 1 d . . .
H35B H 0.5121 0.9550 0.6293 0.161 Uiso 1 1 calc R . .
C36B C 0.5636(6) 0.7821(5) 0.6296(5) 0.1016(19) Uani 1 1 d . . .
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C5A 0.0459(17) 0.0393(16) 0.0485(17) 0.0113(13) -0.0146(14) -0.0214(14)
C11A 0.056(2) 0.058(2) 0.0475(18) 0.0092(15) -0.0219(16) -0.0248(17)
C12A 0.137(5) 0.066(3) 0.053(2) 0.012(2) -0.029(3) -0.035(3)
C13A 0.173(7) 0.103(5) 0.052(3) 0.019(3) -0.040(4) -0.051(5)
C14A 0.110(4) 0.108(4) 0.056(3) -0.008(3) -0.023(3) -0.042(4)
C15A 0.082(3) 0.071(3) 0.080(3) -0.013(2) -0.035(3) -0.022(2)
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C22A 0.058(2) 0.051(2) 0.066(2) 0.0151(17) -0.0288(18) -0.0203(17)
C23A 0.076(3) 0.047(2) 0.076(3) 0.0146(19) -0.033(2) -0.013(2)
C24A 0.096(3) 0.046(2) 0.093(3) 0.024(2) -0.048(3) -0.033(2)
C25A 0.078(3) 0.061(3) 0.121(4) 0.029(3) -0.049(3) -0.039(2)
C26A 0.061(2) 0.048(2) 0.102(3) 0.021(2) -0.043(2) -0.0249(18)
C31A 0.0504(19) 0.0498(19) 0.061(2) 0.0149(16) -0.0227(16) -0.0251(16)
C32A 0.070(3) 0.086(3) 0.060(2) 0.015(2) -0.016(2) -0.040(2)
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C34A 0.058(3) 0.105(4) 0.123(5) 0.036(4) -0.026(3) -0.039(3)
C35A 0.071(3) 0.101(4) 0.120(5) 0.020(4) -0.048(3) -0.041(3)
C36A 0.059(2) 0.070(3) 0.087(3) 0.011(2) -0.037(2) -0.028(2)
Cu2 0.0934(5) 0.0631(4) 0.0408(3) 0.0133(2) -0.0220(3) -0.0495(3)
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N4B 0.071(2) 0.0455(16) 0.0494(16) 0.0041(13) -0.0150(14) -0.0293(15)
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C2B 0.070(2) 0.0479(18) 0.0483(18) 0.0144(15) -0.0225(17) -0.0357(18)
C3B 0.073(3) 0.059(2) 0.051(2) -0.0010(17) -0.0045(18) -0.037(2)
C4B 0.066(2) 0.0443(17) 0.0442(17) 0.0114(14) -0.0229(15) -0.0318(16)
C5B 0.065(2) 0.0439(17) 0.0391(15) 0.0101(13) -0.0158(15) -0.0314(16)
C11B 0.073(3) 0.073(3) 0.062(2) 0.003(2) -0.013(2) -0.039(2)
C12B 0.089(4) 0.110(4) 0.070(3) -0.013(3) -0.006(3) -0.053(3)
C13B 0.079(4) 0.138(6) 0.103(5) -0.032(5) 0.007(4) -0.048(4)
C14B 0.076(4) 0.121(6) 0.167(8) -0.020(6) -0.023(5) -0.032(4)
C15B 0.078(4) 0.138(7) 0.141(7) 0.030(5) -0.034(4) -0.034(4)
C16B 0.078(4) 0.120(5) 0.092(4) 0.028(4) -0.028(3) -0.040(3)
C21B 0.061(2) 0.072(3) 0.0469(19) 0.0153(17) -0.0233(17) -0.028(2)
C22B 0.080(3) 0.076(3) 0.061(2) 0.020(2) -0.029(2) -0.036(2)
C23B 0.098(4) 0.099(4) 0.088(4) 0.046(3) -0.053(3) -0.054(3)
C24B 0.069(3) 0.132(5) 0.072(3) 0.051(3) -0.027(3) -0.041(3)
C25B 0.066(3) 0.113(5) 0.061(3) 0.024(3) -0.015(2) -0.023(3)
C26B 0.068(3) 0.078(3) 0.052(2) 0.012(2) -0.0175(19) -0.020(2)
C31B 0.083(3) 0.075(3) 0.052(2) -0.0105(19) -0.010(2) -0.046(2)
C32B 0.129(5) 0.125(5) 0.068(3) 0.006(3) -0.033(3) -0.087(4)
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C34B 0.156(8) 0.112(6) 0.124(6) -0.027(5) 0.000(5) -0.093(6)
C35B 0.146(7) 0.075(4) 0.186(8) -0.012(5) -0.055(6) -0.055(4)
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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)
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N1A C5A 1.362(5) . ?
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S1A Cu1 S1A 109.40(3) 2_755 . ?
N1A Cu1 Cu1 95.56(8) . 2_755 ?
P1A Cu1 Cu1 130.27(4) . 2_755 ?
S1A Cu1 Cu1 58.70(3) 2_755 2_755 ?
S1A Cu1 Cu1 50.70(3) . 2_755 ?
C4A S1A Cu1 100.70(11) . 2_755 ?
C4A S1A Cu1 89.85(13) . . ?
Cu1 S1A Cu1 70.60(3) 2_755 . ?
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C31A P1A C21A 103.08(17) . . ?
C11A P1A C21A 103.71(17) . . ?
C31A P1A Cu1 111.21(12) . . ?
C11A P1A Cu1 118.48(13) . . ?
C21A P1A Cu1 115.01(11) . . ?
C1A N1A C5A 102.1(3) . . ?
C1A N1A Cu1 144.9(3) . . ?
C5A N1A Cu1 112.5(2) . . ?
C1A N2A C2A 103.6(3) . . ?
C3A N3A C2A 112.9(3) . . ?
C3A N4A C4A 122.9(3) . . ?
C3A N4A H4AA 118.5 . . ?
C4A N4A H4AA 118.5 . . ?
N1A C1A N2A 116.1(3) . . ?
N1A C1A H1AA 121.9 . . ?
N2A C1A H1AA 121.9 . . ?
N3A C2A N2A 127.7(3) . . ?
N3A C2A C5A 124.6(4) . . ?
N2A C2A C5A 107.8(3) . . ?
N3A C3A N4A 125.6(4) . . ?
N3A C3A H3AA 117.2 . . ?
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N4A C4A C5A 113.2(3) . . ?
N4A C4A S1A 123.8(3) . . ?
C5A C4A S1A 122.9(3) . . ?
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N1A C5A C2A 110.4(3) . . ?
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C16A C15A H15A 120.1 . . ?
C11A C16A C15A 120.8(4) . . ?
C11A C16A H16A 119.6 . . ?
C15A C16A H16A 119.6 . . ?
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C26A C21A P1A 117.5(3) . . ?
C22A C21A P1A 123.9(3) . . ?
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C21A C22A H22A 120.1 . . ?
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C22A C23A H23A 119.8 . . ?
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P1B Cu2 Cu2 137.96(4) . 2_666 ?
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C3B N4B C4B 118.7(3) . . ?
N1B C1B N2B 113.3(4) . . ?
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C13B C12B C11B 120.0(7) . . ?
C13B C12B H12B 120.0 . . ?
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C33B C32B H32B 120.6 . . ?
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C34B C33B H33B 119.7 . . ?
C32B C33B H33B 119.7 . . ?
C33B C34B C35B 120.7(7) . . ?
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C34B C35B C36B 119.5(9) . . ?
C34B C35B H35B 120.2 . . ?
C36B C35B H35B 120.2 . . ?
C31B C36B C35B 121.3(7) . . ?
C31B C36B H36B 119.3 . . ?
C35B C36B H36B 119.3 . . ?

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Cu1 Cu1 S1A C4A -101.41(11) 2_755 . . . ?
N1A Cu1 S1A Cu1 100.66(8) . . . 2_755 ?
P1A Cu1 S1A Cu1 -131.62(4) . . . 2_755 ?
S1A Cu1 S1A Cu1 0.0 2_755 . . 2_755 ?
N1A Cu1 P1A C31A -1.28(18) . . . . ?
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Cu1 Cu1 P1A C11A 94.39(16) 2_755 . . . ?
N1A Cu1 P1A C21A 115.38(17) . . . . ?
S1A Cu1 P1A C21A -103.28(13) 2_755 . . . ?
S1A Cu1 P1A C21A 20.28(14) . . . . ?
Cu1 Cu1 P1A C21A -29.03(14) 2_755 . . . ?
P1A Cu1 N1A C1A 86.9(4) . . . . ?
S1A Cu1 N1A C1A -60.5(4) 2_755 . . . ?
S1A Cu1 N1A C1A -169.4(4) . . . . ?
Cu1 Cu1 N1A C1A -119.6(4) 2_755 . . . ?
P1A Cu1 N1A C5A -103.4(2) . . . . ?
S1A Cu1 N1A C5A 109.2(2) 2_755 . . . ?
S1A Cu1 N1A C5A 0.3(2) . . . . ?
Cu1 Cu1 N1A C5A 50.1(2) 2_755 . . . ?
C5A N1A C1A N2A 0.4(4) . . . . ?
Cu1 N1A C1A N2A 170.7(3) . . . . ?
C2A N2A C1A N1A -0.5(4) . . . . ?
C3A N3A C2A N2A 178.2(4) . . . . ?
C3A N3A C2A C5A -0.3(6) . . . . ?
C1A N2A C2A N3A -178.4(4) . . . . ?
C1A N2A C2A C5A 0.3(4) . . . . ?
C2A N3A C3A N4A -0.3(7) . . . . ?
C4A N4A C3A N3A -2.3(7) . . . . ?
C3A N4A C4A C5A 5.0(5) . . . . ?
C3A N4A C4A S1A -173.2(3) . . . . ?
Cu1 S1A C4A N4A 109.0(3) 2_755 . . . ?
Cu1 S1A C4A N4A 179.3(3) . . . . ?
Cu1 S1A C4A C5A -68.9(3) 2_755 . . . ?
Cu1 S1A C4A C5A 1.3(3) . . . . ?
C1A N1A C5A C4A 174.5(4) . . . . ?
Cu1 N1A C5A C4A 0.6(5) . . . . ?
C1A N1A C5A C2A -0.2(4) . . . . ?
Cu1 N1A C5A C2A -174.2(2) . . . . ?
N4A C4A C5A N1A -179.7(3) . . . . ?
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N4A C4A C5A C2A -5.4(5) . . . . ?
S1A C4A C5A C2A 172.7(3) . . . . ?
N3A C2A C5A N1A 178.7(4) . . . . ?
N2A C2A C5A N1A -0.1(4) . . . . ?
N3A C2A C5A C4A 3.5(6) . . . . ?
N2A C2A C5A C4A -175.3(3) . . . . ?
C31A P1A C11A C16A -97.8(4) . . . . ?
C21A P1A C11A C16A 154.8(3) . . . . ?
Cu1 P1A C11A C16A 26.0(4) . . . . ?
C31A P1A C11A C12A 81.5(5) . . . . ?
C21A P1A C11A C12A -25.9(5) . . . . ?
Cu1 P1A C11A C12A -154.7(4) . . . . ?
C16A C11A C12A C13A 0.1(9) . . . . ?
P1A C11A C12A C13A -179.2(6) . . . . ?
C11A C12A C13A C14A 0.5(12) . . . . ?
C12A C13A C14A C15A -1.5(12) . . . . ?
C13A C14A C15A C16A 1.9(10) . . . . ?
C12A C11A C16A C15A 0.3(7) . . . . ?
P1A C11A C16A C15A 179.6(4) . . . . ?
C14A C15A C16A C11A -1.3(8) . . . . ?
C31A P1A C21A C26A 168.5(3) . . . . ?
C11A P1A C21A C26A -83.7(3) . . . . ?
Cu1 P1A C21A C26A 47.3(3) . . . . ?
C31A P1A C21A C22A -10.7(4) . . . . ?
C11A P1A C21A C22A 97.2(3) . . . . ?
Cu1 P1A C21A C22A -131.9(3) . . . . ?
C26A C21A C22A C23A -0.9(6) . . . . ?
P1A C21A C22A C23A 178.2(3) . . . . ?
C21A C22A C23A C24A 1.1(7) . . . . ?
C22A C23A C24A C25A -0.2(8) . . . . ?
C23A C24A C25A C26A -0.9(9) . . . . ?
C24A C25A C26A C21A 1.1(8) . . . . ?
C22A C21A C26A C25A -0.2(7) . . . . ?
P1A C21A C26A C25A -179.4(4) . . . . ?
C11A P1A C31A C36A 4.8(4) . . . . ?
C21A P1A C31A C36A 112.6(4) . . . . ?
Cu1 P1A C31A C36A -123.6(3) . . . . ?
C11A P1A C31A C32A -177.7(3) . . . . ?
C21A P1A C31A C32A -69.8(4) . . . . ?
Cu1 P1A C31A C32A 54.0(4) . . . . ?
C36A C31A C32A C33A -2.0(7) . . . . ?
P1A C31A C32A C33A -179.7(4) . . . . ?
C31A C32A C33A C34A 2.4(9) . . . . ?
C32A C33A C34A C35A -0.7(10) . . . . ?
C33A C34A C35A C36A -1.4(10) . . . . ?
C32A C31A C36A C35A -0.1(7) . . . . ?
P1A C31A C36A C35A 177.5(4) . . . . ?
C34A C35A C36A C31A 1.8(9) . . . . ?
N1B Cu2 S1B C4B 5.12(16) . . . . ?
P1B Cu2 S1B C4B -113.67(13) . . . . ?
S1B Cu2 S1B C4B 111.33(13) 2_666 . . . ?
Cu2 Cu2 S1B C4B 111.33(13) 2_666 . . . ?
N1B Cu2 S1B Cu2 -106.21(11) . . . 2_666 ?
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S1B Cu2 P1B C11B 163.96(18) 2_666 . . . ?
S1B Cu2 P1B C11B 31.83(18) . . . . ?
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S1B Cu2 N1B C1B -174.2(6) . . . . ?
Cu2 Cu2 N1B C1B 134.4(6) 2_666 . . . ?
P1B Cu2 N1B C5B 105.5(3) . . . . ?
S1B Cu2 N1B C5B -119.8(3) 2_666 . . . ?
S1B Cu2 N1B C5B -7.1(3) . . . . ?
Cu2 Cu2 N1B C5B -58.5(3) 2_666 . . . ?
C5B N1B C1B N2B -0.1(5) . . . . ?
Cu2 N1B C1B N2B 167.4(4) . . . . ?
C2B N2B C1B N1B -0.4(6) . . . . ?
C3B N3B C2B N2B -178.6(4) . . . . ?
C3B N3B C2B C5B 1.5(6) . . . . ?
C1B N2B C2B N3B -179.2(4) . . . . ?
C1B N2B C2B C5B 0.7(5) . . . . ?
C2B N3B C3B N4B -0.9(7) . . . . ?
C4B N4B C3B N3B -0.2(7) . . . . ?
C3B N4B C4B C5B 0.8(6) . . . . ?
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Cu2 S1B C4B N4B 174.3(3) . . . . ?
Cu2 S1B C4B C5B 63.4(3) 2_666 . . . ?
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C1B N1B C5B C2B 0.6(5) . . . . ?
Cu2 N1B C5B C2B -171.9(3) . . . . ?
C1B N1B C5B C4B -179.2(4) . . . . ?
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N3B C2B C5B N1B 179.1(4) . . . . ?
N2B C2B C5B N1B -0.8(5) . . . . ?
N3B C2B C5B C4B -1.0(6) . . . . ?
N2B C2B C5B C4B 179.0(4) . . . . ?
N4B C4B C5B N1B 179.6(4) . . . . ?
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N4B C4B C5B C2B -0.2(5) . . . . ?
S1B C4B C5B C2B 177.2(3) . . . . ?
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C31B P1B C11B C16B 81.8(5) . . . . ?
Cu2 P1B C11B C16B -152.6(5) . . . . ?
C21B P1B C11B C12B 152.8(4) . . . . ?
C31B P1B C11B C12B -96.4(4) . . . . ?
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C16B C11B C12B C13B -1.1(9) . . . . ?
P1B C11B C12B C13B 177.2(5) . . . . ?
C11B C12B C13B C14B 0.4(11) . . . . ?
C12B C13B C14B C15B 0.1(13) . . . . ?
C13B C14B C15B C16B 0.1(14) . . . . ?
C12B C11B C16B C15B 1.2(10) . . . . ?
P1B C11B C16B C15B -176.9(6) . . . . ?
C14B C15B C16B C11B -0.8(13) . . . . ?
C11B P1B C21B C22B -60.9(4) . . . . ?
C31B P1B C21B C22B -168.6(4) . . . . ?
Cu2 P1B C21B C22B 67.4(4) . . . . ?
C11B P1B C21B C26B 127.0(4) . . . . ?
C31B P1B C21B C26B 19.3(4) . . . . ?
Cu2 P1B C21B C26B -104.7(4) . . . . ?
C26B C21B C22B C23B -1.1(7) . . . . ?
P1B C21B C22B C23B -173.5(4) . . . . ?
C21B C22B C23B C24B 0.5(7) . . . . ?
C22B C23B C24B C25B 0.1(8) . . . . ?
C23B C24B C25B C26B -0.2(8) . . . . ?
C22B C21B C26B C25B 1.0(7) . . . . ?
P1B C21B C26B C25B 172.9(4) . . . . ?
C24B C25B C26B C21B -0.3(8) . . . . ?
C21B P1B C31B C36B -108.9(5) . . . . ?
C11B P1B C31B C36B 141.5(5) . . . . ?
Cu2 P1B C31B C36B 13.2(5) . . . . ?
C21B P1B C31B C32B 75.9(5) . . . . ?
C11B P1B C31B C32B -33.7(5) . . . . ?
Cu2 P1B C31B C32B -162.1(4) . . . . ?
C36B C31B C32B C33B 0.9(8) . . . . ?
P1B C31B C32B C33B 176.1(4) . . . . ?
C31B C32B C33B C34B -1.4(10) . . . . ?
C32B C33B C34B C35B 1.8(13) . . . . ?
C33B C34B C35B C36B -1.6(14) . . . . ?
C32B C31B C36B C35B -0.7(10) . . . . ?
P1B C31B C36B C35B -176.2(6) . . . . ?
C34B C35B C36B C31B 1.1(13) . . . . ?

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N2B H2BA N2A  0.86 1.88 2.730(4) 170.7 1_565

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;
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 'H'  'H'   0.0000   0.0000
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 '-x, -y, -z'

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_cell_angle_gamma                 67.452(7)
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;
CrysAlisRED; Oxford Diffraction, 2010.
;

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_computing_cell_refinement     '<i>CrysAlisPRO</i> (Oxford Diffraction,
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_computing_data_reduction      '<i>CrysAlisRED</i> (Oxford Diffraction,
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_computing_structure_solution   '<i>SHELXS97</i> (Sheldrick, 2008)'
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Refinement of <i>F</i>^2^ against ALL reflections. The weighted <i>R</i>-
factor
<i>wR</i> and goodness of fit <i>S</i> are based on <i>F</i>^2^,
conventional
<i>R</i>-factors <i>R</i> are based on <i>F</i>, with <i>F</i> set to zero
for
negative <i>F</i>^2^. The threshold expression of <i>F</i>^2^ >
\s(<i>F</i>^2^) is used only for calculating <i>R</i>-factors(gt)
<i>etc</i>.
and is not relevant to the choice of reflections for refinement.
<i>R</i>-factors based on <i>F</i>^2^ are statistically about twice as
large
as those based on <i>F</i>, and <i>R</i>- factors based on ALL data will
be
even larger.
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 'calc w=1/[\s^2^(Fo^2^)+(0.0379P)^2^+1.7543P] 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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S1 S 0.78764(6) 0.29375(5) 0.07007(5) 0.03739(14) Uani 1 1 d . . .
Cl1 Cl 0.93989(6) 0.47712(5) 0.14088(5) 0.04125(14) Uani 1 1 d . . .
P1 P 0.88347(6) 0.23300(5) 0.30971(4) 0.03462(14) Uani 1 1 d . . .
P2 P 0.58964(6) 0.52003(5) 0.20602(4) 0.02970(12) Uani 1 1 d . . .
O1 O 1.1525(2) 0.00303(18) -0.0618(2) 0.0796(8) Uani 1 1 d . . .
N1 N 0.9940(2) 0.14344(18) 0.00026(19) 0.0468(6) Uani 1 1 d D . .
H1NA H 0.944(3) 0.105(2) 0.012(2) 0.056 Uiso 1 1 d D . .
N2 N 1.0313(2) 0.29761(17) 0.01491(16) 0.0396(5) Uani 1 1 d D . .
H2NA H 0.998(3) 0.3585(18) 0.0361(19) 0.048 Uiso 1 1 d D . .
C1 C 1.1208(3) 0.0949(2) -0.0406(2) 0.0524(7) Uani 1 1 d . . .
C2 C 1.2041(3) 0.1592(2) -0.0518(2) 0.0558(8) Uani 1 1 d . . .
H2A H 1.2926 0.1326 -0.0793 0.067 Uiso 1 1 calc R . .
C3 C 1.1572(3) 0.2571(2) -0.0234(2) 0.0474(6) Uani 1 1 d . . .
H3A H 1.2136 0.2992 -0.0303 0.057 Uiso 1 1 calc R . .
C4 C 0.9457(2) 0.24351(18) 0.02768(16) 0.0325(5) Uani 1 1 d . . .
C5 C 1.0480(3) 0.1323(2) 0.28131(17) 0.0381(5) Uani 1 1 d . . .
C6 C 1.1447(3) 0.1749(3) 0.2400(3) 0.0609(8) Uani 1 1 d . . .
H6A H 1.1228 0.2540 0.2235 0.073 Uiso 1 1 calc R . .
C7 C 1.2735(3) 0.1035(3) 0.2223(3) 0.0801(12) Uani 1 1 d . . .
H7A H 1.3402 0.1339 0.1953 0.096 Uiso 1 1 calc R . .
C8 C 1.3062(4) -0.0101(3) 0.2430(3) 0.0757(11) Uani 1 1 d . . .
H8A H 1.3948 -0.0586 0.2293 0.091 Uiso 1 1 calc R . .
C9 C 1.2113(4) -0.0538(3) 0.2835(3) 0.0811(12) Uani 1 1 d . . .
H9A H 1.2339 -0.1330 0.2987 0.097 Uiso 1 1 calc R . .
C10 C 1.0821(3) 0.0168(2) 0.3026(3) 0.0662(9) Uani 1 1 d . . .
H10A H 1.0161 -0.0142 0.3305 0.079 Uiso 1 1 calc R . .
C11 C 0.7865(3) 0.14173(19) 0.35332(19) 0.0405(5) Uani 1 1 d . . .
C12 C 0.7444(3) 0.1030(3) 0.2883(2) 0.0577(8) Uani 1 1 d . . .
H12A H 0.7667 0.1238 0.2238 0.069 Uiso 1 1 calc R . .
C13 C 0.6701(4) 0.0343(3) 0.3170(3) 0.0673(9) Uani 1 1 d . . .
H13A H 0.6416 0.0081 0.2721 0.081 Uiso 1 1 calc R . .
C14 C 0.6376(3) 0.0041(3) 0.4101(3) 0.0682(10) Uani 1 1 d . . .
H14A H 0.5863 -0.0428 0.4296 0.082 Uiso 1 1 calc R . .
C15 C 0.6788(3) 0.0412(3) 0.4747(3) 0.0642(9) Uani 1 1 d . . .
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H15A H 0.6562 0.0198 0.5391 0.077 Uiso 1 1 calc R . .
C16 C 0.7535(3) 0.1102(2) 0.4471(2) 0.0495(7) Uani 1 1 d . . .
H16A H 0.7819 0.1358 0.4925 0.059 Uiso 1 1 calc R . .
C17 C 0.9152(2) 0.2693(2) 0.41382(17) 0.0385(5) Uani 1 1 d . . .
C18 C 0.8450(3) 0.3762(3) 0.4300(2) 0.0609(8) Uani 1 1 d . . .
H18A H 0.7819 0.4289 0.3869 0.073 Uiso 1 1 calc R . .
C19 C 0.8645(4) 0.4081(3) 0.5072(3) 0.0812(12) Uani 1 1 d . . .
H19A H 0.8141 0.4820 0.5174 0.097 Uiso 1 1 calc R . .
C20 C 0.9555(4) 0.3346(3) 0.5692(3) 0.0734(10) Uani 1 1 d . . .
H20A H 0.9695 0.3572 0.6221 0.088 Uiso 1 1 calc R . .
C21 C 1.0268(4) 0.2278(3) 0.5549(3) 0.0711(10) Uani 1 1 d . . .
H21A H 1.0901 0.1760 0.5982 0.085 Uiso 1 1 calc R . .
C22 C 1.0070(3) 0.1954(3) 0.4778(2) 0.0592(8) Uani 1 1 d . . .
H22A H 1.0571 0.1211 0.4684 0.071 Uiso 1 1 calc R . .
C23 C 0.5478(2) 0.63355(19) 0.10303(16) 0.0324(5) Uani 1 1 d . . .
C24 C 0.4723(3) 0.7442(2) 0.1099(2) 0.0478(6) Uani 1 1 d . . .
H24A H 0.4439 0.7628 0.1697 0.057 Uiso 1 1 calc R . .
C25 C 0.4383(3) 0.8273(2) 0.0309(2) 0.0553(7) Uani 1 1 d . . .
H25A H 0.3869 0.9027 0.0366 0.066 Uiso 1 1 calc R . .
C26 C 0.4780(3) 0.8019(3) -0.0555(2) 0.0520(7) Uani 1 1 d . . .
H26A H 0.4529 0.8593 -0.1098 0.062 Uiso 1 1 calc R . .
C27 C 0.5545(3) 0.6932(3) -0.06365(19) 0.0519(7) Uani 1 1 d . . .
H27A H 0.5836 0.6755 -0.1237 0.062 Uiso 1 1 calc R . .
C28 C 0.5893(3) 0.6091(2) 0.01550(17) 0.0405(5) Uani 1 1 d . . .
H28A H 0.6422 0.5340 0.0094 0.049 Uiso 1 1 calc R . .
C29 C 0.5788(2) 0.59792(18) 0.29615(17) 0.0350(5) Uani 1 1 d . . .
C30 C 0.6722(3) 0.6483(2) 0.2894(2) 0.0488(6) Uani 1 1 d . . .
H30A H 0.7383 0.6418 0.2390 0.059 Uiso 1 1 calc R . .
C31 C 0.6701(4) 0.7079(3) 0.3554(3) 0.0640(9) Uani 1 1 d . . .
H31A H 0.7336 0.7432 0.3500 0.077 Uiso 1 1 calc R . .
C32 C 0.5757(4) 0.7159(3) 0.4291(2) 0.0708(10) Uani 1 1 d . . .
H32A H 0.5742 0.7567 0.4746 0.085 Uiso 1 1 calc R . .
C33 C 0.4845(4) 0.6658(3) 0.4372(2) 0.0685(10) Uani 1 1 d . . .
H33A H 0.4205 0.6708 0.4888 0.082 Uiso 1 1 calc R . .
C34 C 0.4845(3) 0.6072(2) 0.37043(19) 0.0498(7) Uani 1 1 d . . .
H34A H 0.4195 0.5735 0.3759 0.060 Uiso 1 1 calc R . .
C35 C 0.4411(2) 0.4826(2) 0.23304(16) 0.0361(5) Uani 1 1 d . . .
C36 C 0.3194(3) 0.5494(2) 0.1941(2) 0.0509(7) Uani 1 1 d . . .
H36A H 0.3117 0.6172 0.1504 0.061 Uiso 1 1 calc R . .
C37 C 0.2097(3) 0.5174(3) 0.2189(3) 0.0661(9) Uani 1 1 d . . .
H37A H 0.1271 0.5629 0.1912 0.079 Uiso 1 1 calc R . .
C38 C 0.2187(3) 0.4207(3) 0.2829(2) 0.0659(9) Uani 1 1 d . . .
H38A H 0.1418 0.4006 0.3009 0.079 Uiso 1 1 calc R . .
C39 C 0.3388(4) 0.3527(3) 0.3210(2) 0.0637(9) Uani 1 1 d . . .
H39A H 0.3458 0.2849 0.3646 0.076 Uiso 1 1 calc R . .
C40 C 0.4500(3) 0.3836(3) 0.29561(19) 0.0487(6) Uani 1 1 d . . .
H40A H 0.5333 0.3361 0.3215 0.058 Uiso 1 1 calc R . .

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0.00983(11)
S1 0.0289(3) 0.0379(3) 0.0504(4) -0.0206(3) 0.0022(2) -0.0123(2)
Cl1 0.0396(3) 0.0349(3) 0.0557(4) -0.0121(3) 0.0015(3) -0.0202(2)
P1 0.0348(3) 0.0274(3) 0.0413(3) -0.0040(2) -0.0028(2) -0.0124(2)
P2 0.0292(3) 0.0295(3) 0.0320(3) -0.0108(2) -0.0017(2) -0.0097(2)
O1 0.0470(12) 0.0483(12) 0.154(3) -0.0570(15) 0.0311(14) -0.0196(10)
N1 0.0323(11) 0.0332(11) 0.0810(17) -0.0258(11) 0.0116(11) -0.0152(9)
N2 0.0362(11) 0.0285(10) 0.0585(13) -0.0164(9) 0.0072(9) -0.0156(8)
C1 0.0364(14) 0.0351(13) 0.086(2) -0.0241(14) 0.0117(14) -0.0113(11)
C2 0.0349(14) 0.0417(14) 0.091(2) -0.0203(15) 0.0152(14) -0.0161(11)
C3 0.0376(13) 0.0375(13) 0.0707(18) -0.0143(12) 0.0099(12) -0.0201(11)
C4 0.0320(11) 0.0256(10) 0.0400(12) -0.0081(9) -0.0022(9) -0.0096(9)
C5 0.0413(13) 0.0323(12) 0.0403(13) -0.0073(10) -0.0011(10) -0.0134(10)
C6 0.0421(16) 0.0436(16) 0.090(2) -0.0058(15) 0.0054(15) -0.0152(13)
C7 0.0439(18) 0.067(2) 0.116(3) -0.012(2) 0.0191(19) -0.0173(16)
C8 0.0494(19) 0.067(2) 0.094(3) -0.030(2) 0.0160(18) -0.0016(16)
C9 0.072(2) 0.0394(17) 0.116(3) -0.0271(19) 0.015(2) -0.0031(16)
C10 0.0573(19) 0.0376(15) 0.098(3) -0.0183(16) 0.0173(18) -0.0155(13)
C11 0.0379(13) 0.0282(11) 0.0520(15) -0.0017(10) -0.0039(11) -0.0116(10)
C12 0.070(2) 0.0529(17) 0.0599(18) 0.0014(14) -0.0112(15) -0.0377(16)
C13 0.067(2) 0.0583(19) 0.089(3) -0.0039(17) -0.0163(19) -0.0386(17)
C14 0.0489(18) 0.0526(18) 0.104(3) -0.0040(18) 0.0070(18) -0.0308(15)
C15 0.0555(19) 0.0593(19) 0.072(2) -0.0060(16) 0.0200(16) -0.0268(16)
C16 0.0436(15) 0.0439(14) 0.0565(17) -0.0075(12) 0.0088(12) -0.0169(12)
C17 0.0368(12) 0.0367(12) 0.0409(13) -0.0048(10) -0.0039(10) -0.0136(10)
C18 0.064(2) 0.0467(16) 0.0644(19) -0.0189(14) -0.0236(16) 0.0003(14)
C19 0.091(3) 0.060(2) 0.083(3) -0.0388(19) -0.029(2) 0.0057(19)
C20 0.079(2) 0.078(2) 0.067(2) -0.0325(19) -0.0197(19) -0.016(2)
C21 0.074(2) 0.064(2) 0.068(2) -0.0140(17) -0.0330(18) -0.0068(18)
C22 0.0626(19) 0.0420(15) 0.0653(19) -0.0128(14) -0.0235(16) -0.0025(14)
C23 0.0317(11) 0.0338(11) 0.0321(11) -0.0071(9) -0.0027(9) -0.0117(9)
C24 0.0514(16) 0.0386(13) 0.0449(14) -0.0108(11) -0.0038(12) -0.0052(12)
C25 0.0559(18) 0.0365(14) 0.0619(18) -0.0025(13) -0.0120(14) -0.0057(12)
C26 0.0487(16) 0.0543(17) 0.0497(16) 0.0069(13) -0.0131(13) -0.0218(13)
C27 0.0595(18) 0.0633(18) 0.0368(14) -0.0071(12) -0.0038(12) -0.0280(15)
C28 0.0453(14) 0.0401(13) 0.0384(13) -0.0123(10) -0.0018(10) -0.0157(11)
C29 0.0362(12) 0.0278(11) 0.0381(12) -0.0108(9) -0.0054(10) -0.0051(9)
C30 0.0486(15) 0.0476(15) 0.0581(17) -0.0231(13) -0.0025(13) -0.0188(12)
C31 0.073(2) 0.0537(18) 0.079(2) -0.0276(16) -0.0209(18) -0.0247(16)
C32 0.107(3) 0.0546(19) 0.0549(19) -0.0263(15) -0.0206(19) -0.0191(19)
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C38 0.0565(19) 0.102(3) 0.067(2) -0.037(2) 0.0128(16) -0.053(2)
C39 0.077(2) 0.085(2) 0.0493(17) -0.0074(16) 0.0000(16) -0.057(2)
C40 0.0518(16) 0.0582(17) 0.0443(15) -0.0085(12) -0.0062(12) -0.0289(14)

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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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P2 C35 1.819(2) . ?
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N1 C1 1.387(3) . ?
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N2 C4 1.338(3) . ?
N2 C3 1.350(3) . ?
N2 H2NA 0.857(17) . ?
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O1 C1 C2 126.1(3) . . ?
N1 C1 C2 114.3(2) . . ?
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_cell_measurement_temperature     173(2)
_cell_measurement_reflns_used   18388
_cell_measurement_theta_min     3.20
_cell_measurement_theta_max     32.28

_exptl_crystal_description        plate
_exptl_crystal_colour             yellow
_exptl_crystal_size_max           0.24
_exptl_crystal_size_mid           0.18
_exptl_crystal_size_min           0.12
_exptl_crystal_density_meas       ?
_exptl_crystal_density_diffrn     1.368
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              2800
_exptl_absorpt_coefficient_mu     0.893
_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_correction_T_min   0.8142
_exptl_absorpt_correction_T_max   0.9004
_exptl_absorpt_process_details
'CrysAlisRED; Oxford Diffraction, 2007.'

_exptl_special_details
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;

_diffrn_ambient_temperature       173(2)
_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source 'Enhance (Mo) X-ray Source'
_diffrn_radiation_monochromator 'graphite'
_diffrn_measurement_device_type 'Xcalibur, Eos, Gemini'
_diffrn_detector_area_resol_mean 16.1500
_diffrn_measurement_method        ' \w scans'

_diffrn_reflns_number             77752
_diffrn_reflns_av_R_equivalents   0.0475
_diffrn_reflns_av_sigmaI/netI     0.0717
_diffrn_reflns_limit_h_min        -23
_diffrn_reflns_limit_h_max        23
_diffrn_reflns_limit_k_min        -24
_diffrn_reflns_limit_k_max        24
_diffrn_reflns_limit_l_min        -30
_diffrn_reflns_limit_l_max        28
_diffrn_reflns_theta_min          3.21
_diffrn_reflns_theta_max          27.88
_reflns_number_total              31317
_reflns_number_gt                 19640
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection   '<i>CrysAlisPRO</i> (Oxford Diffraction,
2010)'
_computing_cell_refinement     '<i>CrysAlisPRO</i> (Oxford Diffraction,
2010)'
_computing_data_reduction      '<i>CrysAlisRED</i> (Oxford Diffraction,
2010)'
_computing_structure_solution   '<i>SHELXS97</i> (Sheldrick, 2008)'
_computing_structure_refinement  '<i>SHELXL97</i> (Sheldrick, 2008)'
_computing_molecular_graphics   '<i>SHELXTL</i> (Bruker, 2000)'
_computing_publication_material    '<i>SHELXTL</i> (Bruker, 2000)'

_refine_special_details
;
Refinement of <i>F</i>^2^ against ALL reflections. The weighted <i>R</i>-
factor
<i>wR</i> and goodness of fit <i>S</i> are based on <i>F</i>^2^,
conventional
<i>R</i>-factors <i>R</i> are based on <i>F</i>, with <i>F</i> set to zero
for
negative <i>F</i>^2^. The threshold expression of <i>F</i>^2^ >
\s(<i>F</i>^2^) is used only for calculating <i>R</i>-factors(gt)
<i>etc</i>.
and is not relevant to the choice of reflections for refinement.
<i>R</i>-factors based on <i>F</i>^2^ are statistically about twice as
large
as those based on <i>F</i>, and <i>R</i>- factors based on ALL data will
be
```

```
even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0449P)^2^+1.9596P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          31317
_refine_ls_number_parameters      1573
_refine_ls_number_restraints      2
_refine_ls_R_factor_all           0.1037
_refine_ls_R_factor_gt            0.0542
_refine_ls_wR_factor_ref          0.1234
_refine_ls_wR_factor_gt           0.1041
_refine_ls_goodness_of_fit_ref    1.016
_refine_ls_restrained_S_all       1.016
_refine_ls_shift/su_max           0.001
_refine_ls_shift/su_mean          0.000

loop_
 _atom_site_label
 _atom_site_type_symbol
 _atom_site_fract_x
 _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
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
Cu1 Cu 0.66897(2) 0.99612(2) 0.147577(18) 0.03256(9) Uani 1 1 d . . .
Cu2 Cu 0.50575(2) 0.81293(2) 0.341779(18) 0.03244(9) Uani 1 1 d . . .
Cl1 Cl 0.61996(4) 0.87849(5) 0.24295(4) 0.03981(19) Uani 1 1 d . . .
S1 S 0.56195(5) 1.06555(5) 0.11185(4) 0.0432(2) Uani 1 1 d . . .
S2 S 0.40372(5) 0.90315(5) 0.36308(4) 0.0415(2) Uani 1 1 d . . .
P1 P 0.72329(5) 1.05499(5) 0.19377(4) 0.03383(18) Uani 1 1 d . . .
P2 P 0.74673(5) 0.95201(5) 0.06491(4) 0.03309(18) Uani 1 1 d . . .
P3 P 0.45571(5) 0.74268(5) 0.30176(4) 0.03232(18) Uani 1 1 d . . .
P4 P 0.56278(5) 0.75509(5) 0.42429(4) 0.03051(17) Uani 1 1 d . . .
N1 N 0.46692(14) 0.98950(15) 0.23477(13) 0.0342(6) Uani 1 1 d D . .
H1N H 0.5115(14) 0.9617(16) 0.2391(15) 0.041 Uiso 1 1 d D . .
N2 N 0.32813(18) 1.0077(2) 0.28247(18) 0.0606(9) Uani 1 1 d . . .
C1 C 0.39838(18) 0.97056(19) 0.28893(16) 0.0357(7) Uani 1 1 d . . .
C2 C 0.3325(2) 1.0610(2) 0.2206(2) 0.0656(12) Uani 1 1 d . . .
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H2B H 0.2834 1.0866 0.2148 0.079 Uiso 1 1 calc R . .
C3 C 0.4002(2) 1.0808(2) 0.16665(18) 0.0455(9) Uani 1 1 d . . .
H3A H 0.3982 1.1187 0.1250 0.055 Uiso 1 1 calc R . .
C4 C 0.47168(18) 1.04469(18) 0.17387(16) 0.0364(7) Uani 1 1 d . . .
C5 C 0.78709(19) 1.13640(19) 0.13354(15) 0.0372(7) Uani 1 1 d . . .
C6 C 0.8668(2) 1.1419(2) 0.12809(19) 0.0611(11) Uani 1 1 d . . .
H6A H 0.8916 1.1017 0.1565 0.073 Uiso 1 1 calc R . .
C7 C 0.9104(3) 1.2059(3) 0.0812(2) 0.0843(15) Uani 1 1 d . . .
H7A H 0.9648 1.2096 0.0786 0.101 Uiso 1 1 calc R . .
C8 C 0.8777(3) 1.2634(3) 0.0389(2) 0.0727(13) Uani 1 1 d . . .
H8A H 0.9091 1.3065 0.0063 0.087 Uiso 1 1 calc R . .
C9 C 0.7993(3) 1.2589(2) 0.0436(2) 0.0630(11) Uani 1 1 d . . .
H9A H 0.7754 1.2993 0.0146 0.076 Uiso 1 1 calc R . .
C10 C 0.7544(2) 1.1957(2) 0.09051(18) 0.0510(9) Uani 1 1 d . . .
H10E H 0.6998 1.1930 0.0931 0.061 Uiso 1 1 calc R . .
C11 C 0.65187(19) 1.09670(19) 0.25249(15) 0.0376(7) Uani 1 1 d . . .
C12 C 0.6676(2) 1.1624(2) 0.2587(2) 0.0610(11) Uani 1 1 d . . .
H12E H 0.7171 1.1882 0.2311 0.073 Uiso 1 1 calc R . .
C13 C 0.6118(3) 1.1905(3) 0.3048(2) 0.0729(13) Uani 1 1 d . . .
H13J H 0.6237 1.2349 0.3093 0.087 Uiso 1 1 calc R . .
C14 C 0.5393(3) 1.1545(3) 0.3441(2) 0.0653(11) Uani 1 1 d . . .
H14E H 0.5003 1.1747 0.3748 0.078 Uiso 1 1 calc R . .
C15 C 0.5237(2) 1.0896(2) 0.33864(18) 0.0549(10) Uani 1 1 d . . .
H15A H 0.4740 1.0641 0.3663 0.066 Uiso 1 1 calc R . .
C16 C 0.5797(2) 1.0605(2) 0.29307(16) 0.0439(8) Uani 1 1 d . . .
H16A H 0.5682 1.0151 0.2899 0.053 Uiso 1 1 calc R . .
C17 C 0.78814(19) 0.99225(19) 0.24163(16) 0.0391(8) Uani 1 1 d . . .
C18 C 0.7807(2) 0.9858(2) 0.30564(19) 0.0588(10) Uani 1 1 d . . .
H18A H 0.7408 1.0155 0.3269 0.071 Uiso 1 1 calc R . .
C19 C 0.8312(3) 0.9360(3) 0.3391(2) 0.0756(13) Uani 1 1 d . . .
H19A H 0.8250 0.9313 0.3835 0.091 Uiso 1 1 calc R . .
C20 C 0.8890(3) 0.8940(3) 0.3094(2) 0.0685(12) Uani 1 1 d . . .
H20A H 0.9244 0.8613 0.3324 0.082 Uiso 1 1 calc R . .
C21 C 0.8969(2) 0.8985(2) 0.2463(2) 0.0657(11) Uani 1 1 d . . .
H21A H 0.9367 0.8680 0.2258 0.079 Uiso 1 1 calc R . .
C22 C 0.8465(2) 0.9476(2) 0.2125(2) 0.0536(10) Uani 1 1 d . . .
H22A H 0.8521 0.9507 0.1686 0.064 Uiso 1 1 calc R . .
C23 C 0.79345(17) 1.0259(2) -0.01629(15) 0.0358(7) Uani 1 1 d . . .
C24 C 0.8356(2) 1.0088(2) -0.07368(17) 0.0498(9) Uani 1 1 d . . .
H24A H 0.8385 0.9576 -0.0719 0.060 Uiso 1 1 calc R . .
C25 C 0.8731(2) 1.0666(3) -0.13325(18) 0.0618(11) Uani 1 1 d . . .
H25A H 0.9024 1.0548 -0.1721 0.074 Uiso 1 1 calc R . .
C26 C 0.8682(2) 1.1410(3) -0.13663(19) 0.0630(12) Uani 1 1 d . . .
H26A H 0.8948 1.1802 -0.1775 0.076 Uiso 1 1 calc R . .
C27 C 0.8253(2) 1.1584(2) -0.0815(2) 0.0613(11) Uani 1 1 d . . .
H27A H 0.8205 1.2101 -0.0842 0.074 Uiso 1 1 calc R . .
C28 C 0.7886(2) 1.1008(2) -0.02124(18) 0.0480(9) Uani 1 1 d . . .
H28A H 0.7596 1.1133 0.0173 0.058 Uiso 1 1 calc R . .
C29 C 0.8323(2) 0.8883(2) 0.08036(16) 0.0401(8) Uani 1 1 d . . .
C30 C 0.8178(2) 0.8191(2) 0.13351(19) 0.0572(10) Uani 1 1 d . . .
H30A H 0.7639 0.8064 0.1625 0.069 Uiso 1 1 calc R . .
C31 C 0.8812(3) 0.7679(3) 0.1451(2) 0.0709(12) Uani 1 1 d . . .
H31A H 0.8701 0.7193 0.1803 0.085 Uiso 1 1 calc R . .
C32 C 0.9588(3) 0.7871(3) 0.1063(2) 0.0853(16) Uani 1 1 d . . .
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H32A H 1.0020 0.7520 0.1143 0.102 Uiso 1 1 calc R . .
C33 C 0.9746(3) 0.8563(3) 0.0562(2) 0.0844(15) Uani 1 1 d . . .
H33A H 1.0292 0.8700 0.0298 0.101 Uiso 1 1 calc R . .
C34 C 0.9120(2) 0.9076(3) 0.04293(19) 0.0602(11) Uani 1 1 d . . .
H34A H 0.9240 0.9563 0.0079 0.072 Uiso 1 1 calc R . .
C35 C 0.68943(18) 0.8983(2) 0.04303(15) 0.0378(7) Uani 1 1 d . . .
C36 C 0.6268(2) 0.9356(2) 0.0204(2) 0.0576(10) Uani 1 1 d . . .
H36A H 0.6154 0.9878 0.0155 0.069 Uiso 1 1 calc R . .
C37 C 0.5796(2) 0.8982(3) 0.0046(2) 0.0663(12) Uani 1 1 d . . .
H37A H 0.5356 0.9248 -0.0103 0.080 Uiso 1 1 calc R . .
C38 C 0.5951(2) 0.8251(3) 0.0102(2) 0.0656(12) Uani 1 1 d . . .
H38A H 0.5631 0.8005 -0.0020 0.079 Uiso 1 1 calc R . .
C39 C 0.6562(3) 0.7861(3) 0.0331(3) 0.0967(17) Uani 1 1 d . . .
H39A H 0.6668 0.7339 0.0379 0.116 Uiso 1 1 calc R . .
C40 C 0.7036(3) 0.8235(3) 0.0498(3) 0.0824(15) Uani 1 1 d . . .
H40A H 0.7465 0.7961 0.0662 0.099 Uiso 1 1 calc R . .
C41 C 0.52670(19) 0.6847(2) 0.25773(16) 0.0408(8) Uani 1 1 d . . .
C42 C 0.5110(2) 0.6635(2) 0.21179(19) 0.0578(10) Uani 1 1 d . . .
H42A H 0.4620 0.6798 0.2013 0.069 Uiso 1 1 calc R . .
C43 C 0.5668(3) 0.6182(3) 0.1808(2) 0.0735(13) Uani 1 1 d . . .
H43A H 0.5561 0.6040 0.1489 0.088 Uiso 1 1 calc R . .
C44 C 0.6370(3) 0.5941(3) 0.1961(3) 0.0802(14) Uani 1 1 d . . .
H44A H 0.6750 0.5630 0.1751 0.096 Uiso 1 1 calc R . .
C45 C 0.6524(3) 0.6149(3) 0.2416(2) 0.0831(15) Uani 1 1 d . . .
H45A H 0.7013 0.5981 0.2522 0.100 Uiso 1 1 calc R . .
C46 C 0.5980(2) 0.6600(2) 0.2722(2) 0.0586(11) Uani 1 1 d . . .
H46A H 0.6097 0.6742 0.3036 0.070 Uiso 1 1 calc R . .
C47 C 0.37506(18) 0.67782(19) 0.36579(15) 0.0367(7) Uani 1 1 d . . .
C48 C 0.3666(2) 0.6044(2) 0.37052(19) 0.0523(9) Uani 1 1 d . . .
H48A H 0.4060 0.5831 0.3408 0.063 Uiso 1 1 calc R . .
C49 C 0.2999(2) 0.5617(2) 0.4192(2) 0.0637(11) Uani 1 1 d . . .
H49A H 0.2937 0.5114 0.4222 0.076 Uiso 1 1 calc R . .
C50 C 0.2435(2) 0.5915(2) 0.46264(19) 0.0565(10) Uani 1 1 d . . .
H50A H 0.1984 0.5618 0.4957 0.068 Uiso 1 1 calc R . .
C51 C 0.2517(2) 0.6637(2) 0.45869(18) 0.0507(9) Uani 1 1 d . . .
H51A H 0.2121 0.6844 0.4887 0.061 Uiso 1 1 calc R . .
C52 C 0.31725(18) 0.7064(2) 0.41109(16) 0.0417(8) Uani 1 1 d . . .
H52A H 0.3231 0.7562 0.4092 0.050 Uiso 1 1 calc R . .
C53 C 0.40547(18) 0.80304(19) 0.24075(15) 0.0356(7) Uani 1 1 d . . .
C54 C 0.32352(19) 0.7986(2) 0.25184(17) 0.0508(9) Uani 1 1 d . . .
H54A H 0.2920 0.7599 0.2906 0.061 Uiso 1 1 calc R . .
C55 C 0.2877(2) 0.8506(3) 0.20626(19) 0.0656(12) Uani 1 1 d . . .
H55A H 0.2315 0.8474 0.2140 0.079 Uiso 1 1 calc R . .
C56 C 0.3321(2) 0.9060(2) 0.15063(19) 0.0607(11) Uani 1 1 d . . .
H56A H 0.3067 0.9420 0.1202 0.073 Uiso 1 1 calc R . .
C57 C 0.4137(2) 0.9100(2) 0.13848(18) 0.0566(10) Uani 1 1 d . . .
H57A H 0.4451 0.9481 0.0991 0.068 Uiso 1 1 calc R . .
C58 C 0.4500(2) 0.8587(2) 0.18347(17) 0.0491(9) Uani 1 1 d . . .
H58A H 0.5065 0.8618 0.1749 0.059 Uiso 1 1 calc R . .
C59 C 0.65690(18) 0.70284(18) 0.39852(15) 0.0343(7) Uani 1 1 d . . .
C60 C 0.72183(19) 0.7457(2) 0.34796(16) 0.0426(8) Uani 1 1 d . . .
H60A H 0.7172 0.7999 0.3308 0.051 Uiso 1 1 calc R . .
C61 C 0.7932(2) 0.7101(2) 0.32226(18) 0.0501(9) Uani 1 1 d . . .
H61A H 0.8376 0.7401 0.2883 0.060 Uiso 1 1 calc R . .
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C62 C 0.8004(2) 0.6320(2) 0.34548(19) 0.0533(10) Uani 1 1 d . . .
H62A H 0.8490 0.6078 0.3268 0.064 Uiso 1 1 calc R . .
C63 C 0.7374(2) 0.5889(2) 0.3955(2) 0.0535(10) Uani 1 1 d . . .
H63A H 0.7423 0.5347 0.4116 0.064 Uiso 1 1 calc R . .
C64 C 0.6659(2) 0.62418(19) 0.42307(18) 0.0440(8) Uani 1 1 d . . .
H64A H 0.6232 0.5939 0.4590 0.053 Uiso 1 1 calc R . .
C65 C 0.49911(18) 0.68388(18) 0.49905(16) 0.0374(7) Uani 1 1 d . . .
C66 C 0.4662(2) 0.6282(2) 0.4906(2) 0.0548(10) Uani 1 1 d . . .
H66A H 0.4790 0.6272 0.4469 0.066 Uiso 1 1 calc R . .
C67 C 0.4150(3) 0.5740(3) 0.5449(3) 0.0828(15) Uani 1 1 d . . .
H67A H 0.3940 0.5354 0.5385 0.099 Uiso 1 1 calc R . .
C68 C 0.3947(3) 0.5763(3) 0.6083(3) 0.0927(17) Uani 1 1 d . . .
H68A H 0.3589 0.5397 0.6456 0.111 Uiso 1 1 calc R . .
C69 C 0.4261(3) 0.6313(3) 0.6171(2) 0.0799(14) Uani 1 1 d . . .
H69A H 0.4121 0.6326 0.6609 0.096 Uiso 1 1 calc R . .
C70 C 0.4778(2) 0.6850(2) 0.56343(17) 0.0509(9) Uani 1 1 d . . .
H70A H 0.4991 0.7231 0.5704 0.061 Uiso 1 1 calc R . .
C71 C 0.59529(17) 0.81549(18) 0.45674(14) 0.0311(7) Uani 1 1 d . . .
C72 C 0.64838(19) 0.7885(2) 0.49388(16) 0.0412(8) Uani 1 1 d . . .
H72A H 0.6689 0.7374 0.5030 0.049 Uiso 1 1 calc R . .
C73 C 0.6716(2) 0.8354(2) 0.51771(18) 0.0474(9) Uani 1 1 d . . .
H73A H 0.7078 0.8165 0.5433 0.057 Uiso 1 1 calc R . .
C74 C 0.6423(2) 0.9096(2) 0.50452(17) 0.0481(9) Uani 1 1 d . . .
H74A H 0.6580 0.9417 0.5213 0.058 Uiso 1 1 calc R . .
C75 C 0.5906(2) 0.9372(2) 0.46721(17) 0.0489(9) Uani 1 1 d . . .
H75A H 0.5709 0.9886 0.4578 0.059 Uiso 1 1 calc R . .
C76 C 0.56677(18) 0.89024(19) 0.44316(16) 0.0384(7) Uani 1 1 d . . .
H76A H 0.5308 0.9095 0.4173 0.046 Uiso 1 1 calc R . .
Cu3 Cu 0.19219(2) 0.47216(2) 0.157014(18) 0.03515(10) Uani 1 1 d . . .
Cu4 Cu -0.00899(2) 0.31592(2) 0.344553(18) 0.03411(9) Uani 1 1 d . . .
Cl2 Cl 0.12184(5) 0.36378(5) 0.25593(4) 0.0438(2) Uani 1 1 d . . .
S3 S 0.10305(5) 0.53649(6) 0.09817(4) 0.0506(2) Uani 1 1 d . . .
S4 S -0.09540(5) 0.42375(5) 0.34660(4) 0.0490(2) Uani 1 1 d . . .
P5 P 0.28133(5) 0.40793(5) 0.09373(4) 0.0387(2) Uani 1 1 d . . .
P6 P 0.23353(4) 0.54404(5) 0.20044(4) 0.03054(17) Uani 1 1 d . . .
P7 P 0.03013(4) 0.25618(5) 0.43748(4) 0.02957(17) Uani 1 1 d . . .
P8 P -0.06553(5) 0.25143(5) 0.30380(4) 0.03462(19) Uani 1 1 d . . .
N3 N -0.01053(15) 0.48745(16) 0.21751(14) 0.0386(6) Uani 1 1 d D . .
H3N H 0.0273(16) 0.4551(16) 0.2308(15) 0.046 Uiso 1 1 d D . .
N4 N -0.14784(19) 0.5200(2) 0.24499(18) 0.0674(10) Uani 1 1 d . . .
C77 C -0.0846(2) 0.48010(19) 0.26466(17) 0.0416(8) Uani 1 1 d . . .
C78 C -0.1296(2) 0.5637(3) 0.1779(2) 0.0711(13) Uani 1 1 d . . .
H78A H -0.1733 0.5913 0.1630 0.085 Uiso 1 1 calc R . .
C79 C -0.0556(2) 0.5715(2) 0.13109(18) 0.0491(9) Uani 1 1 d . . .
H79A H -0.0479 0.6036 0.0855 0.059 Uiso 1 1 calc R . .
C80 C 0.00683(19) 0.53188(19) 0.15136(16) 0.0387(7) Uani 1 1 d . . .
C81 C 0.3426(2) 0.4682(2) 0.01008(16) 0.0437(8) Uani 1 1 d . . .
C82 C 0.4261(2) 0.4588(2) -0.01736(18) 0.0548(10) Uani 1 1 d . . .
H82A H 0.4542 0.4178 0.0073 0.066 Uiso 1 1 calc R . .
C83 C 0.4682(3) 0.5087(3) -0.0801(2) 0.0699(12) Uani 1 1 d . . .
H83A H 0.5250 0.5012 -0.0983 0.084 Uiso 1 1 calc R . .
C84 C 0.4297(3) 0.5682(3) -0.1160(2) 0.0717(13) Uani 1 1 d . . .
H84A H 0.4591 0.6016 -0.1594 0.086 Uiso 1 1 calc R . .
C85 C 0.3480(3) 0.5800(3) -0.0893(2) 0.0716(13) Uani 1 1 d . . .
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H85A H 0.3209 0.6222 -0.1139 0.086 Uiso 1 1 calc R . .
C86 C 0.3052(2) 0.5305(2) -0.02662(18) 0.0606(11) Uani 1 1 d . . .
H86A H 0.2488 0.5395 -0.0084 0.073 Uiso 1 1 calc R . .
C87 C 0.35201(18) 0.34304(19) 0.13249(16) 0.0389(8) Uani 1 1 d . . .
C88 C 0.4051(2) 0.2932(2) 0.10454(18) 0.0486(9) Uani 1 1 d . . .
H88A H 0.4051 0.2922 0.0632 0.058 Uiso 1 1 calc R . .
C89 C 0.4572(2) 0.2457(2) 0.1367(2) 0.0579(10) Uani 1 1 d . . .
H89A H 0.4943 0.2134 0.1165 0.070 Uiso 1 1 calc R . .
C90 C 0.4561(2) 0.2443(2) 0.1971(2) 0.0607(11) Uani 1 1 d . . .
H90A H 0.4924 0.2114 0.2189 0.073 Uiso 1 1 calc R . .
C91 C 0.4023(2) 0.2908(2) 0.2265(2) 0.0611(11) Uani 1 1 d . . .
H91A H 0.4005 0.2892 0.2691 0.073 Uiso 1 1 calc R . .
C92 C 0.3508(2) 0.3399(2) 0.19427(18) 0.0487(9) Uani 1 1 d . . .
H92A H 0.3139 0.3720 0.2149 0.058 Uiso 1 1 calc R . .
C93 C 0.2296(2) 0.3446(2) 0.0770(2) 0.0523(10) Uani 1 1 d . . .
C94 C 0.2059(3) 0.3678(3) 0.0211(3) 0.0824(14) Uani 1 1 d . . .
H94A H 0.2205 0.4169 -0.0127 0.099 Uiso 1 1 calc R . .
C95 C 0.1599(4) 0.3190(4) 0.0137(4) 0.109(2) Uani 1 1 d . . .
H95A H 0.1413 0.3359 -0.0241 0.131 Uiso 1 1 calc R . .
C96 C 0.1426(3) 0.2485(4) 0.0603(4) 0.110(2) Uani 1 1 d . . .
H96A H 0.1137 0.2150 0.0541 0.131 Uiso 1 1 calc R . .
C97 C 0.1656(3) 0.2239(4) 0.1162(3) 0.105(2) Uani 1 1 d . . .
H97A H 0.1525 0.1740 0.1489 0.126 Uiso 1 1 calc R . .
C98 C 0.2086(3) 0.2726(3) 0.1249(2) 0.0765(13) Uani 1 1 d . . .
H98A H 0.2236 0.2562 0.1644 0.092 Uiso 1 1 calc R . .
C99 C 0.29249(17) 0.49179(18) 0.25666(14) 0.0327(7) Uani 1 1 d . . .
C100 C 0.25543(19) 0.43046(19) 0.31407(15) 0.0403(8) Uani 1 1 d . . .
H10C H 0.2007 0.4192 0.3236 0.048 Uiso 1 1 calc R . .
C101 C 0.2975(2) 0.3861(2) 0.35715(17) 0.0520(9) Uani 1 1 d . . .
H10A H 0.2715 0.3450 0.3967 0.062 Uiso 1 1 calc R . .
C102 C 0.3772(2) 0.4014(2) 0.34274(19) 0.0580(10) Uani 1 1 d . . .
H10B H 0.4064 0.3704 0.3722 0.070 Uiso 1 1 calc R . .
C103 C 0.4147(2) 0.4610(2) 0.2861(2) 0.0579(10) Uani 1 1 d . . .
H10D H 0.4699 0.4710 0.2763 0.070 Uiso 1 1 calc R . .
C104 C 0.37264(19) 0.5068(2) 0.24305(17) 0.0435(8) Uani 1 1 d . . .
H10F H 0.3987 0.5485 0.2042 0.052 Uiso 1 1 calc R . .
C105 C 0.29875(17) 0.62255(18) 0.13623(14) 0.0331(7) Uani 1 1 d . . .
C106 C 0.3317(2) 0.6212(2) 0.07278(17) 0.0495(9) Uani 1 1 d . . .
H10J H 0.3209 0.5794 0.0640 0.059 Uiso 1 1 calc R . .
C107 C 0.3804(2) 0.6796(3) 0.02119(18) 0.0604(11) Uani 1 1 d . . .
H10I H 0.4025 0.6778 -0.0226 0.073 Uiso 1 1 calc R . .
C108 C 0.3967(2) 0.7395(2) 0.03325(19) 0.0545(10) Uani 1 1 d . . .
H10H H 0.4295 0.7799 -0.0023 0.065 Uiso 1 1 calc R . .
C109 C 0.3657(2) 0.7414(2) 0.0967(2) 0.0641(11) Uani 1 1 d . . .
H10G H 0.3784 0.7824 0.1055 0.077 Uiso 1 1 calc R . .
C110 C 0.3160(2) 0.6838(2) 0.14783(19) 0.0566(10) Uani 1 1 d . . .
H11C H 0.2934 0.6861 0.1914 0.068 Uiso 1 1 calc R . .
C111 C 0.15557(18) 0.59360(18) 0.24924(15) 0.0364(7) Uani 1 1 d . . .
C112 C 0.1600(2) 0.6024(2) 0.30518(18) 0.0555(10) Uani 1 1 d . . .
H11A H 0.2048 0.5809 0.3209 0.067 Uiso 1 1 calc R . .
C113 C 0.0996(3) 0.6425(2) 0.33891(19) 0.0687(12) Uani 1 1 d . . .
H11B H 0.1036 0.6485 0.3771 0.082 Uiso 1 1 calc R . .
C114 C 0.0348(2) 0.6731(2) 0.3171(2) 0.0669(12) Uani 1 1 d . . .
H11E H -0.0072 0.6995 0.3406 0.080 Uiso 1 1 calc R . .
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C115 C 0.0307(2) 0.6656(2) 0.2608(2) 0.0613(11) Uani 1 1 d . . .
H11D H -0.0138 0.6879 0.2450 0.074 Uiso 1 1 calc R . .
C116 C 0.08974(19) 0.6263(2) 0.22715(18) 0.0461(8) Uani 1 1 d . . .
H11G H 0.0856 0.6215 0.1885 0.055 Uiso 1 1 calc R . .
C117 C 0.07465(17) 0.31598(18) 0.46278(14) 0.0308(7) Uani 1 1 d . . .
C118 C 0.0546(2) 0.3930(2) 0.44457(16) 0.0433(8) Uani 1 1 d . . .
H11F H 0.0219 0.4150 0.4162 0.052 Uiso 1 1 calc R . .
C119 C 0.0824(2) 0.4385(2) 0.46782(19) 0.0570(10) Uani 1 1 d . . .
H11H H 0.0694 0.4916 0.4549 0.068 Uiso 1 1 calc R . .
C120 C 0.1287(2) 0.4063(3) 0.50945(19) 0.0593(11) Uani 1 1 d . . .
H12I H 0.1462 0.4372 0.5263 0.071 Uiso 1 1 calc R . .
C121 C 0.1499(2) 0.3310(2) 0.52710(18) 0.0510(9) Uani 1 1 d . . .
H12H H 0.1826 0.3096 0.5555 0.061 Uiso 1 1 calc R . .
C122 C 0.12342(18) 0.2854(2) 0.50348(15) 0.0397(8) Uani 1 1 d . . .
H12G H 0.1388 0.2328 0.5153 0.048 Uiso 1 1 calc R . .
C123 C 0.10597(18) 0.17897(18) 0.43361(15) 0.0331(7) Uani 1 1 d . . .
C124 C 0.0955(2) 0.1054(2) 0.48082(18) 0.0484(9) Uani 1 1 d . . .
H12F H 0.0479 0.0935 0.5188 0.058 Uiso 1 1 calc R . .
C125 C 0.1536(2) 0.0490(2) 0.4732(2) 0.0574(10) Uani 1 1 d . . .
H12B H 0.1463 -0.0012 0.5063 0.069 Uiso 1 1 calc R . .
C126 C 0.2219(2) 0.0655(2) 0.4180(2) 0.0538(10) Uani 1 1 d . . .
H12A H 0.2612 0.0264 0.4122 0.065 Uiso 1 1 calc R . .
C127 C 0.2337(2) 0.1381(2) 0.37115(19) 0.0506(9) Uani 1 1 d . . .
H12D H 0.2816 0.1496 0.3334 0.061 Uiso 1 1 calc R . .
C128 C 0.17609(19) 0.1948(2) 0.37861(17) 0.0423(8) Uani 1 1 d . . .
H12C H 0.1845 0.2451 0.3458 0.051 Uiso 1 1 calc R . .
C129 C -0.05131(17) 0.20957(18) 0.51436(15) 0.0327(7) Uani 1 1 d . . .
C130 C -0.10734(19) 0.1683(2) 0.51105(18) 0.0450(8) Uani 1 1 d . . .
H13I H -0.1023 0.1655 0.4692 0.054 Uiso 1 1 calc R . .
C131 C -0.1697(2) 0.1316(2) 0.5668(2) 0.0529(10) Uani 1 1 d . . .
H13E H -0.2073 0.1036 0.5634 0.064 Uiso 1 1 calc R . .
C132 C -0.1780(2) 0.1350(2) 0.62773(19) 0.0535(10) Uani 1 1 d . . .
H13H H -0.2211 0.1094 0.6665 0.064 Uiso 1 1 calc R . .
C133 C -0.1236(2) 0.1756(2) 0.63209(18) 0.0559(10) Uani 1 1 d . . .
H13F H -0.1292 0.1783 0.6741 0.067 Uiso 1 1 calc R . .
C134 C -0.06078(19) 0.2127(2) 0.57605(16) 0.0448(8) Uani 1 1 d . . .
H13C H -0.0236 0.2408 0.5798 0.054 Uiso 1 1 calc R . .
C135 C -0.01065(18) 0.16959(19) 0.28511(16) 0.0382(7) Uani 1 1 d . . .
C136 C -0.0228(2) 0.1421(2) 0.24097(17) 0.0454(8) Uani 1 1 d . . .
H13B H -0.0579 0.1693 0.2156 0.054 Uiso 1 1 calc R . .
C137 C 0.0154(2) 0.0758(2) 0.2336(2) 0.0576(10) Uani 1 1 d . . .
H13G H 0.0060 0.0576 0.2035 0.069 Uiso 1 1 calc R . .
C138 C 0.0668(3) 0.0359(3) 0.2690(2) 0.0743(13) Uani 1 1 d . . .
H13A H 0.0925 -0.0102 0.2641 0.089 Uiso 1 1 calc R . .
C139 C 0.0806(3) 0.0631(3) 0.3115(3) 0.0897(17) Uani 1 1 d . . .
H13D H 0.1167 0.0361 0.3360 0.108 Uiso 1 1 calc R . .
C140 C 0.0426(2) 0.1293(2) 0.3193(2) 0.0655(12) Uani 1 1 d . . .
H14G H 0.0533 0.1477 0.3488 0.079 Uiso 1 1 calc R . .
C141 C -0.16391(18) 0.2106(2) 0.36143(16) 0.0418(8) Uani 1 1 d . . .
C142 C -0.1877(2) 0.1389(2) 0.37298(18) 0.0561(10) Uani 1 1 d . . .
H14H H -0.1523 0.1086 0.3496 0.067 Uiso 1 1 calc R . .
C143 C -0.2622(3) 0.1111(3) 0.4181(2) 0.0739(13) Uani 1 1 d . . .
H14C H -0.2783 0.0622 0.4249 0.089 Uiso 1 1 calc R . .
C144 C -0.3133(2) 0.1537(3) 0.4531(2) 0.0704(13) Uani 1 1 d . . .
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H14D H -0.3644 0.1342 0.4845 0.085 Uiso 1 1 calc R . .
C145 C -0.2906(2) 0.2238(3) 0.4429(2) 0.0722(13) Uani 1 1 d . . .
H14I H -0.3260 0.2534 0.4671 0.087 Uiso 1 1 calc R . .
C146 C -0.2167(2) 0.2524(3) 0.3976(2) 0.0589(10) Uani 1 1 d . . .
H14B H -0.2015 0.3015 0.3910 0.071 Uiso 1 1 calc R . .
C147 C -0.0874(2) 0.3113(2) 0.22606(17) 0.0422(8) Uani 1 1 d . . .
C148 C -0.0244(2) 0.3435(2) 0.16901(18) 0.0566(10) Uani 1 1 d . . .
H14F H 0.0297 0.3331 0.1703 0.068 Uiso 1 1 calc R . .
C149 C -0.0378(3) 0.3904(3) 0.1100(2) 0.0717(12) Uani 1 1 d . . .
H14A H 0.0068 0.4111 0.0707 0.086 Uiso 1 1 calc R . .
C150 C -0.1142(4) 0.4073(3) 0.1075(3) 0.0925(17) Uani 1 1 d . . .
H15C H -0.1235 0.4394 0.0666 0.111 Uiso 1 1 calc R . .
C151 C -0.1771(4) 0.3783(4) 0.1635(3) 0.121(2) Uani 1 1 d . . .
H15B H -0.2308 0.3915 0.1618 0.145 Uiso 1 1 calc R . .
C152 C -0.1656(3) 0.3294(3) 0.2240(2) 0.0860(15) Uani 1 1 d . . .
H15D H -0.2107 0.3089 0.2629 0.103 Uiso 1 1 calc R . .

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Cu2 0.0352(2) 0.0299(2) 0.0343(2) -0.00885(17) -0.01590(16) -0.00281(15)
Cl1 0.0309(4) 0.0349(5) 0.0396(4) -0.0025(4) -0.0068(3) -0.0020(3)
S1 0.0419(5) 0.0412(5) 0.0360(4) -0.0041(4) -0.0122(4) 0.0013(4)
S2 0.0390(4) 0.0406(5) 0.0368(4) -0.0122(4) -0.0055(4) 0.0013(4)
P1 0.0343(4) 0.0358(5) 0.0368(4) -0.0184(4) -0.0103(4) -0.0043(3)
P2 0.0322(4) 0.0380(5) 0.0318(4) -0.0169(4) -0.0085(3) -0.0010(3)
P3 0.0313(4) 0.0343(5) 0.0353(4) -0.0148(4) -0.0114(3) -0.0038(3)
P4 0.0341(4) 0.0257(4) 0.0340(4) -0.0080(3) -0.0159(3) -0.0024(3)
N1 0.0310(14) 0.0345(16) 0.0378(14) -0.0121(13) -0.0150(12) 0.0038(11)
N2 0.0451(18) 0.062(2) 0.078(2) -0.030(2) -0.0246(17) 0.0130(15)
C1 0.0313(16) 0.0380(19) 0.0415(18) -0.0192(16) -0.0111(14) 0.0006(13)
C2 0.055(2) 0.060(3) 0.097(3) -0.033(3) -0.047(3) 0.024(2)
C3 0.051(2) 0.037(2) 0.051(2) -0.0091(17) -0.0318(18) 0.0095(16)
C4 0.0396(17) 0.0334(19) 0.0415(18) -0.0148(15) -0.0181(15) 0.0000(14)
C5 0.0431(18) 0.038(2) 0.0362(17) -0.0178(15) -0.0102(15) -0.0094(14)
C6 0.054(2) 0.063(3) 0.059(2) -0.002(2) -0.026(2) -0.019(2)
C7 0.059(3) 0.090(4) 0.083(3) 0.005(3) -0.024(2) -0.041(3)
C8 0.085(3) 0.060(3) 0.058(3) -0.003(2) -0.014(2) -0.032(2)
C9 0.085(3) 0.042(2) 0.059(2) -0.010(2) -0.026(2) -0.006(2)
C10 0.052(2) 0.042(2) 0.061(2) -0.0167(19) -0.0222(19) -0.0015(17)
C11 0.0403(18) 0.042(2) 0.0379(17) -0.0196(16) -0.0154(15) -0.0002(14)
C12 0.063(3) 0.060(3) 0.069(3) -0.042(2) -0.006(2) -0.013(2)
C13 0.092(3) 0.059(3) 0.080(3) -0.050(3) -0.011(3) -0.006(2)
C14 0.067(3) 0.071(3) 0.057(2) -0.037(2) -0.007(2) 0.011(2)
C15 0.053(2) 0.064(3) 0.046(2) -0.024(2) -0.0082(18) -0.0028(19)
C16 0.048(2) 0.049(2) 0.0388(18) -0.0208(17) -0.0118(16) -0.0034(16)
C17 0.0405(18) 0.037(2) 0.0441(19) -0.0146(16) -0.0162(15) -0.0066(14)
C18 0.058(2) 0.069(3) 0.052(2) -0.026(2) -0.022(2) 0.010(2)
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C19 0.078(3) 0.094(4) 0.055(3) -0.021(3) -0.035(2) 0.013(3)
C20 0.065(3) 0.056(3) 0.082(3) -0.007(2) -0.042(2) 0.001(2)
C21 0.056(2) 0.059(3) 0.094(3) -0.037(3) -0.032(2) 0.011(2)
C22 0.053(2) 0.060(3) 0.064(2) -0.036(2) -0.027(2) 0.0088(19)
C23 0.0292(16) 0.046(2) 0.0350(17) -0.0156(16) -0.0131(13) 0.0010(14)
C24 0.051(2) 0.054(2) 0.042(2) -0.0204(19) -0.0094(17) 0.0022(17)
C25 0.055(2) 0.087(4) 0.034(2) -0.017(2) -0.0073(18) -0.004(2)
C26 0.060(3) 0.077(3) 0.038(2) 0.001(2) -0.0156(19) -0.025(2)
C27 0.068(3) 0.048(3) 0.065(3) -0.008(2) -0.027(2) -0.016(2)
C28 0.049(2) 0.047(2) 0.048(2) -0.0181(19) -0.0143(17) -0.0039(17)
C29 0.049(2) 0.043(2) 0.0364(17) -0.0220(17) -0.0177(16) 0.0075(15)
C30 0.060(2) 0.055(3) 0.050(2) -0.021(2) -0.0124(19) 0.0117(19)
C31 0.087(3) 0.057(3) 0.062(3) -0.022(2) -0.027(3) 0.025(2)
C32 0.079(3) 0.101(4) 0.068(3) -0.031(3) -0.035(3) 0.045(3)
C33 0.047(2) 0.113(4) 0.082(3) -0.027(3) -0.027(2) 0.022(3)
C34 0.042(2) 0.075(3) 0.056(2) -0.014(2) -0.0196(19) 0.0037(19)
C35 0.0380(17) 0.043(2) 0.0365(17) -0.0204(16) -0.0081(14) -0.0047(14)
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C37 0.065(3) 0.080(3) 0.077(3) -0.037(3) -0.040(2) 0.002(2)
C38 0.066(3) 0.077(3) 0.074(3) -0.042(3) -0.024(2) -0.016(2)
C39 0.106(4) 0.068(4) 0.161(5) -0.069(4) -0.069(4) 0.011(3)
C40 0.075(3) 0.074(3) 0.141(5) -0.067(3) -0.060(3) 0.016(2)
C41 0.0391(18) 0.041(2) 0.0440(19) -0.0195(17) -0.0085(15) -0.0055(14)
C42 0.045(2) 0.076(3) 0.067(2) -0.043(2) -0.0159(19) -0.0030(19)
C43 0.068(3) 0.092(4) 0.079(3) -0.065(3) -0.004(2) -0.010(2)
C44 0.059(3) 0.089(4) 0.099(4) -0.063(3) -0.005(3) 0.010(2)
C45 0.056(3) 0.107(4) 0.095(4) -0.059(3) -0.022(3) 0.030(3)
C46 0.047(2) 0.076(3) 0.064(2) -0.038(2) -0.0220(19) 0.015(2)
C47 0.0366(17) 0.0361(19) 0.0395(17) -0.0112(15) -0.0152(15) -0.0060(14)
C48 0.054(2) 0.046(2) 0.058(2) -0.025(2) -0.0080(18) -0.0098(17)
C49 0.074(3) 0.042(2) 0.070(3) -0.020(2) -0.009(2) -0.023(2)
C50 0.053(2) 0.047(2) 0.057(2) -0.010(2) -0.0041(19) -0.0203(18)
C51 0.042(2) 0.050(2) 0.051(2) -0.0165(19) -0.0053(17) -0.0033(17)
C52 0.0398(18) 0.037(2) 0.0487(19) -0.0167(17) -0.0102(16) -0.0072(14)
C53 0.0404(18) 0.041(2) 0.0370(17) -0.0219(16) -0.0162(15) -0.0020(14)
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C55 0.042(2) 0.108(4) 0.044(2) -0.026(2) -0.0189(18) 0.012(2)
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C59 0.0376(17) 0.0368(19) 0.0361(17) -0.0137(15) -0.0204(14) 0.0001(14)
C60 0.0421(19) 0.040(2) 0.0430(19) -0.0109(16) -0.0159(16) 0.0005(15)
C61 0.043(2) 0.058(3) 0.047(2) -0.0199(19) -0.0110(17) 0.0006(17)
C62 0.047(2) 0.065(3) 0.063(2) -0.040(2) -0.0229(19) 0.0146(19)
C63 0.055(2) 0.038(2) 0.082(3) -0.029(2) -0.036(2) 0.0124(18)
C64 0.0429(19) 0.032(2) 0.057(2) -0.0130(17) -0.0183(17) -0.0042(15)
C65 0.0347(17) 0.0295(18) 0.0430(18) -0.0009(15) -0.0193(15) -0.0036(13)
C66 0.056(2) 0.044(2) 0.063(2) -0.0066(19) -0.0245(19) -0.0180(18)
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C68 0.092(4) 0.078(4) 0.071(3) 0.016(3) -0.012(3) -0.048(3)
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C71 0.0309(15) 0.0334(18) 0.0287(15) -0.0088(14) -0.0100(13) -0.0057(13)
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Cl2 0.0343(4) 0.0413(5) 0.0414(4) -0.0009(4) -0.0102(3) -0.0038(3)
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S4 0.0496(5) 0.0433(6) 0.0456(5) -0.0183(4) -0.0076(4) 0.0103(4)
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C77 0.0443(19) 0.035(2) 0.052(2) -0.0218(17) -0.0180(17) 0.0038(15)
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C79 0.045(2) 0.053(2) 0.047(2) -0.0124(18) -0.0250(18) 0.0145(17)
C80 0.0436(18) 0.0323(19) 0.0454(19) -0.0139(16) -0.0219(16) 0.0026(14)
C81 0.0444(19) 0.053(2) 0.0364(18) -0.0185(17) -0.0100(15) -0.0093(16)
C82 0.050(2) 0.059(3) 0.049(2) -0.015(2) -0.0107(18) -0.0084(18)
C83 0.055(2) 0.087(4) 0.054(2) -0.024(3) 0.004(2) -0.019(2)
C84 0.081(3) 0.082(4) 0.042(2) -0.016(2) -0.004(2) -0.030(3)
C85 0.082(3) 0.079(3) 0.045(2) -0.008(2) -0.025(2) -0.008(2)
C86 0.054(2) 0.073(3) 0.045(2) -0.015(2) -0.0126(19) -0.003(2)
C87 0.0354(17) 0.0350(19) 0.0449(19) -0.0173(16) -0.0077(15) -0.0017(14)
C88 0.052(2) 0.041(2) 0.050(2) -0.0241(18) -0.0050(18) -0.0007(17)
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C108 0.044(2) 0.046(2) 0.053(2) 0.0035(19) -0.0103(18) -0.0154(17)
C109 0.076(3) 0.045(3) 0.069(3) -0.020(2) -0.012(2) -0.023(2)
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C114 0.060(3) 0.057(3) 0.063(3) -0.027(2) 0.006(2) 0.012(2)
C115 0.039(2) 0.060(3) 0.082(3) -0.032(2) -0.014(2) 0.0102(18)

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C132 0.040(2) 0.048(2) 0.055(2) -0.0149(19) 0.0045(17) -0.0106(16)
C133 0.054(2) 0.068(3) 0.0392(19) -0.021(2) -0.0014(17) -0.0114(19)
C134 0.0392(18) 0.056(2) 0.0408(18) -0.0215(18) -0.0061(15) -0.0113(16)
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C146 0.038(2) 0.075(3) 0.076(3) -0.043(2) -0.0155(19) -0.0012(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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S1 C4 1.693(3) . ?
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P1 C5 1.826(3) . ?
P1 C11 1.830(3) . ?
P1 C17 1.832(3) . ?
P2 C23 1.826(3) . ?
P2 C29 1.828(3) . ?
P2 C35 1.837(3) . ?
P3 C53 1.827(3) . ?
P3 C47 1.829(3) . ?
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Cu4 S4 2.3618(9) . ?
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S4 C77 1.711(3) . ?
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C123 C124 H12F 119.7 . . ?
C126 C125 C124 120.0(4) . . ?
C126 C125 H12B 120.0 . . ?
C124 C125 H12B 120.0 . . ?
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C128 C127 H12D 120.0 . . ?
C127 C128 C123 120.6(3) . . ?
C127 C128 H12C 119.7 . . ?
C123 C128 H12C 119.7 . . ?
C134 C129 C130 117.7(3) . . ?
C134 C129 P7 124.0(2) . . ?
C130 C129 P7 118.3(2) . . ?
C131 C130 C129 121.4(3) . . ?
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C129 C130 H13I 119.3 . . ?
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C130 C131 H13E 119.9 . . ?
C132 C131 H13E 119.9 . . ?
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C131 C132 H13H 120.3 . . ?
C132 C133 C134 120.6(3) . . ?
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C133 C134 C129 120.7(3) . . ?
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C129 C134 H13C 119.6 . . ?
C140 C135 C136 117.5(3) . . ?
C140 C135 P8 118.7(2) . . ?
C136 C135 P8 123.7(2) . . ?
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C137 C136 H13B 119.6 . . ?
C135 C136 H13B 119.6 . . ?
C138 C137 C136 120.8(3) . . ?
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C136 C137 H13G 119.6 . . ?
C139 C138 C137 119.2(4) . . ?
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C135 C140 H14G 119.3 . . ?
C139 C140 H14G 119.3 . . ?
C142 C141 C146 117.8(3) . . ?
C142 C141 P8 123.7(3) . . ?
C146 C141 P8 118.4(3) . . ?
C143 C142 C141 120.7(4) . . ?
C143 C142 H14H 119.6 . . ?
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C144 C143 C142 120.3(4) . . ?
C144 C143 H14C 119.9 . . ?
C142 C143 H14C 119.9 . . ?
C145 C144 C143 119.7(4) . . ?
C145 C144 H14D 120.1 . . ?
C143 C144 H14D 120.1 . . ?
C144 C145 C146 120.5(4) . . ?
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C146 C145 H14I 119.8 . . ?
C145 C146 C141 121.0(4) . . ?
C145 C146 H14B 119.5 . . ?
C141 C146 H14B 119.5 . . ?
C148 C147 C152 118.6(4) . . ?
C148 C147 P8 119.1(3) . . ?
C152 C147 P8 122.2(3) . . ?
C147 C148 C149 121.2(4) . . ?
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C149 C148 H14F 119.4 . . ?
C150 C149 C148 120.3(5) . . ?
C150 C149 H14A 119.8 . . ?
C148 C149 H14A 119.8 . . ?
C151 C150 C149 119.4(5) . . ?
C151 C150 H15C 120.3 . . ?
C149 C150 H15C 120.3 . . ?
C150 C151 C152 121.7(5) . . ?
C150 C151 H15B 119.1 . . ?
C152 C151 H15B 119.1 . . ?
C147 C152 C151 118.7(5) . . ?
C147 C152 H15D 120.7 . . ?
C151 C152 H15D 120.7 . . ?

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P3 Cu2 Cl1 Cu1 100.22(7) . . . . ?
S2 Cu2 Cl1 Cu1 -11.24(8) . . . . ?
P2 Cu1 S1 C4 135.01(12) . . . . ?
P1 Cu1 S1 C4 -87.97(12) . . . . ?
Cl1 Cu1 S1 C4 24.37(13) . . . . ?
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Cl1 Cu1 P1 C11 -73.89(12) . . . . ?
P2 Cu1 P1 C17 -66.08(12) . . . . ?
S1 Cu1 P1 C17 164.82(12) . . . . ?
Cl1 Cu1 P1 C17 46.85(12) . . . . ?
P1 Cu1 P2 C23 -68.77(11) . . . . ?
S1 Cu1 P2 C23 63.29(11) . . . . ?
Cl1 Cu1 P2 C23 179.20(10) . . . . ?
P1 Cu1 P2 C29 52.69(14) . . . . ?
S1 Cu1 P2 C29 -175.25(13) . . . . ?
Cl1 Cu1 P2 C29 -59.34(13) . . . . ?
P1 Cu1 P2 C35 173.92(12) . . . . ?
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S1 Cu1 P2 C35 -54.03(12) . . . . ?
Cl1 Cu1 P2 C35 61.89(12) . . . . ?
P4 Cu2 P3 C53 175.09(11) . . . . ?
S2 Cu2 P3 C53 43.49(11) . . . . ?
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P4 Cu2 P3 C47 59.64(12) . . . . ?
S2 Cu2 P3 C47 -71.96(12) . . . . ?
Cl1 Cu2 P3 C47 173.92(11) . . . . ?
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S2 Cu2 P3 C41 163.21(13) . . . . ?
Cl1 Cu2 P3 C41 49.08(13) . . . . ?
P3 Cu2 P4 C65 -53.24(13) . . . . ?
S2 Cu2 P4 C65 74.72(13) . . . . ?
Cl1 Cu2 P4 C65 -166.56(12) . . . . ?
P3 Cu2 P4 C59 65.75(12) . . . . ?
S2 Cu2 P4 C59 -166.30(11) . . . . ?
Cl1 Cu2 P4 C59 -47.58(12) . . . . ?
P3 Cu2 P4 C71 -176.23(11) . . . . ?
S2 Cu2 P4 C71 -48.28(11) . . . . ?
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C2 N2 C1 N1 1.0(5) . . . . ?
C2 N2 C1 S2 179.2(3) . . . . ?
C4 N1 C1 N2 1.5(5) . . . . ?
C4 N1 C1 S2 -176.7(2) . . . . ?
Cu2 S2 C1 N2 150.2(3) . . . . ?
Cu2 S2 C1 N1 -31.7(3) . . . . ?
C1 N2 C2 C3 -1.8(6) . . . . ?
N2 C2 C3 C4 0.0(6) . . . . ?
C1 N1 C4 C3 -3.3(5) . . . . ?
C1 N1 C4 S1 176.8(2) . . . . ?
C2 C3 C4 N1 2.4(5) . . . . ?
C2 C3 C4 S1 -177.7(3) . . . . ?
Cu1 S1 C4 N1 -3.9(3) . . . . ?
Cu1 S1 C4 C3 176.3(3) . . . . ?
C11 P1 C5 C10 -71.1(3) . . . . ?
C17 P1 C5 C10 -178.4(3) . . . . ?
Cu1 P1 C5 C10 56.1(3) . . . . ?
C11 P1 C5 C6 109.4(3) . . . . ?
C17 P1 C5 C6 2.2(3) . . . . ?
Cu1 P1 C5 C6 -123.3(3) . . . . ?
C10 C5 C6 C7 0.9(6) . . . . ?
P1 C5 C6 C7 -179.7(4) . . . . ?
C5 C6 C7 C8 -1.4(8) . . . . ?
C6 C7 C8 C9 1.4(8) . . . . ?
C7 C8 C9 C10 -0.9(7) . . . . ?
C6 C5 C10 C9 -0.4(5) . . . . ?
P1 C5 C10 C9 -179.9(3) . . . . ?
C8 C9 C10 C5 0.4(6) . . . . ?
C5 P1 C11 C16 160.4(3) . . . . ?
C17 P1 C11 C16 -91.8(3) . . . . ?
Cu1 P1 C11 C16 34.3(3) . . . . ?
C5 P1 C11 C12 -20.7(3) . . . . ?
C17 P1 C11 C12 87.1(3) . . . . ?
Cu1 P1 C11 C12 -146.7(3) . . . . ?
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C16 C11 C12 C13 0.0(6) . . . . ?
P1 C11 C12 C13 -178.9(3) . . . . ?
C11 C12 C13 C14 -1.3(7) . . . . ?
C12 C13 C14 C15 1.8(7) . . . . ?
C13 C14 C15 C16 -1.1(6) . . . . ?
C12 C11 C16 C15 0.7(5) . . . . ?
P1 C11 C16 C15 179.7(3) . . . . ?
C14 C15 C16 C11 -0.2(5) . . . . ?
C5 P1 C17 C18 103.5(3) . . . . ?
C11 P1 C17 C18 -2.5(3) . . . . ?
Cu1 P1 C17 C18 -130.5(3) . . . . ?
C5 P1 C17 C22 -78.1(3) . . . . ?
C11 P1 C17 C22 175.9(3) . . . . ?
Cu1 P1 C17 C22 47.9(3) . . . . ?
C22 C17 C18 C19 0.5(6) . . . . ?
P1 C17 C18 C19 178.9(3) . . . . ?
C17 C18 C19 C20 1.0(7) . . . . ?
C18 C19 C20 C21 -2.0(7) . . . . ?
C19 C20 C21 C22 1.5(7) . . . . ?
C18 C17 C22 C21 -0.9(6) . . . . ?
P1 C17 C22 C21 -179.4(3) . . . . ?
C20 C21 C22 C17 -0.1(6) . . . . ?
C29 P2 C23 C28 -120.7(3) . . . . ?
C35 P2 C23 C28 131.8(3) . . . . ?
Cu1 P2 C23 C28 8.2(3) . . . . ?
C29 P2 C23 C24 58.0(3) . . . . ?
C35 P2 C23 C24 -49.5(3) . . . . ?
Cu1 P2 C23 C24 -173.1(2) . . . . ?
C28 C23 C24 C25 1.7(5) . . . . ?
P2 C23 C24 C25 -177.0(3) . . . . ?
C23 C24 C25 C26 -0.9(5) . . . . ?
C24 C25 C26 C27 -1.0(6) . . . . ?
C25 C26 C27 C28 2.0(6) . . . . ?
C24 C23 C28 C27 -0.7(5) . . . . ?
P2 C23 C28 C27 178.1(3) . . . . ?
C26 C27 C28 C23 -1.2(5) . . . . ?
C23 P2 C29 C30 -170.8(3) . . . . ?
C35 P2 C29 C30 -64.7(3) . . . . ?
Cu1 P2 C29 C30 61.5(3) . . . . ?
C23 P2 C29 C34 12.3(3) . . . . ?
C35 P2 C29 C34 118.5(3) . . . . ?
Cu1 P2 C29 C34 -115.4(3) . . . . ?
C34 C29 C30 C31 -5.6(6) . . . . ?
P2 C29 C30 C31 177.4(3) . . . . ?
C29 C30 C31 C32 3.6(6) . . . . ?
C30 C31 C32 C33 0.0(7) . . . . ?
C31 C32 C33 C34 -1.5(8) . . . . ?
C30 C29 C34 C33 4.2(6) . . . . ?
P2 C29 C34 C33 -178.9(3) . . . . ?
C32 C33 C34 C29 -0.7(7) . . . . ?
C23 P2 C35 C40 117.0(4) . . . . ?
C29 P2 C35 C40 10.2(4) . . . . ?
Cu1 P2 C35 C40 -118.3(3) . . . . ?
C23 P2 C35 C36 -65.2(3) . . . . ?
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C29 P2 C35 C36 -171.9(3) . . . . ?
Cu1 P2 C35 C36 59.5(3) . . . . ?
C40 C35 C36 C37 -0.3(6) . . . . ?
P2 C35 C36 C37 -178.3(3) . . . . ?
C35 C36 C37 C38 -1.0(6) . . . . ?
C36 C37 C38 C39 1.7(7) . . . . ?
C37 C38 C39 C40 -1.1(8) . . . . ?
C36 C35 C40 C39 1.0(7) . . . . ?
P2 C35 C40 C39 178.8(4) . . . . ?
C38 C39 C40 C35 -0.3(8) . . . . ?
C53 P3 C41 C46 150.0(3) . . . . ?
C47 P3 C41 C46 -103.3(3) . . . . ?
Cu2 P3 C41 C46 25.6(3) . . . . ?
C53 P3 C41 C42 -31.3(3) . . . . ?
C47 P3 C41 C42 75.4(3) . . . . ?
Cu2 P3 C41 C42 -155.7(3) . . . . ?
C46 C41 C42 C43 -0.2(6) . . . . ?
P3 C41 C42 C43 -178.9(3) . . . . ?
C41 C42 C43 C44 0.5(7) . . . . ?
C42 C43 C44 C45 -0.3(8) . . . . ?
C43 C44 C45 C46 0.0(8) . . . . ?
C44 C45 C46 C41 0.3(7) . . . . ?
C42 C41 C46 C45 -0.2(6) . . . . ?
P3 C41 C46 C45 178.6(4) . . . . ?
C53 P3 C47 C48 98.6(3) . . . . ?
C41 P3 C47 C48 -8.7(3) . . . . ?
Cu2 P3 C47 C48 -140.3(3) . . . . ?
C53 P3 C47 C52 -79.2(3) . . . . ?
C41 P3 C47 C52 173.5(2) . . . . ?
Cu2 P3 C47 C52 41.9(3) . . . . ?
C52 C47 C48 C49 1.4(5) . . . . ?
P3 C47 C48 C49 -176.3(3) . . . . ?
C47 C48 C49 C50 -0.7(6) . . . . ?
C48 C49 C50 C51 0.2(6) . . . . ?
C49 C50 C51 C52 -0.5(6) . . . . ?
C50 C51 C52 C47 1.2(5) . . . . ?
C48 C47 C52 C51 -1.7(5) . . . . ?
P3 C47 C52 C51 176.2(3) . . . . ?
C47 P3 C53 C58 -178.4(3) . . . . ?
C41 P3 C53 C58 -69.2(3) . . . . ?
Cu2 P3 C53 C58 59.2(3) . . . . ?
C47 P3 C53 C54 6.1(3) . . . . ?
C41 P3 C53 C54 115.3(3) . . . . ?
Cu2 P3 C53 C54 -116.3(3) . . . . ?
C58 C53 C54 C55 -1.3(5) . . . . ?
P3 C53 C54 C55 174.2(3) . . . . ?
C53 C54 C55 C56 0.1(6) . . . . ?
C54 C55 C56 C57 1.2(6) . . . . ?
C55 C56 C57 C58 -1.3(6) . . . . ?
C56 C57 C58 C53 0.1(6) . . . . ?
C54 C53 C58 C57 1.2(5) . . . . ?
P3 C53 C58 C57 -174.5(3) . . . . ?
C65 P4 C59 C64 13.1(3) . . . . ?
C71 P4 C59 C64 121.1(3) . . . . ?
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Cu2 P4 C59 C64 -111.5(3) . . . . ?
C65 P4 C59 C60 -170.8(2) . . . . ?
C71 P4 C59 C60 -62.8(3) . . . . ?
Cu2 P4 C59 C60 64.6(2) . . . . ?
C64 C59 C60 C61 1.0(5) . . . . ?
P4 C59 C60 C61 -175.4(3) . . . . ?
C59 C60 C61 C62 1.2(5) . . . . ?
C60 C61 C62 C63 -1.7(5) . . . . ?
C61 C62 C63 C64 0.0(5) . . . . ?
C60 C59 C64 C63 -2.7(5) . . . . ?
P4 C59 C64 C63 173.3(2) . . . . ?
C62 C63 C64 C59 2.3(5) . . . . ?
C59 P4 C65 C66 -72.8(3) . . . . ?
C71 P4 C65 C66 -178.8(3) . . . . ?
Cu2 P4 C65 C66 51.0(3) . . . . ?
C59 P4 C65 C70 111.2(3) . . . . ?
C71 P4 C65 C70 5.2(3) . . . . ?
Cu2 P4 C65 C70 -125.0(3) . . . . ?
C70 C65 C66 C67 -1.5(5) . . . . ?
P4 C65 C66 C67 -177.7(3) . . . . ?
C65 C66 C67 C68 1.6(7) . . . . ?
C66 C67 C68 C69 -1.0(8) . . . . ?
C67 C68 C69 C70 0.3(8) . . . . ?
C68 C69 C70 C65 -0.2(7) . . . . ?
C66 C65 C70 C69 0.8(5) . . . . ?
P4 C65 C70 C69 176.8(3) . . . . ?
C65 P4 C71 C76 -111.8(3) . . . . ?
C59 P4 C71 C76 140.1(3) . . . . ?
Cu2 P4 C71 C76 16.0(3) . . . . ?
C65 P4 C71 C72 68.9(3) . . . . ?
C59 P4 C71 C72 -39.2(3) . . . . ?
Cu2 P4 C71 C72 -163.2(2) . . . . ?
C76 C71 C72 C73 0.9(5) . . . . ?
P4 C71 C72 C73 -179.9(3) . . . . ?
C71 C72 C73 C74 -0.2(5) . . . . ?
C72 C73 C74 C75 -0.5(5) . . . . ?
C73 C74 C75 C76 0.7(5) . . . . ?
C72 C71 C76 C75 -0.7(5) . . . . ?
P4 C71 C76 C75 -180.0(2) . . . . ?
C74 C75 C76 C71 -0.1(5) . . . . ?
P5 Cu3 Cl2 Cu4 -144.50(7) . . . . ?
P6 Cu3 Cl2 Cu4 87.67(7) . . . . ?
S3 Cu3 Cl2 Cu4 -34.06(8) . . . . ?
P7 Cu4 Cl2 Cu3 -136.61(7) . . . . ?
P8 Cu4 Cl2 Cu3 94.70(7) . . . . ?
S4 Cu4 Cl2 Cu3 -16.02(8) . . . . ?
P5 Cu3 S3 C80 139.21(13) . . . . ?
P6 Cu3 S3 C80 -83.65(13) . . . . ?
Cl2 Cu3 S3 C80 32.32(13) . . . . ?
P7 Cu4 S4 C77 156.30(12) . . . . ?
P8 Cu4 S4 C77 -67.19(13) . . . . ?
Cl2 Cu4 S4 C77 44.12(13) . . . . ?
P6 Cu3 P5 C87 54.54(13) . . . . ?
S3 Cu3 P5 C87 -173.19(12) . . . . ?
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Cl2 Cu3 P5 C87 -60.19(12) . . . . ?
P6 Cu3 P5 C81 -69.97(12) . . . . ?
S3 Cu3 P5 C81 62.30(12) . . . . ?
Cl2 Cu3 P5 C81 175.30(12) . . . . ?
P6 Cu3 P5 C93 171.48(15) . . . . ?
S3 Cu3 P5 C93 -56.24(15) . . . . ?
Cl2 Cu3 P5 C93 56.76(15) . . . . ?
P5 Cu3 P6 C105 60.24(11) . . . . ?
S3 Cu3 P6 C105 -68.65(11) . . . . ?
Cl2 Cu3 P6 C105 172.87(10) . . . . ?
P5 Cu3 P6 C99 -59.16(11) . . . . ?
S3 Cu3 P6 C99 171.95(11) . . . . ?
Cl2 Cu3 P6 C99 53.47(11) . . . . ?
P5 Cu3 P6 C111 179.13(12) . . . . ?
S3 Cu3 P6 C111 50.24(12) . . . . ?
Cl2 Cu3 P6 C111 -68.24(12) . . . . ?
P8 Cu4 P7 C129 -60.88(12) . . . . ?
S4 Cu4 P7 C129 67.02(12) . . . . ?
Cl2 Cu4 P7 C129 -177.83(11) . . . . ?
P8 Cu4 P7 C117 179.63(10) . . . . ?
S4 Cu4 P7 C117 -52.47(11) . . . . ?
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P8 Cu4 P7 C123 58.63(12) . . . . ?
S4 Cu4 P7 C123 -173.47(11) . . . . ?
Cl2 Cu4 P7 C123 -58.32(12) . . . . ?
P7 Cu4 P8 C135 -54.79(13) . . . . ?
S4 Cu4 P8 C135 173.03(13) . . . . ?
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P7 Cu4 P8 C141 64.77(13) . . . . ?
S4 Cu4 P8 C141 -67.41(12) . . . . ?
Cl2 Cu4 P8 C141 -179.93(12) . . . . ?
P7 Cu4 P8 C147 -177.18(12) . . . . ?
S4 Cu4 P8 C147 50.64(13) . . . . ?
Cl2 Cu4 P8 C147 -61.88(13) . . . . ?
C80 N3 C77 N4 0.2(5) . . . . ?
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C78 N4 C77 N3 0.7(5) . . . . ?
C78 N4 C77 S4 178.9(3) . . . . ?
Cu4 S4 C77 N3 -38.4(3) . . . . ?
Cu4 S4 C77 N4 143.4(3) . . . . ?
C77 N4 C78 C79 -1.3(7) . . . . ?
N4 C78 C79 C80 0.9(7) . . . . ?
C78 C79 C80 N3 0.1(5) . . . . ?
C78 C79 C80 S3 -179.6(3) . . . . ?
C77 N3 C80 C79 -0.7(5) . . . . ?
C77 N3 C80 S3 179.1(3) . . . . ?
Cu3 S3 C80 C79 172.7(3) . . . . ?
Cu3 S3 C80 N3 -7.0(3) . . . . ?
C87 P5 C81 C86 -170.4(3) . . . . ?
C93 P5 C81 C86 81.9(3) . . . . ?
Cu3 P5 C81 C86 -41.2(3) . . . . ?
C87 P5 C81 C82 4.6(3) . . . . ?
C93 P5 C81 C82 -103.1(3) . . . . ?
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C146 C141 C142 C143 1.3(5) . . . . ?
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C128 H12C Cl2  0.95 2.78 3.600(4) 145.4 .
C146 H14B S4  0.95 2.84 3.733(4) 156.7 .
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Version 1.171.34.44 (release 25-10-2010 CrysAlis171 .NET)
(compiled Oct 25 2010,18:11:34)
Empirical absorption correction using spherical harmonics,
 implemented in SCALE3 ABSPACK scaling algorithm.
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(compiled Oct 25 2010,18:11:34)
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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
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based
 on F^2^ are statistically about twice as large as those based on F, and
R-
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Cu2A Cu 0.695755(16) 0.972753(18) 0.653958(15) 0.01764(6) Uani 1 1 d . . .
Br1A Br 0.628566(15) 0.855009(17) 0.752921(14) 0.02828(7) Uani 1 1 d . . .
S1A S 0.40585(4) 0.92578(4) 0.84455(3) 0.02438(13) Uani 1 1 d . A .
S2A S 0.60588(4) 1.03657(4) 0.59540(3) 0.02575(14) Uani 1 1 d . A .
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P1A P 0.53044(3) 0.75549(4) 0.93753(3) 0.01596(11) Uani 1 1 d . . .
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P3A P 0.78683(4) 0.90715(4) 0.59119(3) 0.01971(12) Uani 1 1 d . . .
P4A P 0.73448(3) 1.04384(4) 0.70006(3) 0.01615(11) Uani 1 1 d . . .
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C2A C 0.55511(15) 0.89400(15) 0.94396(13) 0.0223(5) Uani 1 1 d . . .
H2AA H 0.5225 0.9161 0.9153 0.027 Uiso 1 1 calc R . .
C3A C 0.58290(17) 0.93975(17) 0.96743(15) 0.0277(6) Uani 1 1 d . . .
H3AA H 0.5697 0.9934 0.9543 0.033 Uiso 1 1 calc R . .
C4A C 0.62972(17) 0.90784(18) 1.00979(15) 0.0302(6) Uani 1 1 d . . .
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C5A C 0.65164(15) 0.83006(18) 1.02767(14) 0.0256(6) Uani 1 1 d . . .
H5AA H 0.6849 0.8085 1.0558 0.031 Uiso 1 1 calc R . .
C6A C 0.62458(14) 0.78411(16) 1.00405(12) 0.0202(5) Uani 1 1 d . . .
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C2B C 0.44041(15) 0.71213(16) 1.07675(13) 0.0235(5) Uani 1 1 d . . .
H2BA H 0.4784 0.7393 1.0808 0.028 Uiso 1 1 calc R . .
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C5B C 0.32892(16) 0.63256(17) 1.06647(15) 0.0277(6) Uani 1 1 d . . .
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C6B C 0.39192(15) 0.66953(16) 1.00960(14) 0.0237(5) Uani 1 1 d . . .
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C1C C 0.60651(14) 0.67667(15) 0.93467(13) 0.0189(4) Uani 1 1 d . . .
C2C C 0.59360(17) 0.60215(16) 0.98121(14) 0.0261(5) Uani 1 1 d . . .
H2CA H 0.5447 0.5908 1.0182 0.031 Uiso 1 1 calc R . .
C3C C 0.65262(18) 0.54384(17) 0.97369(16) 0.0310(6) Uani 1 1 d . . .
H3CA H 0.6437 0.4931 1.0059 0.037 Uiso 1 1 calc R . .
C4C C 0.72345(16) 0.55915(17) 0.92021(16) 0.0285(6) Uani 1 1 d . . .
H4CA H 0.7626 0.5189 0.9148 0.034 Uiso 1 1 calc R . .
C5C C 0.73751(15) 0.63350(18) 0.87418(15) 0.0262(6) Uani 1 1 d . . .
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C6C C 0.67996(14) 0.69165(16) 0.88097(13) 0.0217(5) Uani 1 1 d . . .
H6CA H 0.6901 0.7424 0.8490 0.026 Uiso 1 1 calc R . .
C1D C 0.33653(14) 0.71073(16) 0.85979(14) 0.0233(5) Uani 1 1 d . . .
C2D C 0.28325(16) 0.75413(19) 0.89634(16) 0.0303(6) Uani 1 1 d . . .
H2DA H 0.2981 0.8038 0.8894 0.036 Uiso 1 1 calc R . .
C3D C 0.20882(16) 0.7254(2) 0.94268(16) 0.0348(7) Uani 1 1 d . . .
H3DA H 0.1730 0.7555 0.9670 0.042 Uiso 1 1 calc R . .
C4D C 0.18686(17) 0.6529(2) 0.95350(16) 0.0369(8) Uani 1 1 d . . .
H4DA H 0.1362 0.6329 0.9855 0.044 Uiso 1 1 calc R . .
C5D C 0.2391(2) 0.6098(2) 0.91746(16) 0.0378(7) Uani 1 1 d . . .
H5DA H 0.2238 0.5603 0.9245 0.045 Uiso 1 1 calc R . .
C6D C 0.31393(18) 0.63773(18) 0.87106(15) 0.0299(6) Uani 1 1 d . . .
H6DA H 0.3495 0.6071 0.8471 0.036 Uiso 1 1 calc R . .
C1E C 0.49247(14) 0.66906(15) 0.78255(13) 0.0210(5) Uani 1 1 d . . .
C2E C 0.54876(19) 0.63032(19) 0.81558(17) 0.0351(7) Uani 1 1 d . . .
H2EA H 0.5596 0.6498 0.8447 0.042 Uiso 1 1 calc R . .
C3E C 0.5890(2) 0.5641(2) 0.8066(2) 0.0450(9) Uani 1 1 d . . .
H3EA H 0.6269 0.5381 0.8298 0.054 Uiso 1 1 calc R . .
C4E C 0.5748(2) 0.53536(19) 0.76423(18) 0.0371(7) Uani 1 1 d . . .
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H4EA H 0.6018 0.4892 0.7588 0.045 Uiso 1 1 calc R . .
C5E C 0.52021(18) 0.57454(18) 0.72934(16) 0.0310(6) Uani 1 1 d . . .
H5EA H 0.5108 0.5555 0.6994 0.037 Uiso 1 1 calc R . .
C6E C 0.47959(16) 0.64145(16) 0.73828(14) 0.0240(5) Uani 1 1 d . . .
H6EA H 0.4430 0.6683 0.7140 0.029 Uiso 1 1 calc R . .
C1F C 0.41325(16) 0.81222(16) 0.72473(14) 0.0232(5) Uani 1 1 d . . .
C2F C 0.33441(19) 0.8354(2) 0.72287(19) 0.0427(8) Uani 1 1 d . . .
H2FA H 0.2893 0.8169 0.7623 0.051 Uiso 1 1 calc R . .
C3F C 0.3215(2) 0.8853(3) 0.6638(2) 0.0545(11) Uani 1 1 d . . .
H3FA H 0.2675 0.9014 0.6632 0.065 Uiso 1 1 calc R . .
C4F C 0.3858(2) 0.9118(2) 0.60616(19) 0.0456(9) Uani 1 1 d . . .
H4FA H 0.3764 0.9451 0.5656 0.055 Uiso 1 1 calc R . .
C5F C 0.4644(2) 0.8898(2) 0.60745(17) 0.0380(7) Uani 1 1 d . . .
H5FA H 0.5092 0.9085 0.5678 0.046 Uiso 1 1 calc R . .
C6F C 0.47808(18) 0.84028(18) 0.66682(16) 0.0316(6) Uani 1 1 d . . .
H6FA H 0.5322 0.8257 0.6676 0.038 Uiso 1 1 calc R . .
C1G C 0.73551(15) 0.84303(18) 0.57422(15) 0.0263(6) Uani 1 1 d . . .
C2G C 0.71782(18) 0.76896(19) 0.62155(17) 0.0345(7) Uani 1 1 d . . .
H2GA H 0.7360 0.7515 0.6597 0.041 Uiso 1 1 calc R . .
C3G C 0.6735(2) 0.7207(2) 0.6127(2) 0.0460(9) Uani 1 1 d . . .
H3GA H 0.6622 0.6701 0.6446 0.055 Uiso 1 1 calc R . .
C4G C 0.6462(2) 0.7455(3) 0.5587(2) 0.0506(10) Uani 1 1 d . . .
H4GA H 0.6166 0.7119 0.5529 0.061 Uiso 1 1 calc R . .
C5G C 0.6616(2) 0.8193(3) 0.5123(2) 0.0520(10) Uani 1 1 d . . .
H5GA H 0.6414 0.8370 0.4752 0.062 Uiso 1 1 calc R . .
C6G C 0.7069(2) 0.8677(2) 0.52000(18) 0.0404(8) Uani 1 1 d . . .
H6GA H 0.7181 0.9181 0.4877 0.048 Uiso 1 1 calc R . .
C1H C 0.84871(14) 0.96670(16) 0.50754(13) 0.0214(5) Uani 1 1 d . . .
C2H C 0.80983(17) 1.02965(18) 0.47041(14) 0.0288(6) Uani 1 1 d . . .
H2HA H 0.7529 1.0382 0.4883 0.035 Uiso 1 1 calc R . .
C3H C 0.85316(19) 1.08016(19) 0.40762(15) 0.0328(6) Uani 1 1 d . . .
H3HA H 0.8257 1.1225 0.3831 0.039 Uiso 1 1 calc R . .
C4H C 0.93639(19) 1.06825(19) 0.38121(15) 0.0336(7) Uani 1 1 d . . .
H4HA H 0.9662 1.1016 0.3381 0.040 Uiso 1 1 calc R . .
C5H C 0.97553(17) 1.00737(19) 0.41824(15) 0.0318(6) Uani 1 1 d . . .
H5HA H 1.0327 0.9997 0.4006 0.038 Uiso 1 1 calc R . .
C6H C 0.93293(15) 0.95742(17) 0.48058(14) 0.0255(5) Uani 1 1 d . . .
H6HA H 0.9613 0.9163 0.5054 0.031 Uiso 1 1 calc R . .
C1I C 0.85749(14) 0.84128(15) 0.63119(13) 0.0205(5) Uani 1 1 d . . .
C2I C 0.85404(15) 0.83881(16) 0.69384(14) 0.0234(5) Uani 1 1 d . . .
H2IA H 0.8163 0.8717 0.7141 0.028 Uiso 1 1 calc R . .
C3I C 0.90525(17) 0.78875(17) 0.72751(15) 0.0276(6) Uani 1 1 d . . .
H3IA H 0.9019 0.7870 0.7707 0.033 Uiso 1 1 calc R . .
C4I C 0.96135(17) 0.74128(16) 0.69775(15) 0.0288(6) Uani 1 1 d . . .
H4IA H 0.9971 0.7077 0.7202 0.035 Uiso 1 1 calc R . .
C5I C 0.96507(16) 0.74296(16) 0.63542(16) 0.0287(6) Uani 1 1 d . . .
H5IA H 1.0035 0.7106 0.6150 0.034 Uiso 1 1 calc R . .
C6I C 0.91277(16) 0.79188(16) 0.60247(15) 0.0248(5) Uani 1 1 d . . .
H6IA H 0.9146 0.7918 0.5602 0.030 Uiso 1 1 calc R . .
C1J C 0.79921(13) 1.12265(14) 0.63673(12) 0.0178(4) Uani 1 1 d . . .
C2J C 0.82846(15) 1.12448(16) 0.57107(13) 0.0220(5) Uani 1 1 d . . .
H2JA H 0.8151 1.0847 0.5606 0.026 Uiso 1 1 calc R . .
C3J C 0.87698(16) 1.18358(18) 0.52037(14) 0.0272(6) Uani 1 1 d . . .
H3JA H 0.8967 1.1841 0.4755 0.033 Uiso 1 1 calc R . .
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C4J C 0.89667(15) 1.24185(16) 0.53514(14) 0.0259(6) Uani 1 1 d . . .
H4JA H 0.9290 1.2829 0.5003 0.031 Uiso 1 1 calc R . .
C5J C 0.86926(16) 1.24024(17) 0.60064(15) 0.0285(6) Uani 1 1 d . . .
H5JA H 0.8842 1.2794 0.6109 0.034 Uiso 1 1 calc R . .
C6J C 0.81983(16) 1.18146(16) 0.65151(14) 0.0257(5) Uani 1 1 d . . .
H6JA H 0.8001 1.1812 0.6963 0.031 Uiso 1 1 calc R . .
C1K C 0.65502(14) 1.09407(14) 0.74897(13) 0.0194(5) Uani 1 1 d . . .
C2K C 0.58899(14) 1.12731(16) 0.72573(14) 0.0234(5) Uani 1 1 d . . .
H2KA H 0.5861 1.1225 0.6864 0.028 Uiso 1 1 calc R . .
C3K C 0.52780(15) 1.16728(18) 0.75992(16) 0.0297(6) Uani 1 1 d . . .
H3KA H 0.4830 1.1897 0.7440 0.036 Uiso 1 1 calc R . .
C4K C 0.53145(17) 1.17477(18) 0.81685(16) 0.0328(7) Uani 1 1 d . . .
H4KA H 0.4890 1.2018 0.8403 0.039 Uiso 1 1 calc R . .
C5K C 0.5972(2) 1.14287(19) 0.84003(16) 0.0347(7) Uani 1 1 d . . .
H5KA H 0.6001 1.1485 0.8790 0.042 Uiso 1 1 calc R . .
C6K C 0.65837(17) 1.10303(17) 0.80623(15) 0.0278(6) Uani 1 1 d . . .
H6KA H 0.7033 1.0814 0.8221 0.033 Uiso 1 1 calc R . .
C1L C 0.79296(14) 0.99116(14) 0.75692(12) 0.0180(4) Uani 1 1 d . . .
C2L C 0.87431(14) 1.00449(15) 0.74333(13) 0.0215(5) Uani 1 1 d . . .
H2LA H 0.9011 1.0453 0.7041 0.026 Uiso 1 1 calc R . .
C3L C 0.91654(15) 0.95818(17) 0.78700(14) 0.0260(6) Uani 1 1 d . . .
H3LA H 0.9721 0.9674 0.7773 0.031 Uiso 1 1 calc R . .
C4L C 0.87805(17) 0.89906(18) 0.84422(15) 0.0289(6) Uani 1 1 d . . .
H4LA H 0.9070 0.8679 0.8741 0.035 Uiso 1 1 calc R . .
C5L C 0.79692(16) 0.88500(17) 0.85830(14) 0.0264(5) Uani 1 1 d . . .
H5LA H 0.7706 0.8441 0.8976 0.032 Uiso 1 1 calc R . .
C6L C 0.75461(14) 0.93043(15) 0.81522(12) 0.0209(5) Uani 1 1 d . . .
H6LA H 0.6992 0.9206 0.8250 0.025 Uiso 1 1 calc R . .
C1M C 0.50903(15) 1.03255(15) 0.64891(13) 0.0204(5) Uani 1 1 d . . .
N3M N 0.44556(15) 1.07371(17) 0.62807(14) 0.0304(7) Uani 0.40(3) 1 d P A 1
C3' C 0.44556(15) 1.07371(17) 0.62807(14) 0.0304(7) Uani 0.60(3) 1 d P A 2
H3'A H 0.4533 1.1058 0.5825 0.037 Uiso 0.60(3) 1 calc PR A 2
C3M C 0.37071(18) 1.0665(2) 0.67568(17) 0.0371(8) Uani 1 1 d . . .
H3MA H 0.329(3) 1.085(3) 0.665(2) 0.062(13) Uiso 1 1 d . . .
N2M N 0.35335(15) 1.02266(17) 0.74200(14) 0.0321(7) Uani 0.60(3) 1 d P A 1
C2' C 0.35335(15) 1.02266(17) 0.74200(14) 0.0321(7) Uani 0.40(3) 1 d P A 2
H2'A H 0.2997 1.0206 0.7726 0.038 Uiso 0.40(3) 1 calc PR A 2
C5M C 0.41677(15) 0.98184(15) 0.76228(14) 0.0210(5) Uani 1 1 d . . .
N1M N 0.49170(12) 0.98815(13) 0.71525(11) 0.0209(4) Uani 1 1 d . A .
H1MA H 0.5323 0.9614 0.7287 0.025 Uiso 1 1 calc R . .
Cu1B Cu 0.171249(17) 0.497624(18) 0.645985(15) 0.01732(6) Uani 1 1 d . . .
Cu2B Cu 0.003954(16) 0.311812(17) 0.842932(15) 0.01628(6) Uani 1 1 d . . .
Br1B Br 0.126383(15) 0.371506(16) 0.741044(14) 0.02547(6) Uani 1 1 d . . .
S1B S 0.06304(4) 0.56417(4) 0.60988(3) 0.02247(12) Uani 1 1 d . B .
S2B S -0.09749(3) 0.40509(4) 0.86188(3) 0.02102(12) Uani 1 1 d . B .
P1B P 0.22359(4) 0.55584(4) 0.69406(3) 0.01843(12) Uani 1 1 d . . .
P2B P 0.25102(4) 0.45334(4) 0.56294(3) 0.01730(12) Uani 1 1 d . . .
P3B P -0.04523(4) 0.24040(4) 0.80266(3) 0.01714(12) Uani 1 1 d . . .
P4B P 0.06202(3) 0.25481(4) 0.92513(3) 0.01541(11) Uani 1 1 d . . .
C1N C 0.15076(15) 0.59722(15) 0.75350(13) 0.0208(5) Uani 1 1 d . . .
C2N C 0.07758(15) 0.56047(16) 0.79399(13) 0.0221(5) Uani 1 1 d . . .
H2NA H 0.0667 0.5151 0.7897 0.026 Uiso 1 1 calc R . .
C3N C 0.02052(16) 0.58886(17) 0.84035(14) 0.0268(6) Uani 1 1 d . . .
H3NA H -0.0292 0.5632 0.8673 0.032 Uiso 1 1 calc R . .
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C4N C 0.03567(18) 0.65460(19) 0.84758(16) 0.0321(6) Uani 1 1 d . . .
H4NA H -0.0038 0.6744 0.8791 0.039 Uiso 1 1 calc R . .
C5N C 0.10872(19) 0.6915(2) 0.80853(17) 0.0365(7) Uani 1 1 d . . .
H5NA H 0.1197 0.7361 0.8139 0.044 Uiso 1 1 calc R . .
C6N C 0.16601(17) 0.66331(18) 0.76141(16) 0.0307(6) Uani 1 1 d . . .
H6NA H 0.2157 0.6891 0.7345 0.037 Uiso 1 1 calc R . .
C1O C 0.28900(15) 0.49245(15) 0.74178(13) 0.0216(5) Uani 1 1 d . . .
C2O C 0.27976(18) 0.48590(18) 0.80746(15) 0.0304(6) Uani 1 1 d . . .
H2OA H 0.2385 0.5154 0.8292 0.036 Uiso 1 1 calc R . .
C3O C 0.3314(2) 0.4359(2) 0.84076(17) 0.0389(7) Uani 1 1 d . . .
H3OA H 0.3251 0.4316 0.8853 0.047 Uiso 1 1 calc R . .
C4O C 0.39167(18) 0.39247(19) 0.80998(17) 0.0348(7) Uani 1 1 d . . .
H4OA H 0.4269 0.3589 0.8330 0.042 Uiso 1 1 calc R . .
C5O C 0.40020(17) 0.39830(18) 0.74559(17) 0.0313(6) Uani 1 1 d . . .
H5OA H 0.4415 0.3685 0.7243 0.038 Uiso 1 1 calc R . .
C6O C 0.34904(16) 0.44722(17) 0.71167(15) 0.0269(6) Uani 1 1 d . . .
H6OA H 0.3549 0.4500 0.6677 0.032 Uiso 1 1 calc R . .
C1P C 0.28715(14) 0.63785(15) 0.63500(13) 0.0205(5) Uani 1 1 d . . .
C2P C 0.36749(16) 0.64265(18) 0.63008(15) 0.0312(7) Uani 1 1 d . . .
H2PA H 0.3921 0.6016 0.6583 0.037 Uiso 1 1 calc R . .
C3P C 0.41216(19) 0.7072(2) 0.58405(17) 0.0407(8) Uani 1 1 d . . .
H3PA H 0.4668 0.7102 0.5817 0.049 Uiso 1 1 calc R . .
C4P C 0.37787(19) 0.76663(18) 0.54203(16) 0.0333(7) Uani 1 1 d . . .
H4PA H 0.4087 0.8103 0.5104 0.040 Uiso 1 1 calc R . .
C5P C 0.29834(18) 0.76222(17) 0.54626(16) 0.0310(6) Uani 1 1 d . . .
H5PA H 0.2742 0.8031 0.5175 0.037 Uiso 1 1 calc R . .
C6P C 0.25338(17) 0.69830(16) 0.59246(15) 0.0265(6) Uani 1 1 d . . .
H6PA H 0.1986 0.6959 0.5950 0.032 Uiso 1 1 calc R . .
C1Q C 0.33886(14) 0.39045(16) 0.57683(13) 0.0206(5) Uani 1 1 d . . .
C2Q C 0.32578(16) 0.32015(16) 0.63118(14) 0.0251(5) Uani 1 1 d . . .
H2QA H 0.2720 0.3067 0.6603 0.030 Uiso 1 1 calc R . .
C3Q C 0.39031(18) 0.27041(19) 0.64277(16) 0.0323(6) Uani 1 1 d . . .
H3QA H 0.3802 0.2224 0.6788 0.039 Uiso 1 1 calc R . .
C4Q C 0.47037(18) 0.2898(2) 0.60212(17) 0.0395(8) Uani 1 1 d . . .
H4QA H 0.5145 0.2549 0.6094 0.047 Uiso 1 1 calc R . .
C5Q C 0.48401(18) 0.3614(2) 0.55085(17) 0.0403(8) Uani 1 1 d . . .
H5QA H 0.5382 0.3764 0.5242 0.048 Uiso 1 1 calc R . .
C6Q C 0.41916(15) 0.41106(18) 0.53817(15) 0.0280(6) Uani 1 1 d . . .
H6QA H 0.4296 0.4596 0.5028 0.034 Uiso 1 1 calc R . .
C1R C 0.29486(13) 0.52838(15) 0.48200(13) 0.0196(5) Uani 1 1 d . . .
C2R C 0.28449(15) 0.60458(16) 0.47890(14) 0.0244(5) Uani 1 1 d . . .
H2RA H 0.2535 0.6162 0.5180 0.029 Uiso 1 1 calc R . .
C3R C 0.31914(16) 0.66401(17) 0.41904(15) 0.0281(6) Uani 1 1 d . . .
H3RA H 0.3113 0.7159 0.4172 0.034 Uiso 1 1 calc R . .
C4R C 0.36456(17) 0.64719(18) 0.36278(15) 0.0303(6) Uani 1 1 d . . .
H4RA H 0.3893 0.6875 0.3223 0.036 Uiso 1 1 calc R . .
C5R C 0.37470(17) 0.57163(19) 0.36453(14) 0.0295(6) Uani 1 1 d . . .
H5RA H 0.4061 0.5605 0.3253 0.035 Uiso 1 1 calc R . .
C6R C 0.33895(15) 0.51239(17) 0.42361(13) 0.0241(5) Uani 1 1 d . . .
H6RA H 0.3444 0.4610 0.4244 0.029 Uiso 1 1 calc R . .
C1S C 0.19332(14) 0.39836(15) 0.54230(13) 0.0199(5) Uani 1 1 d . . .
C2S C 0.13199(17) 0.43825(17) 0.51558(15) 0.0271(6) Uani 1 1 d . . .
H2SA H 0.1234 0.4919 0.5073 0.033 Uiso 1 1 calc R . .
C3S C 0.08360(18) 0.40047(19) 0.50102(16) 0.0314(6) Uani 1 1 d . . .
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H3SA H 0.0425 0.4284 0.4822 0.038 Uiso 1 1 calc R . .
C4S C 0.09466(18) 0.32215(19) 0.51369(16) 0.0331(7) Uani 1 1 d . . .
H4SA H 0.0613 0.2963 0.5036 0.040 Uiso 1 1 calc R . .
C5S C 0.1539(2) 0.2822(2) 0.5408(2) 0.0410(8) Uani 1 1 d . . .
H5SA H 0.1609 0.2283 0.5503 0.049 Uiso 1 1 calc R . .
C6S C 0.20366(19) 0.31957(18) 0.55458(18) 0.0361(7) Uani 1 1 d . . .
H6SA H 0.2453 0.2912 0.5726 0.043 Uiso 1 1 calc R . .
C1T C 0.02662(14) 0.18047(15) 0.75964(13) 0.0208(5) Uani 1 1 d . . .
C2T C 0.09968(16) 0.15801(19) 0.77280(16) 0.0312(6) Uani 1 1 d . . .
H2TA H 0.1118 0.1748 0.8029 0.037 Uiso 1 1 calc R . .
C3T C 0.15539(19) 0.1112(2) 0.7425(2) 0.0469(9) Uani 1 1 d . . .
H3TA H 0.2049 0.0953 0.7526 0.056 Uiso 1 1 calc R . .
C4T C 0.13918(19) 0.0878(2) 0.69756(19) 0.0418(8) Uani 1 1 d . . .
H4TA H 0.1774 0.0553 0.6772 0.050 Uiso 1 1 calc R . .
C5T C 0.06763(18) 0.1114(2) 0.68221(17) 0.0350(7) Uani 1 1 d . . .
H5TA H 0.0570 0.0961 0.6506 0.042 Uiso 1 1 calc R . .
C6T C 0.01103(16) 0.15765(18) 0.71326(15) 0.0270(6) Uani 1 1 d . . .
H6TA H -0.0384 0.1738 0.7029 0.032 Uiso 1 1 calc R . .
C1U C -0.09484(14) 0.30123(15) 0.74103(13) 0.0197(5) Uani 1 1 d . . .
C2U C -0.04814(16) 0.35556(17) 0.68222(14) 0.0258(6) Uani 1 1 d . . .
H2UA H 0.0090 0.3560 0.6730 0.031 Uiso 1 1 calc R . .
C3U C -0.08440(18) 0.40886(17) 0.63714(15) 0.0293(6) Uani 1 1 d . . .
H3UA H -0.0522 0.4457 0.5974 0.035 Uiso 1 1 calc R . .
C4U C -0.16801(18) 0.40826(19) 0.65032(15) 0.0311(6) Uani 1 1 d . . .
H4UA H -0.1933 0.4454 0.6202 0.037 Uiso 1 1 calc R . .
C5U C -0.21383(17) 0.3536(2) 0.70726(15) 0.0347(7) Uani 1 1 d . . .
H5UA H -0.2707 0.3525 0.7157 0.042 Uiso 1 1 calc R . .
C6U C -0.17784(15) 0.30007(18) 0.75253(14) 0.0272(6) Uani 1 1 d . . .
H6UA H -0.2102 0.2625 0.7915 0.033 Uiso 1 1 calc R . .
C1V C -0.12675(14) 0.17692(15) 0.86627(12) 0.0189(4) Uani 1 1 d . . .
C2V C -0.13531(16) 0.10262(17) 0.87062(15) 0.0273(6) Uani 1 1 d . . .
H2VA H -0.0961 0.0811 0.8403 0.033 Uiso 1 1 calc R . .
C3V C -0.20182(18) 0.05973(18) 0.91972(16) 0.0321(6) Uani 1 1 d . . .
H3VA H -0.2073 0.0088 0.9229 0.038 Uiso 1 1 calc R . .
C4V C -0.25968(17) 0.09082(17) 0.96377(15) 0.0295(6) Uani 1 1 d . . .
H4VA H -0.3051 0.0616 0.9965 0.035 Uiso 1 1 calc R . .
C5V C -0.25129(15) 0.16445(17) 0.96010(14) 0.0266(6) Uani 1 1 d . . .
H5VA H -0.2909 0.1859 0.9904 0.032 Uiso 1 1 calc R . .
C6V C -0.18450(15) 0.20721(16) 0.91185(13) 0.0230(5) Uani 1 1 d . . .
H6VA H -0.1783 0.2574 0.9100 0.028 Uiso 1 1 calc R . .
C1W C -0.00173(14) 0.18333(14) 0.99994(13) 0.0193(5) Uani 1 1 d . . .
C2W C -0.03474(16) 0.12807(16) 0.98973(15) 0.0261(6) Uani 1 1 d . . .
H2WA H -0.0218 0.1274 0.9457 0.031 Uiso 1 1 calc R . .
C3W C -0.0866(2) 0.07380(19) 1.04399(19) 0.0406(8) Uani 1 1 d . . .
H3WA H -0.1081 0.0356 1.0369 0.049 Uiso 1 1 calc R . .
C4W C -0.1070(2) 0.0751(2) 1.10799(19) 0.0474(9) Uani 1 1 d . . .
H4WA H -0.1425 0.0380 1.1449 0.057 Uiso 1 1 calc R . .
C5W C -0.07569(19) 0.1307(2) 1.11835(16) 0.0368(7) Uani 1 1 d . . .
H5WA H -0.0901 0.1318 1.1624 0.044 Uiso 1 1 calc R . .
C6W C -0.02326(15) 0.18491(16) 1.06472(13) 0.0235(5) Uani 1 1 d . . .
H6WA H -0.0021 0.2230 1.0722 0.028 Uiso 1 1 calc R . .
C1X C 0.09384(13) 0.31621(14) 0.95744(12) 0.0168(4) Uani 1 1 d . . .
C2X C 0.14719(14) 0.28885(15) 0.99542(13) 0.0207(5) Uani 1 1 d . . .
H2XA H 0.1671 0.2369 1.0051 0.025 Uiso 1 1 calc R . .
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C3X C 0.17127(15) 0.33622(17) 1.01898(14) 0.0236(5) Uani 1 1 d . . .
H3XA H 0.2071 0.3169 1.0451 0.028 Uiso 1 1 calc R . .
C4X C 0.14265(15) 0.41265(17) 1.00427(14) 0.0245(5) Uani 1 1 d . . .
H4XA H 0.1593 0.4457 1.0201 0.029 Uiso 1 1 calc R . .
C5X C 0.09003(16) 0.44028(16) 0.96672(14) 0.0245(5) Uani 1 1 d . . .
H5XA H 0.0706 0.4923 0.9569 0.029 Uiso 1 1 calc R . .
C6X C 0.06526(14) 0.39240(15) 0.94323(13) 0.0200(5) Uani 1 1 d . . .
H6XA H 0.0289 0.4117 0.9176 0.024 Uiso 1 1 calc R . .
C1Y C 0.15749(13) 0.20210(14) 0.89934(12) 0.0170(4) Uani 1 1 d . . .
C2Y C 0.16654(15) 0.12236(15) 0.92152(14) 0.0227(5) Uani 1 1 d . . .
H2YA H 0.1228 0.0920 0.9559 0.027 Uiso 1 1 calc R . .
C3Y C 0.23828(16) 0.08636(16) 0.89432(15) 0.0259(5) Uani 1 1 d . . .
H3YA H 0.2430 0.0317 0.9095 0.031 Uiso 1 1 calc R . .
C4Y C 0.30336(15) 0.13006(17) 0.84488(14) 0.0247(5) Uani 1 1 d . . .
H4YA H 0.3525 0.1055 0.8261 0.030 Uiso 1 1 calc R . .
C5Y C 0.29589(15) 0.20953(17) 0.82335(14) 0.0242(5) Uani 1 1 d . . .
H5YA H 0.3405 0.2396 0.7901 0.029 Uiso 1 1 calc R . .
C6Y C 0.22356(14) 0.24590(15) 0.84998(12) 0.0199(5) Uani 1 1 d . . .
H6YA H 0.2190 0.3005 0.8347 0.024 Uiso 1 1 calc R . .
C1Z C -0.02889(14) 0.54443(15) 0.67189(13) 0.0203(5) Uani 1 1 d . . .
N2Z N -0.09993(17) 0.58215(16) 0.66337(16) 0.0325(7) Uani 0.43(3) 1 d P B
1
C2" C -0.09993(17) 0.58215(16) 0.66337(16) 0.0325(7) Uani 0.57(3) 1 d P B
2
H2"A H -0.1013 0.6202 0.6216 0.039 Uiso 0.57(3) 1 calc PR B 2
C3Z C -0.16891(19) 0.56254(19) 0.7177(2) 0.0389(8) Uani 1 1 d . . .
H3ZA H -0.2184 0.5882 0.7117 0.047 Uiso 1 1 calc R B 1
N3Z N -0.17321(14) 0.50979(17) 0.77957(15) 0.0307(6) Uani 0.57(3) 1 d P B
1
C3" C -0.17321(14) 0.50979(17) 0.77957(15) 0.0307(6) Uani 0.43(3) 1 d P B
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H3"A H -0.2230 0.5001 0.8157 0.037 Uiso 0.43(3) 1 calc PR B 2
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N1Z N -0.03303(12) 0.48914(12) 0.73277(11) 0.0189(4) Uani 1 1 d . B .
H1ZA H 0.0120 0.4629 0.7376 0.023 Uiso 1 1 calc R . .

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Br1A 0.02255(11) 0.02670(14) 0.02541(14) 0.00098(11) -0.00603(9) -
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P1A 0.0166(2) 0.0152(3) 0.0161(3) -0.0046(2) -0.0064(2) 0.0002(2)
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C4Y 0.0210(11) 0.0307(15) 0.0269(14) -0.0157(12) -0.0092(9) 0.0050(10)
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C3" 0.0192(10) 0.0338(15) 0.0440(17) -0.0185(13) -0.0139(10) 0.0068(10)
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_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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Cu2A P4A 2.2815(7) . ?
Cu2A P3A 2.2835(8) . ?
Cu2A S2A 2.3110(7) . ?
Cu2A Br1A 2.5528(4) . ?
S1A C5M 1.717(3) . ?
S2A C1M 1.700(3) . ?
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P1A C1B 1.826(2) . ?
P1A C1C 1.832(3) . ?
P2A C1E 1.822(3) . ?
P2A C1D 1.834(3) . ?
P2A C1F 1.836(3) . ?
P3A C1I 1.826(3) . ?
P3A C1H 1.832(3) . ?
P3A C1G 1.833(3) . ?
P4A C1J 1.822(2) . ?
P4A C1L 1.824(2) . ?
P4A C1K 1.833(3) . ?
C1A C2A 1.388(4) . ?
C1A C6A 1.405(3) . ?
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C1I P3A C1G 102.52(13) . . ?
C1H P3A C1G 103.83(13) . . ?
C1I P3A Cu2A 115.34(9) . . ?
C1H P3A Cu2A 115.62(9) . . ?
C1G P3A Cu2A 111.58(9) . . ?
C1J P4A C1L 104.36(11) . . ?
C1J P4A C1K 101.81(11) . . ?
C1L P4A C1K 102.77(12) . . ?
C1J P4A Cu2A 112.41(9) . . ?
C1L P4A Cu2A 115.42(9) . . ?
C1K P4A Cu2A 118.25(8) . . ?
C2A C1A C6A 119.5(2) . . ?
C2A C1A P1A 118.86(18) . . ?
C6A C1A P1A 121.46(19) . . ?
C1A C2A C3A 119.7(3) . . ?
C1A C2A H2AA 120.1 . . ?
C3A C2A H2AA 120.1 . . ?
C4A C3A C2A 120.5(3) . . ?
C4A C3A H3AA 119.7 . . ?
C2A C3A H3AA 119.7 . . ?
C3A C4A C5A 120.3(3) . . ?
C3A C4A H4AA 119.8 . . ?
C5A C4A H4AA 119.8 . . ?
C6A C5A C4A 119.5(3) . . ?
C6A C5A H5AA 120.3 . . ?
C4A C5A H5AA 120.3 . . ?
C5A C6A C1A 120.4(3) . . ?
C5A C6A H6AA 119.8 . . ?
C1A C6A H6AA 119.8 . . ?
C2B C1B C6B 118.7(2) . . ?
C2B C1B P1A 123.79(18) . . ?
C6B C1B P1A 117.5(2) . . ?
C3B C2B C1B 120.4(2) . . ?
C3B C2B H2BA 119.8 . . ?
C1B C2B H2BA 119.8 . . ?
C2B C3B C4B 120.4(3) . . ?
C2B C3B H3BA 119.8 . . ?
C4B C3B H3BA 119.8 . . ?
C5B C4B C3B 119.6(2) . . ?
C5B C4B H4BA 120.2 . . ?
C3B C4B H4BA 120.2 . . ?
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C4B C5B C6B 120.6(2) . . ?
C4B C5B H5BA 119.7 . . ?
C6B C5B H5BA 119.7 . . ?
C5B C6B C1B 120.2(3) . . ?
C5B C6B H6BA 119.9 . . ?
C1B C6B H6BA 119.9 . . ?
C2C C1C C6C 118.5(2) . . ?
C2C C1C P1A 123.21(19) . . ?
C6C C1C P1A 118.2(2) . . ?
C1C C2C C3C 120.1(3) . . ?
C1C C2C H2CA 120.0 . . ?
C3C C2C H2CA 120.0 . . ?
C4C C3C C2C 120.7(3) . . ?
C4C C3C H3CA 119.7 . . ?
C2C C3C H3CA 119.7 . . ?
C3C C4C C5C 119.7(3) . . ?
C3C C4C H4CA 120.1 . . ?
C5C C4C H4CA 120.1 . . ?
C6C C5C C4C 120.3(3) . . ?
C6C C5C H5CA 119.9 . . ?
C4C C5C H5CA 119.9 . . ?
C5C C6C C1C 120.7(3) . . ?
C5C C6C H6CA 119.6 . . ?
C1C C6C H6CA 119.6 . . ?
C6D C1D C2D 118.8(2) . . ?
C6D C1D P2A 123.4(2) . . ?
C2D C1D P2A 117.8(2) . . ?
C3D C2D C1D 120.7(3) . . ?
C3D C2D H2DA 119.6 . . ?
C1D C2D H2DA 119.6 . . ?
C4D C3D C2D 120.1(3) . . ?
C4D C3D H3DA 119.9 . . ?
C2D C3D H3DA 119.9 . . ?
C5D C4D C3D 119.4(3) . . ?
C5D C4D H4DA 120.3 . . ?
C3D C4D H4DA 120.3 . . ?
C4D C5D C6D 121.1(3) . . ?
C4D C5D H5DA 119.5 . . ?
C6D C5D H5DA 119.5 . . ?
C5D C6D C1D 119.9(3) . . ?
C5D C6D H6DA 120.1 . . ?
C1D C6D H6DA 120.1 . . ?
C6E C1E C2E 118.8(3) . . ?
C6E C1E P2A 122.8(2) . . ?
C2E C1E P2A 118.3(2) . . ?
C3E C2E C1E 120.9(3) . . ?
C3E C2E H2EA 119.6 . . ?
C1E C2E H2EA 119.6 . . ?
C4E C3E C2E 120.4(3) . . ?
C4E C3E H3EA 119.8 . . ?
C2E C3E H3EA 119.8 . . ?
C3E C4E C5E 119.5(3) . . ?
C3E C4E H4EA 120.3 . . ?
C5E C4E H4EA 120.3 . . ?
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C6E C5E C4E 120.2(3) . . ?
C6E C5E H5EA 119.9 . . ?
C4E C5E H5EA 119.9 . . ?
C1E C6E C5E 120.1(2) . . ?
C1E C6E H6EA 119.9 . . ?
C5E C6E H6EA 119.9 . . ?
C6F C1F C2F 118.9(3) . . ?
C6F C1F P2A 118.3(2) . . ?
C2F C1F P2A 122.7(2) . . ?
C3F C2F C1F 120.3(3) . . ?
C3F C2F H2FA 119.9 . . ?
C1F C2F H2FA 119.9 . . ?
C4F C3F C2F 120.7(3) . . ?
C4F C3F H3FA 119.7 . . ?
C2F C3F H3FA 119.7 . . ?
C3F C4F C5F 119.6(3) . . ?
C3F C4F H4FA 120.2 . . ?
C5F C4F H4FA 120.2 . . ?
C4F C5F C6F 120.1(3) . . ?
C4F C5F H5FA 119.9 . . ?
C6F C5F H5FA 119.9 . . ?
C1F C6F C5F 120.4(3) . . ?
C1F C6F H6FA 119.8 . . ?
C5F C6F H6FA 119.8 . . ?
C6G C1G C2G 118.9(3) . . ?
C6G C1G P3A 122.4(2) . . ?
C2G C1G P3A 118.4(2) . . ?
C3G C2G C1G 119.9(3) . . ?
C3G C2G H2GA 120.1 . . ?
C1G C2G H2GA 120.1 . . ?
C4G C3G C2G 120.6(4) . . ?
C4G C3G H3GA 119.7 . . ?
C2G C3G H3GA 119.7 . . ?
C3G C4G C5G 120.2(3) . . ?
C3G C4G H4GA 119.9 . . ?
C5G C4G H4GA 119.9 . . ?
C4G C5G C6G 119.8(4) . . ?
C4G C5G H5GA 120.1 . . ?
C6G C5G H5GA 120.1 . . ?
C1G C6G C5G 120.6(3) . . ?
C1G C6G H6GA 119.7 . . ?
C5G C6G H6GA 119.7 . . ?
C6H C1H C2H 117.7(2) . . ?
C6H C1H P3A 124.6(2) . . ?
C2H C1H P3A 117.50(19) . . ?
C3H C2H C1H 121.3(3) . . ?
C3H C2H H2HA 119.4 . . ?
C1H C2H H2HA 119.4 . . ?
C4H C3H C2H 119.7(3) . . ?
C4H C3H H3HA 120.1 . . ?
C2H C3H H3HA 120.1 . . ?
C5H C4H C3H 119.3(3) . . ?
C5H C4H H4HA 120.3 . . ?
C3H C4H H4HA 120.3 . . ?
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C4H C5H C6H 121.1(3) . . ?
C4H C5H H5HA 119.4 . . ?
C6H C5H H5HA 119.4 . . ?
C5H C6H C1H 120.8(3) . . ?
C5H C6H H6HA 119.6 . . ?
C1H C6H H6HA 119.6 . . ?
C2I C1I C6I 118.9(3) . . ?
C2I C1I P3A 118.0(2) . . ?
C6I C1I P3A 123.1(2) . . ?
C1I C2I C3I 120.8(3) . . ?
C1I C2I H2IA 119.6 . . ?
C3I C2I H2IA 119.6 . . ?
C4I C3I C2I 119.8(3) . . ?
C4I C3I H3IA 120.1 . . ?
C2I C3I H3IA 120.1 . . ?
C5I C4I C3I 119.9(3) . . ?
C5I C4I H4IA 120.1 . . ?
C3I C4I H4IA 120.1 . . ?
C4I C5I C6I 120.2(3) . . ?
C4I C5I H5IA 119.9 . . ?
C6I C5I H5IA 119.9 . . ?
C5I C6I C1I 120.4(3) . . ?
C5I C6I H6IA 119.8 . . ?
C1I C6I H6IA 119.8 . . ?
C2J C1J C6J 118.9(2) . . ?
C2J C1J P4A 118.14(19) . . ?
C6J C1J P4A 122.9(2) . . ?
C1J C2J C3J 120.9(2) . . ?
C1J C2J H2JA 119.5 . . ?
C3J C2J H2JA 119.5 . . ?
C4J C3J C2J 119.9(3) . . ?
C4J C3J H3JA 120.0 . . ?
C2J C3J H3JA 120.0 . . ?
C5J C4J C3J 120.0(2) . . ?
C5J C4J H4JA 120.0 . . ?
C3J C4J H4JA 120.0 . . ?
C4J C5J C6J 120.2(3) . . ?
C4J C5J H5JA 119.9 . . ?
C6J C5J H5JA 119.9 . . ?
C5J C6J C1J 120.0(3) . . ?
C5J C6J H6JA 120.0 . . ?
C1J C6J H6JA 120.0 . . ?
C6K C1K C2K 118.8(2) . . ?
C6K C1K P4A 123.71(19) . . ?
C2K C1K P4A 117.5(2) . . ?
C3K C2K C1K 120.1(3) . . ?
C3K C2K H2KA 120.0 . . ?
C1K C2K H2KA 120.0 . . ?
C4K C3K C2K 120.5(3) . . ?
C4K C3K H3KA 119.8 . . ?
C2K C3K H3KA 119.8 . . ?
C3K C4K C5K 120.1(3) . . ?
C3K C4K H4KA 120.0 . . ?
C5K C4K H4KA 120.0 . . ?
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C6K C5K C4K 119.8(3) . . ?
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C4K C5K H5KA 120.1 . . ?
C5K C6K C1K 120.8(3) . . ?
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C1K C6K H6KA 119.6 . . ?
C2L C1L C6L 118.9(2) . . ?
C2L C1L P4A 123.64(19) . . ?
C6L C1L P4A 117.33(17) . . ?
C3L C2L C1L 120.3(2) . . ?
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C1L C2L H2LA 119.9 . . ?
C4L C3L C2L 120.3(2) . . ?
C4L C3L H3LA 119.9 . . ?
C2L C3L H3LA 119.9 . . ?
C3L C4L C5L 120.1(3) . . ?
C3L C4L H4LA 120.0 . . ?
C5L C4L H4LA 120.0 . . ?
C6L C5L C4L 120.1(3) . . ?
C6L C5L H5LA 119.9 . . ?
C4L C5L H5LA 119.9 . . ?
C5L C6L C1L 120.4(2) . . ?
C5L C6L H6LA 119.8 . . ?
C1L C6L H6LA 119.8 . . ?
N1M C1M N3M 117.1(2) . . ?
N1M C1M S2A 120.68(19) . . ?
N3M C1M S2A 122.2(2) . . ?
C3M N3M C1M 116.9(3) . . ?
N2M C3M N3M 126.1(3) . . ?
N2M C3M H3MA 113(3) . . ?
N3M C3M H3MA 120(3) . . ?
C3M N2M C5M 116.6(3) . . ?
N1M C5M N2M 117.9(2) . . ?
N1M C5M S1A 119.48(19) . . ?
N2M C5M S1A 122.5(2) . . ?
C5M N1M C1M 125.3(2) . . ?
C5M N1M H1MA 117.3 . . ?
C1M N1M H1MA 117.3 . . ?
P1B Cu1B P2B 122.35(2) . . ?
P1B Cu1B S1B 115.02(3) . . ?
P2B Cu1B S1B 105.38(3) . . ?
P1B Cu1B Br1B 101.44(2) . . ?
P2B Cu1B Br1B 100.23(2) . . ?
S1B Cu1B Br1B 111.122(19) . . ?
P4B Cu2B P3B 121.31(3) . . ?
P4B Cu2B S2B 114.96(3) . . ?
P3B Cu2B S2B 105.86(2) . . ?
P4B Cu2B Br1B 101.897(19) . . ?
P3B Cu2B Br1B 100.40(2) . . ?
S2B Cu2B Br1B 111.21(2) . . ?
Cu1B Br1B Cu2B 140.944(15) . . ?
C1Z S1B Cu1B 112.94(9) . . ?
C5Z S2B Cu2B 109.76(9) . . ?
C1N P1B C1P 101.86(12) . . ?
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C1N P1B C1O 103.42(12) . . ?
C1P P1B C1O 103.95(11) . . ?
C1N P1B Cu1B 116.88(8) . . ?
C1P P1B Cu1B 114.85(9) . . ?
C1O P1B Cu1B 114.14(9) . . ?
C1R P2B C1Q 103.32(11) . . ?
C1R P2B C1S 102.64(11) . . ?
C1Q P2B C1S 104.33(12) . . ?
C1R P2B Cu1B 114.72(9) . . ?
C1Q P2B Cu1B 118.08(9) . . ?
C1S P2B Cu1B 112.06(8) . . ?
C1T P3B C1V 105.62(12) . . ?
C1T P3B C1U 103.42(12) . . ?
C1V P3B C1U 102.24(11) . . ?
C1T P3B Cu2B 118.39(8) . . ?
C1V P3B Cu2B 113.77(9) . . ?
C1U P3B Cu2B 111.70(8) . . ?
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C1X P4B C1Y 100.98(11) . . ?
C1W P4B C1Y 104.40(11) . . ?
C1X P4B Cu2B 118.13(8) . . ?
C1W P4B Cu2B 113.71(8) . . ?
C1Y P4B Cu2B 113.40(8) . . ?
C2N C1N C6N 118.4(2) . . ?
C2N C1N P1B 118.7(2) . . ?
C6N C1N P1B 122.9(2) . . ?
C3N C2N C1N 121.2(2) . . ?
C3N C2N H2NA 119.4 . . ?
C1N C2N H2NA 119.4 . . ?
C2N C3N C4N 120.2(2) . . ?
C2N C3N H3NA 119.9 . . ?
C4N C3N H3NA 119.9 . . ?
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C5N C4N H4NA 120.2 . . ?
C4N C5N C6N 120.3(3) . . ?
C4N C5N H5NA 119.9 . . ?
C6N C5N H5NA 119.9 . . ?
C5N C6N C1N 120.3(3) . . ?
C5N C6N H6NA 119.8 . . ?
C1N C6N H6NA 119.8 . . ?
C6O C1O C2O 118.9(3) . . ?
C6O C1O P1B 118.1(2) . . ?
C2O C1O P1B 122.9(2) . . ?
C3O C2O C1O 119.6(3) . . ?
C3O C2O H2OA 120.2 . . ?
C1O C2O H2OA 120.2 . . ?
C4O C3O C2O 121.0(3) . . ?
C4O C3O H3OA 119.5 . . ?
C2O C3O H3OA 119.5 . . ?
C5O C4O C3O 119.4(3) . . ?
C5O C4O H4OA 120.3 . . ?
C3O C4O H4OA 120.3 . . ?
C4O C5O C6O 120.6(3) . . ?
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C6O C5O H5OA 119.7 . . ?
C5O C6O C1O 120.4(3) . . ?
C5O C6O H6OA 119.8 . . ?
C1O C6O H6OA 119.8 . . ?
C6P C1P C2P 118.3(2) . . ?
C6P C1P P1B 118.10(18) . . ?
C2P C1P P1B 123.6(2) . . ?
C1P C2P C3P 120.5(3) . . ?
C1P C2P H2PA 119.8 . . ?
C3P C2P H2PA 119.8 . . ?
C4P C3P C2P 120.6(3) . . ?
C4P C3P H3PA 119.7 . . ?
C2P C3P H3PA 119.7 . . ?
C3P C4P C5P 119.4(3) . . ?
C3P C4P H4PA 120.3 . . ?
C5P C4P H4PA 120.3 . . ?
C4P C5P C6P 120.2(3) . . ?
C4P C5P H5PA 119.9 . . ?
C6P C5P H5PA 119.9 . . ?
C1P C6P C5P 121.1(2) . . ?
C1P C6P H6PA 119.5 . . ?
C5P C6P H6PA 119.5 . . ?
C6Q C1Q C2Q 118.1(2) . . ?
C6Q C1Q P2B 122.9(2) . . ?
C2Q C1Q P2B 118.87(18) . . ?
C3Q C2Q C1Q 120.7(2) . . ?
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C1Q C2Q H2QA 119.6 . . ?
C2Q C3Q C4Q 120.9(3) . . ?
C2Q C3Q H3QA 119.6 . . ?
C4Q C3Q H3QA 119.6 . . ?
C5Q C4Q C3Q 118.6(3) . . ?
C5Q C4Q H4QA 120.7 . . ?
C3Q C4Q H4QA 120.7 . . ?
C4Q C5Q C6Q 120.7(3) . . ?
C4Q C5Q H5QA 119.6 . . ?
C6Q C5Q H5QA 119.6 . . ?
C5Q C6Q C1Q 120.8(3) . . ?
C5Q C6Q H6QA 119.6 . . ?
C1Q C6Q H6QA 119.6 . . ?
C2R C1R C6R 119.0(2) . . ?
C2R C1R P2B 118.2(2) . . ?
C6R C1R P2B 122.8(2) . . ?
C1R C2R C3R 120.7(3) . . ?
C1R C2R H2RA 119.7 . . ?
C3R C2R H2RA 119.7 . . ?
C4R C3R C2R 119.7(3) . . ?
C4R C3R H3RA 120.2 . . ?
C2R C3R H3RA 120.2 . . ?
C3R C4R C5R 120.6(3) . . ?
C3R C4R H4RA 119.7 . . ?
C5R C4R H4RA 119.7 . . ?
C6R C5R C4R 120.0(3) . . ?
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C4R C5R H5RA 120.0 . . ?
C5R C6R C1R 120.0(3) . . ?
C5R C6R H6RA 120.0 . . ?
C1R C6R H6RA 120.0 . . ?
C6S C1S C2S 118.2(2) . . ?
C6S C1S P2B 124.8(2) . . ?
C2S C1S P2B 116.9(2) . . ?
C3S C2S C1S 120.6(3) . . ?
C3S C2S H2SA 119.7 . . ?
C1S C2S H2SA 119.7 . . ?
C2S C3S C4S 120.4(3) . . ?
C2S C3S H3SA 119.8 . . ?
C4S C3S H3SA 119.8 . . ?
C5S C4S C3S 119.6(3) . . ?
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C3S C4S H4SA 120.2 . . ?
C4S C5S C6S 120.7(3) . . ?
C4S C5S H5SA 119.6 . . ?
C6S C5S H5SA 119.6 . . ?
C5S C6S C1S 120.6(3) . . ?
C5S C6S H6SA 119.7 . . ?
C1S C6S H6SA 119.7 . . ?
C2T C1T C6T 119.0(3) . . ?
C2T C1T P3B 118.5(2) . . ?
C6T C1T P3B 122.5(2) . . ?
C1T C2T C3T 120.6(3) . . ?
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C3T C2T H2TA 119.7 . . ?
C4T C3T C2T 120.2(3) . . ?
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C2T C3T H3TA 119.9 . . ?
C3T C4T C5T 120.1(3) . . ?
C3T C4T H4TA 119.9 . . ?
C5T C4T H4TA 119.9 . . ?
C4T C5T C6T 119.8(3) . . ?
C4T C5T H5TA 120.1 . . ?
C6T C5T H5TA 120.1 . . ?
C5T C6T C1T 120.2(3) . . ?
C5T C6T H6TA 119.9 . . ?
C1T C6T H6TA 119.9 . . ?
C6U C1U C2U 118.8(2) . . ?
C6U C1U P3B 122.8(2) . . ?
C2U C1U P3B 118.22(18) . . ?
C3U C2U C1U 120.7(2) . . ?
C3U C2U H2UA 119.7 . . ?
C1U C2U H2UA 119.7 . . ?
C2U C3U C4U 119.8(3) . . ?
C2U C3U H3UA 120.1 . . ?
C4U C3U H3UA 120.1 . . ?
C5U C4U C3U 119.7(3) . . ?
C5U C4U H4UA 120.2 . . ?
C3U C4U H4UA 120.2 . . ?
C4U C5U C6U 120.8(3) . . ?
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C6U C5U H5UA 119.6 . . ?
C1U C6U C5U 120.3(3) . . ?
C1U C6U H6UA 119.9 . . ?
C5U C6U H6UA 119.9 . . ?
C2V C1V C6V 119.2(2) . . ?
C2V C1V P3B 124.3(2) . . ?
C6V C1V P3B 116.45(19) . . ?
C1V C2V C3V 119.9(3) . . ?
C1V C2V H2VA 120.1 . . ?
C3V C2V H2VA 120.1 . . ?
C4V C3V C2V 120.5(3) . . ?
C4V C3V H3VA 119.7 . . ?
C2V C3V H3VA 119.7 . . ?
C5V C4V C3V 120.0(2) . . ?
C5V C4V H4VA 120.0 . . ?
C3V C4V H4VA 120.0 . . ?
C4V C5V C6V 119.8(3) . . ?
C4V C5V H5VA 120.1 . . ?
C6V C5V H5VA 120.1 . . ?
C5V C6V C1V 120.6(2) . . ?
C5V C6V H6VA 119.7 . . ?
C1V C6V H6VA 119.7 . . ?
C2W C1W C6W 119.2(2) . . ?
C2W C1W P4B 116.9(2) . . ?
C6W C1W P4B 123.77(19) . . ?
C3W C2W C1W 120.1(3) . . ?
C3W C2W H2WA 119.9 . . ?
C1W C2W H2WA 119.9 . . ?
C4W C3W C2W 120.4(3) . . ?
C4W C3W H3WA 119.8 . . ?
C2W C3W H3WA 119.8 . . ?
C3W C4W C5W 119.8(3) . . ?
C3W C4W H4WA 120.1 . . ?
C5W C4W H4WA 120.1 . . ?
C4W C5W C6W 120.5(3) . . ?
C4W C5W H5WA 119.8 . . ?
C6W C5W H5WA 119.8 . . ?
C5W C6W C1W 120.0(3) . . ?
C5W C6W H6WA 120.0 . . ?
C1W C6W H6WA 120.0 . . ?
C6X C1X C2X 119.2(2) . . ?
C6X C1X P4B 119.22(18) . . ?
C2X C1X P4B 121.58(19) . . ?
C3X C2X C1X 120.9(2) . . ?
C3X C2X H2XA 119.6 . . ?
C1X C2X H2XA 119.6 . . ?
C2X C3X C4X 119.6(2) . . ?
C2X C3X H3XA 120.2 . . ?
C4X C3X H3XA 120.2 . . ?
C5X C4X C3X 120.0(2) . . ?
C5X C4X H4XA 120.0 . . ?
C3X C4X H4XA 120.0 . . ?
C4X C5X C6X 120.5(3) . . ?
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C4X C5X H5XA 119.8 . . ?
C6X C5X H5XA 119.8 . . ?
C1X C6X C5X 119.8(2) . . ?
C1X C6X H6XA 120.1 . . ?
C5X C6X H6XA 120.1 . . ?
C2Y C1Y C6Y 118.5(2) . . ?
C2Y C1Y P4B 124.39(18) . . ?
C6Y C1Y P4B 116.88(19) . . ?
C3Y C2Y C1Y 121.1(2) . . ?
C3Y C2Y H2YA 119.5 . . ?
C1Y C2Y H2YA 119.5 . . ?
C2Y C3Y C4Y 120.1(3) . . ?
C2Y C3Y H3YA 119.9 . . ?
C4Y C3Y H3YA 119.9 . . ?
C5Y C4Y C3Y 119.4(2) . . ?
C5Y C4Y H4YA 120.3 . . ?
C3Y C4Y H4YA 120.3 . . ?
C4Y C5Y C6Y 120.6(2) . . ?
C4Y C5Y H5YA 119.7 . . ?
C6Y C5Y H5YA 119.7 . . ?
C5Y C6Y C1Y 120.2(2) . . ?
C5Y C6Y H6YA 119.9 . . ?
C1Y C6Y H6YA 119.9 . . ?
N1Z C1Z N2Z 117.6(2) . . ?
N1Z C1Z S1B 119.62(18) . . ?
N2Z C1Z S1B 122.8(2) . . ?
C3Z N2Z C1Z 116.9(3) . . ?
N3Z C3Z N2Z 126.0(3) . . ?
N3Z C3Z H3ZA 117.0 . . ?
N2Z C3Z H3ZA 117.0 . . ?
C3Z N3Z C5Z 116.5(3) . . ?
N3Z C5Z N1Z 118.4(2) . . ?
N3Z C5Z S2B 122.1(2) . . ?
N1Z C5Z S2B 119.45(18) . . ?
C1Z N1Z C5Z 124.5(2) . . ?
C1Z N1Z H1ZA 117.8 . . ?
C5Z N1Z H1ZA 117.8 . . ?

loop_
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 _geom_torsion_atom_site_label_2
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 _geom_torsion_atom_site_label_4
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 _geom_torsion_site_symmetry_2
 _geom_torsion_site_symmetry_3
 _geom_torsion_site_symmetry_4
 _geom_torsion_publ_flag
P4A Cu2A Br1A Cu1A 82.14(3) . . . . ?
P3A Cu2A Br1A Cu1A -151.14(3) . . . . ?
S2A Cu2A Br1A Cu1A -41.26(4) . . . . ?
P1A Cu1A Br1A Cu2A -131.75(3) . . . . ?
P2A Cu1A Br1A Cu2A 100.69(3) . . . . ?
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S1A Cu1A Br1A Cu2A -9.44(4) . . . . ?
P1A Cu1A S1A C5M 156.18(9) . . . . ?
P2A Cu1A S1A C5M -66.16(9) . . . . ?
Br1A Cu1A S1A C5M 42.78(9) . . . . ?
P4A Cu2A S2A C1M -82.05(10) . . . . ?
P3A Cu2A S2A C1M 139.52(10) . . . . ?
Br1A Cu2A S2A C1M 35.92(10) . . . . ?
P2A Cu1A P1A C1A 179.02(8) . . . . ?
S1A Cu1A P1A C1A -51.90(9) . . . . ?
Br1A Cu1A P1A C1A 66.02(9) . . . . ?
P2A Cu1A P1A C1B -61.33(10) . . . . ?
S1A Cu1A P1A C1B 67.75(10) . . . . ?
Br1A Cu1A P1A C1B -174.33(9) . . . . ?
P2A Cu1A P1A C1C 58.13(9) . . . . ?
S1A Cu1A P1A C1C -172.79(9) . . . . ?
Br1A Cu1A P1A C1C -54.87(9) . . . . ?
P1A Cu1A P2A C1E -55.23(10) . . . . ?
S1A Cu1A P2A C1E 171.09(10) . . . . ?
Br1A Cu1A P2A C1E 57.20(10) . . . . ?
P1A Cu1A P2A C1D 64.66(10) . . . . ?
S1A Cu1A P2A C1D -69.02(10) . . . . ?
Br1A Cu1A P2A C1D 177.10(10) . . . . ?
P1A Cu1A P2A C1F -177.35(10) . . . . ?
S1A Cu1A P2A C1F 48.97(10) . . . . ?
Br1A Cu1A P2A C1F -64.91(10) . . . . ?
P4A Cu2A P3A C1I 53.66(9) . . . . ?
S2A Cu2A P3A C1I -172.35(9) . . . . ?
Br1A Cu2A P3A C1I -59.49(9) . . . . ?
P4A Cu2A P3A C1H -71.57(10) . . . . ?
S2A Cu2A P3A C1H 62.42(9) . . . . ?
Br1A Cu2A P3A C1H 175.29(9) . . . . ?
P4A Cu2A P3A C1G 170.09(11) . . . . ?
S2A Cu2A P3A C1G -55.92(11) . . . . ?
Br1A Cu2A P3A C1G 56.95(11) . . . . ?
P3A Cu2A P4A C1J 61.44(9) . . . . ?
S2A Cu2A P4A C1J -69.26(9) . . . . ?
Br1A Cu2A P4A C1J 170.27(8) . . . . ?
P3A Cu2A P4A C1L -58.10(9) . . . . ?
S2A Cu2A P4A C1L 171.19(8) . . . . ?
Br1A Cu2A P4A C1L 50.73(9) . . . . ?
P3A Cu2A P4A C1K 179.67(9) . . . . ?
S2A Cu2A P4A C1K 48.96(10) . . . . ?
Br1A Cu2A P4A C1K -71.51(9) . . . . ?
C1B P1A C1A C2A -100.8(2) . . . . ?
C1C P1A C1A C2A 153.4(2) . . . . ?
Cu1A P1A C1A C2A 25.3(2) . . . . ?
C1B P1A C1A C6A 74.6(2) . . . . ?
C1C P1A C1A C6A -31.2(2) . . . . ?
Cu1A P1A C1A C6A -159.28(17) . . . . ?
C6A C1A C2A C3A -1.1(4) . . . . ?
P1A C1A C2A C3A 174.4(2) . . . . ?
C1A C2A C3A C4A -0.7(4) . . . . ?
C2A C3A C4A C5A 2.0(4) . . . . ?
C3A C4A C5A C6A -1.6(4) . . . . ?
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C4A C5A C6A C1A -0.2(4) . . . . ?
C2A C1A C6A C5A 1.5(4) . . . . ?
P1A C1A C6A C5A -173.85(19) . . . . ?
C1A P1A C1B C2B -11.9(3) . . . . ?
C1C P1A C1B C2B 93.9(2) . . . . ?
Cu1A P1A C1B C2B -139.1(2) . . . . ?
C1A P1A C1B C6B 168.8(2) . . . . ?
C1C P1A C1B C6B -85.4(2) . . . . ?
Cu1A P1A C1B C6B 41.7(2) . . . . ?
C6B C1B C2B C3B 0.1(4) . . . . ?
P1A C1B C2B C3B -179.2(2) . . . . ?
C1B C2B C3B C4B 0.5(4) . . . . ?
C2B C3B C4B C5B -1.0(5) . . . . ?
C3B C4B C5B C6B 0.9(4) . . . . ?
C4B C5B C6B C1B -0.3(4) . . . . ?
C2B C1B C6B C5B -0.2(4) . . . . ?
P1A C1B C6B C5B 179.1(2) . . . . ?
C1A P1A C1C C2C 109.4(2) . . . . ?
C1B P1A C1C C2C 3.5(2) . . . . ?
Cu1A P1A C1C C2C -122.5(2) . . . . ?
C1A P1A C1C C6C -73.6(2) . . . . ?
C1B P1A C1C C6C -179.52(19) . . . . ?
Cu1A P1A C1C C6C 54.5(2) . . . . ?
C6C C1C C2C C3C -0.7(4) . . . . ?
P1A C1C C2C C3C 176.3(2) . . . . ?
C1C C2C C3C C4C -0.5(4) . . . . ?
C2C C3C C4C C5C 1.6(4) . . . . ?
C3C C4C C5C C6C -1.5(4) . . . . ?
C4C C5C C6C C1C 0.3(4) . . . . ?
C2C C1C C6C C5C 0.8(4) . . . . ?
P1A C1C C6C C5C -176.4(2) . . . . ?
C1E P2A C1D C6D -10.1(3) . . . . ?
C1F P2A C1D C6D 97.7(2) . . . . ?
Cu1A P2A C1D C6D -138.3(2) . . . . ?
C1E P2A C1D C2D 166.6(2) . . . . ?
C1F P2A C1D C2D -85.6(2) . . . . ?
Cu1A P2A C1D C2D 38.4(2) . . . . ?
C6D C1D C2D C3D -0.5(4) . . . . ?
P2A C1D C2D C3D -177.3(2) . . . . ?
C1D C2D C3D C4D 0.5(5) . . . . ?
C2D C3D C4D C5D -0.6(5) . . . . ?
C3D C4D C5D C6D 0.8(5) . . . . ?
C4D C5D C6D C1D -0.8(5) . . . . ?
C2D C1D C6D C5D 0.7(4) . . . . ?
P2A C1D C6D C5D 177.3(2) . . . . ?
C1D P2A C1E C6E 76.1(2) . . . . ?
C1F P2A C1E C6E -31.5(2) . . . . ?
Cu1A P2A C1E C6E -158.78(19) . . . . ?
C1D P2A C1E C2E -100.9(2) . . . . ?
C1F P2A C1E C2E 151.4(2) . . . . ?
Cu1A P2A C1E C2E 24.2(3) . . . . ?
C6E C1E C2E C3E -2.3(5) . . . . ?
P2A C1E C2E C3E 174.8(3) . . . . ?
C1E C2E C3E C4E 0.5(6) . . . . ?
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C2E C3E C4E C5E 1.2(6) . . . . ?
C3E C4E C5E C6E -1.1(5) . . . . ?
C2E C1E C6E C5E 2.4(4) . . . . ?
P2A C1E C6E C5E -174.6(2) . . . . ?
C4E C5E C6E C1E -0.7(5) . . . . ?
C1E P2A C1F C6F -61.0(3) . . . . ?
C1D P2A C1F C6F -168.0(2) . . . . ?
Cu1A P2A C1F C6F 68.7(2) . . . . ?
C1E P2A C1F C2F 123.6(3) . . . . ?
C1D P2A C1F C2F 16.5(3) . . . . ?
Cu1A P2A C1F C2F -106.8(3) . . . . ?
C6F C1F C2F C3F 0.4(5) . . . . ?
P2A C1F C2F C3F 175.8(3) . . . . ?
C1F C2F C3F C4F 0.9(7) . . . . ?
C2F C3F C4F C5F -1.5(6) . . . . ?
C3F C4F C5F C6F 0.8(6) . . . . ?
C2F C1F C6F C5F -1.1(5) . . . . ?
P2A C1F C6F C5F -176.8(2) . . . . ?
C4F C5F C6F C1F 0.5(5) . . . . ?
C1I P3A C1G C6G -149.1(3) . . . . ?
C1H P3A C1G C6G -38.3(3) . . . . ?
Cu2A P3A C1G C6G 86.9(3) . . . . ?
C1I P3A C1G C2G 37.4(3) . . . . ?
C1H P3A C1G C2G 148.2(2) . . . . ?
Cu2A P3A C1G C2G -86.6(2) . . . . ?
C6G C1G C2G C3G 1.5(5) . . . . ?
P3A C1G C2G C3G 175.2(3) . . . . ?
C1G C2G C3G C4G -0.9(5) . . . . ?
C2G C3G C4G C5G -0.7(6) . . . . ?
C3G C4G C5G C6G 1.6(6) . . . . ?
C2G C1G C6G C5G -0.5(5) . . . . ?
P3A C1G C6G C5G -174.0(3) . . . . ?
C4G C5G C6G C1G -1.0(6) . . . . ?
C1I P3A C1H C6H 3.8(3) . . . . ?
C1G P3A C1H C6H -104.0(2) . . . . ?
Cu2A P3A C1H C6H 133.4(2) . . . . ?
C1I P3A C1H C2H -170.8(2) . . . . ?
C1G P3A C1H C2H 81.4(2) . . . . ?
Cu2A P3A C1H C2H -41.1(2) . . . . ?
C6H C1H C2H C3H 2.0(4) . . . . ?
P3A C1H C2H C3H 176.9(2) . . . . ?
C1H C2H C3H C4H -0.1(5) . . . . ?
C2H C3H C4H C5H -1.4(5) . . . . ?
C3H C4H C5H C6H 1.1(5) . . . . ?
C4H C5H C6H C1H 0.7(5) . . . . ?
C2H C1H C6H C5H -2.3(4) . . . . ?
P3A C1H C6H C5H -176.8(2) . . . . ?
C1H P3A C1I C2I 126.4(2) . . . . ?
C1G P3A C1I C2I -124.9(2) . . . . ?
Cu2A P3A C1I C2I -3.4(2) . . . . ?
C1H P3A C1I C6I -55.6(2) . . . . ?
C1G P3A C1I C6I 53.1(2) . . . . ?
Cu2A P3A C1I C6I 174.57(18) . . . . ?
C6I C1I C2I C3I 0.7(4) . . . . ?
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P3A C1I C2I C3I 178.8(2) . . . . ?
C1I C2I C3I C4I 0.8(4) . . . . ?
C2I C3I C4I C5I -1.2(4) . . . . ?
C3I C4I C5I C6I -0.1(4) . . . . ?
C4I C5I C6I C1I 1.7(4) . . . . ?
C2I C1I C6I C5I -2.0(4) . . . . ?
P3A C1I C6I C5I -180.0(2) . . . . ?
C1L P4A C1J C2J 115.8(2) . . . . ?
C1K P4A C1J C2J -137.6(2) . . . . ?
Cu2A P4A C1J C2J -10.0(2) . . . . ?
C1L P4A C1J C6J -64.9(2) . . . . ?
C1K P4A C1J C6J 41.8(2) . . . . ?
Cu2A P4A C1J C6J 169.34(19) . . . . ?
C6J C1J C2J C3J -0.4(4) . . . . ?
P4A C1J C2J C3J 179.0(2) . . . . ?
C1J C2J C3J C4J -0.1(4) . . . . ?
C2J C3J C4J C5J 1.3(4) . . . . ?
C3J C4J C5J C6J -2.0(4) . . . . ?
C4J C5J C6J C1J 1.5(4) . . . . ?
C2J C1J C6J C5J -0.3(4) . . . . ?
P4A C1J C6J C5J -179.7(2) . . . . ?
C1J P4A C1K C6K -92.4(2) . . . . ?
C1L P4A C1K C6K 15.5(2) . . . . ?
Cu2A P4A C1K C6K 143.9(2) . . . . ?
C1J P4A C1K C2K 85.3(2) . . . . ?
C1L P4A C1K C2K -166.80(19) . . . . ?
Cu2A P4A C1K C2K -38.4(2) . . . . ?
C6K C1K C2K C3K -0.9(4) . . . . ?
P4A C1K C2K C3K -178.8(2) . . . . ?
C1K C2K C3K C4K 0.1(4) . . . . ?
C2K C3K C4K C5K 0.7(4) . . . . ?
C3K C4K C5K C6K -0.7(5) . . . . ?
C4K C5K C6K C1K -0.2(5) . . . . ?
C2K C1K C6K C5K 1.0(4) . . . . ?
P4A C1K C6K C5K 178.7(2) . . . . ?
C1J P4A C1L C2L -10.4(3) . . . . ?
C1K P4A C1L C2L -116.3(2) . . . . ?
Cu2A P4A C1L C2L 113.5(2) . . . . ?
C1J P4A C1L C6L 174.2(2) . . . . ?
C1K P4A C1L C6L 68.2(2) . . . . ?
Cu2A P4A C1L C6L -61.9(2) . . . . ?
C6L C1L C2L C3L 0.0(4) . . . . ?
P4A C1L C2L C3L -175.4(2) . . . . ?
C1L C2L C3L C4L -0.4(4) . . . . ?
C2L C3L C4L C5L 0.5(5) . . . . ?
C3L C4L C5L C6L -0.3(5) . . . . ?
C4L C5L C6L C1L 0.0(4) . . . . ?
C2L C1L C6L C5L 0.2(4) . . . . ?
P4A C1L C6L C5L 175.9(2) . . . . ?
Cu2A S2A C1M N1M -7.5(2) . . . . ?
Cu2A S2A C1M N3M 171.9(2) . . . . ?
N1M C1M N3M C3M 0.0(4) . . . . ?
S2A C1M N3M C3M -179.3(3) . . . . ?
C1M N3M C3M N2M 0.5(6) . . . . ?
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N3M C3M N2M C5M -0.6(6) . . . . ?
C3M N2M C5M N1M 0.2(4) . . . . ?
C3M N2M C5M S1A 178.2(3) . . . . ?
Cu1A S1A C5M N1M -39.0(2) . . . . ?
Cu1A S1A C5M N2M 143.0(2) . . . . ?
N2M C5M N1M C1M 0.3(4) . . . . ?
S1A C5M N1M C1M -177.8(2) . . . . ?
N3M C1M N1M C5M -0.4(4) . . . . ?
S2A C1M N1M C5M 179.0(2) . . . . ?
P1B Cu1B Br1B Cu2B 88.42(3) . . . . ?
P2B Cu1B Br1B Cu2B -145.34(3) . . . . ?
S1B Cu1B Br1B Cu2B -34.32(4) . . . . ?
P4B Cu2B Br1B Cu1B -130.24(3) . . . . ?
P3B Cu2B Br1B Cu1B 104.41(3) . . . . ?
S2B Cu2B Br1B Cu1B -7.26(3) . . . . ?
P1B Cu1B S1B C1Z -86.06(10) . . . . ?
P2B Cu1B S1B C1Z 136.13(10) . . . . ?
Br1B Cu1B S1B C1Z 28.45(11) . . . . ?
P4B Cu2B S2B C5Z 152.13(9) . . . . ?
P3B Cu2B S2B C5Z -71.14(9) . . . . ?
Br1B Cu2B S2B C5Z 37.01(9) . . . . ?
P2B Cu1B P1B C1N 173.64(10) . . . . ?
S1B Cu1B P1B C1N 43.68(10) . . . . ?
Br1B Cu1B P1B C1N -76.33(10) . . . . ?
P2B Cu1B P1B C1P 54.38(10) . . . . ?
S1B Cu1B P1B C1P -75.57(10) . . . . ?
Br1B Cu1B P1B C1P 164.42(10) . . . . ?
P2B Cu1B P1B C1O -65.54(10) . . . . ?
S1B Cu1B P1B C1O 164.50(9) . . . . ?
Br1B Cu1B P1B C1O 44.49(9) . . . . ?
P1B Cu1B P2B C1R -71.00(9) . . . . ?
S1B Cu1B P2B C1R 62.91(8) . . . . ?
Br1B Cu1B P2B C1R 178.34(8) . . . . ?
P1B Cu1B P2B C1Q 51.22(10) . . . . ?
S1B Cu1B P2B C1Q -174.87(9) . . . . ?
Br1B Cu1B P2B C1Q -59.44(10) . . . . ?
P1B Cu1B P2B C1S 172.48(9) . . . . ?
S1B Cu1B P2B C1S -53.61(10) . . . . ?
Br1B Cu1B P2B C1S 61.82(9) . . . . ?
P4B Cu2B P3B C1T -64.03(10) . . . . ?
S2B Cu2B P3B C1T 162.64(10) . . . . ?
Br1B Cu2B P3B C1T 46.89(10) . . . . ?
P4B Cu2B P3B C1V 60.90(10) . . . . ?
S2B Cu2B P3B C1V -72.43(9) . . . . ?
Br1B Cu2B P3B C1V 171.82(9) . . . . ?
P4B Cu2B P3B C1U 176.03(9) . . . . ?
S2B Cu2B P3B C1U 42.69(9) . . . . ?
Br1B Cu2B P3B C1U -73.06(9) . . . . ?
P3B Cu2B P4B C1X -176.39(8) . . . . ?
S2B Cu2B P4B C1X -46.90(9) . . . . ?
Br1B Cu2B P4B C1X 73.49(9) . . . . ?
P3B Cu2B P4B C1W -53.27(10) . . . . ?
S2B Cu2B P4B C1W 76.22(10) . . . . ?
Br1B Cu2B P4B C1W -163.40(10) . . . . ?
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P3B Cu2B P4B C1Y 65.81(9) . . . . ?
S2B Cu2B P4B C1Y -164.71(8) . . . . ?
Br1B Cu2B P4B C1Y -44.32(9) . . . . ?
C1P P1B C1N C2N 160.4(2) . . . . ?
C1O P1B C1N C2N -91.9(2) . . . . ?
Cu1B P1B C1N C2N 34.4(2) . . . . ?
C1P P1B C1N C6N -21.2(3) . . . . ?
C1O P1B C1N C6N 86.5(3) . . . . ?
Cu1B P1B C1N C6N -147.2(2) . . . . ?
C6N C1N C2N C3N 0.9(4) . . . . ?
P1B C1N C2N C3N 179.4(2) . . . . ?
C1N C2N C3N C4N -0.4(4) . . . . ?
C2N C3N C4N C5N -0.6(5) . . . . ?
C3N C4N C5N C6N 1.1(5) . . . . ?
C4N C5N C6N C1N -0.6(5) . . . . ?
C2N C1N C6N C5N -0.4(5) . . . . ?
P1B C1N C6N C5N -178.8(3) . . . . ?
C1N P1B C1O C6O 175.8(2) . . . . ?
C1P P1B C1O C6O -78.2(2) . . . . ?
Cu1B P1B C1O C6O 47.7(2) . . . . ?
C1N P1B C1O C2O -2.3(2) . . . . ?
C1P P1B C1O C2O 103.7(2) . . . . ?
Cu1B P1B C1O C2O -130.4(2) . . . . ?
C6O C1O C2O C3O 1.3(4) . . . . ?
P1B C1O C2O C3O 179.4(2) . . . . ?
C1O C2O C3O C4O -0.1(5) . . . . ?
C2O C3O C4O C5O -0.6(5) . . . . ?
C3O C4O C5O C6O 0.1(5) . . . . ?
C4O C5O C6O C1O 1.2(4) . . . . ?
C2O C1O C6O C5O -1.9(4) . . . . ?
P1B C1O C6O C5O 180.0(2) . . . . ?
C1N P1B C1P C6P -70.6(2) . . . . ?
C1O P1B C1P C6P -177.8(2) . . . . ?
Cu1B P1B C1P C6P 56.7(2) . . . . ?
C1N P1B C1P C2P 109.9(3) . . . . ?
C1O P1B C1P C2P 2.6(3) . . . . ?
Cu1B P1B C1P C2P -122.8(2) . . . . ?
C6P C1P C2P C3P 0.8(5) . . . . ?
P1B C1P C2P C3P -179.7(3) . . . . ?
C1P C2P C3P C4P -1.0(6) . . . . ?
C2P C3P C4P C5P 0.7(6) . . . . ?
C3P C4P C5P C6P -0.1(5) . . . . ?
C2P C1P C6P C5P -0.2(4) . . . . ?
P1B C1P C6P C5P -179.8(2) . . . . ?
C4P C5P C6P C1P -0.1(5) . . . . ?
C1R P2B C1Q C6Q 12.0(3) . . . . ?
C1S P2B C1Q C6Q 119.1(2) . . . . ?
Cu1B P2B C1Q C6Q -115.8(2) . . . . ?
C1R P2B C1Q C2Q -171.9(2) . . . . ?
C1S P2B C1Q C2Q -64.8(2) . . . . ?
Cu1B P2B C1Q C2Q 60.3(2) . . . . ?
C6Q C1Q C2Q C3Q -4.8(4) . . . . ?
P2B C1Q C2Q C3Q 178.9(2) . . . . ?
C1Q C2Q C3Q C4Q 2.1(5) . . . . ?
```

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C2Q C3Q C4Q C5Q 1.8(5) . . . . ?
C3Q C4Q C5Q C6Q -3.1(5) . . . . ?
C4Q C5Q C6Q C1Q 0.3(5) . . . . ?
C2Q C1Q C6Q C5Q 3.6(4) . . . . ?
P2B C1Q C6Q C5Q 179.7(3) . . . . ?
C1Q P2B C1R C2R -122.8(2) . . . . ?
C1S P2B C1R C2R 128.9(2) . . . . ?
Cu1B P2B C1R C2R 7.1(2) . . . . ?
C1Q P2B C1R C6R 56.4(2) . . . . ?
C1S P2B C1R C6R -51.9(2) . . . . ?
Cu1B P2B C1R C6R -173.70(17) . . . . ?
C6R C1R C2R C3R -1.6(4) . . . . ?
P2B C1R C2R C3R 177.6(2) . . . . ?
C1R C2R C3R C4R -0.6(4) . . . . ?
C2R C3R C4R C5R 1.6(4) . . . . ?
C3R C4R C5R C6R -0.2(4) . . . . ?
C4R C5R C6R C1R -2.0(4) . . . . ?
C2R C1R C6R C5R 2.9(4) . . . . ?
P2B C1R C6R C5R -176.3(2) . . . . ?
C1R P2B C1S C6S 124.0(3) . . . . ?
C1Q P2B C1S C6S 16.5(3) . . . . ?
Cu1B P2B C1S C6S -112.4(2) . . . . ?
C1R P2B C1S C2S -59.5(2) . . . . ?
C1Q P2B C1S C2S -167.0(2) . . . . ?
Cu1B P2B C1S C2S 64.1(2) . . . . ?
C6S C1S C2S C3S -0.8(4) . . . . ?
P2B C1S C2S C3S -177.5(2) . . . . ?
C1S C2S C3S C4S 0.9(5) . . . . ?
C2S C3S C4S C5S 0.0(5) . . . . ?
C3S C4S C5S C6S -1.1(5) . . . . ?
C4S C5S C6S C1S 1.3(6) . . . . ?
C2S C1S C6S C5S -0.3(5) . . . . ?
P2B C1S C6S C5S 176.2(3) . . . . ?
C1V P3B C1T C2T -106.1(2) . . . . ?
C1U P3B C1T C2T 146.9(2) . . . . ?
Cu2B P3B C1T C2T 22.8(3) . . . . ?
C1V P3B C1T C6T 75.0(2) . . . . ?
C1U P3B C1T C6T -32.0(2) . . . . ?
Cu2B P3B C1T C6T -156.16(19) . . . . ?
C6T C1T C2T C3T -2.4(5) . . . . ?
P3B C1T C2T C3T 178.7(3) . . . . ?
C1T C2T C3T C4T 1.3(6) . . . . ?
C2T C3T C4T C5T 0.6(6) . . . . ?
C3T C4T C5T C6T -1.3(5) . . . . ?
C4T C5T C6T C1T 0.3(5) . . . . ?
C2T C1T C6T C5T 1.6(4) . . . . ?
P3B C1T C6T C5T -179.5(2) . . . . ?
C1T P3B C1U C6U 118.1(2) . . . . ?
C1V P3B C1U C6U 8.5(3) . . . . ?
Cu2B P3B C1U C6U -113.5(2) . . . . ?
C1T P3B C1U C2U -67.2(2) . . . . ?
C1V P3B C1U C2U -176.8(2) . . . . ?
Cu2B P3B C1U C2U 61.2(2) . . . . ?
C6U C1U C2U C3U 1.9(4) . . . . ?
```

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C3U C4U C5U C6U 1.4(5) . . . . ?
C2U C1U C6U C5U -2.0(4) . . . . ?
P3B C1U C6U C5U 172.6(2) . . . . ?
C4U C5U C6U C1U 0.3(5) . . . . ?
C1T P3B C1V C2V -9.5(3) . . . . ?
C1U P3B C1V C2V 98.4(2) . . . . ?
Cu2B P3B C1V C2V -141.0(2) . . . . ?
C1T P3B C1V C6V 172.12(19) . . . . ?
C1U P3B C1V C6V -80.0(2) . . . . ?
Cu2B P3B C1V C6V 40.6(2) . . . . ?
C6V C1V C2V C3V 0.8(4) . . . . ?
P3B C1V C2V C3V -177.5(2) . . . . ?
C1V C2V C3V C4V 0.5(5) . . . . ?
C2V C3V C4V C5V -1.0(5) . . . . ?
C3V C4V C5V C6V 0.1(4) . . . . ?
C4V C5V C6V C1V 1.3(4) . . . . ?
C2V C1V C6V C5V -1.7(4) . . . . ?
P3B C1V C6V C5V 176.7(2) . . . . ?
C1X P4B C1W C2W -179.9(2) . . . . ?
C1Y P4B C1W C2W -74.3(2) . . . . ?
Cu2B P4B C1W C2W 49.8(2) . . . . ?
C1X P4B C1W C6W 4.9(2) . . . . ?
C1Y P4B C1W C6W 110.6(2) . . . . ?
Cu2B P4B C1W C6W -125.3(2) . . . . ?
C6W C1W C2W C3W -1.9(4) . . . . ?
P4B C1W C2W C3W -177.3(2) . . . . ?
C1W C2W C3W C4W 1.3(5) . . . . ?
C2W C3W C4W C5W -0.1(6) . . . . ?
C3W C4W C5W C6W -0.4(6) . . . . ?
C4W C5W C6W C1W -0.2(5) . . . . ?
C2W C1W C6W C5W 1.4(4) . . . . ?
P4B C1W C6W C5W 176.5(2) . . . . ?
C1W P4B C1X C6X -112.6(2) . . . . ?
C1Y P4B C1X C6X 139.22(19) . . . . ?
Cu2B P4B C1X C6X 15.0(2) . . . . ?
C1W P4B C1X C2X 68.3(2) . . . . ?
C1Y P4B C1X C2X -39.9(2) . . . . ?
Cu2B P4B C1X C2X -164.11(17) . . . . ?
C6X C1X C2X C3X 0.3(4) . . . . ?
P4B C1X C2X C3X 179.4(2) . . . . ?
C1X C2X C3X C4X -0.6(4) . . . . ?
C2X C3X C4X C5X 0.5(4) . . . . ?
C3X C4X C5X C6X -0.1(4) . . . . ?
C2X C1X C6X C5X 0.1(4) . . . . ?
P4B C1X C6X C5X -179.03(19) . . . . ?
C4X C5X C6X C1X -0.2(4) . . . . ?
C1X P4B C1Y C2Y 124.5(2) . . . . ?
C1W P4B C1Y C2Y 16.2(2) . . . . ?
Cu2B P4B C1Y C2Y -108.1(2) . . . . ?
C1X P4B C1Y C6Y -60.6(2) . . . . ?
C1W P4B C1Y C6Y -168.91(19) . . . . ?
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Cu2B P4B C1Y C6Y 66.80(19) . . . . ?
C6Y C1Y C2Y C3Y -1.9(4) . . . . ?
P4B C1Y C2Y C3Y 172.9(2) . . . . ?
C1Y C2Y C3Y C4Y 1.2(4) . . . . ?
C2Y C3Y C4Y C5Y 0.2(4) . . . . ?
C3Y C4Y C5Y C6Y -1.0(4) . . . . ?
C4Y C5Y C6Y C1Y 0.3(4) . . . . ?
C2Y C1Y C6Y C5Y 1.1(4) . . . . ?
P4B C1Y C6Y C5Y -174.1(2) . . . . ?
Cu1B S1B C1Z N1Z -5.7(2) . . . . ?
Cu1B S1B C1Z N2Z 174.2(2) . . . . ?
N1Z C1Z N2Z C3Z 2.0(4) . . . . ?
S1B C1Z N2Z C3Z -178.0(2) . . . . ?
C1Z N2Z C3Z N3Z 0.9(5) . . . . ?
N2Z C3Z N3Z C5Z -2.2(5) . . . . ?
C3Z N3Z C5Z N1Z 0.7(4) . . . . ?
C3Z N3Z C5Z S2B 178.6(2) . . . . ?
Cu2B S2B C5Z N3Z 149.9(2) . . . . ?
Cu2B S2B C5Z N1Z -32.3(2) . . . . ?
N2Z C1Z N1Z C5Z -3.5(4) . . . . ?
S1B C1Z N1Z C5Z 176.4(2) . . . . ?
N3Z C5Z N1Z C1Z 2.1(4) . . . . ?
S2B C5Z N1Z C1Z -175.8(2) . . . . ?

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 _geom_hbond_distance_DA
 _geom_hbond_angle_DHA
 _geom_hbond_site_symmetry_A
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N1Z H1ZA Br1B  0.88 2.43 3.288(2) 166.6 .

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_diffrn_reflns_theta_full              25.00
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data_6

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_chemical_name_common             ?
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_chemical_melting_point           ?
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 'C39 H33 Cu N3 O0.50 P2 S3'
_chemical_formula_weight          773.34

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'S'  'S'   0.1246   0.1234
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'P'  'P'   0.1023   0.0942
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 'O'  'O'   0.0106   0.0060
 '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'
 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_space_group_IT_number            4
_space_group_name_H-M_alt         'P 21'
_space_group_name_Hall            'P 2yb'

_shelx_space_group_comment
;
The symmetry employed for this shelxl refinement is uniquely defined
by the following loop, which should always be used as a source of
symmetry information in preference to the above space-group names.
They are only intended as comments.
;

loop_
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 'x, y, z'
 '-x, y+1/2, -z'

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_cell_length_c                    17.506(5)
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_cell_angle_beta                  95.271(4)
_cell_angle_gamma                 90
_cell_volume                      3625.4(19)
_cell_formula_units_Z             4
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_exptl_transmission_factor_max    ?
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_exptl_absorpt_correction_T_min   0.763
_exptl_absorpt_correction_T_max   1.000
_exptl_absorpt_process_details    SADABS

_exptl_special_details
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_diffrn_radiation_type            MoK\a
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_diffrn_measurement_device_type   'Bruker CCD SMART1000'
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_diffrn_reflns_av_R_equivalents   0.0473
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_diffrn_reflns_limit_h_max        16
_diffrn_reflns_limit_k_min        -20
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_diffrn_reflns_Laue_measured_fraction_max    1.000
_diffrn_reflns_Laue_measured_fraction_full   1.000
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_reflns_number_gt                 12422
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_reflns_Friedel_coverage          0.928
_reflns_Friedel_fraction_max      1.000
_reflns_Friedel_fraction_full     1.000

_reflns_special_details
;
 Data were apparently pre-merged, so _diffrn_reflns_number
 etc. will have to be added later.

 Reflections were merged by SHELXL according to the crystal
 class for the calculation of statistics and refinement.

 _reflns_Friedel_fraction is defined as the number of unique
 Friedel pairs measured divided by the number that would be
 possible theoretically, ignoring centric projections and
 systematic absences.
;

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_computing_cell_refinement        'SMART Software (Bruker, 1997)'
_computing_data_reduction         'SAINT Software (Bruker, 1997)'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 2008)'
_computing_structure_refinement   'SHELXL-2013 (Sheldrick, 2013)'
_computing_molecular_graphics     'PLATON (Spek, 2009)'
_computing_publication_material   'SHELXL-2013 (Sheldrick, 2013)'

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 Refined as a 2-component inversion twin.
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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
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_atom_sites_solution_secondary    direct
_atom_sites_solution_hydrogens    difmap
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_refine_ls_extinction_method      none
_refine_ls_extinction_coef        .
_refine_ls_abs_structure_details
;
 Refined as an inversion twin.
;
_refine_ls_abs_structure_Flack    0.545(15)
_chemical_absolute_configuration  ?
_refine_ls_number_reflns          14793
_refine_ls_number_parameters      875
_refine_ls_number_restraints      1
_refine_ls_R_factor_all           0.0675
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_refine_ls_restrained_S_all       1.048
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 _atom_site_adp_type
 _atom_site_occupancy
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S12 S -0.24709(15) 0.60432(11) 0.11920(10) 0.0233(4) Uani 1 1 d . . . . .
S14 S -0.25079(15) 0.47783(12) 0.39868(10) 0.0258(4) Uani 1 1 d . . . . .
S16 S -0.35465(16) 0.29412(11) 0.15255(11) 0.0275(4) Uani 1 1 d . . . . .
P11 P -0.13871(14) 0.41607(10) -0.01067(10) 0.0165(4) Uani 1 1 d . . . . .
P12 P -0.42207(14) 0.49650(11) -0.05203(10) 0.0172(4) Uani 1 1 d . . . . .
N11 N -0.2963(4) 0.4509(4) 0.1455(3) 0.0180(12) Uani 1 1 d . . . . .
N13 N -0.2569(5) 0.5319(4) 0.2549(3) 0.0193(12) Uani 1 1 d . . . . .
H13 H -0.2416 0.5797 0.2742 0.023 Uiso 1 1 d R U . . .
N15 N -0.2989(5) 0.3950(4) 0.2684(3) 0.0210(12) Uani 1 1 d . . . . .
H15 H -0.3080 0.3529 0.2970 0.025 Uiso 1 1 d R U . . .
C12 C -0.2673(5) 0.5243(4) 0.1773(4) 0.0180(14) Uani 1 1 d . . . . .
C14 C -0.2694(5) 0.4678(4) 0.3039(4) 0.0206(15) Uani 1 1 d . . . . .
C16 C -0.3149(5) 0.3845(4) 0.1902(4) 0.0183(14) Uani 1 1 d . . . . .
C31 C -0.0381(5) 0.3990(4) 0.0694(4) 0.0184(13) Uani 1 1 d . . . . .
C32 C -0.0658(6) 0.3525(4) 0.1315(4) 0.0212(15) Uani 1 1 d . . . . .
H32 H -0.1334 0.3286 0.1302 0.025 Uiso 1 1 d R U . . .
C33 C 0.0048(6) 0.3409(4) 0.1949(4) 0.0237(16) Uani 1 1 d . . . . .
H33 H -0.0142 0.3085 0.2367 0.028 Uiso 1 1 d R U . . .
C34 C 0.1024(6) 0.3763(5) 0.1979(4) 0.0302(18) Uani 1 1 d . . . . .
H34 H 0.1501 0.3692 0.2421 0.036 Uiso 1 1 d R U . . .
C35 C 0.1308(6) 0.4218(5) 0.1369(4) 0.0281(17) Uani 1 1 d . . . . .
H35 H 0.1986 0.4454 0.1386 0.034 Uiso 1 1 d R U . . .
C36 C 0.0595(6) 0.4335(4) 0.0716(4) 0.0253(17) Uani 1 1 d . . . . .
H36 H 0.0790 0.4651 0.0294 0.030 Uiso 1 1 d R U . . .
C37 C -0.1354(6) 0.3216(4) -0.0689(4) 0.0188(14) Uani 1 1 d . . . . .
C38 C -0.0466(6) 0.2735(4) -0.0702(4) 0.0200(15) Uani 1 1 d . . . . .
H38 H 0.0143 0.2873 -0.0378 0.024 Uiso 1 1 d R U . . .
C39 C -0.0455(6) 0.2048(4) -0.1186(4) 0.0246(16) Uani 1 1 d . . . . .
H39 H 0.0148 0.1708 -0.1178 0.030 Uiso 1 1 d R U . . .
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C40 C -0.1333(6) 0.1866(4) -0.1679(4) 0.0237(16) Uani 1 1 d . . . . .
H40 H -0.1324 0.1405 -0.2014 0.028 Uiso 1 1 d R U . . .
C41 C -0.2218(6) 0.2349(4) -0.1684(4) 0.0220(15) Uani 1 1 d . . . . .
H41 H -0.2816 0.2219 -0.2022 0.026 Uiso 1 1 d R U . . .
C42 C -0.2236(6) 0.3029(4) -0.1194(4) 0.0214(15) Uani 1 1 d . . . . .
H42 H -0.2843 0.3364 -0.1201 0.026 Uiso 1 1 d R U . . .
C43 C -0.0778(5) 0.4929(4) -0.0696(4) 0.0183(14) Uani 1 1 d . . . . .
C44 C -0.0341(5) 0.4723(4) -0.1364(4) 0.0203(15) Uani 1 1 d . . . . .
H44 H -0.0341 0.4164 -0.1531 0.024 Uiso 1 1 d R U . . .
C45 C 0.0103(6) 0.5344(4) -0.1796(4) 0.0222(15) Uani 1 1 d . . . . .
H45 H 0.0399 0.5204 -0.2257 0.027 Uiso 1 1 d R U . . .
C46 C 0.0107(6) 0.6152(5) -0.1551(4) 0.0254(16) Uani 1 1 d . . . . .
H46 H 0.0420 0.6568 -0.1837 0.030 Uiso 1 1 d R U . . .
C47 C -0.0340(6) 0.6357(5) -0.0895(5) 0.0285(18) Uani 1 1 d . . . . .
H47 H -0.0344 0.6919 -0.0736 0.034 Uiso 1 1 d R U . . .
C48 C -0.0785(6) 0.5760(5) -0.0460(4) 0.0271(17) Uani 1 1 d . . . . .
H48 H -0.1093 0.5911 -0.0007 0.033 Uiso 1 1 d R U . . .
C49 C -0.4683(5) 0.4087(4) -0.1110(4) 0.0183(14) Uani 1 1 d . . . . .
C50 C -0.4821(6) 0.3342(5) -0.0718(4) 0.0239(15) Uani 1 1 d . . . . .
H50 H -0.4711 0.3326 -0.0174 0.029 Uiso 1 1 d R U . . .
C51 C -0.5121(6) 0.2626(4) -0.1126(5) 0.0257(17) Uani 1 1 d . . . . .
H51 H -0.5235 0.2128 -0.0859 0.031 Uiso 1 1 d R U . . .
C52 C -0.5252(6) 0.2642(5) -0.1918(5) 0.0288(18) Uani 1 1 d . . . . .
H52 H -0.5428 0.2150 -0.2197 0.035 Uiso 1 1 d R U . . .
C53 C -0.5125(6) 0.3383(5) -0.2306(4) 0.0293(17) Uani 1 1 d . . . . .
H53 H -0.5230 0.3398 -0.2850 0.035 Uiso 1 1 d R U . . .
C54 C -0.4847(5) 0.4096(5) -0.1902(4) 0.0238(15) Uani 1 1 d . . . . .
H54 H -0.4766 0.4598 -0.2172 0.029 Uiso 1 1 d R U . . .
C55 C -0.3725(5) 0.5733(4) -0.1163(4) 0.0181(14) Uani 1 1 d . . . . .
C56 C -0.3029(5) 0.5499(5) -0.1688(4) 0.0216(15) Uani 1 1 d . . . . .
H56 H -0.2883 0.4929 -0.1754 0.026 Uiso 1 1 d R U . . .
C57 C -0.2548(6) 0.6079(5) -0.2113(4) 0.0257(16) Uani 1 1 d . . . . .
H57 H -0.2082 0.5907 -0.2474 0.031 Uiso 1 1 d R U . . .
C58 C -0.2746(6) 0.6915(5) -0.2012(5) 0.0316(18) Uani 1 1 d . . . . .
H58 H -0.2416 0.7319 -0.2302 0.038 Uiso 1 1 d R U . . .
C59 C -0.3425(7) 0.7154(5) -0.1489(5) 0.0325(18) Uani 1 1 d . . . . .
H59 H -0.3557 0.7725 -0.1417 0.039 Uiso 1 1 d R U . . .
C60 C -0.3912(6) 0.6577(5) -0.1072(4) 0.0265(17) Uani 1 1 d . . . . .
H60 H -0.4382 0.6754 -0.0717 0.032 Uiso 1 1 d R U . . .
C61 C -0.5445(5) 0.5411(4) -0.0258(4) 0.0183(14) Uani 1 1 d . . . . .
C62 C -0.6189(6) 0.5716(4) -0.0816(4) 0.0241(16) Uani 1 1 d . . . . .
H62 H -0.6045 0.5713 -0.1339 0.029 Uiso 1 1 d R U . . .
C63 C -0.7122(6) 0.6020(4) -0.0625(5) 0.0266(16) Uani 1 1 d . . . . .
H63 H -0.7619 0.6226 -0.1014 0.032 Uiso 1 1 d R U . . .
C64 C -0.7346(6) 0.6029(4) 0.0138(5) 0.0268(17) Uani 1 1 d . . . . .
H64 H -0.7997 0.6233 0.0273 0.032 Uiso 1 1 d R U . . .
C65 C -0.6604(6) 0.5734(5) 0.0699(4) 0.0263(17) Uani 1 1 d . . . . .
H65 H -0.6743 0.5745 0.1222 0.032 Uiso 1 1 d R U . . .
C66 C -0.5658(6) 0.5423(4) 0.0497(4) 0.0234(16) Uani 1 1 d . . . . .
H66 H -0.5157 0.5217 0.0883 0.028 Uiso 1 1 d R U . . .
Cu2 Cu 0.25602(6) 0.39798(5) -0.42137(5) 0.01910(19) Uani 1 1 d . . . . .
S22 S 0.23190(15) 0.53686(12) -0.29855(12) 0.0278(4) Uani 1 1 d . . . . .
S24 S 0.23028(15) 0.33677(12) -0.05895(10) 0.0256(4) Uani 1 1 d . . . . .
S26 S 0.23006(14) 0.21455(11) -0.34040(10) 0.0225(4) Uani 1 1 d . . . . .
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P21 P 0.40950(13) 0.40898(12) -0.47259(10) 0.0185(4) Uani 1 1 d . . . . .
P22 P 0.09530(13) 0.40513(11) -0.48683(9) 0.0152(3) Uani 1 1 d . . . . .
N21 N 0.2416(5) 0.3753(4) -0.3097(3) 0.0195(13) Uani 1 1 d . . . . .
N23 N 0.2305(5) 0.4265(3) -0.1859(3) 0.0206(13) Uani 1 1 d . . . . .
H23 H 0.2286 0.4690 -0.1565 0.025 Uiso 1 1 d R U . . .
N25 N 0.2256(5) 0.2868(4) -0.2044(3) 0.0191(12) Uani 1 1 d . . . . .
H25 H 0.2181 0.2373 -0.1877 0.023 Uiso 1 1 d R U . . .
C22 C 0.2349(5) 0.4401(4) -0.2635(4) 0.0192(15) Uani 1 1 d . . . . .
C24 C 0.2291(5) 0.3493(4) -0.1527(4) 0.0214(15) Uani 1 1 d . . . . .
C26 C 0.2332(5) 0.2970(4) -0.2818(4) 0.0195(15) Uani 1 1 d . . . . .
C67 C 0.4821(5) 0.5036(4) -0.4442(4) 0.0192(15) Uani 1 1 d . . . . .
C68 C 0.4754(6) 0.5335(5) -0.3707(4) 0.0234(16) Uani 1 1 d . . . . .
H68 H 0.4302 0.5072 -0.3382 0.028 Uiso 1 1 d R U . . .
C69 C 0.5336(6) 0.6010(5) -0.3441(4) 0.0295(18) Uani 1 1 d . . . . .
H69 H 0.5298 0.6202 -0.2932 0.035 Uiso 1 1 d R U . . .
C70 C 0.5978(6) 0.6408(5) -0.3925(4) 0.0268(17) Uani 1 1 d . . . . .
H70 H 0.6358 0.6887 -0.3751 0.032 Uiso 1 1 d R U . . .
C71 C 0.6064(6) 0.6112(4) -0.4651(4) 0.0253(16) Uani 1 1 d . . . . .
H71 H 0.6528 0.6369 -0.4971 0.030 Uiso 1 1 d R U . . .
C72 C 0.5469(6) 0.5433(4) -0.4918(4) 0.0231(16) Uani 1 1 d . . . . .
H72 H 0.5506 0.5241 -0.5428 0.028 Uiso 1 1 d R U . . .
C73 C 0.5095(6) 0.3295(4) -0.4493(4) 0.0214(15) Uani 1 1 d . . . . .
C74 C 0.4816(6) 0.2569(4) -0.4115(4) 0.0248(16) Uani 1 1 d . . . . .
H74 H 0.4115 0.2486 -0.4004 0.030 Uiso 1 1 d R U . . .
C75 C 0.5573(7) 0.1971(5) -0.3904(5) 0.0302(18) Uani 1 1 d . . . . .
H75 H 0.5386 0.1484 -0.3647 0.036 Uiso 1 1 d R U . . .
C76 C 0.6592(6) 0.2089(4) -0.4069(5) 0.0294(18) Uani 1 1 d . . . . .
H76 H 0.7105 0.1682 -0.3923 0.035 Uiso 1 1 d R U . . .
C77 C 0.6872(6) 0.2799(5) -0.4449(5) 0.0317(19) Uani 1 1 d . . . . .
H77 H 0.7573 0.2879 -0.4564 0.038 Uiso 1 1 d R U . . .
C78 C 0.6112(6) 0.3396(5) -0.4662(5) 0.0274(17) Uani 1 1 d . . . . .
H78 H 0.6301 0.3878 -0.4926 0.033 Uiso 1 1 d R U . . .
C79 C 0.3992(5) 0.4145(4) -0.5775(4) 0.0180(14) Uani 1 1 d . . . . .
C80 C 0.4526(6) 0.3623(4) -0.6238(4) 0.0227(16) Uani 1 1 d . . . . .
H80 H 0.4962 0.3201 -0.6006 0.027 Uiso 1 1 d R U . . .
C81 C 0.4433(6) 0.3709(5) -0.7027(4) 0.0263(17) Uani 1 1 d . . . . .
H81 H 0.4797 0.3344 -0.7335 0.032 Uiso 1 1 d R U . . .
C82 C 0.3804(6) 0.4333(5) -0.7369(4) 0.0270(17) Uani 1 1 d . . . . .
H82 H 0.3755 0.4408 -0.7910 0.032 Uiso 1 1 d R U . . .
C83 C 0.3252(6) 0.4842(5) -0.6918(4) 0.0287(17) Uani 1 1 d . . . . .
H83 H 0.2810 0.5259 -0.7152 0.034 Uiso 1 1 d R U . . .
C84 C 0.3337(6) 0.4751(4) -0.6131(4) 0.0238(16) Uani 1 1 d . . . . .
H84 H 0.2948 0.5102 -0.5828 0.029 Uiso 1 1 d R U . . .
C85 C 0.0606(5) 0.3138(4) -0.5452(4) 0.0142(13) Uani 1 1 d . . . . .
C86 C 0.1393(6) 0.2611(4) -0.5628(4) 0.0222(15) Uani 1 1 d . . . . .
H86 H 0.2097 0.2718 -0.5440 0.027 Uiso 1 1 d R U . . .
C87 C 0.1144(6) 0.1914(4) -0.6089(5) 0.0282(17) Uani 1 1 d . . . . .
H87 H 0.1684 0.1552 -0.6217 0.034 Uiso 1 1 d R U . . .
C88 C 0.0131(6) 0.1752(4) -0.6354(4) 0.0259(17) Uani 1 1 d . . . . .
H88 H -0.0028 0.1278 -0.6663 0.031 Uiso 1 1 d R U . . .
C89 C -0.0668(6) 0.2277(4) -0.6175(4) 0.0233(16) Uani 1 1 d . . . . .
H89 H -0.1371 0.2160 -0.6358 0.028 Uiso 1 1 d R U . . .
C90 C -0.0432(6) 0.2975(4) -0.5726(4) 0.0202(15) Uani 1 1 d . . . . .
H90 H -0.0973 0.3339 -0.5605 0.024 Uiso 1 1 d R U . . .
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C91 C 0.0707(5) 0.4902(4) -0.5541(4) 0.0170(14) Uani 1 1 d . . . . .
C92 C 0.0358(6) 0.4792(4) -0.6314(4) 0.0195(15) Uani 1 1 d . . . . .
H92 H 0.0235 0.4250 -0.6512 0.023 Uiso 1 1 d R U . . .
C93 C 0.0191(6) 0.5471(4) -0.6796(4) 0.0215(15) Uani 1 1 d . . . . .
H93 H -0.0025 0.5389 -0.7324 0.026 Uiso 1 1 d R U . . .
C94 C 0.0336(6) 0.6266(4) -0.6513(4) 0.0250(17) Uani 1 1 d . . . . .
H94 H 0.0193 0.6728 -0.6841 0.030 Uiso 1 1 d R U . . .
C95 C 0.0690(6) 0.6387(4) -0.5751(4) 0.0270(17) Uani 1 1 d . . . . .
H95 H 0.0803 0.6933 -0.5561 0.032 Uiso 1 1 d R U . . .
C96 C 0.0883(6) 0.5719(4) -0.5261(4) 0.0212(15) Uani 1 1 d . . . . .
H96 H 0.1132 0.5807 -0.4740 0.025 Uiso 1 1 d R U . . .
C97 C -0.0112(5) 0.4118(4) -0.4245(4) 0.0156(13) Uani 1 1 d . . . . .
C98 C -0.0918(5) 0.4701(4) -0.4325(4) 0.0180(14) Uani 1 1 d . . . . .
H98 H -0.0926 0.5108 -0.4717 0.022 Uiso 1 1 d R U . . .
C99 C -0.1700(5) 0.4689(4) -0.3838(4) 0.0197(14) Uani 1 1 d . . . . .
H99 H -0.2258 0.5073 -0.3911 0.024 Uiso 1 1 d R U . . .
C100 C -0.1683(5) 0.4120(5) -0.3240(4) 0.0239(15) Uani 1 1 d . . . . .
H100 H -0.2211 0.4128 -0.2895 0.029 Uiso 1 1 d R U . . .
C101 C -0.0883(6) 0.3539(4) -0.3153(4) 0.0227(15) Uani 1 1 d . . . . .
H101 H -0.0869 0.3145 -0.2750 0.027 Uiso 1 1 d R U . . .
C102 C -0.0109(5) 0.3531(4) -0.3652(4) 0.0178(14) Uani 1 1 d . . . . .
H102 H 0.0428 0.3127 -0.3593 0.021 Uiso 1 1 d R U . . .
O1 O -0.3331(5) 0.2366(4) 0.3366(4) 0.0561(19) Uani 1 1 d . . . . .
H1A H -0.2801 0.2100 0.3216 0.084 Uiso 1 1 d R U . . .
H1B H -0.3807 0.2017 0.3476 0.084 Uiso 1 1 d R U . . .

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S14 0.0320(10) 0.0297(10) 0.0155(8) 0.0001(7) 0.0008(7) -0.0030(8)
S16 0.0386(11) 0.0186(9) 0.0254(10) -0.0042(7) 0.0035(8) -0.0045(8)
P11 0.0191(9) 0.0159(9) 0.0144(8) 0.0005(7) 0.0012(7) -0.0008(7)
P12 0.0197(9) 0.0155(8) 0.0163(9) -0.0010(7) 0.0005(7) 0.0006(7)
N11 0.022(3) 0.015(3) 0.017(3) 0.001(2) 0.002(2) 0.001(2)
N13 0.025(3) 0.016(3) 0.016(3) -0.003(2) 0.001(2) -0.003(2)
N15 0.030(3) 0.016(3) 0.018(3) 0.005(2) 0.003(2) -0.002(3)
C12 0.022(4) 0.012(3) 0.019(4) 0.000(3) -0.001(3) -0.001(3)
C14 0.019(3) 0.020(4) 0.023(4) -0.001(3) 0.005(3) 0.001(3)
C16 0.019(3) 0.013(3) 0.022(4) 0.000(3) 0.002(3) 0.001(3)
C31 0.023(3) 0.017(3) 0.015(3) 0.000(3) 0.001(3) 0.001(3)
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C34 0.035(5) 0.029(4) 0.024(4) -0.004(3) -0.011(3) 0.011(3)
C35 0.024(4) 0.032(4) 0.027(4) 0.003(3) -0.004(3) -0.004(3)
C36 0.027(4) 0.029(4) 0.020(4) 0.003(3) -0.003(3) 0.002(3)
C37 0.025(4) 0.015(3) 0.016(3) 0.003(3) 0.003(3) -0.001(3)
C38 0.021(4) 0.024(4) 0.015(3) 0.002(3) 0.001(3) 0.002(3)
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C39 0.030(4) 0.019(4) 0.025(4) 0.003(3) 0.005(3) 0.007(3)
C40 0.033(4) 0.016(3) 0.023(4) -0.002(3) 0.008(3) -0.002(3)
C41 0.027(4) 0.020(4) 0.020(4) -0.004(3) 0.004(3) -0.005(3)
C42 0.022(4) 0.017(3) 0.025(4) 0.001(3) -0.001(3) 0.000(3)
C43 0.020(4) 0.017(3) 0.017(3) 0.003(3) -0.002(3) -0.002(3)
C44 0.025(4) 0.016(4) 0.020(3) 0.004(3) 0.004(3) 0.003(3)
C45 0.025(4) 0.021(4) 0.021(4) 0.007(3) 0.004(3) 0.005(3)
C46 0.023(4) 0.025(4) 0.028(4) 0.009(3) -0.001(3) -0.007(3)
C47 0.038(5) 0.017(4) 0.030(4) 0.002(3) 0.000(4) -0.006(3)
C48 0.043(5) 0.019(4) 0.020(4) -0.004(3) 0.006(3) -0.007(3)
C49 0.015(3) 0.017(3) 0.023(3) -0.005(3) 0.003(3) 0.003(3)
C50 0.024(4) 0.020(4) 0.027(4) -0.001(3) 0.001(3) 0.001(3)
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C53 0.033(4) 0.031(4) 0.022(4) -0.007(3) -0.002(3) 0.004(4)
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C55 0.022(4) 0.016(3) 0.015(3) -0.001(3) -0.003(3) -0.001(3)
C56 0.016(4) 0.025(4) 0.022(4) 0.001(3) -0.005(3) 0.000(3)
C57 0.020(4) 0.036(4) 0.020(4) 0.005(3) -0.005(3) -0.004(3)
C58 0.030(4) 0.033(4) 0.030(4) 0.007(3) -0.006(3) -0.009(4)
C59 0.042(5) 0.019(4) 0.036(4) 0.003(3) -0.003(4) -0.004(3)
C60 0.030(4) 0.023(4) 0.027(4) -0.004(3) 0.005(3) 0.000(3)
C61 0.023(4) 0.009(3) 0.023(4) -0.002(3) 0.004(3) 0.000(3)
C62 0.027(4) 0.021(4) 0.024(4) 0.000(3) 0.000(3) -0.004(3)
C63 0.026(4) 0.016(4) 0.036(4) 0.000(3) -0.003(3) 0.001(3)
C64 0.027(4) 0.016(4) 0.039(4) -0.003(3) 0.007(3) 0.003(3)
C65 0.030(4) 0.025(4) 0.024(4) -0.007(3) 0.008(3) -0.006(3)
C66 0.030(4) 0.016(3) 0.024(4) 0.000(3) 0.002(3) 0.001(3)
Cu2 0.0203(4) 0.0202(4) 0.0165(4) 0.0009(4) 0.0001(3) -0.0014(4)
S22 0.0284(10) 0.0214(9) 0.0344(11) 0.0096(8) 0.0073(8) 0.0012(8)
S24 0.0300(10) 0.0300(10) 0.0170(9) 0.0028(8) 0.0034(7) 0.0026(8)
S26 0.0276(10) 0.0220(9) 0.0172(8) 0.0002(7) -0.0011(7) 0.0008(7)
P21 0.0197(9) 0.0196(9) 0.0159(8) 0.0010(7) 0.0004(7) -0.0014(8)
P22 0.0185(8) 0.0117(8) 0.0152(8) -0.0002(7) 0.0007(6) -0.0002(7)
N21 0.024(3) 0.023(3) 0.012(3) 0.005(2) 0.002(2) 0.003(2)
N23 0.029(3) 0.012(3) 0.021(3) -0.001(2) 0.000(3) 0.002(2)
N25 0.026(3) 0.015(3) 0.016(3) 0.005(2) 0.002(2) -0.001(2)
C22 0.016(3) 0.018(4) 0.023(4) 0.003(3) 0.003(3) 0.002(3)
C24 0.016(4) 0.022(4) 0.026(4) 0.003(3) 0.004(3) 0.001(3)
C26 0.020(4) 0.019(4) 0.019(4) 0.004(3) 0.001(3) 0.002(3)
C67 0.018(4) 0.025(4) 0.015(3) 0.001(3) 0.000(3) 0.002(3)
C68 0.021(4) 0.027(4) 0.022(4) 0.000(3) -0.001(3) 0.001(3)
C69 0.028(4) 0.033(4) 0.027(4) -0.012(3) -0.004(3) 0.004(3)
C70 0.029(4) 0.018(4) 0.031(4) -0.005(3) -0.008(3) 0.001(3)
C71 0.026(4) 0.015(4) 0.034(4) 0.006(3) -0.004(3) 0.000(3)
C72 0.030(4) 0.018(4) 0.021(4) -0.001(3) 0.001(3) -0.001(3)
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C75 0.048(5) 0.014(4) 0.029(4) -0.001(3) 0.003(4) 0.000(3)
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C77 0.026(4) 0.023(4) 0.045(5) 0.002(4) -0.005(4) -0.003(3)
C78 0.026(4) 0.018(4) 0.038(5) 0.009(3) 0.000(3) 0.001(3)
C79 0.014(3) 0.021(4) 0.019(3) 0.003(3) 0.000(3) -0.004(3)
C80 0.023(4) 0.021(4) 0.023(4) -0.003(3) 0.000(3) 0.001(3)

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C81 0.024(4) 0.030(4) 0.025(4) -0.007(3) 0.005(3) 0.001(3)
C82 0.030(4) 0.034(4) 0.017(4) 0.003(3) -0.001(3) -0.003(3)
C83 0.031(4) 0.028(4) 0.026(4) 0.005(3) -0.006(3) 0.000(3)
C84 0.025(4) 0.021(4) 0.025(4) -0.005(3) 0.001(3) 0.000(3)
C85 0.018(3) 0.012(3) 0.013(3) 0.003(2) 0.002(3) -0.001(2)
C86 0.023(4) 0.015(3) 0.028(4) -0.003(3) 0.000(3) -0.001(3)
C87 0.038(5) 0.013(3) 0.034(5) -0.006(3) 0.007(4) 0.005(3)
C88 0.045(5) 0.013(4) 0.019(4) -0.001(3) 0.001(3) -0.002(3)
C89 0.032(4) 0.017(3) 0.020(4) 0.002(3) -0.004(3) -0.007(3)
C90 0.029(4) 0.009(3) 0.022(4) 0.001(3) 0.001(3) 0.004(3)
C91 0.021(4) 0.011(3) 0.019(3) -0.001(3) 0.004(3) -0.002(3)
C92 0.030(4) 0.008(3) 0.020(3) 0.003(3) 0.004(3) 0.001(3)
C93 0.032(4) 0.015(3) 0.018(3) 0.005(3) 0.002(3) -0.001(3)
C94 0.032(4) 0.017(4) 0.027(4) 0.009(3) 0.008(3) 0.001(3)
C95 0.043(5) 0.010(3) 0.029(4) -0.002(3) 0.010(4) -0.005(3)
C96 0.030(4) 0.010(3) 0.024(4) 0.001(3) 0.006(3) -0.003(3)
C97 0.024(3) 0.008(3) 0.015(3) -0.002(3) -0.001(3) -0.002(3)
C98 0.028(4) 0.012(3) 0.013(3) 0.000(3) -0.005(3) 0.000(3)
C99 0.020(3) 0.015(4) 0.024(4) -0.002(3) 0.000(3) 0.005(3)
C100 0.025(4) 0.022(4) 0.027(4) -0.005(3) 0.009(3) 0.000(3)
C101 0.030(4) 0.016(3) 0.022(4) 0.002(3) 0.000(3) -0.004(3)
C102 0.021(4) 0.009(3) 0.022(4) 0.000(3) -0.003(3) -0.001(3)
O1 0.046(4) 0.033(4) 0.091(6) 0.013(4) 0.014(4) -0.001(3)

_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 S12 2.879(2) . y
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S14 C14 1.663(7) . ?
S16 C16 1.664(7) . ?
P11 C43 1.835(7) . ?
P11 C37 1.838(7) . ?
P11 C31 1.839(7) . ?
P12 C49 1.823(7) . ?
P12 C61 1.828(7) . ?
P12 C55 1.829(7) . ?
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N11 C16 1.362(9) . ?
N13 C12 1.358(9) . ?
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N13 H13 0.8599 . ?
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N15 C16 1.376(9) . ?
N15 H15 0.8600 . ?
C31 C36 1.371(10) . ?
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C37 C42 1.406(10) . ?
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C55 C60 1.397(10) . ?
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Cu2 P22 2.2729(19) . y
Cu2 S22 3.144(2) . y
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S24 C24 1.652(7) . ?
S26 C26 1.680(7) . ?
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P21 C73 1.837(7) . ?
P21 C67 1.837(7) . ?
P22 C91 1.820(7) . ?
P22 C85 1.827(7) . ?
P22 C97 1.832(7) . ?
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N21 C26 1.364(9) . ?
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N23 C22 1.382(9) . ?
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N25 H25 0.8600 . ?
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C67 C72 1.389(10) . ?
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C85 C90 1.401(10) . ?
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O1 H1A 0.8672 . ?
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O1 H1B 0.8682 . ?

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P12 Cu1 S12 101.91(7) . . y
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C12 S12 Cu1 69.4(2) . . ?
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N21 Cu2 P22 109.75(17) . . y
P21 Cu2 P22 125.88(7) . . y
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P21 Cu2 S22 111.20(7) . . y
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C22 S22 Cu2 65.4(2) . . ?
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C75 C74 H74 120.0 . . ?
C73 C74 H74 120.0 . . ?
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Cu2 S22 C22 N23 177.8(6) . . . . ?
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 CrysAlisRED; Oxford Diffraction, 2010.
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_computing_data_reduction      '<i>CrysAlisRED</i> (Oxford Diffraction,
2010)'
_computing_structure_solution   '<i>SHELXS97</i> (Sheldrick, 2008)'
_computing_structure_refinement  '<i>SHELXL97</i> (Sheldrick, 2008)'
_computing_molecular_graphics   '<i>SHELXL97</i> (Sheldrick, 2008)'
_computing_publication_material   '<i>SHELXL97</i> (Sheldrick, 2008)'

_refine_special_details
;
Refinement of <i>F</i>^2^ against ALL reflections. The weighted <i>R</i>-
factor
<i>wR</i> and goodness of fit <i>S</i> are based on <i>F</i>^2^,
conventional
<i>R</i>-factors <i>R</i> are based on <i>F</i>, with <i>F</i> set to zero
for
negative <i>F</i>^2^. The threshold expression of <i>F</i>^2^ >
\s(<i>F</i>^2^) is used only for calculating <i>R</i>-factors(gt)
<i>etc</i>.
and is not relevant to the choice of reflections for refinement.
<i>R</i>-factors based on <i>F</i>^2^ are statistically about twice as
large
as those based on <i>F</i>, and <i>R</i>- factors based on ALL data will
be
even larger.
;
_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0378P)^2^+12.1610P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
_refine_ls_number_reflns          23304
_refine_ls_number_parameters      1124
_refine_ls_number_restraints      4
_refine_ls_R_factor_all           0.0932
_refine_ls_R_factor_gt            0.0679
_refine_ls_wR_factor_ref          0.1475
_refine_ls_wR_factor_gt           0.1345
_refine_ls_goodness_of_fit_ref    1.102
_refine_ls_restrained_S_all       1.102
_refine_ls_shift/su_max           0.002
_refine_ls_shift/su_mean          0.000
```

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 _atom_site_fract_x
 _atom_site_fract_y
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 _atom_site_symmetry_multiplicity
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Br1 Br 0.53954(5) 0.57429(5) 0.637695(14) 0.04840(13) Uani 1 1 d . . .
Br2 Br 0.41187(5) 0.46718(4) 0.872759(14) 0.04234(12) Uani 1 1 d . . .
Cu1 Cu 0.35823(5) 0.59362(5) 0.620570(14) 0.03110(12) Uani 1 1 d . . .
Cu2 Cu 0.34982(5) 0.85628(5) 0.738684(18) 0.03795(13) Uani 1 1 d . A .
Cu3 Cu 0.40843(5) 0.64939(5) 0.891825(15) 0.03339(12) Uani 1 1 d . . .
S1 S 0.37069(11) 0.72393(10) 0.67611(3) 0.0359(2) Uani 1 1 d . . .
S2 S 0.35399(11) 0.71570(11) 0.83094(3) 0.0384(3) Uani 1 1 d . . .
S3 S 0.57577(15) 0.52248(14) 0.76204(4) 0.0569(4) Uani 1 1 d . . .
P1 P 0.37198(9) 0.67477(10) 0.56190(3) 0.0296(2) Uani 1 1 d . . .
P2 P 0.19499(10) 0.41767(10) 0.62650(3) 0.0313(2) Uani 1 1 d . . .
P3 P 0.16636(11) 0.82941(11) 0.74267(4) 0.0394(3) Uani 1 1 d . . .
P4 P 0.51497(10) 1.03259(10) 0.73684(3) 0.0330(2) Uani 1 1 d D . .
P5 P 0.59689(10) 0.79901(10) 0.91948(3) 0.0322(2) Uani 1 1 d . . .
P6 P 0.24218(10) 0.58893(10) 0.92277(3) 0.0329(2) Uani 1 1 d . . .
N1 N 0.3844(3) 0.7240(3) 0.75433(9) 0.0294(7) Uani 1 1 d . . .
N2 N 0.4570(4) 0.6196(3) 0.79083(10) 0.0343(8) Uani 1 1 d D . .
H2N H 0.462(4) 0.587(4) 0.8115(10) 0.041 Uiso 1 1 d D . .
N3 N 0.4684(3) 0.6245(3) 0.72311(10) 0.0328(8) Uani 1 1 d D . .
H3N H 0.489(4) 0.609(4) 0.7013(9) 0.039 Uiso 1 1 d D . .
C1 C 0.4017(4) 0.6853(3) 0.78981(11) 0.0284(8) Uani 1 1 d . A .
C2 C 0.4992(4) 0.5911(4) 0.75867(12) 0.0344(9) Uani 1 1 d . A .
C3 C 0.4102(4) 0.6866(3) 0.72061(11) 0.0292(8) Uani 1 1 d . A .
C4 C 0.2603(4) 0.7181(4) 0.54553(13) 0.0334(9) Uani 1 1 d . . .
C5 C 0.2452(5) 0.7903(5) 0.57296(15) 0.0515(13) Uani 1 1 d . . .
H5A H 0.2917 0.8149 0.5994 0.062 Uiso 1 1 calc R . .
C6 C 0.1632(6) 0.8273(6) 0.5624(2) 0.0683(17) Uani 1 1 d . . .
H6A H 0.1550 0.8784 0.5813 0.082 Uiso 1 1 calc R . .
C7 C 0.0946(5) 0.7904(6) 0.5251(2) 0.0650(16) Uani 1 1 d . . .
H7A H 0.0367 0.8140 0.5182 0.078 Uiso 1 1 calc R . .
C8 C 0.1080(5) 0.7200(5) 0.49746(19) 0.0629(16) Uani 1 1 d . . .
H8A H 0.0609 0.6960 0.4711 0.075 Uiso 1 1 calc R . .
C9 C 0.1900(5) 0.6834(5) 0.50759(15) 0.0492(12) Uani 1 1 d . . .
H9A H 0.1984 0.6336 0.4882 0.059 Uiso 1 1 calc R . .
C10 C 0.3563(4) 0.5777(4) 0.51775(12) 0.0326(9) Uani 1 1 d . . .
C11 C 0.4381(5) 0.6058(5) 0.49170(17) 0.0546(14) Uani 1 1 d . . .
H11D H 0.5089 0.6803 0.4964 0.066 Uiso 1 1 calc R . .
C12 C 0.4194(6) 0.5273(6) 0.45857(18) 0.0664(17) Uani 1 1 d . . .
H12A H 0.4772 0.5484 0.4408 0.080 Uiso 1 1 calc R . .
C13 C 0.3186(5) 0.4202(5) 0.45148(16) 0.0564(14) Uani 1 1 d . . .
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H13A H 0.3052 0.3669 0.4286 0.068 Uiso 1 1 calc R . .
C14 C 0.2377(5) 0.3900(5) 0.47722(18) 0.0632(16) Uani 1 1 d . . .
H14A H 0.1676 0.3149 0.4725 0.076 Uiso 1 1 calc R . .
C15 C 0.2561(5) 0.4683(5) 0.51066(16) 0.0558(14) Uani 1 1 d . . .
H15A H 0.1989 0.4458 0.5287 0.067 Uiso 1 1 calc R . .
C16 C 0.5110(4) 0.8117(4) 0.56036(13) 0.0362(9) Uani 1 1 d . . .
C17 C 0.6026(4) 0.8556(5) 0.59353(17) 0.0518(13) Uani 1 1 d . . .
H17A H 0.5948 0.8134 0.6162 0.062 Uiso 1 1 calc R . .
C18 C 0.7056(5) 0.9613(6) 0.5933(2) 0.0738(19) Uani 1 1 d . . .
H18A H 0.7683 0.9917 0.6160 0.089 Uiso 1 1 calc R . .
C19 C 0.7185(5) 1.0229(6) 0.5608(2) 0.0741(19) Uani 1 1 d . . .
H19A H 0.7894 1.0959 0.5612 0.089 Uiso 1 1 calc R . .
C20 C 0.6296(5) 0.9793(5) 0.5278(2) 0.0611(15) Uani 1 1 d . . .
H20A H 0.6394 1.0206 0.5048 0.073 Uiso 1 1 calc R . .
C21 C 0.5250(4) 0.8749(4) 0.52781(16) 0.0478(12) Uani 1 1 d . . .
H21A H 0.4620 0.8462 0.5052 0.057 Uiso 1 1 calc R . .
C22 C 0.0496(4) 0.4121(4) 0.61840(13) 0.0379(10) Uani 1 1 d . . .
C23 C -0.0540(4) 0.3237(5) 0.62932(16) 0.0509(13) Uani 1 1 d . . .
H23A H -0.0522 0.2607 0.6412 0.061 Uiso 1 1 calc R . .
C24 C -0.1600(5) 0.3273(6) 0.62293(19) 0.0684(18) Uani 1 1 d . . .
H24A H -0.2307 0.2662 0.6303 0.082 Uiso 1 1 calc R . .
C25 C -0.1647(6) 0.4168(7) 0.6062(2) 0.0717(18) Uani 1 1 d . . .
H25A H -0.2384 0.4176 0.6016 0.086 Uiso 1 1 calc R . .
C26 C -0.0633(6) 0.5051(6) 0.5961(2) 0.0704(17) Uani 1 1 d . . .
H26A H -0.0656 0.5687 0.5850 0.084 Uiso 1 1 calc R . .
C27 C 0.0434(5) 0.5026(5) 0.60209(15) 0.0478(12) Uani 1 1 d . . .
H27A H 0.1137 0.5646 0.5948 0.057 Uiso 1 1 calc R . .
C28 C 0.1751(4) 0.2912(4) 0.59361(13) 0.0376(10) Uani 1 1 d . . .
C29 C 0.2743(6) 0.2958(6) 0.5819(2) 0.080(2) Uani 1 1 d . . .
H29A H 0.3509 0.3625 0.5914 0.096 Uiso 1 1 calc R . .
C30 C 0.2662(7) 0.2049(6) 0.5562(2) 0.090(2) Uani 1 1 d . . .
H30A H 0.3374 0.2095 0.5489 0.108 Uiso 1 1 calc R . .
C31 C 0.1598(6) 0.1112(5) 0.54172(18) 0.0641(16) Uani 1 1 d . . .
H31A H 0.1547 0.0502 0.5236 0.077 Uiso 1 1 calc R . .
C32 C 0.0605(6) 0.1040(5) 0.55300(19) 0.0688(17) Uani 1 1 d . . .
H32A H -0.0154 0.0368 0.5432 0.083 Uiso 1 1 calc R . .
C33 C 0.0669(5) 0.1942(5) 0.57894(18) 0.0602(15) Uani 1 1 d . . .
H33A H -0.0047 0.1880 0.5865 0.072 Uiso 1 1 calc R . .
C34 C 0.2004(4) 0.3766(4) 0.67729(13) 0.0396(10) Uani 1 1 d . . .
C35 C 0.2459(6) 0.3053(5) 0.68864(17) 0.0627(15) Uani 1 1 d . . .
H35A H 0.2696 0.2691 0.6690 0.075 Uiso 1 1 calc R . .
C36 C 0.2570(7) 0.2867(7) 0.7295(2) 0.090(2) Uani 1 1 d . . .
H36A H 0.2857 0.2354 0.7371 0.109 Uiso 1 1 calc R . .
C37 C 0.2277(7) 0.3399(6) 0.75828(19) 0.080(2) Uani 1 1 d . . .
H37A H 0.2384 0.3279 0.7859 0.096 Uiso 1 1 calc R . .
C38 C 0.1834(6) 0.4100(6) 0.74767(16) 0.0668(18) Uani 1 1 d . . .
H38A H 0.1616 0.4466 0.7678 0.080 Uiso 1 1 calc R . .
C39 C 0.1692(5) 0.4291(5) 0.70739(14) 0.0493(12) Uani 1 1 d . . .
H39A H 0.1378 0.4787 0.7003 0.059 Uiso 1 1 calc R . .
C40 C 0.0877(5) 0.8541(5) 0.69871(15) 0.0461(12) Uani 1 1 d . . .
C41 C 0.1554(5) 0.9432(5) 0.67672(16) 0.0556(14) Uani 1 1 d . . .
H41A H 0.2407 0.9844 0.6833 0.067 Uiso 1 1 calc R . .
C42 C 0.1000(7) 0.9723(6) 0.64542(18) 0.0713(18) Uani 1 1 d . . .
H42A H 0.1470 1.0344 0.6309 0.086 Uiso 1 1 calc R . .
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C43 C -0.0236(8) 0.9113(9) 0.6351(2) 0.090(2) Uani 1 1 d . . .
H43A H -0.0616 0.9304 0.6131 0.108 Uiso 1 1 calc R . .
C44 C -0.0912(7) 0.8235(8) 0.6564(3) 0.092(2) Uani 1 1 d . . .
H44A H -0.1764 0.7816 0.6492 0.111 Uiso 1 1 calc R . .
C45 C -0.0366(6) 0.7955(6) 0.6883(2) 0.0712(17) Uani 1 1 d . . .
H45A H -0.0845 0.7353 0.7033 0.085 Uiso 1 1 calc R . .
C46 C 0.1740(4) 0.9325(4) 0.78330(14) 0.0408(10) Uani 1 1 d . . .
C47 C 0.2413(5) 0.9478(5) 0.82097(16) 0.0587(14) Uani 1 1 d . . .
H47A H 0.2765 0.9001 0.8260 0.070 Uiso 1 1 calc R . .
C48 C 0.2570(6) 1.0316(7) 0.85097(18) 0.0750(19) Uani 1 1 d . . .
H48A H 0.3028 1.0414 0.8767 0.090 Uiso 1 1 calc R . .
C49 C 0.2071(6) 1.1014(6) 0.84420(19) 0.0713(18) Uani 1 1 d . . .
H49A H 0.2199 1.1606 0.8649 0.086 Uiso 1 1 calc R . .
C50 C 0.1391(6) 1.0851(5) 0.8077(2) 0.0647(16) Uani 1 1 d . . .
H50A H 0.1028 1.1320 0.8032 0.078 Uiso 1 1 calc R . .
C51 C 0.1221(5) 1.0016(5) 0.77701(17) 0.0516(13) Uani 1 1 d . . .
H51A H 0.0747 0.9916 0.7516 0.062 Uiso 1 1 calc R . .
C52 C 0.0559(5) 0.6857(4) 0.75307(17) 0.0495(12) Uani 1 1 d . . .
C53 C 0.0158(7) 0.6652(6) 0.7898(2) 0.088(2) Uani 1 1 d . . .
H53A H 0.0464 0.7273 0.8114 0.105 Uiso 1 1 calc R . .
C54 C -0.0704(9) 0.5524(7) 0.7950(3) 0.122(4) Uani 1 1 d . . .
H54A H -0.0989 0.5376 0.8203 0.147 Uiso 1 1 calc R . .
C55 C -0.1139(8) 0.4628(7) 0.7640(3) 0.106(3) Uani 1 1 d . . .
H55A H -0.1750 0.3868 0.7672 0.127 Uiso 1 1 calc R . .
C56 C -0.0701(8) 0.4828(6) 0.7290(3) 0.102(3) Uani 1 1 d . . .
H56A H -0.0981 0.4198 0.7080 0.122 Uiso 1 1 calc R . .
C57 C 0.0146(7) 0.5930(5) 0.7231(2) 0.080(2) Uani 1 1 d . . .
H57A H 0.0449 0.6053 0.6981 0.096 Uiso 1 1 calc R . .
C58 C 0.5528(4) 1.1464(4) 0.77826(14) 0.0368(10) Uani 1 1 d . A .
C59 C 0.6644(5) 1.2085(5) 0.80163(15) 0.0489(12) Uani 1 1 d . . .
H59A H 0.7250 1.1895 0.7976 0.059 Uiso 1 1 calc R A .
C60 C 0.6896(6) 1.2991(5) 0.83118(17) 0.0617(15) Uani 1 1 d . A .
H60A H 0.7668 1.3409 0.8476 0.074 Uiso 1 1 calc R . .
C61 C 0.6025(6) 1.3286(5) 0.83673(18) 0.0621(16) Uani 1 1 d . . .
H61A H 0.6205 1.3924 0.8562 0.075 Uiso 1 1 calc R A .
C62 C 0.4914(6) 1.2661(5) 0.81423(17) 0.0554(14) Uani 1 1 d . A .
H62A H 0.4312 1.2857 0.8182 0.066 Uiso 1 1 calc R . .
C63 C 0.4652(5) 1.1747(5) 0.78569(16) 0.0477(12) Uani 1 1 d . . .
H63A H 0.3861 1.1301 0.7708 0.057 Uiso 1 1 calc R A .
C64 C 0.5109(4) 1.1046(4) 0.69187(14) 0.0404(10) Uani 1 1 d . A .
C65 C 0.4877(5) 1.0419(5) 0.65424(16) 0.0603(15) Uani 1 1 d . . .
H65A H 0.4712 0.9632 0.6526 0.072 Uiso 1 1 calc R A .
C66 C 0.4882(6) 1.0922(7) 0.6189(2) 0.081(2) Uani 1 1 d . A .
H66A H 0.4736 1.0490 0.5932 0.098 Uiso 1 1 calc R . .
C67 C 0.5100(7) 1.2052(8) 0.6215(2) 0.087(2) Uani 1 1 d . . .
H67A H 0.5100 1.2399 0.5973 0.104 Uiso 1 1 calc R A .
C68 C 0.5317(7) 1.2683(7) 0.6583(3) 0.083(2) Uani 1 1 d . A .
H68A H 0.5462 1.3462 0.6597 0.099 Uiso 1 1 calc R . .
C69 C 0.5324(6) 1.2186(5) 0.69358(19) 0.0604(15) Uani 1 1 d . . .
H69A H 0.5478 1.2628 0.7192 0.072 Uiso 1 1 calc R A .
C70 C 0.6625(6) 1.0404(9) 0.7348(3) 0.0728(11) Uani 0.50 1 d PGD A 1
C71 C 0.7545(7) 1.1334(7) 0.7203(3) 0.0728(11) Uani 0.50 1 d PG A 1
H71A H 0.7427 1.1945 0.7112 0.087 Uiso 0.50 1 calc PR A 1
C72 C 0.8637(6) 1.1370(7) 0.7190(3) 0.0728(11) Uani 0.50 1 d PG A 1
```

```
H72A H 0.9265 1.2006 0.7090 0.087 Uiso 0.50 1 calc PR A 1
C73 C 0.8809(6) 1.0476(8) 0.7323(3) 0.0728(11) Uani 0.50 1 d PG A 1
H73A H 0.9556 1.0501 0.7314 0.087 Uiso 0.50 1 calc PR A 1
C74 C 0.7890(7) 0.9546(7) 0.7468(3) 0.0728(11) Uani 0.50 1 d PG A 1
H74A H 0.8008 0.8935 0.7559 0.087 Uiso 0.50 1 calc PR A 1
C75 C 0.6798(6) 0.9510(7) 0.7481(3) 0.0728(11) Uani 0.50 1 d PG A 1
H75A H 0.6169 0.8874 0.7581 0.087 Uiso 0.50 1 calc PR A 1
C70A C 0.6486(7) 1.0221(9) 0.7397(3) 0.0728(11) Uani 0.50 1 d PGD A 2
C71A C 0.7357(8) 1.0687(8) 0.7147(3) 0.0728(11) Uani 0.50 1 d PG A 2
H71B H 0.7323 1.1190 0.6960 0.087 Uiso 0.50 1 calc PR A 2
C72A C 0.8279(7) 1.0419(9) 0.7172(3) 0.0728(11) Uani 0.50 1 d PG A 2
H72B H 0.8875 1.0738 0.7002 0.087 Uiso 0.50 1 calc PR A 2
C73A C 0.8330(7) 0.9685(9) 0.7446(3) 0.0728(11) Uani 0.50 1 d PG A 2
H73B H 0.8960 0.9502 0.7463 0.087 Uiso 0.50 1 calc PR A 2
C74A C 0.7458(7) 0.9218(8) 0.7696(3) 0.0728(11) Uani 0.50 1 d PG A 2
H74B H 0.7493 0.8716 0.7883 0.087 Uiso 0.50 1 calc PR A 2
C75A C 0.6536(7) 0.9486(9) 0.7671(3) 0.0728(11) Uani 0.50 1 d PG A 2
H75B H 0.5941 0.9167 0.7842 0.087 Uiso 0.50 1 calc PR A 2
C76 C 0.7142(4) 0.8244(4) 0.88893(13) 0.0381(10) Uani 1 1 d . . .
C77 C 0.8120(5) 0.9349(5) 0.88877(19) 0.0598(15) Uani 1 1 d . . .
H7B H 0.8158 1.0012 0.9030 0.072 Uiso 1 1 calc R . .
C78 C 0.9041(6) 0.9486(6) 0.8679(2) 0.0750(19) Uani 1 1 d . . .
H8B H 0.9699 1.0244 0.8673 0.090 Uiso 1 1 calc R . .
C79 C 0.9003(6) 0.8526(6) 0.8480(2) 0.078(2) Uani 1 1 d . . .
H9B H 0.9645 0.8618 0.8343 0.093 Uiso 1 1 calc R . .
C80 C 0.8044(5) 0.7442(6) 0.8479(2) 0.0644(16) Uani 1 1 d . . .
H80A H 0.8015 0.6784 0.8337 0.077 Uiso 1 1 calc R . .
C81 C 0.7111(4) 0.7288(5) 0.86838(15) 0.0466(12) Uani 1 1 d . . .
H81A H 0.6451 0.6527 0.8683 0.056 Uiso 1 1 calc R . .
C82 C 0.6705(4) 0.8002(4) 0.96986(13) 0.0369(10) Uani 1 1 d . . .
C83 C 0.6023(5) 0.7617(4) 1.00067(14) 0.0446(11) Uani 1 1 d . . .
H83A H 0.5192 0.7383 0.9956 0.054 Uiso 1 1 calc R . .
C84 C 0.6536(6) 0.7569(5) 1.03890(16) 0.0593(15) Uani 1 1 d . . .
H84A H 0.6059 0.7312 1.0598 0.071 Uiso 1 1 calc R . .
C85 C 0.7730(7) 0.7891(6) 1.04635(17) 0.0705(19) Uani 1 1 d . . .
H85A H 0.8080 0.7848 1.0724 0.085 Uiso 1 1 calc R . .
C86 C 0.8411(6) 0.8272(6) 1.01676(19) 0.0712(18) Uani 1 1 d . . .
H86A H 0.9240 0.8501 1.0222 0.085 Uiso 1 1 calc R . .
C87 C 0.7914(5) 0.8331(5) 0.97854(17) 0.0573(14) Uani 1 1 d . . .
H87A H 0.8406 0.8600 0.9581 0.069 Uiso 1 1 calc R . .
C88 C 0.5979(4) 0.9381(4) 0.92351(14) 0.0354(9) Uani 1 1 d . . .
C89 C 0.6132(6) 1.0013(5) 0.95965(16) 0.0601(15) Uani 1 1 d . . .
H89A H 0.6349 0.9786 0.9843 0.072 Uiso 1 1 calc R . .
C90 C 0.5979(7) 1.0979(6) 0.9609(2) 0.078(2) Uani 1 1 d . . .
H90A H 0.6082 1.1404 0.9864 0.094 Uiso 1 1 calc R . .
C91 C 0.5679(6) 1.1324(5) 0.9259(2) 0.0639(16) Uani 1 1 d . . .
H91A H 0.5564 1.1983 0.9269 0.077 Uiso 1 1 calc R . .
C92 C 0.5546(5) 1.0728(5) 0.88962(19) 0.0561(14) Uani 1 1 d . . .
H92A H 0.5347 1.0974 0.8651 0.067 Uiso 1 1 calc R . .
C94 C 0.5701(5) 0.9760(4) 0.88822(16) 0.0501(12) Uani 1 1 d . . .
H94A H 0.5616 0.9351 0.8626 0.060 Uiso 1 1 calc R . .
C95 C 0.1141(4) 0.4472(4) 0.89996(14) 0.0400(10) Uani 1 1 d . . .
C96 C 0.0972(5) 0.4157(5) 0.85882(17) 0.0569(14) Uani 1 1 d . . .
H96A H 0.1510 0.4680 0.8428 0.068 Uiso 1 1 calc R . .
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C97 C 0.0023(6) 0.3083(6) 0.8403(2) 0.0694(17) Uani 1 1 d . . .
H97A H -0.0084 0.2875 0.8118 0.083 Uiso 1 1 calc R . .
C98 C -0.0748(6) 0.2333(5) 0.8628(2) 0.0711(19) Uani 1 1 d . . .
H98A H -0.1392 0.1597 0.8501 0.085 Uiso 1 1 calc R . .
C99 C -0.0606(6) 0.2632(5) 0.9042(2) 0.0733(19) Uani 1 1 d . . .
H99A H -0.1158 0.2107 0.9198 0.088 Uiso 1 1 calc R . .
C100 C 0.0339(5) 0.3691(5) 0.92279(18) 0.0569(14) Uani 1 1 d . . .
H10H H 0.0445 0.3890 0.9513 0.068 Uiso 1 1 calc R . .
C101 C 0.2633(4) 0.5632(4) 0.97532(13) 0.0335(9) Uani 1 1 d . . .
C102 C 0.2169(5) 0.5938(5) 1.00647(16) 0.0507(13) Uani 1 1 d . . .
H10E H 0.1712 0.6317 1.0012 0.061 Uiso 1 1 calc R . .
C103 C 0.2376(6) 0.5685(6) 1.04552(17) 0.0653(16) Uani 1 1 d . . .
H10B H 0.2059 0.5897 1.0667 0.078 Uiso 1 1 calc R . .
C104 C 0.3028(6) 0.5136(5) 1.05380(16) 0.0626(16) Uani 1 1 d . . .
H10A H 0.3154 0.4957 1.0805 0.075 Uiso 1 1 calc R . .
C105 C 0.3496(6) 0.4847(5) 1.02334(17) 0.0593(15) Uani 1 1 d . . .
H10D H 0.3963 0.4479 1.0290 0.071 Uiso 1 1 calc R . .
C106 C 0.3297(5) 0.5087(4) 0.98441(15) 0.0466(12) Uani 1 1 d . . .
H10G H 0.3622 0.4873 0.9635 0.056 Uiso 1 1 calc R . .
C107 C 0.1793(4) 0.6861(4) 0.92535(14) 0.0397(10) Uani 1 1 d . . .
C108 C 0.0589(5) 0.6484(5) 0.9257(2) 0.076(2) Uani 1 1 d . . .
H10F H 0.0027 0.5671 0.9221 0.091 Uiso 1 1 calc R . .
C109 C 0.0191(7) 0.7280(7) 0.9313(3) 0.100(3) Uani 1 1 d . . .
H10C H -0.0640 0.7008 0.9315 0.121 Uiso 1 1 calc R . .
C110 C 0.0986(7) 0.8446(6) 0.9367(2) 0.079(2) Uani 1 1 d . . .
H11A H 0.0709 0.8988 0.9404 0.094 Uiso 1 1 calc R . .
C111 C 0.2175(6) 0.8839(5) 0.93667(18) 0.0631(16) Uani 1 1 d . . .
H11C H 0.2733 0.9654 0.9408 0.076 Uiso 1 1 calc R . .
C112 C 0.2569(5) 0.8041(4) 0.93061(15) 0.0465(11) Uani 1 1 d . . .
H11B H 0.3400 0.8322 0.9301 0.056 Uiso 1 1 calc R . .

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Cu2 0.0423(3) 0.0308(3) 0.0468(3) 0.0069(2) 0.0090(2) 0.0223(3)
Cu3 0.0406(3) 0.0311(3) 0.0297(3) 0.0017(2) 0.0091(2) 0.0182(2)
S1 0.0569(7) 0.0366(6) 0.0217(5) 0.0028(4) 0.0016(4) 0.0300(6)
S2 0.0599(7) 0.0465(7) 0.0246(5) 0.0049(4) 0.0092(5) 0.0379(6)
S3 0.0861(10) 0.0791(10) 0.0430(7) 0.0098(7) 0.0101(7) 0.0696(9)
P1 0.0314(5) 0.0305(6) 0.0223(5) 0.0021(4) 0.0021(4) 0.0125(5)
P2 0.0322(5) 0.0276(6) 0.0286(5) 0.0012(4) 0.0008(4) 0.0115(5)
P3 0.0420(6) 0.0365(7) 0.0461(7) 0.0072(5) 0.0121(5) 0.0230(6)
P4 0.0359(6) 0.0294(6) 0.0369(6) 0.0023(5) 0.0022(5) 0.0196(5)
P5 0.0385(6) 0.0279(6) 0.0317(5) 0.0040(4) 0.0082(4) 0.0170(5)
P6 0.0356(6) 0.0308(6) 0.0331(5) 0.0044(4) 0.0078(4) 0.0165(5)
N1 0.0419(19) 0.0288(18) 0.0230(16) 0.0039(13) 0.0039(14) 0.0219(16)
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N2 0.052(2) 0.037(2) 0.0248(17) 0.0067(15) 0.0053(16) 0.0311(19)
N3 0.046(2) 0.037(2) 0.0244(17) 0.0014(15) 0.0057(15) 0.0285(18)
C1 0.036(2) 0.026(2) 0.0241(18) 0.0014(15) 0.0026(16) 0.0167(18)
C2 0.049(3) 0.035(2) 0.029(2) 0.0027(17) 0.0026(18) 0.028(2)
C3 0.040(2) 0.023(2) 0.0226(18) 0.0008(15) 0.0006(16) 0.0153(18)
C4 0.034(2) 0.032(2) 0.031(2) 0.0076(17) 0.0070(17) 0.0138(19)
C5 0.071(4) 0.052(3) 0.040(3) -0.001(2) 0.003(2) 0.039(3)
C6 0.085(4) 0.067(4) 0.076(4) 0.005(3) 0.016(4) 0.056(4)
C7 0.045(3) 0.061(4) 0.096(5) 0.018(4) 0.007(3) 0.031(3)
C8 0.052(3) 0.066(4) 0.065(4) 0.002(3) -0.018(3) 0.031(3)
C9 0.050(3) 0.059(3) 0.037(3) -0.005(2) -0.005(2) 0.029(3)
C10 0.038(2) 0.035(2) 0.027(2) 0.0038(17) 0.0048(17) 0.020(2)
C11 0.052(3) 0.046(3) 0.055(3) -0.004(2) 0.019(2) 0.014(3)
C12 0.068(4) 0.069(4) 0.059(4) -0.004(3) 0.032(3) 0.028(3)
C13 0.068(4) 0.064(4) 0.041(3) -0.010(3) 0.005(3) 0.039(3)
C14 0.062(3) 0.045(3) 0.057(3) -0.015(3) 0.014(3) 0.008(3)
C15 0.054(3) 0.049(3) 0.046(3) -0.007(2) 0.019(2) 0.011(3)
C16 0.031(2) 0.035(2) 0.038(2) 0.0023(19) 0.0038(18) 0.0143(19)
C17 0.038(3) 0.044(3) 0.056(3) 0.006(2) -0.005(2) 0.010(2)
C18 0.043(3) 0.062(4) 0.082(5) 0.002(3) -0.011(3) 0.005(3)
C19 0.044(3) 0.049(4) 0.107(6) 0.020(4) 0.009(3) 0.006(3)
C20 0.055(3) 0.046(3) 0.077(4) 0.026(3) 0.017(3) 0.017(3)
C21 0.044(3) 0.042(3) 0.051(3) 0.015(2) 0.005(2) 0.016(2)
C22 0.036(2) 0.042(3) 0.030(2) -0.0014(19) -0.0010(17) 0.016(2)
C23 0.042(3) 0.053(3) 0.051(3) 0.010(2) 0.007(2) 0.018(2)
C24 0.037(3) 0.078(5) 0.067(4) -0.004(3) 0.007(3) 0.012(3)
C25 0.048(3) 0.102(6) 0.074(4) 0.012(4) 0.005(3) 0.045(4)
C26 0.066(4) 0.085(5) 0.079(4) 0.023(4) 0.008(3) 0.052(4)
C27 0.045(3) 0.055(3) 0.049(3) 0.013(2) 0.007(2) 0.028(3)
C28 0.040(2) 0.032(2) 0.035(2) 0.0021(18) -0.0004(18) 0.015(2)
C29 0.057(4) 0.051(4) 0.107(5) -0.037(4) 0.018(4) 0.011(3)
C30 0.084(5) 0.063(5) 0.113(6) -0.031(4) 0.021(4) 0.033(4)
C31 0.090(5) 0.048(4) 0.056(3) -0.012(3) -0.008(3) 0.042(4)
C32 0.072(4) 0.043(3) 0.065(4) -0.017(3) -0.015(3) 0.016(3)
C33 0.052(3) 0.048(3) 0.063(4) -0.015(3) -0.002(3) 0.015(3)
C34 0.037(2) 0.033(2) 0.033(2) 0.0029(18) -0.0030(18) 0.008(2)
C35 0.082(4) 0.060(4) 0.049(3) 0.009(3) -0.004(3) 0.040(3)
C36 0.116(6) 0.079(5) 0.076(5) 0.030(4) -0.016(4) 0.052(5)
C37 0.095(5) 0.065(4) 0.040(3) 0.019(3) -0.008(3) 0.011(4)
C38 0.071(4) 0.060(4) 0.036(3) 0.006(3) 0.004(3) 0.007(3)
C39 0.053(3) 0.046(3) 0.034(2) 0.006(2) 0.008(2) 0.013(2)
C40 0.049(3) 0.052(3) 0.045(3) -0.001(2) 0.005(2) 0.032(3)
C41 0.055(3) 0.065(4) 0.050(3) 0.010(3) 0.008(2) 0.033(3)
C42 0.093(5) 0.090(5) 0.046(3) 0.018(3) 0.015(3) 0.055(4)
C43 0.099(6) 0.139(8) 0.060(4) 0.011(5) -0.003(4) 0.083(6)
C44 0.060(4) 0.114(7) 0.099(6) 0.009(5) -0.012(4) 0.046(5)
C45 0.056(4) 0.083(5) 0.077(4) 0.013(4) 0.007(3) 0.036(4)
C46 0.043(2) 0.040(3) 0.041(2) 0.006(2) 0.014(2) 0.020(2)
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C49 0.088(5) 0.063(4) 0.055(4) -0.007(3) 0.030(3) 0.029(4)
C50 0.086(4) 0.054(4) 0.072(4) 0.013(3) 0.037(4) 0.043(3)
C51 0.062(3) 0.056(3) 0.049(3) 0.010(2) 0.016(2) 0.038(3)
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C78 0.062(4) 0.057(4) 0.112(6) 0.026(4) 0.045(4) 0.027(3)
C79 0.074(4) 0.080(5) 0.102(5) 0.030(4) 0.055(4) 0.046(4)
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C81 0.043(3) 0.046(3) 0.051(3) 0.002(2) 0.009(2) 0.023(2)
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C83 0.055(3) 0.043(3) 0.042(3) 0.004(2) 0.005(2) 0.030(2)
C84 0.089(4) 0.062(4) 0.040(3) 0.004(3) 0.011(3) 0.048(4)
C85 0.101(5) 0.090(5) 0.040(3) -0.007(3) -0.010(3) 0.068(4)
C86 0.061(4) 0.096(5) 0.059(4) 0.001(3) -0.010(3) 0.046(4)
C87 0.057(3) 0.069(4) 0.050(3) 0.005(3) 0.003(3) 0.036(3)
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C96 0.049(3) 0.054(4) 0.053(3) -0.003(3) 0.000(2) 0.017(3)
C97 0.061(4) 0.069(4) 0.060(4) -0.015(3) -0.014(3) 0.025(3)
C98 0.061(4) 0.037(3) 0.094(5) -0.001(3) -0.023(4) 0.016(3)
C99 0.066(4) 0.035(3) 0.096(5) 0.018(3) 0.003(4) 0.009(3)
C100 0.058(3) 0.038(3) 0.060(3) 0.007(2) 0.007(3) 0.012(3)
C101 0.039(2) 0.028(2) 0.032(2) 0.0048(17) 0.0075(17) 0.0154(19)

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C104 0.097(5) 0.044(3) 0.039(3) 0.012(2) 0.006(3) 0.029(3)
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C106 0.066(3) 0.042(3) 0.043(3) 0.009(2) 0.012(2) 0.033(3)
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C109 0.063(4) 0.070(5) 0.187(9) 0.011(5) 0.017(5) 0.048(4)
C110 0.087(5) 0.063(4) 0.112(6) 0.018(4) 0.013(4) 0.058(4)
C111 0.089(5) 0.036(3) 0.068(4) 0.007(3) 0.005(3) 0.036(3)
C112 0.053(3) 0.041(3) 0.049(3) 0.008(2) 0.007(2) 0.025(2)

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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 P1 2.2696(11) . ?
Cu1 P2 2.2926(12) . ?
Cu1 S1 2.3946(11) . ?
Cu2 N1 2.080(3) . ?
Cu2 P3 2.2340(13) . ?
Cu2 P4 2.2762(13) . ?
Cu2 S1 2.7694(12) . ?
Cu3 P6 2.2858(12) . ?
Cu3 P5 2.2966(13) . ?
Cu3 S2 2.4226(12) . ?
S1 C3 1.693(4) . ?
S2 C1 1.672(4) . ?
S3 C2 1.631(4) . ?
P1 C10 1.824(4) . ?
P1 C4 1.831(4) . ?
P1 C16 1.833(5) . ?
P2 C34 1.814(5) . ?
P2 C22 1.827(5) . ?
P2 C28 1.837(5) . ?
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P3 C40 1.824(5) . ?
P3 C46 1.827(5) . ?
P4 C70A 1.785(5) . ?
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P5 C82 1.831(5) . ?
P6 C101 1.822(4) . ?
P6 C107 1.823(5) . ?
P6 C95 1.832(5) . ?
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N2 C2 1.370(5) . ?
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N3 C2 1.373(5) . ?
N3 H3N 0.853(19) . ?
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C4 C5 1.382(6) . ?
C5 C6 1.383(7) . ?
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C6 C7 1.356(9) . ?
C6 H6A 0.9500 . ?
C7 C8 1.356(9) . ?
C7 H7A 0.9500 . ?
C8 C9 1.377(7) . ?
C8 H8A 0.9500 . ?
C9 H9A 0.9500 . ?
C10 C11 1.367(6) . ?
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C11 C12 1.387(7) . ?
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C12 C13 1.360(8) . ?
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C23 C24 1.382(8) . ?
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C88 C89 C90 121.1(5) . . ?
C88 C89 H89A 119.5 . . ?
C90 C89 H89A 119.5 . . ?
C91 C90 C89 120.3(6) . . ?
C91 C90 H90A 119.9 . . ?
C89 C90 H90A 119.9 . . ?
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C91 C92 C94 119.9(5) . . ?
C91 C92 H92A 120.0 . . ?
C94 C92 H92A 120.0 . . ?
C88 C94 C92 120.9(5) . . ?
C88 C94 H94A 119.5 . . ?
C92 C94 H94A 119.5 . . ?
C96 C95 C100 118.6(5) . . ?
C96 C95 P6 118.8(4) . . ?
C100 C95 P6 122.6(4) . . ?
C95 C96 C97 120.8(6) . . ?
C95 C96 H96A 119.6 . . ?
C97 C96 H96A 119.6 . . ?
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C97 C98 H98A 119.8 . . ?
C99 C98 H98A 119.8 . . ?
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C95 C100 H10H 119.9 . . ?
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C106 C101 P6 117.1(3) . . ?
C102 C101 P6 124.7(4) . . ?
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C101 C102 H10E 120.1 . . ?
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C104 C103 C102 121.1(5) . . ?
C104 C103 H10B 119.5 . . ?
C102 C103 H10B 119.5 . . ?
C105 C104 C103 119.3(5) . . ?
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C103 C104 H10A 120.4 . . ?
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C104 C105 H10D 119.8 . . ?
C106 C105 H10D 119.8 . . ?
C101 C106 C105 121.2(5) . . ?
C101 C106 H10G 119.4 . . ?
C105 C106 H10G 119.4 . . ?
C112 C107 C108 117.5(5) . . ?
C112 C107 P6 118.2(4) . . ?
C108 C107 P6 124.0(4) . . ?
C107 C108 C109 120.8(6) . . ?
C107 C108 H10F 119.6 . . ?
C109 C108 H10F 119.6 . . ?
C110 C109 C108 120.2(6) . . ?
C110 C109 H10C 119.9 . . ?
C108 C109 H10C 119.9 . . ?
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C111 C110 H11A 119.9 . . ?
C109 C110 H11A 119.9 . . ?
C110 C111 C112 119.5(6) . . ?
C110 C111 H11C 120.3 . . ?
C112 C111 H11C 120.3 . . ?
C107 C112 C111 121.8(5) . . ?
C107 C112 H11B 119.1 . . ?
C111 C112 H11B 119.1 . . ?

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P4 Cu2 S1 C3 105.75(16) . . . . ?
P6 Cu3 S2 C1 -142.46(17) . . . . ?
P5 Cu3 S2 C1 86.65(17) . . . . ?
Br2 Cu3 S2 C1 -32.57(17) . . . . ?
P2 Cu1 P1 C10 -54.73(16) . . . . ?
S1 Cu1 P1 C10 -177.38(15) . . . . ?
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S1 Cu1 P1 C4 -58.21(17) . . . . ?
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S1 Cu1 P1 C16 60.61(17) . . . . ?
Br1 Cu1 P1 C16 -52.96(17) . . . . ?
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S1 Cu1 P2 C34 -50.38(18) . . . . ?
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S1 Cu1 P2 C28 -169.78(16) . . . . ?
Br1 Cu1 P2 C28 -59.54(16) . . . . ?
N1 Cu2 P3 C52 -7.6(2) . . . . ?
P4 Cu2 P3 C52 -169.1(2) . . . . ?
S1 Cu2 P3 C52 64.4(2) . . . . ?
N1 Cu2 P3 C40 -130.3(2) . . . . ?
P4 Cu2 P3 C40 68.2(2) . . . . ?
S1 Cu2 P3 C40 -58.3(2) . . . . ?
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S1 Cu2 P3 C46 -175.56(17) . . . . ?
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P3 Cu2 P4 C64 -65.53(19) . . . . ?
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S1 Cu2 P4 C70 -48.0(4) . . . . ?
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S2 Cu3 P5 C76 -65.64(17) . . . . ?
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S2 Cu3 P5 C82 171.76(17) . . . . ?
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S2 Cu3 P6 C101 -166.91(16) . . . . ?
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S2 Cu3 P6 C107 -45.63(18) . . . . ?
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P5 Cu3 P6 C95 -165.78(17) . . . . ?
S2 Cu3 P6 C95 76.53(17) . . . . ?
Br2 Cu3 P6 C95 -37.17(17) . . . . ?
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P4 Cu2 N1 C3 -78.3(3) . . . . ?
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P4 Cu2 N1 C1 90.6(4) . . . . ?
S1 Cu2 N1 C1 178.9(4) . . . . ?
C3 N1 C1 N2 7.0(6) . . . . ?
Cu2 N1 C1 N2 -160.8(3) . . . . ?
C3 N1 C1 S2 -171.9(3) . . . . ?
Cu2 N1 C1 S2 20.3(6) . . . . ?
C2 N2 C1 N1 1.4(7) . . . . ?
C2 N2 C1 S2 -179.7(4) . . . . ?
Cu3 S2 C1 N1 -175.7(3) . . . . ?
Cu3 S2 C1 N2 5.4(4) . . . . ?
C1 N2 C2 N3 -6.9(6) . . . . ?
C1 N2 C2 S3 174.2(4) . . . . ?
C3 N3 C2 N2 4.6(6) . . . . ?
C3 N3 C2 S3 -176.5(4) . . . . ?
C1 N1 C3 N3 -9.2(6) . . . . ?
Cu2 N1 C3 N3 161.7(3) . . . . ?
C1 N1 C3 S1 172.5(3) . . . . ?
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C2 N3 C3 S1 -178.6(3) . . . . ?
Cu1 S1 C3 N1 -159.2(3) . . . . ?
Cu2 S1 C3 N1 12.5(3) . . . . ?
Cu1 S1 C3 N3 22.6(4) . . . . ?
Cu2 S1 C3 N3 -165.7(4) . . . . ?
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C16 P1 C4 C9 105.8(4) . . . . ?
Cu1 P1 C4 C9 -126.9(4) . . . . ?
C10 P1 C4 C5 177.8(4) . . . . ?
C16 P1 C4 C5 -74.2(4) . . . . ?
Cu1 P1 C4 C5 53.1(4) . . . . ?
C9 C4 C5 C6 -0.6(8) . . . . ?
P1 C4 C5 C6 179.3(5) . . . . ?
C4 C5 C6 C7 1.5(10) . . . . ?
C5 C6 C7 C8 -1.9(10) . . . . ?
C6 C7 C8 C9 1.4(10) . . . . ?
C7 C8 C9 C4 -0.6(9) . . . . ?
C5 C4 C9 C8 0.2(8) . . . . ?
P1 C4 C9 C8 -179.8(4) . . . . ?
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C16 P1 C10 C15 -178.1(4) . . . . ?
Cu1 P1 C10 C15 53.6(4) . . . . ?
C15 C10 C11 C12 1.4(8) . . . . ?
P1 C10 C11 C12 -179.6(5) . . . . ?
C10 C11 C12 C13 -0.1(10) . . . . ?
C11 C12 C13 C14 -1.0(10) . . . . ?
C12 C13 C14 C15 0.7(10) . . . . ?
C11 C10 C15 C14 -1.7(8) . . . . ?
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C13 C14 C15 C10 0.6(10) . . . . ?
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C4 P1 C16 C21 -45.9(4) . . . . ?
Cu1 P1 C16 C21 -173.7(4) . . . . ?
C10 P1 C16 C17 -122.7(4) . . . . ?
C4 P1 C16 C17 131.4(4) . . . . ?
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C21 C16 C17 C18 0.1(8) . . . . ?
P1 C16 C17 C18 -177.3(5) . . . . ?
C16 C17 C18 C19 -0.3(10) . . . . ?
C17 C18 C19 C20 -0.8(11) . . . . ?
C18 C19 C20 C21 2.1(11) . . . . ?
C19 C20 C21 C16 -2.3(9) . . . . ?
C17 C16 C21 C20 1.2(8) . . . . ?
P1 C16 C21 C20 178.5(4) . . . . ?
C34 P2 C22 C27 134.6(4) . . . . ?
C28 P2 C22 C27 -117.1(4) . . . . ?
Cu1 P2 C22 C27 12.1(4) . . . . ?
C34 P2 C22 C23 -42.8(5) . . . . ?
C28 P2 C22 C23 65.6(4) . . . . ?
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Cu1 P2 C22 C23 -165.2(4) . . . . ?
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P2 C22 C23 C24 178.6(4) . . . . ?
C22 C23 C24 C25 -0.3(9) . . . . ?
C23 C24 C25 C26 -1.0(10) . . . . ?
C24 C25 C26 C27 1.4(10) . . . . ?
C23 C22 C27 C26 -0.9(8) . . . . ?
P2 C22 C27 C26 -178.4(4) . . . . ?
C25 C26 C27 C22 -0.4(9) . . . . ?
C34 P2 C28 C29 -97.1(5) . . . . ?
C22 P2 C28 C29 156.1(5) . . . . ?
Cu1 P2 C28 C29 27.0(5) . . . . ?
C34 P2 C28 C33 85.3(5) . . . . ?
C22 P2 C28 C33 -21.5(5) . . . . ?
Cu1 P2 C28 C33 -150.6(4) . . . . ?
C33 C28 C29 C30 -0.6(11) . . . . ?
P2 C28 C29 C30 -178.4(6) . . . . ?
C28 C29 C30 C31 1.3(13) . . . . ?
C29 C30 C31 C32 -1.6(12) . . . . ?
C30 C31 C32 C33 1.3(11) . . . . ?
C29 C28 C33 C32 0.2(9) . . . . ?
P2 C28 C33 C32 177.8(5) . . . . ?
C31 C32 C33 C28 -0.6(10) . . . . ?
C22 P2 C34 C35 140.8(5) . . . . ?
C28 P2 C34 C35 31.3(5) . . . . ?
Cu1 P2 C34 C35 -94.7(4) . . . . ?
C22 P2 C34 C39 -46.2(4) . . . . ?
C28 P2 C34 C39 -155.8(4) . . . . ?
Cu1 P2 C34 C39 78.2(4) . . . . ?
C39 C34 C35 C36 1.2(9) . . . . ?
P2 C34 C35 C36 174.1(5) . . . . ?
C34 C35 C36 C37 -2.2(11) . . . . ?
C35 C36 C37 C38 2.0(12) . . . . ?
C36 C37 C38 C39 -0.9(10) . . . . ?
C35 C34 C39 C38 -0.1(8) . . . . ?
P2 C34 C39 C38 -173.4(4) . . . . ?
C37 C38 C39 C34 0.0(9) . . . . ?
C52 P3 C40 C45 21.0(5) . . . . ?
C46 P3 C40 C45 -88.5(5) . . . . ?
Cu2 P3 C40 C45 150.1(4) . . . . ?
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C46 P3 C40 C41 85.8(4) . . . . ?
Cu2 P3 C40 C41 -35.5(5) . . . . ?
C45 C40 C41 C42 0.1(9) . . . . ?
P3 C40 C41 C42 -174.5(5) . . . . ?
C40 C41 C42 C43 -1.3(10) . . . . ?
C41 C42 C43 C44 1.3(12) . . . . ?
C42 C43 C44 C45 0.0(13) . . . . ?
C43 C44 C45 C40 -1.2(12) . . . . ?
C41 C40 C45 C44 1.1(10) . . . . ?
P3 C40 C45 C44 175.5(6) . . . . ?
C52 P3 C46 C51 -105.0(5) . . . . ?
C40 P3 C46 C51 2.7(5) . . . . ?
Cu2 P3 C46 C51 128.7(4) . . . . ?
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C52 P3 C46 C47 79.6(5) . . . . ?
C40 P3 C46 C47 -172.6(4) . . . . ?
Cu2 P3 C46 C47 -46.7(5) . . . . ?
C51 C46 C47 C48 -1.0(9) . . . . ?
P3 C46 C47 C48 174.5(5) . . . . ?
C46 C47 C48 C49 -0.2(10) . . . . ?
C47 C48 C49 C50 1.6(10) . . . . ?
C48 C49 C50 C51 -1.6(10) . . . . ?
C49 C50 C51 C46 0.4(9) . . . . ?
C47 C46 C51 C50 1.0(8) . . . . ?
P3 C46 C51 C50 -174.4(4) . . . . ?
C40 P3 C52 C57 60.2(6) . . . . ?
C46 P3 C52 C57 167.6(5) . . . . ?
Cu2 P3 C52 C57 -69.7(6) . . . . ?
C40 P3 C52 C53 -122.4(6) . . . . ?
C46 P3 C52 C53 -14.9(6) . . . . ?
Cu2 P3 C52 C53 107.7(6) . . . . ?
C57 C52 C53 C54 -3.4(12) . . . . ?
P3 C52 C53 C54 179.2(7) . . . . ?
C52 C53 C54 C55 0.4(15) . . . . ?
C53 C54 C55 C56 2.7(16) . . . . ?
C54 C55 C56 C57 -2.7(16) . . . . ?
C55 C56 C57 C52 -0.3(14) . . . . ?
C53 C52 C57 C56 3.4(11) . . . . ?
P3 C52 C57 C56 -179.0(7) . . . . ?
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C64 P4 C58 C59 -105.2(4) . . . . ?
C70 P4 C58 C59 -4.7(5) . . . . ?
Cu2 P4 C58 C59 127.1(4) . . . . ?
C70A P4 C58 C63 -177.9(5) . . . . ?
C64 P4 C58 C63 72.4(4) . . . . ?
C70 P4 C58 C63 173.0(5) . . . . ?
Cu2 P4 C58 C63 -55.3(4) . . . . ?
C63 C58 C59 C60 -1.6(8) . . . . ?
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C61 C62 C63 C58 -2.1(9) . . . . ?
C59 C58 C63 C62 3.2(8) . . . . ?
P4 C58 C63 C62 -174.6(4) . . . . ?
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C58 P4 C64 C65 178.0(4) . . . . ?
C70 P4 C64 C65 73.6(5) . . . . ?
Cu2 P4 C64 C65 -54.1(4) . . . . ?
C70A P4 C64 C69 -108.0(6) . . . . ?
C58 P4 C64 C69 -0.4(5) . . . . ?
C70 P4 C64 C69 -104.8(5) . . . . ?
Cu2 P4 C64 C69 127.5(4) . . . . ?
C69 C64 C65 C66 1.3(9) . . . . ?
P4 C64 C65 C66 -177.2(5) . . . . ?
C64 C65 C66 C67 -1.2(10) . . . . ?
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C66 C67 C68 C69 0.3(12) . . . . ?
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C58 P4 C70 C71 -71.9(5) . . . . ?
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C71 C72 C73 C74 0.0 . . . . ?
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C71 C70 C75 C74 0.0 . . . . ?
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C82 P5 C76 C77 -78.7(5) . . . . ?
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P5 C76 C77 C78 174.5(5) . . . . ?
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C77 C78 C79 C80 1.7(12) . . . . ?
C78 C79 C80 C81 -1.2(11) . . . . ?
C77 C76 C81 C80 -0.3(8) . . . . ?
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C79 C80 C81 C76 0.5(9) . . . . ?
C76 P5 C82 C83 -167.8(4) . . . . ?
C88 P5 C82 C83 85.3(4) . . . . ?
Cu3 P5 C82 C83 -39.1(4) . . . . ?
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C88 P5 C82 C87 -97.6(5) . . . . ?
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C83 C82 C87 C86 0.1(8) . . . . ?
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C76 P5 C88 C89 -124.3(5) . . . . ?
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C76 P5 C88 C94 62.2(4) . . . . ?
C82 P5 C88 C94 167.4(4) . . . . ?
Cu3 P5 C88 C94 -61.1(4) . . . . ?
C94 C88 C89 C90 2.0(9) . . . . ?
P5 C88 C89 C90 -171.6(5) . . . . ?
C88 C89 C90 C91 -0.6(11) . . . . ?
C89 C90 C91 C92 -0.8(11) . . . . ?
C90 C91 C92 C94 0.7(10) . . . . ?
C89 C88 C94 C92 -2.1(8) . . . . ?
P5 C88 C94 C92 171.9(4) . . . . ?
C91 C92 C94 C88 0.7(9) . . . . ?
C101 P6 C95 C96 -156.6(4) . . . . ?
C107 P6 C95 C96 96.1(4) . . . . ?
Cu3 P6 C95 C96 -32.5(5) . . . . ?
C101 P6 C95 C100 22.4(5) . . . . ?
C107 P6 C95 C100 -84.9(5) . . . . ?
Cu3 P6 C95 C100 146.5(4) . . . . ?
C100 C95 C96 C97 0.0(8) . . . . ?
P6 C95 C96 C97 179.0(5) . . . . ?
C95 C96 C97 C98 0.0(10) . . . . ?
C96 C97 C98 C99 0.5(10) . . . . ?
C97 C98 C99 C100 -1.1(10) . . . . ?
C98 C99 C100 C95 1.1(10) . . . . ?
C96 C95 C100 C99 -0.5(8) . . . . ?
P6 C95 C100 C99 -179.5(5) . . . . ?
C107 P6 C101 C106 -168.9(4) . . . . ?
C95 P6 C101 C106 83.2(4) . . . . ?
Cu3 P6 C101 C106 -40.7(4) . . . . ?
C107 P6 C101 C102 11.5(5) . . . . ?
C95 P6 C101 C102 -96.4(5) . . . . ?
Cu3 P6 C101 C102 139.7(4) . . . . ?
C106 C101 C102 C103 -0.3(8) . . . . ?
P6 C101 C102 C103 179.2(4) . . . . ?
C101 C102 C103 C104 -0.2(9) . . . . ?
C102 C103 C104 C105 0.9(10) . . . . ?
C103 C104 C105 C106 -1.2(10) . . . . ?
C102 C101 C106 C105 0.1(8) . . . . ?
P6 C101 C106 C105 -179.5(4) . . . . ?
C104 C105 C106 C101 0.7(9) . . . . ?
C101 P6 C107 C112 91.9(4) . . . . ?
C95 P6 C107 C112 -162.5(4) . . . . ?
Cu3 P6 C107 C112 -35.2(4) . . . . ?
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C101 P6 C107 C108 -82.5(6) . . . . ?
C95 P6 C107 C108 23.1(6) . . . . ?
Cu3 P6 C107 C108 150.4(5) . . . . ?
C112 C107 C108 C109 -0.2(10) . . . . ?
P6 C107 C108 C109 174.2(6) . . . . ?
C107 C108 C109 C110 -0.1(13) . . . . ?
C108 C109 C110 C111 -0.3(14) . . . . ?
C109 C110 C111 C112 1.0(11) . . . . ?
C108 C107 C112 C111 0.9(8) . . . . ?
P6 C107 C112 C111 -173.9(4) . . . . ?
C110 C111 C112 C107 -1.3(9) . . . . ?

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
N2 H2N Br2  0.849(19) 2.60(2) 3.424(4) 164(4) .
N3 H3N Br1  0.853(19) 2.37(2) 3.223(3) 175(4) .

_diffrn_measured_fraction_theta_max    0.998
_diffrn_reflns_theta_full              25.00
_diffrn_measured_fraction_theta_full   0.998
_refine_diff_density_max    1.529
_refine_diff_density_min   -1.227
_refine_diff_density_rms    0.087


#===end
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