

Supplementary material:

Least-squares planes (x,y,z in crystal coordinates) and deviations
from them (* indicates atom used to define plane)

- 18.3899 (0.0145) x + 5.0321 (0.0144) y + 15.0829 (0.0107) z = 2.6898
(0.0044)

- * 0.0665 (0.0014) O1A
- * 0.0629 (0.0013) N1A
- * -0.0771 (0.0016) N2A
- * -0.0523 (0.0011) N3B_\$5
- 0.1366 (0.0014) Cu1

Rms deviation of fitted atoms = 0.0653

- 10.7592 (0.0199) x + 4.7543 (0.0138) y - 10.7746 (0.0148) z = 0.6580
(0.0049)

Angle to previous plane (with approximate esd) = 88.30 (0.06)

- * -0.0802 (0.0013) O1B
- * 0.0619 (0.0010) N3A
- * -0.0751 (0.0013) N1B
- * 0.0934 (0.0016) N2B
- 0.0745 (0.0014) Cu2

Rms deviation of fitted atoms = 0.0785