

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

$$1) \quad 8.649 \text{ (0.018)} \quad x - 1.568 \text{ (0.024)} \quad y + 3.045 \text{ (0.046)} \quad z = 9.822 \text{ (0.022)}$$

\* 0.000 (0.000) N1  
 \* 0.000 (0.000) H11  
 \* 0.000 (0.000) H12

Rms deviation of fitted atoms = 0.000

$$2) \quad 6.975 \text{ (0.004)} \quad x - 2.788 \text{ (0.002)} \quad y + 5.589 \text{ (0.006)} \quad z = 8.133 \text{ (0.005)}$$

Angle to previous plane (with approximate esd) = 19.29 ( 0.34 )

\* 0.012 (0.001) C1  
 \* -0.015 (0.001) C2  
 \* 0.005 (0.001) C3  
 \* 0.008 (0.001) C4  
 \* -0.011 (0.001) C5  
 \* 0.001 (0.001) C6

Rms deviation of fitted atoms = 0.010

$$3) \quad 6.217 \text{ (0.014)} \quad x - 3.131 \text{ (0.006)} \quad y + 6.335 \text{ (0.031)} \quad z = 7.789 \text{ (0.011)}$$

Angle to previous plane (with approximate esd) = 6.54 ( 0.22 )

\* 0.000 (0.000) N2  
 \* 0.000 (0.000) O1  
 \* 0.000 (0.000) O2

Rms deviation of fitted atoms = 0.000

4) 7.393 (0.009) x - 2.691 (0.011) y + 4.712 (0.035) z = 8.328 (0.013)

Angle to previous plane (with approximate esd) = 10.74 ( 0.31 )

\* 0.000 (0.000) C1  
\* 0.000 (0.000) H11  
\* 0.000 (0.000) H12  
0.142 (0.002) N1

Rms deviation of fitted atoms = 0.000

5) 6.975 (0.004) x + 2.788 (0.002) y + 5.589 (0.006) z = 3.731 (0.003)

Angle to previous plane (with approximate esd) = 59.20 ( 0.11 )

\* -0.012 (0.001) C1\_\$4  
\* 0.015 (0.001) C2\_\$4  
\* -0.005 (0.001) C3\_\$4  
\* -0.008 (0.001) C4\_\$4  
\* 0.011 (0.001) C5\_\$4  
\* -0.001 (0.001) C6\_\$4

Rms deviation of fitted atoms = 0.010

6) 6.975 (0.004) x - 2.788 (0.002) y + 5.589 (0.006) z = 8.133 (0.005)

Angle to previous plane (with approximate esd) = 60.15 ( 0.04 )

\* 0.012 (0.001) C1  
\* -0.015 (0.001) C2  
\* 0.005 (0.001) C3  
\* 0.008 (0.001) C4  
\* -0.011 (0.001) C5  
\* 0.001 (0.001) C6

Rms deviation of fitted atoms = 0.010

7) 6.975 (0.004) x + 2.788 (0.002) y + 5.589 (0.006) z = 10.220 (0.007)

Angle to previous plane (with approximate esd) = 60.15 ( 0.04 )

\* 0.012 (0.001) C1\_\$1  
\* -0.015 (0.001) C2\_\$1  
\* 0.005 (0.001) C3\_\$1  
\* 0.008 (0.001) C4\_\$1  
\* -0.011 (0.001) C5\_\$1  
\* 0.001 (0.001) C6\_\$1

Rms deviation of fitted atoms = 0.010