

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: omer19

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Bond precision:    C-C = 0.0067 Å

Wavelength=0.71073

Cell:                a=8.7544(8)                b=11.0084(10)                c=11.8464(10)  
                      alpha=62.551(6)                beta=70.781(7)                gamma=70.947(7)  
Temperature:        293 K

|                | Calculated          | Reported            |
|----------------|---------------------|---------------------|
| Volume         | 935.65(16)          | 935.65(14)          |
| Space group    | P -1                | P -1                |
| Hall group     | -P 1                | ?                   |
| Moiety formula | C30 H36 Cl6 Cu3 N12 | ?                   |
| Sum formula    | C30 H36 Cl6 Cu3 N12 | C30 H36 Cl6 Cu3 N12 |
| Mr             | 968.06              | 968.03              |
| Dx, g cm-3     | 1.718               | 1.718               |
| Z              | 1                   | 1                   |
| Mu (mm-1)      | 2.160               | 2.160               |
| F000           | 489.0               | 489.0               |
| F000'          | 490.92              |                     |
| h, k, lmax     | 11, 14, 15          | 11, 13, 15          |
| Nref           | 4036                | 3983                |
| Tmin, Tmax     | 0.220, 0.378        | 0.301, 0.436        |
| Tmin'          | 0.178               |                     |

Correction method= INTEGRATION

Data completeness= 0.987

Theta(max)= 26.920

R(reflections)= 0.0458( 3581)

wR2(reflections)= 0.1354( 3983)

S = 1.669

Npar= 227

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

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### Alert level C

ABSTY02\_ALERT\_1\_C An \_exptl\_absorpt\_correction\_type has been given without a literature citation. This should be contained in the \_exptl\_absorpt\_process\_details field.

Absorption correction given as integration

DIFMN02\_ALERT\_2\_C The minimum difference density is < -0.1\*ZMAX\*0.75  
\_refine\_diff\_density\_min given = -2.371

Test value = -2.175  
 DIFMN03\_ALERT\_1\_C The minimum difference density is < -0.1\*ZMAX\*0.75  
 The relevant atom site should be identified.

|                   |                                                  |            |
|-------------------|--------------------------------------------------|------------|
| PLAT098_ALERT_2_C | Large Reported Min. (Negative) Residual Density  | -2.37 eA-3 |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) Cu2 -- Cl1 ..          | 7.67 su    |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for Average U(i,j) Tensor .... | 2.01       |
| PLAT341_ALERT_3_C | Low Bond Precision on C-C Bonds (x 1000) Ang ..  | 7          |
| PLAT152_ALERT_1_C | The Supplied and Calc. Volume s.u. Differ by ... | 2 Units    |
| PLAT194_ALERT_1_C | Missing _cell_measurement_reflns_used datum .... | ?          |
| PLAT195_ALERT_1_C | Missing _cell_measurement_theta_max datum ....   | ?          |
| PLAT196_ALERT_1_C | Missing _cell_measurement_theta_min datum ....   | ?          |

## ● Alert level G

|                   |                                                  |         |
|-------------------|--------------------------------------------------|---------|
| PLAT063_ALERT_4_G | Crystal Size Likely too Large for Beam Size .... | 0.76 mm |
| PLAT199_ALERT_1_G | Check the Reported _cell_measurement_temperature | 293 K   |
| PLAT200_ALERT_1_G | Check the Reported _diffrn_ambient_temperature   | 293 K   |
| PLAT710_ALERT_4_G | Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # | 3       |
|                   | CL1 -CU1 -CL1 -CU2 9.00 0.00 2.656 1.555 1.555   | 1.555   |
| PLAT710_ALERT_4_G | Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # | 12      |
|                   | CL3 -CU2 -CL2 -CU1 164.20 1.00 1.555 1.555 1.555 | 1.555   |
| PLAT710_ALERT_4_G | Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # | 18      |
|                   | CL2 -CU1 -CL2 -CU2 13.00 0.00 2.656 1.555 1.555  | 1.555   |
| PLAT710_ALERT_4_G | Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # | 19      |
|                   | N1 -CU1 -N1 -C3 15.00 0.00 2.656 1.555 1.555     | 1.555   |
| PLAT710_ALERT_4_G | Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... # | 24      |
|                   | N1 -CU1 -N1 -C1 3.00 0.00 2.656 1.555 1.555      | 1.555   |
| PLAT794_ALERT_5_G | Note: Tentative Bond Valency for Cu1 .....       | 1.92    |
| PLAT794_ALERT_5_G | Note: Tentative Bond Valency for Cu2 .....       | 2.00    |

0 ALERT level A = In general: serious problem

0 ALERT level B = Potentially serious problem

11 ALERT level C = Check and explain

10 ALERT level G = General alerts; check

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

4 ALERT type 2 Indicator that the structure model may be wrong or deficient

1 ALERT type 3 Indicator that the structure quality may be low

6 ALERT type 4 Improvement, methodology, query or suggestion

2 ALERT type 5 Informative message, check

## Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

## Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Datablock omer19 - ellipsoid plot

