# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelxl

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

# Datablock: shelxl

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Bond precision:  C-C = 0.0081 A          Wavelength=0.71073

Cell:              a=10.627(5)      b=10.627(5)      c=18.048(5)
                   alpha=90         beta=90          gamma=90
Temperature:       293 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 2038(2) | 2038.2(15) |
| Space group | P 43 | P43 |
| Hall group | P 4cw | ? |
| Moiety formula | C18 H29 Cu N3 O3 | C18 H29 Cu N3 O3 |
| Sum formula | C18 H29 Cu N3 O3 | C18 H29 Cu N3 O3 |
| Mr | 398.99 | 398.98 |
| Dx,g cm-3 | 1.300 | 1.300 |
| Z | 4 | 4 |
| Mu (mm-1) | 1.092 | 1.091 |
| F000 | 844.0 | 844.0 |
| F000′ | 845.54 | |
| h,k,lmax | 14,14,24 | 14,14,24 |
| Nref | 5064[ 2611] | 4720 |
| Tmin,Tmax | 0.770,0.804 | 0.979,0.983 |
| Tmin′ | 0.761 | |

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Correction method= # Reported T Limits: Tmin=0.979 Tmax=0.983
AbsCorr = MULTI-SCAN

Data completeness= 1.81/0.93      Theta(max)= 28.330

R(reflections)= 0.0491( 3169)     wR2(reflections)= 0.1249( 4720)

S = 1.169                 Npar= 233
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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.

## Alert level B

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PLAT019_ALERT_1_B _diffrn_measured_fraction_theta_full/*_max < 1.0      0.976 Report
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......         4 Report
PLAT911_ALERT_3_B Missing # FCF Refl Between THmin & STh/L=  0.600       156 Report
PLAT926_ALERT_1_B Reported and Calculated   R1 Differ by .........    0.0127 Check
PLAT927_ALERT_1_B Reported and Calculated  wR2 Differ by .........    0.0366 Check
PLAT928_ALERT_1_B Reported and Calculated    S value   Differ by .     0.343
```

## Alert level C

```
STRVA01_ALERT_2_C           Chirality of atom sites is inverted?
          From the CIF: _refine_ls_abs_structure_Flack    0.960
          From the CIF: _refine_ls_abs_structure_Flack_su    0.020
PLAT147_ALERT_1_C s.u. on Symmetry Constrained Cell Angle(s) .....     Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference N3     --  C18     ..      0.20 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        N3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C10 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............   0.00809 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond   C10    -   C11    ..      1.41 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H18C   ..  H16D    ..      1.87 Ang.
PLAT907_ALERT_2_C Flack x > 0.5, Structure needs to be Inverted? .      0.96 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers ....         1 Check
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## Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         4 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found  in the CIF     Please Do !
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.960 Note
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as      mixed Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...         5 Units
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)       293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)       293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ............ Percentage =        16 Note
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        55 Do !
            C1  -O1  -CU1 -O3    -70.40  1.10   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        62 Do !
            C7  -N1  -CU1 -N2    138.30  1.50   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        63 Do !
            C8  -N1  -CU1 -N2    -42.80  1.80   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        66 Do !
            C9  -O3  -CU1 -O1     68.90  1.10   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        76 Do !
            C15A-N2  -CU1 -N1    113.40  1.80   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        77 Do !
            C13B-N2  -CU1 -N1    -87.40  1.80   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        78 Do !
            C13A-N2  -CU1 -N1   -119.70  1.60   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        79 Do !
            C14B-N2  -CU1 -N1     43.30  1.90   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        80 Do !
            C14A-N2  -CU1 -N1     -1.00  1.90   1.555   1.555   1.555   1.555
PLAT710_ALERT_4_G Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #        81 Do !
            C15B-N2  -CU1 -N1    155.40  1.60   1.555   1.555   1.555   1.555
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       109 Check
              C13B -N2   -C13A    1.555   1.555   1.555             29.60 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       116 Check
              C14B -N2   -C14A    1.555   1.555   1.555             41.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       117 Check
              C15A -N2   -C15B    1.555   1.555   1.555             40.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #       131 Check
              C16B -N3   -C16A    1.555   1.555   1.555             24.40 Deg.
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PLAT791_ALERT_4_G The Model has Chirality at C8      (Chiral SPGR)          R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          4 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density           4 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  27 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
  19 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

**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* or *IUCrData*, 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.

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**PLATON version of 30/03/2016; check.def file version of 30/03/2016**

**Datablock shelxl** - ellipsoid plot