# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) CAN_1dClBenz

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: CAN_1dClBenz

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Bond precision:  C-C = 0.0055 A          Wavelength=0.71073

Cell:            a=10.2944(16)     b=16.272(3)        c=15.248(3)
                 alpha=90          beta=95.232(4)     gamma=90
Temperature:     173 K

                Calculated                Reported
Volume          2543.6(8)                 2543.6(7)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C24 H16 Co N2 O4, C6 H5 Cl?
Sum formula     C30 H21 Cl Co N2 O4       C30 H21 Cl Co N2 O4
Mr              567.87                    567.87
Dx,g cm-3       1.483                     1.483
Z               4                         4
Mu (mm-1)       0.820                     0.820
F000            1164.0                    1164.0
F000'           1166.42
h,k,lmax        13,21,20                  13,21,20
Nref            6303                      6296
Tmin,Tmax       0.880,0.921               0.849,0.921
Tmin'           0.849

Correction method= # Reported T Limits: Tmin=0.849 Tmax=0.921
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 28.263

R(reflections)= 0.0550( 4493)     wR2(reflections)= 0.1571( 6296)

S = 1.038                 Npar= 343
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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 C

```
PLAT243_ALERT_4_C High   'Solvent' Ueq as Compared to Neighbors of        C5C Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C1C Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT480_ALERT_4_C Long H...A H-Bond Reported H9A      ..CL1C     .       2.96 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H12B     ..CL1C     .       2.92 Ang.
```

## Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C1C      --C6C      .        5.2 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C2C      --C3C      .        6.3 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent)   C3C      --C4C      .        8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --O2B_d    .        6.1 s.u.
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.13 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       1.82 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          8 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          5 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  11 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   9 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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 03/05/2019; check.def file version of 29/04/2019**

**Datablock CAN_1dClBenz** - ellipsoid plot