checkCIF/PLATON report

Structure factors have been supplied for datablock(s) crjplc-2_gaussian_twin1_hklf4

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: crjplc-2_gaussian_twin1_hklf4

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Bond precision:   C-C = 0.0020 A          Wavelength=1.54184

Cell:             a=3.6688(2)     b=12.1030(5)        c=7.0628(3)
                  alpha=90        beta=94.236(4)      gamma=90
Temperature:      120 K

                 Calculated                Reported
Volume           312.76(3)                 312.76(3)
Space group      P 21/m                    P 1 21/m 1
Hall group       -P 2yb                    -P 2yb
Moiety formula   C4 H4 Cl2 Cr N2           C4 H4 Cl2 Cr N2
Sum formula      C4 H4 Cl2 Cr N2           C4 H4 Cl2 Cr N2
Mr               202.99                    202.99
Dx,g cm-3        2.155                     2.156
Z                2                         2
Mu (mm-1)        22.054                    22.054
F000             200.0                     200.0
F000'            201.51
h,k,lmax         4,15,8                    4,14,8
Nref             660                       709
Tmin,Tmax        0.340,0.564               0.276,0.695
Tmin'            0.053

Correction method= # Reported T Limits: Tmin=0.276 Tmax=0.695
AbsCorr = GAUSSIAN

Data completeness= 1.074           Theta(max)= 72.918

R(reflections)= 0.0247( 673)                wR2(reflections)=
                                            0.0719( 709)
S = 1.153                  Npar= 47
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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

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S . 11.78 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cr1 (II) . 2.03 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 5 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.1 Low

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 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.

PLATON version of 18/05/2022; check.def file version of 17/05/2022