checkCIF/PLATON report

Structure factors have been supplied for datablock(s) seyf255

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: seyf255

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Bond precision:   C-C = 0.0131 A          Wavelength=0.71073

Cell:             a=18.0033(10)     b=10.9202(7)         c=8.6309(4)
                  alpha=90          beta=100.774(5)      gamma=90
Temperature:      294 K

                 Calculated                  Reported
Volume           1666.92(16)                 1666.93(16)
Space group      P 21/c                      P 1 21/c 1
Hall group       -P 2ybc                     -P 2ybc
Moiety formula   C11 H17 Br Cl2 N2 Ni O3     C11 H17 Br Cl2 N2 Ni O3
Sum formula      C11 H17 Br Cl2 N2 Ni O3     C11 H17 Br Cl2 N2 Ni O3
Mr               434.76                      434.78
Dx,g cm-3        1.732                       1.732
Z                4                           4
Mu (mm-1)        3.887                       3.887
F000             872.0                       872.0
F000'            873.68
h,k,lmax         23,14,11                    23,14,11
Nref             3824                        3821
Tmin,Tmax        0.257,0.460                 0.080,1.000
Tmin'            0.138

Correction method= # Reported T Limits: Tmin=0.080 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 27.500

R(reflections)= 0.0783( 2069)                wR2(reflections)=
                                             0.2033( 3821)
S = 0.985                 Npar= 186
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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

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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.160
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .....      0.160 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.4 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range       4.1 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C9 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01311 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor  N1       --H1B      .     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     16.992 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.277 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.033 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
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
             H1A   H1B   H2
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          2 Report
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1       (II)      .       2.01 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
               1  0  0,   1  1  0,   2  0  0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        4.2 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       55.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       1.59 Note
             Predicted wR2: Based on SigI**2 12.83 or SHELX Weight 21.17
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 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
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
6 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 06/01/2024; check.def file version of 05/01/2024

Datablock seyf255 - ellipsoid plot