

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

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: 2

Bond precision: C-C = 0.0021 A Wavelength=1.54178

Cell: a=8.1672(1) b=9.3837(1) c=17.2612(2)
 alpha=96.939(1) beta=95.617(1) gamma=112.373(1)

Temperature: 100 K

| | Calculated | Reported |
|----------------|--------------------|--------------------|
| Volume | 1199.33(3) | 1199.33(3) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C23 H40 B Cu N P S | C23 H40 B Cu N P S |
| Sum formula | C23 H40 B Cu N P S | C23 H40 B Cu N P S |
| Mr | 467.95 | 467.94 |
| Dx,g cm-3 | 1.296 | 1.296 |
| Z | 2 | 2 |
| Mu (mm-1) | 2.773 | 2.773 |
| F000 | 500.0 | 500.0 |
| F000' | 498.17 | |
| h,k,lmax | 9,11,21 | 9,11,21 |
| Nref | 4532 | 4471 |
| Tmin,Tmax | 0.704,0.895 | 0.696,1.000 |
| Tmin' | 0.578 | |

Correction method= # Reported T Limits: Tmin=0.696 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 70.033

R(reflections)= 0.0236(4402) wR2(reflections)= 0.0628(4471)

S = 1.052 Npar= 285

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**

| | | | | | |
|-------------------|---|-----|------------|---|--------------|
| PLAT413_ALERT_2_C | Short Inter XH3 .. XHn | H18 | ..H1BC | . | 2.07 Ang. |
| | | | -1+x,y,z = | | 1_455 Check |
| PLAT420_ALERT_2_C | D-H Without Acceptor | Cu1 | --H1AA | . | Please Check |
| PLAT420_ALERT_2_C | D-H Without Acceptor | Cu1 | --H1AB | . | Please Check |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= | | 0.600 | | 28 Report |

● **Alert level G**

| | | | | | |
|-------------------|--|-----|-------|-----------|--------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | | | | 15 Note |
| PLAT154_ALERT_1_G | The s.u.'s on the Cell Angles are Equal ..(Note) | | | | 0.001 Degree |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records | | | | 2 Report |
| PLAT176_ALERT_4_G | The CIF-Embedded .res File Contains SADI Records | | | | 9 Report |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Cu1 | --S1A | . | 6.5 s.u. |
| PLAT301_ALERT_3_G | Main Residue Disorder | | | (Resd 1) | 14% Note |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | | | | 6 Note |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | | | | 37 Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= | | 0.600 | | 34 Note |
| PLAT961_ALERT_5_G | Dataset Contains no Negative Intensities | | | | Please Check |
| PLAT978_ALERT_2_G | Number C-C Bonds with Positive Residual Density. | | | | 17 Info |

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
11 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 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 03/05/2019; check.def file version of 29/04/2019

