# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) asm226

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: asm226

---

```
Bond precision:   C-C = 0.0042 A          Wavelength=0.71073

Cell:             a=8.15286(19)     b=18.9330(4)       c=28.0248(7)
                  alpha=90          beta=95.618(2)     gamma=90
Temperature:      100 K
```

| | Calculated | Reported |
|---|---|---|
| Volume | 4305.08(17) | 4305.07(17) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C39 H38 Br2 N6 Pd2 S, C H Cl3 | C39 H38 Br2 N6 Pd2 S, C H Cl3 |
| Sum formula | C40 H39 Br2 Cl3 N6 Pd2 S | C40 H39 Br2 Cl3 N6 Pd2 S |
| Mr | 1114.78 | 1114.80 |
| Dx,g cm-3 | 1.720 | 1.720 |
| Z | 4 | 4 |
| Mu (mm-1) | 2.963 | 2.963 |
| F000 | 2200.0 | 2200.0 |
| F000' | 2192.55 | |
| h,k,lmax | 10,24,36 | 10,24,36 |
| Nref | 9905 | 9898 |
| Tmin,Tmax | 0.558,0.553 | 0.888,1.000 |
| Tmin' | 0.547 | |

```
Correction method= # Reported T Limits: Tmin=0.888 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999           Theta(max)= 27.500

R(reflections)= 0.0264( 8712)                    wR2(reflections)=
                                                 0.0600( 9898)
S = 1.072                  Npar= 495
```

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

```
PLAT213_ALERT_2_C Atom C16             has ADP max/min Ratio .....       3.2 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.6 Ratio
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of       C1S Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).         8 Note
```

## Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      6.66 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1      --Br1      .      12.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd1      --C3       .       7.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd2      --Br2      .      21.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Pd2      --C4       .       5.9 s.u.
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C11 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Pd1       (II)      .      2.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pd2       (II)      .      2.00 Info
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..      55.0 Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        3 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
  10 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 10/05/2023; check.def file version of 10/05/2023**

**Datablock asm226** - ellipsoid plot