

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_50614b_sq

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: mo_50614b_sq

| | | |
|------------------------|---|-----------------------------------|
| Bond precision: | C-C = 0.0101 Å | Wavelength=0.71073 |
| Cell: | a=12.740(2) | b=21.291(4) c=25.440(5) |
| | alpha=90 | beta=100.263(3) gamma=90 |
| Temperature: | 296 K | |
| | Calculated | Reported |
| Volume | 6790(2) | 6790(2) |
| Space group | P 21/n | P 21/n |
| Hall group | -P 2yn | -P 2yn |
| Moiety formula | C54 H60 B20 N2 P2 Pd2 S2 [+ solvent] | ? |
| Sum formula | C54 H60 B20 N2 P2 Pd2 S2 [+ solvent] | C59 H72 B20 Cl2 N2 O P2 Pd2 S2 |
| Mr | 1292.10 | 1451.14 |
| Dx, g cm ⁻³ | 1.264 | 1.419 |
| Z | 4 | 4 |
| Mu (mm ⁻¹) | 0.674 | 0.759 |
| F000 | 2608.0 | 2944.0 |
| F000' | 2602.37 | |
| h,k,lmax | 16,27,33 | 16,27,32 |
| Nref | 15626 | 15445 |
| Tmin,Tmax | 0.947,0.955 | 0.518,0.746 |
| Tmin' | 0.913 | |

Correction method= # Reported T Limits: Tmin=0.518 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.988 Theta(max)= 27.512

R(reflections)= 0.0566(8785) wR2(reflections)= 0.1761(15445)

S = 0.974 Npar= 787

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 A

CHEMW03_ALERT_2_A ALERT: The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.90 <> 1.10

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_weight 1451.14

TEST: Calculate formula weight from _atom_site_*

| atom | mass | num | sum |
|------|--------|-------|--------|
| C | 12.01 | 54.00 | 648.59 |
| H | 1.01 | 60.00 | 60.48 |
| B | 10.81 | 20.00 | 216.22 |
| N | 14.01 | 2.00 | 28.01 |
| P | 30.97 | 2.00 | 61.95 |
| S | 32.07 | 2.00 | 64.13 |
| Pd | 106.42 | 2.00 | 212.84 |
| Cl | 35.45 | 0.00 | 0.00 |
| O | 16.00 | 0.00 | 0.00 |

Calculated formula weight 1292.23

Alert level C

PLAT234_ALERT_4_C Large Hirshfeld Difference C17 -- C18 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C51 -- C52 .. 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C35 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C53 Check
PLAT332_ALERT_2_C Large Phenyl C-C Range C13 -C18' 0.20 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01009 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -7.906 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.265 Report
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 78 Report
PLAT973_ALERT_2_C Check Calcd Positive Residual Density on Pd2 1.23 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Note

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the _chemical_formula_sum and the formula from the _atom_site* data.

Atom count from _chemical_formula_sum: C59 H72 B20 Cl2 N2 O1 P2 Pd2 S

Atom count from the _atom_site data: C54 H60 B20 N2 P2 Pd2 S2

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum C59 H72 B20 Cl2 N2 O P2 Pd2 S2

TEST: Compare cell contents of formula and atom_site data

| atom | Z*formula | cif sites | diff |
|------|-----------|-----------|-------|
| C | 236.00 | 216.00 | 20.00 |
| H | 288.00 | 240.00 | 48.00 |
| B | 80.00 | 80.00 | 0.00 |
| Cl | 8.00 | 0.00 | 8.00 |
| N | 8.00 | 8.00 | 0.00 |
| O | 4.00 | 0.00 | 4.00 |
| P | 8.00 | 8.00 | 0.00 |
| Pd | 8.00 | 8.00 | 0.00 |
| S | 8.00 | 8.00 | 0.00 |

| | | | |
|-------------------|--|--------|--------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 11 | Note |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 9 | Report |
| PLAT041_ALERT_1_G | Calc. and Reported SumFormula Strings Differ | Please | Check |
| PLAT051_ALERT_1_G | Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . | 11.26 | % |
| PLAT068_ALERT_1_G | Reported F000 Differs from Calcd (or Missing)... | Please | Check |
| PLAT164_ALERT_4_G | Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. | 2 | Note |
| PLAT171_ALERT_4_G | The CIF-Embedded .res File Contains EADP Records | 1 | Report |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | 3 | Report |
| PLAT174_ALERT_4_G | The CIF-Embedded .res File Contains FLAT Records | 1 | Report |
| PLAT186_ALERT_4_G | The CIF-Embedded .res File Contains ISOR Records | 1 | Report |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 1).. | 6 | % Note |
| PLAT343_ALERT_2_G | Unusual sp? Angle Range in Main Residue for | C1 | Check |
| PLAT343_ALERT_2_G | Unusual sp? Angle Range in Main Residue for | C2 | Check |
| PLAT343_ALERT_2_G | Unusual sp? Angle Range in Main Residue for | C10 | Check |
| PLAT343_ALERT_2_G | Unusual sp? Angle Range in Main Residue for | C11 | Check |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C1 - C2 .. | 1.68 | Ang. |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C1 - C3 .. | 1.53 | Ang. |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C10 - C11 .. | 1.67 | Ang. |
| PLAT367_ALERT_2_G | Long? C(sp?)-C(sp?) Bond C10 - C12 .. | 1.52 | Ang. |
| PLAT606_ALERT_4_G | VERY LARGE Solvent Accessible VOID(S) in Structure | ! | Info |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | 64 | Note |
| PLAT869_ALERT_4_G | ALERTS Related to the use of SQUEEZE Suppressed | ! | Info |
| PLAT910_ALERT_3_G | Missing # of FCF Reflection(s) Below Theta(Min) | 3 | Note |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | 99 | Note |
| PLAT913_ALERT_3_G | Missing # of Very Strong Reflections in FCF | 2 | Note |
| PLAT933_ALERT_2_G | Number of OMIT Records in Embedded .res File ... | 8 | Note |

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 18 ALERT type 2 Indicator that the structure model may be wrong or deficient
 8 ALERT type 3 Indicator that the structure quality may be low
 10 ALERT type 4 Improvement, methodology, query or suggestion
 0 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.

