

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh099_raj_sad

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: deh099_raj_sad

Bond precision: C-C = 0.0066 A

Wavelength=0.71073

Cell: a=10.7942(7) b=11.7649(7) c=13.8990(9)
 alpha=93.592(4) beta=109.419(4) gamma=98.850(4)
Temperature: 150 K

| | Calculated | Reported |
|----------------|--------------------------------|--------------------------------|
| Volume | 1632.53(19) | 1632.54(18) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C36 H35 Br Fe N P, C H2 Cl2 | C36 H35 Br Fe N P, C H2 Cl2 |
| Sum formula | C37 H37 Br Cl2 Fe N P | C37 H37 Br Cl2 Fe N P |
| Mr | 733.30 | 733.30 |
| Dx,g cm-3 | 1.492 | 1.492 |
| Z | 2 | 2 |
| Mu (mm-1) | 1.926 | 1.926 |
| F000 | 752.0 | 752.0 |
| F000' | 753.10 | |
| h,k,lmax | 14,15,18 | 14,15,18 |
| Nref | 8437 | 8389 |
| Tmin,Tmax | 0.758,0.908 | 0.579,0.746 |
| Tmin' | 0.749 | |

Correction method= # Reported T Limits: Tmin=0.579 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta(max)= 28.703

R(reflections)= 0.0626(5604)

wR2(reflections)= 0.1517(8389)

S = 1.069

Npar= 394

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 B

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers 2 Check



Alert level C

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C37 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.00657 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 4.690 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 12 Report
PLAT977_ALERT_2_C Check the Negative Difference Density on H35C -0.40 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density 0 Note



Alert level G

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.004 Degree
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 32 Note

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

- 1 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
5 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
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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.

