# checkCIF/PLATON report

**No syntax errors found.** **CIF dictionary** **Interpreting this report**

## Datablock: c__frames_383_work_383s

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**Bond precision: C-C = 0.0036 A Wavelength=0.71073**

**Cell:** **a=11.8398(12)** **b=12.0290(12)** **c=14.8387(15)**
**alpha=75.089(2)** **beta=82.148(2)** **gamma=89.399(2)**
**Temperature:** **173 K**

| | Calculated | Reported |
|---|---|---|
| Volume | 2022.4(4) | 2022.4(4) |
| Space group | P -1 | P-1 |
| Hall group | -P 1 | ? |
| Moiety formula | C16 H35 P S2 | ? |
| Sum formula | C16 H35 P S2 | C16 H35 P S2 |
| Mr | 322.55 | 322.53 |
| Dx,g cm-3 | 1.059 | 1.059 |
| Z | 4 | 4 |
| Mu (mm-1) | 0.332 | 0.332 |
| F000 | 712.0 | 712.0 |
| F000’ | 713.56 | |
| h,k,lmax | 15,16,19 | 15,16,19 |
| Nref | 10086 | 10021 |
| Tmin,Tmax | 0.946,0.974 | 0.893,0.974 |
| Tmin’ | 0.890 | |

**Correction method= MULTI-SCAN**

**Data completeness= 0.994** **Theta(max)= 28.340**

**R(reflections)= 0.0552( 7127)** **wR2(reflections)= 0.1536( 10021)**

**S = 0.995** **Npar= 367**

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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.

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**Alert level C**

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.68
PLAT194_ALERT_1_C Missing _cell_measurement_reflns_used datum .... ?
PLAT195_ALERT_1_C Missing _cell_measurement_theta_max datum .... ?
PLAT196_ALERT_1_C Missing _cell_measurement_theta_min datum .... ?
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.24 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 4.34 Ratio

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PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C12
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for        C20
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**Alert level G**

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PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)        200 Deg.
PLAT793_ALERT_4_G The Model has Chirality at C2      (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C10     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C18     (Verify) ....          R
PLAT793_ALERT_4_G The Model has Chirality at C26     (Verify) ....          R
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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
  8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  5 ALERT level G = General information/check it is not something unexpected

  4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  4 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
  4 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*, 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.**

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**PLATON version of 16/02/2011; check.def file version of 16/02/2011**

**Datablock c__frames_383_work_383s - ellipsoid plot**