

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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: I

| | | |
|-----------------|-----------------------------------------------------|----------------------------|
| Bond precision: | C-C = 0.0062 A | Wavelength=1.54180 |
| Cell: | a=14.0474(11) b=17.4236(14) c=18.3028(13) | |
| | alpha=90 beta=109.786(2) gamma=90 | |
| Temperature: | 123 K | |
| | Calculated | Reported |
| Volume | 4215.3(6) | 4215.2(6) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C45 H41 Cu N O P2 S, F6 P | C45 H41 Cu1 F6 N1 O1 P3 S1 |
| Sum formula | C45 H41 Cu F6 N O P3 S | C45 H41 Cu1 F6 N1 O1 P3 S1 |
| Mr | 914.31 | 914.35 |
| Dx,g cm-3 | 1.441 | 1.441 |
| Z | 4 | 4 |
| Mu (mm-1) | 2.810 | 2.810 |
| F000 | 1880.0 | 1880.0 |
| F000' | 1882.13 | |
| h,k,lmax | 17,21,22 | 17,20,22 |
| Nref | 8034 | 7650 |
| Tmin,Tmax | 0.651,0.656 | 0.570,0.660 |
| Tmin' | 0.591 | |

Correction method= # Reported T Limits: Tmin=0.570 Tmax=0.660
AbsCorr = MULTI-SCAN

Data completeness= 0.952 Theta(max)= 70.226

R(reflections)= 0.0743(7275) wR2(reflections)= 0.1728(7603)

S = 0.994 Npar= 541

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

| | | | | |
|-------------------|-----------|-------------------------------------------|----|-------|
| PLAT241_ALERT_2_B | High | 'MainMol' Ueq as Compared to Neighbors of | C8 | Check |
| PLAT910_ALERT_3_B | Missing # | of FCF Reflection(s) Below Theta(Min). | 34 | Note |

Alert level C

| | | | |
|-------------------|--------------------------------------------------|---------|--------|
| PLAT094_ALERT_2_C | Ratio of Maximum / Minimum Residual Density | 2.09 | Report |
| PLAT213_ALERT_2_C | Atom C8 has ADP max/min Ratio | 3.2 | prolat |
| PLAT215_ALERT_3_C | Disordered C7 has ADP max/min Ratio | 3.1 | Note |
| PLAT220_ALERT_2_C | Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range | 4.0 | Ratio |
| PLAT341_ALERT_3_C | Low Bond Precision on C-C Bonds | 0.00617 | Ang. |
| PLAT911_ALERT_3_C | Missing FCF Refl Between Thmin & STh/L= 0.600 | 140 | Report |

Alert level G

| | | | |
|-------------------|--------------------------------------------------|--------|--------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 9 | Note |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 71 | Report |
| PLAT042_ALERT_1_G | Calc. and Reported MoietyFormula Strings Differ | Please | Check |
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for C7 --C8 .. | 5.1 | s.u. |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) Cul --S1 . | 5.3 | s.u. |
| PLAT244_ALERT_4_G | Low 'Solvent' Ueq as Compared to Neighbors of | P3 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of N1 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of N2 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C1 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C2 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C3 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C4 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C5 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C6 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C7 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C40 Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C41 Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C42 Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C43 Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C44 Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C45 Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C52 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C53 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C54 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C55 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C56 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C57 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C58 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C46 Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C47 Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C48 Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C49 Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C50 Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of C51 Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H11 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H21 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H31 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H41 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H61 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H62 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H71 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H81 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H82 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H83 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H84 Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H85 Constrained at | 0.5 | Check |

| | | | | |
|-------------------|--------------------------------------------------|----------------|------|--------------|
| PLAT300_ALERT_4_G | Atom Site Occupancy of H86 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H91 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H92 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H93 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H94 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H95 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H96 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H411 | Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H421 | Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H431 | Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H441 | Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H451 | Constrained at | 0.65 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H521 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H522 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H531 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H541 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H561 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H571 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H581 | Constrained at | 0.5 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H461 | Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H471 | Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H481 | Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H491 | Constrained at | 0.35 | Check |
| PLAT300_ALERT_4_G | Atom Site Occupancy of H501 | Constrained at | 0.35 | Check |
| PLAT301_ALERT_3_G | Main Residue Disorder(Resd 1) | | 27% | Note |
| PLAT432_ALERT_2_G | Short Inter X...Y Contact C24 ..C47 | | 3.14 | Ang. |
| PLAT808_ALERT_5_G | No Parseable SHELXL Style Weighting Scheme Found | | | Please Check |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | | 599 | Note |
| PLAT882_ALERT_1_G | No Datum for _diffn_reflns_av_unetI/netI | | | Please Do ! |
| PLAT912_ALERT_4_G | Missing # of FCF Reflections Above STh/L= 0.600 | | 243 | Note |
| PLAT913_ALERT_3_G | Missing # of Very Strong Reflections in FCF | | 2 | Note |
| PLAT929_ALERT_5_G | No Weight Pars,Obs and Calc R1,wR2,S not Checked | | | ! Info |
| PLAT960_ALERT_3_G | Number of Intensities with I < - 2*sig(I) ... | | 4 | Check |

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 9 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
 66 ALERT type 4 Improvement, methodology, query or suggestion
 2 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```

# start Validation Reply Form
_vrf_PLAT094_I
;
PROBLEM: Ratio of Maximum / Minimum Residual Density ....      2.09 Report
RESPONSE: ...
;
_vrf_PLAT213_I
;
PROBLEM: Atom C8                      has ADP max/min Ratio .....      3.2 prolat
RESPONSE: ...

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;
_vrf_PLAT215_I
;
PROBLEM: Disordered C7          has ADP max/min Ratio .....    3.1 Note
RESPONSE: ...
;
_vrf_PLAT220_I
;
PROBLEM: Non-Solvent Resd 1  C   Ueq(max)/Ueq(min) Range          4.0 Ratio
RESPONSE: ...
;
_vrf_PLAT341_I
;
PROBLEM: Low Bond Precision on  C-C Bonds .....    0.00617 Ang.
RESPONSE: ...
;
_vrf_PLAT911_I
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600      140 Report
RESPONSE: ...
;
# end Validation Reply Form

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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.

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