

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2

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: 2

Bond precision:	C-C = 0.0040 Å	Wavelength=0.71073	
Cell:	a=10.3369(5)	b=9.5051(5)	c=12.2558(6)
	alpha=90	beta=90.203(4)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	1204.17(10)	1204.17(10)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C8 H7 Cd N5 O S2	?	
Sum formula	C8 H7 Cd N5 O S2	C8 H7 Cd N5 O S2	
Mr	365.72	365.71	
Dx,g cm-3	2.017	2.017	
Z	4	4	
Mu (mm-1)	2.149	2.149	
F000	712.0	712.0	
F000'	709.92		
h,k,lmax	12,11,14	12,11,14	
Nref	2128	2111	
Tmin,Tmax	0.558,0.898	0.604,1.000	
Tmin'	0.438		

Correction method= # Reported T Limits: Tmin=0.604 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 24.996

R(reflections)= 0.0225(1932) wR2(reflections)= 0.0500(2111)

S = 1.064 Npar= 163

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 11 Note

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.317 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 6 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 3 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for S1 --C1 . 7.6 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for N1 --C1 . 7.0 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Cd1 (II) . 2.07 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 3 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 85% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 6 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.9 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
1 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_PLAT910_2
;
PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min). 11 Note
RESPONSE: ...
;
_vrf_PLAT906_2
;
PROBLEM: Large K Value in the Analysis of Variance ..... 2.317 Check
RESPONSE: ...
;
_vrf_PLAT911_2
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.595 6 Report
RESPONSE: ...
;
# end Validation Reply Form
```

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.

