

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rod140\_150k\_

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: rod140\_150k\_

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Bond precision:	C-C = 0.0031 A	Wavelength=1.34050
Cell:	a=9.9697(1)	b=17.2090(2)      c=14.3819(2)
	alpha=90	beta=105.999(2)      gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2371.91(5)	2371.91(5)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C56 H36 Cl2 Co N8 S2	C56 H36 Cl2 Co N8 S2
Sum formula	C56 H36 Cl2 Co N8 S2	C56 H36 Cl2 Co N8 S2
Mr	1014.88	1014.88
Dx,g cm-3	1.421	1.421
Z	2	2
Mu (mm-1)	3.467	3.411
F000	1042.0	1042.0
F000'	1044.93	
h,k,lmax	12,21,18	12,21,18
Nref	5057	5023
Tmin,Tmax	0.474,0.560	0.454,1.000
Tmin'	0.358	

Correction method= # Reported T Limits: Tmin=0.454 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.993      Theta(max)= 58.159

R(reflections)= 0.0507( 4752)      wR2(reflections)= 0.1399( 5023)

S = 1.047      Npar= 313

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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**

RADNW01\_ALERT\_1\_C The radiation wavelength lies outside the expected range  
for the supplied radiation type. Expected range 1.34130-1.34150  
Wavelength given = 1.34050  
PLAT051\_ALERT\_1\_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.65 %  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report

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● **Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.  
PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info  
PLAT230\_ALERT\_2\_G Hirshfeld Test Diff for S1 --C28 . 5.2 s.u.  
PLAT794\_ALERT\_5\_G Tentative Bond Valency for Col (II) . 1.85 Info  
PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 33 Note  
PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 1 Note  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 11 Info  
PLAT984\_ALERT\_1\_G The C-f'= 0.0147 Deviates from the B&C-Value 0.0137 Check  
PLAT984\_ALERT\_1\_G The Cl-f'= 0.3292 Deviates from the B&C-Value 0.3281 Check  
PLAT984\_ALERT\_1\_G The N-f'= 0.0253 Deviates from the B&C-Value 0.0241 Check  
PLAT985\_ALERT\_1\_G The Cl-f'= 0.5397 Deviates from the B&C-Value 0.5435 Check  
PLAT985\_ALERT\_1\_G The Co-f'= 2.8797 Deviates from the B&C-Value 2.9049 Check  
PLAT985\_ALERT\_1\_G The S-f'= 0.4242 Deviates from the B&C-Value 0.4295 Check

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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  
3 **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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 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  
1 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

