

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rod010aa\_130k

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: rod010aa\_130k

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Bond precision:	C-C = 0.0110 A	Wavelength=1.34143	
Cell:	a=25.3093(5)	b=25.3093(5)	c=18.1347(5)
	alpha=90	beta=90	gamma=90
Temperature:	130 K		
	Calculated	Reported	
Volume	11616.4(6)	11616.4(6)	
Space group	P 4/n c c	P 4/n c c	
Hall group	-P 4a 2ac	-P 4a 2ac	
Moiety formula	C48 H38 Co N8 O2 S2, 4(C0.20 H0.20 Cl0.60)	0.25(C192 H152 Co4 N32 O8 S8), 2.4(C H Cl3)	
Sum formula	C50.40 H40.40 Cl7.20 Co N8 O2 S2	C50.40 H40.40 Cl7.20 Co N8 O2 S2	
Mr	1168.40	1168.39	
Dx, g cm <sup>-3</sup>	1.336	1.336	
Z	8	8	
Mu (mm <sup>-1</sup> )	4.327	4.267	
F000	4769.6	4770.0	
F000'	4795.26		
h,k,lmax	31,31,22	30,31,22	
Nref	6061	6020	
Tmin,Tmax	0.440,0.599	0.010,0.201	
Tmin'	0.389		

Correction method= # Reported T Limits: Tmin=0.010 Tmax=0.201  
AbsCorr = MULTI-SCAN

Data completeness= 0.993      Theta(max)= 57.467

R(reflections)= 0.0963( 3155)      wR2(reflections)= 0.3398( 6020)

S = 1.028      Npar= 330

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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 B**

PLAT230\_ALERT\_2\_B Hirshfeld Test Diff for C23 --C24 . 13.4 s.u.

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**Alert level C**

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.146

PLAT020\_ALERT\_3\_C The Value of Rint is Greater Than 0.12 ..... 0.146 Report

PLAT051\_ALERT\_1\_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.41 %

PLAT084\_ALERT\_3\_C High wR2 Value (i.e. > 0.25) ..... 0.34 Report

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference O1 --C20 . 0.19 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference Cl9 --C20 . 0.21 Ang.

PLAT241\_ALERT\_2\_C High MainMol Ueq as Compared to Neighbors of C4 Check

PLAT241\_ALERT\_2\_C High MainMol Ueq as Compared to Neighbors of C23 Check

PLAT244\_ALERT\_4\_C Low Solvent Ueq as Compared to Neighbors of C25 Check

PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including C11 0.152 Check

PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including C14 0.159 Check

PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.01105 Ang.

PLAT601\_ALERT\_2\_C Structure Contains Solvent Accessible VOIDS of . 62 Ang\*\*3

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 6.714 Check

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 2.133 Check

PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check

PLAT978\_ALERT\_2\_C Number C-C Bonds with Positive Residual Density. 0 Info

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**Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 8 Note

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 2 Info

PLAT042\_ALERT\_1\_G Calc. and Reported MoietyFormula Strings Differ Please Check

PLAT068\_ALERT\_1\_G Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT072\_ALERT\_2\_G SHELXL First Parameter in WGHT Unusually Large 0.17 Report

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 22.89 Why ?

PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 1 Report

PLAT176\_ALERT\_4\_G The CIF-Embedded .res File Contains SADI Records 1 Report

PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 1 Report

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Cl4 Constrained at 0.2 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Cl5 Constrained at 0.2 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of Cl6 Constrained at 0.2 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of C26 Constrained at 0.2 Check

PLAT300\_ALERT\_4\_G Atom Site Occupancy of H26 Constrained at 0.2 Check

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 100% Note

PLAT432\_ALERT\_2\_G Short Inter X...Y Contact Cl6 ..C26 3.24 Ang.  
-1/2+y,1-x,1-z = 11\_566 Check

PLAT434\_ALERT\_2\_G Short Inter HL..HL Contact Cl1 ..Cl1 3.03 Ang.  
-1/2+y,1/2+x,3/2-z = 7\_456 Check

PLAT794\_ALERT\_5\_G Tentative Bond Valency for Co1 (II) . 1.96 Info

PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 39 Note

PLAT910\_ALERT\_3\_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note

PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 40 Note

PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 5 Note

PLAT984\_ALERT\_1\_G The C-f'= 0.0148 Deviates from the B&C-Value 0.0137 Check

PLAT984\_ALERT\_1\_G The Cl-f'= 0.3294 Deviates from the B&C-Value 0.3281 Check

PLAT984\_ALERT\_1\_G The Co-f'= -0.6673 Deviates from the B&C-Value -0.6628 Check

PLAT984_ALERT_1_G	The N-f'='	0.0253	Deviates from the B&C-Value	0.0241	Check
PLAT984_ALERT_1_G	The O-f'='	0.0412	Deviates from the B&C-Value	0.0389	Check
PLAT985_ALERT_1_G	The Cl-f"='	0.5404	Deviates from the B&C-Value	0.5435	Check
PLAT985_ALERT_1_G	The Co-f"='	2.8829	Deviates from the B&C-Value	2.9049	Check

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
14 ALERT type 2 Indicator that the structure model may be wrong or deficient  
9 ALERT type 3 Indicator that the structure quality may be low  
13 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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## 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_RINTA01_rod010aa_130k
;
PROBLEM: The value of Rint is greater than 0.12
RESPONSE: ...
;
_vrf_PLAT020_rod010aa_130k
;
PROBLEM: The Value of Rint is Greater Than 0.12 ..... 0.146 Report
RESPONSE: ...
;
_vrf_PLAT051_rod010aa_130k
;
PROBLEM: Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 1.41 %
RESPONSE: ...
;
_vrf_PLAT084_rod010aa_130k
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.34 Report
RESPONSE: ...
;
_vrf_PLAT234_rod010aa_130k
;
PROBLEM: Large Hirshfeld Difference O1 --C20 . 0.19 Ang.
RESPONSE: ...
;
_vrf_PLAT241_rod010aa_130k
;
PROBLEM: High MainMol Ueq as Compared to Neighbors of C4 Check
RESPONSE: ...
;
_vrf_PLAT244_rod010aa_130k
;
PROBLEM: Low Solvent Ueq as Compared to Neighbors of C25 Check
RESPONSE: ...
;
_vrf_PLAT260_rod010aa_130k
;
PROBLEM: Large Average Ueq of Residue Including C11 0.152 Check
```

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RESPONSE: ...
;
_vrf_PLAT341_rod010aa_130k
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.01105 Ang.
RESPONSE: ...
;
_vrf_PLAT601_rod010aa_130k
;
PROBLEM: Structure Contains Solvent Accessible VOIDS of . 62 Ang**3
RESPONSE: ...
;
_vrf_PLAT906_rod010aa_130k
;
PROBLEM: Large K Value in the Analysis of Variance ..... 6.714 Check
RESPONSE: ...
;
_vrf_PLAT918_rod010aa_130k
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) . 2 Check
RESPONSE: ...
;
_vrf_PLAT978_rod010aa_130k
;
PROBLEM: Number C-C Bonds with Positive Residual Density. 0 Info
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.

PLATON version of 22/12/2019; check.def file version of 13/12/2019

Datablock rod010aa\_130k - ellipsoid plot

