

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 4

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Bond precision: C-C = 0.0042 Å

Wavelength=0.71070

Cell: a=11.8562(4) b=15.6902(7) c=11.9620(3)  
alpha=90 beta=94.515(3) gamma=90  
Temperature: 150 K

	Calculated	Reported
Volume	2218.34(14)	2218.34(14)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	?
Moiety formula	C15 H17 Co N10 O3, N O3, H2 O, 0.161(O)	(C15 H17 Co N1 O3)+, (N1 O3)-, (H2 O), 0.161(O)
Sum formula	C15 H19 Co N11 O7.16	C15 H19 Co N11 O7.16
Mr	526.92	526.92
Dx,g cm-3	1.578	1.578
Z	4	4
Mu (mm-1)	0.837	0.837
F000	1081.2	1081.0
F000'	1082.98	
h,k,lmax	16,21,16	16,21,16
Nref	5934	5929
Tmin,Tmax	0.747,0.846	0.935,1.000
Tmin'	0.708	

Correction method= # Reported T Limits: Tmin=0.935 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.999

Theta(max)= 29.070

R(reflections)= 0.0534( 4738)

wR2(reflections)= 0.1464( 5929)

S = 1.042

Npar= 329

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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.

### Alert level B

<a href="#">PLAT430_ALERT_2_B</a>	Short Inter D...A Contact	O4	..02W	.	2.74 Ang.
			-1-x,-1/2+y,1/2-z =		2_445 Check
<a href="#">PLAT430_ALERT_2_B</a>	Short Inter D...A Contact	O6	..02W	.	2.65 Ang.
			-1-x,-1/2+y,1/2-z =		2_445 Check
<a href="#">PLAT430_ALERT_2_B</a>	Short Inter D...A Contact	N11	..02W	.	2.62 Ang.
			1+x,y,z =		1_655 Check

### Alert level C

<a href="#">PLAT077_ALERT_4_C</a>	Unitcell Contains Non-integer Number of Atoms ..	Please Check
<a href="#">PLAT244_ALERT_4_C</a>	Low 'Solvent' Ueq as Compared to Neighbors of	N2 Check
<a href="#">PLAT790_ALERT_4_C</a>	Centre of Gravity not Within Unit Cell: Resd. #	1 Note
	C15 H17 Co N10 O3	

### Alert level G

<a href="#">FORMU01_ALERT_1_G</a>	There is a discrepancy between the atom counts in the _chemical_formula_sum and _chemical_formula_moiety. This is usually due to the moiety formula being in the wrong format. Atom count from _chemical_formula_sum: C15 H19 Co1 N11 O7.16 Atom count from _chemical_formula_moiety:H2 O1.161				
<a href="#">PLAT002_ALERT_2_G</a>	Number of Distance or Angle Restraints on AtSite	3	Note		
<a href="#">PLAT003_ALERT_2_G</a>	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report		
<a href="#">PLAT005_ALERT_5_G</a>	No Embedded Refinement Details Found in the CIF	Please	Do !		
<a href="#">PLAT007_ALERT_5_G</a>	Number of Unrefined Donor-H Atoms .....	6	Report		
<a href="#">PLAT042_ALERT_1_G</a>	Calc. and Reported MoietyFormula Strings Differ	Please	Check		
<a href="#">PLAT068_ALERT_1_G</a>	Reported F000 Differs from Calcd (or Missing)...	Please	Check		
<a href="#">PLAT302_ALERT_4_G</a>	Anion/Solvent/Minor-Residue Disorder (Resd 4 )	100%	Note		
<a href="#">PLAT304_ALERT_4_G</a>	Non-Integer Number of Atoms in ..... Resd 4	0.16	Check		
<a href="#">PLAT311_ALERT_2_G</a>	Isolated Disordered Oxygen Atom (No H's ?) .....	02W	Check		
<a href="#">PLAT790_ALERT_4_G</a>	Centre of Gravity not Within Unit Cell: Resd. #	2	Note		
	N O3				
<a href="#">PLAT790_ALERT_4_G</a>	Centre of Gravity not Within Unit Cell: Resd. #	4	Note		
	O				
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Co1 (II)	1.81	Info		
<a href="#">PLAT860_ALERT_3_G</a>	Number of Least-Squares Restraints .....	15	Note		
<a href="#">PLAT899_ALERT_4_G</a>	SHELXL97 is Deprecated and Succeeded by SHELXL	2018	Note		

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

- 3 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  
 1 ALERT type 3 Indicator that the structure quality may be low  
 8 ALERT type 4 Improvement, methodology, query or suggestion  
 3 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_PLAT430_4
;
PROBLEM: Short Inter D...A Contact O4 ..O2W . 2.74 Ang.
RESPONSE: It is H-bond. We cannot localize H atoms at O2w atom with site occupation 0.16
;
# 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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**PLATON version of 07/08/2019; check.def file version of 30/07/2019**



