

# 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: 2

---

Bond precision:    C-C = 0.0041 Å                      Wavelength=0.71070

Cell:                      a=7.9941(3)              b=17.2119(5)              c=15.0758(5)  
                            alpha=90              beta=103.260(3)              gamma=90  
Temperature:              150 K

	Calculated	Reported
Volume	2019.03(12)	2019.04(11)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	?
Moiety formula	2(C13 H15 Co N9 O2 Se2), C2 H6 O	?
Sum formula	C28 H36 Co2 N18 O5 Se4	C28 H36 Co2 N18 O5 Se4
Mr	1138.45	1138.45
Dx, g cm <sup>-3</sup>	1.873	1.873
Z	2	2
Mu (mm <sup>-1</sup> )	4.489	4.489
F000	1120.0	1120.0
F000'	1121.00	
h,k,lmax	10,23,20	10,23,20
Nref	5406	5397
Tmin,Tmax	0.450,0.638	0.618,1.000
Tmin'	0.258	

Correction method= # Reported T Limits: Tmin=0.618 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.998                      Theta(max)= 29.070

R(reflections)= 0.0354( 4213)              wR2(reflections)= 0.0805( 5397)

S = 1.032                      Npar= 272

---

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 C

PLAT420_ALERT_2_C	D-H Without Acceptor	N8	--H8B	.	Please Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N9	--H9B	.	Please Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd.	#			1 Note
	C13 H15 Co N9 O2 Se2				

### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				2 Note
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF				Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....				7 Report
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as				mixed Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14A	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14B	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3A	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14A	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14B	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14C	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14D	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14E	Constrained at			0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )				100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... Resd 2				4.50 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O3 ..C8				2.97 Ang.
		-x,-y,1-z =			3_556 Check
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #				13 Do !
	N2 -CO1 -N1 -C12 62.60 1.40 1.555 1.555 1.555				1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #				43 Do !
	SE2 -C13 -N2 -CO1 -54.00 47.00 1.555 1.555 1.555				1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #				44 Do !
	N1 -CO1 -N2 -C13 132.20 0.90 1.555 1.555 1.555				1.555
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #				66 Do !
	CO1 -N1 -C12 -SE1 106.00 7.00 1.555 1.555 1.555				1.555
PLAT789_ALERT_4_G	Atoms with Negative atom_site_disorder_group #				9 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (II)				1.75 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....				1 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL				2018 Note

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  
24 **ALERT level G** = General information/check it is not something unexpected

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

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.

