

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ip1\_167

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: ip1\_167

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Bond precision:	C-C = 0.0070 A	Wavelength=0.71073
Cell:	a=7.8532(16)	b=10.000(2)      c=13.192(3)
	alpha=90	beta=105.06(3)      gamma=90
Temperature:	210 K	
	Calculated	Reported
Volume	1000.4(4)	1000.4(3)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C2 H11 Co N3 O5, N O3, H2 O	?
Sum formula	C2 H13 Co N4 O9	C2 H13 Co N4 O9
Mr	296.09	296.09
Dx,g cm-3	1.966	1.966
Z	4	4
Mu (mm-1)	1.764	1.764
F000	608.0	608.0
F000'	609.76	
h,k,lmax	10,13,17	10,13,17
Nref	2433	2403
Tmin,Tmax	0.535,0.884	0.424,0.593
Tmin'	0.489	

Correction method= MULTI-SCAN

Data completeness= 0.988      Theta(max)= 28.080

R(reflections)= 0.0525( 1520)      wR2(reflections)= 0.1327( 2403)

S = 0.881      Npar= 197

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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**

PLAT242\_ALERT\_2\_B Low

Ueq as Compared to Neighbors for .....

N4 Check

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**Alert level C**

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ....	3.1	Note
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.0070	Ang.
PLAT417_ALERT_2_C	Short Inter D-H..H-D H2B .. H8A ..	2.11	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H1C .. O8 ..	2.66	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H2A .. O6 ..	2.63	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H3A .. O1 ..	2.65	Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance .....	2.928	Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	6	Report
PLAT976_ALERT_2_C	Check Calcd Residual Density 0.57A From O6	-0.44	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density 0.82A From O7	-0.43	eA-3
PLAT976_ALERT_2_C	Check Calcd Residual Density 0.99A From O5	-0.42	eA-3

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	18	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3	Report
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	Please	Do !
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	3	Do !
	N2 -CO1 -O1 -C1 5.00 3.00 1.555 1.555 1.555	1.555	
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	9	Do !
	N3 -CO1 -O2 -C2 -7.00 2.00 1.555 1.555 1.555	1.555	
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3	Note
	H2 O		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	33	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	24	Note

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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

11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

8 ALERT type 2 Indicator that the structure model may be wrong or deficient

4 ALERT type 3 Indicator that the structure quality may be low

8 ALERT type 4 Improvement, methodology, query or suggestion

1 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*, 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.

