

# 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: AM\_Co1

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Bond precision:	C-C = 0.0054 A	Wavelength=0.71073
Cell:	a=19.6105(6)	b=15.8275(5)      c=20.3903(6)
	alpha=90	beta=90      gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	6328.9(3)	6328.9(3)
Space group	P b c a	Pbca
Hall group	-P 2ac 2ab	?
Moiety formula	C25 H20 Co N8 O4, C2 H3 N, 2(C H4 O)	C25 H20 Co N8 O4, C2 H3 N, 2(C H4 O)
Sum formula	C29 H31 Co N9 O6	C29 H31 Co N9 O6
Mr	660.56	660.56
Dx,g cm-3	1.387	1.387
Z	8	8
Mu (mm-1)	0.598	0.598
F000	2744.0	2744.0
F000'	2747.82	
h,k,lmax	26,21,27	26,21,27
Nref	7777	7676
Tmin,Tmax	0.879,0.909	0.869,0.919
Tmin'	0.764	

Correction method= # Reported T Limits: Tmin=0.869 Tmax=0.919  
AbsCorr = MULTI-SCAN

Data completeness= 0.987      Theta(max)= 28.180

R(reflections)= 0.0607( 5767)      wR2(reflections)= 0.1970( 7676)

S = 1.095      Npar= 410

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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 C

PLAT414\_ALERT\_2\_C Short Intra D-H..H-X            H2A3    ..   H32A    ..            1.96 Ang.



### Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	45	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details found in the CIF		Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	5	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	10.96	Why ?
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	13	Do !
	N3 -CO1 -N1 -C24 -28.00 2.00 1.555 1.555 1.555 1.555		
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	19	Do !
	N1 -CO1 -N3 -C25 -43.00 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 ... #	20	Do !
	N8 -CO1 -N3 -C25 95.00 2.00 1.555 1.555 1.555 1.555		
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	21	Do !
	O3 -CO1 -N3 -C25 23.00 2.00 1.555 1.555 1.555 1.555		
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	22	Do !
	N7 -CO1 -N3 -C25 166.00 2.00 1.555 1.555 1.555 1.555		
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	23	Do !
	N5 -CO1 -N3 -C25 -125.00 2.00 1.555 1.555 1.555 1.555		
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	24	Do !
	O1 -CO1 -N3 -C25 -54.00 2.00 1.555 1.555 1.555 1.555		
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	133	Do !
	CO1 -N1 -C24 -N2 -139.00 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 ... #	134	Do !
	C25 -N2 -C24 -N1 160.00 3.00 7.655 1.555 1.555 1.555		
PLAT710_ALERT_4_G	Delete 1-2-3 or 2-3-4 Linear Torsion Angle ... #	135	Do !
	CO1 -N3 -C25 -N2 72.00 5.00 1.555 1.555 1.555 7.665		
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	3	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	127	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2014	Note

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

3 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  
12 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.

