

## 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.

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**Alert level C**

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

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**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

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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

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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 06/05/2016; check.def file version of 05/05/2016**

