

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tr005

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: tr005

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Bond precision:	C-C = 0.0084 Å	Wavelength=0.71073
Cell:	a=11.4217(10)      b=16.5963(15)      c=12.9749(11)	
	alpha=90      beta=112.100(2)      gamma=90	
Temperature:	173 K	
	Calculated	Reported
Volume	2278.8(3)	2278.8(3)
Space group	P n	P n
Hall group	P -2yac	P -2yac
Moiety formula	C34 H34 Co N10, 3(B F4), 3(C2 H3 N)	?
Sum formula	C40 H43 B3 Co F12 N13	C40 H43 B3 Co F12 N13
Mr	1025.23	1025.23
Dx,g cm-3	1.494	1.494
Z	2	2
Mu (mm-1)	0.473	0.473
F000	1048.0	1048.0
F000'	1049.29	
h,k,lmax	15,21,17	15,21,17
Nref	10981[ 5501]	10797
Tmin,Tmax	0.783,0.901	0.888,1.179
Tmin'	0.708	

Correction method= # Reported T Limits: Tmin=0.888 Tmax=1.179  
AbsCorr = MULTI-SCAN

Data completeness= 1.96/0.98      Theta(max)= 27.987

R(reflections)= 0.0473( 9040)      wR2(reflections)= 0.1094( 10797)

S = 0.958      Npar= 675

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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

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	8.11	Note
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C2L	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C5L	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C8L	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00841	Ang.



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	5	Report
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size ....	0.73	mm
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B1	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >F9 is Constrained at	0.87	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >F10 is Constrained at	0.87	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >F11 is Constrained at	0.87	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >F12 is Constrained at	0.87	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >B3 is Constrained at	0.87	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F9A is Constrained at	0.13	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F10A is Constrained at	0.13	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F11A is Constrained at	0.13	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <F12A is Constrained at	0.13	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <B3A is Constrained at	0.13	Check
PLAT302_ALERT_4_G	Anion/Solvent Disorder ..... Percentage =	21	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms ( 4.35) in Resd. #	4	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms ( 0.65) in Resd. #	5	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	9	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	42	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	24	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density	3	Note

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

0 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  
4 ALERT type 3 Indicator that the structure quality may be low  
23 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

