

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo\_b1959\_0m

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: mo\_b1959\_0m

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Bond precision:	C-C = 0.0033 A	Wavelength=0.71073	
Cell:	a=12.5987(10)	b=8.9773(9)	c=27.953(2)
	alpha=90	beta=96.829(3)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	3139.1(5)	3139.2(5)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H15 Co3 O11 P, C3 Co O3	C29 H15 Co4 O14 P	
Sum formula	C29 H15 Co4 O14 P	C29 H15 Co4 O14 P	
Mr	854.10	854.10	
Dx,g cm-3	1.807	1.807	
Z	4	4	
Mu (mm-1)	2.198	2.198	
F000	1696.0	1696.0	
F000'	1702.75		
h,k,lmax	19,13,43	19,13,42	
Nref	11973	11959	
Tmin,Tmax	0.605,0.719	0.479,0.566	
Tmin'	0.432		

Correction method= # Reported T Limits: Tmin=0.479 Tmax=0.566  
AbsCorr = MULTI-SCAN

Data completeness= 0.999      Theta(max)= 33.147

R(reflections)= 0.0360( 10539)      wR2(reflections)= 0.1008( 11959)

S = 1.035      Npar= 433

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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 B

PLAT094_ALERT_2_B	Ratio of Maximum / Minimum Residual Density ....	4.95	Report
PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density	3.32	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.41A From Co4	3.43	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.24A From Co4	3.10	eA-3
PLAT971_ALERT_2_B	Check Calcd Resid. Dens. 1.23A From Co2	3.01	eA-3

### ● Alert level C

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	5	Report
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### ● Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1 --C20 .	7.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co1 --C21 .	6.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co2 --C22 .	8.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co2 --C25 .	7.9 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co3 --C23 .	9.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Co3 --C29 .	6.0 s.u.
PLAT233_ALERT_4_G	Hirshfeld (M-X Solvent) Co4 --C26 .	8.5 s.u.
PLAT233_ALERT_4_G	Hirshfeld (M-X Solvent) Co4 --C27 .	9.4 s.u.
PLAT233_ALERT_4_G	Hirshfeld (M-X Solvent) Co4 --C28 .	9.8 s.u.
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C19 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C21 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C24 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C19 ..C28	2.92 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C20 ..C28	3.12 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C21 ..C27	2.92 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C24 ..C26	2.87 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C25 ..C27	3.11 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C26 ..C29	3.08 Ang.
	x,y,z =	1_555 Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.12 Ratio
PLAT794_ALERT_5_G	Tentative Bond Valency for Co2 (III) .	2.13 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Co3 (III) .	2.14 Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	6 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	1 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	12 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

5 **ALERT level B** = A potentially serious problem, consider carefully

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

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

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

22 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
5 ALERT type 4 Improvement, methodology, query or suggestion  
2 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 10/08/2020; check.def file version of 06/08/2020**

