

# 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: 20141029lzd497\_0m

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Bond precision:    C-C = 0.0044 A

Wavelength=0.71073

Cell:            a=9.6429(13)        b=11.4136(15)        c=12.5954(17)  
                  alpha=99.797(2)    beta=106.340(2)     gamma=104.907(2)  
Temperature:    293 K

	Calculated	Reported
Volume	1240.7(3)	1240.7(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H46 Cl4 Co3 N4 O14	C44 H46 Cl4 Co3 N4 O14
Sum formula	C44 H46 Cl4 Co3 N4 O14	C44 H46 Cl4 Co3 N4 O14
Mr	1173.44	1173.44
Dx,g cm-3	1.571	1.570
Z	1	1
Mu (mm-1)	1.274	1.274
F000	599.0	599.0
F000'	600.87	
h,k,lmax	11,13,14	11,13,14
Nref	4379	4359
Tmin,Tmax	0.735,0.795	0.741,0.803
Tmin'	0.720	

Correction method= # Reported T Limits: Tmin=0.741 Tmax=0.803  
AbsCorr = MULTI-SCAN

Data completeness= 0.995

Theta(max)= 25.008

R(reflections)= 0.0376( 3803)

wR2(reflections)= 0.1096( 4359)

S = 1.046

Npar= 316

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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

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	04	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C10	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C18	Check
PLAT250_ALERT_2_C	Large	U3/U1	Ratio for Average U(i,j) Tensor ...	2.1	Note

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### ● Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002	Degree
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293	Check
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O3	111.6	Degree
PLAT395_ALERT_2_G	Deviating X-O-Y Angle From 120 for O4	115.6	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2	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  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
6 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
6 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

PLATON version of 13/12/2017; check.def file version of 12/12/2017

Datablock 20141029lz1\_0m - ellipsoid plot

