

# 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: k149

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Bond precision:	C-C = 0.0027 A	Wavelength=0.71069
Cell:	a=12.4441(8)	b=22.9975(10)      c=13.9971(8)
	alpha=90	beta=92.297(5)      gamma=90
Temperature:	193 K	
	Calculated	Reported
Volume	4002.5(4)	4002.5(4)
Space group	P 21/n	P21/n
Hall group	-P 2yn	?
Moiety formula	C40 H59 Cl2 N2 O2 Sc	?
Sum formula	C40 H59 Cl2 N2 O2 Sc	C40 H59 Cl2 N2 O2 Sc
Mr	715.75	715.75
Dx,g cm-3	1.188	1.188
Z	4	4
Mu (mm-1)	0.351	0.351
F000	1536.0	1536.0
F000'	1538.67	
h,k,lmax	15,28,17	15,27,17
Nref	7635	7530
Tmin,Tmax	0.900,0.932	
Tmin'	0.900	

Correction method= Not given

Data completeness= 0.986      Theta(max)= 25.730

R(reflections)= 0.0376( 6557)      wR2(reflections)= 0.0966( 7530)

S = 1.025      Npar= 424

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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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	4.8	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min) Range	4.8	Ratio
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C23	Check	
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C27	Check	
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C15	Check	
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #				1	Note
C40 H59 C12 N2 O2 Sc						

### ● Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found	in the CIF	Please Do !
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as		mixed Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Sc1 --Cl2 .	5.7 s.u.
PLAT794_ALERT_5_G	Tentative Bond Valency for Sc1	(III) .	3.59 Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL/		2018 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  
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
5 **ALERT level G** = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 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  
2 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.

PLATON version of 16/07/2020; check.def file version of 12/07/2020

Datablock k149 - ellipsoid plot

