

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1-Sm

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: 1-Sm

Bond precision:	C-C = 0.0047 Å	Wavelength=1.54184	
Cell:	a=10.1136 (1)	b=18.0304 (2)	c=24.2334 (2)
	alpha=90	beta=98.587 (1)	gamma=90
Temperature:	120 K		

	Calculated	Reported
Volume	4369.48 (8)	4369.48 (8)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C42 H66 O3 P3 Sm	C42 H66 O3 P3 Sm
Sum formula	C42 H66 O3 P3 Sm	C42 H66 O3 P3 Sm
Mr	862.22	862.20
Dx, g cm-3	1.311	1.311
Z	4	4
Mu (mm-1)	11.385	11.385
F000	1796.0	1796.0
F000'	1782.50	
h, k, lmax	12, 23, 30	12, 23, 30
Nref	9557	9493
Tmin, Tmax	0.594, 0.796	0.377, 1.000
Tmin'	0.539	

Correction method= # Reported T Limits: Tmin=0.377 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.993                      Theta (max)= 80.439

R(reflections)= 0.0470( 9054)	wR2(reflections)= 0.1205( 9493)
S = 1.074	Npar= 460

---

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	3.01	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.74Ang From Sml	2.49	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.75Ang From Sml	2.34	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.76Ang From Sml	2.25	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.79Ang From Sml	2.19	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.80Ang From Sml	2.16	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.79Ang From Sml	1.96	eA-3

---



### Alert level G

PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing .....	0.00020	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Sml (III) .	3.04	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	64	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	4.427	Note
	Predicted wR2: Based on SigI**2 2.72 or SHELX Weight 11.21		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

---

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
7 **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
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 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  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

