

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20210127\_SM\_QE1509\_2\_0m\_a

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: 20210127\_SM\_QE1509\_2\_0m\_a

---

Bond precision:	C-C = 0.0085 A	Wavelength=0.71073	
Cell:	a=15.1358 (12) alpha=90	b=14.5032 (12) beta=96.323 (4)	c=27.104 (2) gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	5913.6 (8)	5913.6 (8)	
Space group	P 21/n	P 21/n	
Hall group	-P 2yn	-P 2yn	
Moiety formula			
Sum formula	C96 H114 B2 F40 O20 Sn12	C96 H114 B2 F40 O20 Sn12	
Mr	3794.02	3793.77	
Dx, g cm <sup>-3</sup>	2.131	2.131	
Z	2	2	
Mu (mm <sup>-1</sup> )	2.612	2.612	
F000	3640.0	3640.0	
F000'	3626.58		
h, k, lmax	22, 21, 40	22, 21, 40	
Nref	20661	20597	
Tmin, Tmax	0.710, 0.760	0.712, 0.744	
Tmin'	0.696		
Correction method=	# Reported T Limits: Tmin=0.712 Tmax=0.744		
AbsCorr =	MULTI-SCAN		
Data completeness=	0.997	Theta (max)=	32.071
R(reflections)=	0.0669 ( 18008)	wR2(reflections)=	0.1099 ( 20597)
S =	1.328	Npar=	827

---

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

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: C48 H114 O20 Sn12, 2(C24 B F20)  
Rep.:

PLAT220_ALERT_2_C	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 1 Sn	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Sn1B	--O3A_a	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Sn6B	--O7A	0.16	Ang.
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....	0.00848	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....		12.616	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....		2.562	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).			7	Note
	1 1 0, -1 0 1, -1 1 1, 0 1 1, 1 0 1,			0 0 2,	
	0 1 2,				
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		3	Report
	-1 1 2, 1 1 2, -1 0 3,				
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc)			1	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.09Ang	From C22A	1.58	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.58Ang	From C41A	-2.09	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.85Ang	From F6E	-1.78	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.37Ang	From Sn5A	-1.76	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.98Ang	From C14A	-1.73	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.15Ang	From F4E	-1.73	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.97Ang	From C4E	-1.68	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.20Ang	From O6A	-1.58	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.20Ang	From O8A	-1.58	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.87Ang	From C12A	-1.57	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.07Ang	From Sn1B	-1.56	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.42Ang	From Sn4B	-1.54	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.92Ang	From Sn4B	-1.51	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.82Ang	From O9A	1.03	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H5A		-0.58	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H12A		-0.35	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H12B		-0.41	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H21A		-0.38	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H23B		-0.34	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H34A		-0.36	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H41A		-0.44	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H42B		-0.42	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H53A		-0.32	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on	H62B		-0.48	eA-3

---



### Alert level G

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C96 H114 B2 F40 O20 Sn12  
Atom count from \_chemical\_formula\_moiety:

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	1	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	3	Report

	H5A	H9A	H10A			
PLAT083_ALERT_2_G	SHELXL	Second	Parameter	in	WGHT	Unusually Large 69.17 Why ?
PLAT186_ALERT_4_G	The	CIF-Embedded	.res	File	Contains	ISOR Records 1 Report
PLAT301_ALERT_3_G	Main	Residue	Disorder	.....	(Resd 1)	15% Note
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF ...	12.00 Deg.
	SN2A	-O4A	-SN2B	3_666	1_555	3_666 ..... # 265 Check
PLAT860_ALERT_3_G	Number	of	Least-Squares	Restraints	.....	6 Note
PLAT912_ALERT_4_G	Missing	#	of	FCF	Reflections	Above STh/L= 0.600 55 Note
PLAT933_ALERT_2_G	Number	of	HKL-OMIT	Records	in	Embedded .res File 5 Note
	1	1	0,	-1	1	1, -1 0 3, 0 1 2, 1 1 2,
PLAT969_ALERT_5_G	The	'Henn et al.'	R-Factor-gap	value	.....	5.60 Note
	Predicted	wR2:	Based	on	SigI**2	1.96 or SHELX Weight 8.45
PLAT978_ALERT_2_G	Number	C-C	Bonds	with	Positive	Residual Density. 0 Info

---

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 30 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 8 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

---

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 06/01/2024; check.def file version of 05/01/2024**

