

# 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: 29\_publ

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Bond precision:	C-C = 0.0084 Å	Wavelength=1.54180	
Cell:	a=10.8434(4)	b=39.2330(17)	c=8.4367(5)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	3589.2(3)	3589.1(3)	
Space group	P b c a	P b c a	
Hall group	-P 2ac 2ab	?	
Moiety formula	C15 H24 O6 S2	?	
Sum formula	C15 H24 O6 S2	C15 H24 O6 S2	
Mr	364.46	364.47	
Dx,g cm-3	1.349	0.000	
Z	8	8	
Mu (mm-1)	2.926	0.000	
F000	1552.0	0.0	
F000'	1561.77		
h,k,lmax	10,39,8	11,40,8	
Nref	1861	1861	
Tmin,Tmax		1.000,1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000  
AbsCorr = ?

Data completeness= 1.000      Theta(max)= 50.053

R(reflections)=      wR2(reflections)=

S =      Npar=

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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

PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	S1	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	S2	Check
PLAT340_ALERT_3_C	Low	Bond Precision on	C-C Bonds .....	0.00843	Ang.
PLAT390_ALERT_3_C	Deviating	Methyl C15	X-C-H Bond Angle .....	102	Degree
PLAT411_ALERT_2_C	Short	Inter H...H Contact	H2 .. H11A ..	2.04	Ang.
PLAT412_ALERT_2_C	Short	Intra XH3 .. XHn	H12B .. H13A ..	1.86	Ang.
PLAT413_ALERT_2_C	Short	Inter XH3 .. XHn	H7A .. H13A ..	2.06	Ang.
PLAT413_ALERT_2_C	Short	Inter XH3 .. XHn	H13B .. H14B ..	2.02	Ang.
PLAT752_ALERT_4_C	Angle	Calc	120.00, Rep	119.9(5) .....	Senseless s.u.
	C8	-C10 -H10	1.555 1.555	1.555 ....	# 62 Check
PLAT752_ALERT_4_C	Angle	Calc	119.00, Rep	118.7(6) .....	Senseless s.u.
	C11	-C10 -H10	1.555 1.555	1.555 ....	# 63 Check

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### ● Alert level G

PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle from 120 Deg for	O1	120.9 Degree
PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle from 120 Deg for	O4	124.0 Degree
PLAT793_ALERT_4_G	The Model has	Chirality at C1	(Centro SPGR)		R Verify
PLAT793_ALERT_4_G	The Model has	Chirality at C2	(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	The Model has	Chirality at C6	(Centro SPGR)		S Verify
PLAT793_ALERT_4_G	The Model has	Chirality at C8	(Centro SPGR)		S Verify
PLAT860_ALERT_3_G	Number of	Least-Squares	Restraints .....	93	Note
PLAT981_ALERT_1_G	No non-zero f"	Anomalous	Scattering Values Found		Please Check
PLAT986_ALERT_1_G	No non-zero f'	Anomalous	Scattering Values Found		Please Check

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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  
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
9 **ALERT level G** = General information/check it is not something unexpected
- 2 **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  
3 **ALERT type 3** Indicator that the structure quality may be low  
6 **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.

