

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision:	C-C = 0.0077 Å	Wavelength=0.71073	
Cell:	a=10.81504(14)	b=10.81504(14)	c=12.7901(3)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1496.00(5)	1495.99(5)	
Space group	P 43	P 43	
Hall group	P 4cw	P 4cw	
Moiety formula	C10 H11 N7 S2 Zn	C10 H11 N7 S2 Zn	
Sum formula	C10 H11 N7 S2 Zn	C10 H11 N7 S2 Zn	
Mr	358.77	358.75	
Dx,g cm-3	1.593	1.593	
Z	4	4	
Mu (mm-1)	1.921	1.921	
F000	728.0	728.0	
F000'	730.22		
h,k,lmax	14,14,17	14,13,17	
Nref	3978[2073]	3528	
Tmin,Tmax	0.555,0.631	0.859,1.000	
Tmin'	0.313		

Correction method= # Reported T Limits: Tmin=0.859 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.70/0.89 Theta(max)= 29.016

R(reflections)= 0.0305(3283) wR2(reflections)= 0.0745(3528)

S = 1.127 Npar= 195

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	2.51	Report
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C9	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C10	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00767	Ang.
PLAT414_ALERT_2_C	Short Intra D-H..H-X H2 .. H8B ..	1.96	Ang.
PLAT420_ALERT_2_C	D-H Without Acceptor N4 -- H4B ...		Please Check
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4A .. S1 ..	2.98	Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H4B .. S2 ..	2.89	Ang.
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	85	%
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	1	Check

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	156	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

- 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
8 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
4 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.

