

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tgs146\_1

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: tgs146\_1

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Bond precision:	C-C = 0.0041 A	Wavelength=0.71073	
Cell:	a=6.4235(2)	b=15.4396(5)	c=19.2190(7)
	alpha=90	beta=90.755(1)	gamma=90
Temperature:	296 K		
	Calculated	Reported	
Volume	1905.90(11)	1905.90(11)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	2(C13 H12 N6 O4 S Zn), C3 H7 N O	C13 H12 N6 O4 S Zn, 0.5(C3 H7 N O)	
Sum formula	C29 H31 N13 O9 S2 Zn2	C14.50 H15.50 N6.50 O4.50 S Zn	
Mr	900.57	450.26	
Dx, g cm <sup>-3</sup>	1.569	1.569	
Z	2	4	
Mu (mm <sup>-1</sup> )	1.436	1.436	
F000	920.0	920.0	
F000'	921.94		
h,k,lmax	7,18,23	7,18,23	
Nref	3665	3640	
Tmin,Tmax	0.602,0.866	0.592,0.745	
Tmin'	0.557		

Correction method= # Reported T Limits: Tmin=0.592 Tmax=0.745  
AbsCorr = MULTI-SCAN

Data completeness= 0.993      Theta(max)= 25.801

R(reflections)= 0.0356( 3405)      wR2(reflections)= 0.1084( 3640)

S = 1.060      Npar= 244

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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**

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	011	Check
PLAT911_ALERT_3_C	Missing #	FCF Refl Between THmin & STh/L= 0.600	2	Report

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	5	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	4	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O1S is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N3S is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2S is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4S is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5S is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SB is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SC is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5SA is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5SB is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5SC is Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)..	100%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	6	Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	12	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	8	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	22	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	3	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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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  
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
28 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
4 ALERT type 3 Indicator that the structure quality may be low  
19 ALERT type 4 Improvement, methodology, query or suggestion  
1 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.

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**PLATON version of 13/08/2017; check.def file version of 27/07/2017**

