

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tgs185_sqd

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: tgs185_sqd

Bond precision:	C-C = 0.0035 A	Wavelength=0.71073
Cell:	a=9.3189(3) b=11.5387(3) c=37.2569(11)	alpha=90 beta=90 gamma=90
Temperature:	298 K	
	Calculated	Reported
Volume	4006.2(2)	4006.2(2)
Space group	P b c m	P b c m
Hall group	-P 2c 2b	-P 2c 2b
Moiety formula	C11 H8 N6 O4 S Zn [+ solvent]	C11 H8 N6 O4 S Zn
Sum formula	C11 H8 N6 O4 S Zn [+ solvent]	C11 H8 N6 O4 S Zn
Mr	385.68	385.66
Dx, g cm ⁻³	1.279	1.279
Z	8	8
Mu (mm ⁻¹)	1.352	1.352
F000	1552.0	1552.0
F000'	1555.77	
h,k,lmax	11,14,45	11,14,45
Nref	3918	3900
Tmin,Tmax	0.784,0.897	0.672,0.745
Tmin'	0.784	

Correction method= # Reported T Limits: Tmin=0.672 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 25.798

R(reflections)= 0.0356(3201) wR2(reflections)= 0.0871(3900)

S = 1.048 Npar= 210

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 B

PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE job ... ! Note

Alert level C

PLAT001_ALERT_1_C	No _shelx_res_file DataName found in SHELXL CIF	Please Do !
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	011 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	022 Check
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	3.944 Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	5 Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0 Info

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum found in CIF	Please Check
PLAT013_ALERT_1_G	N.O.K. _shelx_hkl_checksum found in CIF	Please Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure	! Info
PLAT869_ALERT_4_G	ALERTS Related to the use of SQUEEZE Suppressed	! Info
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	13 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	6 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
6 **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
- 4 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
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

