

## 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

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Bond precision:	C-C = 0.0045 A	Wavelength=0.56076	
Cell:	a=17.4796(16) alpha=90	b=17.4796(16) beta=90	c=10.1256(14) gamma=120
Temperature:	100 K		
	Calculated	Reported	
Volume	2679.3(6)	2679.3(6)	
Space group	P 63/m	P 63/m	
Hall group	-P 6c	-P 6c	
Moiety formula	C27 H6 F3 K2 O19 Zn3 [+ solvent]	(C27 H6 F3 K2 O18 Zn3), (O)	
Sum formula	C27 H6 F3 K2 O19 Zn3 [+ solvent]	C27 H6 F3 K2 O19 Zn3	
Mr	965.69	965.66	
Dx, g cm <sup>-3</sup>	1.197	1.197	
Z	2	2	
Mu (mm <sup>-1</sup> )	0.814	0.815	
F000	950.0	950.0	
F000'	952.71		
h, k, lmax	28, 28, 16	22, 28, 15	
Nref	4416	3909	
Tmin, Tmax	0.907, 0.922	0.925, 1.000	
Tmin'	0.850		

Correction method= # Reported T Limits: Tmin=0.925 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.885

Theta(max)= 27.590

R(reflections)= 0.0575( 1930)

wR2(reflections)=  
0.1752( 3908)

S = 1.047

Npar= 98

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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

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	49% Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.16 Report
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	021 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Zn1 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	K1 Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-7.107 Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.01Ang From O1 .	1.26 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.64Ang From O1 .	0.73 eA-3

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### ● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.	
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ Calc: C27 H6 F3 K2 O19 Zn3 Rep.: (C27 H6 F3 K2 O18 Zn3), (O)	Please Check
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at ..... F3 H3	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1 Constrained at	0.3333 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	8% Note
PLAT606_ALERT_4_G	Tentative Accessible VOID(S) in Structure .....	! Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Zn1 (II) .	1.90 Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	! Info
PLAT899_ALERT_4_G	SHELXL2018 is Outdated and Succeeded by SHELXL	2019/3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	472 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File -1 2 1,	1 Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	6 Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value ..... Predicted wR2: Based on SigI**2 9.78 or SHELX Weight 16.81	1.791 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 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  
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
15 **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  
4 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 22/08/2024; check.def file version of 21/08/2024**

Datablock shelx - ellipsoid plot

