

## 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: zincorietveldite

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Bond precision:	S- O = 0.0088 A	Wavelength=0.71075	
Cell:	a=12.8712 (9) alpha=90	b=8.3148 (4) beta=90	c=11.2959 (4) gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1208.90 (11)	1208.90 (11)	
Space group	P m n 21	P m n 21	
Hall group	P 2ac -2	P 2ac -2	
Moiety formula	Mg0.54 O60 S8 U4 Zn3.46	?	
Sum formula	Mg0.54 O60 S8 U4 Zn3.46	H10 Mg0.12 O15 S2 U Zn0.88	
Mr	2408.06	612.47	
Dx, g cm <sup>-3</sup>	3.308	3.365	
Z	1	4	
Mu (mm <sup>-1</sup> )	15.533	15.553	
F000	1086.3	1127.0	
F000'	1051.00		
h, k, lmax	16, 10, 14	16, 10, 14	
Nref	2900 [ 1523]	2485	
Tmin, Tmax	0.234, 0.733	0.402, 1.000	
Tmin'	0.050		

Correction method= # Reported T Limits: Tmin=0.402 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 1.63/0.86      Theta(max)= 27.483

R(reflections)= 0.0308 ( 2174)	wR2(reflections)= 0.0716 ( 2485)
S = 1.074	Npar= 189

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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 B

PLAT043_ALERT_1_B	Calculated and Reported Mol. Weight Differ by ..	41.82	Check
PLAT094_ALERT_2_B	Ratio of Maximum / Minimum Residual Density ....	4.49	Report

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#### Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT213_ALERT_2_C	Atom O4	has ADP max/min Ratio .....	4.0 oblate
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Ow2	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Ow4	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Ow6	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	Ow8	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	S2	Check

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#### Alert level G

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
Atom count from \_chemical\_formula\_sum: H10 Mg0.12 O15 S2 U1 Zn0.88  
Atom count from the \_atom\_site data: Mg0.1345 O15 S2 U1 Zn0.8655  
CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G WARNING: H atoms missing from atom site list. Is this intentional?  
From the CIF: \_cell\_formula\_units\_Z 4  
From the CIF: \_chemical\_formula\_sum H10 Mg0.12 O15 S2 U Zn0.88  
TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
H	40.00	0.00	40.00
Mg	0.48	0.54	-0.06
O	60.00	60.00	0.00
S	8.00	8.00	0.00
U	4.00	4.00	0.00
Zn	3.52	3.46	0.06

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	2	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .....	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .....	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	9%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	9	Note
PLAT850_ALERT_4_G	Check Flack Parameter Exact Value 0.00 with s.u.	0.01	Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	4.6	Low

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0 **ALERT level A** = Most likely a serious problem - resolve or explain

2 **ALERT level B** = A potentially serious problem, consider carefully  
9 **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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
5 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 18/05/2022; check.def file version of 17/05/2022**

