

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s)  
linhuishi\_TB\_xunchengkuangwu\_lvse\_20230803\_S1

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: linhuishi\_TB\_xunchengkuangwu\_lvse\_20230803\_S1

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Bond precision:      P- O = 0.0020 Å      Wavelength=0.71073

Cell:                      a=9.3801(3)                      b=9.3801(3)                      c=6.8748(3)  
                                    alpha=90                      beta=90                      gamma=120

Temperature:              300 K

	Calculated	Reported
Volume	523.85(4)	523.85(4)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	3(O4 P), H O, 5(Ca)	?
Sum formula	Ca5 H O13 P3	Ca10 H2 O26 P6
Mr	502.32	1004.63
Dx, g cm <sup>-3</sup>	3.185	3.185
Z	2	1
Mu (mm <sup>-1</sup> )	3.094	3.094
F000	500.0	500.0
F000'	503.15	
h, k, lmax	12, 12, 8	12, 12, 8
Nref	438	438
Tmin, Tmax	0.743, 0.831	0.660, 0.746
Tmin'	0.734	

Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 1.000                      Theta(max)= 27.500

R(reflections)= 0.0207( 401)

wR2(reflections)=  
0.0501( 438)

S = 1.137

Npar= 41

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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

PLAT420\_ALERT\_2\_B D-H Bond Without Acceptor O4 --H1 . Please Check

**Author Response: This problem may arise from the disordered nature of O4 and H1 atoms.**

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#### Alert level C

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc.: Ca5 H O13 P3  
Rep.: Ca10 H2 O26 P6  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.70Ang From O4 . 0.51 eA-3  
PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.54Ang From O4 . 0.49 eA-3

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#### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 2 Note  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 2 Check  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
PLAT299\_ALERT\_4\_G Atom Site Occupancy Constrained at ..... 0.5 Check  
O4 H1  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 2) 0.33 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 3) 0.33 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 4) 0.50 Check  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 1 Note  
PLAT883\_ALERT\_1\_G Absent Datum for \_atom\_sites\_solution\_primary .. Please Do !  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 4.768 Note  
Predicted wR2: Based on SigI\*\*2 1.05 or SHELX Weight 4.40

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

- 3 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  
1 ALERT type 3 Indicator that the structure quality may be low  
6 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.

