



## 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: nu-6000-oh-4\_auto

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Bond precision: Wavelength=

Cell: a= b= c=  
alpha= beta= gamma=  
Temperature: ?

Calculated Reported

Volume  
Space group  
Hall group  
Moietiy formula  
Sum formula  
Mr  
Dx, g cm<sup>-3</sup>  
Z  
Mu (mm<sup>-1</sup>)  
F000  
F000'  
h, k, lmax  
Nref  
Tmin, Tmax  
Tmin'

Correction method= Not given

Data completeness=

Theta (max)=

R(reflections)=

wR2 (reflections)=

S =

Npar=

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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 A**

RINTA01\_ALERT\_3\_A The value of Rint is greater than 0.25  
Rint given 0.389

**Author Response: Powder crystal collected by Micro-ED.**

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 **Alert level G**

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

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1 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
1 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
0 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  
0 ALERT type 4 Improvement, methodology, query or suggestion  
0 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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**PLATON version of ; check.def file version of**

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# duplicate check

No duplication found

Datablock nu-6000-oh-4\_auto - ellipsoid plot

