



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: exp_878-long_auto

Bond precision:

Wavelength=

Cell:

a=

b=

c=

alpha=

beta=

gamma=

Temperature:

?

Calculated

Reported

Volume

Space group

Hall group

Moiety formula

Sum formula

Mr

Dx, g cm⁻³

Z

Mu (mm⁻¹)

F000

F000'

h, k, lmax

Nref

Tmin, Tmax

Tmin'

Correction method= Not given

Data completeness=

Theta (max) =

R(reflections)=

wR2(reflections)=

S =

Npar=

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 A

RINTA01_ALERT_3_A The value of Rint is greater than 0.25

Rint given 0.451

Author Response: Powder crystal collected by Micro-ED



Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

- 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.

PLATON version of ; check.def file version of

No duplication found

Datablock exp_878-long_auto - ellipsoid plot

