checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20241004_a

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: 20241004_a

```
Bond precision:   La-Ni = 0.0031 A          Wavelength=0.71073

Cell:             a=10.0995(18)      b=10.0995(18)      c=6.4490(16)
                  alpha=90           beta=90            gamma=120
Temperature:      300 K

                 Calculated                  Reported
Volume           569.7(2)                    569.7(2)
Space group      P 63 m c                    P 63 m c
Hall group       P 6c -2c                    P 6c -2c
Moiety formula   La7 Ni3                     ?
Sum formula      La7 Ni3                     La1.75 Ni0.75
Mr               1148.44                     287.12
Dx,g cm-3        6.695                       6.696
Z                2                           8
Mu (mm-1)        30.370                      30.372
F000             966.0                       966.0
F000'            964.59
h,k,lmax         12,12,7                     12,12,7
Nref             396[ 218]                   388
Tmin,Tmax        0.068,0.545                 0.347,0.746
Tmin'            0.038

Correction method= # Reported T Limits: Tmin=0.347 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.78/0.98        Theta(max)= 24.976

R(reflections)= 0.0316( 337)                    wR2(reflections)=
                                                0.0615( 388)
S = 1.094                  Npar= 22
```

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 C

```
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           gray
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
STRVA01_ALERT_4_C          Flack parameter is too small
          From the CIF: _refine_ls_abs_structure_Flack   -1.000
          From the CIF: _refine_ls_abs_structure_Flack_su    0.600
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.37Ang From Ni1             1.61 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  2.14Ang From La3             1.51 eA-3
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High .      0.600 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.250 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      13.26 Why ?
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        88% Note
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by .       0.10 Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      1.478 Note
             Predicted wR2: Based on SigI**2  4.16 or SHELX Weight  5.62
```

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

4 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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.

PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock 20241004_a - ellipsoid plot