## checkCIF (basic structural check) running

*Checking for embedded fcf data in CIF ...*
*Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait* **. . . .**

## checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) iam

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
Please wait while processing .... Interpreting this report

Structure factor report

# Datablock: iam

Bond precision: C–C = 0.0005 A Wavelength=0.71073

Cell: a=6.5784(3) b=7.3916(9) c=13.2645(7)
alpha=74.252(6) beta=88.589(5) gamma=77.892(6)

Temperature: 100 K

| | Calculated | Reported |
|---|---|---|
| Volume | 606.61(9) | 606.61(8) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | 2(C7 H5 O6 S), H12 Ni O6, 2(H2 O) | 2(C7 H5 O6 S), H12 Ni O6, 2(H2 O) |
| Sum formula | C14 H26 Ni O20 S2 | C14 H26 Ni O20 S2 |
| Mr | 637.16 | 637.18 |
| Dx,g cm-3 | 1.744 | 1.744 |
| Z | 1 | 1 |
| Mu (mm-1) | 1.065 | 1.065 |
| F000 | 330.0 | 330.0 |
| F000' | 330.81 | |
| h,k,lmax | 15,17,31 | 15,17,31 |
| Nref | 17538 | 17461 |
| Tmin,Tmax | 0.734,0.791 | 0.643,0.743 |
| Tmin' | 0.719 | |

Correction method= # Reported T Limits: Tmin=0.643 Tmax=0.743
AbsCorr = GAUSSIAN

Data completeness= 0.996 Theta(max)= 58.497

R(reflections)= 0.0266( 15967) wR2(reflections)= 0.0760( 17461)

S = 1.147 Npar= 209

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 B

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density .... 4.43 Report

**Author Response: the reason is the high resolution; at standard resolution, max/min densities are 0.52/-0.37 eA-3, with a ratio of 1.4**

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 8 Check
1 3 0, 1 3 1, -2 1 2, 1 3 2, 1 4 3, 2 1 5,
2 2 6, -1 -4 7,

**Author Response: the reason is the high resolution; at standard resolution, all reflections have (Iobs-Icalc)/Sigma(W) < 10**

## Alert level C

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report
2 0 0, 0 1 3, 5 -1 9, 6 0 9,
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.44Ang From Ni1 1.96 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.35Ang From Ni1 1.88 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.48Ang From O10 . 0.56 eA-3

## Alert level G

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ni1 --O1 . 21.0 s.u.
**And 2 other PLAT232 Alerts**
More ...
PLAT480_ALERT_4_G Long H...A H-Bond Reported H2WA ..S2 . 3.00 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
H1WA H1WB H2WA H2WB H3WA H3WB
PLAT794_ALERT_5_G Tentative Bond Valency for Ni1 (II) . 2.08 Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 72 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
2 0 0,
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 117.0 Degree
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 4.001 Note
Predicted wR2: Based on SigI**2 1.90 or SHELX Weight 6.63
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
4 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**

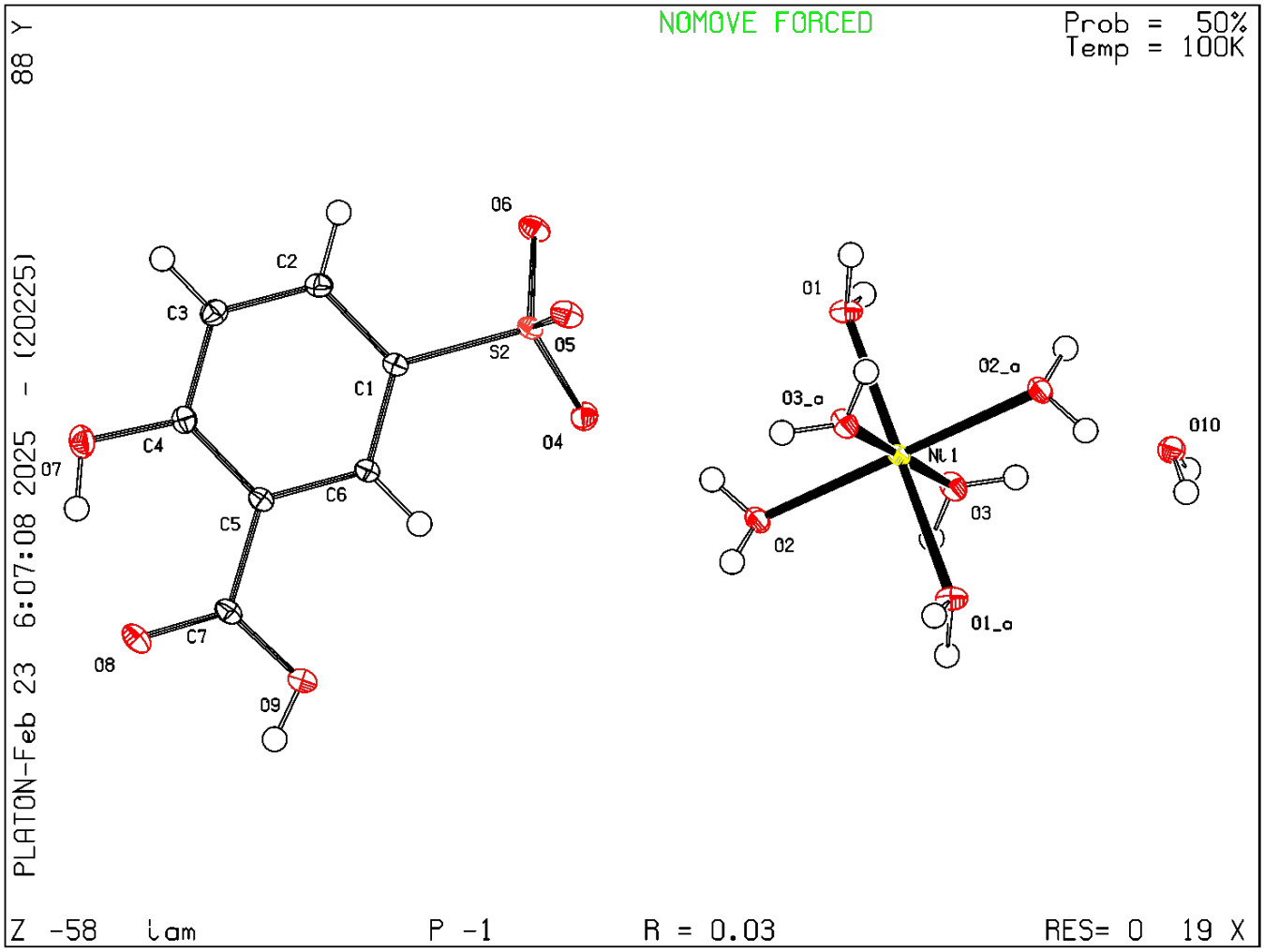
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 02/02/2025; check.def file version of 02/02/2025**

# **Datablock iam** - ellipsoid plot

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