# 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: shinarumpite

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Bond precision: Co- O = 0.0062 A Wavelength=0.71075

Cell: a=21.0549(15) b=6.8708(3) c=12.9106(5)
alpha=90 beta=96.678(7) gamma=90
Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1855.03(17) | 1855.03(17) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | H4 O22 S4 U2, 2(Co H12 O6), 8(H2 O) | ? |
| Sum formula | Co2 H44 O42 S4 U2 | Co H22 O21 S2 U |
| Mr | 1438.51 | 719.25 |
| Dx,g cm-3 | 2.575 | 2.575 |
| Z | 2 | 4 |
| Mu (mm-1) | 9.934 | 9.934 |
| F000 | 1364.0 | 1364.0 |
| F000' | 1329.09 | |
| h,k,lmax | 25,8,15 | 25,8,15 |
| Nref | 3271 | 3045 |
| Tmin,Tmax | 0.438,0.820 | 0.522,1.000 |
| Tmin' | 0.367 | |

Correction method= # Reported T Limits: Tmin=0.522 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.931 Theta(max)= 25.028

R(reflections)= 0.0336( 2623) wR2(reflections)= 0.0774( 3045)

S = 1.065 Npar= 295

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.931 Why?

## Alert level B

PLAT417_ALERT_2_B Short Inter D-H..H-D H14B ..H20A . 2.03 Ang.
x,3/2-y,-1/2+z = 4_575 Check

## Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.07 Report
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of Co2 Check

## Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 33 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.44 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 6 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 11 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 33 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 7 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.1 Low

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

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

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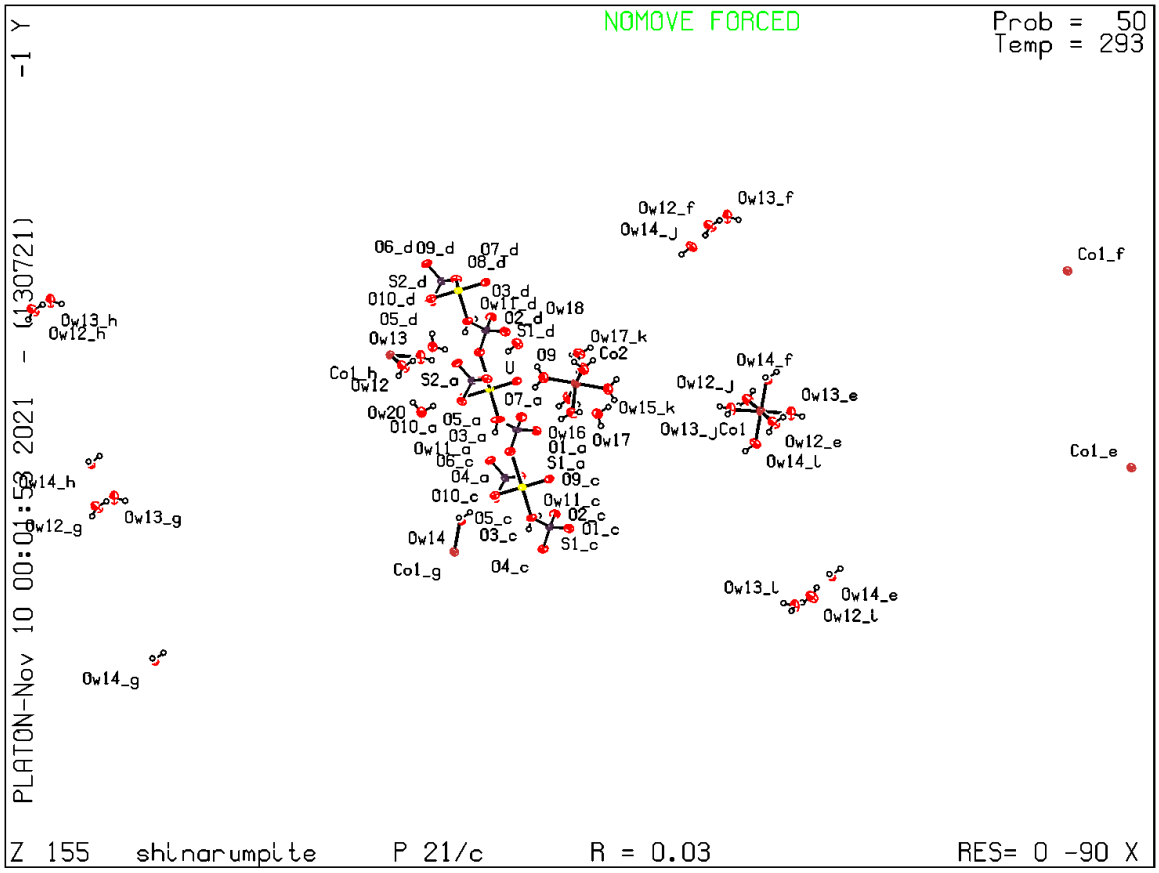
**PLATON version of 13/07/2021; check.def file version of 13/07/2021**

**Datablock shinarumpite** - ellipsoid plot