# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) pov3

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: pov3

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Bond precision: O- B = 0.0050 A Wavelength=0.71073

Cell: a=16.2165(4) b=16.2165(4) c=7.4609(4)
alpha=90 beta=90 gamma=120
Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1699.17(12) | 1699.17(12) |
| Space group | R 3 m | R 3 m :H |
| Hall group | R 3 -2" | R 3 -2" |
| Moiety formula | Al6.17 B9 Fe19.62 H9 Mg1.21 O93 Si18, 3(K0.10), 2.7(Na) | ? |
| Sum formula | Al6.17 B9 Fe19.62 H9 K0.30 Mg1.21 Na2.70 O93 Si18 | H3 Al2.06 B3 Fe6.54 K0.10 Mg0.40 Na0.90 O31 Si6 |
| Mr | 3465.45 | 1155.02 |
| Dx,g cm-3 | 3.387 | 3.386 |
| Z | 1 | 3 |
| Mu (mm-1) | 4.672 | 4.672 |
| F000 | 1690.3 | 1876.0 |
| F000' | 1699.86 | |
| h,k,lmax | 27,27,12 | 27,27,10 |
| Nref | 2123[ 1068] | 1704 |
| Tmin,Tmax | 0.242,0.358 | 0.579,0.747 |
| Tmin' | 0.179 | |

Correction method= # Reported T Limits: Tmin=0.579 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 1.60/0.80 Theta(max)= 37.286

R(reflections)= 0.0268( 1547)

wR2(reflections)= 0.0590( 1704)

S = 1.095 Npar= 94

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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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.897 Why?

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## Alert level C

PLAT031_ALERT_4_C Refined Extinction Parameter Within Range of ... 2.556 Sigma
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 40 Report
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by ..... -0.0024 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.48Ang From O3 . 0.45 eA-3

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## Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of T as SI
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.333 Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 3 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1 ) 19% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 100% Note
PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O5 . 132.9 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 5 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 73 Note
PLAT915_ALERT_3_G No Flack x Check Done: Low Friedel Pair Coverage 75 %
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 2 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 2 Units
PLAT982_ALERT_1_G The O-f'= 0.0080 Deviates from IT-value = 0.0106 Check

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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
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20 **ALERT level G** = General information/check it is not something unexpected

10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  3 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
  9 ALERT type 4 Improvement, methodology, query or suggestion
  2 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. 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.

## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT029_pov3
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low .      0.897 Why?
RESPONSE: ...
;
_vrf_PLAT031_pov3
;
PROBLEM: Refined Extinction Parameter Within Range of ...      2.556 Sigma
RESPONSE: ...
;
_vrf_PLAT041_pov3
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
```

```
_vrf_PLAT068_pov3
;
PROBLEM: Reported F000 Differs from Calcd (or Missing)...     Please Check
RESPONSE: ...
;
_vrf_PLAT077_pov3
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT911_pov3
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=    0.600         40 Report
RESPONSE: ...
;
_vrf_PLAT927_pov3
;
PROBLEM: Reported and Calculated  wR2 Differ by .........    -0.0024 Check
RESPONSE: ...
;
_vrf_PLAT975_pov3
;
PROBLEM: Check Calcd Resid. Dens.  0.48Ang From O3      .       0.45 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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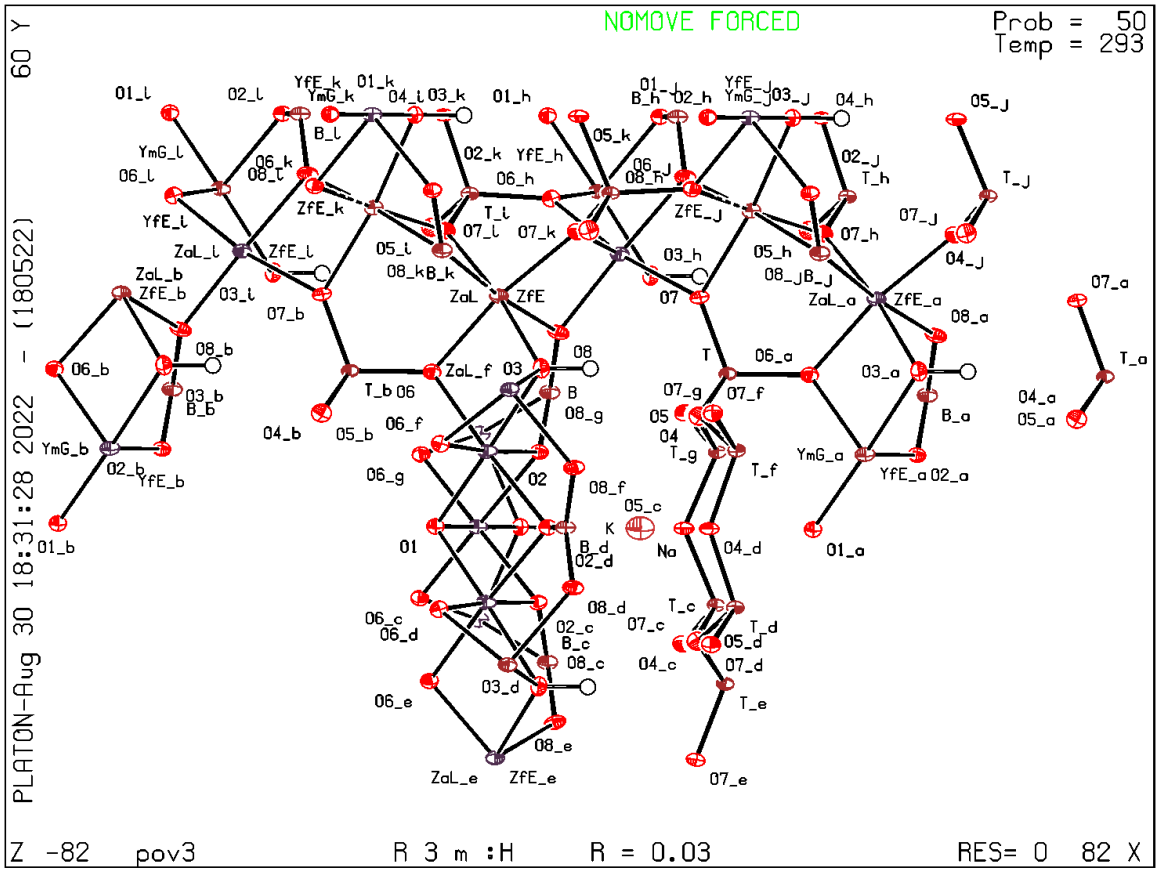
**PLATON version of 18/05/2022; check.def file version of 17/05/2022**

**Datablock pov3** - ellipsoid plot