# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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

Cell: a=15.1359(10) b=7.2035(3) c=9.9876(6)
alpha=90 beta=110.361(5) gamma=90
Temperature: 293 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1020.92(11) | 1020.92(11) |
| Space group | P 2/a | P 1 2/a 1 |
| Hall group | -P 2ya | -P 2ya |
| Moiety formula | Al0.12 Fe3.78 H36 Mg0.58 Mn5.53 O52 P8, 0.76(Ca), 1.24(Na) | ? |
| Sum formula | Al0.12 Ca0.76 Fe3.78 H36 Mg0.58 Mn5.53 Na1.24 O52 P8 | Al0.06 H18 Ca0.38 Fe2.21 Mg0.29 Mn2.45 Na0.62 O26 P4 |
| Mr | 1707.08 | 850.18 |
| Dx,g cm-3 | 2.777 | 2.766 |
| Z | 1 | 2 |
| Mu (mm-1) | 3.539 | 3.561 |
| F000 | 845.8 | 843.0 |
| F000' | 850.49 | |
| h,k,lmax | 19,9,13 | 19,9,13 |
| Nref | 2440 | 2406 |
| Tmin,Tmax | 0.899,0.931 | 0.899,1.000 |
| Tmin' | 0.766 | |

Correction method= # Reported T Limits: Tmin=0.899 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.986 Theta(max)= 27.877

R(reflections)= 0.0570( 1587)  wR2(reflections)= 0.1490( 2406)

S = 0.862  Npar= 199

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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 B

PLAT005_ALERT_5_B No Embedded Refinement Details Found in the CIF Please Do !
PLAT214_ALERT_2_B Atom CaX (Anion/Solvent) ADP max/min Ratio 5.2 prolat
PLAT214_ALERT_2_B Atom NaX (Anion/Solvent) ADP max/min Ratio 5.2 prolat
PLAT420_ALERT_2_B D-H Bond Without Acceptor Ow12 --H12B . Please Check
PLAT964_ALERT_2_B SHELXL WEIGHT Par. Values in CIF & RES Differ .. Please Check

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### Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.158
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 6.72 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
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ow10 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ow11 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 12.964 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.662 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 21 Report
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by ..... -0.0015 Check
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by ..... -0.0037 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.79Ang From O8 . 0.48 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.82Ang From O4 . 0.44 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 1.07Ang From Ow12 . -0.51 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.78Ang From Ow13 . -0.46 eA-3

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### Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:H18 Al.06 Ca0.38 Fe2.21 Mg0.29 M
Atom count from the _atom_site data: H18 Al.06 Ca0.38 Fe1.89 Mg0.288
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum Al0.06 H18 Ca0.38 Fe2.21 Mg0.29 Mn
TEST: Compare cell contents of formula and atom_site data

atom Z*formula cif sites diff

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          Al         0.12      0.12   -0.00
          H         36.00     36.00    0.00
          Ca         0.76      0.76    0.00
          Fe         4.42      3.78    0.64
          Mg         0.58      0.58    0.00
          Mn         4.90      5.53   -0.63
          Na         1.24      1.24    0.00
          O         52.00     52.00    0.00
          P          8.00      8.00    0.00
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         14 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of FE1      as         MN
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .....      0.158 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.500 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      12.89 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe3A       Constrained at      0.766 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe3B       Constrained at      0.846 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mn1        Constrained at       0.68 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mn2A       Constrained at      0.716 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mn2B       Constrained at      0.718 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe2A       Constrained at      0.142 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe2B       Constrained at      0.136 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fe1        Constrained at       0.32 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mn3A       Constrained at       0.21 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mn3B       Constrained at       0.12 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al3A       Constrained at      0.026 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Al3B       Constrained at      0.034 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mg2A       Constrained at      0.142 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mg2B       Constrained at      0.146 Check
PLAT300_ALERT_4_G Atom Site Occupancy of CaX        Constrained at       0.38 Check
PLAT300_ALERT_4_G Atom Site Occupancy of NaX        Constrained at       0.62 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )        25% 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
PLAT480_ALERT_4_G Long H...A H-Bond Reported H12B     ..OW10     .       2.63 Ang.
PLAT480_ALERT_4_G Long H...A H-Bond Reported H13B     ..O6       .       2.63 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          8 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         13 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          9 Note
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
5 **ALERT level B** = A potentially serious problem, consider carefully
18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
38 **ALERT level G** = General information/check it is not something unexpected

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

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**PLATON version of 10/05/2023; check.def file version of 10/05/2023**

**Datablock shelx** - ellipsoid plot