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) 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
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: shelx

```
Bond precision:        Si- O = 0.0030 A              Wavelength=0.71073

Cell:      a=8.8483(4)        b=5.7307(3)       c=10.0314(5)
           alpha=90           beta=113.3659(15) gamma=90

Temperature: 293 K
```

	Calculated	Reported
Volume	466.95(4)	466.95(4)
Space group	P 21/m	P 21/m
Hall group	-P 2yb	-P 2yb
Moiety formula	Al1.96 Ce1.91 Fe0.94 H2 Mg1.11 Mn3.26 O24 Si6, 1.3(O), 0.7(F),	?
Sum formula	Al1.96 Ca0.82 Ce1.91 F0.70 Fe0.94 H2 Mg1.11 Mn3.26 O25.30 Si6	Al0.98 Ca0.41 Ce0.955 F0.35 Fe0.47 H Mg0.555 Mn1.63 O12.65 Si3
Mr	1200.68	600.34
Dx,g cm-3	4.270	4.270
Z	1	2
Mu (mm-1)	8.297	8.297
F000	566.7	566.7
F000'	568.68	
h,k,lmax	13,8,15	13,8,15
Nref	1939	1921
Tmin,Tmax	0.584,0.718	0.554,0.747
Tmin'	0.381	

```
Correction method= # Reported T Limits: Tmin=0.554 Tmax=0.747 AbsCorr =
MULTI-SCAN

Data completeness= 0.991        Theta(max)= 33.157

R(reflections)= 0.0210( 1910)              wR2(reflections)= 0.0533(
                                           1921)

 S = 1.325             Npar= 127
```

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

PLAT430_ALERT_2_B Short Inter D...A Contact O1   ..O4   .   2.79 Ang.
                          x,1+y,z =   1_565 Check
PLAT430_ALERT_2_B Short Inter D...A Contact O4   ..O5   .   2.74 Ang.
                        -x,-1/2+y,-z =   2_545 Check

🔵 Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..   Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.18 Report

PLAT430_ALERT_2_C Short Inter D...A Contact O1   ..O4   .   2.86 Ang.
                              -x,1/2+y,-z =   2_555 Check
And 2 other PLAT430 Alerts
More ...
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   2 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.27Ang From CeA2   1.51 eA-3

⦿ Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.500 Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records   6 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP 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
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   35% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)   100% Note
And 3 other PLAT302 Alerts
More ...
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O4 Check
PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O9   .   137.5 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact Si1   ..O4   .   3.32 Ang.
                              -x,1/2+y,-z =   2_555 Check
And 2 other PLAT432 Alerts
More ...
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   4 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....   ! Info
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   17 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   1 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ....   Please Check

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

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 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
  9 ALERT type 4 Improvement, methodology, query or suggestion
  3 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.

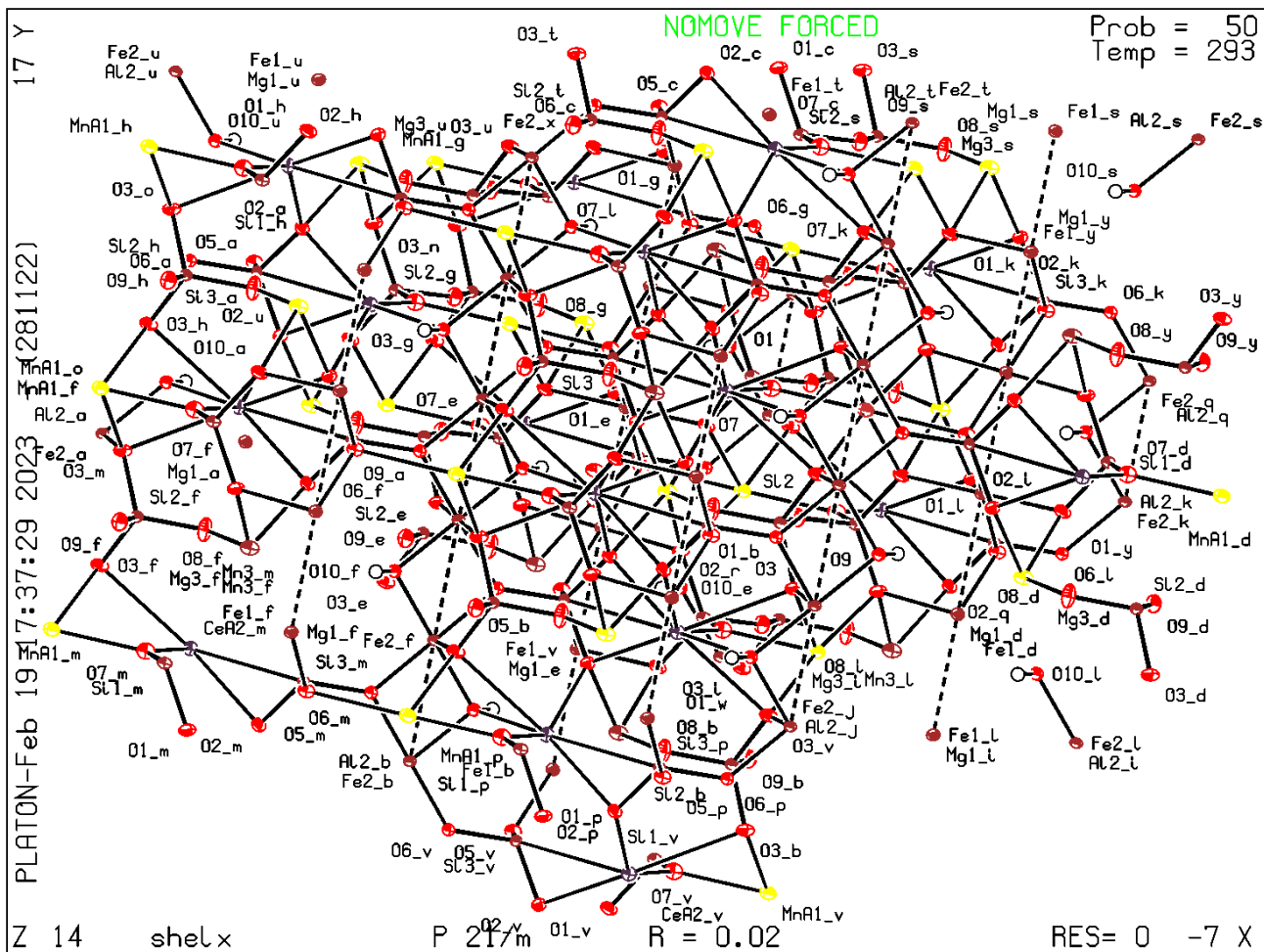**Publication of your CIF in IUCr journals**

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 28/11/2022; check.def file version of 28/11/2022

Datablock shelx - ellipsoid plot