

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: shen-allanite-2-1

Bond precision:	Si- O = 0.0027 A	Wavelength=0.71073
Cell:	a=8.9599 (5)	b=5.8062 (3) c=10.1742 (5)
	alpha=90	beta=114.720 (6) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	480.79 (5)	480.79 (5)
Space group	P 21/m	P 1 21/m 1
Hall group	-P 2yb	-P 2yb
Moiety formula	Al ₂ Ce _{1.10} Fe _{3.16} H ₂ La _{0.56} Mg _{0.36} Nd _{0.12} O ₂₆ Pr _{0.08} Si ₆ Ti _{0.30}	Al Ca _{0.917} Ce _{0.01} Fe _{1.58} H La _{0.28} Mg _{0.18} Nd _{0.06} O ₁₃ Pr _{0.04} Si ₃
Sum formula	Al ₂ Ca _{1.83} Ce _{1.10} Fe _{3.16} H ₂ La _{0.56} Mg _{0.36} Nd _{0.12} O ₂₆ Pr _{0.08} Si ₆	Al Ca _{0.92} H Ce _{0.55} Fe _{1.58} La _{0.28} Mg _{0.18} Nd _{0.06} O ₁₃ Pr _{0.04} Si ₃ T
Mr	1174.12	587.19
Dx, g cm ⁻³	4.055	4.056
Z	1	2
Mu (mm ⁻¹)	7.838	7.840
F000	557.4	558.0
F000'	559.39	
h, k, lmax	13, 9, 15	12, 8, 15
Nref	2053	1791
Tmin, Tmax	0.760, 0.822	0.839, 1.000
Tmin'	0.760	

Correction method= # Reported T Limits: Tmin=0.839 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.872

Theta(max)= 33.580

R(reflections)= 0.0258(1663)

wR2(reflections)=
0.0750(1791)

S = 1.064

Npar= 122

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 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
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	02 Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	07 Check



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the _chemical_formula_sum and _chemical_formula_moiety. This is usually due to the moiety formula being in the wrong format. Atom count from _chemical_formula_sum: H1 Al1 Ca0.92 Ce0.55 Fe1.58 L Atom count from _chemical_formula_moiety:H1 Al1 Ca0.917 Ce00000000 Fe1		
PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2 Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please Check
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	4 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4 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
PLAT300_ALERT_4_G	Atom Site Occupancy of Nd2 Constrained at	0.06 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ce2 Constrained at	0.54 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Pr2 Constrained at	0.04 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ce1 Constrained at	0.01 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of La2 Constrained at	0.28 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fe1 Constrained at	0.76 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fe3 Constrained at	0.82 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ti1 Constrained at	0.15 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mg3 Constrained at	0.18 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.91 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.007 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	21% 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
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

29 **ALERT level G** = General information/check it is not something unexpected

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

3 ALERT type 2 Indicator that the structure model may be wrong or deficient

2 ALERT type 3 Indicator that the structure quality may be low

18 ALERT type 4 Improvement, methodology, query or suggestion

2 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.

