checkCIF/PLATON report

Structure factors have been supplied for datablock(s) fluorbritholite-Nd

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: fluorbritholite-Nd

```
Bond precision:   Si- O = 0.0088 A          Wavelength=0.71073

Cell:               a=9.5994(3)      b=9.5994(3)      c=6.9892(4)
                    alpha=90         beta=90          gamma=120
Temperature:        273 K
```

	Calculated	Reported
Volume	557.76(5)	557.76(5)
Space group	P 63/m	P 63/m
Hall group	-P 6c	-P 6c
Moiety formula	La6.86 O24 Si6, 0.38(Cl), 1.62(O), 3.138(Ca)	La6.86 O24 Si6, 0.38(Cl), 1.62(O), 3.138(Ca)
Sum formula	Ca3.14 Cl0.38 La6.86 O25.62 Si6	Ca3.14 Cl0.38 La6.86 O25.62 Si6
Mr	1670.90	1670.90
Dx,g cm-3	4.975	4.975
Z	1	1
Mu (mm-1)	14.050	14.050
F000	749.3	750.0
F000'	748.96	
h,k,lmax	14,14,10	14,14,10
Nref	702	704
Tmin,Tmax	0.448,0.531	0.619,0.706
Tmin'	0.414	

```
Correction method= # Reported T Limits: Tmin=0.619 Tmax=0.706
AbsCorr = MULTI-SCAN

Data completeness= 1.003           Theta(max)= 32.029
```

R(reflections)= 0.0429(578)

wR2(reflections)= 0.1081(704)

S = 1.102 Npar= 42

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

PLAT972_ALERT_2_B Check Calcd Resid. Dens. 0.65Ang From Re2 -2.99 eA-3

Alert level C

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.57Ang From Re2 2.49 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.52Ang From O2 . 1.02 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.00Ang From O4 . 0.86 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.77Ang From O2 . 0.77 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.76Ang From O4 . -1.10 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of RE1as LA
PLAT017_ALERT_1_G Check Scattering Type Consistency of RE2as LA
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.76 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 273 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 273 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1 Constrained at 0.095 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at 0.81 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 32% 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) ..... O1 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 2 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 !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check

---

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

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

```
 10 ALERT type 2 Indicator that the structure model may be wrong or deficient
  1 ALERT type 3 Indicator that the structure quality may be low
 10 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.

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

Datablock fluorbritholite-Nd - ellipsoid plot