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

```
Bond precision:    = 0.0000 A                    Wavelength=0.71073

Cell:              a=10.0031(2)       b=10.0031(2)       c=7.5382(2)
                   alpha=90           beta=90            gamma=120
Temperature:       293 K

                   Calculated                 Reported
Volume             653.23(3)                  653.23(3)
Space group        P 63/m                     P 63/m
Hall group         -P 6c                      -P 6c
                   O P0.93 V0.07, 0.037(Ba2),
Moiety formula     0.037(Cl), 3(O), 0.28(F),  ?
                   1.259(Ba),
                   Ba1.33 Ca0.33 Cl0.04 F0.28 Ba8 Ca1.99 Cl0.22 F1.69 O24
Sum formula
                   O4 P0.93 V0.07             P5.60 V0.40
Mr                 299.30                     1796.20
Dx,g cm-3          4.565                      4.566
Z                  6                          1
Mu (mm-1)          12.850                     12.853
F000               791.8                      792.0
F000'              790.84
h,k,lmax           16,16,12                   15,16,12
Nref               1030                       1009
Tmin,Tmax          0.545,0.680                0.588,1.000
Tmin'              0.521

Correction method= # Reported T Limits: Tmin=0.588 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.980              Theta(max)= 35.064
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R(reflections)= 0.0192(890)

wR2(reflections)= 0.0405(1009)

S = 1.074   Npar= 64

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
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of   O1 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.01Ang From O1   .   0.49 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.03Ang From O2   .   0.48 eA-3

⚪ **Alert level G**
PLAT017_ALERT_1_G Check Scattering Type Consistency of   M2as   BA
PLAT017_ALERT_1_G Check Scattering Type Consistency of   M2Aas   BA
PLAT017_ALERT_1_G Check Scattering Type Consistency of   M1as   BA
PLAT017_ALERT_1_G Check Scattering Type Consistency of   M1Aas   CA
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   6 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   2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   2 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 V1   Constrained at   0.066 Check
PLAT300_ALERT_4_G Atom Site Occupancy of P1   Constrained at   0.934 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O2   Constrained at   0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   50% Note
PLAT301_ALERT_3_G Main 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 8)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10)   100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11)   100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 2)   0.07 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 3)   0.02 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 4)   0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 5)   0.71 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 6)   0.08 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 7)   0.06 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 8)   0.29 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 9)   0.46 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 10)   0.17 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd 11)   0.17 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O2 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O3 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O3A Check

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........      4 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      6 Note
          F
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #      7 Note
          F
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     20 Note
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   0 ALERT level A = Most likely a serious problem – resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  43 ALERT level G = General information/check it is not something unexpected

  10 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 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
  29 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.

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

Datablock shelx - ellipsoid plot

NOMOVE FORCED

Prob = 50
Temp = 293

-30 Y

PLATON-May 23 10:17:20 2023 - (100523)

O2

M1
M1A

M2

M2A

M2A_a

V1 P1

O3

O3A

O1

Cl

F

F1

Z -40   shelx   P 63/m   R = 0.02   RES= 0   12 X