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=6.72970(12) b=15.5109(3) c=10.1147(2)
alpha=90 beta=90 gamma=90
Temperature: 288 K

	Calculated	Reported
Volume	1055.81(3)	1055.81(3)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	O16 P3.60 V0.40, O32 P3.60 Si4 V0.40, 20(Ca)	?
Sum formula	Ca20 O48 P7.20 Si4 V0.80	Ca5 O12 P1.80 Si V0.20
Mr	1945.70	486.42
Dx,g cm-3	3.060	3.060
Z	1	4
Mu (mm-1)	3.155	3.155
F000	966.4	966.0
F000'	972.72	
h,k,lmax	12,28,18	12,28,18
Nref	3510	3446
Tmin,Tmax	0.746,0.910	0.769,1.000
Tmin'	0.722	

Correction method= # Reported T Limits: Tmin=0.769 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max)= 40.721

R(reflections)= 0.0192(3155) wR2(reflections)= 0.0525(3446)

S = 1.083 Npar= 103

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

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PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
                  2  1  3,
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Alert level G

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          1 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.250 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          3 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
                  Si2
PLAT300_ALERT_4_G Atom Site Occupancy of V1         Constrained at        0.1 Check
PLAT300_ALERT_4_G Atom Site Occupancy of P1         Constrained at        0.9 Check
PLAT300_ALERT_4_G Atom Site Occupancy of V2         Constrained at       0.05 Check
PLAT300_ALERT_4_G Atom Site Occupancy of P2         Constrained at       0.45 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)         31% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    2)         20% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)        100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    6)        100% Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
                  0  2  0,   0  1  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         62 Note
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       3.212 Note
                  Predicted wR2: Based on SigI**2  1.63 or SHELX Weight  4.85
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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
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  18 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
  11 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 22/08/2024; check.def file version of 21/08/2024

Datablock shelx - ellipsoid plot

