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: naalasite

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Bond precision:   Al- O = 0.0089 A         Wavelength=0.71075

Cell:               a=8.4796(6)      b=8.4796(6)      c=26.399(3)
                    alpha=90         beta=90          gamma=120
Temperature:        293 K
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	Calculated	Reported
Volume	1643.9(3)	1643.9(3)
Space group	R 3 2	R 3 2 :H
Hall group	R 3 2"	R 3 2"
Moiety formula	Al9 As18 O72, 1.755(Na2 O2), 6(O), 5.22(Na)	?
Sum formula	Al9 As18 Na8.73 O81.51	Al As2 H4.11 Na0.97 O9.06
Mr	3096.24	348.17
Dx,g cm-3	3.128	3.165
Z	1	9
Mu (mm-1)	9.349	9.350
F000	1459.1	1496.0
F000'	1461.76	
h,k,lmax	10,10,31	10,10,31
Nref	656[398]	655
Tmin,Tmax	0.515,0.627	0.747,1.000
Tmin'	0.427	

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Correction method= # Reported T Limits: Tmin=0.747 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.65/1.00        Theta(max)= 25.017

R(reflections)= 0.0378( 641)                    wR2(reflections)=
                                                0.0934( 655)
S = 1.117                  Npar= 70
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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

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 37.29 Check
PLAT090_ALERT_3_B Poor Data / Parameter Ratio (Zmax > 18) ..... 5.69 Note
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... Ow Check

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Alert level C

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Na1 0.121 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Ow 0.110 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Na2 0.120 Check

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Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:H4.11 Al1 As2 Na0.97 O9.06
Atom count from the _atom_site data: Al1 As2 Na0.97 O9.056666
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 9
From the CIF: _chemical_formula_sum Al As2 H4.11 Na0.97 O9.06
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Al	9.00	9.00	0.00
As	18.00	18.00	0.00
H	36.99	0.00	36.99
Na	8.73	8.73	0.00
O	81.54	81.51	0.03

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.111 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.67 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 3 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Al2 (III) . 2.78 Info
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 with s.u. 0.02 Check
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

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

  8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  7 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
  7 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 28/11/2022; check.def file version of 28/11/2022

Datablock naalasite - ellipsoid plot