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: As- O = 0.0106 A   Wavelength=0.71073

Cell: a=6.6379(13)   b=9.6849(19)   c=12.666(3)
               alpha=108.86(3)   beta=90.97(3)   gamma=104.49(3)
Temperature: 298 K

	Calculated	Reported
Volume	741.8(3)	741.8(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	As8 Fe4 H4 O32 Sr0.28, 0.225(Sr2), 3.28(Sr)	?
Sum formula	As8 Fe4 H4 O32 Sr4	As2 H Fe O8 Sr
Mr	1690.15	422.32
Dx,g cm-3	3.783	3.782
Z	1	4
Mu (mm-1)	18.023	18.006
F000	780.4	780.0
F000'	776.78	
h,k,lmax	7,11,15	7,11,15
Nref	2609	2590
Tmin,Tmax	0.656,0.835	0.589,0.758
Tmin'	0.577	

Correction method= # Reported T Limits: Tmin=0.589 Tmax=0.758
AbsCorr = MULTI-SCAN

Data completeness= 0.993   Theta(max)= 25.026

R(reflections)= 0.0623(2042)   wR2(reflections)= 0.1408(2590)

S = 1.102   Npar= 254

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 A**
PLAT213_ALERT_2_A Atom O32   has ADP max/min Ratio .....   7.4 prolat

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🟡 **Alert level C**
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   7.345 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.595   17 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.01A   From O22   0.86 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H24   -0.42 eA-3

⚪ **Alert level G**
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ....   3 Report
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.25 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   25.02 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.03 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H34   Constrained at   0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H44   Constrained at   0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder ....(Resd 1)   1% Note
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
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
PLAT303_ALERT_2_G Full Occupancy Atom H24   with # Connections   1.14 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1   (III)   .   3.03 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Fe2   (III)   .   3.15 Info
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON   4 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   1 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still   59% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...   19 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   2.0 Low

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   1 **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
  29 **ALERT level G** = General information/check it is not something unexpected

   5 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
   7 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   5 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 05/12/2020; check.def file version of 05/12/2020

NOMOVE FORCED

Prob = 50
Temp = 298

Z -96   shelx   P -1   R = 0.06   RES= 0   -5 X