

# 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

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Bond precision:	As- O = 0.0122 A	Wavelength=0.71073
Cell:	a=9.0719(15)      b=12.227(2)      c=7.5457(15)	
	alpha=90      beta=114.575(6)      gamma=90	
Temperature:	295 K	
	Calculated	Reported
Volume	761.2(2)	761.2(2)
Space group	P m	P m
Hall group	P -2y	P -2y
	As8 Fe6.38 H6.38 O38.38	
Moiety formula	Sr0.01, 0.074(Sr2), 5.455(Sr)	?
Sum formula	As8 Fe6.38 H6.38 O38.38 Sr5.62	As2 H1.60 Fe1.60 O9.60 Sr1.40
Mr	2068.59	517.08
Dx,g cm-3	4.513	4.512
Z	1	4
Mu (mm-1)	21.470	21.449
F000	956.9	957.0
F000'	951.80	
h,k,lmax	12,17,10	12,17,10
Nref	4841[ 2429]	4785
Tmin,Tmax	0.604,0.651	0.781,0.827
Tmin'	0.520	

Correction method= # Reported T Limits: Tmin=0.781 Tmax=0.827  
AbsCorr = NUMERICAL

Data completeness= 1.97/0.99      Theta(max)= 30.468

R(reflections)= 0.0280( 4001)      wR2(reflections)= 0.0603( 4785)

S = 1.045      Npar= 315

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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.

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### Alert level A

PLAT213\_ALERT\_2\_A Atom O53 has ADP max/min Ratio ..... 6.8 prolat

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### Alert level C

ABSTY02\_ALERT\_1\_C An \_exptl\_absorpt\_correction\_type has been given without  
a literature citation. This should be contained in the  
\_exptl\_absorpt\_process\_details field.

Absorption correction given as numerical

CRYSC01\_ALERT\_1\_C The word below has not been recognised as a standard  
identifier.

ruby

STRVA01\_ALERT\_4\_C Flack test results are ambiguous.

From the CIF: \_refine\_ls\_abs\_structure\_Flack 0.569

From the CIF: \_refine\_ls\_abs\_structure\_Flack\_su 0.018

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
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) .....	7.70 Note
PLAT213_ALERT_2_C Atom O12 has ADP max/min Ratio .....	3.6 oblate
PLAT213_ALERT_2_C Atom O54 has ADP max/min Ratio .....	3.5 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	3.4 Ratio
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .	0.57 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.67A From O24	0.43 eA-3

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### Alert level G

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.

From the CIF: \_cell\_formula\_units\_Z 4

From the CIF: \_chemical\_formula\_sum As2 H1.60 Fe1.60 O9.60 Sr1.40

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
As	8.00	8.00	0.00
H	6.40	6.38	0.02
Fe	6.40	6.38	0.02
O	38.40	38.38	0.02
Sr	5.60	5.62	-0.02

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite	16 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	3 Info
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
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records	6 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	6 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records	18 Report
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1 )	26% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2 )	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
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....	! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....	18 Note

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	3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...	4 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged	Please Check

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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  
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
23 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
13 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.

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**PLATON version of 22/03/2021; check.def file version of 19/03/2021**

