checkCIF/PLATON report

Structure factors have been supplied for datablock(s) P_rich_gurimite

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: P_rich_gurimite

```
Bond precision:   = 0.0000 A                Wavelength=0.70848

Cell:               a=5.7186(1)      b=5.7186(1)      c=21.2436(4)
                    alpha=90         beta=90          gamma=120
Temperature:        293 K
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	Calculated	Reported
Volume	601.64(2)	601.642(19)
Space group	R -3 m	R -3 m
Hall group	-R 3 2"	?
Moiety formula	O8 P0.96 V1.04, 2.577(Ba), 0.423(K)	?
Sum formula	Ba2.58 K0.42 O8 P0.96 V1.04	Ba2.58 K0.42 O8 P0.96 V1.04
Mr	581.19	581.20
Dx,g cm-3	4.812	4.812
Z	3	3
Mu (mm-1)	13.859	13.859
F000	764.1	764.0
F000'	763.75	
h,k,lmax	9,9,33	8,9,33
Nref	369	357
Tmin,Tmax	0.847,0.871	0.846,0.870
Tmin'	0.758	

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Correction method= # Reported T Limits: Tmin=0.846 Tmax=0.870
AbsCorr = MULTI-SCAN

Data completeness= 0.967            Theta(max)= 34.750

                                                    wR2(reflections)=
R(reflections)= 0.0140( 339)                        wR= 0.0231( 357)
S = 1.730                  Npar= 21
```

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

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.
GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

Alert level C

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. 0.89Ang From O1 .	0.64 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.60Ang From O2 .	-0.41 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	? Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.70848 Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	43% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-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
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
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	12 Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked	! Info
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities	Please Check
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0 Sig(I)
PLAT984_ALERT_1_G	The Ba-f'= -0.2823 Deviates from the B&C-Value	-0.2860 Check
PLAT984_ALERT_1_G	The K-f'= 0.2016 Deviates from the B&C-Value	0.2005 Check
PLAT984_ALERT_1_G	The P-f'= 0.1035 Deviates from the B&C-Value	0.1021 Check
PLAT985_ALERT_1_G	The Ba-f"= 2.2981 Deviates from the B&C-Value	2.2830 Check
PLAT985_ALERT_1_G	The K-f"= 0.2519 Deviates from the B&C-Value	0.2493 Check
PLAT985_ALERT_1_G	The V-f"= 0.5335 Deviates from the B&C-Value	0.5303 Check

3 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
25 **ALERT level G** = General information/check it is not something unexpected

14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  3 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
  7 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 10/05/2023; check.def file version of 10/05/2023

Datablock P_rich_gurimite - ellipsoid plot