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: test

```
Bond precision:   As- O = 0.0088 A         Wavelength=0.71073

Cell:             a=14.5957(2)     b=14.5957(2)     c=8.34370(18)
                  alpha=90         beta=90          gamma=90
Temperature:      293 K
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	Calculated	Reported
Volume	1777.50(6)	1777.51(6)
Space group	P 4 b m	P 4 b m
Hall group	P 4 -2ab	P 4 -2ab
Moiety formula	As14.94 Cl2 Cu13.73 O64 P1.06, 2(Cl), 3.04(F), 0.96(O), 31(Na0.	?
Sum formula	As14.94 Cl4 Cu13.73 F3.04 Na29.49 O64.96 P1.06	As3.73 Cl Cu3.43 F0.76 Na7.37 O16.24 P0.26
Mr	3941.66	985.36
Dx,g cm-3	3.682	3.682
Z	1	4
Mu (mm-1)	11.408	11.407
F000	1846.6	1847.0
F000'	1854.14	
h,k,lmax	19,19,11	19,19,11
Nref	2338[1247]	2330
Tmin,Tmax	0.509,0.710	0.608,0.776
Tmin'	0.499	

```
Correction method= # Reported T Limits: Tmin=0.608 Tmax=0.776
AbsCorr = GAUSSIAN

Data completeness= 1.87/1.00        Theta(max)= 28.264
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R(reflections)= 0.0450(2247)

wR2(reflections)= 0.0972(2330)

S = 1.163 Npar= 175

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

```
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 gaussian
STRVA01_ALERT_4_C          Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack    0.560
          From the CIF: _refine_ls_abs_structure_Flack_su    0.030
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) ........       7.13 Note
PLAT213_ALERT_2_C Atom O6              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom O7              has ADP max/min Ratio .....        3.1 prolat
PLAT220_ALERT_2_C NonSolvent   Resd 1 Cu   Ueq(max)/Ueq(min) Range        5.9 Ratio
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .       0.56 Check
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Alert level G

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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  As3.73 Cl Cu3.43 F0.76 Na7.37 O16.
          TEST: Compare cell contents of formula and atom_site data

          atom    Z*formula  cif sites diff
          As        14.92     14.94   -0.02
          Cl         4.00      4.00    0.00
          Cu        13.72     13.73   -0.01
          F          3.04      3.04    0.00
          Na        29.48     29.49   -0.01
          O         64.96     64.96    0.00
          P          1.04      1.06   -0.02
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.250 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      12.17 Why ?
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          4 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          4 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F          Constrained at       0.76 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O          Constrained at       0.24 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na6        Constrained at       0.95 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na'        Constrained at       0.25 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        28% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
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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 10  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 12  )       100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....          0 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          1 Note
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 !
PLAT933_ALERT_2_G Number of HKL-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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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   9 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  27 ALERT level G = General information/check it is not something unexpected

   9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or deficient
   2 ALERT type 3 Indicator that the structure quality may be low
  15 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 12/09/2022; check.def file version of 09/08/2022

Datablock test - ellipsoid plot