checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Al12Pb4

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: Al12Pb4

```
Bond precision:   C-C = 0.0112 A          Wavelength=1.34050

Cell:             a=23.5670(2)     b=18.7552(1)         c=24.7399(1)
                  alpha=90         beta=107.235(1)      gamma=90
Temperature:      100 K
```

	Calculated	Reported
Volume	10444.12(13)	10444.12(13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C36 H51 Al6 N O21 Pb2 [+ solvent]	C72 H102 Al12 O36 Pb4, 2(N O3)
Sum formula	C36 H51 Al6 N O21 Pb2 [+ solvent]	C72 H102 Al12 N2 O42 Pb4
Mr	1410.06	2820.07
Dx,g cm-3	1.793	1.793
Z	8	4
Mu (mm-1)	9.355	9.355
F000	5472.0	5472.0
F000'	5419.17	
h,k,lmax	27,22,29	27,22,29
Nref	8917	8884
Tmin,Tmax		1.000,1.000
Tmin'		

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Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000
AbsCorr = SPHERE

Data completeness= 0.996           Theta(max)= 52.048
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R(reflections)= 0.0332(8570)

wR2(reflections)= 0.0832(8884)

S = 1.027 Npar= 632

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

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.80Ang From Pb1 3.76 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

PLAT971_ALERT_2_A Check Calcd Resid. Dens. 0.88Ang From Pb1 3.54 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

Alert level B

PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Author Response: : It h as been checked that all the atoms form a connected set.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.13Ang From Pb2 2.72 eA-3

Author Response: These alerts are generated because of residual density peaks near the heaviest atoms in the structure, due to fourier termination ripples. After inspection, the residual electron density peak does not make chemical sense and will not affect the correct identification of the structure.

Alert level C

RADNW01_ALERT_1_C The radiation wavelength lies outside the expected range
for the supplied radiation type. Expected range 1.34130-1.34150
Wavelength given = 1.34050
THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5882
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio

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PLAT220_ALERT_2_C NonSolvent   Resd 1  O   Ueq(max)/Ueq(min) Range        3.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        5.6 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C35 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         N1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01118 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.588         33 Report
                  2  0  0,   4  4  0,   5  3  0,  -4  2  1,  -3  1  1,  -2  4  1,
                 -1  1  1,   1  1  1,   5  1  1,  -2  2  2,   0  0  2,   5  1  2,
                  7  1  2, -18 12  3, -20  0  4, -10  4  4,   2  8  4, -18 14  5,
                 -3  1  7,   1  3  8,  16  8  9, -18  0 12,  12 10 12,   9 11 14,
                  8  0 16,  11  3 17,  -6  8 18,  -8 12 20,  -7 11 20,   0 10 20,
                  4  0 22,  -4  4 24,  -4  0 28,
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.80Ang From Pb1            -2.37 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.65Ang From Pb1            -1.67 eA-3
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                   not performed for this radiation type.
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H Atoms          41 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
                  H4
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
                  Calc: C36 H51 Al6 N O21 Pb2
                  Rep.: C72 H102 Al12 O36 Pb4, 2(N O3)
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          2 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      126.26 Why ?
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..............    0.00010 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............    0.00010 Ang.
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used     0.0100 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar     0.0200 Report
PLAT299_ALERT_4_G Atom Site Occupancy Constrained at .............        0.5 Check
                  O9      O22     C22     C23     C24     C25     H21     H21A
                  H22     H23     H24     H25
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd    1)          5% Note
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ........          ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2       (II)      .       1.97 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al1       (III)     .       2.80 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al2       (III)     .       2.78 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al3       (III)     .       2.76 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al5       (III)     .       2.81 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Al6       (III)     .       2.71 Info
PLAT795_ALERT_4_G C-Atom in CIF Coordinate List Out-of-Sequence ..         C2 Note
PLAT796_ALERT_4_G O-Atom in CIF Coordinate List Out-of-Sequence ..        O11 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        314 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed          ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still         91% Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                  2  0  0,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         22 Note
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```
               11   9 21,  -3  1  1,  15  3 21,   0  0  2,  -2  2  2,   1  1  1,
               15   9 19,   5  1  2,  20  6 13,  22 14  3,  18  6 15,  -3  1  7,
               -8 12 20,  -2  4  1,   7  1  2,   4  4  0,   5  1  1,  -4  2  1,
              -10   4  4,   1  3  8,   5  3  0,   2  8  4,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........      4.704 Note
             Predicted wR2: Based on SigI**2  1.77 or SHELX Weight  8.10
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
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2 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
34 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
12 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
9 ALERT type 5 Informative message, check

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checkCIF publication errors

Alert level A

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
            _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
            _publ_contact_author_phone are all missing.
            At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
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7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

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Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
```

```
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 15/07/2024; check.def file version of 15/07/2024

Datablock Al12Pb4 - ellipsoid plot