checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Pna21_a

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: Pna21_a

```
Bond precision:    C-C = 0.0042 A              Wavelength=0.71073

Cell:              a=34.914(7)        b=11.175(2)        c=17.505(4)
                   alpha=90           beta=90            gamma=90
Temperature:       100 K

                 Calculated        Reported
Volume           6830(2)           6830(2)
Space group      P n a 21          P n a 21
Hall group       P 2c -2n          P 2c -2n
                 C15.99 Al
Moiety           F35.97 O4, C16
formula          H31 Al2 N2,       [(TMEDA)AL(ALCP*)3][AL(OC4F9)4]
                 2(C10 H15 Al)
                 C51.99 H61 Al5
Sum formula      F35.97 N2 O4      C52 H61 Al5 F36 N2 O4
Mr               1596.22           1596.37
Dx,g cm-3        1.552             1.552
Z                4                 4
Mu (mm-1)        0.223             0.223
F000             3230.6            3231.0
F000'            3234.84
h,k,lmax         49,15,25          49,15,25
Nref             20873[ 10748]     20768
Tmin,Tmax        0.941,0.964       0.723,0.746
Tmin'            0.906

Correction method= # Reported T Limits: Tmin=0.723 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.93/0.99        Theta(max)= 30.530
```

R(reflections)= 0.0373(17167)

wR2(reflections)=
0.0933(20768)

S = 1.018   Npar= 1675

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

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings  Differ    Please Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........      6.40 Note
PLAT213_ALERT_2_C Atom F4_7           has ADP max/min Ratio .....       3.1 prolat
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of    Al02 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....      2.8 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00416 Ang.
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .     39 Ang**3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600      8 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....      6 Note
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⚪ Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C52 H61 Al5 F36 N2 O4
            Atom count from _chemical_formula_moiety:
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:C52 H61 Al5 F36 N2 O4
            Atom count from the _atom_site data:  C51.988 H61 Al5 F35.97297 N2 O4.
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  C52 H61 Al5 F36 N2 O4
        TEST: Compare cell contents of formula and atom_site data

        atom    Z*formula  cif sites diff
        C        208.00    207.95    0.05
        H        244.00    244.00    0.00
        Al        20.00     20.00    0.00
        F        144.00    143.89    0.11
        N          8.00      8.00    0.00
        O         16.00     15.99    0.01
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite     170 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...     170 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ  Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...  Please Check
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records      1 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records      2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records     11 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records      7 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records      6 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )     98% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  1 )   56.96 Check
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PLAT432_ALERT_2_G Short Inter X...Y Contact  F6_12    ..C9_10              2.95 Ang.
                                             1/2+x,1/2-y,z  =      3_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F9_12    ..C6_10              2.92 Ang.
                                             1-x,1-y,-1/2+z  =    2_664 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........     220 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....       ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............   18750 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      19 Note
PLAT955_ALERT_1_G Reported (CIF) and Actual (FCF) Lmax Differ by .       1 Units
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       3 Info
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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
  24 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   8 ALERT type 4 Improvement, methodology, query or suggestion
   1 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
```

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.

```
# 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 18/12/2021; check.def file version of 18/12/2021

Datablock Pna21_a - ellipsoid plot