

## checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait .....  
 .....

## checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) C2c\_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](#)

Please wait while processing .... [Interpreting this report](#)

[Structure factor report](#)

## Datablock: C2c\_a

|                 |                                                  |                    |
|-----------------|--------------------------------------------------|--------------------|
| Bond precision: | C-C = 0.0051 Å                                   | Wavelength=0.71073 |
| Cell:           | a=43.085 (9)      b=34.018 (9)      c=26.753 (6) |                    |
|                 | alpha=90      beta=97.625 (7)      gamma=90      |                    |
| Temperature:    | 100 K                                            |                    |

  

|                | Calculated                                                         | Reported                        |
|----------------|--------------------------------------------------------------------|---------------------------------|
| Volume         | 38864 (16)                                                         | 38864 (16)                      |
| Space group    | C 2/c                                                              | C 2/c                           |
| Hall group     | -C 2yc                                                             | -C 2yc                          |
| Moiety formula | 3(C15.98 Al F35.95 O4), C15.94 Al<br>F35.86 O3.98, 2(C31.73 H47.60 | [Al8C70H105][AlO4C16F36]        |
| Sum formula    | C344.25 H420.60 Al36 F143.66<br>O15.96                             | C86.02 H105.09 Al9 F35.97 O3.99 |
| Mr             | 8514.70                                                            | 2129.16                         |
| Dx, g cm-3     | 1.455                                                              | 1.455                           |
| Z              | 4                                                                  | 16                              |
| Mu (mm-1)      | 0.210                                                              | 0.210                           |
| F000           | 17499.1                                                            | 17493.0                         |
| F000'          | 17520.90                                                           |                                 |
| h, k, lmax     | 58, 46, 36                                                         | 58, 45, 36                      |
| Nref           | 50351                                                              | 50268                           |
| Tmin, Tmax     | 0.947, 0.978                                                       | 0.710, 0.746                    |
| Tmin'          | 0.947                                                              |                                 |

Correction method= # Reported T Limits: Tmin=0.710 Tmax=0.746  
 AbsCorr = MULTI-SCAN

Data completeness= 0.998      Theta(max)= 28.729

R(reflections)= 0.0713 ( 27318)      wR2(reflections)= 0.2309 ( 50268)

S = 1.019      Npar= 5201

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

[PLAT068\\_ALERT\\_1\\_C](#) Reported F000 Differs from Calcd (or Missing)... Please Check

[PLAT088\\_ALERT\\_3\\_C](#) Poor Data / Parameter Ratio ..... 9.67 Note

PLAT213\_ALERT\_2\_C Atom F9\_17 has ADP max/min Ratio ..... 3.5 prolat

#### And 2 other PLAT213 Alerts

More ...

PLAT214\_ALERT\_2\_C Atom C10\_5 (Anion/Solvent) ADP max/min Ratio 4.3 prolat

PLAT221\_ALERT\_2\_C Solv./Anion Resd 4 C Ueq(max)/Ueq(min) Range 4.2 Ratio

PLAT340\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00505 Ang.

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 5.601 Check

PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 6 Note

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 24 Report

PLAT913\_ALERT\_3\_C Missing # of Very Strong Reflections in FCF .... 7 Note

PLAT918\_ALERT\_3\_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check

PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

## Alert level G

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: C86.02 H105.09 Al9 F35.97 O3.

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: C86.02 H105.09 Al9 F35.97 O3.99

Atom count from the \_atom\_site data: C86.06264 H105.1499 Al9 F35.9158

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

CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests

From the CIF: \_cell\_formula\_units\_Z 16

From the CIF: \_chemical\_formula\_sum C86.02 H105.09 Al9 F35.97 O3.99

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

| atom | Z*formula | cif sites | diff  |
|------|-----------|-----------|-------|
| C    | 1376.32   | 1377.00   | -0.68 |
| H    | 1681.44   | 1682.40   | -0.96 |
| Al   | 144.00    | 144.00    | 0.00  |
| F    | 575.52    | 574.65    | 0.87  |
| O    | 63.84     | 63.85     | -0.01 |

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 540 Note

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 540 Report

PLAT042\_ALERT\_1\_G Calc. and Reported Moiety Formula Strings Differ Please Check

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 0.25 Check

PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 153.66 Why ?

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 24 Report

PLAT187\_ALERT\_4\_G The CIF-Embedded .res File Contains RIGU Records 23 Report

PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 1 ) 98% Note

PLAT301\_ALERT\_3\_G Main Residue Disorder .....(Resd 2 ) 98% Note

PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 98% Note

#### And 7 other PLAT302 Alerts

More ...

PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 1 ) 56.89 Check

#### And 5 other PLAT304 Alerts

More ...

PLAT380\_ALERT\_4\_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C10\_10 Check

#### And 6 other PLAT380 Alerts

More ...

PLAT412\_ALERT\_2\_G Short Intra XH3 .. XHn H7A\_6 ..H8C\_37 . 2.14 Ang.

x,y,z = 1\_555 Check

PLAT412\_ALERT\_2\_G Short Intra XH3 .. XHn H7C\_15 ..H9B\_43 . 1.91 Ang.

x,y,z = 1\_555 Check

PLAT412\_ALERT\_2\_G Short Intra XH3 .. XHn H9B\_15 ..H10C\_42 . 1.91 Ang.

x,y,z = 1\_555 Check

PLAT413\_ALERT\_2\_G Short Inter XH3 .. XHn H9A\_6 ..H10C\_36 . 1.91 Ang.

x,y,z = 1\_555 Check

PLAT413\_ALERT\_2\_G Short Inter XH3 .. XHn H6B\_15 ..H8A\_44 . 1.99 Ang.

x,y,z = 1\_555 Check

PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 930 Note

PLAT789\_ALERT\_4\_G Atoms with Negative \_atom\_site\_disorder\_group # 112 Check  
 PLAT790\_ALERT\_4\_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note  
 C15.98 Al F35.95 O4  
 PLAT811\_ALERT\_5\_G No ADDSYM Analysis: Too Many Excluded Atoms .... ! Info  
 PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 126060 Note  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 48 Note  
 PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 3 Note  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 1 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  
 15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 50 **ALERT level G** = General information/check it is not something unexpected

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

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### 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\_PLAT041\_C2c\_a

;

PROBLEM: Calc. and Reported SumFormula Strings Differ Please Check

RESPONSE: ...

;

\_vrf\_PLAT068\_C2c\_a

;

PROBLEM: Reported F000 Differs from Calcd (or Missing)... Please Check

RESPONSE: ...

;

\_vrf\_PLAT088\_C2c\_a

;

PROBLEM: Poor Data / Parameter Ratio ..... 9.67 Note

RESPONSE: ...

;

\_vrf\_PLAT213\_C2c\_a

;

PROBLEM: Atom F9\_17 has ADP max/min Ratio ..... 3.5 prolat

RESPONSE: ...

;

\_vrf\_PLAT214\_C2c\_a

;

PROBLEM: Atom C10\_5 (Anion/Solvent) ADP max/min Ratio 4.3 prolat

RESPONSE: ...

;

\_vrf\_PLAT221\_C2c\_a

;

PROBLEM: Solv./Anion Resd 4 C Ueq(max)/Ueq(min) Range 4.2 Ratio

RESPONSE: ...

;

\_vrf\_PLAT340\_C2c\_a

;

PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00505 Ang.

RESPONSE: ...

;

\_vrf\_PLAT906\_C2c\_a

;

PROBLEM: Large K Value in the Analysis of Variance ..... 5.601 Check

RESPONSE: ...

;

\_vrf\_PLAT910\_C2c\_a

;

PROBLEM: Missing # of FCF Reflection(s) Below Theta(Min). 6 Note

RESPONSE: ...

```
;
_vrf_PLAT911_C2c_a
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 24 Report
RESPONSE: ...
;
_vrf_PLAT913_C2c_a
;
PROBLEM: Missing # of Very Strong Reflections in FCF .... 7 Note
RESPONSE: ...
;
_vrf_PLAT918_C2c_a
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
RESPONSE: ...
;
_vrf_PLAT934_C2c_a
;
PROBLEM: Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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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 13/07/2021; check.def file version of 13/07/2021

## Datablock C2c\_a - ellipsoid plot



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