checkCIF/PLATON report

Structure factors have been supplied for datablock(s) P-1_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: P-1_a

Bond precision: C-C = 0.0049 A Wavelength=0.71073

Cell: a=16.596(6) b=19.883(6) c=22.100(7)
alpha=90.590(7) beta=107.669(13) gamma=104.381(19)
Temperature: 100 K

	Calculated	Reported
Volume	6702(4)	6702(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 Al F36 O4, C30 H45 Al4, C6 H4 F2	[AL(ALCP*)3][AL(ORF)4]
Sum formula	C52 H49 Al5 F38 O4	C52 O4 F38 Al5 H49
Mr	1594.81	1594.81
Dx,g cm-3	1.581	1.581
Z	4	4
Mu (mm-1)	0.230	0.230
F000	3200.0	3200.0
F000'	3204.33	
h,k,lmax	19,23,26	19,23,26
Nref	23875	23831
Tmin,Tmax	0.932,0.967	0.706,0.745
Tmin'	0.914	

Correction method= # Reported T Limits: Tmin=0.706 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 25.095

R(reflections)= 0.0494(17667) wR2(reflections)= 0.1269(23831)

S = 1.070 Npar= 2309

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

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C1_13    --C5_13    .        5.3 s.u.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Al4 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.4 Note
PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.00487 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     Hn_13    ..Hn_13    .       2.09 Ang.
                                              2-x,1-y,-z  =      2_765 Check
PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of .         35 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.604 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.597         43 Report
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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 H49 Al5 F38 O4
           Atom count from _chemical_formula_moiety:
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        242 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        190 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       8.96 Why ?
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records          2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records          3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         15 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         11 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records         13 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C2_2 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C3_2 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C4_2 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C2_3 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C3_3 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C4_3 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C2_4 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C2_6 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C3_6 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C4_6 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C2_8 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C3_8 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C4_8 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C2_24 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C3_24 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C4_24 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        25% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2  )        25% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        29% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
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PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  5  )      10.61 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  6  )       8.75 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  7  )       3.25 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  8  )       1.39 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F7_4     ..F3_16           2.76 Ang.
                                              1-x,1-y,1-z  =      2_666 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F9_6     ..F1_20           2.82 Ang.
                                                x,1+y,z  =      1_565 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F5_24    ..F5_24           2.68 Ang.
                                               -x,2-y,-z  =      2_575 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....        365 Note
PLAT722_ALERT_1_G Angle   Calc      121.00, Rep      119.90 Dev...       1.10 Degree
              C2_21   -C3_21   -H_21       1_555  1_555  1_555     #  712 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      22815 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        47% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
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
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
47 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
32 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
15 ALERT type 4 Improvement, methodology, query or suggestion
1 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 18/12/2021; check.def file version of 18/12/2021

Datablock P-1_a - ellipsoid plot