checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
No extractable fcf data in found in CIF

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) xstr0887

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: xstr0887

Bond precision: C-C = 0.0027 A Wavelength=1.54184
Cell: a=11.3290(3) b=11.3991(3) c=14.1862(3)
alpha=90 beta=94.627(2) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	1826.04(8)	1826.04(7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C16 H28 Al Cl N2 O2	C16 H28 Al Cl N2 O2
Sum formula	C16 H28 Al Cl N2 O2	C16 H28 Al Cl N2 O2
Mr	342.83	342.85
Dx,g cm-3	1.247	1.247
Z	4	4
Mu (mm-1)	2.381	2.381
F000	736.0	740.2
F000'	740.00	
h,k,lmax	12,12,15	12,12,15
Nref	1272	1267
Tmin,Tmax	0.593,0.827	0.703,1.000
Tmin'	0.414	

Correction method= # Reported T Limits: Tmin=0.703 Tmax=1.000
AbsCorr = MULTI-SCAN
Data completeness= 0.996 Theta(max)= 57.880
R(reflections)= 0.0246(1199) wR2(reflections)= 0.0686(1267)
S = 1.075 Npar= 157

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

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5493
PLAT027_ALERT_3_A _diffrn_reflns_theta_full value (too) Low ..... 57.88 Degree

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Alert level C

PLAT088_ALERT_3_C Poor Data / Parameter Ratio ..... 8.07 Note
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.2 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.549 5 Report
4 4 3, 11 1 6, -2 0 8, 8 4 10, -6 6 12,

Alert level G

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT769_ALERT_4_G CIF Embedded Explicitly Supplied Scattering Data Please Note
PLAT794_ALERT_5_G Tentative Bond Valency for Al2 (III) . 3.00 Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 100% Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note
-2 0 8, 4 4 3,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 6.460 Note
Predicted wR2: Based on SigI**2 1.06 or SHELX Weight 6.38
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info
PLAT982_ALERT_1_G The C-f'= 0.0192 Deviates from IT-value = 0.0181 Check
And 3 other PLAT982 Alerts
More ...
PLAT983_ALERT_1_G The Al-f"= 0.2420 Deviates from IT-Value = 0.2455 Check
And 2 other PLAT983 Alerts
More ...

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2 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
14 ALERT level G = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

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_THETM01_xstr0887
;
PROBLEM: The value of sine(theta_max)/wavelength is less than 0.550
RESPONSE: ...
;
_vrf_PLAT027_xstr0887
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ......      57.88 Degree
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock xstr0887 - ellipsoid plot

Download CIF editor (publCIF) from the IUCr
Download CIF editor (enCIFer) from the CCDC
Test a new CIF entry