

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: mc21033

Bond precision:	C-C = 0.0018 A	Wavelength=0.71073
Cell:	a=13.2338(13) b=16.0297(14) c=17.3617(19)	
	alpha=90 beta=105.344(4) gamma=90	
Temperature:	100 K	
	Calculated	Reported
Volume	3551.7(6)	3551.7(6)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C74 H106 Al2, 2(C D2 Cl2)	2(C Cl2 D2), C74 H106 Al2
Sum formula	C76 H106 D4 Al2 Cl4	C76 H106 Al2 Cl4 D4
Mr	1223.41	1223.42
Dx,g cm-3	1.144	1.144
Z	2	2
Mu (mm-1)	0.232	0.232
F000	1320.0	1320.0
F000'	1321.79	
h,k,lmax	17,21,23	17,21,23
Nref	8820	8798
Tmin,Tmax	0.928,0.964	0.712,0.746
Tmin'	0.928	

Correction method= # Reported T Limits: Tmin=0.712 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 28.287

R(reflections)= 0.0424(7626) wR2(reflections)= 0.1174(8798)

S = 1.048 Npar= 520

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
PLAT213_ALERT_2_C	Atom C30A	has ADP max/min Ratio	3.1 prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C Ueq(max)/Ueq(min) Range	3.8 Ratio



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	40	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	20	Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ		Please Check
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	1	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	7	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	41	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) All --C37	9.4	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	42%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H with # Connections	2.00	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	4.27	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	0.73	Check
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	1	Info
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	310	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	5	Note

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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
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
11 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
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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.

