

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: i12444z

Bond precision: C-C = 0.0028 Å

Wavelength=0.71073

Cell: a=10.3063(2) b=11.3760(2) c=15.3201(3)
 alpha=89.290(1) beta=89.348(1) gamma=72.542(1)
Temperature: 150 K

	Calculated	Reported
Volume	1713.27(6)	1713.27(6)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C34 H58 Al N5	?
Sum formula	C34 H58 Al N5	C34 H58 Al N5
Mr	563.83	563.83
Dx, g cm-3	1.093	1.093
Z	2	2
Mu (mm-1)	0.088	0.088
F000	620.0	620.0
F000'	620.29	
h, k, lmax	12, 14, 19	12, 14, 19
Nref	7014	6925
Tmin, Tmax	0.983, 0.993	0.983, 0.993
Tmin'	0.983	

Correction method= MULTI-SCAN

Data completeness= 0.987

Theta(max)= 26.410

R(reflections)= 0.0476(4778)

wR2(reflections)= 0.1212(6925)

S = 1.063

Npar= 373

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

PLAT220_ALERT_2_C Large Non-Solvent	C	Ueq(max)/Ueq(min)	...	3.8	Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for	C24	--	C25	..	6.5 su
PLAT411_ALERT_2_C Short Inter H...H Contact	H23A	..	H30B	..	2.13 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor	N3	-	H3N	...	?

● Alert level G

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF	?
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal	0.00100 Deg.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Al -- C1 ..	7.2 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Al -- C2 ..	5.4 su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Al -- C3 ..	6.7 su

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected
- 1 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
0 ALERT type 3 Indicator that the structure quality may be low
0 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*, 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.

