

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 35-dnba_300k

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 35-dnba_300k

Bond precision: C-C = 0.0018 A

Wavelength=0.71073

Cell: a=21.042(3) b=8.7285(9) c=9.7693(10)
 alpha=90 beta=111.118(4) gamma=90
Temperature: 300 K

	Calculated	Reported
Volume	1673.8(3)	1673.8(3)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C7 H4 N2 O6	?
Sum formula	C7 H4 N2 O6	C7 H4 N2 O6
Mr	212.12	212.12
Dx,g cm-3	1.684	1.684
Z	8	8
Mu (mm-1)	0.152	0.152
F000	864.0	864.0
F000'	864.63	
h,k,lmax	27,11,12	27,11,12
Nref	1917	1916
Tmin,Tmax	0.947,0.970	0.888,1.000
Tmin'	0.941	

Correction method= MULTI-SCAN

Data completeness= 0.999

Theta(max)= 27.480

R(reflections)= 0.0345(1543)

wR2(reflections)= 0.1059(1916)

S = 1.104

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 B

PLAT430_ALERT_2_B Short Inter D...A Contact O5 .. N1 .. 2.85 Ang.



Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF ?
PLAT432_ALERT_2_G Short Inter X...Y Contact O6 .. C7 .. 3.02 Ang.

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

0 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
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

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.

PLATON version of 19/04/2012; check.def file version of 14/04/2012

