

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dnba\_200

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: dnba\_200

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Bond precision:    C-C = 0.0015 A                      Wavelength=0.71073

Cell:                      a=20.690(5)              b=8.750(5)              c=9.730(5)  
                                alpha=90              beta=110.45(1)              gamma=90

Temperature:              200 K

	Calculated	Reported
Volume	1650.5(13)	1650.5(13)
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	212.00
Dx,g cm-3	1.707	1.706
Z	8	8
Mu (mm-1)	0.154	0.000
F000	864.0	68.0
F000'	864.63	
h,k,lmax	35,14,16	30,13,14
Nref	4306	1901
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.441                      Theta(max)= 37.360

R(reflections)= 0.0370( 1491)              wR2(reflections)= 0.0708( 1901)

S = 1.255                      Npar= 173

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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.

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### Alert level A

TYPE031\_ALERT\_1\_A \_diffn\_radiation\_wavelength is not of type numb.  
PLAT027\_ALERT\_3\_A \_diffn\_reflns\_theta\_full (too) Low ..... 0.00 Deg.  
PLAT029\_ALERT\_3\_A \_diffn\_measured\_fraction\_theta\_full Low ..... 0.000  
PLAT091\_ALERT\_1\_A No Wavelength found in CIF - 0.71073 Ang Assumed ?

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## Alert level B

PLAT430\_ALERT\_2\_B Short Inter D...A Contact O5 .. N1 .. 2.82 Ang.

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## Alert level G

ABSMU\_01 Radiation type not identified. Calculation of  
\_exptl\_absorpt\_correction\_mu not performed.

PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF ....	?
PLAT153_ALERT_1_G	The su's on the Cell Axes are Equal .....	0.00500 Ang.
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3
PLAT195_ALERT_1_G	Missing _cell_measurement_theta_max datum ...	?
PLAT196_ALERT_1_G	Missing _cell_measurement_theta_min datum ...	?
PLAT432_ALERT_2_G	Short Inter X...Y Contact O6 .. C7 ..	2.97 Ang.
PLAT950_ALERT_5_G	Reported and Calculated Hmax Values Differ by ..	5
PLAT952_ALERT_5_G	Reported and Calculated Lmax Values Differ by ..	2
PLAT981_ALERT_1_G	No non-zero f" Anomalous Scattering Values Found	?
PLAT982_ALERT_1_G	The C-f' = 0.000 Deviates from the IT-value	0.003
PLAT982_ALERT_1_G	The N-f' = 0.000 Deviates from the IT-value	0.006
PLAT982_ALERT_1_G	The O-f' = 0.000 Deviates from the IT-value	0.011
PLAT983_ALERT_1_G	The C-f" = 0.000 Deviates from the IT-Value	0.002
PLAT983_ALERT_1_G	The N-f" = 0.000 Deviates from the IT-Value	0.003
PLAT983_ALERT_1_G	The O-f" = 0.000 Deviates from the IT-Value	0.006

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4 **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  
15 **ALERT level G** = General information/check it is not something unexpected

12 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  
2 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

