

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cs3_300

No syntax errors found. CIF dictionary Interpreting this report

Datablock: cs3_300

Bond precision:	C-C = 0.0066 A	Wavelength=0.71073	
Cell:	a=14.430(6)	b=6.950(2)	c=16.920(8)
	alpha=90	beta=99.650(16)	gamma=90
Temperature:	300 K		
	Calculated	Reported	
Volume	1672.9(12)	1672.9(12)	
Space group	P 21/c	P21/c	
Hall group	-P 2ybc	?	
Moiety formula	C9 H11 N O2, C7 H3 N2 O6, H	?	
Sum formula	C16 H15 N3 O8	C16 H15 N3 O8	
Mr	377.31	377.31	
Dx,g cm-3	1.498	1.498	
Z	4	4	
Mu (mm-1)	0.122	0.002	
F000	784.0	499.0	
F000'	784.49		
h,k,lmax		15,7,17	
Nref		1651	
Tmin,Tmax	0.998,0.999		
Tmin'	0.996		

Correction method= Not given

Data completeness= Theta(max)= 0.000

R(reflections)= 0.0547(1001) wR2(reflections)= 0.0995(1651)

S = 1.142 Npar= 379

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

TYPE031_ALERT_1_A _diffn_radiation_wavelength is not of type numb.

RINTA01_ALERT_3_A The value of Rint is greater than 0.25

Rint given 0.475

PLAT029_ALERT_3_A	_diffn_measured_fraction_theta_full Low	0.000
PLAT051_ALERT_1_A	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	6023.02 Perc.
PLAT088_ALERT_3_A	Poor Data / Parameter Ratio	4.36
PLAT091_ALERT_1_A	No Wavelength found in CIF - 0.71073 Ang Assumed	?
PLAT305_ALERT_2_A	Isolated Hydrogen Atom (Outside Bond Range ??)	H14

Alert level B

PLAT430_ALERT_2_B	Short Inter D...A Contact	O3 .. O4 ..	2.66 Ang.
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Alert level C

PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	?
PLAT213_ALERT_2_C	Atom H5 has ADP max/min Ratio	3.2 prola
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C10 -- C12 ..	6.0 su
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	N3
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.3
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0066 Ang
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C7 - H8 ...	1.11 Ang.
PLAT351_ALERT_3_C	Long C-H Bond (0.96A) C8 - H9 ...	1.11 Ang.
PLAT355_ALERT_3_C	Long O-H Bond (0.82A) O1 - H11 ...	1.01 Ang.
PLAT391_ALERT_3_C	Deviating Methyl C6 H-C-H Bond Angle	102 Deg.
PLAT776_ALERT_1_C	Suspect D-H Dist in CIF: O3 -- H14 ..	1.32 Ang.

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	?
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	1.80 mm
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	4
PLAT195_ALERT_1_G	Missing _cell_measurement_theta_max datum	?
PLAT196_ALERT_1_G	Missing _cell_measurement_theta_min datum	?
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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- 7 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 12 **ALERT level G** = General information/check it is not something unexpected
- 14 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
 6 **ALERT type 2** Indicator that the structure model may be wrong or deficient
 8 **ALERT type 3** Indicator that the structure quality may be low
 2 **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.

