

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Compound_4_mo_tdv9_n_0m

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: Compound_4_mo_tdv9_n_0m

Bond precision: N- C = 0.0050 A Wavelength=0.71073

Cell: a=5.7104(5) b=7.6993(7) c=10.2304(9)
 alpha=78.072(2) beta=75.750(2) gamma=75.623(2)
Temperature: 100 K

	Calculated	Reported
Volume	417.19(6)	417.19(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	H4 N2 O10 U, 2(N O3), 2(C H6 N)	H4 N2 O10 U, 2(N O3), 2(C H6 N)
Sum formula	C2 H16 N6 O16 U	C2 H16 N6 O16 U
Mr	618.24	618.24
Dx,g cm-3	2.461	2.461
Z	1	1
Mu (mm-1)	9.821	9.821
F000	290.0	290.0
F000'	280.63	
h,k,lmax	8,10,14	8,10,14
Nref	2424	2336
Tmin,Tmax	0.320,0.906	0.310,0.462
Tmin'	0.296	

Correction method= # Reported T Limits: Tmin=0.310 Tmax=0.462
AbsCorr = MULTI-SCAN

Data completeness= 0.964 Theta(max)= 30.000

R(reflections)= 0.0172(2336) wR2(reflections)= 0.0446(2336)

S = 1.040 Npar= 118

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

PLAT430_ALERT_2_C	Short Inter D...A Contact	O4	..04	.	2.85 Ang.
			-x,-y,-z	=	2_555 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			15 Report
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on		U1		1.21 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.69A	From O1		0.46 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H2B				-0.46 eA-3



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms			5 Report
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)				0.002 Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	U1	--O3	.	8.6 s.u.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O1	..N1		2.86 Ang.
			-x,l-y,-z	=	2_565 Check
PLAT794_ALERT_5_G	Tentative Bond Valency for U1		(VI)	.	6.10 Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary				Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			73 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			2.0 Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities			Please Check

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

2 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
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

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.

