

# 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: WO3\_phen

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Bond precision:    C-C = 0.0134 Å                      Wavelength=1.54178

Cell:                      a=22.6294(4)              b=7.5779(1)              c=14.7923(10)  
                                alpha=90                      beta=90                      gamma=90

Temperature:              293 K

	Calculated	Reported
Volume	2536.63(18)	2536.63(18)
Space group	C m c a	C m c a
Hall group	-C 2bc 2	?
Moiety formula	C6 H4 N O3 W	C6 H4 N1 O3 W1
Sum formula	C6 H4 N O3 W	C6 H4 N1 O3 W1
Mr	321.94	321.94
Dx,g cm-3	3.372	3.372
Z	16	16
Mu (mm-1)	33.384	33.384
F000	2320.0	2320.0
F000'	2237.95	
h,k,lmax	26,8,16	26,8,17
Nref	1048	1039
Tmin,Tmax	0.235,0.716	0.537,1.000
Tmin'	0.151	

Correction method= EMPIRICAL

Data completeness= 0.991                      Theta(max)= 62.340

R(reflections)= 0.0316( 856)                      wR2(reflections)= 0.0810( 1039)

S = 1.101                      Npar= 101

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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 B

THETM01\_ALERT\_3\_B The value of sine(theta\_max)/wavelength is less than 0.575

Calculated sin(theta\_max)/wavelength = 0.5745

PLAT093\_ALERT\_1\_B No su's on H-atoms, but refinement reported as .                      mixed



### Alert level C

PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	W1
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds .....	0.0134 Ang



### Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained Atom Sites ....	11
PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension .	3
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF ...	?
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	86.53
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature	293 K
PLAT200_ALERT_1_G	Check the Reported _diffrn_ambient_temperature	293 K
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) W1 -- O1 ..	5.7 su
PLAT333_ALERT_2_G	Check Large Av C6-Ring C-C Dist. C3 -C3_f	1.42 Ang.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.20 Ratio
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	66

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 2 **ALERT level B** = A potentially serious problem, consider carefully  
 2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 10 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 5 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 3 ALERT type 3 Indicator that the structure quality may be low  
 1 ALERT type 4 Improvement, methodology, query or suggestion  
 2 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.

Datablock WO3\_phen - ellipsoid plot

