

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4CNPY-H\_Tos

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: 4CNPY-H\_Tos

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Bond precision:	C-C = 0.0020 A	Wavelength=1.54184
Cell:	a=7.8849 (1) alpha=90	b=11.4201 (1) beta=90
Temperature:	120 K	c=27.8681 (2) gamma=90
	Calculated	Reported
Volume	2509.42 (4)	2509.42 (4)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C7 H7 O3 S, C6 H5 N2	C7 H7 O3 S, C6 H5 N2
Sum formula	C13 H12 N2 O3 S	C13 H12 N2 O3 S
Mr	276.31	276.31
Dx, g cm <sup>-3</sup>	1.463	1.463
Z	8	8
Mu (mm <sup>-1</sup> )	2.361	2.361
F000	1152.0	1152.0
F000'	1158.05	
h, k, lmax	9, 13, 33	9, 13, 33
Nref	2226	2226
Tmin, Tmax	0.753, 0.846	0.868, 1.000
Tmin'	0.753	

Correction method= # Reported T Limits: Tmin=0.868 Tmax=1.000  
AbsCorr = GAUSSIAN

Data completeness= 1.000      Theta(max)= 66.722

R(reflections)= 0.0277 ( 2135)	wR2(reflections)= 0.0749 ( 2226)
S = 1.035	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 C**

PLAT353\_ALERT\_3\_C Long N-H (N0.87,N1.01A) N1 - H1 . 1.04 Ang.

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#### **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	1	Report
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing .....	0.00010	Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing .....	0.00020	Ang.
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	95%	Note
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	1	Units
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..	133.5	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	15	Info

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

