

**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) pdmn\_0m

No syntax errors found. CIF dictionary Interpreting this report

**Datablock: pdmn\_0m**

Bond precision: C-C = 0.0019 Å Wavelength=0.71073

Cell: a=22.5974(6) b=7.1916(2) c=21.4416(6)  
 alpha=90 beta=117.848(1) gamma=90

Temperature: 89 K

	Calculated	Reported
Volume	3080.97(15)	3080.96(15)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C10 H4 Mn2 O10 S2, 2(C6 H16 N)	C10 H4 Mn2 O10 S2, 2(C6 H16 N)
Sum formula	C22 H36 Mn2 N2 O10 S2	C22 H36 Mn2 N2 O10 S2
Mr	662.55	662.53
Dx, g cm <sup>-3</sup>	1.428	1.428
Z	4	4
Mu (mm <sup>-1</sup> )	1.005	1.005
F000	1376.0	1376.0
F000'	1380.26	
h,k,lmax	29,9,28	29,9,28
Nref	3717	3712
Tmin,Tmax	0.845,0.869	0.674,0.872
Tmin'	0.740	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 27.950

R(reflections)= 0.0216( 3448) wR2(reflections)= 0.0606( 3712)

S = 1.048 Npar= 179

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 B**

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O3	--	C3	..	8.29	su
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O4	--	C4	..	7.86	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Mn1	--	C3	..	17.00	su

PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Mn1	--	C4	..	16.60	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Mn1	--	C5	..	15.80	su

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● **Alert level C**

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	....				2.49	
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O5	--	C5	..	6.14	su
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of	.				32	A**3
PLAT912_ALERT_4_C	Missing # of FCF Reflections Above STh/L=	0.600				9	

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● **Alert level G**

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mn1	--	S1	..	7.87	su
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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
5 **ALERT level B** = A potentially serious problem, consider carefully  
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
1 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
0 ALERT type 3 Indicator that the structure quality may be low  
1 ALERT type 4 Improvement, methodology, query or suggestion  
0 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.

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